Electronic Supplementary Material (ESI) for Chemical Science.

Supporting information for:

Phosphinoborylenes as Stable Sources of Fleeting Borylenes

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Contents:

Synthetic procedures

General considerations: All manipulations were performed under an inert atmosphere of dry argon using either standard Schlenk-line or glovebox techniques. Deuterated solvents were degassed by three freeze-pump-thaw cycles and dried over activated molecular sieves prior to use. All other solvents were distilled from appropriate drying agents,[1] and were stored under argon over activated molecular sieves. NMR spectra were acquired on a Bruker Avance 500 NMR spectrometer or a Bruker Avance 400 NMR spectrometer. Chemical shifts (δ) are given in ppm. ^{1}H and ^{13}C{^{1}H} NMR spectra were referenced to residual protio solvent (^{1}H) or the solvent itself (^{13}C). In some cases, ^{13}C resonances were observed indirectly by HSQC or HMBC experiments. ^{11}B NMR spectra were referenced to external $BF_3{\cdot}OEt_2$ (15% in $CDCl_3$). ^{31}P NMR were referenced to external H_3PO_4 (85% in H_2O). HRMS were measured on an Exactive Plus Orbitrap-HRMS manufactured by Thermo Scientific, and samples were measured using a LIFDI 700 Ion source from Linden CMS. Compound [(^{Me}CAAC)B(NMe_2)BBr(NMe_2)][BAr^{Cl}_4] was synthesized according to a literature procedure.[2] Trimethylphosphine, 2,6-dimethylphenylisocyanide, N,N-dimethylaminopyridine, N,N'-diisopropylcarbodiimide, N,N'-dicyclohexylcarbodiimide, diphenyl ditelluride, diphenyl diselenide, and carbon monoxide (Grade 5.0) were purchased from Sigma-Aldrich or Acros and used as received.

Improved synthesis of the *E*-isomer (^{Me}CAAC)B(PMe_3)-B(NMe_2)$_2$ (1a) and a mixture of isomers 1a and 1b: THF (5 mL) was added to a solid mixture of [(^{Me}CAAC)B(NMe_2)BBr(NMe_2)][BAr^{Cl}_4] (688 mg, 0.644 mmol) and KC_8 (305 mg, 2.25 mmol) at –80 °C over the course of three minutes. After the mixture was stirred for 15 minutes at this temperature, PMe_3 (70 µL, 0.683 mmol) was added to the solution. The stirred mixture was allowed to warm to room temperature over the course of 30 minutes. Volatiles were removed under high vacuum, and the residue was extracted with pentane (20 mL). The obtained orange solution was filtered off and the solvent was rapidly removed under vacuum in such a manner that the crystallization of the product was largely avoided. This yields a mixture of **1a** and **1b** in an approximate 1:1 ratio. However, if slow crystallization is allowed to occur, more of isomer **1a** is obtained. This mixture was recrystallized overnight from pentane (2 mL) at –30 °C to yield a yellow solid consisting solely of isomer **1a** (225 mg, 74%). **1b** was not isolated in pure form. Data for **1a:** ^{1}H NMR (C_6D_6, 23 °C): 7.14 (s, 3H, *m*-Dipp + *p*-Dipp), 3.85-1.76 (br m, 15H, 4x NCH_3 + 2x C***H***(CH_3)$_2$ + C***H***$_2$C(CH_3)$_2$), 1.57 (br s, 6H, CH_2C(C***H***$_3$)$_2$), 1.51 (d, 6H, $^{3}J_{H\text{-}H}$ = 7 Hz, CH(C***H***$_3$)$_2$), 1.30 (d, 6H, $^{3}J_{H\text{-}H}$ = 7 Hz, CH(C***H***$_3$)$_2$), 0.98 (d, 9H, $^{2}J_{H\text{-}p}$ = 9 Hz, P(C***H***$_3$)$_3$). ^{1}H NMR (toluene-d_8, –40 °C): 7.11-7.06 (m, 3H, *m*-Dipp + *p*-Dipp), 3.64 (septet, 1H, $^{3}J_{H\text{-}H}$ = 7 Hz, C***H***(CH_3)$_2$), 3.28 (septet, 1H, $^{3}J_{H\text{-}H}$ = 7 Hz, C***H***(CH_3)$_2$), 2.97 (s, 3H, NCH_3), 2.58 (s, 3H, NCH_3), 2.43 (s, 3H, NCH_3), 2.28 (s, 3H, NCH_3), 2.13 (d, 1H, $^{2}J_{H\text{-}H}$ = 12 Hz, C***H***$_2$C(CH_3)$_2$), 1.91 (d, 1H, $^{2}J_{H\text{-}H}$ = 12 Hz, C***H***$_2$C(CH_3)$_2$), 1.68 (s, 3H, CH_2C(C***H***$_3$)$_2$), 1.64 (s, 3H, CH_2C(C***H***$_3$)$_2$), 1.57 (d, 3H, $^{3}J_{H\text{-}H}$ = 7 Hz, CH(C***H***$_3$)$_2$), 1.53 (d, 3H, $^{3}J_{H\text{-}H}$ = 7 Hz, CH(C***H***$_3$)$_2$), 1.48 (s, 3H, CH_2C(C***H***$_3$)$_2$), 1.32 (d, 3H, $^{3}J_{H\text{-}H}$ = 7 Hz, CH(C***H***$_3$)$_2$), 1.31 (d, 3H, $^{3}J_{H\text{-}H}$ = 7 Hz, CH(C***H***$_3$)$_2$), 1.04 (s, 3H, CH_2C(C***H***$_3$)$_2$), 0.92 (d, 9H, $^{2}J_{H\text{-}p}$ = 9 Hz, P(C***H***$_3$)$_3$). ^{31}P{^{1}H} NMR (C_6D_6, 23 °C): –27.1 - –29.0 (m). ^{11}B NMR (C_6D_6, 23 °C): 40.3 (B(NMe_2)$_2$), 0.8 (B-PMe_3). ^{13}C{^{1}H} NMR (C_6D_6, 23 °C): 149.2, 145.23, 145.22, 125.3, 62.40, 62.38, 61.0, 45.24, 45.18, 28.2, 18.4 (d, $^{1}J_{C\text{-}P}$ = 40 Hz, PMe_3). Extrapolated NMR data for **1b**: ^{1}H NMR (C_6D_6, 23 °C) 7.11 (s, 3H, *m*-Dipp + *p*-Dipp), 3.73 (septet, 2H, $^{3}J_{H\text{-}H}$ = 7 Hz, C***H***(CH_3)$_2$), 2.89 (br s, 12H, 2x NMe_2), 1.96 (s, 2H, C***H***$_2$C(CH_3)$_2$), 1.70 (s, 6H, C(CH_3)$_2$), 1.33 (d, 6H, $^{3}J_{H\text{-}H}$ = 7 Hz, CH(C***H***$_3$)$_2$), 1.30 (d, 6H, $^{3}J_{H\text{-}H}$ = 7 Hz, CH(C***H***$_3$)$_2$), 1.26 (s, 6H, C(CH_3)$_2$), 0.60 (d, 9H, $^{2}J_{H\text{-}p}$ = 10 Hz, P(C***H***$_3$)$_3$).

^{11}B NMR (C_6D_6, 23 °C): 42.3 ($B(NMe_2)_2$), –1.7 (CAAC-B) ppm. $^{31}P\{^1H\}$ NMR (C_6D_6, 23 °C): –27.1 - –29.0 (m). HRMS (LIFDI) for $C_{27}H_{52}N_3B_2P$ (M^+): 471.4079. Found: 471.4076.

Synthesis of 2a from 1a. C_6D_6 (0.5 mL) was added to a mixture of **1a** (10 mg, 21.2 µmol) and 2,6-dimethylphenylisocyanide (8.4 mg, 64.0 µmol) in a J.-Young-style NMR tube. The mixture was heated to 60 °C for 6 h, resulting in complete conversion to **2a** and free PMe_3 as evidenced by ^{1}H and ^{11}B NMR spectroscopy. Spectroscopic data are identical to those reported previously.[2]

Synthesis of 2b from 1a. Toluene-d_8 (0.5 mL) was added to a sample of **1a** (5 mg, 10,6 µmol) in a J.-Young-style NMR tube with a total internal volume of 2.7 mL. The mixture was degassed and backfilled with 1 bar of CO. The sample was heated to 60 °C for 10 h, resulting in complete conversion to **2b** and free PMe_3 as evidenced by ^{1}H and ^{11}B NMR spectroscopy. Spectroscopic data are identical to those reported previously.[2]

Synthesis & further discussion of DMAP-borylene 2c:

As in the case of the phosphinoborylenes **1a**/**1b**, isomerism is observed in the case of the DMAP-borylene **2c**. Crystallization from pentane as described in this procedure yields the *Z* isomer (**2c**-**I**), which partially converts in solution at room temperature overnight to another isomer (**2c**-**II**) alongside traces of decomposition. Recrystallization of any mixture of isomers leads only to crystals of isomer **2c**-**I**. While unfortunately a molecular structure of **2c**-**II** was not determined, it is likely that these isomers are also similarly derived from rotation around the CAAC-B bond, as maintaining a mixture of **2c-I** and **2c-II** with 3 equiv of 2,6-dimethylphenylisocyanide resulted in clean quantitative conversion to the corresponding isocyanide-stabilized borylene **2a**.

Synthesis of (^{Me}CAAC)B(DMAP)-B(NMe_2)$_2$ (2c) by reduction: THF (4 mL) was added to a solid mixture of [(^{Me}CAAC)B(NMe_2)BBr(NMe_2)][BAr^{Cl}_4] (350 mg, 0.328 mmol) and KC_8 (156 mg, 1.15 mmol) at –80 °C over the course of three minutes. After the mixture was stirred for 15 minutes at this temperature, 4-(N,N-dimethylamino)pyridine (44.1 mg, 0.361 mmol) was added to the solution, resulting in a rapid colour change to dark green. The mixture was subsequently allowed to warm to room temperature and the solvent was removed under high vacuum. The residue was extracted with pentane (4 x 10 mL), filtered and concentrated under vacuum, yielding a dark green crystalline powder, which was washed with a minimum of cold pentane (−30°C, 3 x 1 mL) and dried under high vacuum (61 mg, 36%). Data for **2c**-**I**: 8.09 (d, $^3J_{H-H}$ = 6 Hz, 2H, DMAP–H_{Ar}), 7.29 (d, $^3J_{H-H}$ = 6 Hz, 1H, *m*-Dipp), 7.29 (d, $^3J_{H-H}$ = 9 Hz, 1H, *m*-Dipp), 7.23 (dd, $^3J_{H-H}$ = 6 Hz, $^3J_{H-H}$ = 9 Hz, 1H, *p*-Dipp), 5.51 (d, $^3J_{H-H}$ = 6 Hz, 2H, DMAP–H_{Ar}), 4.10 – 1.15 (multiple very broad low-intensity signals, total of 34H, 3x $N(CH_3)_2$, 1x $C(CH_3)_2$, CH_2, 2x C***H***$(CH_3)_2$, 1x $CH(CH_3)_2$), 1.92 (s, 6H, $C(CH_3)_2$), 1.49 (d, 6H, $^3J_{H-H}$ = 6 Hz, $CH(CH_3)_2$). ^{11}B NMR (C_6D_6, 23 °C): 40.5 (s, $B(NMe_2)$), 28.2 (s, CAAC–B). Due to the rapid isomerization of **2c-I**, adequate $^{13}C\{^1H\}$ NMR data could not be obtained. Data for **2c**-**II**: ^{1}H NMR (C_6D_6, 23 °C): 7.56 (d, $^3J_{H-H}$ = 6 Hz, 2H, DMAP–H_{Ar}), 7.07 (dd, $^3J_{H-H}$ = 6 Hz, $^3J_{H-H}$ = 9 Hz, 1H, *p*-Dipp), 7.03 (d, $^3J_{H-H}$ = 6 Hz, 1H, *m*-Dipp), 7.02 (d, $^3J_{H-H}$ = 9 Hz, 1H, *m*-Dipp), 5.43 (d, $^3J_{H-H}$ = 6 Hz, 2H, DMAP–H_{Ar}), 4.01 (septet, $^3J_{H-H}$ = 6 Hz, 2H, C***H***$(CH_3)_2$), 3.09 (s, 12H, $N(CH_3)_2$), 2.19 (s, 2H, C***H*****$_2$**$C(CH_3)_2$), 1.92 (s, 6H, $N(CH_3)_2$), 1.91 (s, 6H, C*H*$_2$C(C***H***$_3)_2$), 1.47 (s, 6H, C*H*$_2$C(C***H***$_3)_2$), 1.35 (d, 6H, $^3J_{H-H}$ = 6 Hz, $CH(CH_3)_2$),

1.15 (d, 6H, $^{3}J_{H-H}$ = 6 Hz, CH(C***H***$_3$)$_2$). ^{11}B NMR (C_6D_6, 23 °C): 42.5 (s, B(NMe_2)), 23.7 (s, CAAC–B). ^{11}C{^{1}H} NMR (C_6D_6, 23 °C): HRMS (LIFDI) for $C_{31}H_{53}B_2N_5$ (M^+): 517.4482. Found: 517.4474.

