Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Transition-metal-like coordination chemistry of dicoordinate borylenes with organic azides

Robert Witte,[ab] Sourav Kar,[ab] Krzysztof Radacki,[ab] Marcel Härterich,[ab] Maximilian Rang,[ab] Maximilian Michel,[ab] Cornelius Mihm,[ab] Corinna Czernetzki,[ab] Tobias Brückner,[ab] Eva Beck,[ab] Sarah Lutz,[ab] Rian D. Dewhurst,[ab] and Holger Braunschweig*[ab]

[a]*Institute for Inorganic Chemistry, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany.*

[b]*Institute for Sustainable Chemistry & Catalysis with Boron, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany.*

Contents

Methods and materials

All manipulations were performed either under an atmosphere of dry argon or *in vacuo* using standard Schlenk line or glovebox techniques. Deuterated solvents were dried over molecular sieves and degassed by three freeze-pump-thaw cycles prior to use. All other solvents were distilled and degassed from appropriate drying agents. Both deuterated and non-deuterated solvents were stored under argon over activated 4 Å molecular sieves. NMR spectra were acquired either on a Bruker Avance 500 or a Bruker Avance 400 NMR spectrometer. Chemical shifts (δ) are provided in ppm and internally referenced to the carbon nuclei ($^{13}C\{^{1}H\}$) or residual protons (^{1}H) of the solvent. Heteronuclei NMR spectra are referenced to external standards (^{11}B: $BF_3{\cdot}OEt_2$). Solid-state IR spectra were recorded on a Bruker FT-IR spectrometer ALPHA II inside a glovebox. Microanalyses (C, H, N, S) were performed on an Elementar vario MICRO cube elemental analyzer. High-resolution mass spectrometry (HRMS) data were obtained from a Thermo Scientific Exactive Plus spectrometer in LIFDI (*Linden CMS*) or ASAP mode. UV-vis spectra were measured on a Metler Toledo UV-vis-Excellence UV5 spectrophotometer.

Solvents and reagents (phenylazide) were purchased from Sigma-Aldrich, Alfa Aesar and Merck. Reagents were used without further purification. The borylenes (Tip-CO-Borylene (**1**),[1] [{(CAAC)TipB}$_2$(μ_2-N_4K_2)] (**2**),[2] (CAAC^{Me})B(TMP) (**5**)[3]) as well as the arylazides (1-azido-2,6-dichlorobenzene,[4] 1-azido-4-methoxybenzene,[5] mesitylazide[6]) were synthesized using literature procedures.

Synthetic procedures

Synthesis of 4a

Release of borylene by photolysis of a borylene carbonyl:

A solution of **1** (20.0 mg, 37.9 µmol) and phenylazide (25 mg, 200 µmol) in 1 mL benzene was irradiated with an LED (average wavelength: 365 nm) for 5 h at room temperature. A color change from orange to red was observed. The solvent was removed *in vacuo* and the resulting residue was rinsed with 1 mL of hexane to afford **4a** as a red powder (17 mg, 69%).

Release of borylene by N_2 elimination:

A solution of **2** (50.0 mg, 44.1 µmol) in 5 mL Toluene was stirred and rapidly treated with phenylazide (30.5 mg, 250 µmol), after which immediate gas evolution concomitant with a color change from deep blue to red was observed. The reaction mixture was stirred for 30 min at room temperature and the solvent subsequently removed *in vacuo*. The residue was washed with 2 mL of pentane to afford compound **4a** as a red powder (41.2 mg, 75%). Single crystals suitable for single-crystal X-ray analysis were obtained by slow evaporation of a saturated pentane solution at room temperature.

^{1}H NMR (500.1 MHz, benzene-d_6): δ = 7.42 – 7.37 (m, 2H, *o*-C*H*^{Phenyl}), 7.08 – 6.99 (m, 5H, *m*-C*H*^{Dip}, *m*-C*H*^{Phenyl}, *p*-C*H*^{Phenyl}), 6.80 – 6.75 (m, 1H, *p*-C*H*^{Dip}), 3.33 (sept, ^3J = 6.7 Hz, 2H, C*H*$(CH_3)_2^{Tip}$), 2.86 (sept, ^3J = 6.9 Hz, 1H, C*H*$(CH_3)_2^{Tip}$), 2.71 (sept, ^3J = 6.6 Hz, 2H, C*H*$(CH_3)_2^{Dip}$), 1.81 (d, ^3J = 6.6 Hz, 6H, CH(C*H*$_3)_2^{Dip}$), 1.59 (d, ^3J = 6.5 Hz, 6H, CH(C*H*$_3)_2^{Tip}$), 1.52 (d, ^3J = 6.8 Hz, 6H, CH(C*H*$_3)_2^{Tip}$), 1.35 (s, 2H, C*H*$_2^{CAAC}$), 1.26 (d, ^3J = 6.9 Hz, 6H, CH(C*H*$_3)_2^{Tip}$), 1.23 (d, ^3J = 6.6 Hz, 6H, CH(C*H*$_3)_2^{Dip}$), 1.13 (s, 6H, C*H*$_3^{CAAC}$), 0.87 (s, 6H, C*H*$_3^{CAAC}$) ppm. *Two aromatic meta-CH protons of the Tip moiety are overlapping with the deuterated solvent resonance.*

^{13}C{^{1}H} NMR (125.8 MHz, benzene-d_6): δ = 210.9 (*C*$_q^{Carbene}$), 154.0 (*i*-*C*$_q^{Phenyl}$), 151.9 (*o*-*C*$_q^{Tip}$), 148.0 (*p*-*C*$_q^{Tip}$), 143.6 (*o*-*C*$_q^{Dip}$), 134.4(*i*-*C*$_q^{Dip}$), 128.9 (*p*-*C*H^{Dip}), 128.5 (*m*-*C*H^{Phenyl}), 125.1 (*m*-*C*H^{Dip}), 123.6 (*p*-*C*H^{Phenyl}), 121.3 (*o*-*C*H^{Phenyl}), 120.0 (*m*-*C*H^{Tip}), 77.1 (*C*$_q^{CAAC}$), 51.8 (*C*$_q^{CAAC}$), 51.7 (*C*H$_2^{CAAC}$), 36.0 (*C*H$(CH_3)_2^{Tip}$), 34.7 (*C*H$(CH_3)_2^{Tip}$), 30.0 (*C*H$(CH_3)_2^{Dip}$), 28.9 (*C*H$_3^{CAAC}$), 28.2 (CH(*C*H$_3)_2^{Tip}$), 26.9 (CH(*C*H$_3)_2^{Dip}$), 24.6 (CH(*C*H$_3)_2^{Dip}$), 24.4 (CH(*C*H$_3)_2^{Tip}$),

23.2 ($CH(CH_3)_2^{Tip}$) ppm. *The ipso carbon atom of the Tip substituent could not be detected due to quadrupole broadening*.

^{11}B NMR (160.5 MHz): δ = 16.1 (s) ppm.

HRMS (LIFDI): calcd. for $[C_{41}H_{60}BN_4]^+ = [M + H]^+$: 619.4906; found: 619.4903.

UV/vis (THF): λ_{max} = 324 nm, λ_2 = 448 nm.

Synthesis of 4b

Release of borylene by photolysis of a borylene carbonyl:

A solution of **1** (20.0 mg, 37.9 µmol) and mesityl azide (12 mg, 74.4 µmol) in 1 mL benzene was irradiated with a LED (average wavelength: 365 nm) for 5 h at room temperature. A color change from orange to red was observed. The solvent was removed *in vacuo* and the resulting residue was washed with 1 mL of hexane to afford **4b** as a red powder (19 mg, 76%).

Release of borylene by N_2 elimination:

A solution of **2** (50.0 mg, 44.1 µmol) in 5 mL toluene was stirred and rapidly treated with mesityl azide (42.0 mg, 261 µmol), after which immediate gas evolution concomitant with a color change from deep blue to green was observed. The reaction mixture was stirred for 2 h at room temperature whereupon another color change from green to dark red was observed, and the solvent was subsequently removed *in vacuo*. The residue was washed with 2 mL of pentane to afford compound **4b** as a red powder (54.1 mg, 93%). Single crystals suitable for single-crystal X-ray analysis were obtained by slow evaporation of a saturated pentane solution at room temperature.

^{1}H NMR (500.1 MHz, C_6D_6): δ = 7.09 (s, 1H, C*H*^{Dip}), 7.08 (m, 1H, C*H*^{Dip}), 6.71 (m, 2H, *m*-C*H*^{Mes}), 3.22 (sept, ^3J = 6.7 Hz, 2H, C*H*$(CH_3)_2^{Tip}$), 2.90 (sept, ^3J = 6.9 Hz, 1H, C*H*$(CH_3)_2^{Tip}$), 2.71 (sept, ^3J = 6.6 Hz, 2H, C*H*$(CH_3)_2^{Dip}$), 2.12 (s, 3H, *p*-C*H*$_3^{Mes}$), 1.78 (s, 6H, *o*-C*H*$_3^{Mes}$), 1.68 (d, ^3J = 6.6 Hz, 6H, CH(C*H*$_3)_2^{Dip}$), 1.51 (d, ^3J = 6.6 Hz, 6H, CH(C*H*$_3)_2^{Tip}$), 1.48 (d, ^3J = 6.8 Hz, 6H, CH(C*H*$_3)_2^{Tip}$), 1.39 (s, 2H, C*H*$_2^{CAAC}$), 1.33 (d, ^3J = 6.9 Hz, 6H, CH(C*H*$_3)_2^{Tip}$), 1.23 – 1.21 (m, 6H, CH(C*H*$_3)_2^{Dip}$), 1.21 (s, 6H, C*H*$_3^{CAAC}$), 0.89 (s, 6H, C*H*$_3^{CAAC}$) ppm. *Two meta-CH protons of the Tip moiety and one aromatic CH of the Dip moiety are overlapping with the deuterated solvent resonance*.

$^{13}C\{^1H\}$ NMR (125.8 MHz, C_6D_6): δ = 210.8 ($C_q^{Carbene}$), 151.6 (*o*-C_q^{Tip}), 150.0 (*i*-C_q^{Mes}), 148.0 (*p*-C_q^{Tip}), 143.9 (*o*-C_q^{Dip}), 134.8 (*i*-C_q^{Dip}), 132.3 (*o*-C_q^{Mes}), 130.6 (*p*-C_q^{Mes}), 128.7 (*m*-CH^{Mes}), 128.4 (*p*-CH^{Dip}), 125.0 (*m*-CH^{Dip}), 120.5 (*m*-CH^{Tip}), 77.1 (C_q^{CAAC}), 51.8 (C_q^{CAAC}), 51.8 (CH_2^{CAAC}), 35.8 ($CH(CH_3)_2^{Tip}$), 35.0 ($CH(CH_3)_2^{Tip}$), 30.1 ($CH(CH_3)_2^{Dip}$), 29.1 (CH_3^{CAAC}), 28.9 (CH_3^{CAAC}), 27.7 ($CH(CH_3)_2^{Tip}$), 27.2 ($CH(CH_3)_2^{Dip}$), 24.6 ($CH(CH_3)_2^{Tip}$), 24.4 ($CH(CH_3)_2^{Dip}$), 23.9 ($CH(CH_3)_2^{Tip}$), 21.0 (*p*-CH_3^{Mes}), 18.0 (*o*-CH_3^{Mes}) ppm.

^{11}B NMR (160.5 MHz): δ = 15.5 (s) ppm.

HRMS (LIFDI): calcd. for $[C_{44}H_{66}BN_4]^+ = [M + H]^+$: 661.5375; found: 661.5363.

UV/vis (THF): λ_{max} = 434 nm, λ_2 = 601 nm (weak)).

Synthesis of 6a and conversion to 7a

A solution of **5** (50 mg, 114.5 µmol) in 5 mL hexane was stirred and treated with phenyl azide (13.6 mg, 114.5 µmol), after which an immediate color change from orange to dark red could be observed. The reaction mixture was then stored at –30 °C for 48 h yielding compound **6a** (32 mg, 71%) as red crystals. The residual solvent was removed *in vacuo*. Suitable crystals for X-ray diffraction were obtained by crystallization from a saturated hexane solution at –30 °C.

^1H NMR (500.1 MHz, toluene-d_8, –30 °C): δ = 7.63 – 7.59 (m, 2H, *o*-CH^{Phenyl}), 7.23 – 7.17 (m, 2H, *m*-CH^{Phenyl}), 6.93 – 6.88 (m, 4H, *p*-CH^{Phenyl}, CH^{Dip}), 2.54 – 2.45 (sept, ^3J = 6.5 Hz, 2H, $CH(CH_3)_2^{Dip}$), 1.71 (d, ^3J = 6.5 Hz, 6H, $CH(CH_3)_2^{Dip}$), 1.60 (s, 6H, CH_3^{CAAC}), 1.51 (s br, 12H, CH_3^{TMP}), 1.31 (s, 2H, CH_2^{CAAC}), 1.16 (d, ^3J = 6.6 Hz, 6H, $CH(CH_3)_2^{Dip}$), 0.76 (s, 6H, CH_3^{CAAC}), 1.88 – 1.15 (br m, 8 H, CH_2^{TMP} assigned *via* HSQC) ppm.

^{13}C NMR (125.8 MHz, toluene-d_8, –30 °C): δ = 213.9 (C_q-$Carbene^{CAAC}$), 154.5 (*i*-C_q^{Phenyl}), 142.9 (C_q^{Dip}), 134.9 (*i*-C_q^{Dip}), 128.26 (CH^{Dip}), 125.42 (CH^{Dip}), 123.18 (*p*-CH^{Phenyl}), 120.89 (*o*-CH^{Phenyl}), 76.0 (C_q^{CAAC}), 53.0 (C_q^{TMP}), 52.1 (C_q^{CAAC}), 51.8 (CH_2^{CAAC}), 39.1 (CH_2^{TMP}), 32.2 (CH_2^{TMP}), 30.8 (CH_3^{CAAC}), 29.2 ($CH(CH_3)_2^{Dip}$), 28.8 (CH_3^{CAAC}), 27.1 ($CH(CH_3)_2^{Dip}$), 24.5 ($CH(CH_3)_2^{Dip}$), 19.2 (CH_2^{TMP}) ppm.

^{11}B NMR (160.5 MHz, toluene-d_8, –30 °C): δ = 13.2 (br s) ppm.

Elemental analysis (%) calcd. for $C_{35}H_{54}BN_5$: C 75.65, H 9.80, N 12.60; found: C 75.41, H 9.69, N 12.69.

UV/vis (hexane): λ_{max} = 341 nm, λ_2= 465 nm.

After 3 h at room temperature in solution, compound **6a** rearranges to compound **7a**. Suitable crystals for X-ray diffraction were obtained by storing the solution at −30 °C. Due to further decomposition as well as different rotational isomers of compound **7a**, it was not possible to obtain clean ^{1}H or ^{13}C NMR spectra.

^{11}B NMR (160.5 MHz, toluene-d_8): δ= 36.4 (br s) ppm.

Synthesis of 6b and conversion to 7b

A solution of **5** (100 mg, 229.1 µmol) in 10 mL hexane was stirred and treated with 1-azido-4-methoxybenzene (34.2 mg, 229.1 µmol) after which an immediate color change from orange to dark red was observed. The reaction mixture was then stored at −30 °C for 48 h, yielding compound **6b** (98 mg, 73%) as red crystals. The residual solvent was removed *in vacuo*. Suitable crystals for X-ray diffraction were obtained by crystallization from a saturated hexane solution at −30 °C.

^{1}H NMR (500.1 MHz, toluene-d_8, −30 °C): δ = 7.58 – 7.56 (m, 2H, *m*-C*H*^{Phenyl}), 6.97 – 6.91 (m, 3H, C*H*^{Dip}), 6.73 – 6.70 (m, 2H, *o*-C*H*^{Phenyl}), 3.22 (s, 3H, OC*H*$_3$), 2.54 (sept., ^3J = 6.6 Hz, 2H, C*H*(CH$_3$)$_2^{Dip}$), 1.73 (d, ^3J = 6.5 Hz, 6H, CH(C*H*$_3$)$_2^{Dip}$), 1.63 (s, 6H, C*H*$_3^{CAAC}$), 1.54 (br s, 12H, C*H*$_3^{TMP}$), 1.33 (s, 2H, C*H*$_2^{CAAC}$), 1.19 (d, ^3J = 6.6 Hz, CH(C*H*$_3$)$_2^{Dip}$), 0.78 (s, 6H, C*H*$_3^{CAAC}$), 1.88 – 1.15 (br m, 8 H, C*H*$_2^{TMP}$ assigned *via* HSQC) ppm.

^{13}C NMR (125.8 MHz, toluene-d_8, −30 °C): δ = 213.7 (*C*$_q$-Carbene^{CAAC}), 156.5 (*i*-*C*$_q^{Ar}$), 148.1 (*C*$_q^{Ar}$), 142.9 (*C*$_q^{Dip}$), 134.8 (*C*$_q^{Dip}$), 121.6 (*o*-*C*H^{Ar}), 113.7 (*m*-*C*H^{Ar}), 75.9 (*C*$_q^{CAAC}$), 54.4 (*C*H$_3^{Ar}$), 52.9 (*C*$_q^{TMP}$), 52.0 (*C*$_q^{CAAC}$), 51.9 (*C*H$_2^{CAAC}$), 39.0 (*C*H$_2^{TMP}$), 33.3 – 31.5 (br, *C*H$_3^{TMP}$), 30.8 (*C*H$_3^{CAAC}$), 29.2 (*C*H(CH$_3$)$_2^{Dip}$), 27.1 (CH(*C*H$_3$)$_2^{Dip}$), 19.2 (*C*H$_2^{TMP}$) ppm.

^{11}B NMR (160.5 MHz, toluene-d_8, −30 °C): δ= 14.0 (br s) ppm.

Elemental analysis (%) calcd. for $C_{36}H_{56}BN_5O$: C 73.83, H 9.64, N 11.96; found: C 73.75, H 10.00, N 11.92.

UV/vis (hexane): λ_{max} = 345 nm, λ_2 = 468 nm.

After 3 h at room temperature in solution, compound **6b** rearranges to compound **7b**. Suitable crystals for X-ray diffraction were obtained by storing a hexane solution of compound **7b** at −30 °C. Due to further decomposition as well as different rotational isomers of compound **7b**, it was not possible to obtain clean ^{1}H or ^{13}C NMR spectra.

^{11}B NMR (160.5 MHz, toluene-d_8): δ = 36.5 (br s) ppm.

Synthesis of 6c

A solution of **5** (50 mg, 114.5 µmol) in 5 mL hexane was stirred and treated with 1-azido-2,6-dichlorbenzene (21.5 mg, 114.5 µmol) after which a color change from orange to dark red could be observed. The reaction mixture was stirred for 30 min at room temperature and the solvent subsequently removed *in vacuo* to afford compound **6c** as a dark red powder (69 mg, 97%). Single crystals suitable for single-crystal X-ray analysis could be obtained from slow evaporation of a saturated hexane solution.

^{1}H NMR (500.1 MHz, benzene-d_6): δ = 7.15 – 7.09 (m, 3H, C*H*^{Dip}), 7.06 (d, ^{3}J = 8.0 Hz, 2H, *m*-C*H*^{Ar}), 6.28 (t, ^{3}J = 8.0 Hz, 1H, *p*-C*H*^{Ar}), 2.54 (sept, ^{3}J = 6.7 Hz, 2H, C*H*(*C*H$_3$)$_2^{Dip}$), 1.86-1.78 (m, 2H, C*H*$_2^{TMP}$), 1.72 (d, ^{3}J = 6.6 Hz, 6H, CH(C*H*$_3$)$_2^{Dip}$), 1.66 (s, 6H, C*H*$_3^{CAAC}$), 1.52 (s, 12H, C*H*$_3^{TMP}$), 1.41 (s, 2H, C*H*$_2^{CAAC}$), 1.29-1.25 (m, 4H, C*H*$_2^{TMP}$), 1.14 (d, ^{3}J = 6.6 Hz, 6H, CH(C*H*$_3$)$_2^{Dip}$), 0.79 (s, 6H, C*H*$_3^{CAAC}$) ppm.

^{13}C NMR (125.8 MHz, benzene-d_6): δ = 215.1 (*C*$_q^{Carbene}$), 148.6 (C$_q^{Ar}$), 143.2 (C$_q^{Dip}$), 134.4 (C$_q^{Dip}$), 129.3 (*C*H^{Dip}), 129.18 (*o*-*C*H^{Ar}), 128.8 (*m*-*C*H^{Ar}), 125.7 (*C*H^{Dip}), 123.2 (*m*-*C*H^{Ar}), 77.0 (C$_q^{CAAC}$), 53.4 (C$_q^{TMP}$), 52.8 (C$_q^{CAAC}$), 52.4 (*C*H$_2^{CAAC}$), 39.3 (*C*H$_2^{TMP}$), 32.5 (*C*H$_3^{TMP}$), 31.2 (*C*H$_3^{CAAC}$), 29.5 (*C*H(CH$_3$)$_2^{Dip}$), 28.8 (*C*H$_3^{CAAC}$), 27.1 (CH(*C*H$_3$)$_2^{Dip}$), 24.7 (CH(*C*H$_3$)$_2^{Dip}$), 24.1 (*C*H$_2^{TMP}$), 19.4 (*C*H$_2^{TMP}$) ppm.

^{11}B NMR (160.5 MHz, benzene-d_6): δ = 12.6 (s) ppm.

Elemental analysis (%) calcd. for $C_{35}H_{52}BN_5Cl_2$: C 67.31, H 8.39, N 11.21; found: C 67.33, H 8.70, N 11.10.

UV/vis (hexane): λ_{max} = 326 nm, λ_2 = 476 nm.

NMR spectra of isolated compounds

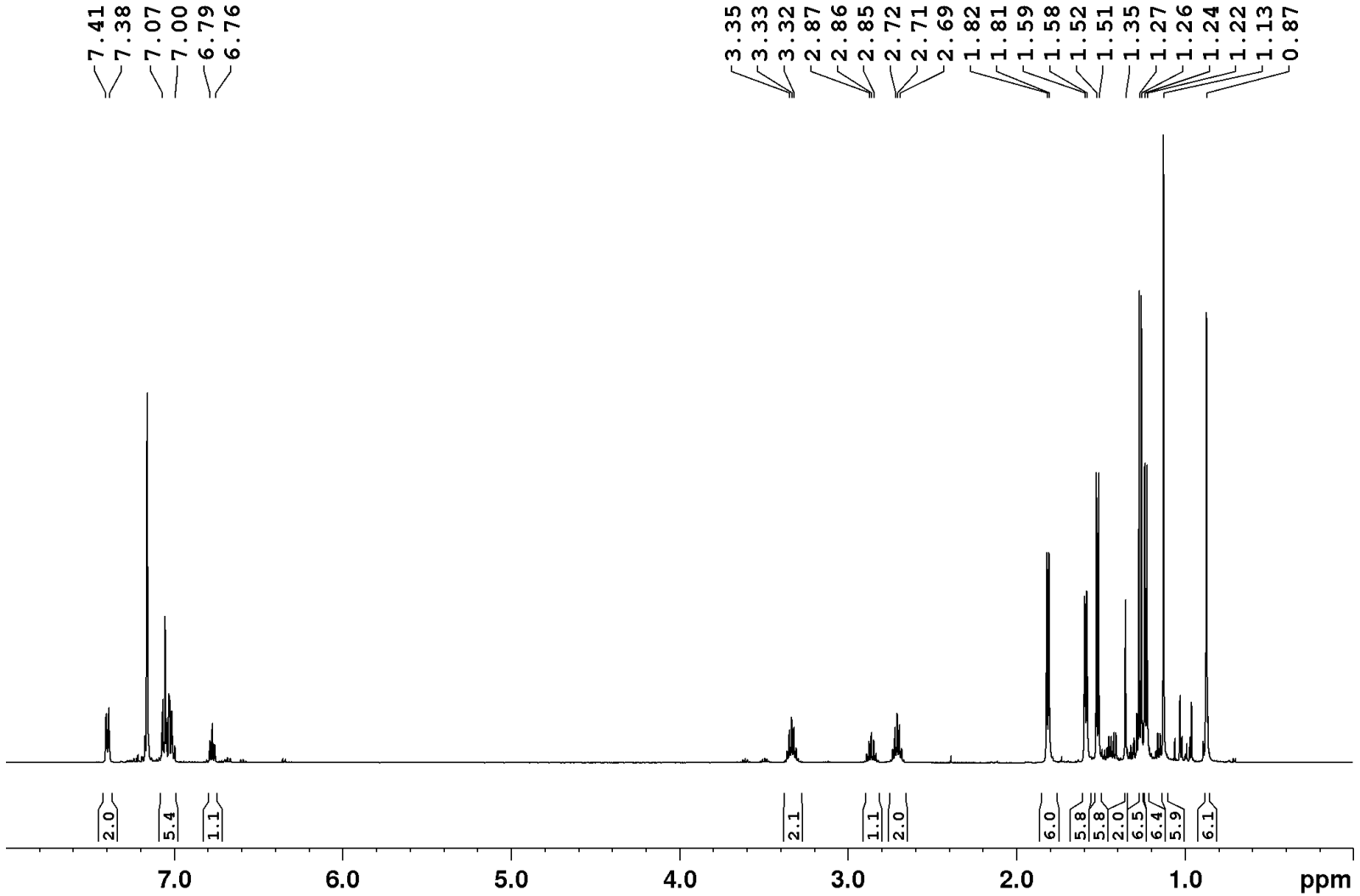


Fig. S1 $^{1}H\{^{11}B\}$ NMR spectrum of **4a** in benzene-d_6.

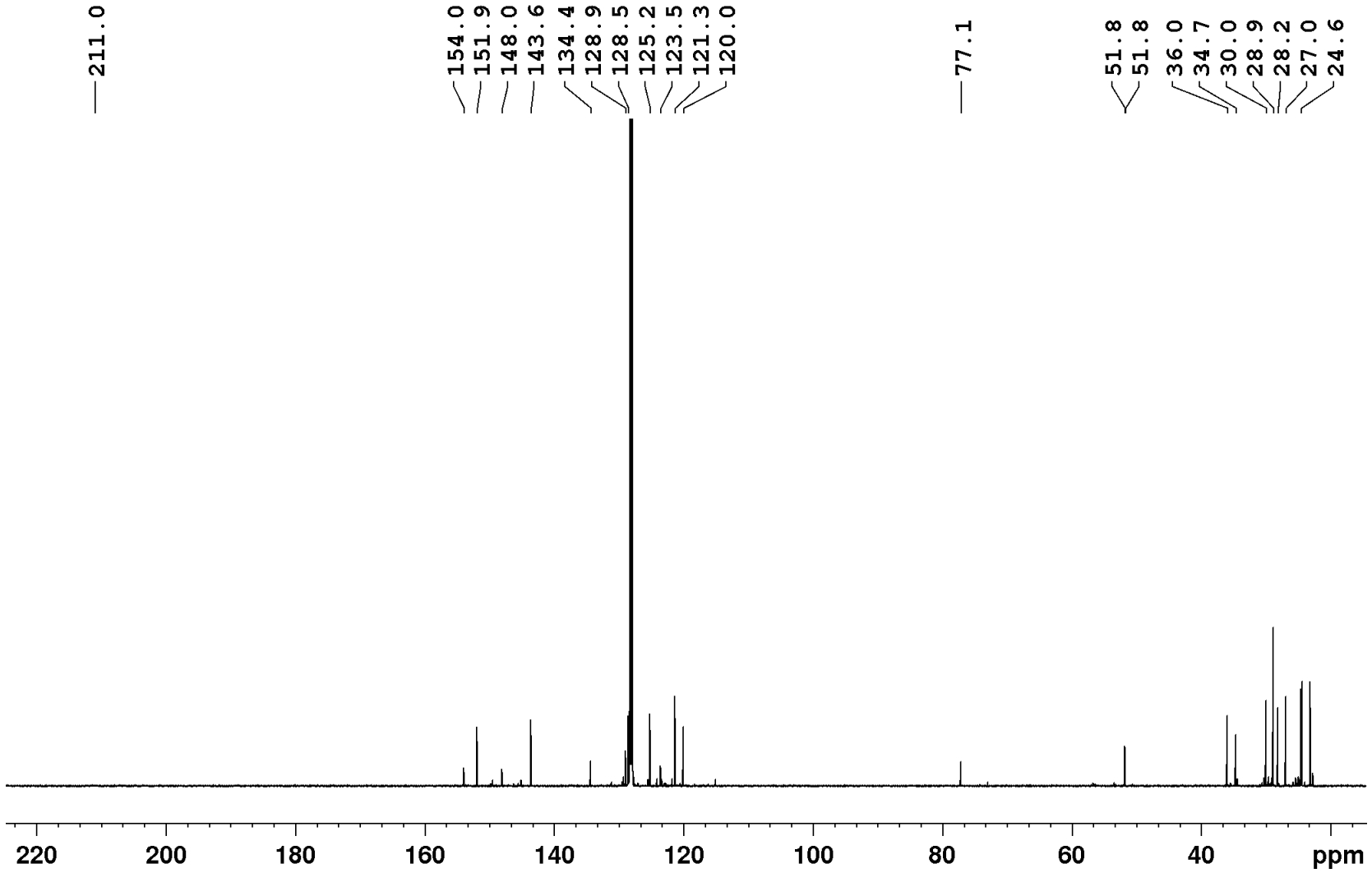


Fig. S2 $^{13}C\{^{1}H\}$ NMR spectrum of **4a** in benzene-d_6.

