Supporting Information for:

Intramolecular B/N Frustrated Lewis Pairs and the Hydrogenation of Carbon Dioxide

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Contents

S1....General Experimental..........................................................S2
S2....Preparation of 1, 2 and precursors........................................S3
S3....HD scrambling experiments with 1.......................................S5
S4....Synthesis of 3 from 1..........................................................S6
S5....Hydrogenation of CO2 using 1 and 2 J Young NMR Tube Experiments ..........S9
S6.... Preparation of 4.................................................................S24
S7....Additional computational details and figures...........................S29
S8....Cartesian coordinates of optimized structures..........................S35
S9....Crystallographic details ......................................................S71
S10....References .......................................................................S77

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**S1: General experimental:**

Unless otherwise specified, all the manipulations were conducted under an inert atmosphere of dinitrogen, using standard Schlenk and glovebox techniques. Reactions were carried either in a sealed J-Young NMR tube, in which case NMR conversions are indicated, or in standard oven dried Schlenk vessels. Benzene-$d_6$ was purified by vacuum distillation from Na/K alloy, or by degassing by three subsequent freeze pump thaw cycles followed by standing over activated 3 Å molecular sieves. Acetonitrile-$d_3$ and bromobenzene-$d_5$ were dried over 3 Å molecular sieves. Dry CO$_2$ was purchased from Praxair and used as received. $^{13}$CO$_2$ (99% isotope label) was purchased from Cambridge Isotope Laboratories or Aldrich. Ultra high purity hydrogen (5.0 grade) was purchased from Praxair and used as received. 5-Bromo,1,2,4-trimethylbenzene, 2-Bromo-1,3,5-trimethylbenzene and BF$_3$.Et$_2$O were purchased from Aldrich or TCI and used as received. FBMes$_2^{-}$ was synthesized according to a literature procedure$^1$ and further purified by sublimation. (2-(dimethylamino)phenyl)lithium was synthesized according to a literature procedure.$^2$ Benzaldehyde was purchased from Aldrich and distilled under reduced pressure before use.

NMR spectra were recorded on Agilent DD2-600 at 600 MHz ($^1$H), 150.84 MHz ($^{13}$C), 192.45 MHz ($^{11}$B), Agilent Technologies NMR spectrometer at 500 MHz ($^1$H), 125.758 MHz ($^{13}$C), 160.462 MHz ($^{11}$B), a Varian Inova NMR AS400 spectrometer, at 400.0 MHz ($^1$H), 100.580 MHz ($^{13}$C), 128.378 MHz ($^{11}$B). $^1$H NMR and $^{13}$C{$^1$H} NMR chemical shifts are referenced to residual protons in deuterated solvent. Multiplicities are reported as singlet (s), broad singlet (s, br) doublet (d), triplet (t), multiplet (m). Chemical shifts are reported in ppm. Coupling constants are reported in Hz. gHSQC experiments were performed in order to confirm C-H correlations. Mass spectroscopy analysis were performed on a JMS T100-LC using AccuTOF DART.

**WARNING:** Condensation of high pressure of H$_2$ and CO$_2$ might lead to an explosion of the glassware. Care should be taken.
S2: Synthesis of compounds 1, 2 and precursors

dimethylbis(2,4,5-trimethylphenyl)stannane

This compound was synthesized with a slightly modified approach from a known procedure.\(^3\)

Ca. 50 mL of THF and 3.48 g (143 mmol, 4.0 equivalents) of magnesium turnings were combined in a Schlenk flask. To the resulting mixture, 25.9 g (130 mmol, 3.7 equivalents) of 1-bromo-2,4,5-trimethylbenzene were added and heated at 40°C for 2 hours. \(\text{Me}_2\text{SnCl}_2\) (7.7 g, 35 mmol, 1.0 equivalent) was dissolved in ca. 20 mL of THF in a separate Schlenk flask. The solution containing the tin compound was then cannulated into the Schlenk flask containing the Grignard reagent. The resulting mixture was heated at 50°C for 4 hours.

Work-up: The solution was cooled down in an ice bath and 20 mL of a saturated solution of NH\(_4\)Cl was added. The contents were transferred to a separatory funnel and extracted three times with a mixture of Et\(_2\)O/Hexanes (50/50). The organic layer was then washed with water and with brine. The organic layer was dried with Na\(_2\)SO\(_4\) and the solvents removed by rotary evaporation. The compound was then passed through a silica plug using hexanes as an eluent which was then removed by rotary evaporation yielding 11.3 g of white crystals. Yield = 83%.