Synthesis of 2c from 1a. C_6D_6 (0.5 mL) was added to a mixture of **1a** (12 mg, 25.5 µmol) and 4-(N,N-dimethylamino)pyridine (8.0 mg, 65.5 µmol) in a J.-Young-style NMR tube. The mixture was heated to 60 °C for 6 h, resulting in a mixture consisting of **1a** (9%), **1b** (20%), **2c-I** (7%), and **2c-II** (24%), alongside other identified decomposition products.

Synthesis of 2a from 2c. C_6D_6 (0.5 mL) was added to a mixture of **2c** (10 mg, 19.3 µmol) and 2,6-dimethylphenylisocyanide (10 mg, 76.2 µmol) in a J.-Young-style NMR tube. The mixture was maintained at ambient temperature for 3 h, resulting in complete conversion to **2a** and free DMAP as evidenced by ^{1}H and ^{11}B NMR spectroscopy.

Synthesis of 3a: N,N'-di*iso*propylcarbodiimide (26.7 mg, 0.21 mmol) was added to a solution of **1a** (25.0 mg, 53.0 µmol) in toluene (3 mL). The mixture was stirred for three hours at 60 °C, resulting in a clear, colourless solution, and all volatiles were removed under vacuum. The was residue crystallized from pentane at −30 °C, affording colourless crystals of **3a** suitable for X-ray diffraction (10 mg, 36%). ^{1}H NMR (C_6D_6): 7.23 (dd, $^{3}J_{H-H}$ = 7 Hz, $^{4}J_{H-H}$ = 2 Hz, 1H, *m*-Dipp), 7.20-7.14 (m, multiplicity obscured by C_6D_5H resonance, 2H, m-Dipp; *p*-Dipp), 4.44 (septet, $^{3}J_{H-H}$ = 6 Hz, 2H, C***H***$(CH_3)_2$), 4.35 (septet, $^{3}J_{H-H}$ = 6 Hz, 2H, C***H***$(CH_3)_2$), 4.21 (septet, $^{3}J_{H-H}$ = 6 Hz, 2H, C***H***$(CH_3)_2$), 3.90 (septet, $^{3}J_{H-H}$ = 6 Hz, 2H, C***H***$(CH_3)_2$), 2.78 (d, 1H, $^{2}J_{H-H}$ = 12 Hz, C***H*****$_2$**C$(CH_3)_2$), 2.59 (s, 6H, N$(CH_3)_2$), 2.35 (br s, 3H, N$(CH_3)_2$), 1.89 (d, 1H, $^{2}J_{H-H}$ = 12 Hz, C***H*****$_2$**C$(CH_3)_2$), 1.71 (s, 3H, C$(CH_3)_2$), 1.66 (s, 3H, C$(CH_3)_2$), 1.37 (d, 6H, $^{3}J_{H-H}$ = 6 Hz, CH(C***H***$_3$)$_2$), 1.36 (d, 3H, $^{3}J_{H-H}$ = 6 Hz, CH(C***H***$_3$)$_2$), 1.32 (s, 3H, C$(CH_3)_2$), 1.32 (d, 3H, $^{3}J_{H-H}$ = 6 Hz, CH(C***H***$_3$)$_2$), 1.30 (s, 3H, C$(CH_3)_2$), 1.30 (d, 3H, $^{3}J_{H-H}$ = 6 Hz, CH(C***H***$_3$)$_2$), 1.20 (d, 3H, $^{3}J_{H-H}$ = 6 Hz, CH(C***H***$_3$)$_2$), 1.12 (d, 3H, $^{3}J_{H-H}$ = 6 Hz, CH(C***H***$_3$)$_2$), 1.06 (d, 3H, $^{3}J_{H-H}$ = 6 Hz, CH(C***H***$_3$)$_2$). ^{11}B NMR (C_6D_6): 61.3 (B-C), 34.2 (B(NMe_2)$_2$). ^{13}C{^{1}H} NMR (C_6D_6): 163.0 (NCN), 154.2 (*o*-Dipp), 153.6 (*o*-Dipp), 141.1 (*ipso*-Dipp), 127.1 (*p*-Dipp), 125.5 (*m*-Dipp), 82.2 (NC(***C***)N), 62.9 (***C***$(CH_3)_2$), 56.6 (CH_2), 48.8 (N***C***H$(CH_3)_2$), 46.6 (N***C***H$(CH_3)_2$), 44.1 (***C***$(CH_3)_2$), 42.8 (NCH_3), 40.8 (NCH_3), 32.7, 30.0, 29.4, 27.5, 27.4, 26.6, 26.3, 25.7, 25.5, 25.2, 25.1, 22.3. HRMS (LIFDI) for $C_{31}H_{57}B_2N_5$ (M^+): 521.4795. Found: 521.4787.

Synthesis of 3b. **3b** was prepared in an identical manner to **3a** employing N,N'-di*iso*propylcarbodiimide. Yield: 38% as colourless crystals. ^{1}H NMR (C_6D_6): 7.24 (dd, $^{3}J_{H-H}$ = 7 Hz, $^{4}J_{H-H}$ = 2 Hz, 1H, *m*-Dipp), 7.21-7.15 (m, multiplicity obscured by C_6D_5H resonance, 2H, *m*-Dipp; *p*-Dipp), 4.53 (septet, $^{3}J_{H-H}$ = 6 Hz, 2H, C***H***$(CH_3)_2$), 4.37 (septet, $^{3}J_{H-H}$ = 6 Hz, 2H, C***H***$(CH_3)_2$), 3.98 (apparent tt, $^{3}J_{H-H}$ = 9 Hz, $^{4}J_{H-H}$ = 4 Hz, 1H, $CH_{cyclohexyl}$), 3.60 (apparent tt, $^{3}J_{H-H}$ = 11 Hz, $^{4}J_{H-H}$ = 4 Hz, 1H, $CH_{cyclohexyl}$), 2.79 (d, 1H, $^{2}J_{H-H}$ = 12 Hz, C***H*****$_2$**C$(CH_3)_2$), 2.62 (s, 6H, N$(CH_3)_2$), 2.38 (br s, 3H, N$(CH_3)_2$), 2.11-0.92 (multiple broad overlapping resonances, 20H, $CH_{2cyclohexyl}$), 1.92 (d, 1H, $^{2}J_{H-H}$ = 12 Hz, C***H*****$_2$**C$(CH_3)_2$), 1.75 (s, 3H, C$(CH_3)_2$), 1.68 (s, 3H, C$(CH_3)_2$), 1.38 (d, 3H, $^{3}J_{H-H}$ = 6 Hz, CH(C***H***$_3$)$_2$), 1.37 1.36 (s, 3H, C$(CH_3)_2$), (d, 3H, $^{3}J_{H-H}$ = 6 Hz, CH(C***H***$_3$)$_2$), 1.33 (d, 3H, $^{3}J_{H-H}$ = 6 Hz, CH(C***H***$_3$)$_2$), 1.32 (s, 3H, C$(CH_3)_2$), 1.26 (d, 3H, $^{3}J_{H-H}$ = 6 Hz, CH(C***H***$_3$)$_2$). ^{11}B NMR (C_6D_6): 60.8 (B-C), 34.3 (B(NMe_2)$_2$). ^{13}C{^{1}H} NMR (C_6D_6): 163.3 (NCN), 154.2 (*o*-Dipp), 153.7 (*o*-Dipp), 141.1 (*ipso*-Dipp), 127.2 (*p*-Dipp), 125.5 (*m*-Dipp), 125.4 (*m*-Dipp), 82.6 (NC(***C***)N), 62.9 (***C***$(CH_3)_2$), 57.3 (NCH), 56.6 (***C***H$_2$$(CH_3)_2$), 55.2 (NCH), 44.1 (***C***$(CH_3)_2$), 42.9 (NCH_3), 40.8 (NCH_3), 36.2, 36.1, 35.6, 34.5, 33.4, 32.6, 30.0,

29.5, 27.6, 27.4, 26.9, 26.7, 26.6, 26.5, 26.4, 26.0, 25.19, 25,16, 25.13, 24.8, 22.7, 14.3. HRMS (LIFDI) for $C_{37}H_{65}B_2N_5$ (M^+): 601.5421. Found: 601.5412.

Synthesis of 4a. Toluene (2 mL) was added to a solid mixture of **1a** (25.0 mg, 53.0 µmol) and diphenyl ditelluride (10.9 mg, 26.5 µmol), resulting in an immediate colour change to dark red. After removal of volatiles under high vacuum, the residue was crystallized from slow evaporation of a pentane solution, affording **4a** as dark red crystals suitable for X-ray diffraction (22.1 mg, 70 %). HRMS (LIFDI) for $C_{30}H_{48}B_2N_3Te$ (M^+): 602.3091. Found: 602.3078.

Synthesis of 4b. 4b was prepared in an identical manner to **3a** employing diphenyl diselenide. Yield: 48% as bright orange crystals. HRMS (LIFDI) for $C_{30}H_{48}B_2N_3Se$ (M^+): 552.3194. Found: 552.3186.