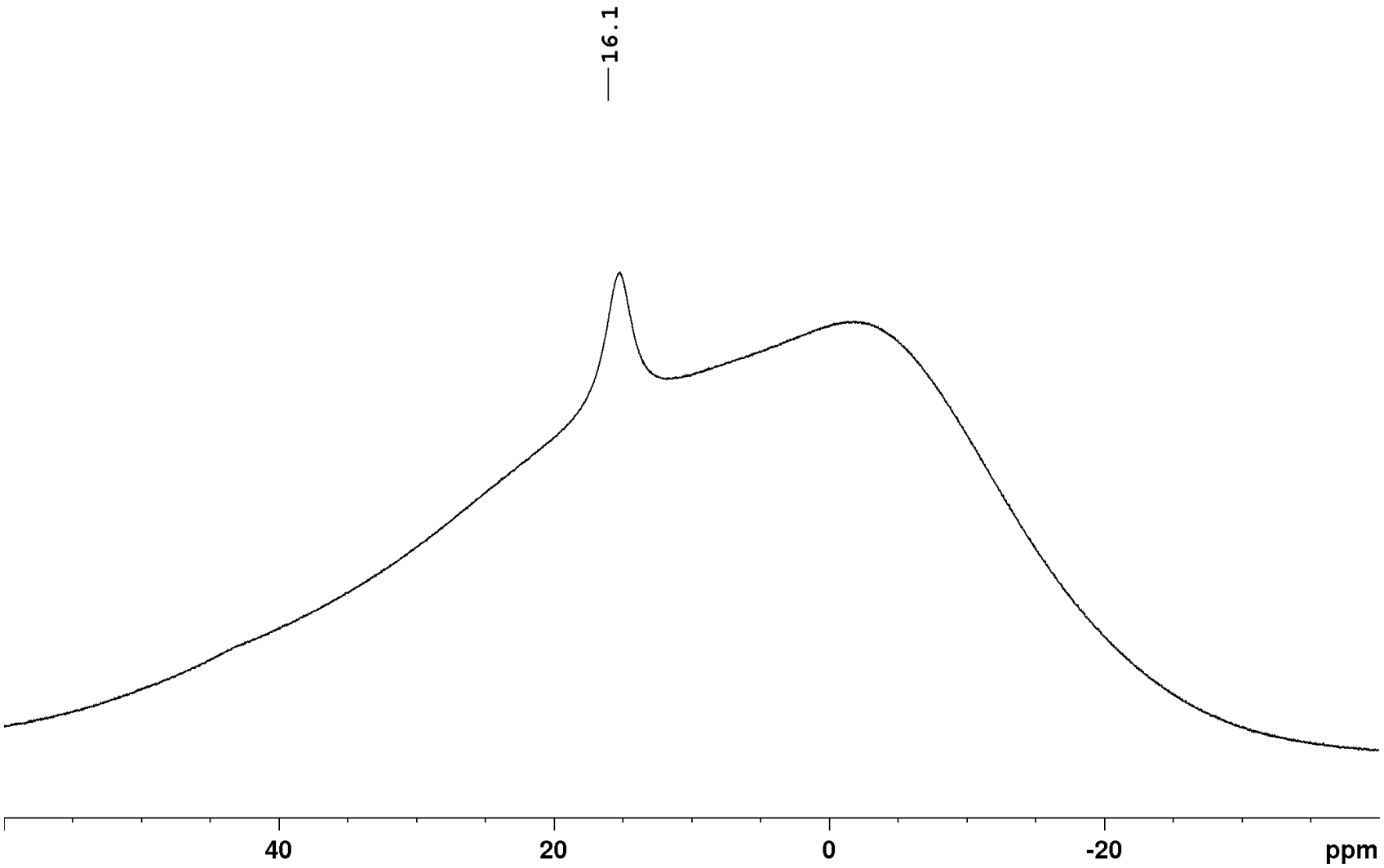


Fig. S3 $^{11}B\{^{1}H\}$ NMR spectrum of **4a** in benzene-d_6.

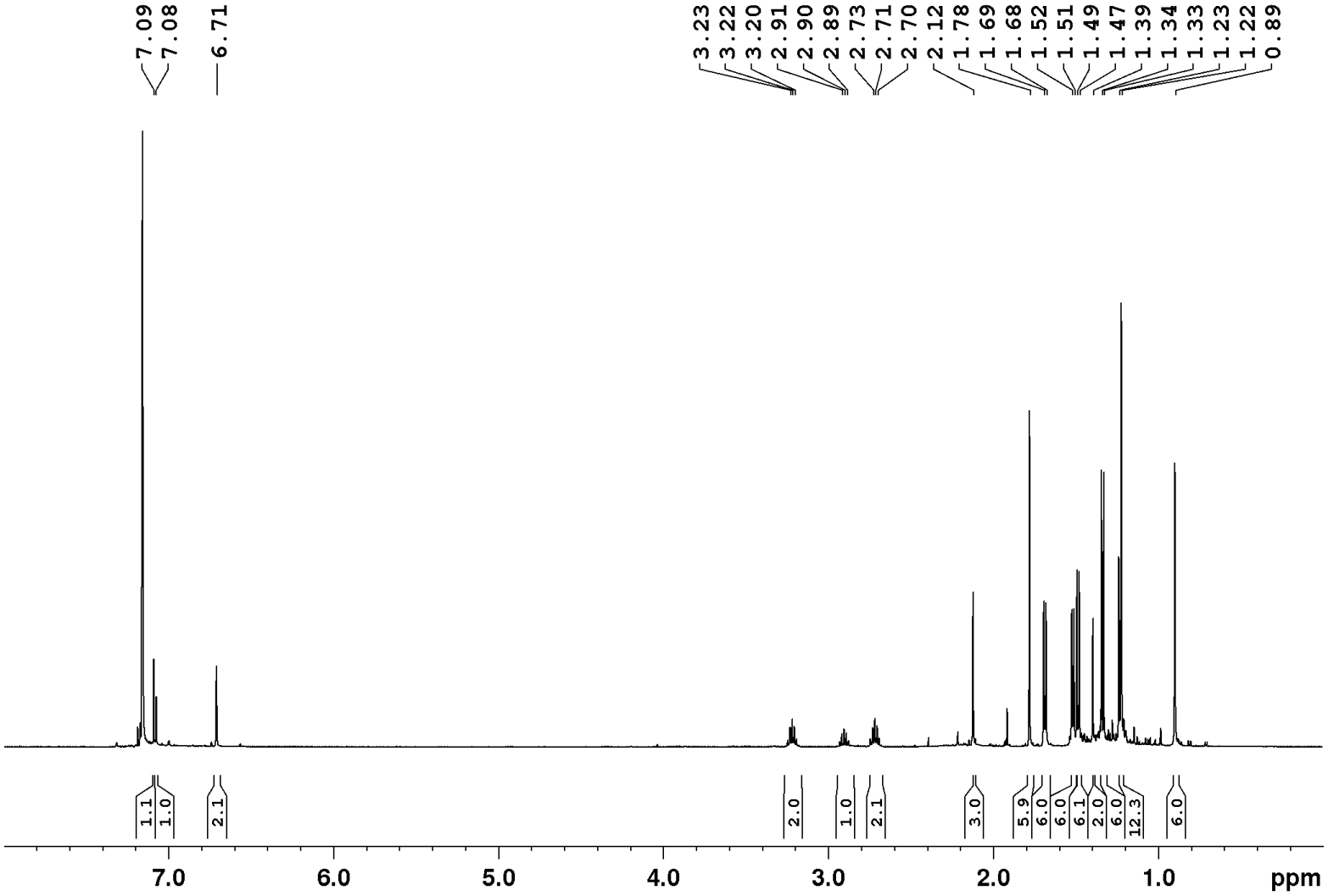


Fig. S4 $^{1}H\{^{11}B\}$ NMR spectrum of **4b** in benzene-d_6.

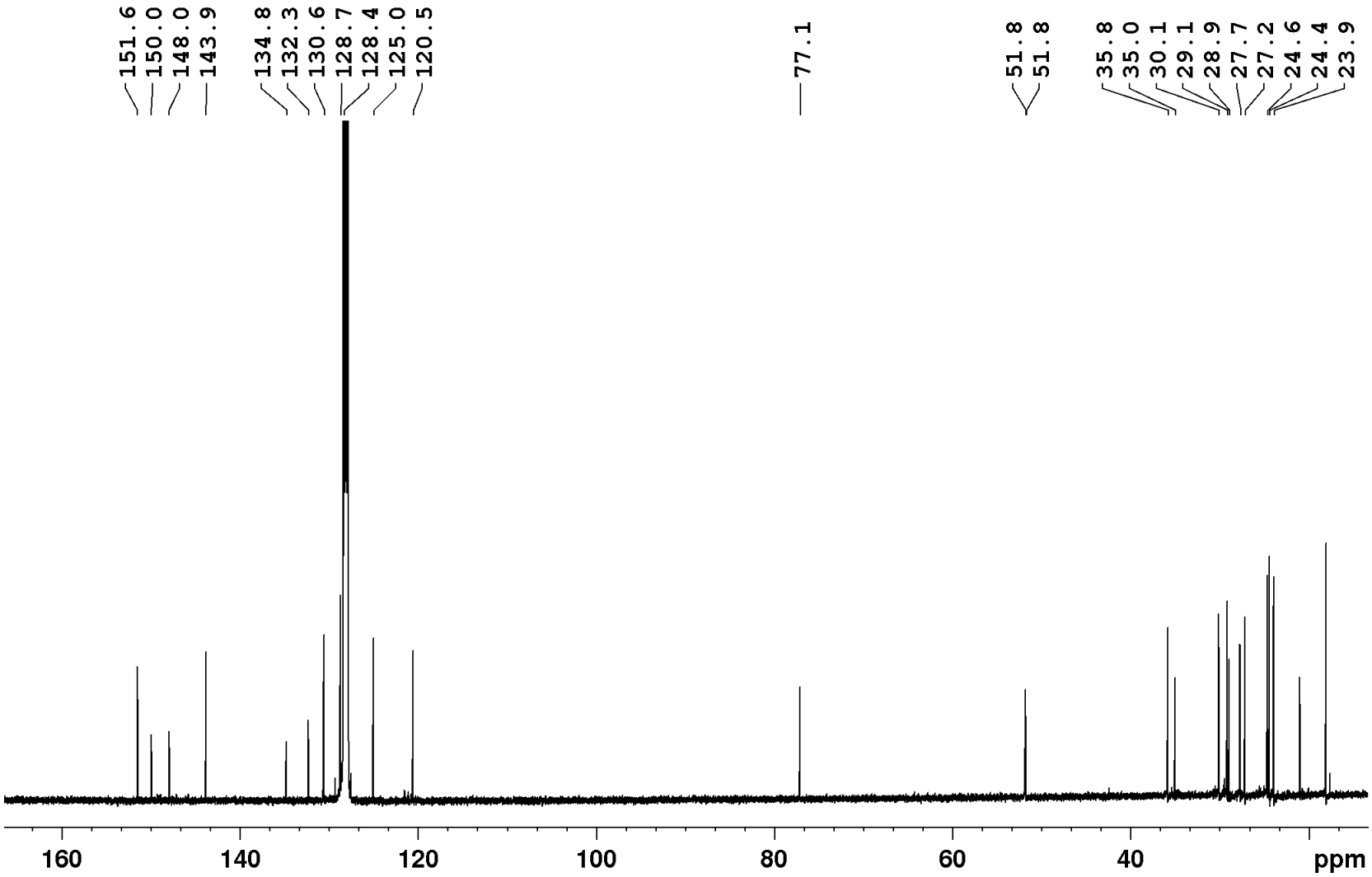


Fig. S5 $^{13}C\{^{1}H\}$ NMR spectrum of **4b** in benzene-d_6.

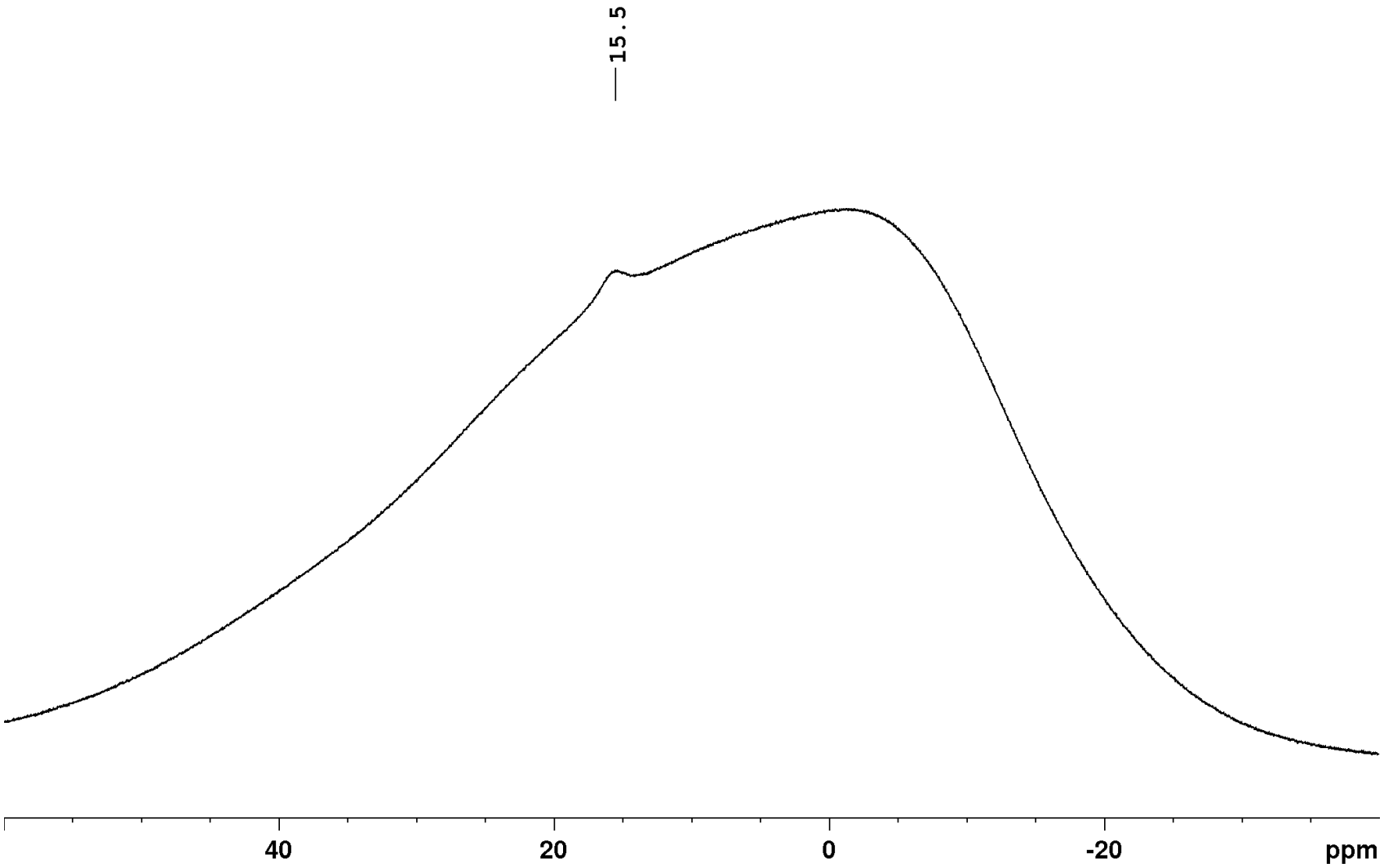


Fig. S6 $^{11}B\{^{1}H\}$ NMR spectrum of **4b** in benzene-d_6.

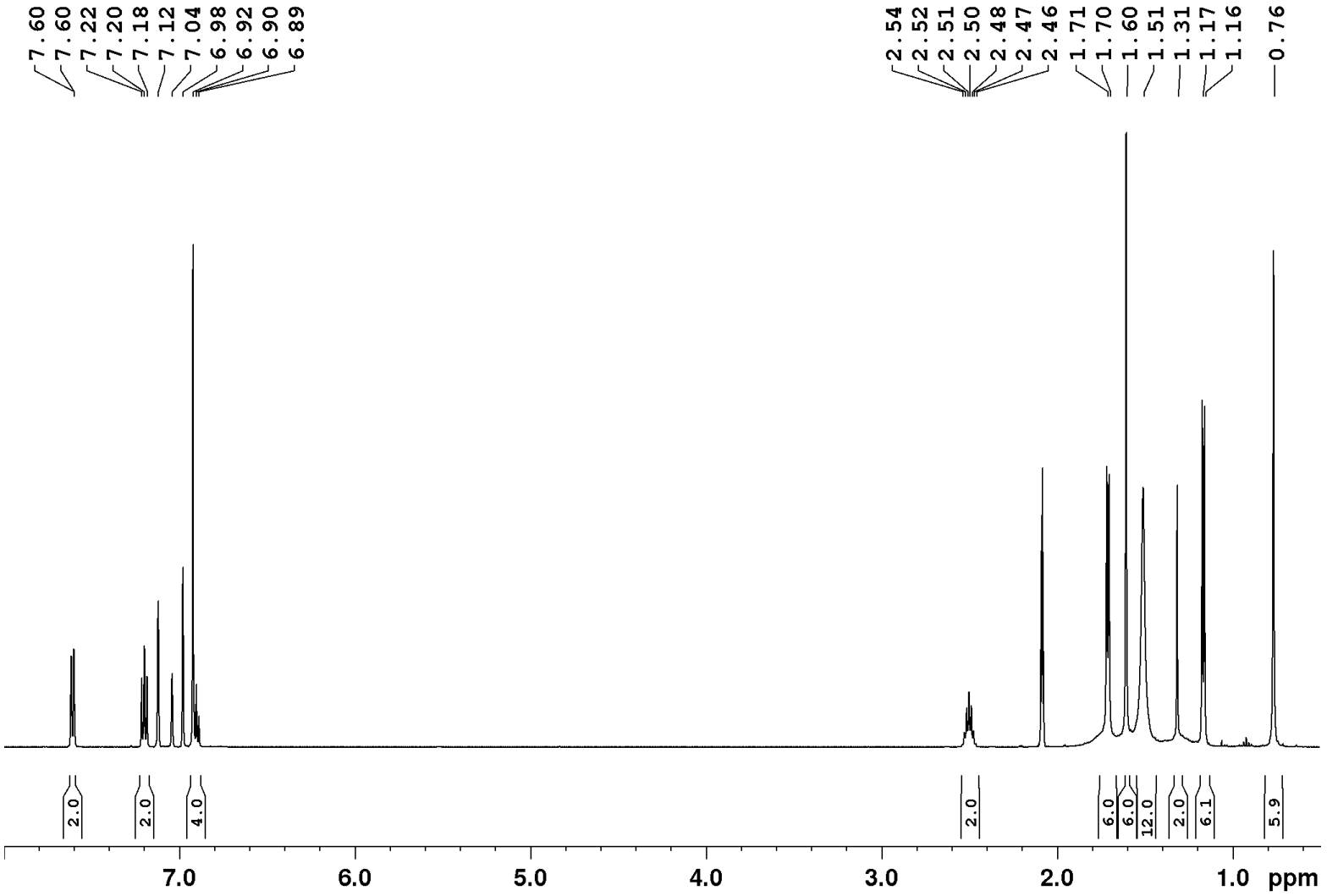


Fig. S7 $^{1}H\{^{11}B\}$ NMR spectrum of **6a** in toluene-d_8 at –30 °C.

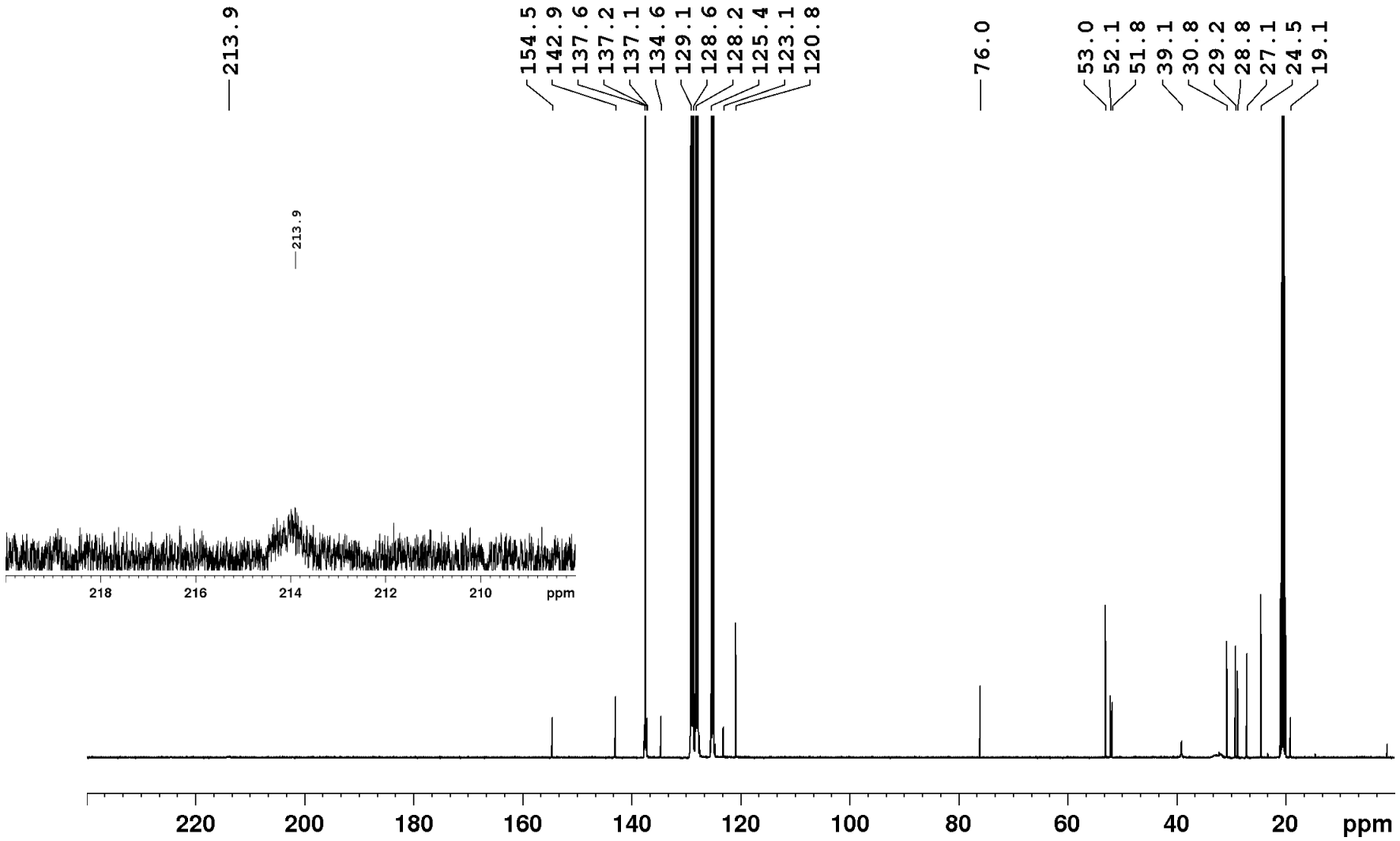


Fig. S8 $^{13}C\{^{1}H\}$ NMR spectrum of **6a** in toluene-d_8 at –30 °C.

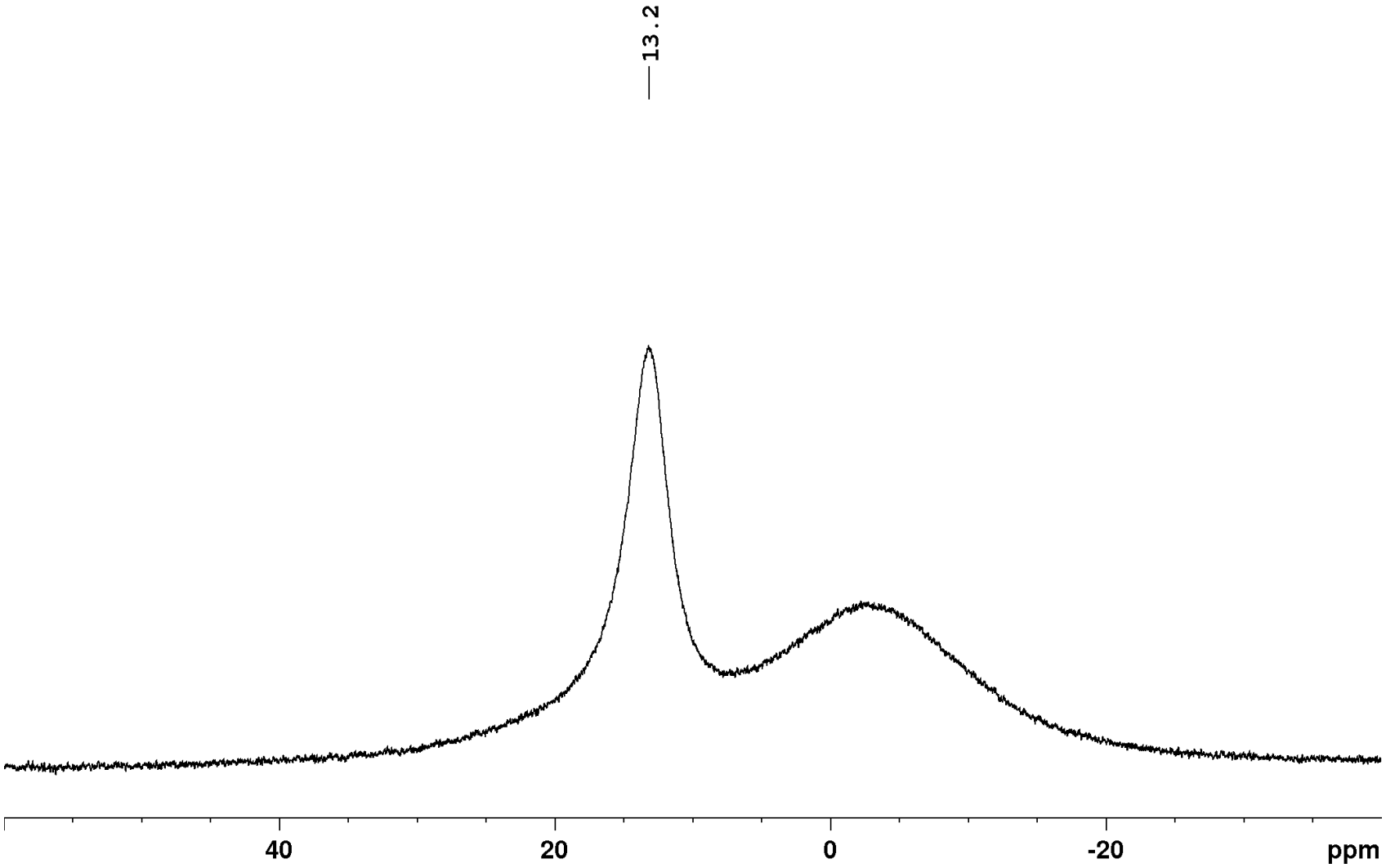


Fig. S9 $^{11}B\{^{1}H\}$ NMR spectrum of **6a** in toluene-d_8 at −30 °C.