\(^1\)H NMR 400 MHz: \(\delta\) 7.20 (s, 2H, m-Ar); 7.05 (s, 2H, o-Ar); 2.35 (s, 6H, m-Me); 2.27 (s, 6H, p-Me); 2.25 (s, 6H, o-Me); 0.55 (s, 6H, Sn-Me). \(^{13}\)C \(^1\)H (101 MHz): \(\delta\) 142.3 (m-Ar); 137.8 (m-Ar\(_{\text{quat}}\)); 137.2 (p-Ar); 136.7 (o-Ar); 133.3 (o-Ar\(_{\text{quat}}\)); 130.7 (Sn-Ar); 24.4 (m-Me); 19.8 (p-Me); 19.3 (o-Me); -8.03 (Sn-Me).

chlorobis(2,4,5-trimethylphenyl)borane

This compound was synthesized with a slightly modified approach from a known procedure\(^4\).

In a Schlenk flask, 11.1 g of dimethylbis(2,4,5-trimethylphenyl)stannane (0.029 mol, 1 equivalent) was dissolved in ca. 10 mL of hexanes in a teflon capped Schlenk flask with a magnetic stir bar. 29 mL (0.029 mol, 1 equivalent) of a 1.0 molar solution of BCl\(_3\) in heptane was added at once. The resulting mixture was heated for 40 hours at 100 °C with vigorous stirring. Upon reaction completion, the Schlenk flask was allowed to cool to r.t. naturally after which it was placed in a cold bath. The solution containing the title compound was filtered from the precipitated \(\text{Me}_2\text{SnCl}_2\). The resulting solution was then evaporated until the title compound started precipitating out. The flask was then stored at -35 °C for 4 hours after which the hexanes were filtered by keeping the solution at -35 °C. The compound was then further purified by sublimation at 80 °C at 0.1 Tor. 6.43 g of white crystals, yield = 80%. Recrystallization from hexanes yielded monocrystals suitable for X-ray crystallography. (The structure is reported in S9).

\(^1\)H NMR 400MHz: \(\delta\) 7.62 (s, 2H, o-Ar); 6.8 (s, 2H, m-Ar); 2.28 (s, 6H, o-Me); 1.98 (s, 6H, p-Me); 1.97 (s, 6H, m-Me); \(^{13}\)C \(^1\)H (101 MHz): \(\delta\) 140.8 (m-Ar\(_{\text{quat}}\)); 140.5 (p-Ar\(_{\text{quat}}\)); 139.3 (s, br., Ar-B); 136.8 (m-Ar); 133.5 (o-Ar\(_{\text{quat}}\)); 132.3 (o-Ar); 22.7 (o-Me); 19.8 (p-Me); 19.1 (m-Me).
1-(dimesitylboryl)-2-NMe_2-C_6H_4 (1)

This compound was synthesized with a slightly modified approach from a known procedure.⁵

1.5 g (5.5 mmol, 1.0 equivalent) of dimesitylboron fluoride was dissolved in toluene and cannulated to a -78°C solution of 700 mg (5.5 mmol, 1.0 equivalent) of (2-(dimethylamino)phenyl)lithium in 10mL of toluene. The resulting mixture was then left to warm to r.t. naturally and to stir for 16 hours. Upon reaction completion the solution was bright, fluorescent green.

Work-up: The salts were left to separate without agitation and the solution was filtered via cannula. The residue was washed once with toluene (10mL). The volatiles were then removed in vacuo. Upon cooling, 1.8 g of a green solid was recovered: yield= 91%. The compound can be further purified by recrystallization from a saturated hexane solution at -35°C. Using this method, 1.46 g of pure compound was recovered. Yield = 72%

The characterization of this compound is conform to that previously reported.⁶

1-(bis(2,4,5-trimethylphenyl)boryl)-2-NMe_2-C_6H_4 (2)

This compound was synthesized with a slightly modified approach from a known procedure⁵

967 mg (3.4 mmol, 1.0 equivalent) of chlorobis(2,4,5-trimethylphenyl)borane was dissolved in toluene and cannulated to a -78°C solution of 432 mg (3.4 mmol, 1.0 equivalent) of (2-(dimethylamino)phenyl)lithium in 10mL of toluene. The resulting mixture was then left to warm to r.t. naturally and to stir for 16 hours. Upon reaction completion the solution was bright, fluorescent green.

Work-up: The salts were left to separate without agitation and the solution was filtered via cannula. The residue was washed once with toluene (10 mL). The volatiles were then removed in vacuo and left under vacuum at 110 °C for 2 hours. Upon cooling, 1.1 g of a sticky green solid was recovered: yield= 88 %. The compound can be further purified by recrystallization from a saturated hexane solution at -35°C. Using this method, 807 mg of pure compound was recovered. Yield = 64%

The characterizations of this compound conform to those that were previously reported⁶
S3: HD scrambling with 1

In a glove box, 5.2 mg (0.014 mmol) of 1 was dissolved in benzene-d$_6$ (0.5 ml) and the green solution transferred to a J Young NMR tube. The solution was degassed via three freeze-pump-thaw cycles in liquid nitrogen. The tube was charged with HD (4 atm) and $^1$H NMR recorded. The reaction was heated at 80 °C for 14 h, cooled and $^1$H-NMR recorded.