Experimental spectra

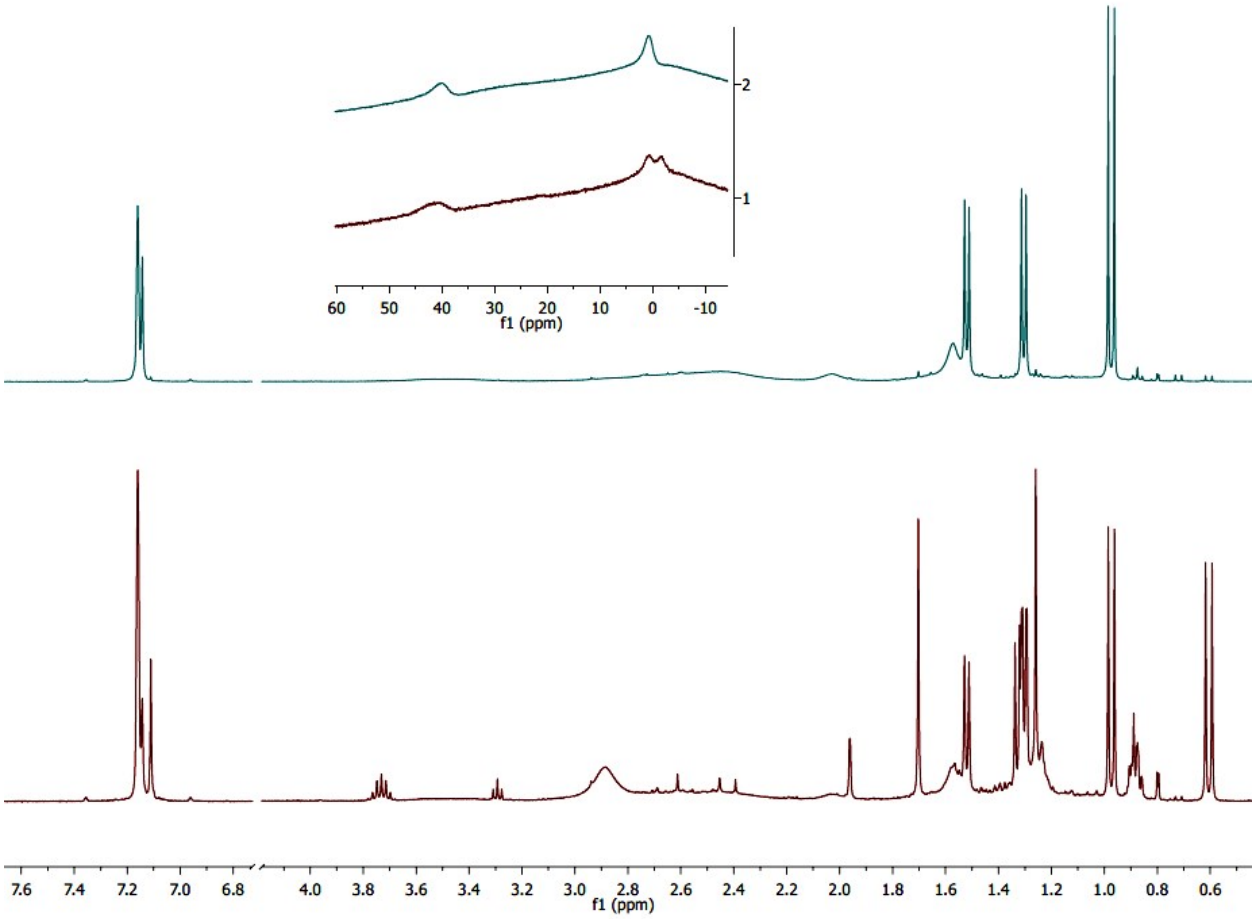


Figure S1: ^{1}H and ^{11}B (inset) NMR spectra of recrystallized **1a** (top) and crude mixture consisting of isomers **1a** and **1b** (bottom).

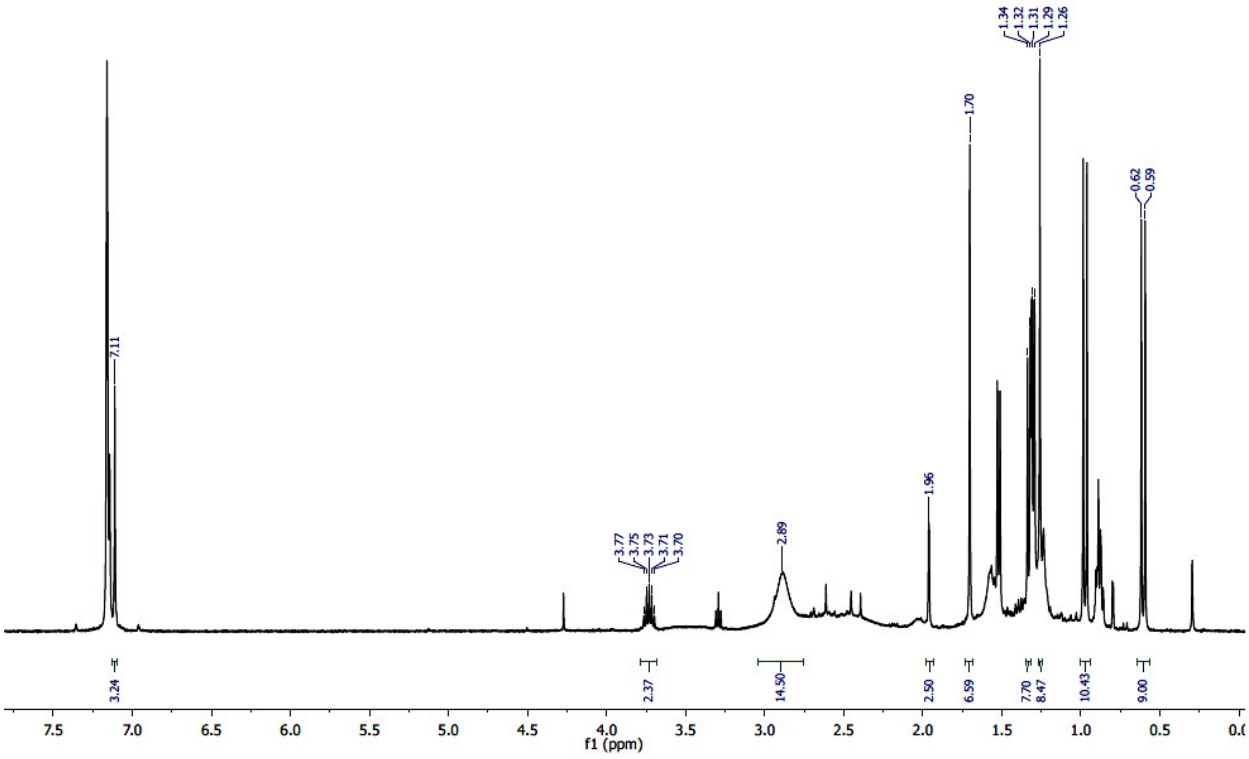


Figure S2. ^{1}H NMR spectrum of a crude mixture of isomers **1a** and **1b** with the signals for compound **1b** integrated and peak-picked.

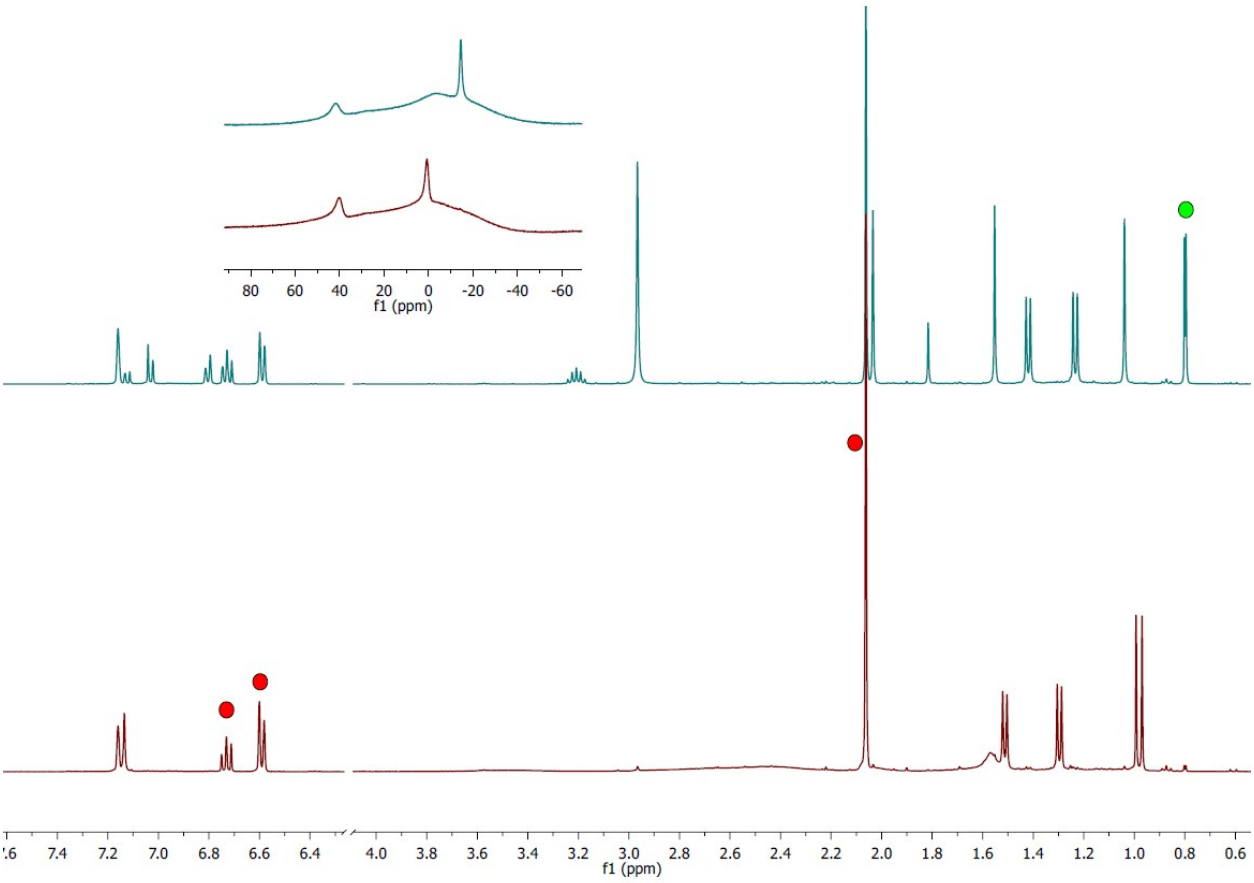


Figure S3. ^{1}H and ^{11}B (inset) NMR spectra of (bottom) compound **1a** and 3.0 equivalents of 2,6-dimethylphenylisocyanide (red dots) at ambient temperature. Top: the same sample after heating at 60 °C for 6 h, revealing complete conversion to **2a** and release of free PMe_3 (green dot).

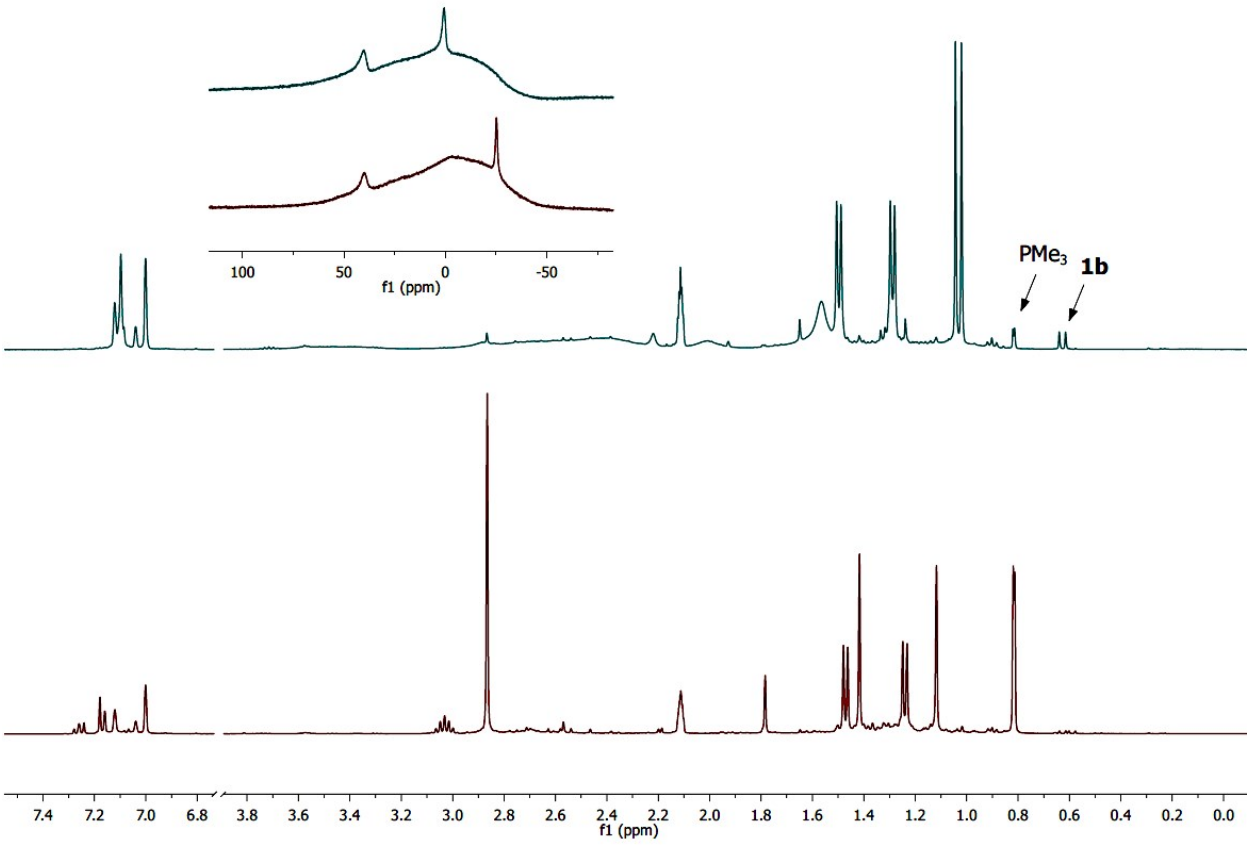


Figure S4. ^{1}H and ^{11}B (inset) NMR spectra of compound **1a** under an atmosphere of CO in toluene-d_8. Top: Compound **1a** immediately after backfilling with CO at ambient temperature. Small amounts (<5%) of isomer **1b** and PMe_3 are present, as are traces of **2a**. Bottom: the same sample after heating at 60 °C for 10 h, revealing complete conversion to **2a** and release of free PMe_3.