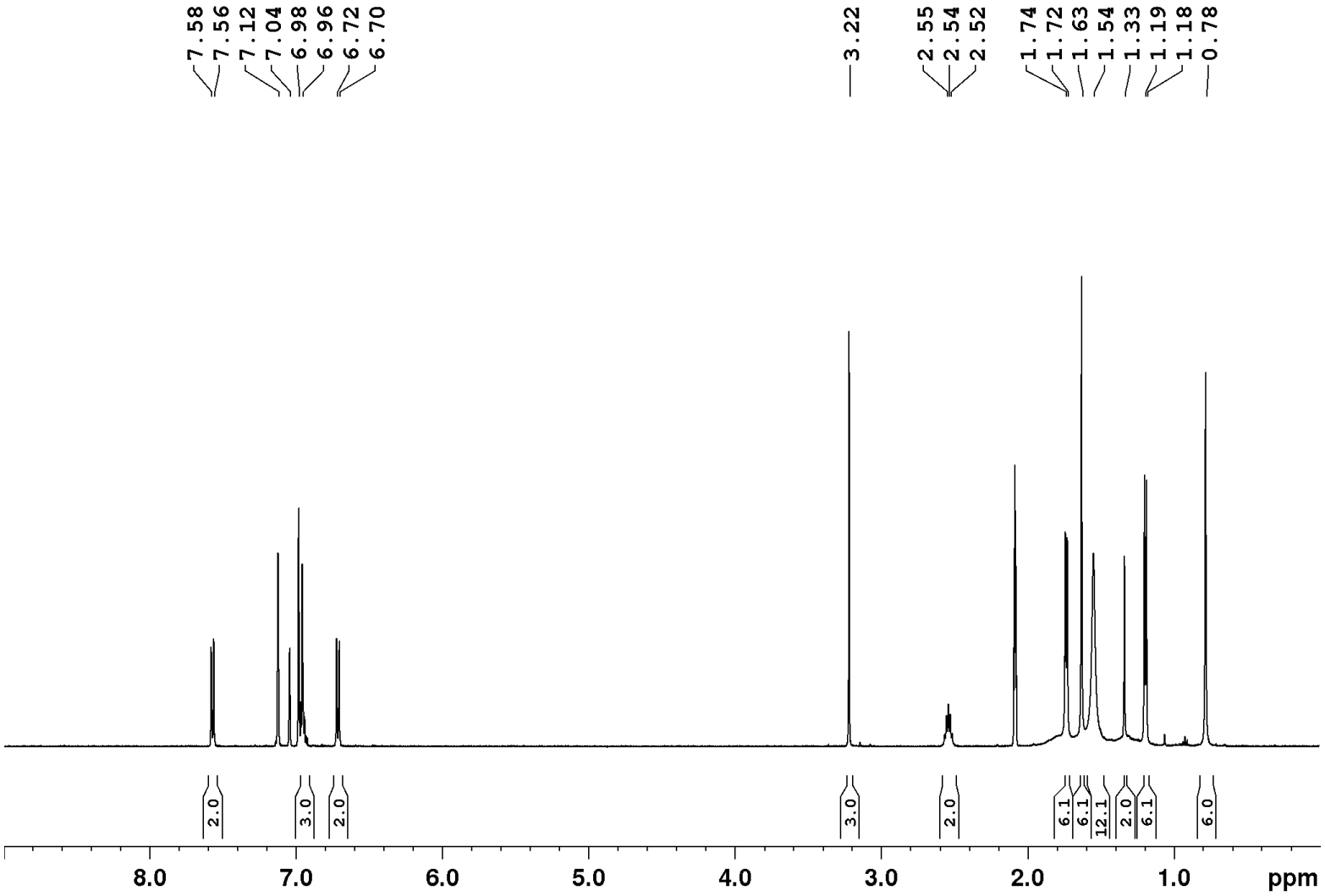


Fig. S10 $^{1}H\{^{11}B\}$ NMR spectrum of **6b** in toluene-d_8 at –30 °C.

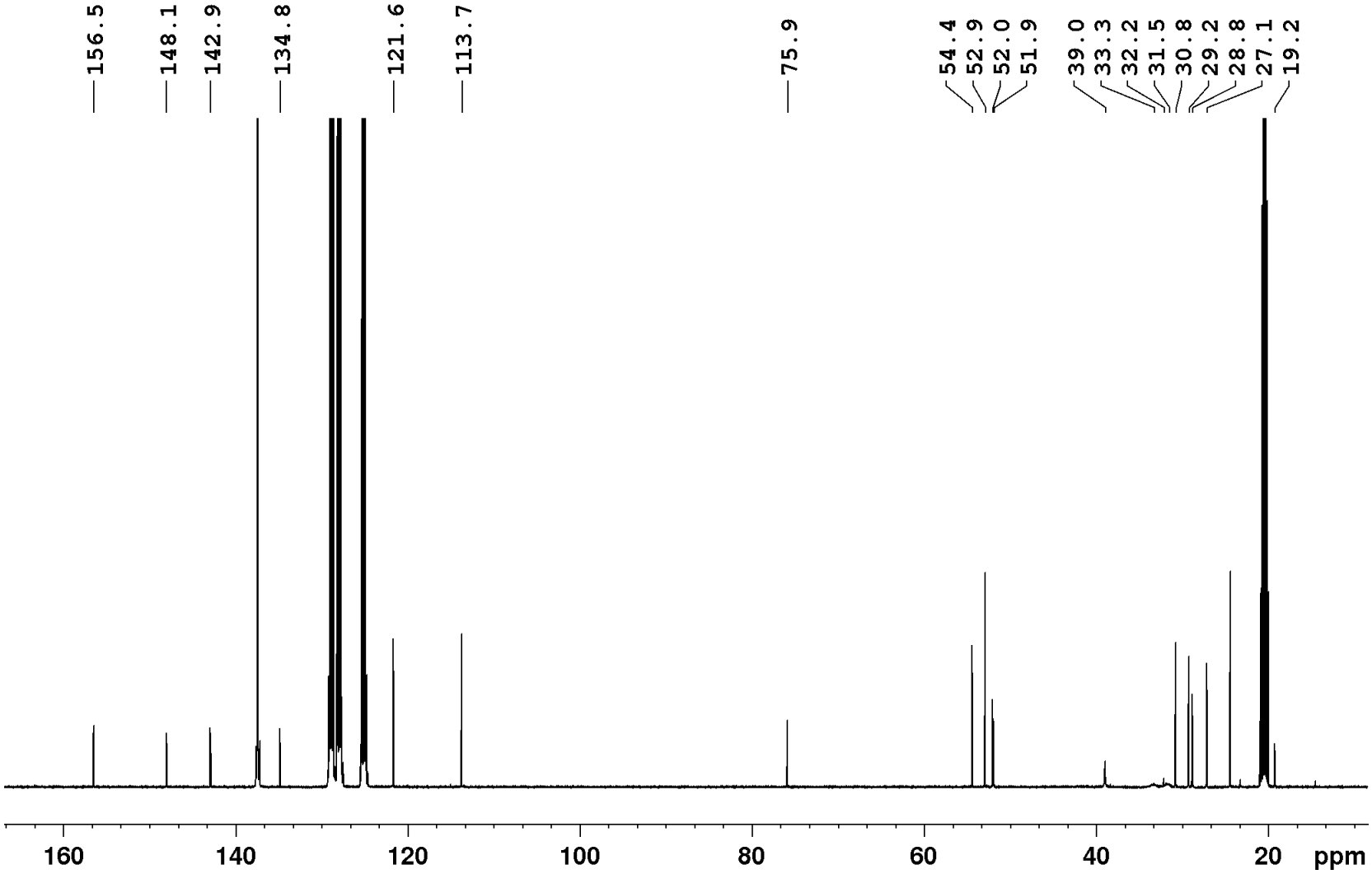


Fig. S11 $^{13}C\{^{1}H\}$ NMR spectrum of **6b** in toluene-d_8 at –30 °C.

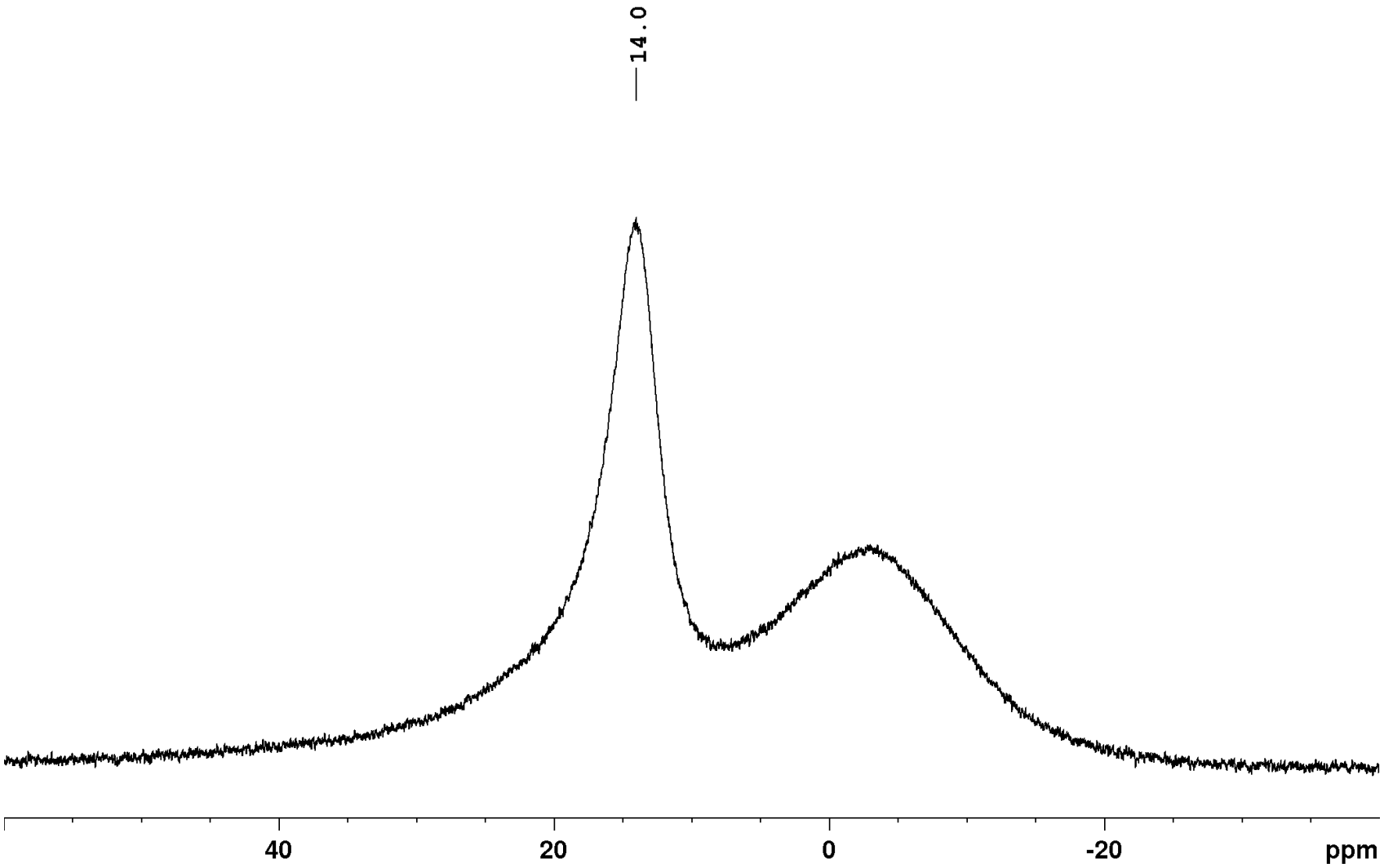


Fig. S12 $^{11}B\{^{1}H\}$ NMR spectrum of **6b** in toluene-d_8 at –30 °C.

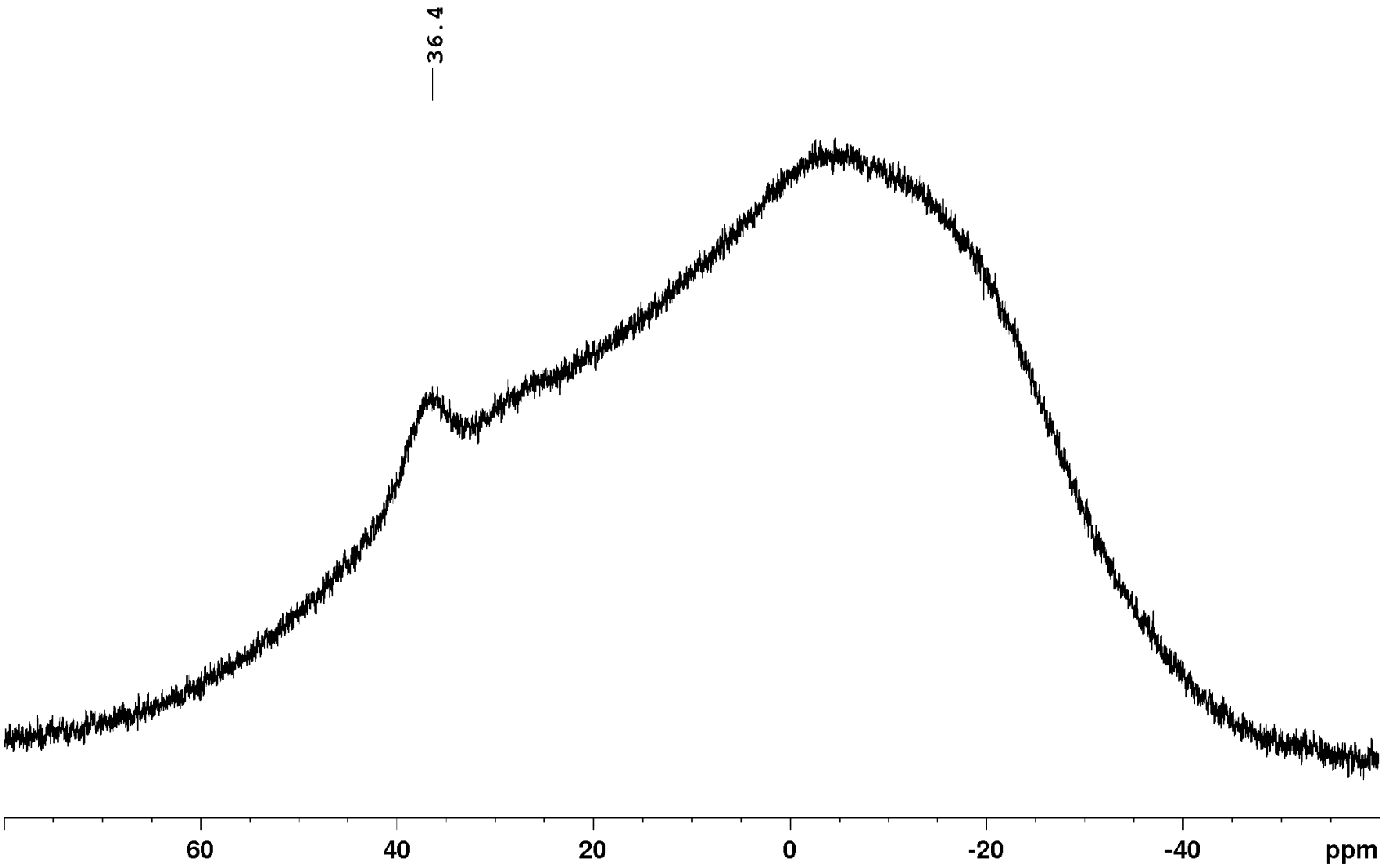


Fig. S13 $^{11}B\{^{1}H\}$ NMR spectrum of **7a** in benzene-d_6 at room temperature.

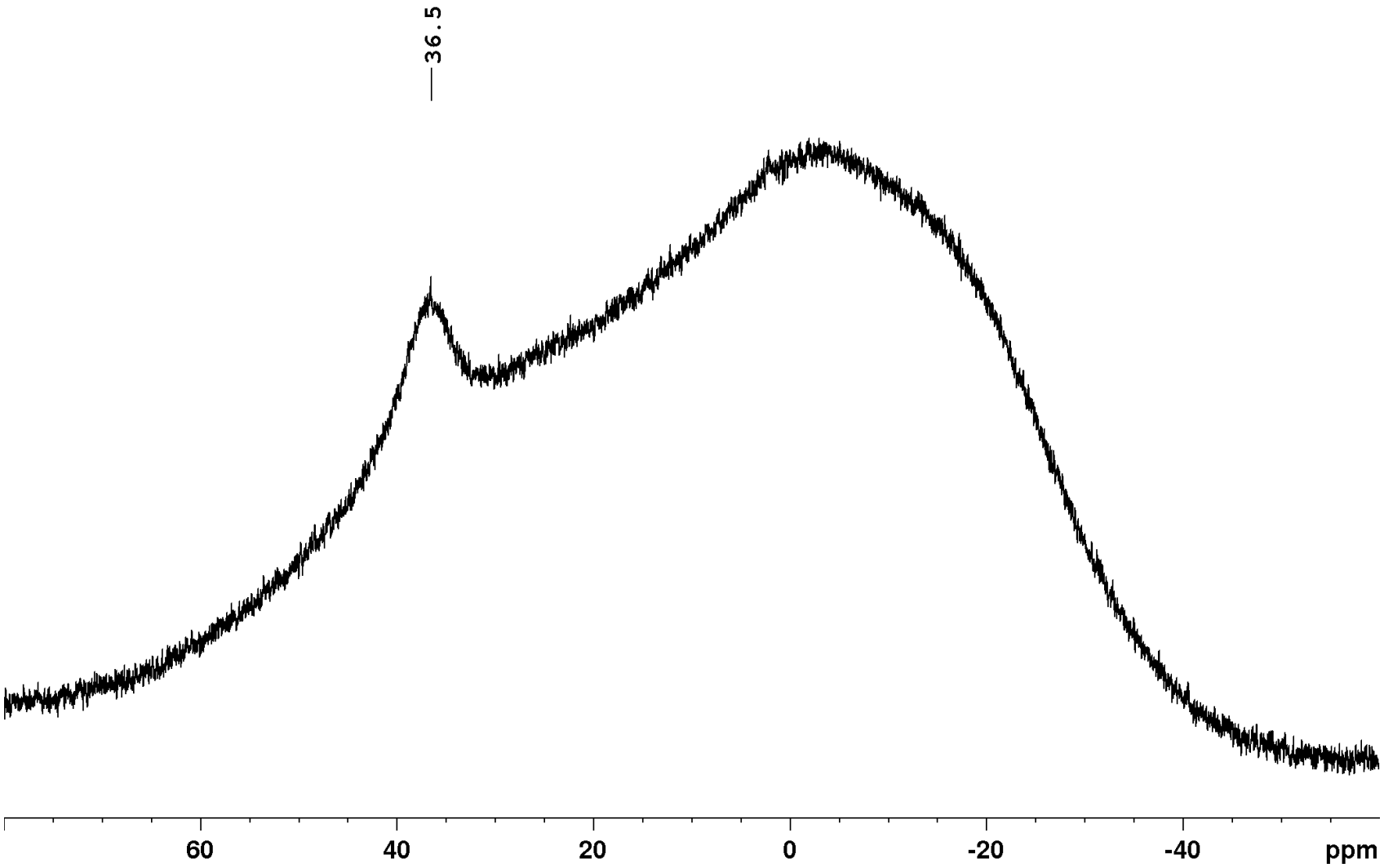


Fig. S14 $^{11}B\{^{1}H\}$ NMR spectrum of **7b** in benzene-d_6 at room temperature.

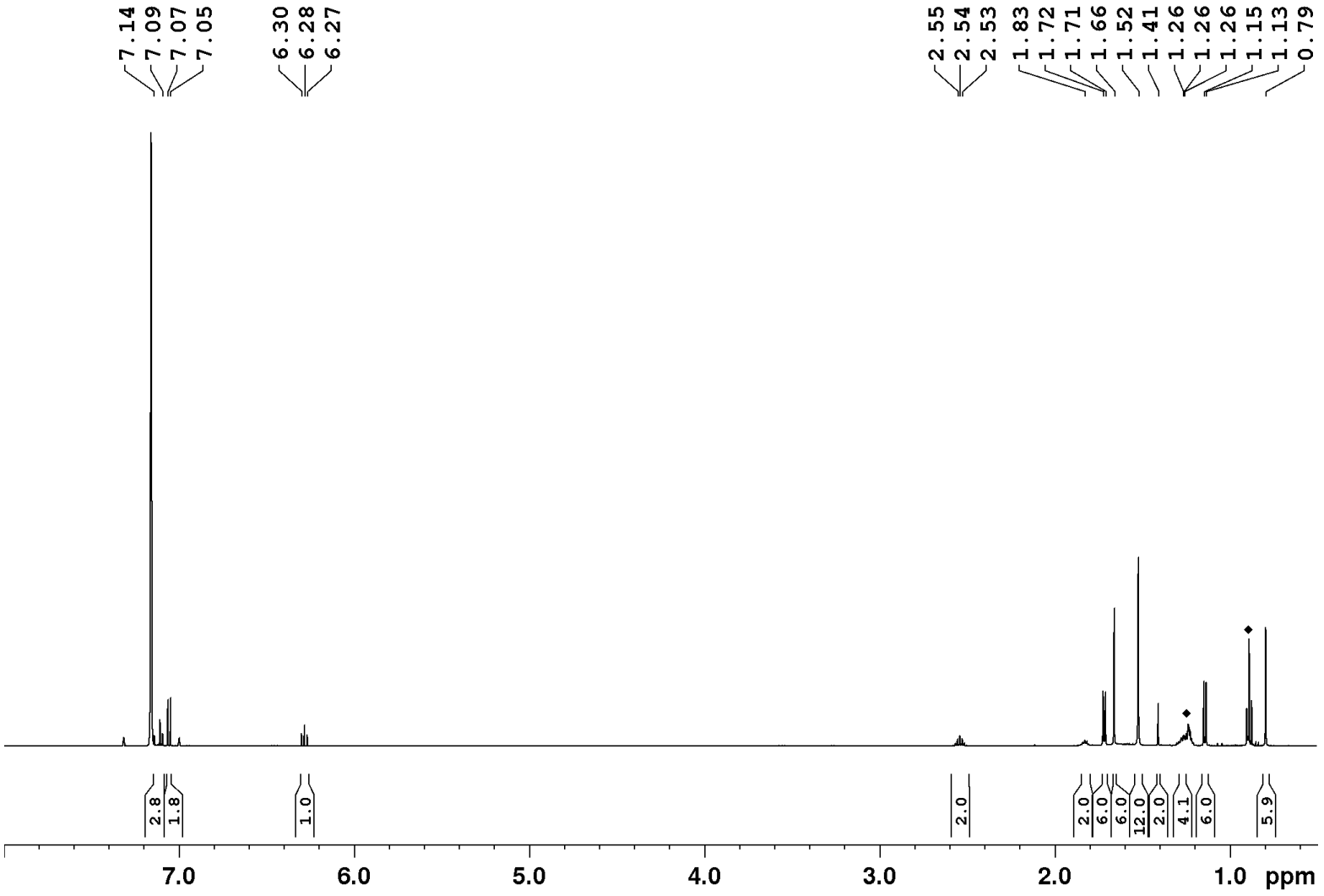


Fig. S15 $^{1}H\{^{11}B\}$ NMR spectrum of **6c** in benzene-d_6 (The resonances indicated with ◆ originate from hexane used for crystallization).

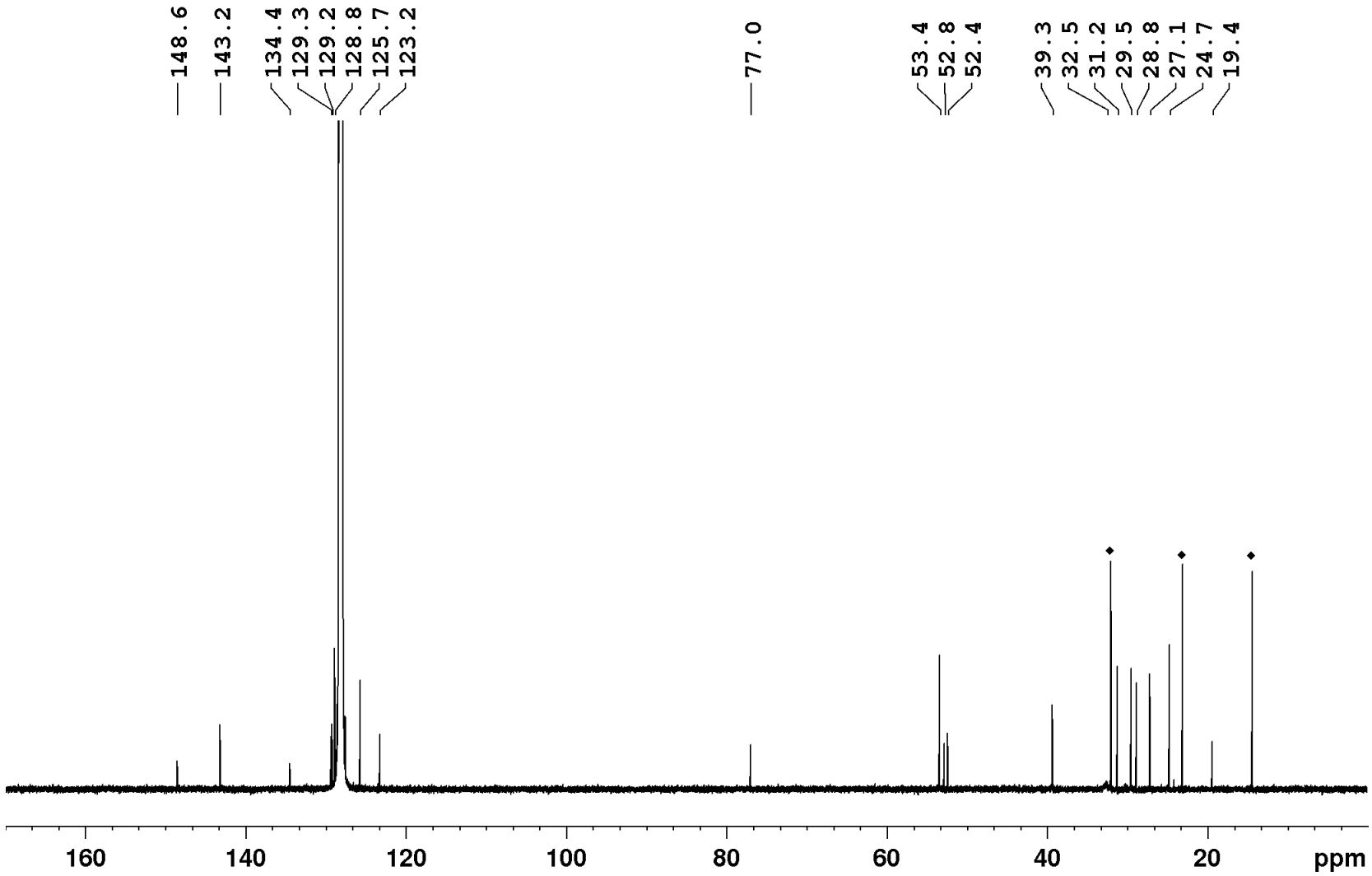


Fig. S16 $^{13}C\{^{1}H\}$ NMR spectrum of **6c** in benzene-d_6 (The resonances indicated with ◆ originate from hexane used for crystallization).