Figure S3. 600 MHz $^1$H-NMR during isotope scrambling of HD by 1. a) Expansion of reaction mixture at t = 0 h. b) Expansion reaction mixture after 14 h at 80 °C. c) Full spectra of reaction mixture after 14 h at 80 °C.
S4: Synthesis of 3 from 1

In a glove box, 1 (46 mg, 0.13 mmol) was dissolved in benzene (4 ml) and the green solution transferred to a J Young flask (bomb) equipped with a teflon coated magnetic stir bar. The solution was degassed via three freeze-pump-thaw cycles in liquid nitrogen. The flask was charged with H₂ (4 atm) and the mixture was stirred and heated at 80 °C for 48 h. The volatiles were removed in vacuo to give a pale green solid. The product was crystallised from hot n-hexane (2 ml), which after decantation of the supernatant and washing the solid with n-hexane (0.5 ml) gave 3 as white feathery crystals (9 mg, 54%).

*The H atoms are numbered based on the carbon atom to which they are attached

\[^{1}H\text{ NMR (600 MHz, benzene-}d_{6}\text{):} \delta\ 7.76\ (dd, J = 7.3, 1.5 Hz, 1H, H7), 7.16\ (td, J = 7.3, 1.0 Hz, 1H, H5), 6.99\ (ddd, J = 8.0, 7.3, 1.5 Hz, 1H, H6), 6.62\ (dd, J = 8.0, 1.0 Hz, 1H, H4), 3.54\ (app. br. d, J = 96 Hz, 1H, BH), 2.77\ (s, 3H, C2), 2.55\ (s, 3H, C1).\]

\[^{13}C[^{1}H]\text{ NMR (151 MHz, benzene-}d_{6}\text{):} \delta\ 158.1\ (C3), 137.3\ (C7), 126.6\ (H5), 126.5\ (H6), 116.9\ (C4), 59.3\ (C1), 48.2\ (C2).\]

\[^{11}B[^{1}H]\text{ NMR (193 MHz, benzene-}d_{6}\text{):} \delta\ +2.5.\]

HRMS (DART-TOF+): mass [M–H] calc’d for \(C_{16}H_{23}B_{2}N_{2}\) 265.20473 Da, measured 265.20539 Da.
Figure S4-1. 600Mz $^1$H-NMR of isolated 3 in C$_6$D$_6$ showing an expansion of the BH signal (top, red) superimposed on the $^{11}$B decoupled spectra (bottom, blue).
Figure S4-2. 151 MHz $^{13}$C-NMR of isolated 3 in C$_6$D$_6$. 
SS: Hydrogenation of CO\textsubscript{2} - J Young NMR Tube Experiments

General procedure

In a glove box, the solvent (0.5 ml) and cyclohexane (~1 µl) was added to 0.014 mmol of aminoborane. The bright green solution was transferred to a J Young NMR tube and the mixture was degassed via three freeze-pump-thaw cycles in liquid nitrogen. The tube was charged with the stated pressure of CO\textsubscript{2} or \textsuperscript{13}C labelled CO\textsubscript{2} (99% \textsuperscript{13}C). The mixture was frozen in liquid nitrogen and the tube charged with H\textsubscript{2} (4 atm). The \textsuperscript{1}H NMR was recorded and the tube heated at the stated temperature. The reaction was periodically monitored by \textsuperscript{1}H-, \textsuperscript{13}C- and \textsuperscript{11}B-NMR. When stated, at the end of the reaction, the reaction solution was colourless and contained a white precipitate. The mixture was homogenised by cooling to −20 °C and then adding acetonitrile-d\textsubscript{3} (0.15 ml) followed by shaking of the tube. The final \textsuperscript{1}H-, \textsuperscript{13}C- and \textsuperscript{11}B-NMRs were then recorded. For the experiments involving 2, the solution remained homogeneous throughout the entire process.
Table S5. Hydrogenation of CO$_2$ with 1 and 2