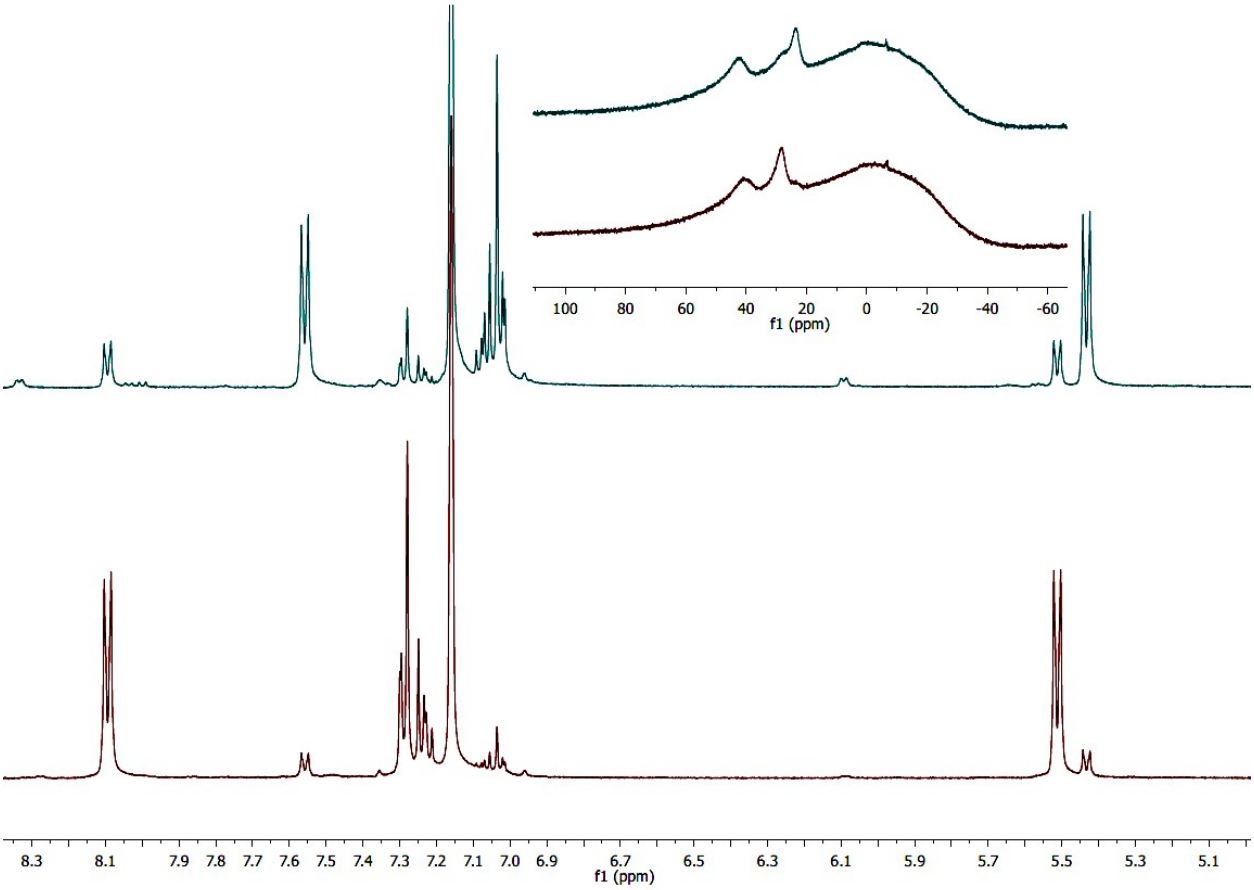


Figure S5: Detail of the aromatic region of the ^{1}H NMR spectrum of a mixture of isomers **2c-I** and **2c-II** with inset ^{11}B NMR in C_6D_6. Bottom: Initial mixture of isomers form upon dissolving crystals of **2c-I** in C_6D_6 consisting of approximately 89% **2c-I** and 11% **2c-II**. Top: the same sample left at 25 °C for 24 h, now consisting of approximately 20% **2c-I** and 80% **2c-II**, alongside traces of other decomposition products.

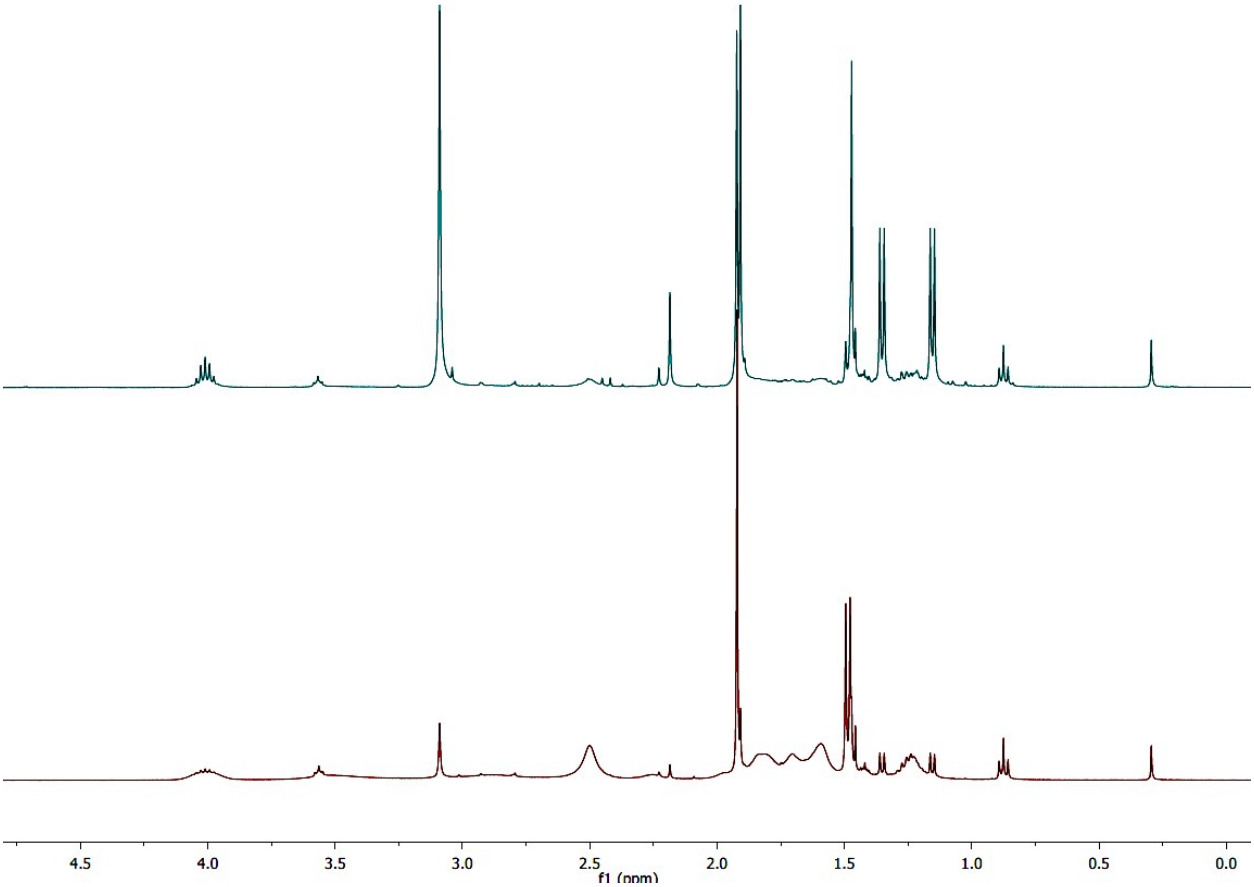


Figure S6: Detail of the aliphatic region of the ^{1}H NMR spectrum of mixture of isomers **2c-I** and **2c-II**. Bottom: Initial mixture of isomers formed upon dissolving crystals of **2c-I** consisting of approximately 89% **2c-I** and 11% **2c-II**. Top: the same sample left at 25 °C for 24 h, now consisting of approximately 20% **2c-I** and 80% **2c-II**, alongside traces of other decomposition products.

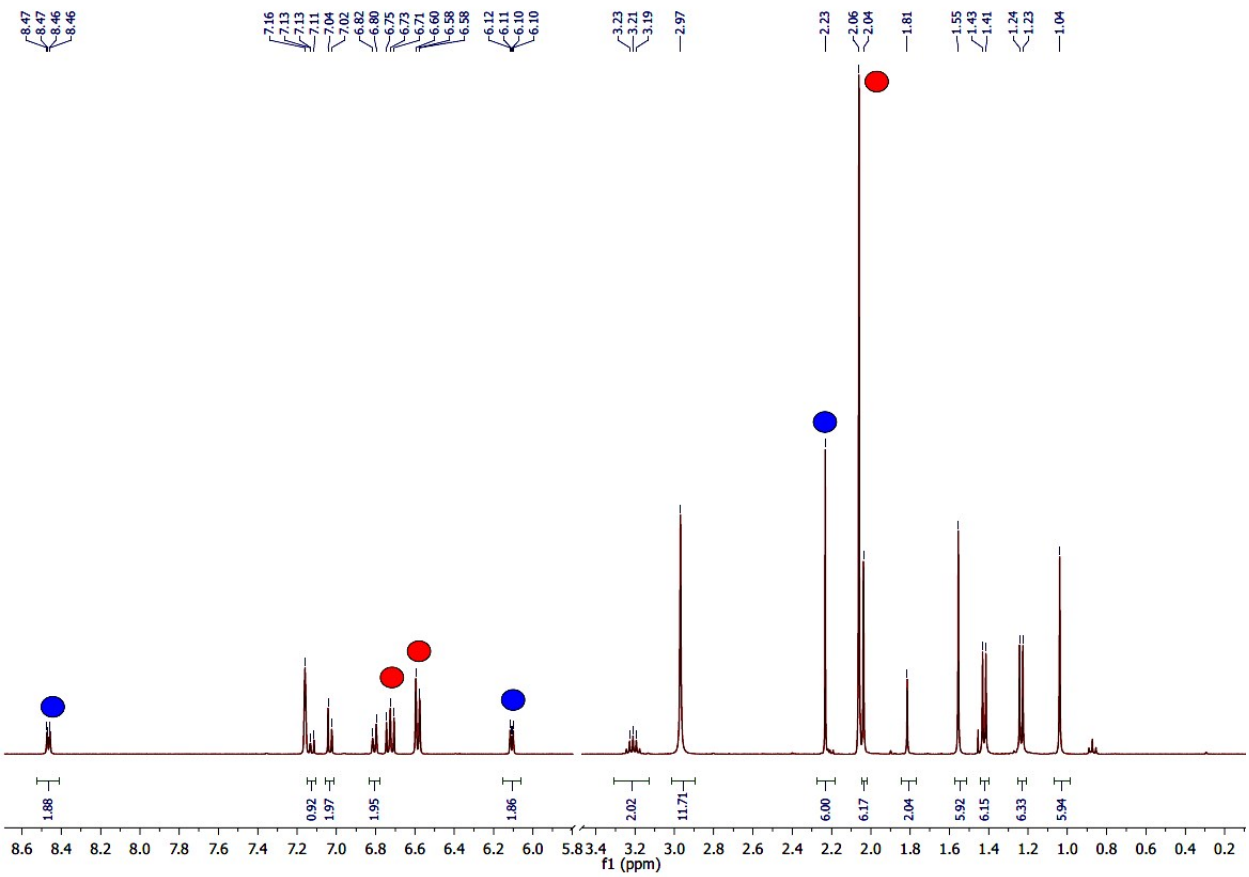


Figure S7. ^{1}H NMR (C_6D_6) spectrum of a reaction mixture initially consisting of **2c** and an excess (4.0 equivalents) of 2,6-dimethylisocyanide after sitting at 25 °C for 3 h, revealing full conversion to **2b**. Signals corresponding to free DMAP (blue) and excess 2,6-dimethylisocyanide (red) are identified.