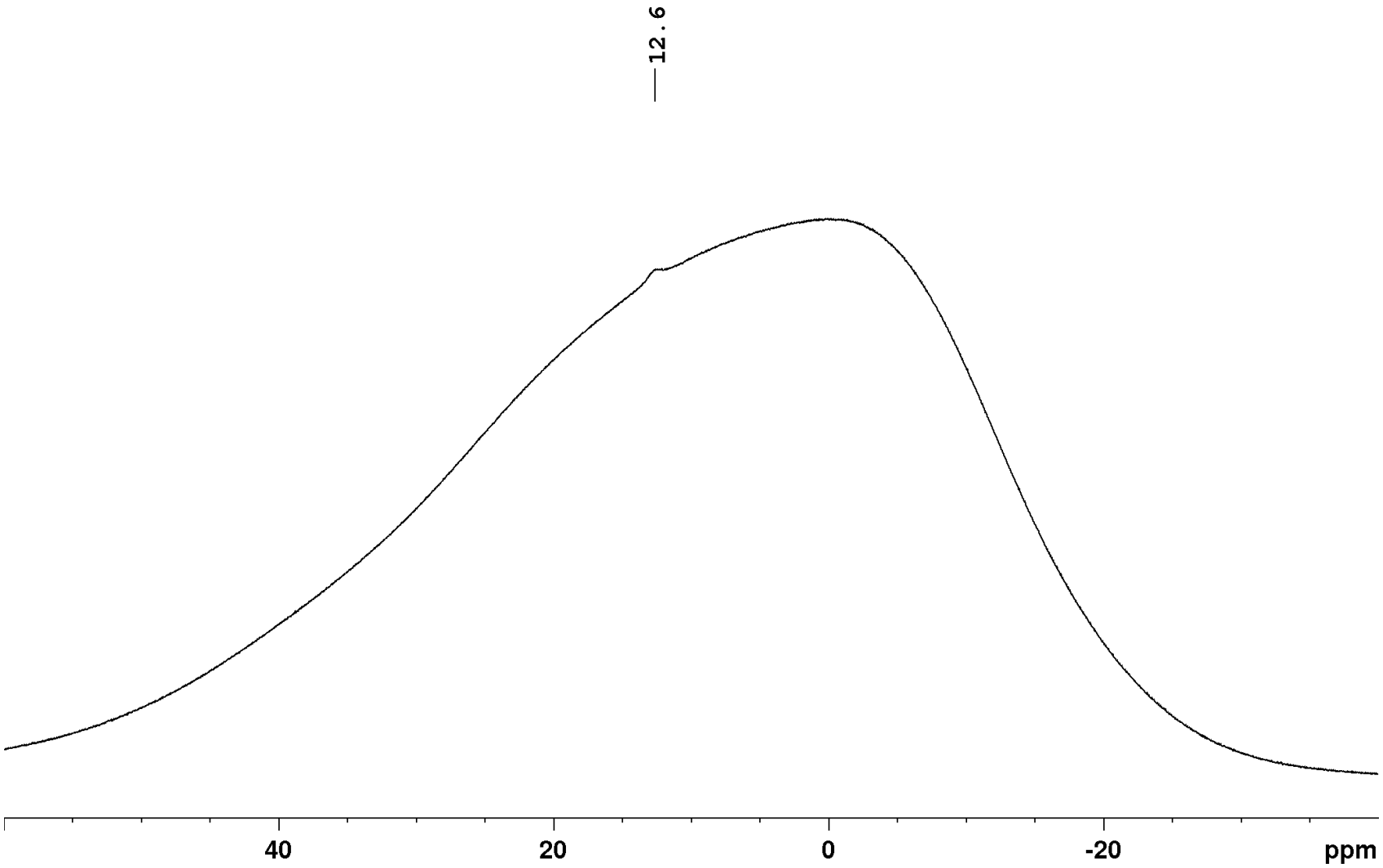


Fig. S17 $^{11}B\{^{1}H\}$ NMR spectrum of **6c** in benzene-d_6.

UV-vis spectra

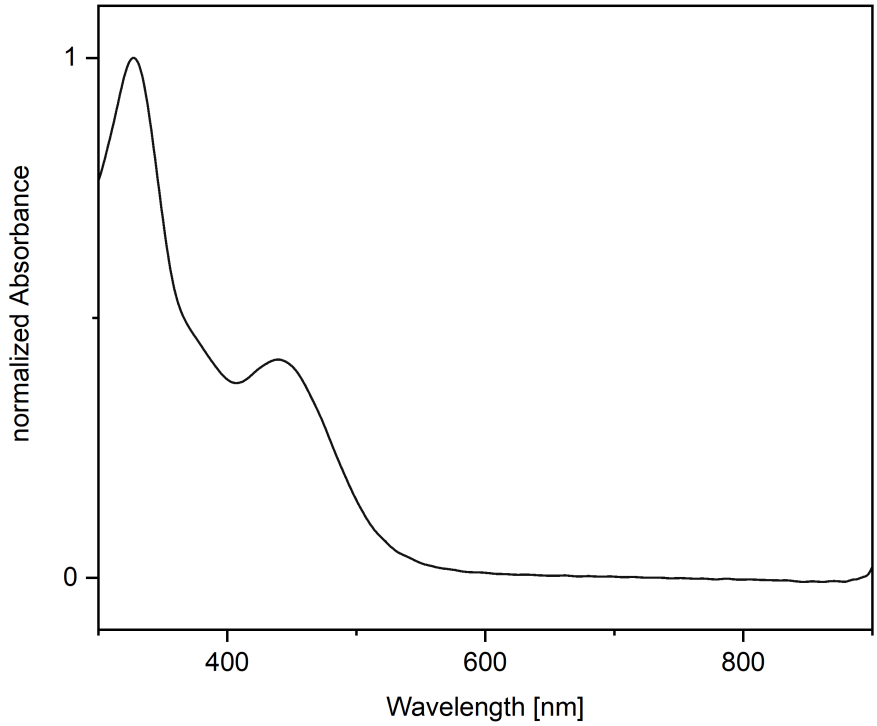


Fig. S18 UV-vis spectrum of compound **4a** in THF (absorption maxima: λ_{max} = 324, λ_2 = 448 nm).

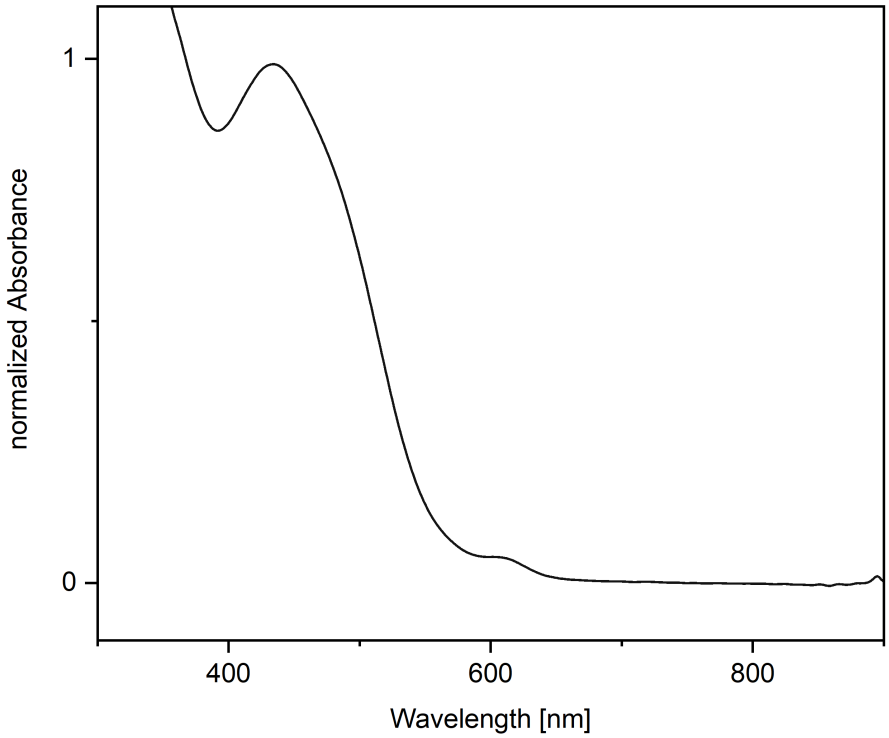


Fig. S19 UV-vis spectrum of compound **4b** in THF (absorption maxima: λ_{max} = 434 nm, λ_2 = 601 nm (weak)).

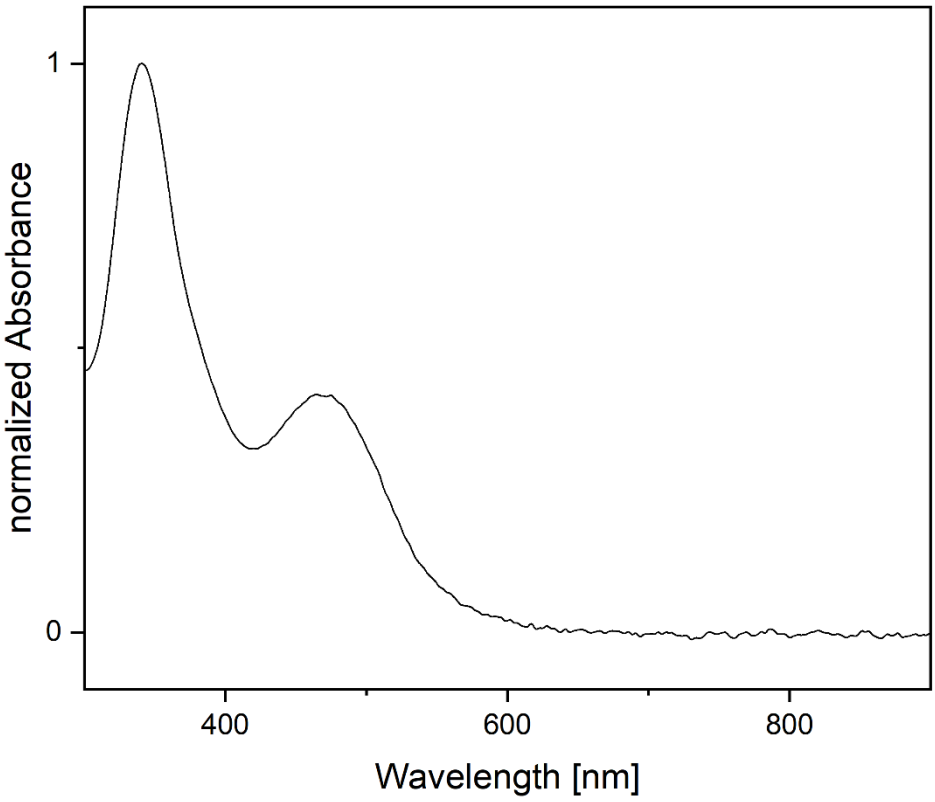


Fig. S20 UV-vis spectrum of compound **6a** in hexane (absorption maxima: λ_{max} = 341, λ_2 = 465 nm).

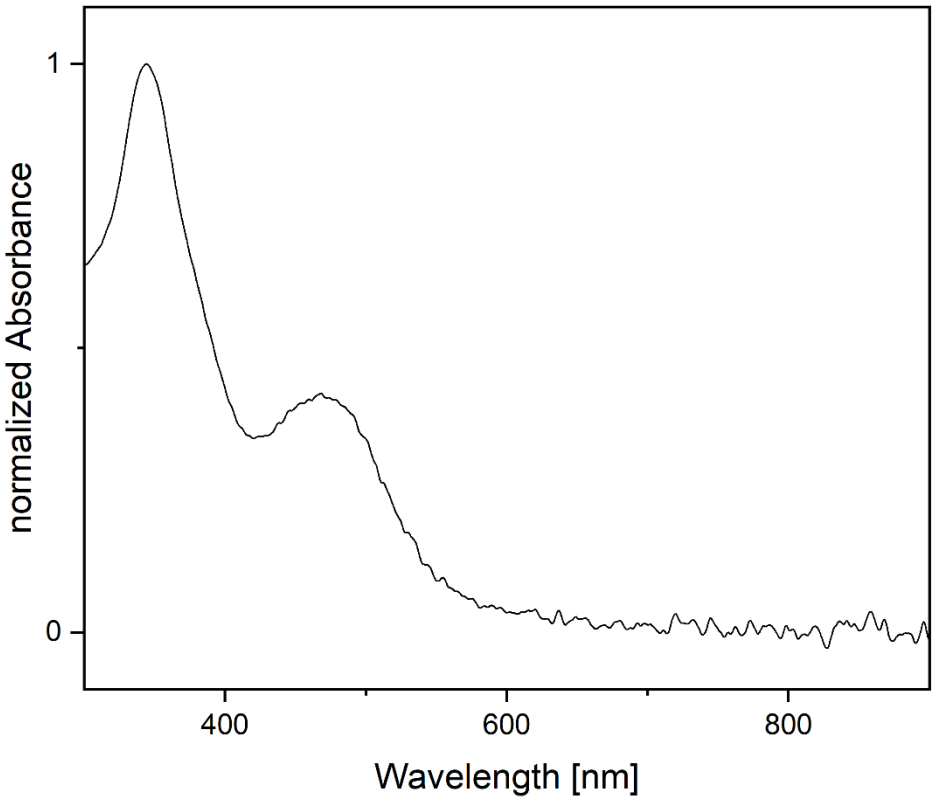


Fig. S21 UV-vis spectrum of compound **6b** in hexane (absorption maxima: λ_{max} = 345, λ_2 = 468 nm).

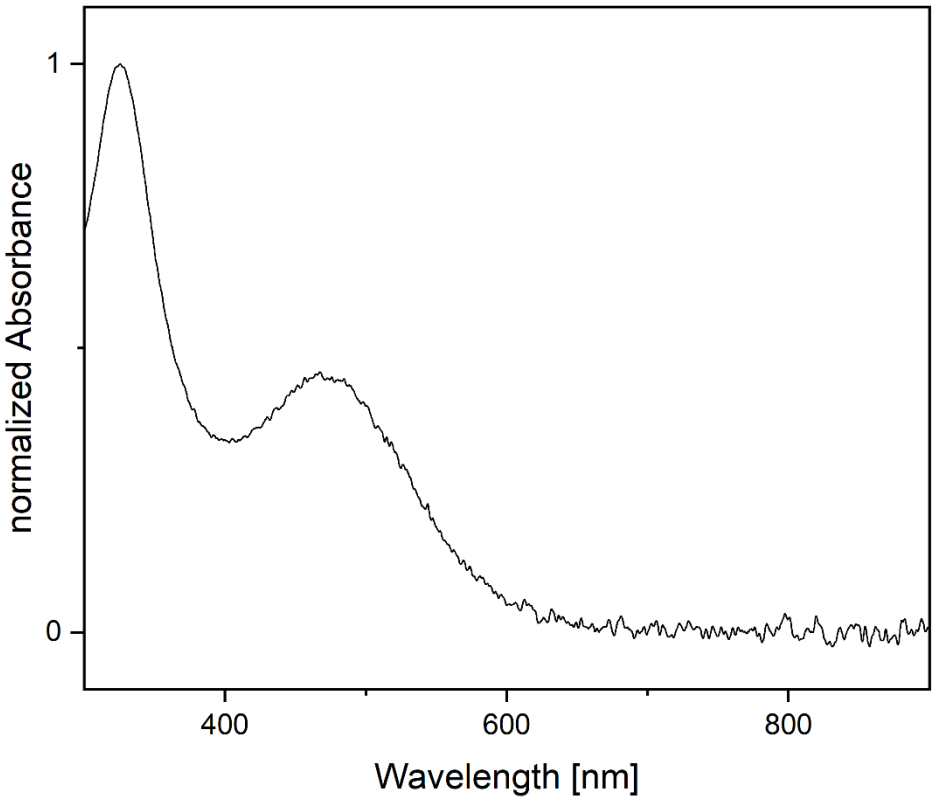


Fig. S22 UV-vis spectrum of compound **6c** in hexane (absorption maxima: λ_{max} = 326, λ_2 = 476 nm).

IR spectra

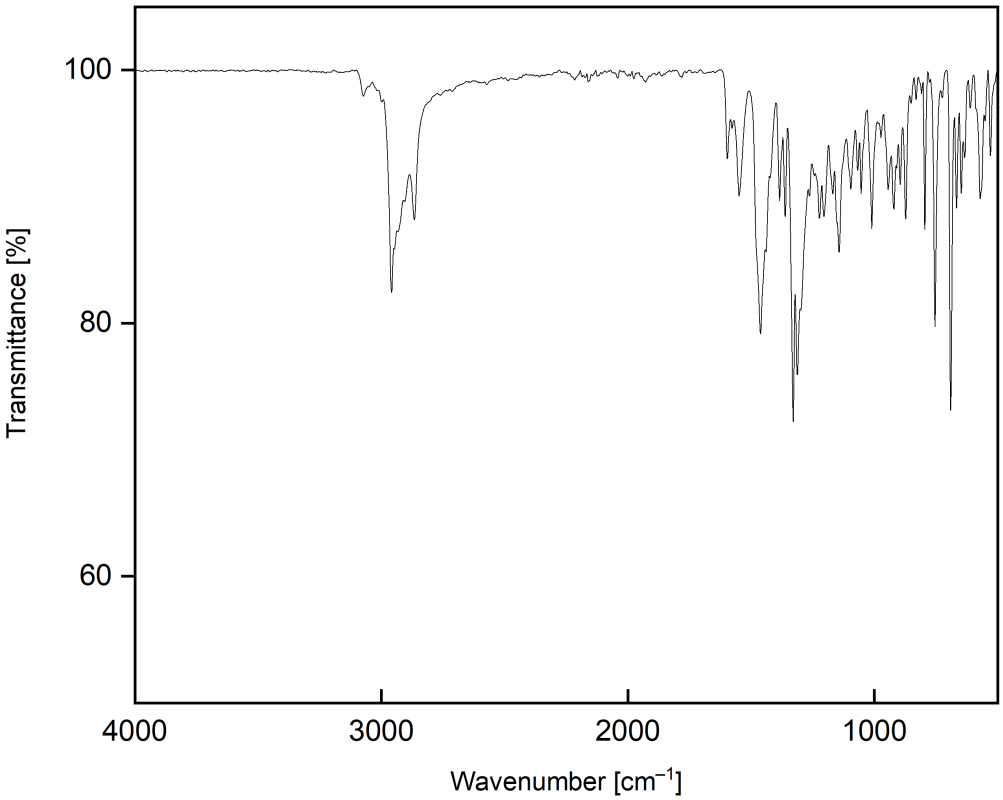


Fig. S23 IR spectrum of compound **4a**.

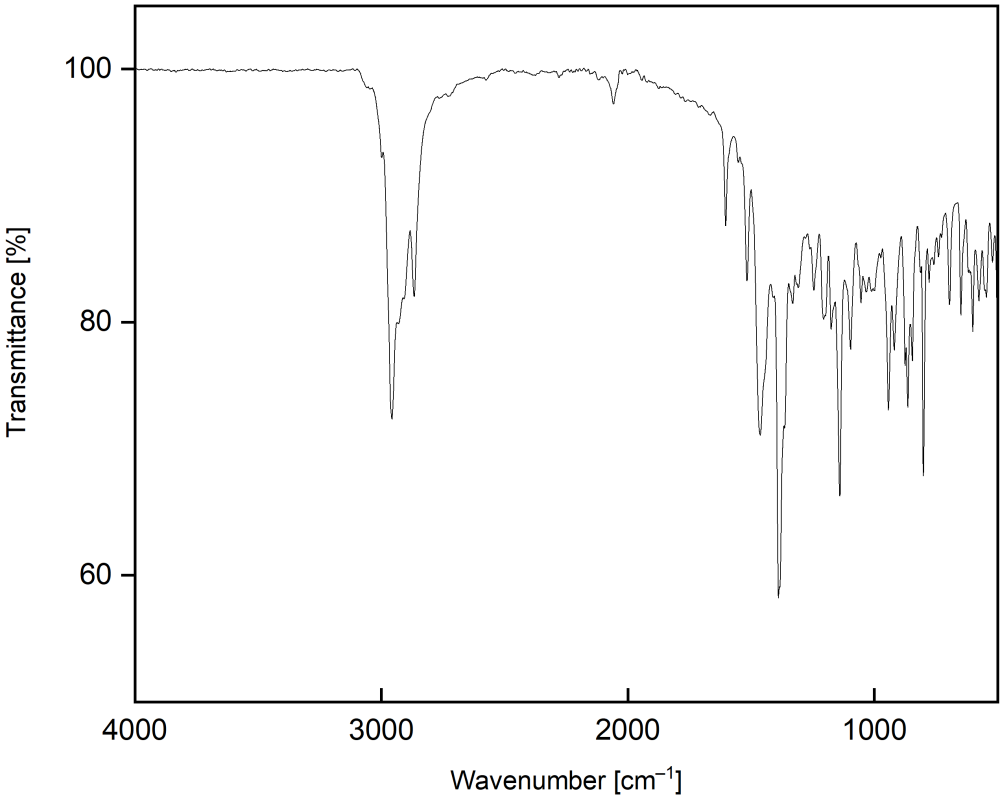


Fig. S24 IR spectrum of compound **4b**.

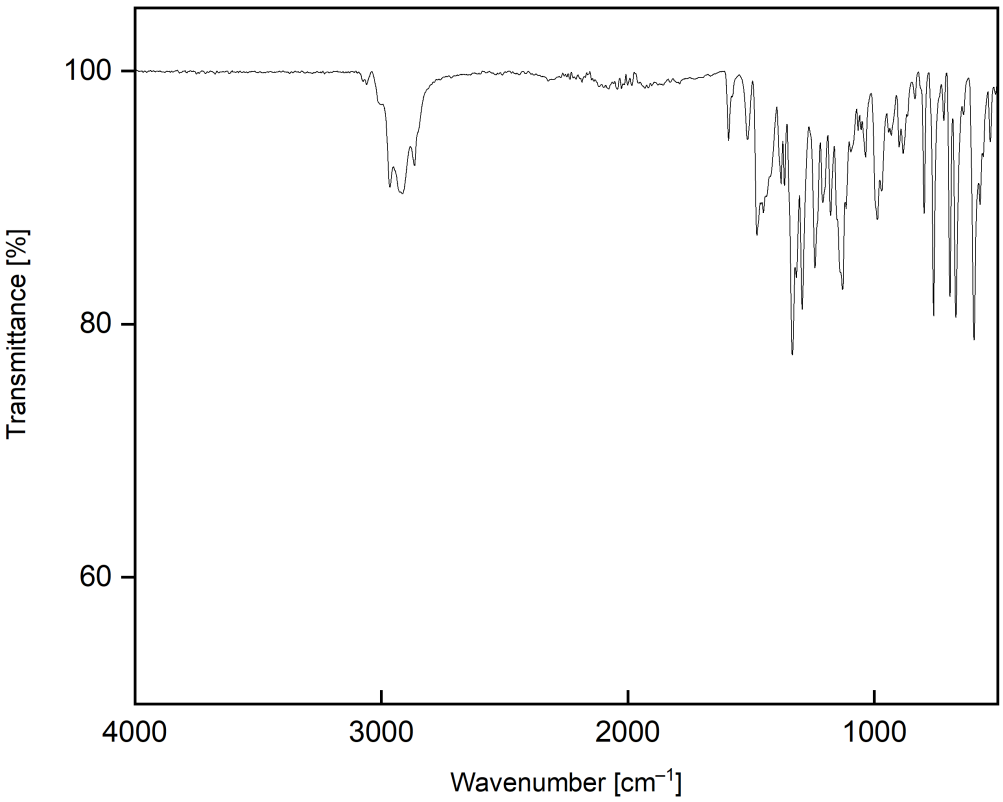


Fig. S25 IR spectrum of compound **6a**.

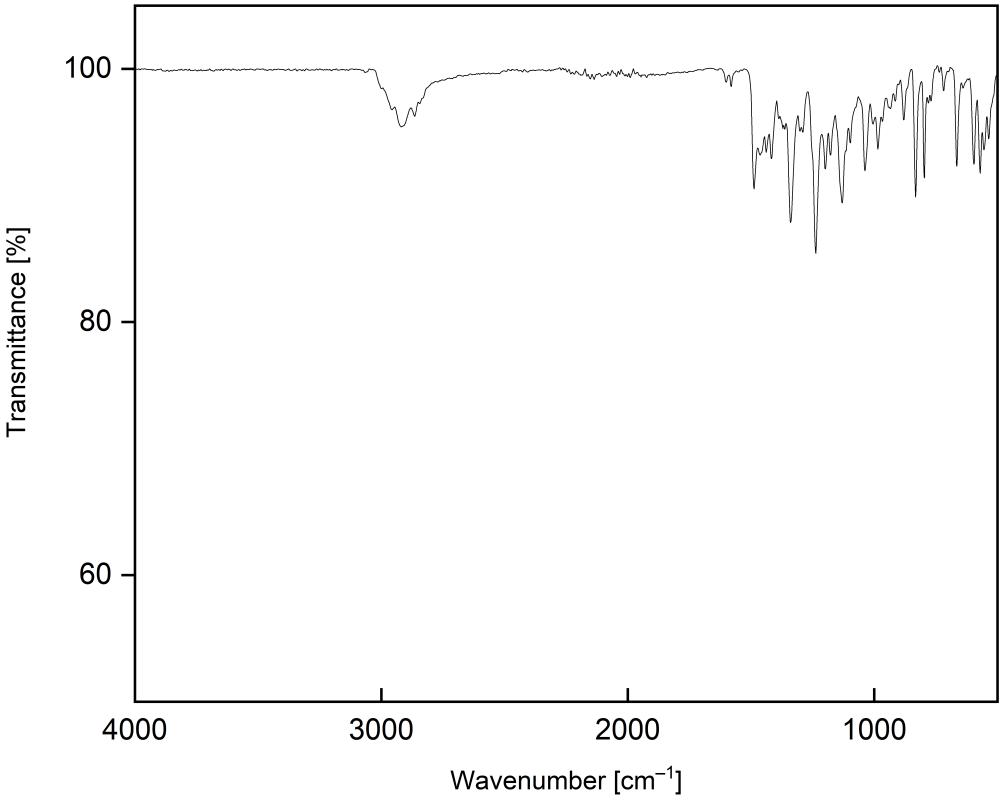


Fig. S26 IR spectrum of compound **6b**.

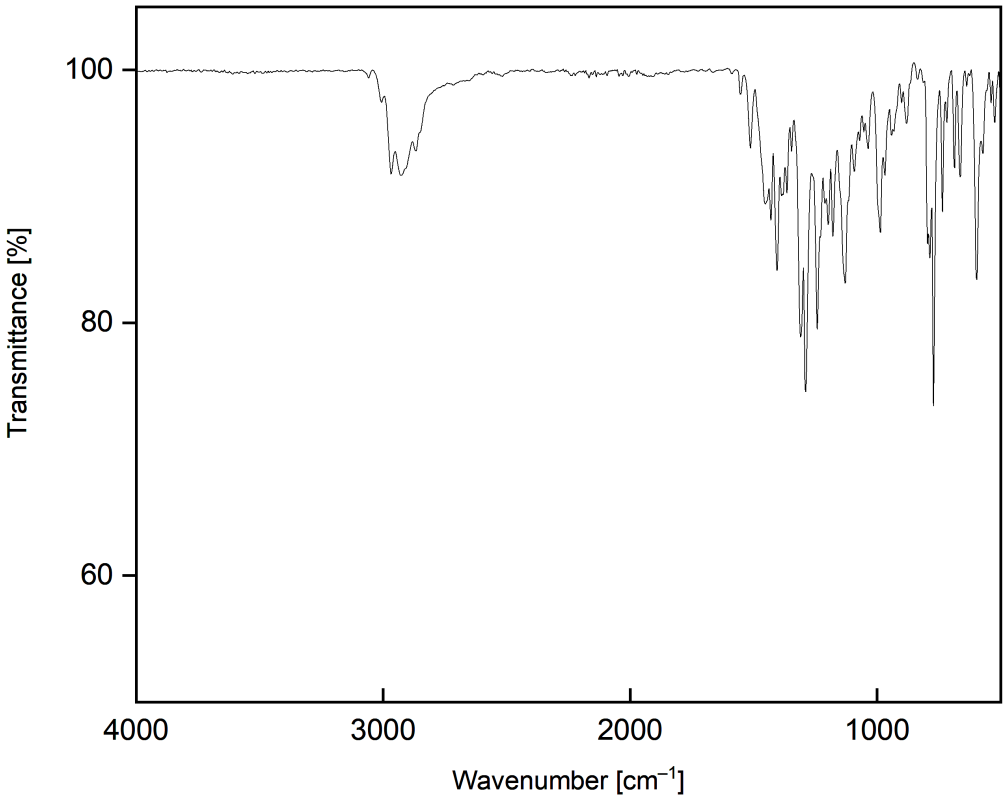


Fig. S27 IR spectrum of compound **6c**.

X-ray crystallographic data

The crystal data of **4a** and **4b** were collected on a BRUKER D8 QUEST diffractometer with a CMOS area detector and multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The crystal data of **6a**, **6b**, **6c**, **7a** and **7b** were collected on a RIGAKU XTALAB SYNERGY-R diffractometer with a HPA area detector and multi-layer mirror monochromated $Cu_{K\alpha}$ radiation. The structure was solved using intrinsic phasing method,[7] refined with the SHELXL program[8] and expanded using Fourier techniques. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were included in structure factor calculations. All hydrogen atoms were assigned to idealized geometric positions.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC-2362579 (**4a**), 2362580 (**4b**), 2362581 (**6a**), 2362582 (**6b**), 2362584 (**6c**), 2362592 (**7a**), 2362586 (**7b**). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via http://www.ccdc.cam.ac.uk/data_request/cif*.