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*a After addition of acetonitrile-d$_3$
Figure S5-1. 600Mz $^1$H-NMR of the reaction between 1, $^{13}$CO$_2$ (1 atm) and H$_2$ (4 atm) in benzene-d$_6$ after 9 days at 80 °C, after the addition of acetonitrile-d$_3$. a) Full spectra. b) Formate region [$J_{CH} = 211-213$ Hz]. c) (OCH$_2$O) region [$J_{CH} = 165$ Hz]. d) Methoxide region [$J_{CH} = 143$ Hz].
Figure S5-2. 151 MHz $^{13}$C-NMR of the reaction between 1, $^{13}$CO$_2$ (1 atm) and H$_2$ (4 atm) in benzene-d$_6$ after 9 days at 80 °C, after the addition of acetonitrile-d$_3$. 
Figure S5-3. HSQC-NMR of the reaction between 1, $^{13}$CO$_2$ (1 atm) and H$_2$ (4 atm) in benzene-d$_6$ after 9 days at 80 °C, after the addition of acetonitrile-d$_3$. 
Figure S5-4. 600Mz $^1$H-NMR of the reaction between 1, $^{13}$CO$_2$ (0.1 atm) and H$_2$ (4 atm) in benzene-d$_6$ after 9 days at 80 °C. a) Full spectra. b) Methoxide region [$J_{CH} = 141-143$ Hz]. c) Methane [$J_{CH} = 126$ Hz].
Figure S5-5. 151 MHz $^{13}$C-NMR of the reaction between 1, $^{13}$CO$_2$ (0.1 atm) and H$_2$ (4 atm) in benzene-d$_6$ after 9 days at 80 °C.
Figure S5-6. 600Mz $^1$H-NMR of the reaction between 1, $^{13}$CO$_2$ (1 atm) and H$_2$ (4 atm) in BrC$_6$D$_5$ after 1 day at 130 °C, after the addition of acetonitrile-d$_3$. a) Full spectra. b) Formate region [$\delta_{CH} = 212-213$ Hz]. c) (OCH$_2$O) region [$\delta_{CH} = 165-167$ Hz]. d) Methoxide region [$\delta_{CH} = 140-143$ Hz].
Figure S5-7. 151 MHz $^{13}$C-NMR of the reaction between 1, $^{13}$CO$_2$ (1 atm) and H$_2$ (4 atm) in BrC$_6$D$_5$ after 1 day at 130 °C, after the addition of acetonitrile-d3.
Figure S5-8. 600Mz $^1$H-NMR of the reaction between 2, $^{13}$CO$_2$ (1 atm) and H$_2$ (4 atm) in C$_6$D$_6$ after 6 h at 80 °C after the addition of acetonitrile-d3. a) Full spectra. b) Formate region [$J_{CH}$ = 204-212 Hz]. c) (OCH$_2$O) region [$J_{CH}$ = 163-165 Hz].
**Figure S5-9.** 151 MHz $^{13}$C-NMR of the reaction between 2, $^{13}$CO$_2$ (1 atm) and H$_2$ (4 atm) in C$_6$D$_6$ after 6 h at 80 °C after the addition of acetonitrile-d$_3$. 
**Figure S5-10** $^1$H-NMR of the reaction between 2, $^{13}$CO$_2$ (1 atm) and H$_2$ (4 atm) in benzene-d$_6$ after 72 h at r.t. in benzene-d6.
**Figure S5-11** $^1$H-NMR of the reaction between 2, $^{13}$CO$_2$ (1 atm) and H$_2$ (4 atm) in C$_6$D$_6$ after 72 h at r.t. in benzene-d6. Zoom on aromatic region.
Figure S5-12 $^1$H-NMR of the reaction between 2, $^{13}$CO$_2$ (1 atm) and H$_2$ (4 atm) in C$_6$D$_6$ after 72 h at r.t. in benzene-d6. Zoom on aliphatic region.
**Figure S5-13** $^{13}$C-NMR of the reaction between 2, $^{13}$CO$_2$ (1 atm) and H$_2$ (4 atm) in benzene-d$_6$ after 72 h at r.t. in benzene-d6. Zoom on aliphatic region.
In a glove box, 2 (200 mg, 0.54 mmol) was dissolved in toluene (4 ml) and the green solution transferred to a teflon capped Schlenk flask equipped with a teflon coated magnetic stir bar. The solution was degassed via three freeze-pump-thaw cycles in liquid nitrogen. The flask was charged with CO₂ (1 atm) and H₂ (1 atm) and the mixture was stirred at r.t. for 72 h after which the bright green coloration had almost completely disappeared and white precipitate had formed. The volatiles were removed in vacuo and left under vacuum at 60°C for one hour to ensure complete removal of 1,2,4-trimethylbenzene. The residue was dissolved in hot hexanes (ca 4mL) and filtered hot. The hexane solution was stored at -35°C for 72 hours, yielding the title compound as colorless crystals (90 mg, 60%). Note that the crystals readily re-dissolve upon warming of the hexanes solution. The crystals were isolated by cold filtration at -35°C followed by rapid evacuation of the remaining traces of hexanes in vacuo.
*The H atoms are numbered based on the carbon atom to which they are attached

11: $^1$H NMR (500 MHz, benzene-d$_6$) $\delta$ 7.69 (s, 2H, H$_{13}$), 7.29 (d, $J = 7.2$ Hz, 2H, H$_6$), 7.19 (t, $J = 7.8$ Hz, 2H, H$_4$), 6.99 (s, 2H, H$_{10}$), 6.80 (t, $J = 7.3$ Hz, 2H, H$_5$), 6.66 (m, 2H,H$_3$), 5.72 (s, 2H, H$_{17}$), 2.82 (s, 6H, H$_{14}$), 2.48 (s, 12H, H$_1$), 2.04 (s, 6H, H$_{15}$), 1.97 (s, 6H, H$_{16}$).