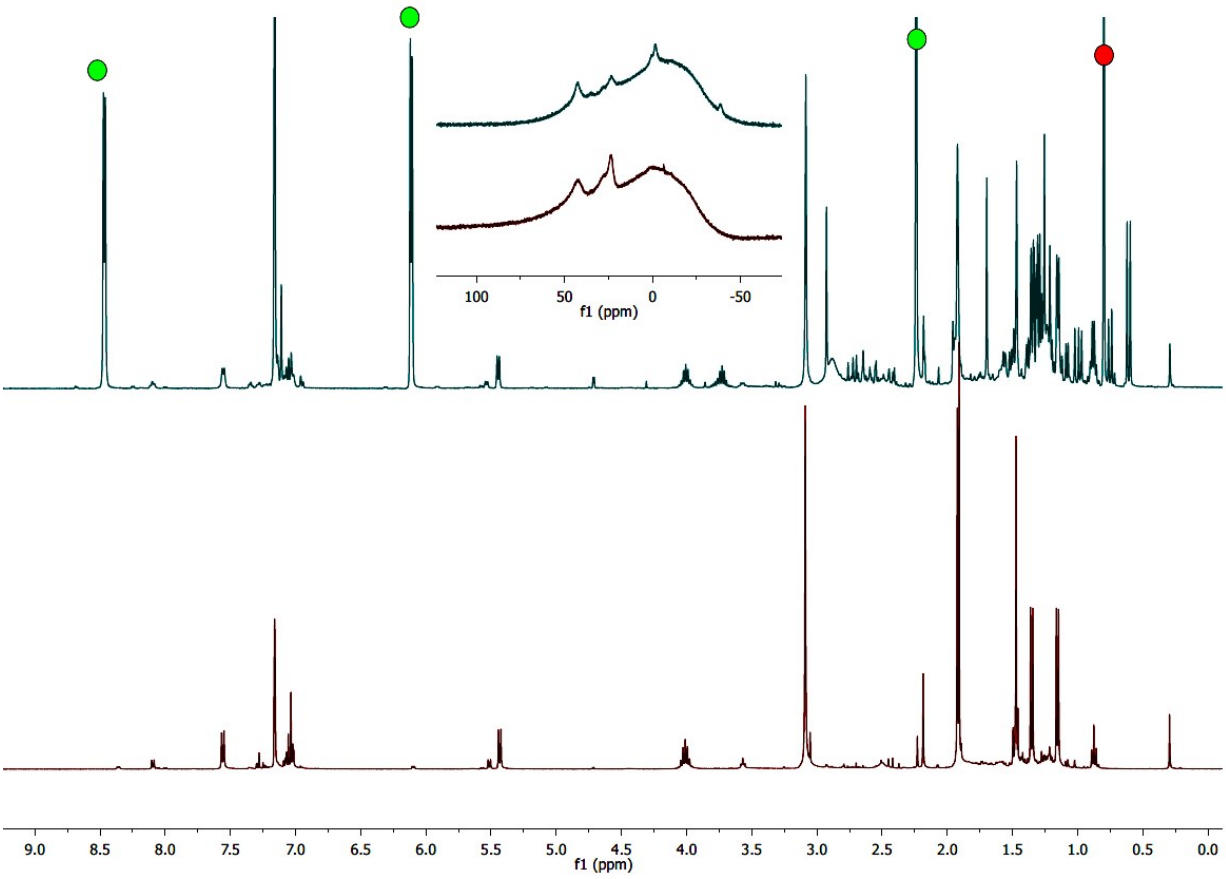


Figure S8. ^{1}H NMR (C_6D_6) and ^{11}B (inset) NMR spectra of a crude reaction mixture initially consisting of **1a** and 2.6 equivalents of N,N-dimethylaminopyridine after heating at 60 °C for 6 h, consisting approximately of **1a** (9%), **1b** (20%), **2c-I** (7%), and **2c-II** (24%), alongside other unknown decomposition products. Bottom: For reference, ^{1}H (C_6D_6) and ^{11}B (inset) NMR spectra of a mixture consisting of approximately 20% **2c-I** and 80% **2c-II**, alongside traces of other decomposition products. Signals corresponding to free DMAP (green) and excess PMe_3 (red) are identified.

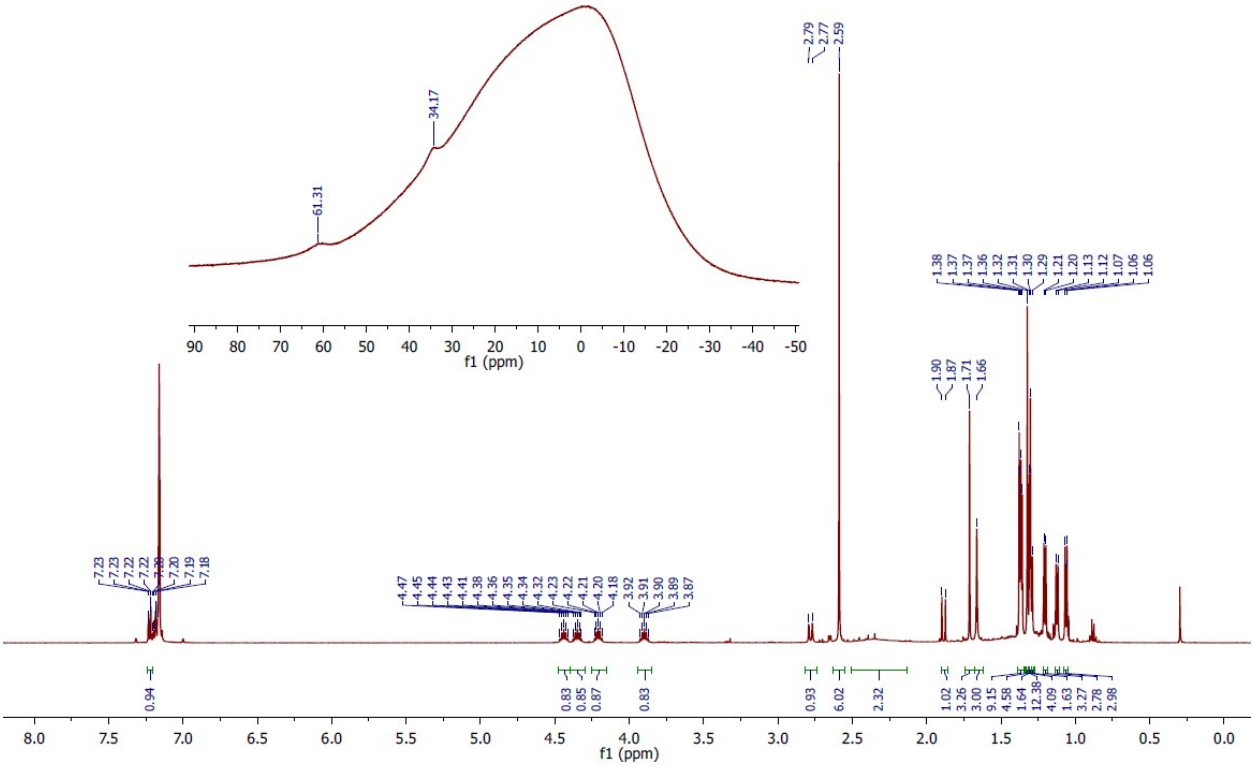


Figure S9. ^{1}H and ^{11}B (inset) NMR spectra of **3a** in C_6D_6.

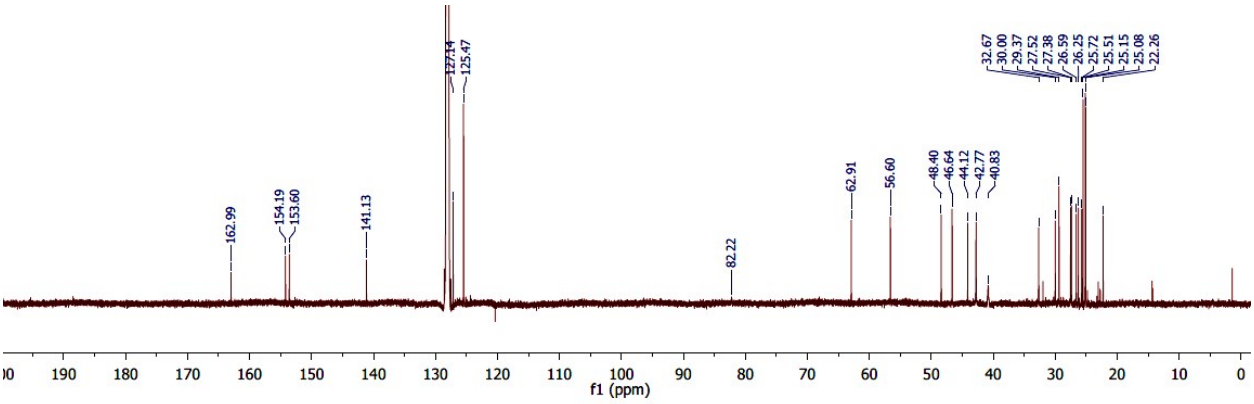


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of **3a** in C_6D_6.