Refinement details for 4a. The azide group was modelled as twofold disordered. The displacement parameters of all atoms of the azide residues (resi 2 and 12) were restrained to the same value with similarity restraints SIMU and RIGU (standard values of 0.004 for both parameters s1 and s2 were used). The Uii displacement parameters within the disorder were restrained with ISOR keyword to approximate isotropic behavior. The 1-2 and 1-3 distances of the azide residues (resi 2 and 12) were restrained to the same values with SAME.

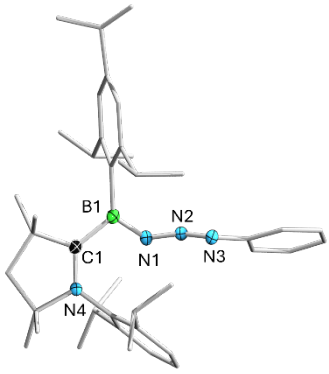


Fig. S28 Crystallographically determined solid-state structure of **4a**. Atomic displacement ellipsoids displayed at 50%. Ellipsoids of ligand periphery and hydrogen atoms omitted for clarity.

Crystal data for 4a. Formula: $C_{41}H_{59}BN_4$, M_r = 618.73, orange block, 0.199×0.109×0.089 mm^3, triclinic space group $P\ \bar{1}$, a = 9.959(2) Å, b = 10.779(4) Å, c = 18.206(6) Å, α = 81.921(18)°, β = 74.267(17)°, γ = 88.188(15)°, V = 1862.4(10) Å^3, Z = 2, ρ_{calcd} = 1.103 g·cm^{-3}, μ = 0.064 mm^{-1}, $F(000)$ = 676, T = 100(2) K, R_1 = 0.0715, wR^2 = 0.1126, 7267 independent reflections [2$\theta \leq$52.044°] and 511 parameters.

Refinement details for 4b. The displacement parameters of atoms of the disordered CAAC ligand were restrained to the same value with similarity restraint SIMU and RIGU.The Uii displacement parameters of atoms of the disordered CAAC ligand were restrained with ISOR keyword to approximate isotropic behavior.

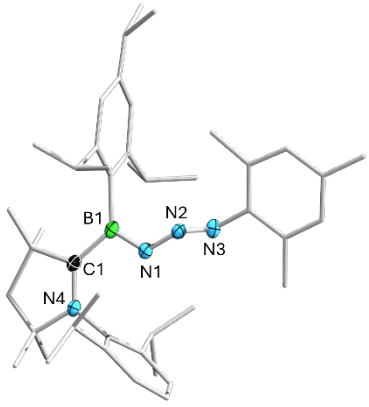


Fig. S29 Crystallographically determined solid-state structure of **4b**. Atomic displacement ellipsoids displayed at 50%. Ellipsoids of ligand periphery and hydrogen atoms omitted for clarity.

Crystal data for 4b. Formula: $C_{44}H_{65}BN_4$, M_r = 660.81, yellow block, 0.165×0.145×0.122 mm^3, monoclinic space group $P2_1/n$, a = 10.5315(2) Å, b = 16.4623(3) Å, c = 23.1574(5) Å, β = 96.2090(10)°, V = 3991.31(14) Å^3, Z = 4, ρ_{calcd} = 1.100 g·cm^{-3}, μ = 0.063 mm^{-1}, F(000) = 1448, T = 100(2) K, R_1 = 0.0708, wR^2 = 0.1208, 7847 independent reflections [2θ≤52.044°] and 499 parameters.

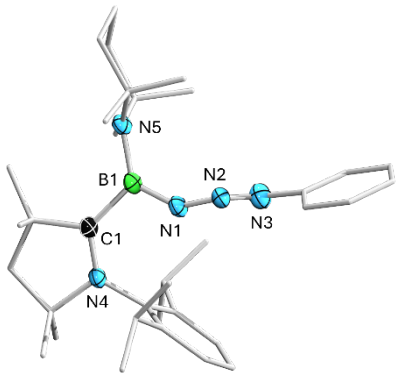


Fig. S30 Crystallographically determined solid-state structure of **6a**. Atomic displacement ellipsoids displayed at 50%. Ellipsoids of ligand periphery and hydrogen atoms omitted for clarity.

Crystal data for 6a. Formula: $C_{35}H_{54}BN_5$, M_r = 555.64, red block, 0.210×0.150×0.100 mm^3, triclinic space group $P\bar{1}$, a = 10.8020(2) Å, b = 12.3555(3) Å, c = 13.8232(2) Å, α = 76.108(2)°, β = 79.110(2)°, γ = 68.167(2)°, V = 1652.28(6) Å^3, Z = 2, ρ_{calcd} = 1.117 g·cm^{-3}, m = 0.495 mm^{-1}, F(000) = 608, T = 100(2) K, R_1 = 0.0678, wR_2 = 0.1659, 6539 independent reflections [2θ≤149.456°] and 382 parameters.

Refinement details for 6b. The atomic displacement parameters of the azide groups were restrained with the RIGU keyword ('enhanced rigid bond' restraint for all bonds in the connectivity list). The displacement parameters of atoms N1 to C11 of residues 2 and 3 were restrained to the same value with similarity restraint SIMU.

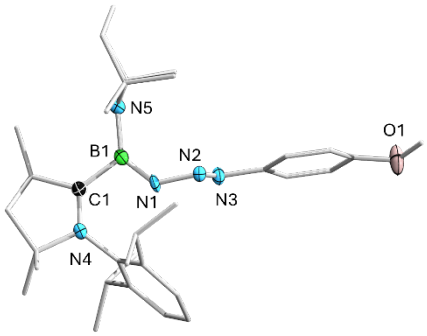


Fig. S31 Crystallographically determined solid-state structure of **6b**. Atomic displacement ellipsoids displayed at 50%. Ellipsoids of ligand periphery and hydrogen atoms omitted for clarity.

Crystal data for 6b: Formula: $C_{36}H_{56}BN_5O$, M_r = 585.66, red block, 0.210×0.120×0.060 mm^3, monoclinic space group $P2_1/n$, a = 9.6634(2) Å, b = 19.2539(2) Å, c = 18.6478(3) Å, α = 90°, β = 103.619(2)°, γ = 90°, V = 3372.02(10) Å^3, Z = 4, ρ_{calcd} = 1.154 g·cm^{-3}, m = 0.532 mm^{-1}, F(000) = 1280, T = 100(2) K, R_1 = 0.0753, wR_2 = 0.1752, 6826 independent reflections [2θ≤150.258°] and 476 parameters.

Refinement details for 6c. Refined as a two-component twin. Component 2 was rotated by –179.9928° around [1.00 0.00 –0.05] (reciprocal) or [1.00 –0.00 0.00] (direct). The BASF parameter was refined to 48.9%.

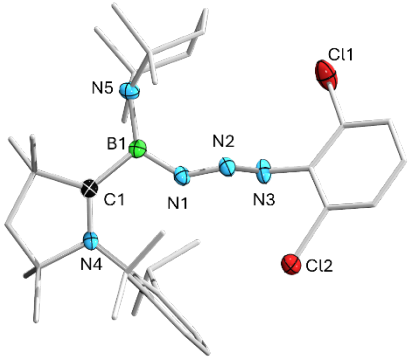


Fig. S32 Crystallographically determined solid-state structure of **6c**. Atomic displacement ellipsoids displayed at 50%. Ellipsoids of ligand periphery and hydrogen atoms omitted for clarity.

Crystal data for 6c: Formula: $C_{35}H_{52}BCl_2N_5$, M_r = 624.52, clear red block, 0.550×0.154×0.078 mm^3, monoclinic space group $P2_1/c$, a = 23.6475(4) Å, b = 15.5802(3) Å, c = 18.9468(2) Å, α = 90°, β = 93.6140(10)°, γ = 90°, V = 6966.74(19) Å^3, Z = 8, ρ_{calcd} = 1.191 g·cm^{-3}, μ = 1.902 mm^{-1}, F(000) = 2688, T = 100.00(10) K, R_1 = 0.0551, wR_2 = 0.1530, 22478 independent reflections [2θ≤140.14°] and 800 parameters.

Refinement detail for 7a. Refined as a two-component twin. Component 2 was rotated by 147.9911° around [0.71 0.52 0.48] (reciprocal) or [0.79 0.55 0.29] (direct) The BASF parameter was refined to 4.9%.

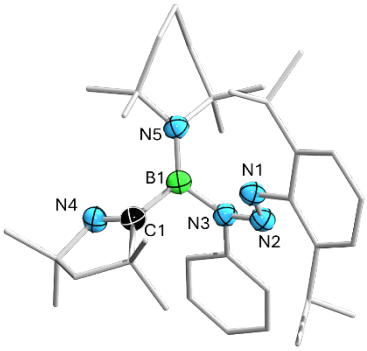


Fig. S33 Crystallographically determined solid-state structure of **7a**. Atomic displacement ellipsoids displayed at 50%. Ellipsoids of ligand periphery and hydrogen atoms omitted for clarity.

Crystal data for 7a: Formula: $C_{35}H_{54}BN_5$, M_r = 555.64, colorless needle, 0.449×0.043×0.036 mm^3, monoclinic space group $P2_1/n$, a = 13.32910(10) Å, b = 13.6009(2) Å, c = 18.6157(3) Å, α = 90°, β = 92.4420(10)°, γ = 90°, V = 3371.73(8) Å^3, Z = 4, ρ_{calcd} = 1.095 g·cm^{-3}, m = 0.485 mm^{-1}, F(000) = 1216, T = 100.00(10) K, R_1 = 0.1078, wR_2 = 0.2601, 15582 independent reflections [2θ≤152.296°] and 383 parameters.

Refinement detail for 7b. Refined as a two-component twin. The BASF parameter was refined to 12.7%.

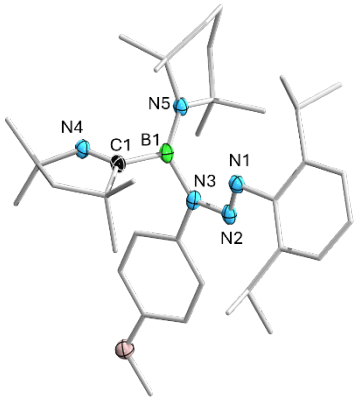


Fig. S34 Crystallographically determined solid-state structure of **7b**. Atomic displacement ellipsoids displayed at 50%. Ellipsoids of ligand periphery and hydrogen atoms omitted for clarity.

Crystal data for 7b: Formula: $C_{36}H_{56}BN_5O$, M_r = 585.66, orange block, 0.378×0.247×0.149 mm^3, triclinic space group $P\bar{1}$, a = 10.16230(10) Å, b = 10.46690(10) Å, c = 17.7919(3) Å, a = 80.9440(10)°, b = 74.9360(10)°, g = 71.0580(10)°, V = 1722.96(4) Å^3, Z = 2, r_{calcd} = 1.129 g·cm^{-3}, m = 0.520 mm^{-1}, F(000) = 640, T = 100(2) K, R_1 = 0.0709, wR_2 = 0.2075, 13828 independent reflections [2q≤150.146°] and 402 parameters.

Computational details

All molecules were fully optimized using the Gaussian 16, Rev. C.01[9] quantum chemistry program package at the ωB97X-D[10]/Def2-SVP level of theory. The model compounds were fully optimized in gaseous state (no solvent effect) starting from the X-ray crystallographic coordinates. Frequency calculations were performed at the same level of theory to verify the nature of the stationary states and the absence of any imaginary frequency to confirm that all structures represent minima on the potential energy hypersurface. Natural bonding analyses were performed with the natural bond orbital (NBO 7.0) partitioning scheme as implemented in the Gaussian 16 suite of programs.[11-13] Natural charges and Wiberg bond indexes (WBI)[14] were obtained from a natural bond orbital analysis. In order to understand the nature of bonding in the synthesised molecules in greater detail, the QTAIM analysis[15, 16] was carried out utilizing the Multiwfn V.3.6 package[17] whereas the wave functions were generated with Gaussian16 at the same level of theory as for geometry optimization.

All calculations of mechanism of reaction of PhN_3 azide with **5** were carried out using Gaussian 16, Rev. C.01[9] quantum chemistry program package at the ωB97X-D[10]/Def2-SVP and re-optimized at the SMD(benzene)/ωB97X-D[10]/Def2-TZVP[18] level of theory. Unfortunately, frequency calculations for one of the transition states using the larger basis set did not converge and thus we obtained no thermal corrections. For this reason, in this study we used results from a lower level of theory. The optimized geometries of intermediates were determined as minima at their respective potential energy surfaces through vibrational frequency calculations, which confirmed the presence of positive eigenvalues in the Hessian matrices. All transition states in the reaction mechanism have one negative eigenvalue (NEv). To ensure the connectivity between corresponding minima and transition states, intrinsic reaction coordinate (IRC) calculations were performed.

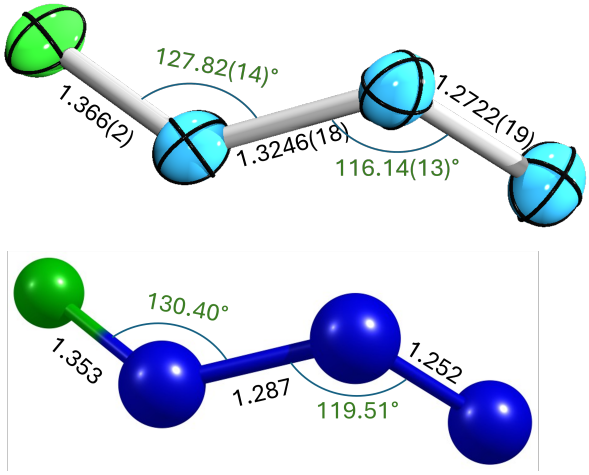


Fig. S35 Structural parameters of the BNNN motif of crystallographically-derived molecular structure and optimized structure of **4b**. Bond distances are in Å.

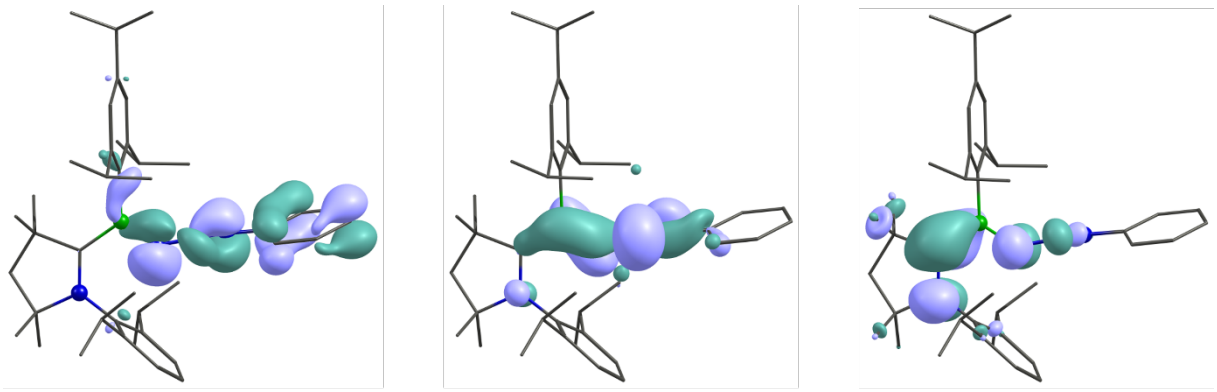


Fig. S36 Selected molecular orbitals of **4a**.

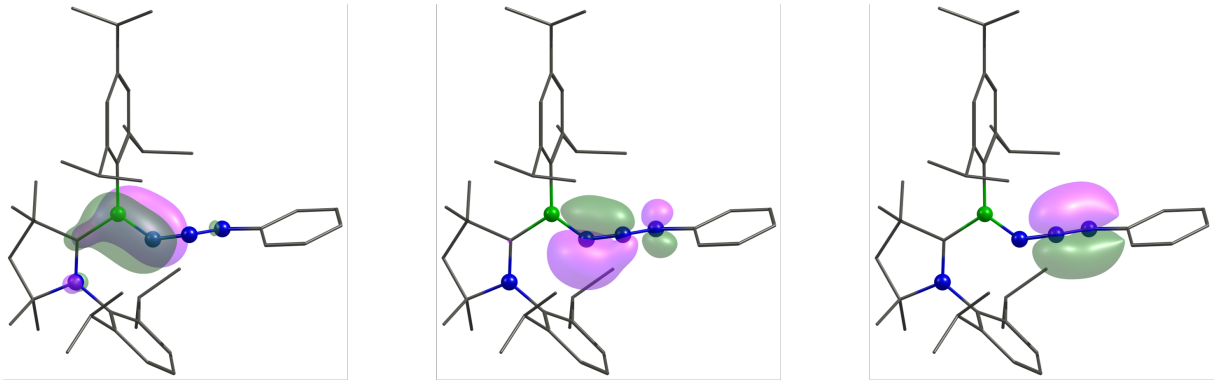
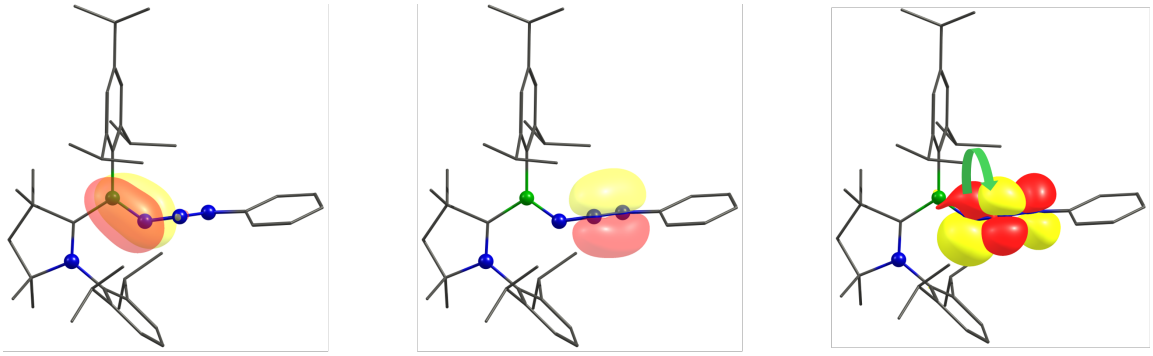


Fig. S37 Selected NLMOs of **4a**.



B1-N1 (π) N2-N3 (π) lp (N1) → π^*(N2-N3): resulted in N1-N2 (π-*interaction*), E(2) = 80.79 Kcal·mol^{-1}

Fig.S38 Selected NBOs of **4a**.

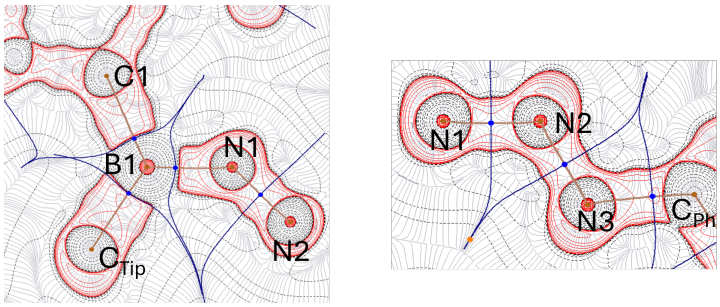
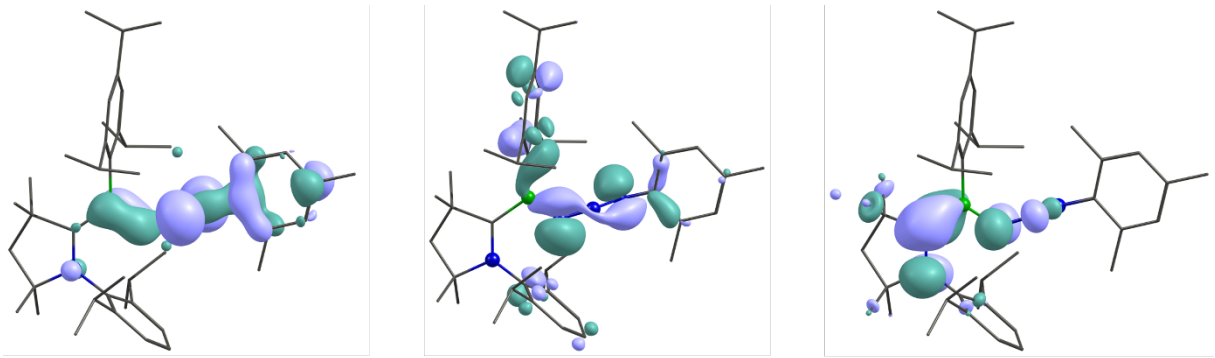


Fig. S39 Contour-line diagram of the Laplacian of the electron density of **4a** in B1-N1-N2 and N1-N2-N3 planes, respectively. Regions of charge depletion and concentration are represented with dashed black and solid red curves, respectively. Bond critical points (BCP) and paths are represented by blue dots, and brown curves, respectively. These Laplacian plots of electron density show bond critical points (BCPs) and bond paths with higher charge concentration, which suggest strong bonding connectivity along the BN_3 unit.



HOMO HOMO-1 LUMO

Fig. S40 Selected molecular orbitals of **4b**.

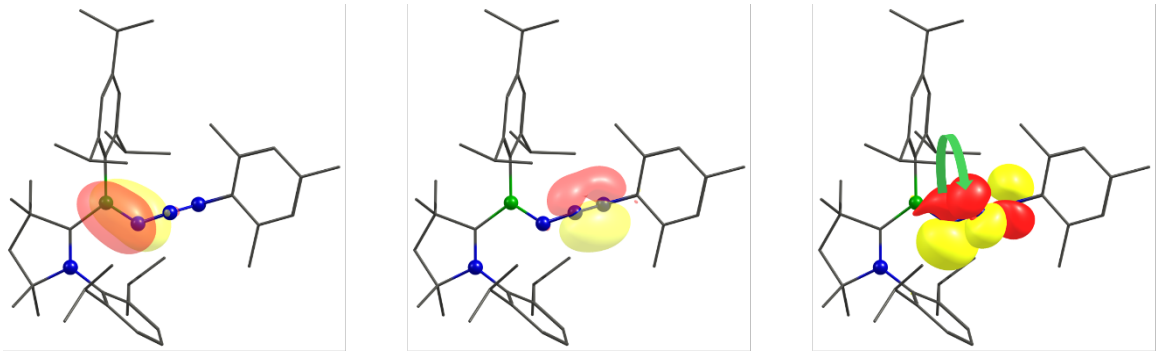


Fig. S41 Selected NBOs of **4b**.

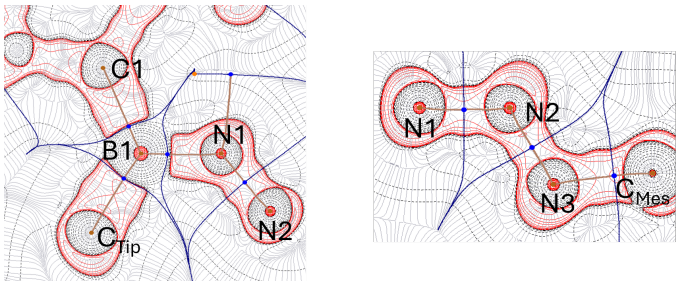


Fig. S42 Contour-line diagram of the Laplacian of the electron density of **4b** in B1-N1-N2 and N1-N2-N3 planes, respectively. Regions of charge depletion and concentration are represented with dashed black and solid red curves, respectively. Bond critical points (BCP) and paths are represented by blue dots, and brown curves, respectively. These Laplacian plots of electron density show bond critical points (BCPs) and bond paths with higher charge concentration, which suggest strong bonding connectivity along the BN_3 unit.

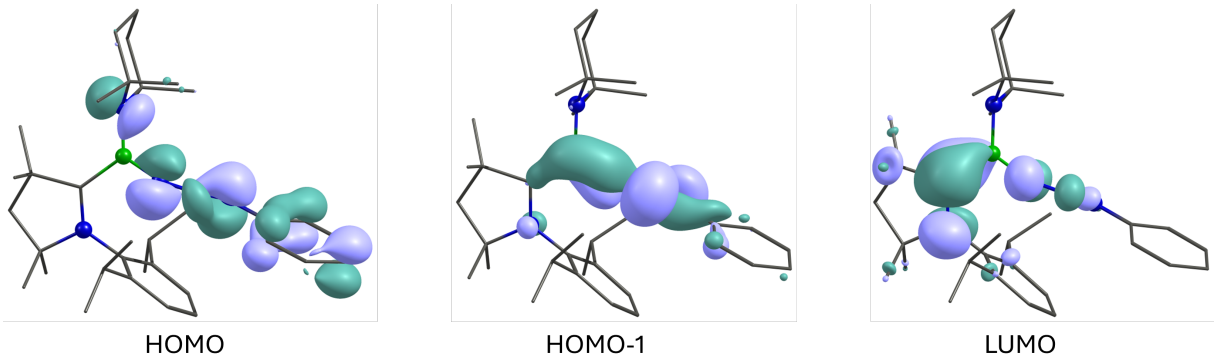
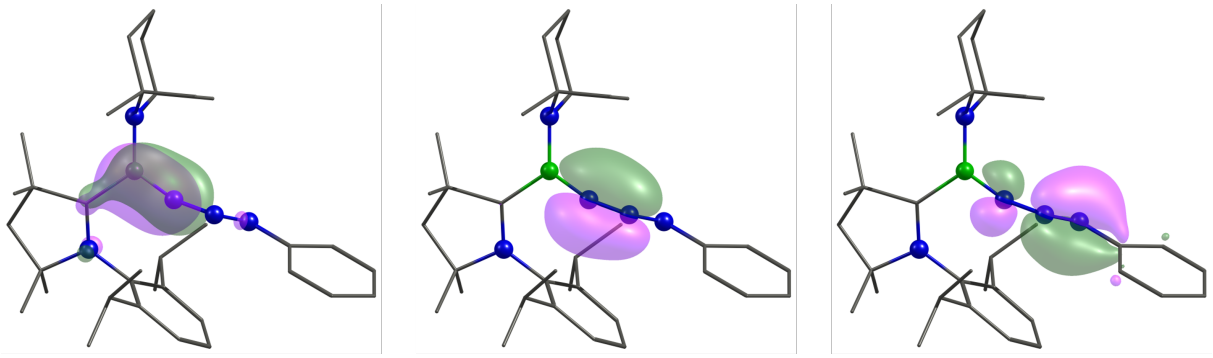


Fig. S43 Selected molecular orbitals of **6a**.

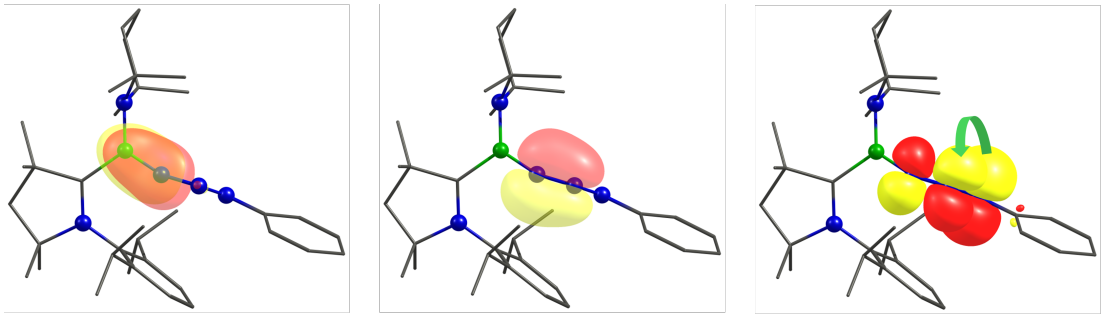


25.3% B1(*p*) + 68.2 % N1(*p*) + 3.4% C1(*p*) + 1.2% N4($sp^{78.76}$)

65.3% N1(*p*) + 32.2% N2(*p*)

19.6% N2(*p*) + 64.7% N3(*p*) + 9.1% N1($sp^{42.39}$)

Fig. S44 Selected NLMOs of **6a**.

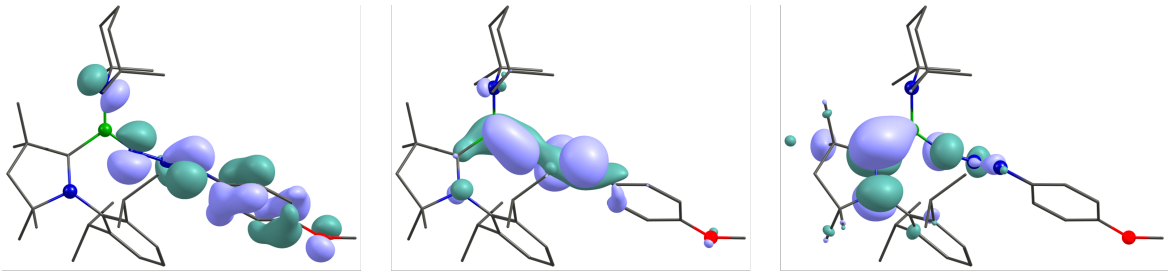


B1-N1 (π)

N1-N2 (π)

lp (N3) → π^*(N1-N2): resulted in N2-N3 (*π-interaction*), E(2) = 276.67 Kcal·mol^{-1}

Fig. S45 Selected NBOs of **6a**.