$^{13}$C ($^1$H) NMR (126 MHz, benzene-d$_6$) $\delta$ (155.7, C$_8$), (143.3, C$_7$), (140.5, C$_9$), (139.6, C$_{13}$), (133.8, C$_6$), (132.7, C$_{11}$) (132.6, C$_{10}$) (130.0, C$_4$), (128.4, C$_{12}$), (119.3,C$_5$), (114.8, C$_3$), (90.9, C$_{17}$), (43.4, C$_1$), (23.2, C$_{14}$), (19.7,C$_{15}$),(19.2, C$_{16}$).

$^{11}$B ($^1$H) NMR (193 MHz, benzene-d$_6$): $\delta$ +46.1.
Figure S6-1: $^1$H NMR spectra of the crystals of 4 in benzene-d6
Figure S6-2: $^{13}$C {H} NMR spectra of the crystals of 4 in benzene-d$_6$. n-hexane was found to co-crystallize with the product, explaining the presence of small amounts of n-hexane in the product.
Figure S6-2: HSQC NMR spectra of the crystals of 4 in benzene-d6. n-hexane was found to co-crystallize with the product, explaining the presence of small amounts of n-hexane in the product
**S7: Additional computational details and figures**

**Computational details:**

All the calculations were performed on the full structures of the reported compounds. Calculations were performed with the GAUSSIAN 03 and GAUSSIAN 09 suite of programs.\cite{7,8} The \(\omega B97XD\) functional\cite{9} was qualified as promising by Grimme\cite{10} and was used to accurately describe the mechanism of FLP mediated hydrogenation of alkynes\cite{11} and was thus used in combination with the 6-31G** basis set for all atoms\cite{12} The transition states were located and confirmed by frequency calculations (single imaginary frequency). The stationary points were characterized as minima by full vibration frequencies calculations (no imaginary frequency). All geometry optimizations were carried out without any symmetry constraints. The energies were then refined by single point calculations to include solvent effects using the SMD solvation model\cite{13} with the experimental solvent (benzene) at the \(\omega B97XD /6-31++G^{**}\) level of theory.\cite{14} All structures with their associated free enthalpy and Gibbs free energies as well as their cartesian coordinates are fully detailed in section S8.
Figure S7-1: Protodeborylation for 1
*Because of the asymmetry in Mes', many conformers can be possible for most of these structures. However, it was assumed that energetic differences between them were negligible and they weren’t all computed. Nevertheless, uncertainty on the values reported might be slightly higher than for NMe₂BMes₂, but still we are confident that the conclusions based on those calculations should not be altered significantly.*
Figure S7-3: Identification of the resting state of 4

NmeB2h_open

18.3 (37.0)

NmeB2h_close

6.7 (22.2)

NmeB2h_H2

17.9 (18.2)

NmeB2h_dimtrans

8.7 (13.3)

NmeB2h_dimcis

7.2 (12.5)

NmeB2h_dimchair

6.4 (4.8)

NmeB2h_dimboat

0 (0)

NmeB2h_olig2

18.2 (22.5)

NmeB2h_olig3

19.0 (17.4)
Figure S7-4: Hydrogenation of CO2 by 1

34.7 (9.4)

12.2 (0.4)

31.7 (19.9)

29.3 (16.3)

24.4 (1.9)

7.6 (-2.4)

0 (0)

0 (0)
S8: Optimized geometries with cartesian coordinates and electronic energies.

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![Chemical Structure](image)

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C  1.23037200 0.25683900 0.12528400  H  5.42412200 0.72249500 -2.11063400
C  2.00561400 1.27317800 -0.40744300  H  6.94220300 0.88536900 -1.21229600
C  1.87425000 -0.89240900 0.20753300  H  6.49976200 -0.67377700 -1.95067300
C  3.41244700 1.19876000 -0.49035800  C  6.06794300 -1.27275300 0.48142500
H  1.52770700 2.18999500 -0.74247800  H  5.92180100 -2.25357900 -0.00067600
C  3.24972700 -1.03737400 0.47735300  H  7.14213200 -1.06982300 0.50963800
H  1.52770700 2.18999500 -0.74247800  H  6.49976200 -1.27275300 -1.95067300
C  1.29315100 -1.70659300 1.00680500  C  5.41071100 -0.19124400 -0.21951800
H  3.70126100 -1.96810000 0.79966900  H  3.52152600 3.45436400 -1.17216300
B  4.14721300 2.51509300 -0.76345000  H  5.30981400 2.66745900 -0.52231200

NmeB2h_close

Sum of electronic and thermal Enthalpies= -391.371616
Sum of electronic and thermal Free Energies= -391.414550