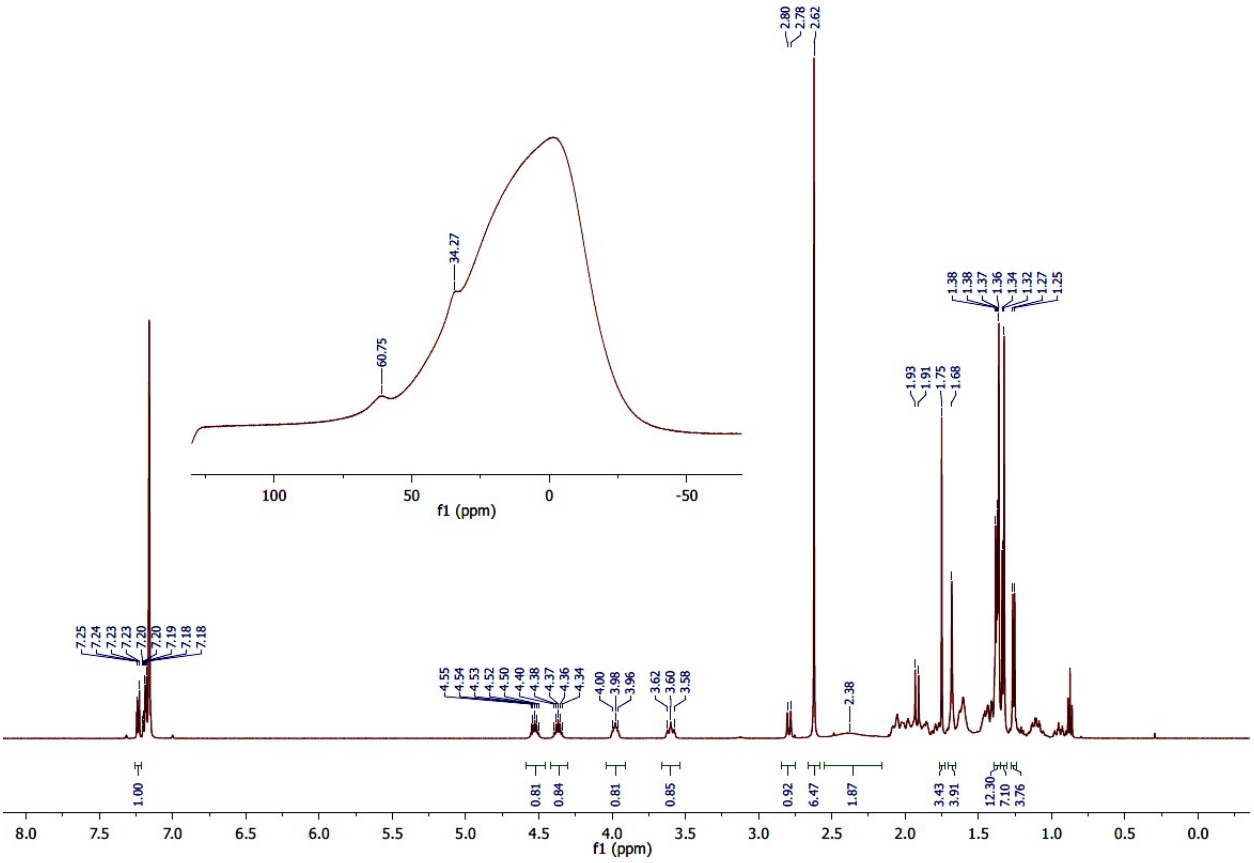


Figure S11. ^{1}H and ^{11}B (inset) NMR spectra of **3b** in C_6D_6.

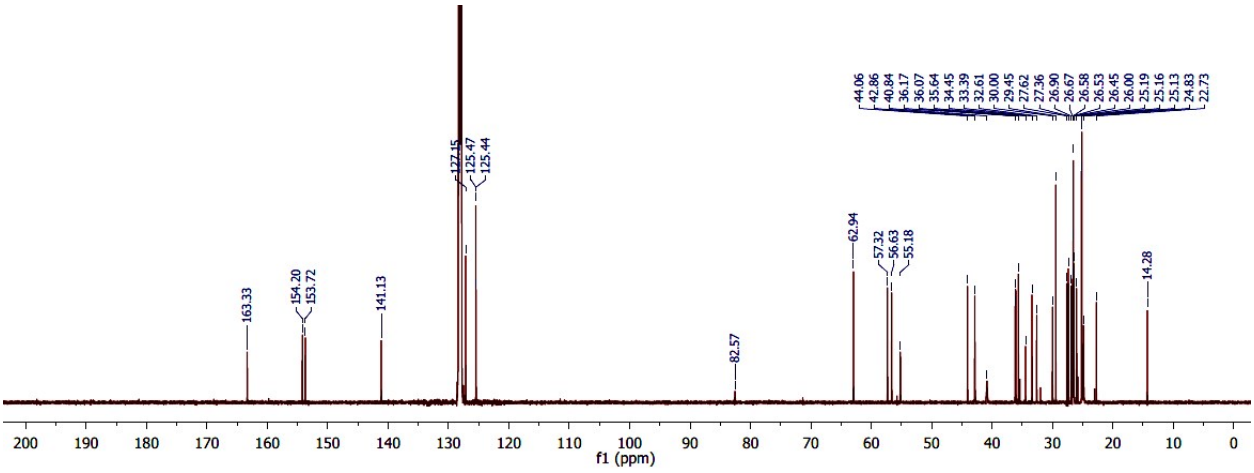


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of **3b** in C_6D_6.

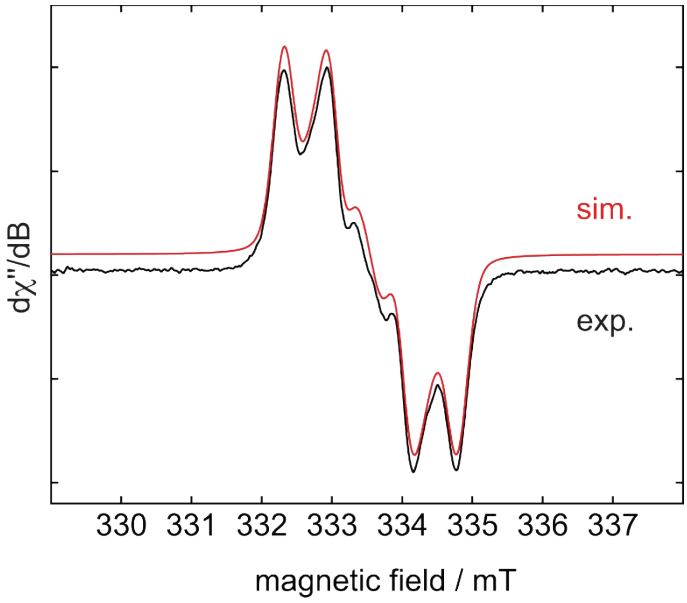


Figure S13. Experimental (black) and simulated (red) continuous-wave (CW) X-band EPR spectra of **4a** in hexane at room temperature. Experimental parameters: microwave frequency = 9.38 GHz; microwave power = 0.4 mW; modulation amplitude = 0.5 G; conversion time = 20 ms; modulation frequency = 100 kHz. Simulation parameters: g_{iso} = 2.0097, a(B) = 9.2 MHz, a(B) = 2.3 MHz, and a(N) = 17.0 MHz.

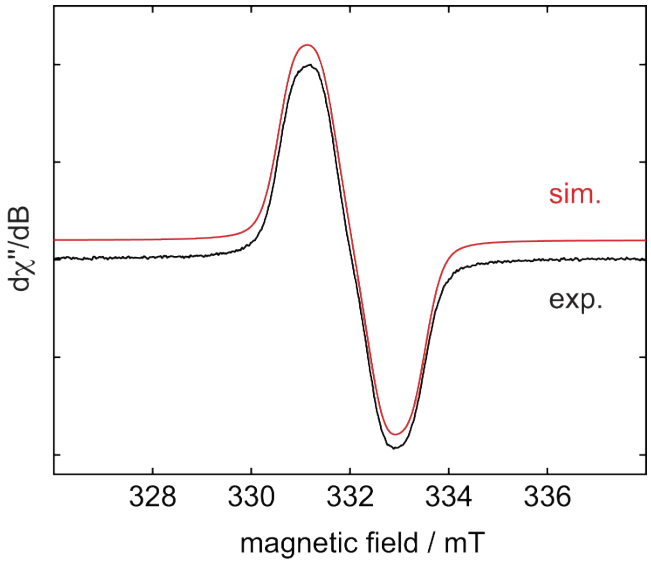


Figure S14. Experimental (black) and simulated (red) continuous-wave (CW) X-band EPR spectra of **4b** in hexane at room temperature. Experimental parameters: microwave frequency = 9.38 GHz; microwave power = 1 mW; modulation amplitude = 0.5 G; conversion time = 20 ms; modulation frequency = 100 kHz. Simulation parameters: g_{iso} = 2.0188, a(B) = 9.1 MHz, a(B) = 2.1 MHz, and a(N) = 17.0 MHz.

Kinetic Studies

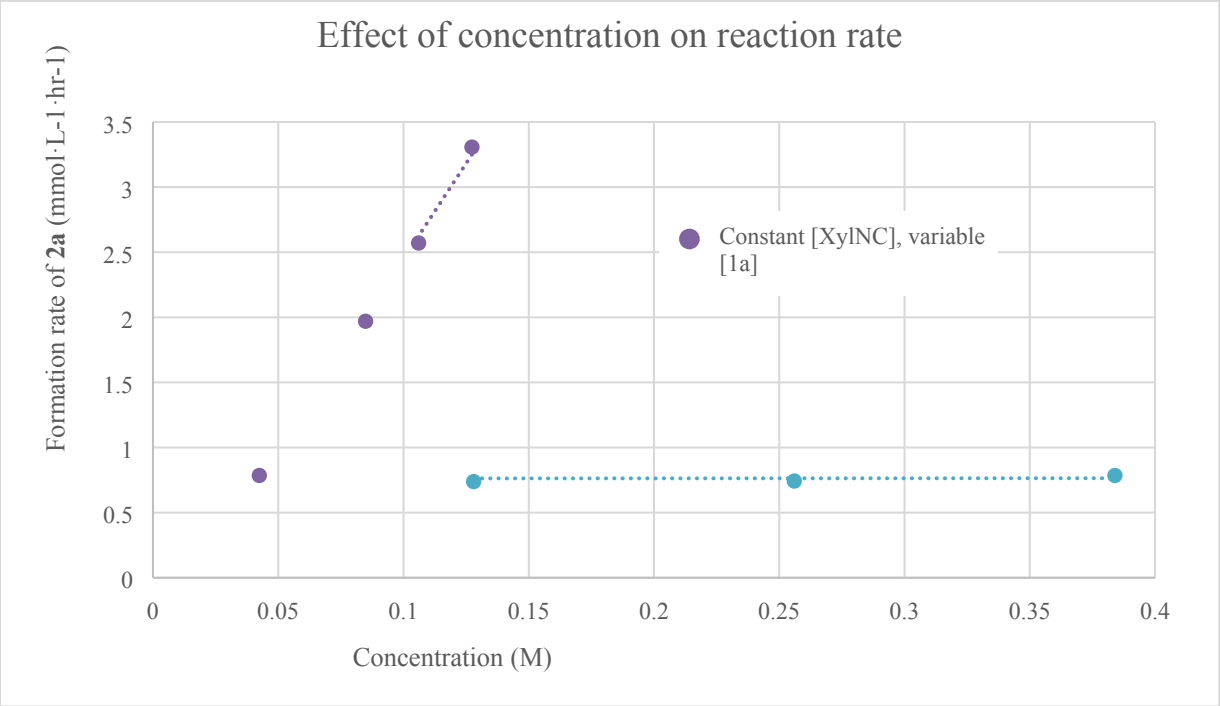


Figure S15: Effect of concentration of each reagent in the formation of **2a** from **1a** in the presence of 2,6-dimethylisocyandide (XylNC), indicating the reaction is zeroth-order in [XylNC] and first-order in [**1a**].