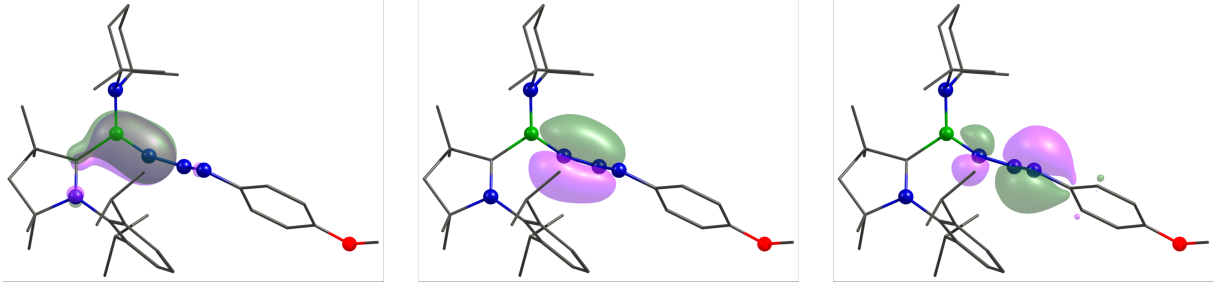


HOMO

HOMO-1

LUMO

Fig. S46 Selected molecular orbitals of **6b**.

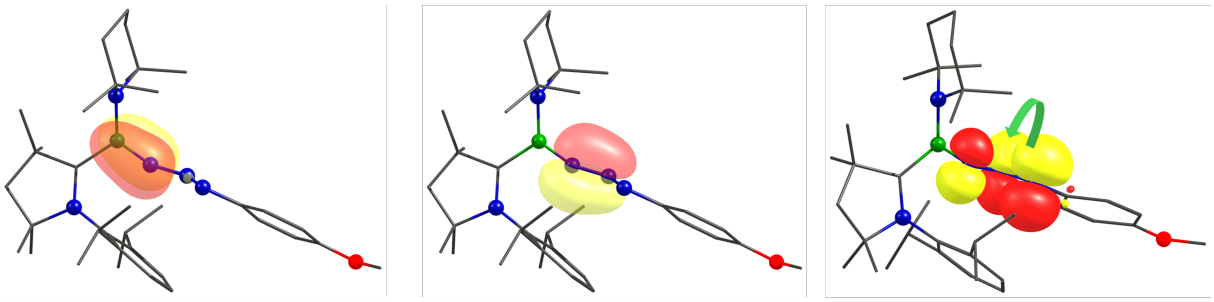


25.4% B1(*p*) + 67.9% N1(*p*) + 3.6% C1(*p*) + 1.2% N4($sp^{82.09}$)

66.0% N1($sp^{80.4}$) + 31.5% N2(*p*)

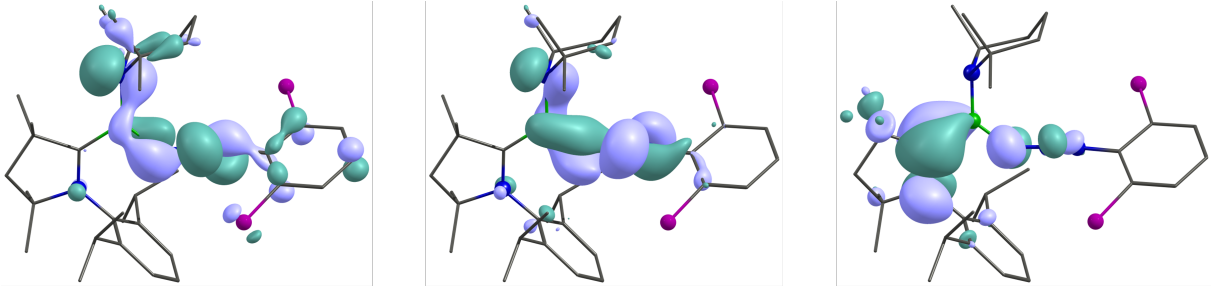
20.7% N2(*p*) + 64.2% N3(*p*) + 9.3% N1($sp^{35.2}$)

Fig.S47 Selected NLMOs of **6b**.



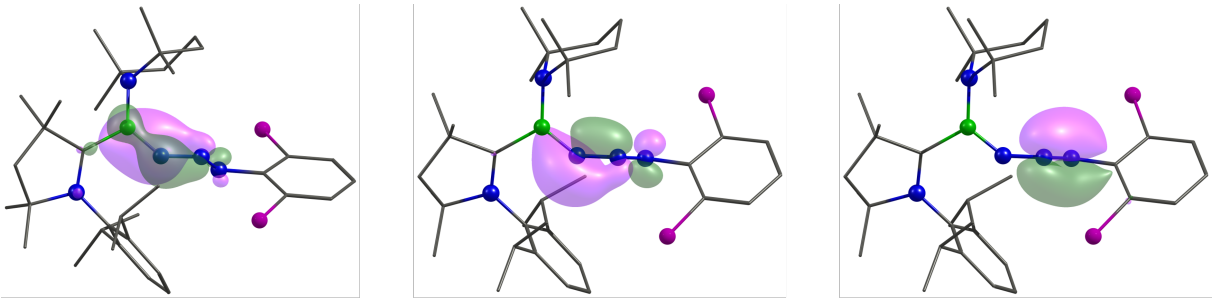
B1-N1 (π) | N1-N2 (π) | lp (N3) → π^*(N1-N2): resulted in N2-N3 (π-*interaction*), E(2) = 292.28 Kcal·mol^{-1}

Fig. S48 Selected NBOs of **6b**.



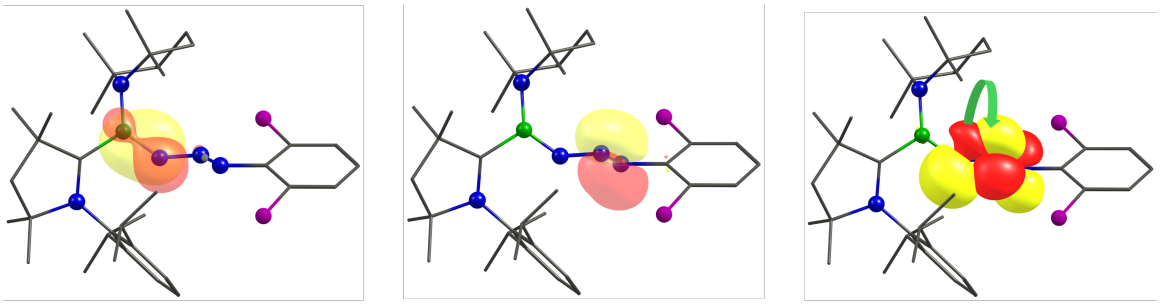
HOMO | HOMO-1 | LUMO

Fig. S49 Selected molecular orbitals of **6c**.



19.8% B1($sp^{10.63}$) + 71.1% N1($sp^{8.84}$) + 3.3% N2($sp^{15.75}$) + 1.9% N3($sp^{20.26}$) | 78.8% N1($sp^{2.18}$) + 8.2% N2(p) + 4.7% N3(p) + 6.2% B1($sp^{5.15}$) | 38.4% N2($sp^{45.29}$) + 58.1% N3(p)

Fig. S50 Selected NLMOs of **6c**.



B1-N1 (π) | N2-N3 (π) | lp (N1) → π^*(N2-N3): resulted in N1-N2 (π-*interaction*), E(2) = 46.51 Kcal·mol^{-1}

Fig. S51 Selected NBOs of **6c**.

Table S1. Details of the B—N_γ unit in compounds **4a**,**b** and **6a**-**c**. Natural charges are denoted by *q*.

	NBO details of B=N_γ			q_B	$q_{N\gamma}$
	occupancy	B contribution	N_γ contribution		
4a	BD(1) 1.95 BD(2) 1.85	23.80% ($sp^{2.23}$) 27.77% (*p*)	76.20% ($sp^{1.28}$) 72.23% (*p*)	0.64	-0.51
4b	BD(1) 1.96 BD(2) 1.84	24.19% ($sp^{2.25}$) 28.23% (*p*)	75.81% ($sp^{1.17}$) 71.77% (*p*)	0.64	-0.54
6a	BD(1) 1.98 BD(2) 1.87	22.89% ($sp^{2.23}$) 26.50% (*p*)	77.11% ($sp^{0.61}$) 73.50% (*p*)	0.83	-0.49
6b	BD(1) 1.98 BD(2) 1.87	22.94% ($sp^{2.16}$) 26.69% (*p*)	77.06% ($sp^{0.61}$) 73.31% (*p*)	0.83	-0.50
6c	BD(1) 1.90 BD(2) 1.80	23.18% ($sp^{3.37}$) 21.93% ($sp^{8.57}$)	76.82% ($sp^{3.63}$) 78.07% ($sp^{14.53}$)	0.86	-0.55

Table S2. Wiberg bond indices (WBIs) of compounds **6a**-**c**.

	B—N_γ	N_γ—N_β	N_β—N_α
6a	1.72	1.66	1.71
6b	1.72	1.64	1.73
6c	1.69	1.62	1.75

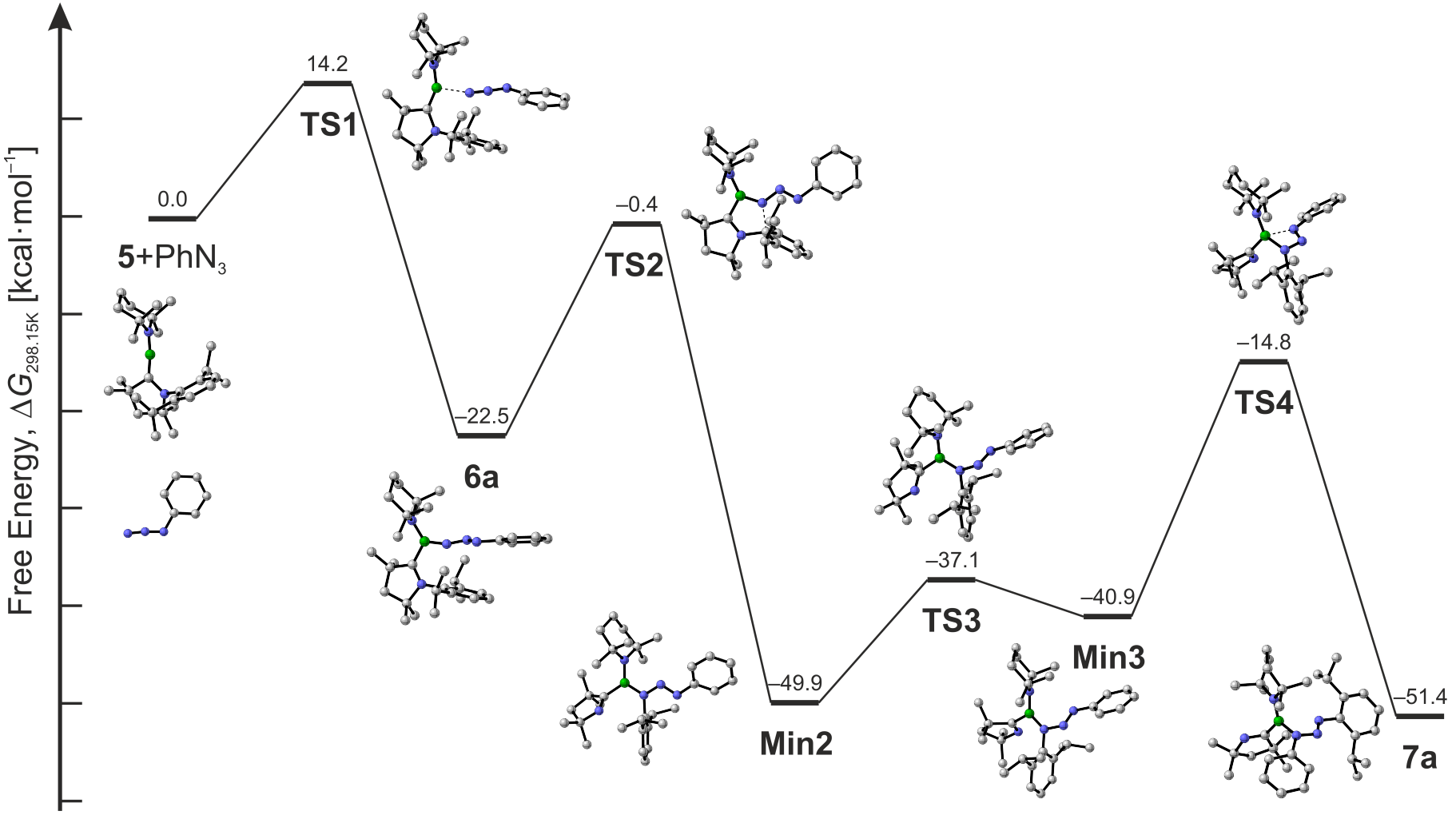
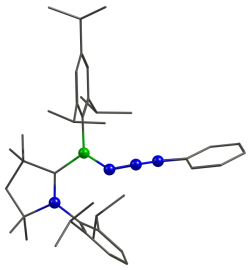


Fig. S52 Free energy profile (kcal·mol^{-1}) of the proposed mechanistic pathway for the formation of **7a** at the ωB97X-D/Def2-SVP level of theory. Energies are referenced to substrates (**5** and PhN_3). Hydrogen atoms are omitted for clarity.

Coordinates of computed molecules 4a-b and 6a-c

4a (Coordinates in Å), NEv = 0

E = –1839.931418



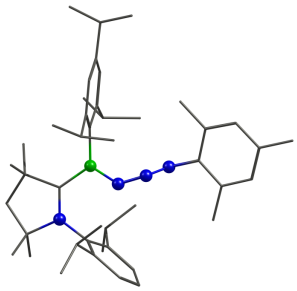
B	0.131447000000	-0.497851000000	0.074274000000
N	-0.431196000000	0.734051000000	-0.049387000000
N	-0.025724000000	1.917801000000	-0.295445000000
N	0.132298000000	2.730080000000	0.653952000000
C	0.460138000000	4.036999000000	0.235702000000
C	0.249223000000	4.528865000000	-1.061860000000
H	-0.190898000000	3.870091000000	-1.811761000000
C	0.594277000000	5.840184000000	-1.374640000000
H	0.425608000000	6.213800000000	-2.387802000000
C	1.146102000000	6.681291000000	-0.406332000000
H	1.412862000000	7.710067000000	-0.658068000000
C	1.345980000000	6.198131000000	0.886807000000
H	1.773313000000	6.848359000000	1.653942000000
C	1.001221000000	4.887710000000	1.207350000000
H	1.148091000000	4.494396000000	2.215389000000
C	1.707178000000	-0.748490000000	0.121019000000
C	2.397235000000	-0.776026000000	1.351196000000
C	3.781750000000	-0.971119000000	1.368119000000
H	4.313340000000	-0.990907000000	2.323767000000
C	4.516267000000	-1.134903000000	0.194832000000
C	3.829879000000	-1.078256000000	-1.019124000000
H	4.392891000000	-1.178381000000	-1.951207000000
C	2.448808000000	-0.877785000000	-1.074357000000
C	-2.941637000000	-0.284329000000	-0.080750000000
C	-3.212923000000	0.220317000000	-1.368243000000
C	-3.990988000000	1.376993000000	-1.458429000000
H	-4.214649000000	1.791983000000	-2.443523000000
C	-4.452791000000	2.030751000000	-0.324098000000
H	-5.053794000000	2.937147000000	-0.420362000000
C	-4.111524000000	1.551203000000	0.933180000000
H	-4.430127000000	2.100819000000	1.821184000000
C	-3.343777000000	0.394927000000	1.086885000000
C	-0.938378000000	-1.692262000000	0.146106000000
C	-0.598023000000	-3.171518000000	0.238917000000
C	-1.960604000000	-3.834284000000	0.512556000000
H	-2.070539000000	-4.791269000000	-0.016158000000
H	-2.052790000000	-4.045018000000	1.588442000000
C	-3.036974000000	-2.828169000000	0.097142000000

N	-2.239307000000	-1.543667000000	0.060829000000
C	0.383795000000	-3.507752000000	1.365583000000
H	1.386413000000	-3.109889000000	1.168958000000
H	0.456686000000	-4.602710000000	1.456802000000
H	0.034883000000	-3.111030000000	2.330625000000
C	0.008548000000	-3.600459000000	-1.109675000000
H	0.155613000000	-4.691039000000	-1.112420000000
H	0.985377000000	-3.122497000000	-1.258547000000
H	-0.636230000000	-3.338739000000	-1.961877000000
C	-3.629325000000	-3.135951000000	-1.277467000000
H	-2.861466000000	-3.217599000000	-2.057349000000
H	-4.352456000000	-2.364689000000	-1.570978000000
H	-4.162574000000	-4.095659000000	-1.223856000000
C	-4.172189000000	-2.761089000000	1.114034000000
H	-4.700013000000	-3.725770000000	1.108734000000
H	-4.897182000000	-1.973114000000	0.865803000000
H	-3.796033000000	-2.590658000000	2.130012000000
C	-2.595901000000	-0.331612000000	-2.647875000000
H	-2.033060000000	-1.240757000000	-2.394134000000
C	-1.586524000000	0.670258000000	-3.227141000000
H	-1.039638000000	0.214704000000	-4.067523000000
H	-0.861898000000	0.996606000000	-2.472098000000
H	-2.100177000000	1.566017000000	-3.610509000000
C	-3.634284000000	-0.689893000000	-3.717669000000
H	-3.139769000000	-1.151544000000	-4.586069000000
H	-4.152887000000	0.210695000000	-4.080896000000
H	-4.401442000000	-1.386903000000	-3.354527000000
C	-2.899030000000	0.001279000000	2.489530000000
H	-2.365338000000	-0.958589000000	2.425260000000
C	-1.906013000000	1.030682000000	3.048220000000
H	-1.083210000000	1.228246000000	2.349429000000
H	-1.486204000000	0.674066000000	4.002095000000
H	-2.407684000000	1.991841000000	3.242047000000
C	-4.075942000000	-0.173806000000	3.457465000000
H	-4.841865000000	-0.861793000000	3.072893000000
H	-4.569257000000	0.789401000000	3.658993000000
H	-3.718523000000	-0.561797000000	4.423655000000
C	1.776248000000	-0.707976000000	-2.431606000000
H	0.693621000000	-0.859349000000	-2.285126000000
C	1.965652000000	0.732596000000	-2.925985000000
H	3.035809000000	0.946859000000	-3.078738000000
H	1.572456000000	1.456065000000	-2.197388000000
H	1.446407000000	0.892286000000	-3.884243000000
C	2.239786000000	-1.710772000000	-3.491446000000
H	1.622507000000	-1.618516000000	-4.398799000000
H	2.170504000000	-2.750209000000	-3.136195000000
H	3.283397000000	-1.532181000000	-3.793971000000
C	6.018972000000	-1.350418000000	0.236860000000
H	6.313265000000	-1.355470000000	1.300083000000
C	6.412386000000	-2.707482000000	-0.356108000000
H	6.157306000000	-2.762094000000	-1.426594000000
H	5.889364000000	-3.529861000000	0.154639000000

H	7.496411000000	-2.878271000000	-0.262412000000
C	6.773326000000	-0.203239000000	-0.443723000000
H	7.862247000000	-0.336764000000	-0.346352000000
H	6.503519000000	0.766269000000	0.000353000000
H	6.537668000000	-0.155117000000	-1.518858000000
C	1.661338000000	-0.543168000000	2.665628000000
H	0.589133000000	-0.726778000000	2.477638000000
C	1.790944000000	0.921969000000	3.097373000000
H	2.849965000000	1.181170000000	3.259281000000
H	1.249068000000	1.099091000000	4.040429000000
H	1.378945000000	1.599677000000	2.334938000000
C	2.100069000000	-1.481346000000	3.794113000000
H	2.097098000000	-2.536437000000	3.482240000000
H	1.427159000000	-1.376620000000	4.659572000000
H	3.115287000000	-1.242558000000	4.147612000000

4b (Coordinates in Å), NEv = 0

E = –1957.770851



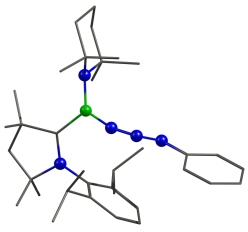
N	3.033850000000	-0.615187000000	0.017642000000
C	1.945584000000	-1.345098000000	-0.060310000000
B	0.451462000000	-0.773534000000	-0.043892000000
N	0.388493000000	0.584633000000	0.049363000000
C	2.316585000000	-2.817621000000	-0.070543000000
N	-1.199746000000	1.873935000000	-0.743209000000
C	4.329567000000	-1.394841000000	0.032651000000
N	-0.619279000000	1.361845000000	0.241277000000
C	1.939647000000	-3.396003000000	1.305569000000
H	0.849994000000	-3.383993000000	1.438304000000
H	2.392946000000	-2.832679000000	2.134809000000
H	2.283104000000	-4.439493000000	1.370187000000
C	1.609382000000	-3.619166000000	-1.166050000000
H	0.528951000000	-3.684628000000	-0.988763000000
H	2.021154000000	-4.640264000000	-1.183955000000
H	1.772876000000	-3.171212000000	-2.157348000000
C	4.988982000000	-1.325335000000	1.409152000000
H	5.272321000000	-0.293695000000	1.653427000000
H	5.905199000000	-1.932408000000	1.391825000000
H	4.340146000000	-1.712739000000	2.205090000000
C	3.082476000000	0.830372000000	0.110156000000
C	5.312953000000	-0.868469000000	-1.008406000000
H	4.904176000000	-0.940775000000	-2.023765000000

H	6.224239000000	-1.482659000000	-0.968451000000
H	5.594822000000	0.175545000000	-0.811518000000
C	3.068043000000	1.446512000000	1.377661000000
C	3.228825000000	2.833418000000	1.425002000000
H	3.219295000000	3.336880000000	2.394054000000
C	3.147948000000	1.580108000000	-1.080801000000
C	3.299667000000	2.964095000000	-0.970966000000
H	3.347624000000	3.568501000000	-1.879117000000
C	3.361029000000	3.588490000000	0.267364000000
H	3.479856000000	4.672082000000	0.329957000000
C	2.944649000000	0.982873000000	-2.466592000000
H	2.899466000000	-0.111802000000	-2.366947000000
C	1.598508000000	1.436930000000	-3.048824000000
H	1.390781000000	0.903770000000	-3.989714000000
H	1.613926000000	2.515266000000	-3.273435000000
H	0.771183000000	1.255302000000	-2.350717000000
C	4.082570000000	1.325635000000	-3.435746000000
H	3.943253000000	0.792797000000	-4.388880000000
H	5.071905000000	1.061973000000	-3.036329000000
H	4.095904000000	2.401950000000	-3.666328000000
C	2.745509000000	0.717601000000	2.676543000000
H	2.662097000000	-0.355816000000	2.456514000000
C	1.380049000000	1.170296000000	3.213960000000
H	0.601876000000	1.109254000000	2.444438000000
H	1.423481000000	2.212838000000	3.566332000000
H	1.082078000000	0.542682000000	4.068434000000
C	-0.868265000000	-1.671973000000	-0.102346000000
C	-1.562167000000	-2.002952000000	1.083638000000
C	-2.790411000000	-2.664465000000	1.012143000000
H	-3.321804000000	-2.902103000000	1.938139000000
C	-3.374558000000	-3.003074000000	-0.208668000000
C	-2.689132000000	-2.664439000000	-1.373565000000
H	-3.145177000000	-2.909526000000	-2.337409000000
C	-1.455920000000	-2.006481000000	-1.341932000000
C	-0.801236000000	-1.617137000000	-2.663547000000
H	0.235574000000	-1.312611000000	-2.438771000000
C	-1.498188000000	-0.400623000000	-3.281974000000
H	-2.552552000000	-0.633932000000	-3.504947000000
H	-1.011827000000	-0.111824000000	-4.227538000000
H	-1.469614000000	0.461572000000	-2.598995000000
C	-0.741017000000	-2.769816000000	-3.672260000000
H	-1.741369000000	-3.015713000000	-4.061379000000
H	-0.323390000000	-3.687635000000	-3.233395000000
H	-0.120435000000	-2.488700000000	-4.537719000000
C	-1.044991000000	-1.572103000000	2.451840000000
H	0.002025000000	-1.250890000000	2.323746000000
C	-1.828977000000	-0.354339000000	2.959146000000
H	-1.760378000000	0.483802000000	2.250636000000
H	-1.439106000000	-0.012952000000	3.931116000000
H	-2.893128000000	-0.608741000000	3.092961000000
C	-1.058937000000	-2.696613000000	3.492055000000
H	-2.086143000000	-2.986043000000	3.763534000000

H	-0.560629000000	-2.368129000000	4.417669000000
H	-0.546402000000	-3.601150000000	3.130926000000
C	-2.238702000000	2.769674000000	-0.369471000000
C	-3.549827000000	2.293556000000	-0.218452000000
C	-4.555283000000	3.216378000000	0.081844000000
H	-5.580578000000	2.853951000000	0.207180000000
C	-4.291009000000	4.580553000000	0.228131000000
C	-2.972851000000	5.017659000000	0.072557000000
H	-2.742428000000	6.081460000000	0.189589000000
C	-1.936252000000	4.131877000000	-0.227149000000
C	-0.511939000000	4.596235000000	-0.383802000000
H	-0.086868000000	4.238756000000	-1.334857000000
H	0.130570000000	4.186877000000	0.411952000000
H	-0.443894000000	5.692935000000	-0.354448000000
C	-3.851146000000	0.825019000000	-0.366456000000
H	-4.929843000000	0.634121000000	-0.278845000000
H	-3.335219000000	0.222152000000	0.396822000000
H	-3.507012000000	0.441647000000	-1.338435000000
C	-5.402433000000	5.558650000000	0.513438000000
H	-5.830719000000	5.955676000000	-0.421849000000
H	-5.042686000000	6.417492000000	1.099063000000
H	-6.221763000000	5.084643000000	1.073543000000
C	3.812359000000	0.906500000000	3.761593000000
H	3.859077000000	1.956151000000	4.090253000000
H	4.819236000000	0.620933000000	3.428672000000
H	3.563009000000	0.301236000000	4.646628000000
C	3.836586000000	-2.803838000000	-0.312869000000
H	4.357554000000	-3.572983000000	0.274085000000
H	4.038229000000	-3.013218000000	-1.373900000000
C	-4.732523000000	-3.679496000000	-0.269941000000
H	-4.931254000000	-3.905892000000	-1.331243000000
C	-5.839331000000	-2.735944000000	0.214270000000
H	-5.840261000000	-1.800522000000	-0.364439000000
H	-6.830644000000	-3.205525000000	0.114451000000
H	-5.696976000000	-2.471368000000	1.274337000000
C	-4.753179000000	-5.006443000000	0.494731000000
H	-5.725193000000	-5.510599000000	0.377246000000
H	-3.967494000000	-5.685956000000	0.131990000000
H	-4.589538000000	-4.849957000000	1.572854000000

6a (Coordinates in Å), NEv = 0

E = –1663.201226



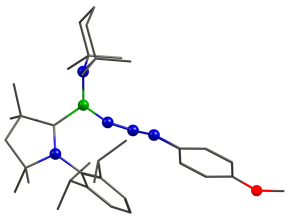
N	-0.806932000000	1.980191000000	0.187633000000