C   -1.26622800 -2.39098400 0.64957700  C   -2.34637500 -0.98487000 -1.06212500
C   0.08192100 -2.12438300 0.80935500  H   -2.51670500 0.06438300 -1.31218800
C   0.91173000 -3.18362200 1.16443300  H   -1.62699000 -1.40672000 -1.76368300
C   0.33764100 -4.44701000 1.33813500  H   -3.29162500 -1.53496200 -1.12536100
C   -1.03264100 -4.66532700 1.16398200  C   -2.70825800 -0.50522100 1.29764200
C   -1.88469400 -3.61733200 0.80791200  H   -2.87465000 0.50099400 1.07597000
H   1.97918600 -3.04959000 1.30885500  H   -3.66512000 -1.03844500 1.28503200
H   0.96874900 -5.28584500 1.61682500  H   -2.25016600 -0.59536900 2.28228200
H   -1.43915000 -5.66185800 1.30884000  B   -0.13012400 -0.56576100 0.45255800
H   -2.95067600 -3.77133200 0.66958100  H   0.24445500 -0.16728000 -0.62610000
N   -1.78618300 -1.06593600 0.29634800  H   -0.06547200 0.24512700 1.34722200
**NmeB2h_H2**

\[
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\text{Sum of electronic and thermal Enthalpies} &= -392.536223 \\
\text{Sum of electronic and thermal Free Energies} &= -392.581801
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C & 3.50611400 & -1.08824100 & 0.31868000 & C & 3.50611400 \\
H & 1.77381100 & 2.37734100 & 0.25768400 & H & 1.77381100 \\
C & 3.50611400 & -1.08824100 & 0.31868000 & C & 3.50611400 \\
B & 4.59878300 & 2.64942300 & -0.26917200 & B & 4.59878300 \\
C & 5.44531400 & 0.40625900 & -2.18719300 & H & 5.44531400 \\
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H & 6.59881000 & 2.51023100 & 0.33138200 & H & 6.59881000 \\
H & 8.10229000 & 1.59421200 & 0.06783400 & H & 8.10229000 \\
H & 5.66338600 & 0.07422400 & -0.13794200 & H & 5.66338600 \\
H & 4.84982000 & 2.67068100 & -1.47092000 & H & 4.84982000
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**NmeB2h_dimtrans**

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\text{Sum of electronic and thermal Free Energies} &= -782.825897
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C & -1.32814100 & -0.46208500 & 1.79808700 & C & -4.29500800 \\
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H & 1.69638200 & 1.08501100 & 1.65239500 & C & -4.99740200 \\
H & -0.59205000 & 1.44201600 & 2.49434800 & C & -6.44928200 \\
N & -2.67299500 & -0.30398900 & 2.25975900 & H & -5.60941100 \\
B & -2.16680500 & -2.70407400 & 0.87237100 & H & -7.04034700 \\
H & -2.59435000 & -3.41313400 & 1.73729400 & H & -7.34984300 \\
H & -3.18949900 & -2.08944200 & 0.31193800 & N & -3.28775000 \\
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NmeB2h_dimcis

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Sum of electronic and thermal Free Energies = -782.828329

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C  0.16951400  -0.41309600  2.49032800  H  -1.34922700  -3.39252700  -0.70320300
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C  -1.44502700  -0.18730800  0.78506900  C  -4.54414800  -3.87827900  -1.82652200
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H  -1.52066200  -2.37613700  3.38222800  H  -5.54016000  -4.72604800  -2.31959400
H  0.24314700  -0.86708200  4.22007900  C  -4.60118400  -6.58605700  -1.10760900
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N  -2.08398300  0.40290000  -0.46967500  H  -6.29516200  -4.34325700  -2.99827600
B  -2.90234300  -2.33960000  0.99210600  H  -4.61892900  -7.6337100  -0.82478100
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H  -2.95774400  -2.20973000  -0.31323100  N  -4.49131800  -2.49592700  -2.17584000
H  -2.42602300  -3.57326000  1.00495600  C  -5.74108400  -1.88653800  -2.58428500
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H  -3.52165000  1.54932400  -0.00266600  H  -3.31494800  -1.05923900  -3.3913200
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### NmeB2h_dimchair

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**Sum of electronic and thermal Free Energies** = -782.829692

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### NmeB2h_dimboat

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**Sum of electronic and thermal Free Energies= -782.839826**

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### NmeB2h_olig2

![Chemical Structure](image)

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**Sum of electronic and thermal Free Energies** = -782.810765

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NMeB1H1Mes_H2CO2TS

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NMeBMes’_H2CO2TS

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NMeB1H1Mes'_CO2TS_inside

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<tr>
<td>H</td>
<td>3.26676800</td>
<td>0.90555900</td>
<td>4.36439500</td>
<td>H</td>
<td>5.08764500</td>
<td>7.03126900</td>
<td>4.03414500</td>
</tr>
<tr>
<td>H</td>
<td>2.08810800</td>
<td>-0.15056600</td>
<td>3.69731700</td>
<td>H</td>
<td>4.98047200</td>
<td>3.78510200</td>
<td>2.82396000</td>
</tr>
</tbody>
</table>
NMeB1H1Mes\textsuperscript{+}H2CO2TS

Sum of electronic and thermal Enthalpies= -929.799215
Sum of electronic and thermal Free Energies= -929.87156