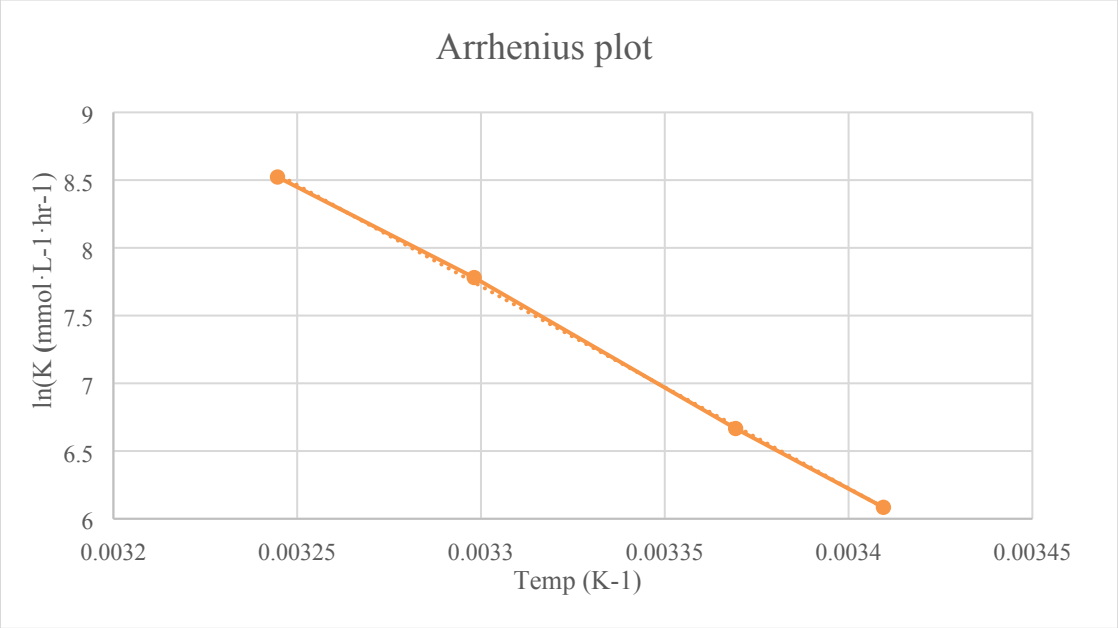


Figure S16: Arrhenius plot for the formation of **2a** from **1a** in the presence of an excess of 2,6-dimethylisocyandide (XylNC). An activation barrier of 29.3 kcal·mol^{-1} can be calculated from the Arrhenius equation.

Crystallographic details

The crystal data were collected on BRUKER X8-APEX II or BRUKER D8-QUEST diffractometers equipped with a CCD area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The structures were solved using intrinsic phasing methods,[3] refined with the SHELXL program[4] and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were assigned to idealized geometric positions, and were included in the structure factor calculations. Specific collection details can be found in the cif files.

Table S1. Crystallographic details.

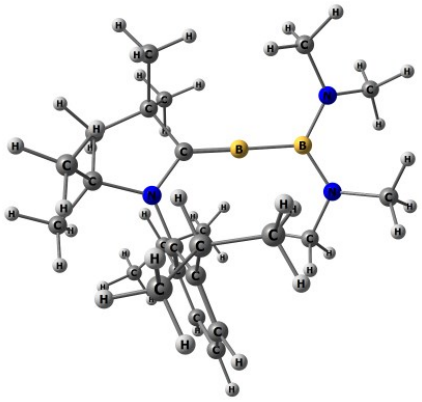
	1b	**2c**	**3a**	**3b**	**5a**	**5b**
Formula	$C_{27}H_{52}B_2N_3P$	$C_{31}H_{53}B_2N_5$	$C_{31}H_{57}B_2N_5$	$C_{37}H_{65}B_2N_5$	$2(C_{30}H_{48}B_2N_3Se)$	$2(C_{30}H_{48}B_2N_3Te)$
wt	471.30	517.40	521.43	601.56	1102.58	1199.86
Cryst. syst.	Monoclinic	Monoclinic	Monoclinic	Triclinic	Triclinic	Triclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	P-1	P-1	P-1
a(Å)	90	90	90	88.070(5)	92.4150(10)	91.628(3)
b(Å)	92.197(2)	109.529(4)	111.276(2)	79.880(5)	90.4870(10)	90.566(3)
c(Å)	90	90	90	65.914(5)	91.6220(10)	91.556(3)
α(deg)	19.3664(10)	12.0336(7)	18.2371(9)	9.710(2)	9.5614(4)	9.5211(10)
β(deg)	9.5507(4)	16.4117(7)	9.7175(4)	11.400(2)	15.9406(5)	15.9810(18)
γ(deg)	15.9131(8)	16.9907(9)	19.5071(9)	18.312(4)	19.9983(8)	20.203(2)
V(Å^3)	2941.2(2)	3162.5(3)	3221.4(3)	1820.1(7)	3044.0(2)	3071.5(6)
Z	4	4	4	2	2	2
d(calc) gcm^{-1}	1.064	1.087	1.075	1.098	1.203	1.297
R(int)	0.0900	0.1052	0.0665	0.0782	0.0794	0.1091
μ, mm^{-1}	0.112	0.063	0.062	0.063	1.256	0.991
Total data	38051	27199	31616	31151	103336	53916
$>2\sigma(F_0^2)$	4268	3578	4850	4924	12389	10359
Parameters	334	357	387	409	673	667
R_1 ($>2\sigma$)	0.0447	0.0523	0.0490	0.0529	0.0303	0.0442
R_w	0.1090	0.1315	0.1279	0.1242	0.0806	0.1000
GOOF	1.012	1.016	1.042	1.012	1.025	0.977
CCDC#	2018686	2018688	2018683	2018685	2018687	2018684

Computational Details

Density functional theory calculations were employed to optimize all the molecules without any geometrical constraints using meta hybrid exchange-correlation energy functional M06[5] in conjunction with the Def2-SVP basis set.[6] Dispersion effects were incorporated by using D3 version of Grimme's dispersion correction coupled with the original D3 damping function with the keyword Empiricaldispersion=GD3.[7] Frequency calculations were carried out at the same level of theory to check the nature of the stationary points and all the structures were characterized as minima with real vibrational frequencies. Bonding analysis was performed with the help of NBO routine[8] as implemented in the Gaussian 09 suit of programs.[9]

Optimized Geometries and Coordinates of the Free Borylborylene [CAAC=B-B(NMe_2)$_2$)] and its Adducts [CAAC=B(L)-B(NMe_2)$_2$] with Different Donors (L) Computed at the M06 (D3)/Def2-SVP Level of Theory

1. Free Borylborylene [CAAC=B-B(NMe_2)$_2$]



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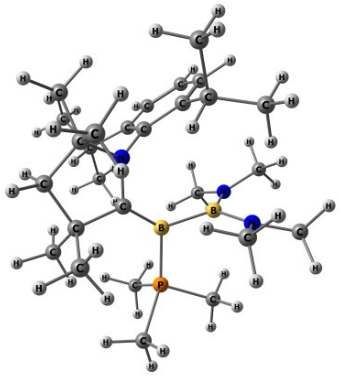
Adducts of Borylborylene with L: [CAAC=B(L)-B(NMe_2)$_2$]

1a (L = PMe_3)



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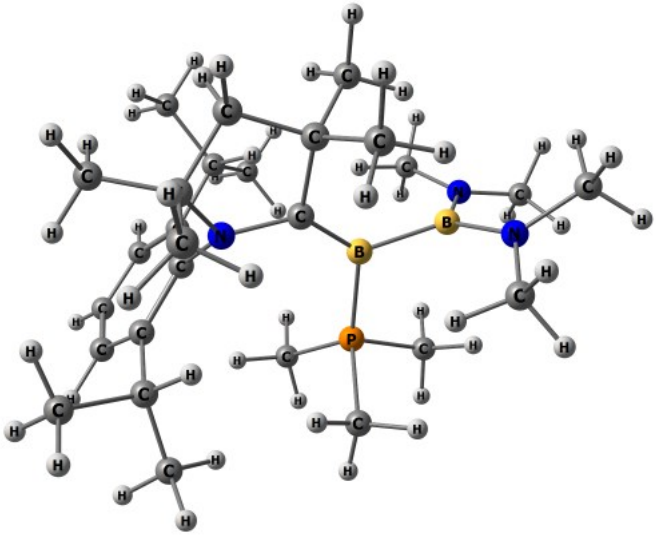
1b (L = PMe_3, *Z* isomer)



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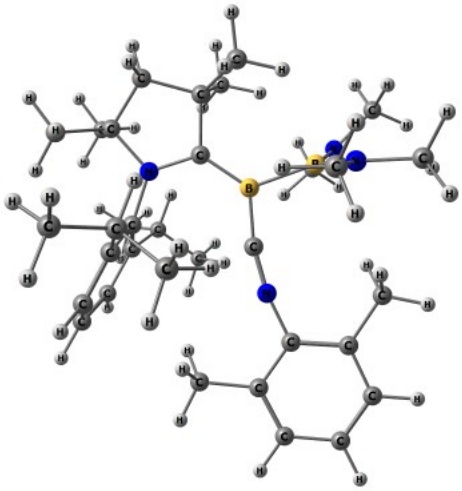
2a (L = 2,6-dimethylphenylisocyanide)



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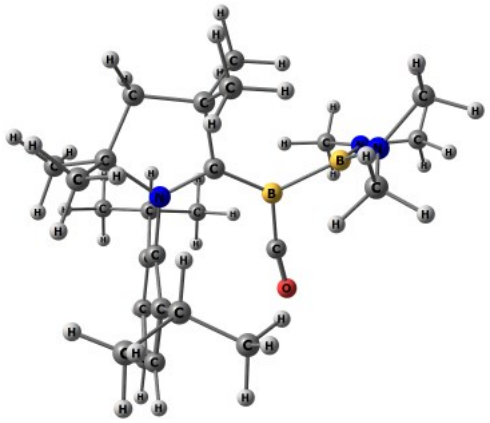
2b (L = CO)



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1	5.631880000	2.016480000	-0.388254000
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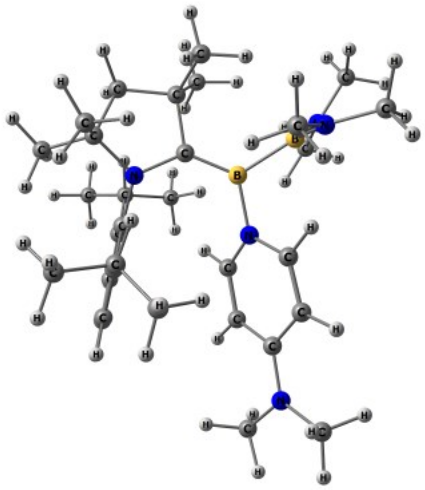
2c (L = (4-dimethylamino)pyridine)



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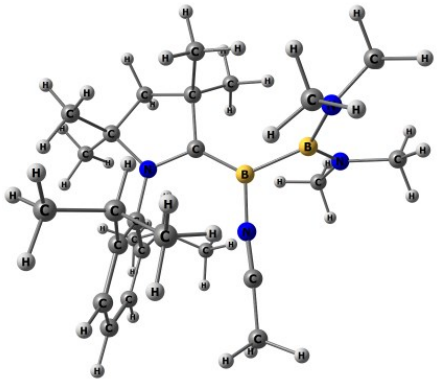
L = NCMe



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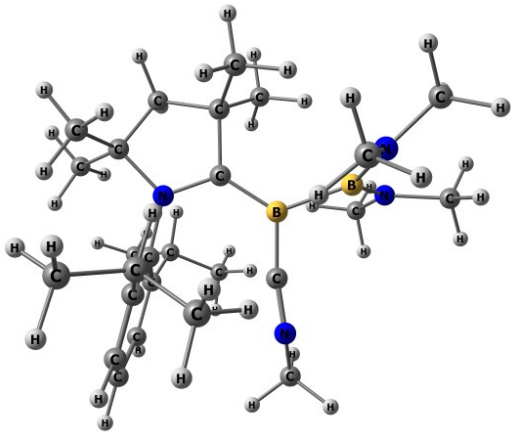

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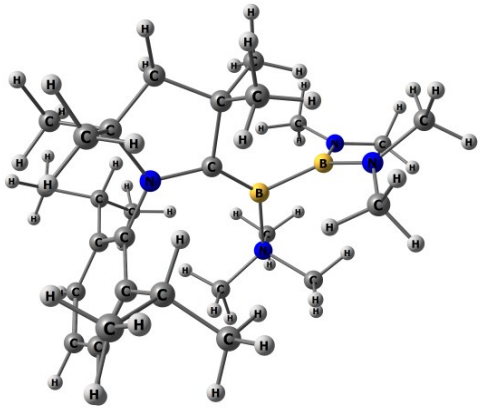