B	-1.184425000000	-0.561858000000	-0.221473000000
N	0.154745000000	-0.697297000000	-0.328563000000
N	-2.155347000000	-1.688153000000	-0.108607000000
N	1.285975000000	-1.161812000000	-0.575678000000
C	0.646035000000	1.883380000000	0.223810000000
C	1.357345000000	2.035845000000	-0.989895000000
C	1.317223000000	1.654868000000	1.442953000000
C	-1.457805000000	3.334536000000	0.388950000000
C	-1.637788000000	1.000825000000	-0.103341000000
C	0.626649000000	1.323818000000	2.760071000000
H	-0.460003000000	1.362632000000	2.592837000000
C	2.716402000000	1.648176000000	1.427469000000
H	3.253852000000	1.454350000000	2.357497000000
C	-2.312287000000	-2.569291000000	-1.291293000000
C	-2.213651000000	-2.314315000000	1.239833000000
C	-3.024365000000	1.593303000000	-0.357141000000
C	0.701281000000	2.129154000000	-2.362975000000
H	-0.381740000000	2.204257000000	-2.218310000000
C	2.750661000000	2.012093000000	-0.938529000000
H	3.318081000000	2.107714000000	-1.866525000000
C	-1.047644000000	4.336663000000	-0.691674000000
H	-1.535704000000	5.297542000000	-0.476017000000
H	-1.343979000000	4.032085000000	-1.701352000000
H	0.038296000000	4.499522000000	-0.677087000000
C	-2.942505000000	2.957565000000	0.343657000000
H	-3.545551000000	3.724948000000	-0.161953000000
H	-3.327475000000	2.860965000000	1.370043000000
C	-4.219150000000	0.772384000000	0.131091000000
H	-4.277542000000	0.762363000000	1.227612000000
H	-4.148003000000	-0.267076000000	-0.213601000000
H	-5.147787000000	1.229007000000	-0.243886000000
C	3.433488000000	1.834882000000	0.257855000000
H	4.524114000000	1.800380000000	0.268750000000
C	-3.156738000000	1.773909000000	-1.887377000000
H	-2.358124000000	2.392634000000	-2.314050000000
H	-4.116205000000	2.267595000000	-2.101869000000
H	-3.144030000000	0.810426000000	-2.405895000000
C	-1.095794000000	-3.473332000000	-1.596667000000
H	-0.175595000000	-2.881660000000	-1.689748000000
H	-1.255560000000	-4.004459000000	-2.548107000000
H	-0.923768000000	-4.233056000000	-0.826588000000
C	-2.319641000000	-1.209289000000	2.299588000000
H	-2.419245000000	-1.656870000000	3.299354000000
H	-3.195278000000	-0.573606000000	2.126302000000
H	-1.419644000000	-0.581584000000	2.314025000000
C	0.966531000000	-0.102417000000	3.214869000000
H	2.020417000000	-0.170988000000	3.526370000000
H	0.833988000000	-0.828911000000	2.404562000000
H	0.341811000000	-0.383730000000	4.076787000000
C	-1.080971000000	3.930613000000	1.741271000000
H	-1.353605000000	3.267171000000	2.571182000000
H	-1.631039000000	4.874279000000	1.868549000000

H	-0.006820000000	4.153369000000	1.796291000000
C	-3.578706000000	-3.430757000000	-1.118791000000
H	-4.457388000000	-2.764450000000	-1.177952000000
H	-3.653228000000	-4.132733000000	-1.965336000000
C	-2.534414000000	-1.693869000000	-2.529474000000
H	-1.682933000000	-1.017904000000	-2.705952000000
H	-3.451378000000	-1.098522000000	-2.419593000000
H	-2.649402000000	-2.322325000000	-3.424820000000
C	1.156217000000	3.363671000000	-3.151771000000
H	1.047883000000	4.294873000000	-2.579075000000
H	0.568558000000	3.461368000000	-4.077766000000
H	2.213354000000	3.278821000000	-3.446659000000
C	-3.484586000000	-3.176861000000	1.348290000000
H	-3.484131000000	-3.693366000000	2.322083000000
H	-4.360128000000	-2.504023000000	1.341962000000
C	-0.971600000000	-3.161510000000	1.606234000000
H	-0.956907000000	-3.354351000000	2.690301000000
H	-0.036838000000	-2.645870000000	1.342553000000
H	-0.962376000000	-4.139644000000	1.110364000000
C	0.980663000000	2.310010000000	3.881489000000
H	0.392959000000	2.082619000000	4.784240000000
H	0.796236000000	3.357529000000	3.609815000000
H	2.043246000000	2.223345000000	4.155509000000
C	3.363984000000	-1.773226000000	0.004944000000
C	0.944262000000	0.864379000000	-3.197951000000
H	2.014512000000	0.746710000000	-3.430205000000
H	0.401989000000	0.935444000000	-4.153941000000
H	0.619736000000	-0.040290000000	-2.670662000000
C	-3.627579000000	-4.173161000000	0.207477000000
H	-2.829671000000	-4.931962000000	0.254189000000
H	-4.577128000000	-4.723829000000	0.299687000000
N	2.053989000000	-1.467447000000	0.395974000000
C	4.190108000000	-2.359045000000	0.975849000000
H	3.756502000000	-2.576906000000	1.954238000000
C	5.520819000000	-2.654127000000	0.694696000000
H	6.146163000000	-3.114791000000	1.463614000000
C	3.913582000000	-1.473313000000	-1.254087000000
H	3.279383000000	-0.999299000000	-2.004104000000
C	6.057909000000	-2.364927000000	-0.560520000000
H	7.102799000000	-2.593764000000	-0.781300000000
C	5.244325000000	-1.773710000000	-1.529005000000
H	5.655877000000	-1.536626000000	-2.513741000000

6b (Coordinates in Å), NEv = 0

E = –1777.60382



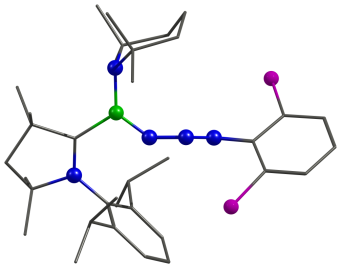
B	-1.406184000000	0.803491000000	-0.220447000000
C	-2.266550000000	-0.579434000000	-0.128374000000
N	-1.733872000000	-1.748592000000	0.163394000000
C	-2.727039000000	-2.880422000000	0.336319000000
C	-4.055225000000	-2.118633000000	0.274804000000
H	-4.416518000000	-1.929400000000	1.296938000000
H	-4.833935000000	-2.692312000000	-0.247456000000
C	-3.756044000000	-0.777567000000	-0.411516000000
C	-3.903985000000	-0.905935000000	-1.945486000000
H	-4.955386000000	-1.128762000000	-2.180604000000
H	-3.287896000000	-1.709244000000	-2.367105000000
H	-3.629486000000	0.024266000000	-2.451952000000
C	-4.695789000000	0.330510000000	0.066601000000
H	-5.705886000000	0.142563000000	-0.328297000000
H	-4.341693000000	1.314775000000	-0.265658000000
H	-4.769421000000	0.348979000000	1.162134000000
C	-2.548107000000	-3.568958000000	1.685420000000
H	-3.333218000000	-4.331629000000	1.791521000000
H	-2.647504000000	-2.864587000000	2.520407000000
H	-1.574049000000	-4.072112000000	1.752874000000
C	-2.581219000000	-3.945413000000	-0.752167000000
H	-3.312504000000	-4.742560000000	-0.557717000000
H	-1.578792000000	-4.392973000000	-0.723790000000
H	-2.766414000000	-3.562542000000	-1.761674000000
C	-0.309111000000	-2.045135000000	0.226380000000
C	0.373291000000	-2.013016000000	1.460231000000
C	1.723122000000	-2.381274000000	1.470766000000
H	2.273188000000	-2.344469000000	2.412839000000
C	2.387936000000	-2.747684000000	0.312727000000
H	3.447054000000	-3.008745000000	0.344154000000
C	1.707427000000	-2.728685000000	-0.897949000000
H	2.247345000000	-2.968744000000	-1.816234000000
C	0.360411000000	-2.376293000000	-0.975343000000
C	-0.266743000000	-2.276923000000	-2.361375000000
H	-1.332051000000	-2.054553000000	-2.237394000000
C	-0.148518000000	-3.581919000000	-3.159020000000
H	-0.717506000000	-3.506325000000	-4.098655000000
H	-0.522169000000	-4.452781000000	-2.603279000000
H	0.898299000000	-3.787855000000	-3.430150000000
C	0.330125000000	-1.119323000000	-3.173771000000
H	-0.194416000000	-1.027053000000	-4.137832000000
H	1.394884000000	-1.299967000000	-3.390583000000

H	0.259536000000	-0.166260000000	-2.636581000000
C	0.469695000000	-0.236269000000	3.244449000000
H	-0.075077000000	0.198822000000	4.096687000000
H	0.555756000000	0.502838000000	2.439214000000
H	1.495949000000	-0.455913000000	3.577809000000
C	-0.231211000000	-1.515962000000	2.767437000000
H	-1.284343000000	-1.259964000000	2.578276000000
C	-0.179656000000	-2.567024000000	3.884645000000
H	-0.704297000000	-2.195020000000	4.778233000000
H	0.860973000000	-2.770483000000	4.180375000000
H	-0.632538000000	-3.525028000000	3.597857000000
N	-2.040707000000	2.150132000000	-0.117918000000
C	-1.956565000000	2.766457000000	1.233363000000
C	-2.951156000000	3.938590000000	1.323278000000
H	-2.833240000000	4.433751000000	2.301059000000
H	-3.974926000000	3.525876000000	1.293501000000
C	-2.795717000000	4.939198000000	0.187886000000
H	-3.563377000000	5.725433000000	0.265227000000
H	-1.823846000000	5.454330000000	0.257008000000
C	-2.919586000000	4.214246000000	-1.143141000000
H	-2.783233000000	4.912338000000	-1.985230000000
H	-3.943862000000	3.809823000000	-1.225902000000
C	-1.928955000000	3.043295000000	-1.296388000000
C	-2.352228000000	2.262812000000	-2.545576000000
H	-2.273719000000	2.900498000000	-3.438359000000
H	-3.398169000000	1.937576000000	-2.458777000000
H	-1.711700000000	1.381933000000	-2.709444000000
C	-0.507417000000	3.586334000000	-1.570403000000
H	-0.496395000000	4.138514000000	-2.523235000000
H	0.221700000000	2.768722000000	-1.644229000000
H	-0.155427000000	4.274088000000	-0.793850000000
C	-2.376629000000	1.728593000000	2.282976000000
H	-2.373315000000	2.184854000000	3.283818000000
H	-1.678192000000	0.882661000000	2.309836000000
H	-3.386721000000	1.351078000000	2.088149000000
C	-0.540785000000	3.248941000000	1.630688000000
H	-0.498332000000	3.429633000000	2.716183000000
H	-0.259176000000	4.189420000000	1.141826000000
H	0.227070000000	2.501995000000	1.382560000000
N	-0.079860000000	0.562827000000	-0.296996000000
N	1.140094000000	0.732986000000	-0.517524000000
N	1.939499000000	0.827079000000	0.468168000000
C	3.776641000000	0.357103000000	-1.145013000000
H	3.059627000000	0.043499000000	-1.904683000000
C	3.293916000000	0.797871000000	0.101660000000
C	4.226825000000	1.169911000000	1.072204000000
H	3.854562000000	1.499704000000	2.044474000000
C	5.599380000000	1.130768000000	0.820407000000
H	6.290691000000	1.436228000000	1.606522000000
C	6.064868000000	0.703146000000	-0.426113000000
C	5.137540000000	0.315841000000	-1.403894000000
H	5.517953000000	-0.024873000000	-2.369070000000

O	7.374485000000	0.621724000000	-0.773535000000
C	8.341060000000	0.999304000000	0.161744000000
H	9.318623000000	0.863266000000	-0.318132000000
H	8.237109000000	2.058268000000	0.460074000000
H	8.303359000000	0.373849000000	1.072229000000

6c (Coordinates in Å), NEv = 0

E = –2582.104419



B	0.662837000000	1.120020000000	-0.350869000000
N	-1.398860000000	-0.232578000000	-0.531598000000
N	-2.185450000000	-0.445930000000	0.443575000000
N	-0.197194000000	0.065306000000	-0.279443000000
C	2.205891000000	0.645224000000	-0.202592000000
N	2.588687000000	-0.514299000000	0.279259000000
C	3.429758000000	1.428293000000	-0.675797000000
C	4.586746000000	0.424812000000	-0.479435000000
H	4.812861000000	-0.081701000000	-1.430623000000
H	5.510814000000	0.912240000000	-0.139527000000
C	4.078267000000	-0.600636000000	0.533070000000
C	3.227530000000	1.738459000000	-2.168607000000
H	2.933253000000	0.843156000000	-2.737561000000
H	4.172747000000	2.115971000000	-2.588180000000
H	2.454228000000	2.505552000000	-2.298674000000
C	3.675683000000	2.754354000000	0.051739000000
H	2.803431000000	3.406607000000	-0.061760000000
H	4.547833000000	3.250195000000	-0.400637000000
H	3.885972000000	2.621444000000	1.121635000000
C	4.645046000000	-1.996908000000	0.314333000000
H	4.192269000000	-2.729010000000	0.997468000000
H	5.726259000000	-1.964986000000	0.512628000000
H	4.502555000000	-2.345763000000	-0.714787000000
C	4.361163000000	-0.162831000000	1.974534000000
H	3.899928000000	0.806310000000	2.207039000000
H	5.447643000000	-0.072386000000	2.117274000000
H	3.987064000000	-0.899908000000	2.693645000000

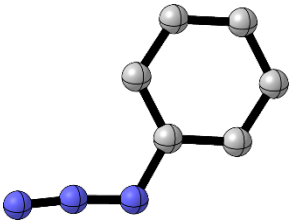
C	1.755257000000	-1.688516000000	0.454585000000
C	1.616382000000	-2.532332000000	-0.669483000000
C	0.880178000000	-3.705693000000	-0.515142000000
H	0.743543000000	-4.367435000000	-1.372396000000
C	0.294611000000	-4.037916000000	0.700024000000
H	-0.289591000000	-4.955157000000	0.793620000000
C	0.430268000000	-3.183900000000	1.782352000000
H	-0.057406000000	-3.433074000000	2.726846000000
C	1.155044000000	-1.991214000000	1.687236000000
C	2.166780000000	-2.194515000000	-2.050310000000
H	2.896980000000	-1.380264000000	-1.941645000000
C	1.054580000000	-1.679002000000	-2.971239000000
H	0.295653000000	-2.457703000000	-3.142145000000
H	1.469183000000	-1.386237000000	-3.948964000000
H	0.541823000000	-0.816803000000	-2.529933000000
C	2.901769000000	-3.371621000000	-2.701853000000
H	2.205622000000	-4.174722000000	-2.987212000000
H	3.657859000000	-3.812467000000	-2.034842000000
H	3.405854000000	-3.040297000000	-3.622565000000
C	1.187067000000	-1.073421000000	2.896587000000
H	1.740312000000	-0.165886000000	2.616301000000
C	-0.230930000000	-0.643600000000	3.299481000000
H	-0.819505000000	-0.303309000000	2.434420000000
H	-0.186147000000	0.161622000000	4.048933000000
H	-0.781227000000	-1.483387000000	3.752182000000
C	1.900641000000	-1.726564000000	4.087482000000
H	2.020093000000	-1.004622000000	4.909987000000
H	2.895238000000	-2.116409000000	3.823800000000
H	1.316178000000	-2.575278000000	4.475227000000
N	0.316983000000	2.559088000000	-0.488572000000
C	-0.524088000000	2.945267000000	-1.660806000000
C	-2.027420000000	3.005952000000	-1.300574000000
H	-2.581728000000	3.434494000000	-2.152126000000
H	-2.392036000000	1.974982000000	-1.173712000000
C	-2.325104000000	3.775518000000	-0.021841000000
H	-2.148534000000	4.855653000000	-0.162507000000
H	-3.390634000000	3.669407000000	0.233412000000
C	-1.470669000000	3.231127000000	1.113521000000
H	-1.759784000000	2.183411000000	1.301343000000
H	-1.660696000000	3.789511000000	2.045714000000
C	0.039362000000	3.264957000000	0.798792000000
C	-0.384933000000	1.916203000000	-2.795708000000
H	-0.942861000000	2.277117000000	-3.672293000000
H	-0.808480000000	0.941320000000	-2.523836000000
H	0.660085000000	1.780869000000	-3.106449000000
C	-0.060853000000	4.296833000000	-2.243577000000
H	-0.529206000000	4.465155000000	-3.225347000000
H	1.031471000000	4.302020000000	-2.377588000000
H	-0.323239000000	5.154415000000	-1.614870000000
C	0.536770000000	4.726863000000	0.816902000000
H	-0.111074000000	5.409735000000	0.256741000000
H	1.549547000000	4.817456000000	0.402016000000

H	0.560321000000	5.095612000000	1.853734000000
C	0.745082000000	2.544353000000	1.956922000000
H	0.503689000000	3.050370000000	2.902743000000
H	1.838595000000	2.550681000000	1.851150000000
H	0.400756000000	1.508185000000	2.043317000000
C	-3.451641000000	-0.888608000000	0.055773000000
Cl	-2.392679000000	-2.847662000000	-1.556364000000
C	-3.706438000000	-1.957473000000	-0.829496000000
Cl	-4.362615000000	1.020208000000	1.769000000000
C	-5.001113000000	-2.384644000000	-1.117935000000
H	-5.140089000000	-3.217800000000	-1.807901000000
C	-6.090901000000	-1.759943000000	-0.521438000000
H	-7.104834000000	-2.094574000000	-0.747212000000
C	-5.882501000000	-0.713419000000	0.371896000000
H	-6.718884000000	-0.208164000000	0.855997000000
C	-4.585126000000	-0.297234000000	0.649788000000

Coordinates of computed molecules involved in the formation of 7a from 5

PhN_3 (Coordinates in Å), NEv = 0

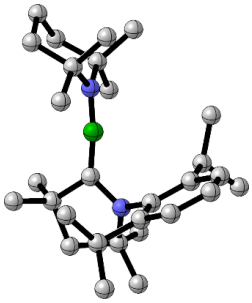
E_{SCF} = –395.407574047, ΔG = –395.334211 Hartree



N	3.230985345253	0.090055550689	-0.181983811536
N	3.703900066300	-0.846150614555	-0.815263823881
N	4.252097643120	-1.659883978157	-1.375925612193
C	1.828214622209	0.170313184910	-0.026097688317
C	1.342078413859	1.258352057427	0.706080277966
H	2.054066935832	1.977669603232	1.113156262414
C	-0.027047125416	1.404107367765	0.901288207905
H	-0.400142707264	2.255760365190	1.473855050746
C	-0.920983439809	0.472045861607	0.371679737620
H	-1.994890518200	0.589824187778	0.527008276656
C	-0.432481534741	-0.610626036308	-0.357237021899
H	-1.122722093626	-1.345860532469	-0.776098320560
C	0.937048343729	-0.767859227105	-0.559829739105
H	1.308865048756	-1.620622790005	-1.133030795814

5 (Coordinates in Å), NEv = 0

E_{SCF} = –1267.73114515, ΔG = –1267.054219 Hartree

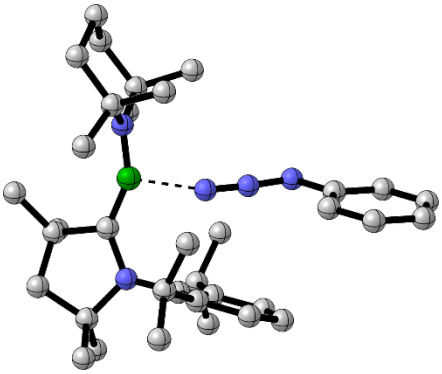


B	1.040299241219	-0.227312958781	-0.969970135066
N	1.168097482341	-1.377925511744	-1.710764944833
C	2.372181085773	-2.261257088837	-1.553374765064
C	1.893014179548	-3.616443258381	-0.999699800605
H	2.755039874036	-4.299190402939	-0.929396108703
H	1.527879404065	-3.453811313703	0.029163099187
C	0.779037682097	-4.240890592683	-1.832034469215
H	0.435257252433	-5.173070357872	-1.357816238608
H	1.158631134184	-4.532021394819	-2.825103824604
C	-0.390216448333	-3.274019645168	-1.972940753322
H	-0.848905533395	-3.124799054415	-0.980139377694
H	-1.171171108399	-3.699889603346	-2.623265717067
C	0.009106189176	-1.888251572894	-2.514190911446
C	3.156206039506	-2.467513814721	-2.863270882274
H	4.146007988898	-2.882551573939	-2.623692732812
H	3.308208776052	-1.516317087896	-3.386902374445
H	2.679611250461	-3.168154915100	-3.556358567606
C	3.342897525224	-1.629728913744	-0.552326810923
H	4.198202495745	-2.306595617838	-0.408471301142
H	2.870166798652	-1.456117960557	0.421307963069
H	3.720504087634	-0.664185421843	-0.919405969230
C	-1.182955468916	-0.944048064840	-2.351357893772
H	-2.042931474445	-1.354782196543	-2.900998539974
H	-0.956999517039	0.054245114425	-2.754658415768
H	-1.467639109297	-0.824299504130	-1.297859107964
C	0.329504293060	-1.934690404589	-4.019111339406
H	-0.606507318797	-2.038755068757	-4.586997273792
H	0.973635383617	-2.771215544830	-4.308849670496
H	0.814933408135	-0.999116220886	-4.333144723561
C	0.762367998025	0.874170572333	-0.132522715664
N	0.927307208984	2.258510009772	-0.397190789674
C	1.356386432702	2.936339296335	0.831521122495
C	0.495286887183	2.188489320465	1.875115525216
H	-0.473749447396	2.703265697872	1.970486619386
H	0.957880887538	2.186438400601	2.874107965341
C	0.278136790600	0.747482822330	1.330166590869

C	2.852619130570	2.709394992426	1.122502749797
H	3.104923057398	3.030107911497	2.145297058080
H	3.482275328202	3.280554333839	0.426560070789
H	3.109827276933	1.644598922562	1.020722208601
C	1.079078886659	4.435167719733	0.799778102632
H	1.409851408641	4.895817027210	1.742479743865
H	0.010224191981	4.650244079287	0.673604976674
H	1.625190063049	4.918674092211	-0.024859297189
C	1.080080592636	-0.281025955704	2.135762966467
H	0.721681552491	-0.328611202212	3.177114702964
H	2.151237138066	-0.034107214474	2.153905571711
H	0.971445326439	-1.288856910904	1.702317475161
C	-1.208079889386	0.364539264015	1.401666447139
H	-1.585417908000	0.422843206655	2.436848466373
H	-1.362977496570	-0.667364545888	1.047032534832
H	-1.819504662753	1.029937364984	0.776516913875
C	0.727489696790	2.843428314780	-1.673130666407
C	1.773220927521	2.879605545076	-2.622486356526
C	1.541319069251	3.441900645191	-3.882253090166
H	2.352573074037	3.476982535400	-4.614165875476
C	0.295391092373	3.952084487252	-4.221022429146
H	0.127479559560	4.384956532069	-5.209915528324
C	-0.737725871044	3.906353052984	-3.292136445804
H	-1.718924639127	4.304570552293	-3.563476919047
C	-0.545561541070	3.363618162968	-2.018986988824
C	3.146377265337	2.312847116530	-2.310605911948
H	3.075850524515	1.828109820885	-1.327640930573
C	3.549811867538	1.237842681981	-3.322416941252
H	4.484500809665	0.742088044804	-3.015259843646
H	3.713730511923	1.658406134719	-4.327284817647
H	2.763719229651	0.473289301957	-3.400719962506
C	4.203687455623	3.418370141689	-2.227707145056
H	5.173289334388	3.010768230140	-1.900507139829
H	3.906563925164	4.205555108023	-1.518790059533
H	4.354432402163	3.898611522542	-3.207994845268
C	-1.716486245738	3.339781144228	-1.050837177126
H	-1.318928884166	2.998476391691	-0.086839194501
C	-2.783657356924	2.331031945827	-1.485367871230
H	-3.607061280983	2.296855240840	-0.754158398983
H	-2.359075228383	1.322410514572	-1.567384070058
H	-3.213858726977	2.599734216554	-2.463780683123
C	-2.333369349289	4.727574336444	-0.846238341365
H	-3.084628229026	4.699156030989	-0.041536214115
H	-2.841579471074	5.084738034389	-1.755977695208
H	-1.572824268926	5.475979959612	-0.578362879919

TS1 (Coordinates in Å), NEv = 1

E_{SCF} = –1663.13861183, ΔG = –1662.365764 Hartree



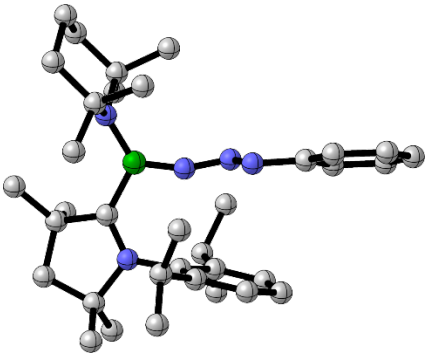
B	-1.564066787870	0.461575306219	-0.052701644866
N	-2.127174151398	1.755599055630	0.003694683381
C	-2.304803863476	2.568364023690	-1.239559654944
C	-3.553507189071	3.463318165660	-1.111464955602
H	-3.613055584663	4.110198781616	-2.001104548930
H	-4.443684997935	2.811245856640	-1.134085896430
C	-3.593754355494	4.283139820627	0.165388961957
H	-4.521950677244	4.873926307999	0.209272498502
H	-2.766287882299	5.011329641410	0.188791624874
C	-3.516878742692	3.336395083120	1.350694204206
H	-4.411267093858	2.689841064380	1.344781154126
H	-3.532179444794	3.891749810682	2.302199751502
C	-2.271027438927	2.431634677411	1.333641445608
C	-1.073139207275	3.428556463594	-1.586501450705
H	-1.259973705528	3.983183525171	-2.518632607358
H	-0.185560062748	2.804543242443	-1.757044095188
H	-0.824602190854	4.164213224346	-0.813560963183
C	-2.557200657147	1.639710552816	-2.429346194637
H	-2.696853803711	2.239084431910	-3.341329376908
H	-3.466644189249	1.046409875374	-2.267983115302
H	-1.724151723969	0.944121026661	-2.594031155971
C	-2.459537728261	1.390244375175	2.441284065314
H	-2.614183629557	1.909609073485	3.398998977004
H	-1.589662250709	0.730581587088	2.539510636739
H	-3.334636108854	0.761538457490	2.243623962020
C	-1.021411245755	3.261540923332	1.698339755976
H	-1.060773565641	3.550752457264	2.759407110394
H	-0.930983247504	4.186090456454	1.115438466234
H	-0.105936251550	2.675310508485	1.542504211809
C	-1.711575902247	-0.968466558162	-0.009396105332
N	-0.807202748272	-2.046240594356	0.167509701846
C	-1.458975100854	-3.358747916130	0.390484930041
C	-2.934509462215	-2.950460204188	0.498174782226

H	-3.181353288415	-2.784371922237	1.558787974359
H	-3.610455853618	-3.733767837632	0.121912760361
C	-3.089186859866	-1.619255417862	-0.255929124295
C	-1.201095566431	-4.362604351094	-0.746713355325
H	-1.682628528361	-5.323898848338	-0.512307531559
H	-0.122060371305	-4.548164134349	-0.852751469123
H	-1.589803491163	-4.023367948380	-1.713699243845
C	-1.002759520284	-4.040277493071	1.685395965841
H	-1.545368451102	-4.989094831753	1.813975004902
H	-1.207214455933	-3.416162163898	2.564431835299
H	0.072792747715	-4.270701603522	1.655613396050
C	-3.317646084740	-1.866631099517	-1.761388863385
H	-4.139863742538	-2.584603508449	-1.916624560665
H	-2.424224308670	-2.258287600438	-2.262335393637
H	-3.585688992787	-0.933098432942	-2.270906282801
C	-4.294067535359	-0.841567058286	0.275879136535
H	-5.227011308869	-1.358726827622	0.000177799403
H	-4.330476471905	0.177101713428	-0.137148288068
H	-4.267422496023	-0.762739391617	1.371408299805
C	0.609093733626	-1.922995810927	0.149165690863
C	1.305583008146	-2.001529424093	-1.083356155590
C	2.699587324438	-1.898978953194	-1.090308793841
H	3.236056149111	-1.945813532710	-2.041071698762
C	3.415761023773	-1.726065536952	0.086915693326
H	4.504689941035	-1.646513829878	0.064754705755
C	2.729861895520	-1.618219593401	1.289460663918
H	3.294844130447	-1.442477863596	2.208536346877
C	1.334594213980	-1.686000527963	1.344267967960
C	0.583219839808	-2.119322186364	-2.416069319953
H	-0.473033791863	-2.289262703113	-2.187774159309
C	0.661605477443	-0.813000733252	-3.214205362664
H	0.128201927612	-0.915691578791	-4.172275957705
H	1.703208147920	-0.529257556640	-3.432917872619
H	0.192505291311	0.011937282172	-2.662294151131
C	1.086289548588	-3.294918152120	-3.259470541654
H	0.452169836857	-3.425000403063	-4.150293634704
H	1.075051433844	-4.237840646316	-2.694460730561
H	2.116237647905	-3.129876127580	-3.613623418507
C	0.661866964223	-1.390172587174	2.677860513920
H	-0.422598707011	-1.472177009210	2.519707777733
C	0.949065384961	0.049485790209	3.125442933715
H	0.386953523552	0.291144098232	4.040775922616
H	0.658686730137	0.773862502365	2.353725629017
H	2.019090525814	0.193159611477	3.348440122381
C	1.083972287816	-2.358336714476	3.789559696704
H	0.496939070071	-2.174028955944	4.702886159324