C  -0.07839600  0.11017100  -0.76596800
C   1.24395700  0.14606200  -1.21700700
C   1.69804000  1.41089900  -1.62119100
C   0.89884500  2.46094200  -1.07820400
C  -0.40413400  2.46004200  -1.07820400
C  -0.90100800  1.22692900  -0.67394000
H   2.71871700  1.49051500  -1.98354500
H   1.29424600  3.50467200  -1.88101600
H  -1.03366500  3.34140700  -1.01915100
H  -1.91707300  1.15507600  -0.29990200
B   2.23335900  -1.1381600  -1.23818000
H   1.78351500  -1.84200700  -2.26568200
H  -0.07382200  -1.93462900  -0.84858000
C   3.76403100  -0.83724600  -1.56486000
C   4.61780600  -0.28565600  -0.59106600
C   4.30382800  -1.08456900  -2.83099200
C   5.94455800  -0.09025000  -0.91780200
C   5.63183400  -0.81420800  -3.16195400
C   6.47071200  -0.26153200  -2.18405100
H   6.59691000  0.41792700  -0.15734200
C   1.13934600  -3.02315300  -2.69645100
O   1.81604800  -3.48649800  -3.55567500
O   0.11175300  -3.13027000  -2.05201300
C  -2.01678000  -1.47227900  -0.70913800
H  -2.12907700  -1.24872500  -1.76840800
H  -2.21667500  -2.52963100  -0.53658000
H  -2.69630500  -0.86319900  -0.11379700
C  -0.38339800  -1.41393000  1.13528700
H   0.67888300  -1.28237100  1.33429800
H  -0.96884400  -0.67850500  1.68878300
H  -0.69174500  -2.42670100  1.39887600
N  -0.60787800  -1.20375600  -0.32007000
C   4.10740800  0.01273200  0.79804000
H   3.30058400  0.75482900  0.77586300
H   3.69949300  -0.88978100  1.26744700
H   4.90111000  0.40049400  1.44265100
C   7.91334400  0.05053300  -2.48942600
H   8.00496600  0.76316600  -3.31740300
H   8.41757300  0.48095200  -1.62038600
H   8.46517400  -0.84934900  -2.78498300
H   2.05117500  -1.88888900  -0.29515300
H   3.66408700  -1.52583600  -3.59292100
C   6.15140800  -1.11421300  -4.54476400
H   6.52530900  -0.21077800  -5.04111500
H   6.98386000  -1.82694600  -4.51599200
H   5.36747800  -1.54300200  -5.17352500
S9: Crystallographic information

S9-1: Crystal structure of chlorobis(2,4,5-trimethylphenyl)borane

The ORTEP of chlorobis(2,4,5-trimethylphenyl)borane with thermal ellipsoids set at the 50% probability level. H atoms are shown as spheres with arbitrary radii. [Symmetry codes: (A) - x+1, y, -z+1/2]
<table>
<thead>
<tr>
<th>Identification code</th>
<th>chlorobis(2,4,5-trimethylphenyl)borane</th>
</tr>
</thead>
<tbody>
<tr>
<td>Empirical formula</td>
<td>C18 H22 B Cl</td>
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<tr>
<td>Formula weight</td>
<td>284.61</td>
</tr>
<tr>
<td>Temperature</td>
<td>296(2) K</td>
</tr>
<tr>
<td>Wavelength</td>
<td>0.71073 Å</td>
</tr>
<tr>
<td>Crystal system</td>
<td>Monoclinic</td>
</tr>
<tr>
<td>Space group</td>
<td>C2/c</td>
</tr>
<tr>
<td>Unit cell dimensions</td>
<td>$a = 14.1030(9)$ Å, $\alpha = 90^\circ$.</td>
</tr>
<tr>
<td></td>
<td>$b = 7.4414(5)$ Å, $\beta = 110.7640(8)^\circ$.</td>
</tr>
<tr>
<td></td>
<td>$c = 16.5975(10)$ Å, $\gamma = 90^\circ$.</td>
</tr>
<tr>
<td>Volume</td>
<td>1628.71(18) Å³</td>
</tr>
<tr>
<td>Z</td>
<td>4</td>
</tr>
<tr>
<td>Density (calculated)</td>
<td>1.161 Mg/m³</td>
</tr>
<tr>
<td>Absorption coefficient</td>
<td>0.222 mm⁻¹</td>
</tr>
<tr>
<td>F(000)</td>
<td>608</td>
</tr>
<tr>
<td>Crystal size</td>
<td>0.520 x 0.360 x 0.300 mm³</td>
</tr>
<tr>
<td>Theta range for data collection</td>
<td>2.625 to 30.498°.</td>
</tr>
<tr>
<td>Index ranges</td>
<td>-20≤h≤20, -10≤k≤10, -23≤l≤23</td>
</tr>
<tr>
<td>Reflections collected</td>
<td>10052</td>
</tr>
<tr>
<td>Independent reflections</td>
<td>2489 [R(int) = 0.0180]</td>
</tr>
<tr>
<td>Completeness to theta</td>
<td>25.242°</td>
</tr>
<tr>
<td>Absorption correction</td>
<td>Semi-empirical from equivalents</td>
</tr>
<tr>
<td>Max. and min. transmission</td>
<td>0.936 and 0.909</td>
</tr>
<tr>
<td>Refinement method</td>
<td>Full-matrix least-squares on F²</td>
</tr>
<tr>
<td>Data / restraints / parameters</td>
<td>2489 / 0 / 95</td>
</tr>
<tr>
<td>Goodness-of-fit on $F^2$</td>
<td>1.064</td>
</tr>
<tr>
<td>Final R indices [$I&gt;2\sigma(I)$]</td>
<td>$R1 = 0.0373$, $wR2 = 0.1149$</td>
</tr>
<tr>
<td>R indices (all data)</td>
<td>$R1 = 0.0410$, $wR2 = 0.1186$</td>
</tr>
<tr>
<td>Extinction coefficient</td>
<td>n/a</td>
</tr>
<tr>
<td>Largest diff. peak and hole</td>
<td>0.396 and -0.281 e.Å$^{-3}$</td>
</tr>
</tbody>
</table>
S9-2: Crystal structure of 4