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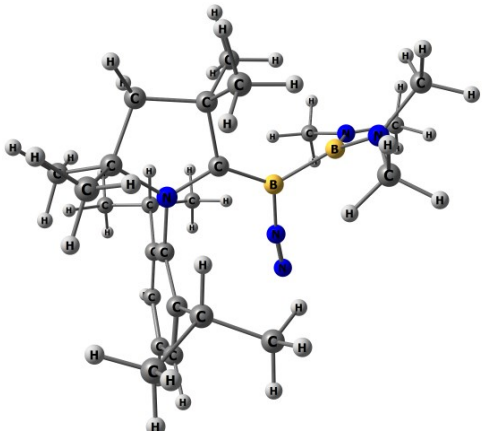

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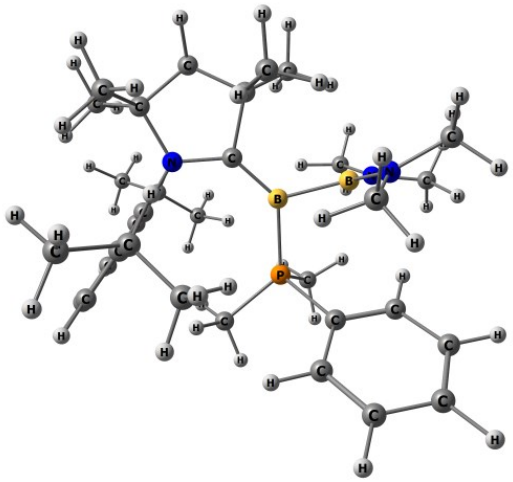

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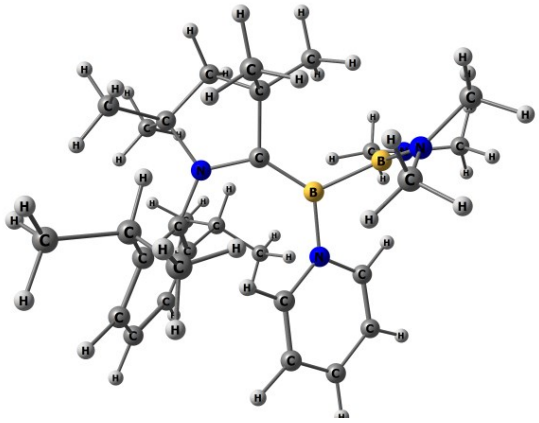

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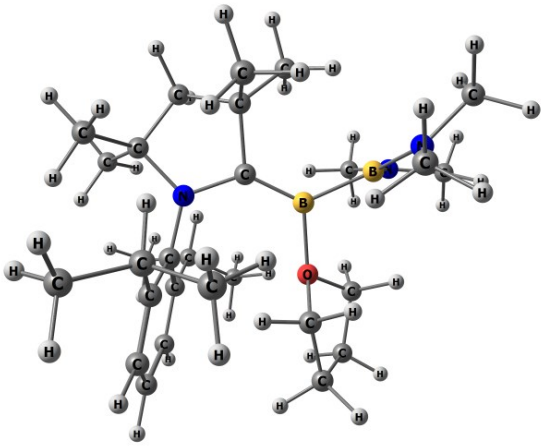

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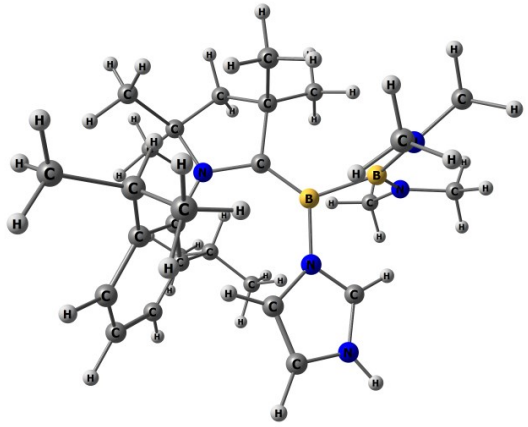

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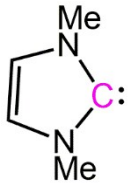

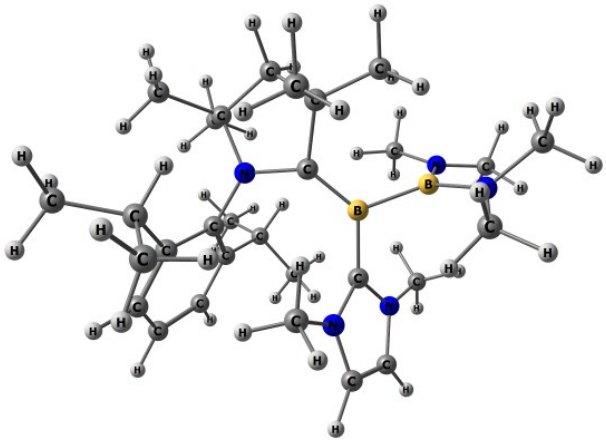

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1	-5.177403000	-0.576552000	1.988266000
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1	-5.711519000	1.239196000	-1.853909000
1	-4.538392000	2.559927000	-2.060794000
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6	0.211181000	3.132191000	-1.252416000
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1	0.232326000	4.237463000	-1.225618000
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1	3.766485000	2.079136000	1.050886000
1	3.111453000	3.540404000	1.805850000
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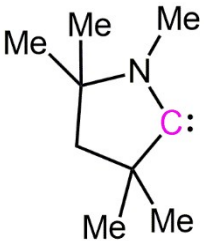

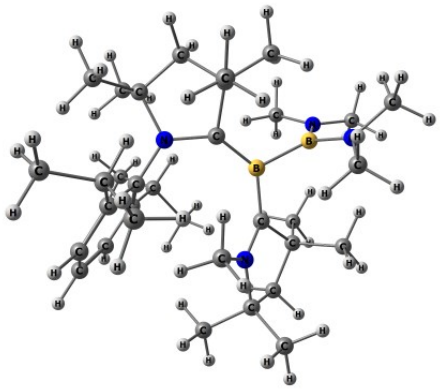

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6	3.576034000	2.021837000	-0.703360000
1	4.093529000	1.051039000	-0.667608000
1	3.228286000	2.163845000	-1.738268000
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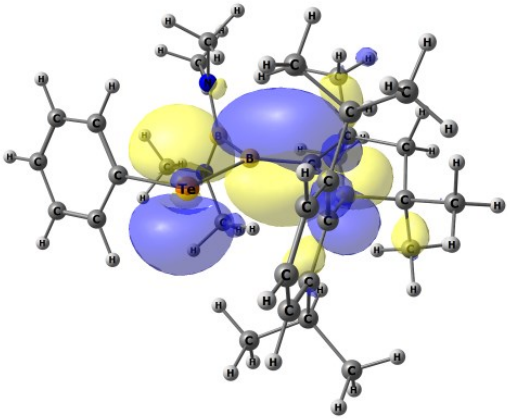
1	-1.340195000	4.149367000	-1.064724000
1	-0.954010000	3.670037000	0.605323000

Optimized Geometries, SOMO, Spin density, and Coordinates of the Telluroborane and selenoborane radicals 4a and 4b computed at the M06 (D3)/Def2-SVP Level of Theory



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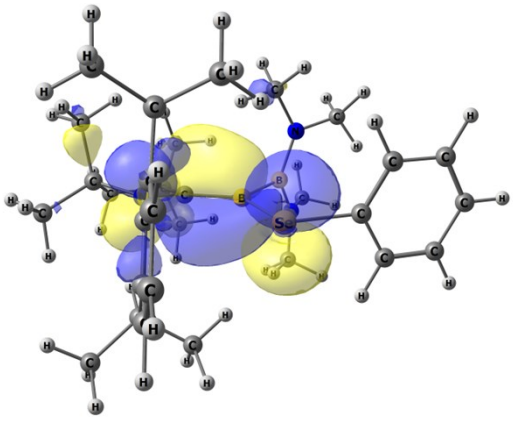

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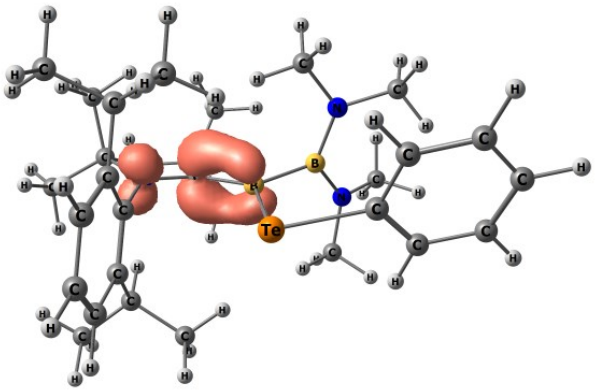

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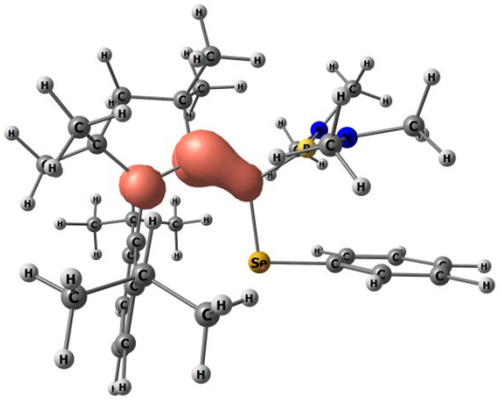

4b

Figure S17. Optimized Geometry of **4a** and **4b** with the corresponding SOMO (top) and spin density (bottom).

Optimized coordinates of **4a**

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7	2.624292000	2.227879000	-0.717458000
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6	3.743100000	-0.863055000	-1.379312000
1	3.319940000	-0.374368000	-2.262838000
6	5.126647000	-0.898805000	-1.208783000
1	5.777100000	-0.427204000	-1.952602000
6	5.679813000	-1.544633000	-0.104350000
1	6.765509000	-1.578784000	0.026108000
6	4.842550000	-2.154286000	0.828100000
1	5.269559000	-2.670384000	1.693958000
6	3.457923000	-2.105496000	0.665309000
1	2.807277000	-2.580492000	1.409410000
6	-0.881619000	1.302569000	0.275451000
6	-1.064458000	2.810862000	0.503585000
6	-2.593121000	2.968015000	0.559249000
1	-2.911025000	3.775599000	1.241133000
1	-2.972456000	3.224710000	-0.446624000
6	-3.160797000	1.610217000	0.965931000
6	-4.535508000	1.353090000	0.374159000
1	-4.554982000	1.496737000	-0.716013000
1	-5.256331000	2.059379000	0.817043000
1	-4.888759000	0.331746000	0.595071000
6	-2.411466000	-0.608887000	-0.085904000
6	-2.684602000	-0.763421000	-1.468030000
6	-2.963258000	-2.043243000	-1.954210000
1	-3.166014000	-2.179250000	-3.021643000
6	-2.993017000	-3.145201000	-1.108668000
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6	-2.129181000	-1.633989000	2.262929000
1	-1.856838000	-0.588249000	2.481657000
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1	-0.756155000	-2.370162000	3.770925000
1	-0.033253000	-2.246528000	2.141015000
6	-3.367222000	-1.999932000	3.079588000
1	-4.262892000	-1.440201000	2.761694000
1	-3.204531000	-1.805298000	4.153205000
1	-3.604897000	-3.072481000	2.971745000

6	-2.704544000	0.406094000	-2.436129000
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5	1.983655000	1.423019000	0.294176000
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1	0.799449000	0.542666000	2.442584000
1	1.951138000	1.276765000	3.589261000
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1	3.394354000	4.160406000	-0.984652000
1	4.644380000	2.896580000	-0.897050000
5	0.474676000	0.670622000	0.004902000

Optimized coordinates of **4b**

34	0.709113000	-1.429104000	-0.397836000
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1	2.191390000	-0.156137000	3.185536000

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