The ORTEP of 4 with thermal ellipsoids set at the 50% probability level. H atoms are shown as spheres with arbitrary radii. [Symmetry codes: (A) -x+1, y, -z+1/2]
Table S9-7. Crystal data and structure refinement for 4

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Identification code</td>
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</tr>
<tr>
<td>Empirical formula</td>
<td>C₃₅H₄₄B₂N₂O₂</td>
</tr>
<tr>
<td>Formula weight</td>
<td>546.34</td>
</tr>
<tr>
<td>Temperature</td>
<td>150(2) K</td>
</tr>
<tr>
<td>Wavelength</td>
<td>0.71073 Å</td>
</tr>
<tr>
<td>Crystal system</td>
<td>Monoclinic</td>
</tr>
<tr>
<td>Space group</td>
<td>P2₁/c</td>
</tr>
<tr>
<td>Unit cell dimensions</td>
<td>( a = 12.8272(10) \text{ Å} ) ( \alpha = 90^\circ )</td>
</tr>
<tr>
<td></td>
<td>( b = 21.1220(16) \text{ Å} ) ( \beta = 93.3920(10)^\circ )</td>
</tr>
<tr>
<td></td>
<td>( c = 14.0969(11) \text{ Å} ) ( \gamma = 90^\circ )</td>
</tr>
<tr>
<td>Volume</td>
<td>3812.7(5) Å³</td>
</tr>
<tr>
<td>( Z )</td>
<td>4</td>
</tr>
<tr>
<td>Density (calculated)</td>
<td>0.952 Mg/m³</td>
</tr>
<tr>
<td>Absorption coefficient</td>
<td>0.057 mm(^{-1})</td>
</tr>
<tr>
<td>( F(000) )</td>
<td>1176</td>
</tr>
<tr>
<td>Crystal size</td>
<td>( 0.520 \times 0.460 \times 0.320 \text{ mm}^3 )</td>
</tr>
<tr>
<td>Theta range for data collection</td>
<td>1.590 to 28.308(^\circ)</td>
</tr>
<tr>
<td>Index ranges</td>
<td>(-17 \leq h \leq 17, -28 \leq k \leq 28, -18 \leq l \leq 18)</td>
</tr>
<tr>
<td>Reflections collected</td>
<td>40253</td>
</tr>
<tr>
<td>Independent reflections</td>
<td>9480 ([R(int) = 0.0307])</td>
</tr>
<tr>
<td>Completeness to theta = 25.242(^\circ)</td>
<td>100.0 %</td>
</tr>
<tr>
<td>Absorption correction</td>
<td>Semi-empirical from equivalents</td>
</tr>
<tr>
<td>Max. and min. transmission</td>
<td>0.979 and 0.969</td>
</tr>
<tr>
<td>Description</td>
<td>Value</td>
</tr>
<tr>
<td>--------------------------------------------------</td>
<td>------------------------------------------------------------</td>
</tr>
<tr>
<td>Refinement method</td>
<td>Full-matrix least-squares on $F^2$</td>
</tr>
<tr>
<td>Data / restraints / parameters</td>
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</tr>
<tr>
<td>Goodness-of-fit on $F^2$</td>
<td>1.101</td>
</tr>
<tr>
<td>Final R indices [$I&gt;2\sigma(I)$]</td>
<td>$R_1 = 0.0570$, $wR_2 = 0.1663$</td>
</tr>
<tr>
<td>R indices (all data)</td>
<td>$R_1 = 0.0720$, $wR_2 = 0.1751$</td>
</tr>
<tr>
<td>Extinction coefficient</td>
<td>n/a</td>
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<tr>
<td>Largest diff. peak and hole</td>
<td>0.581 and -0.192 e.Å$^{-3}$</td>
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</tbody>
</table>
S10: References