H	2.145689984592	-2.222695060075	4.050357396809
H	0.946186169513	-3.408627438018	3.502800921309
N	2.353138224542	1.612027140213	-1.268399961722
N	1.406973462126	1.195061210589	-0.611503772670
N	0.436664805028	0.813529895095	-0.165358633171
C	3.601002472321	1.777665847008	-0.627921940605
C	4.686868100434	2.111264858704	-1.441907738244
H	4.523516831217	2.229271084100	-2.514189890206
C	5.947284651138	2.279784651438	-0.877344954802
H	6.793299429487	2.537446697918	-1.518037785832
C	6.133723397698	2.120818158425	0.496664316215
H	7.124222070664	2.253377872111	0.936027417239
C	5.045753606418	1.793155932265	1.304911091494
H	5.180116300492	1.667300105888	2.381517396977
C	3.780147415889	1.620847540582	0.751045313683
H	2.934407090657	1.351377900297	1.386700578161

6a (Coordinates in Å), NEv = 0

E_{SCF} = –1663.20121945, ΔG = –1662.423890 Hartree



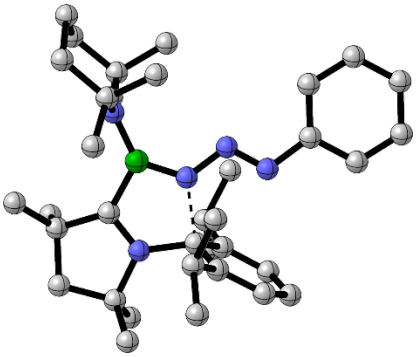
B	0.274458707657	-1.219959450969	0.416810236125
N	0.600684509284	-2.615263669009	0.004155526189
C	2.035926684277	-2.975577646130	-0.094981567102
C	2.170247155274	-4.508705446877	-0.179716872920
H	3.231647540328	-4.768457153640	-0.324406908244
H	1.867136729295	-4.933754845820	0.793429540822
C	1.306619393532	-5.131354254982	-1.265562367833
H	1.398431840828	-6.228785857842	-1.241150083284
H	1.656411643804	-4.818566523618	-2.262803670012
C	-0.142922542627	-4.720045165384	-1.054847671334
H	-0.496888341105	-5.147712724907	-0.100316580541
H	-0.786668168411	-5.132122316660	-1.849112935427
C	-0.333970877104	-3.193152022504	-0.998837030729
C	2.794671949837	-2.312535097012	-1.267540971819
H	3.868775458864	-2.544849775345	-1.195556112442
H	2.682318939082	-1.220559976726	-1.245191568125
H	2.453213515040	-2.659844203957	-2.248636180701
C	2.742105050090	-2.537205368795	1.192648647677
H	3.811986518967	-2.787957850484	1.144794324863
H	2.315787006963	-3.058215266216	2.061052677606
H	2.662966277723	-1.449694833227	1.348149252562
C	-1.776760911707	-2.928706786018	-0.547557664646
H	-2.481274535907	-3.398737248760	-1.249339191528
H	-2.000675507672	-1.854551360467	-0.534467400436
H	-1.965533331244	-3.344638791513	0.448524707703
C	-0.198216335358	-2.595378317957	-2.419787448816
H	-1.082389505818	-2.857462628741	-3.021613150214
H	0.676759964655	-2.976761020745	-2.959858779611
H	-0.121233058517	-1.498761330128	-2.393449273222
C	-0.552501244493	-0.880818906430	1.781375463640
N	-1.184200853565	0.256348825583	1.986355510771
C	-2.008082282999	0.311845322125	3.257856751978

C	-1.909005268599	-1.140458439993	3.736770560159
H	-2.812469743631	-1.689443853087	3.431163590919
H	-1.838827283021	-1.207796783601	4.831641744701
C	-0.686361411069	-1.748394796297	3.033410465176
C	-1.452788523276	1.326142155802	4.259373984029
H	-2.105632299132	1.333153476041	5.143527587099
H	-1.456488885938	2.336606833684	3.829343617744
H	-0.437428942960	1.091702362445	4.597197776947
C	-3.453375284433	0.697287550711	2.960199333451
H	-4.023289425937	0.654652987917	3.899696034588
H	-3.922966305184	0.006241467185	2.249440293190
H	-3.522725850743	1.720386714433	2.566648382172
C	0.593490507942	-1.519360260953	3.870814483786
H	0.498901126804	-2.072672144041	4.816962706671
H	0.759577235400	-0.463172958828	4.114687837717
H	1.483103670426	-1.883980136294	3.348382784939
C	-0.846418492719	-3.253075958022	2.809592679106
H	-0.777381903297	-3.771216020529	3.778214795323
H	-0.075111103045	-3.632046323532	2.127000626530
H	-1.827589508953	-3.492344983736	2.378389723845
C	-1.068988331525	1.455720327868	1.167793567807
C	0.000506199141	2.344593970383	1.429348355355
C	0.064491071569	3.525685926175	0.690703490544
H	0.892650456197	4.216008885799	0.863659922365
C	-0.878294842740	3.828913440218	-0.283018506597
H	-0.795022353750	4.750723362679	-0.861047556433
C	-1.893175412443	2.925626603515	-0.549942848504
H	-2.601087750330	3.140522226235	-1.352468928419
C	-2.010664625940	1.720860035465	0.151928156028
C	1.141731317946	2.052825446088	2.397332145625
H	0.902703559948	1.130831255212	2.938001134350
C	2.462894290832	1.796764659588	1.659032711945
H	3.248461866758	1.519942993341	2.379645089584
H	2.799763113813	2.702966511229	1.131240395188
H	2.365160661113	0.998340031678	0.914185013076
C	1.337198444290	3.166958274469	3.433565947655
H	2.081944983900	2.861280401456	4.184739962281
H	0.407436871214	3.423068460325	3.959691444978
H	1.713170960641	4.087270566244	2.960967786477
C	-3.092778439520	0.747090699974	-0.297480976900
H	-3.037570890516	-0.142448287143	0.347517590320
C	-2.846884614200	0.280414706938	-1.739088943320
H	-3.538256139141	-0.537284724114	-1.995376420329
H	-1.810885046459	-0.045629683438	-1.888593778971

H	-3.020843036014	1.103333848058	-2.449711715587
C	-4.505601703213	1.337164042569	-0.191309525080
H	-5.255088009383	0.570626873920	-0.441846805058
H	-4.636773625032	2.164841636233	-0.905044670237
H	-4.737495400086	1.726315084586	0.808623389885
N	0.358289450138	1.022394706675	-2.160636056846
N	1.035799249566	0.673825539430	-1.137686215185
N	0.525273287703	-0.112331332893	-0.313819067190
C	0.940870963026	2.063695218964	-2.894811665090
C	0.401613338796	2.317816564572	-4.164788288470
H	-0.403700744217	1.670674723712	-4.518889464237
C	0.884105380084	3.362764815527	-4.947191916570
H	0.453584436282	3.540848819682	-5.935839851167
C	1.911539445804	4.181269477328	-4.475851676329
H	2.289015307676	5.003266495113	-5.088009107613
C	2.446798807824	3.940298775249	-3.209063860558
H	3.247233980498	4.579259868530	-2.826559427578
C	1.967499757141	2.898909919850	-2.420020628252
H	2.374192064999	2.716657636560	-1.424617421987

TS2 (Coordinates in Å), NEv = 1

E_{SCF} = –1663.16570417, ΔG = –1662.389103 Hartree



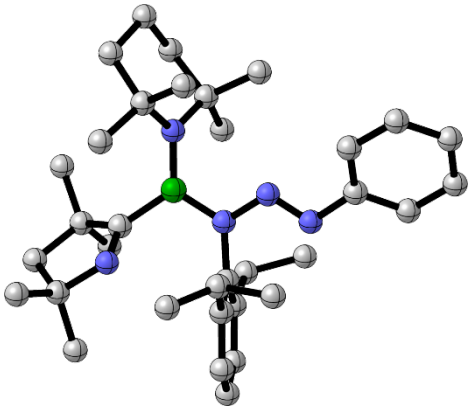
B	1.078421863473	-0.651226844091	-0.038230849305
N	1.555810894304	-2.035695356132	-0.065132189020
C	1.517350173586	-2.779371536534	-1.344752455514
C	2.589931985414	-3.883244985609	-1.306558743611
H	2.514927798544	-4.491210656743	-2.222784310902
H	3.582180580685	-3.399281181024	-1.320776196960
C	2.495592349604	-4.760987451598	-0.065722059892
H	3.314624583741	-5.497141735651	-0.060011609704
H	1.561989813188	-5.346856818104	-0.079816867365
C	2.562861064324	-3.896821190019	1.186514990695
H	3.557774642849	-3.420929845809	1.234431350507
H	2.458757566172	-4.514252305831	2.093650859313
C	1.499088398400	-2.783857285238	1.212896222263
C	0.140691381290	-3.384641950676	-1.694815346785
H	0.153505934208	-3.773617303555	-2.724724072459
H	-0.642491346518	-2.619623028028	-1.612993067380
H	-0.136564493942	-4.218136206737	-1.038439360318
C	1.878700861424	-1.808490088596	-2.472551234286
H	1.854267143057	-2.322128923454	-3.444282911577
H	2.890235563603	-1.411403014874	-2.326516592060
H	1.169068618125	-0.967496137383	-2.530026358352
C	1.851197405332	-1.825938301395	2.359206143109
H	1.880038899578	-2.373840558223	3.312152885666
H	1.102025366603	-1.028472572678	2.467873094261
H	2.836123017400	-1.369904760312	2.201887432421
C	0.110305377071	-3.381233778667	1.530908505735
H	0.065605684112	-3.696811221254	2.584563910881
H	-0.123460915176	-4.260985383511	0.919419534736
H	-0.681706015443	-2.639691647427	1.359148629656
C	1.973383263661	0.691935214889	0.030761552892
N	1.251707598916	1.740394719210	0.263882731043
C	2.029829586427	3.015811102341	0.425343336694

C	3.459956692866	2.451055548261	0.540250271417
H	3.722900585635	2.352512057669	1.604750124439
H	4.200128016933	3.120284397391	0.079743765030
C	3.437643948726	1.050509205373	-0.106775755645
C	1.849126200156	3.937439314482	-0.781160222358
H	2.505252186282	4.811313338974	-0.656818740796
H	0.809110473755	4.281046419558	-0.845692876962
H	2.111537711331	3.445145067040	-1.725174642928
C	1.643478720716	3.777294714839	1.688513738748
H	2.328212256348	4.632615161918	1.791662277325
H	1.748607174125	3.149615298827	2.582317036535
H	0.613247731949	4.150689802554	1.636157358488
C	3.811072419126	1.122066621753	-1.602695859475
H	4.777677301981	1.637563872444	-1.704596424062
H	3.068164002238	1.665917470003	-2.201615953546
H	3.921113273481	0.120420316662	-2.033081438755
C	4.374069820682	0.058744853071	0.585504915501
H	5.421064947007	0.328579359348	0.379313063058
H	4.190978811525	-0.963057837536	0.221790929675
H	4.235457615671	0.067267108303	1.675997931932
C	-0.277082219699	1.665895595396	0.210678597755
C	-0.841280892438	2.210702431470	-1.015439834786
C	-2.005222449817	2.972285856885	-0.951067969239
H	-2.432585500857	3.332975256827	-1.891122049171
C	-2.643906081767	3.293027889802	0.240499237188
H	-3.543890263710	3.909173513149	0.252203461931
C	-2.080034834324	2.810843362248	1.425086988554
H	-2.573546873061	3.041253435638	2.373124504259
C	-0.926745635448	2.051179819893	1.458682193649
C	-0.276572241460	1.827644472605	-2.382733117251
H	0.760653191807	1.475884858141	-2.240788995109
C	-1.052604593083	0.672238178823	-3.037949525133
H	-0.615717168922	0.415745784394	-4.016895199036
H	-2.101381989414	0.966059010970	-3.201315134527
H	-1.060435285515	-0.235676976836	-2.423773666469
C	-0.227475764052	2.993594535133	-3.380938534329
H	0.337993950893	2.705364899600	-4.281316787366
H	0.233905952594	3.896177327654	-2.959582827907
H	-1.239285038198	3.269135711857	-3.716144941505
C	-0.449705976425	1.454639836722	2.777992118776
H	0.618088161214	1.192234614298	2.665845301705
C	-1.199254041958	0.160169388227	3.132595778532
H	-0.831123710585	-0.255472305248	4.084906940358
H	-1.087321723205	-0.608770107934	2.361196920308

H	-2.276156002420	0.362380794072	3.237062574350
C	-0.560800101800	2.416760659812	3.968441599331
H	-0.039437040403	2.003751088551	4.846229569970
H	-1.611746680407	2.562453643002	4.262106867250
H	-0.140867396141	3.408583923248	3.752662071569
N	-2.378007967887	-0.209860742127	0.124887658811
N	-1.332436480315	-0.800093741032	-0.205943423880
N	-0.208286152291	-0.119186283019	0.031077357033
C	-3.567570734985	-0.897270415805	-0.191842092514
C	-4.727540416459	-0.116111630635	-0.209293644240
H	-4.626821752670	0.949044843506	0.011875864518
C	-5.954523078347	-0.699120859648	-0.514849434792
H	-6.857509010785	-0.085023833018	-0.538063107278
C	-6.031491844633	-2.066179867387	-0.782132839033
H	-6.995227744082	-2.526361349464	-1.011353587243
C	-4.874799310438	-2.848755808678	-0.746278156020
H	-4.936312060654	-3.921251794832	-0.945064118656
C	-3.642606464444	-2.272495173045	-0.454981000188
H	-2.733854267952	-2.874804901434	-0.419589072174

Min2 (Coordinates in Å), NEv = 0

E_{SCF} = –1663.24475790, ΔG = –1662.467975 Hartree



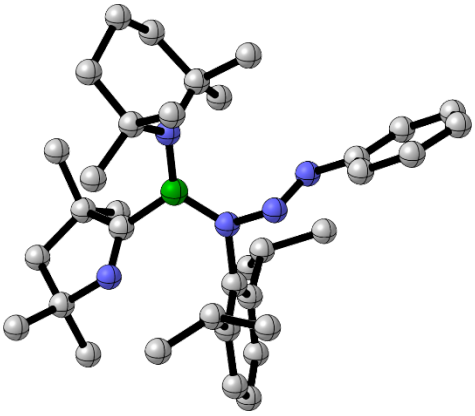
B	0.590929612815	-0.776175010556	-0.058715448777
N	0.128485753003	-2.153221761179	-0.046963721507
C	-0.647775436514	-2.751673862566	-1.175149206439
C	-0.076073085018	-4.156791777979	-1.466618509391
H	-0.677086699511	-4.615158572764	-2.268405977066
H	0.948495529656	-4.048432376826	-1.860272089752
C	-0.042908013893	-5.058341541990	-0.242857883448
H	0.403573617676	-6.031441630141	-0.500476369417
H	-1.066345162764	-5.276401009709	0.103271163337
C	0.762481073671	-4.391208869467	0.859565812467
H	1.816155490511	-4.336661089134	0.539815066781
H	0.741196133870	-4.995784077460	1.780629908379
C	0.295727156775	-2.961707631703	1.192726407823
C	-2.174566719129	-2.877320709755	-0.978102076775
H	-2.645219624380	-3.087289166754	-1.950790055092
H	-2.591906124176	-1.946163120312	-0.585396423267
H	-2.459172106216	-3.698213146546	-0.309370042404
C	-0.435611685298	-1.912420451679	-2.441412785067
H	-0.794175409821	-2.472323423141	-3.316989077313
H	0.631125302852	-1.693729288967	-2.602737835292
H	-0.992784185023	-0.968166997357	-2.407947732894
C	1.340782966498	-2.363048601623	2.143786061707
H	1.390044013008	-2.995988098273	3.041606029881
H	1.087515924872	-1.342672544585	2.466193072384
H	2.343975657674	-2.337354133216	1.701945033981
C	-1.024594428352	-2.982247732631	1.994683799139
H	-0.867195732039	-3.452325544612	2.977480719065
H	-1.828161432910	-3.530781046113	1.493031477001
H	-1.371577697394	-1.950418281339	2.155553963740
C	2.132981986695	-0.357656609310	0.125812427349
N	2.452941902755	0.420429066813	1.083213511166

C	3.886381639433	0.724445518120	1.093134849865
C	4.503931472051	-0.244275887353	0.057228383566
H	4.993618347401	-1.082645291466	0.577303240212
H	5.269932277021	0.239008063803	-0.567415621515
C	3.313726322928	-0.770473809930	-0.775748243692
C	4.037637732790	2.200786947885	0.706518200729
H	5.097846595584	2.497731880797	0.709839254811
H	3.488862690330	2.836558409140	1.416644802179
H	3.619864604938	2.394823626279	-0.292502152590
C	4.437071504617	0.490024754029	2.500042880895
H	5.524686377126	0.660927907351	2.522950076728
H	4.243397573340	-0.543896175057	2.825018033378
H	3.965012556262	1.170137266467	3.224437831527
C	3.211564966835	-0.041367293326	-2.122084609535
H	4.112495651430	-0.227692629763	-2.727317859504
H	3.109590011261	1.043432807829	-1.979687881035
H	2.344941448877	-0.386096768819	-2.705048889356
C	3.406068564122	-2.276939304968	-1.024926943329
H	4.299254688405	-2.505816129671	-1.627814946112
H	2.524507119971	-2.650231053286	-1.563371874739
H	3.483916066673	-2.839920824622	-0.083342343923
C	0.081847753977	1.748348796587	-0.237802930905
C	0.425350977695	2.368038098017	-1.453759199004
C	0.883165448571	3.689279970630	-1.412989380598
H	1.169910191098	4.190257916587	-2.338513344111
C	0.965441450902	4.383531450416	-0.212429460806
H	1.325662329084	5.414638613071	-0.200923345123
C	0.572493208572	3.769151644272	0.969764730558
H	0.618702452054	4.328806337382	1.906697269582
C	0.123065552082	2.447601147330	0.984798274921
C	0.234347919202	1.665286051340	-2.789810057726
H	0.468316006589	0.605417110750	-2.632354143266
C	-1.231271015697	1.747889787645	-3.239159296207
H	-1.385962287516	1.171067734133	-4.164616800390
H	-1.510844618272	2.795070506025	-3.437387201924
H	-1.914462615011	1.367802182747	-2.469397160518
C	1.146667493534	2.173929125604	-3.907357157596
H	1.077316553076	1.504938927625	-4.778512179075
H	2.200863454126	2.219781906598	-3.599817718727
H	0.850345836133	3.177961900954	-4.249488647908
C	-0.352344064402	1.846309883422	2.299848434800
H	-0.532087849815	0.773680702662	2.136199488002
C	-1.680897784847	2.486333133616	2.727178249238
H	-2.090861668991	1.973304238605	3.611218996019

H	-2.426846271962	2.442442609207	1.922456948612
H	-1.535080043750	3.545818800232	2.992832869483
C	0.688191351361	1.955361596264	3.417290753196
H	0.323761215686	1.446232348171	4.323390892695
H	0.884955936212	3.004337714221	3.690874569454
H	1.626494652178	1.485651193277	3.098062288785
N	-2.414079431106	1.034938729975	-0.149577700932
N	-1.638810625267	0.072295943145	-0.055224082751
N	-0.322978140962	0.356504016108	-0.215893800323
C	-3.767412521581	0.713569378822	0.108692865701
C	-4.730889447578	1.528599413472	-0.492691180229
H	-4.396721720716	2.349827441971	-1.129591691507
C	-6.083948196735	1.280630885900	-0.278305352650
H	-6.833948550035	1.912735351544	-0.758540437333
C	-6.480602683832	0.234214353689	0.554691456205
H	-7.541844535167	0.045873220560	0.730215273463
C	-5.517096876290	-0.561494130484	1.176527518357
H	-5.824096472290	-1.370174412914	1.843441566152
C	-4.162683911221	-0.325514408061	0.960848474909
H	-3.401177240378	-0.930597183685	1.454557940614

TS3 (Coordinates in Å), NEv = 1

E_{SCF} = –1663.22165853, ΔG = –1662.447590 Hartree



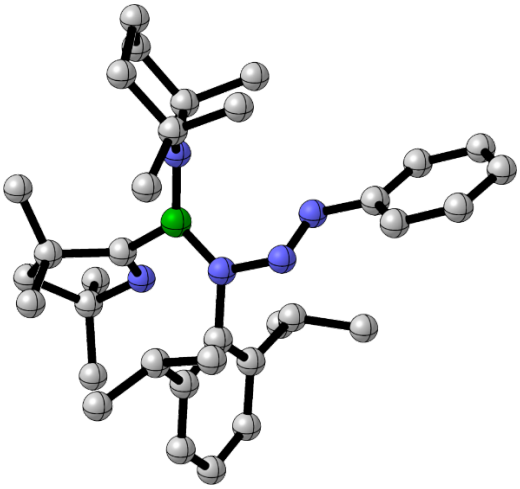
B	0.396145337798	0.761568673913	0.077938160801
N	-0.375705050474	2.006014342434	-0.051958201202
C	-1.272289821773	2.521871699287	1.016341795033
C	-0.965656247616	4.016638344154	1.264448986524
H	-1.684489932332	4.399167814771	2.007689538903
H	0.033912030824	4.108235347917	1.717575162752
C	-1.013214887973	4.855742725067	-0.004305935124
H	-0.728141834643	5.895808996625	0.219154615802
H	-2.041446647198	4.904184027843	-0.398633367441
C	-0.073846101291	4.271726923635	-1.047385103933
H	0.962323673027	4.398090035078	-0.694323703979
H	-0.154153589566	4.825257715396	-1.997164610615
C	-0.297710261988	2.770953819789	-1.322999655219
C	-2.793110635312	2.408481596751	0.723536547106
H	-3.351946204393	2.281766197958	1.662938312362
H	-3.029329499064	1.560821814046	0.078732266394
H	-3.193885910857	3.306889233770	0.235084103773
C	-0.980324966719	1.770778860376	2.322355695082
H	-1.515041664188	2.254080462400	3.153221517012
H	0.093419988372	1.798556451170	2.560810794844
H	-1.309476811649	0.725495002543	2.267673712061
C	0.873204532911	2.305427068789	-2.198901320320
H	0.839632961157	2.855921790854	-3.150225155292
H	0.830257439235	1.231624517196	-2.432014168995
H	1.845508700185	2.506468758786	-1.732972728430
C	-1.575065080988	2.553393015058	-2.164596801730
H	-1.457713305813	2.998978358951	-3.164549278685
H	-2.468584454566	2.997204795737	-1.711727712670
H	-1.758351481844	1.474303572015	-2.286115991821
C	2.013284651197	0.717280060113	0.105626299532

N	2.602976938815	0.020924884215	-0.786592840519
C	4.059355154858	0.037163381291	-0.633235864903
C	4.334171353793	1.144242585090	0.409501622020
H	4.684722382108	2.055807176780	-0.099667724663
H	5.113396279594	0.859794059929	1.132533344544
C	2.973013345431	1.415897364399	1.090007309961
C	4.474633075571	-1.359715680219	-0.154835480533
H	5.569079925636	-1.429997112080	-0.056376828638
H	4.130744470967	-2.121985356429	-0.869570482567
H	4.018220206136	-1.597582548812	0.817410899665
C	4.706690744696	0.343029323350	-1.983874008765
H	5.799986844071	0.423925878053	-1.879313306539
H	4.327425484850	1.293856565219	-2.389139255054
H	4.488094473756	-0.451022426859	-2.713128100694
C	2.899875786808	0.748049824276	2.468814655178
H	3.633072279170	1.202973239858	3.153293943902
H	3.119413493880	-0.325180905390	2.399004789956
H	1.905274563748	0.856998363496	2.925616561172
C	2.708149265518	2.914636439238	1.233976152525
H	3.489523602572	3.378409543116	1.857166342967
H	1.737146351911	3.108422045641	1.706198716158
H	2.711742914691	3.418986247728	0.256413066768
C	0.502332984092	-1.806019509801	0.045244058754
C	0.868397089158	-2.444341646685	1.246851921036
C	1.550475058461	-3.663245553860	1.161840864063
H	1.859417270220	-4.172072129951	2.076219283376
C	1.829148759642	-4.248793882329	-0.066527339773
H	2.357895386129	-5.203636783796	-0.109596519429
C	1.424261704286	-3.621668707679	-1.238623517282
H	1.636547324630	-4.092435149045	-2.201325720217
C	0.761166711023	-2.393924953241	-1.209414485435
C	0.492777043879	-1.881833081167	2.610989473525
H	0.467509928768	-0.788028104664	2.518984478818
C	-0.915222443930	-2.341072628085	3.013584536433
H	-1.188609518415	-1.927773092352	3.997618535320
H	-0.957579833646	-3.440023675753	3.080041339951
H	-1.667699721592	-2.009261070618	2.287645278742
C	1.486060866031	-2.236956001235	3.720648195495
H	1.283089787253	-1.628686651343	4.615138436160
H	2.529171954970	-2.061805525028	3.421565118306
H	1.397909395058	-3.292527302252	4.022544566723
C	0.318178358500	-1.757066275651	-2.516347102223
H	-0.037016138248	-0.744462636652	-2.286881253166
C	-0.861264301020	-2.531139884929	-3.116806497446

H	-1.240243291961	-2.022737975197	-4.017881420241
H	-1.683787094343	-2.614747496912	-2.392385399351
H	-0.559750984755	-3.550019932040	-3.409573461813
C	1.465070596598	-1.612931661187	-3.518578214927
H	1.121741021253	-1.067147457586	-4.411618795950
H	1.843560202184	-2.590172115301	-3.858570955520
H	2.288022220833	-1.051788345990	-3.057780834796
N	-2.371730491655	-0.607970912292	0.547834582692
N	-1.529573928508	-0.785833059333	-0.325892034699
N	-0.200572452607	-0.544754402583	0.096623934619
C	-3.711419221742	-0.858805008871	0.140683519446
C	-4.642463000419	-0.991254761460	1.171772141760
H	-4.298372803639	-0.898232546249	2.203552670569
C	-5.979219956847	-1.240477611785	0.869879084871
H	-6.707840653168	-1.352591570816	1.675190593051
C	-6.384335702444	-1.337459922443	-0.460495289723
H	-7.433486965837	-1.524284389246	-0.699275566481
C	-5.452258189098	-1.184942712348	-1.490251140692
H	-5.774515239781	-1.249667985736	-2.531594088190
C	-4.114506759993	-0.944955015256	-1.197249439330
H	-3.375670832361	-0.814816785564	-1.988702821490

Min3 (Coordinates in Å), NEv = 0

E_{SCF} = –1663.23054339, ΔG = –1662.453678 Hartree



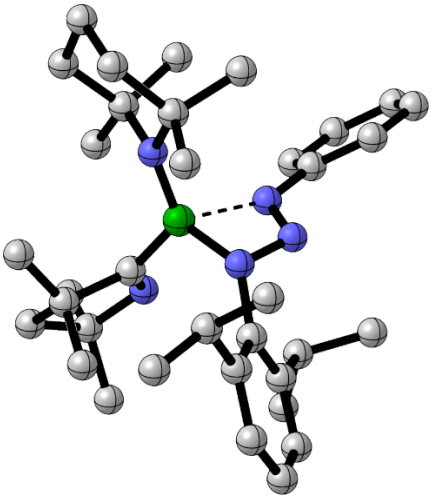
B	0.396145337798	0.761568673913	0.077938160801
N	-0.375705050474	2.006014342434	-0.051958201202
C	-1.272289821773	2.521871699287	1.016341795033
C	-0.965656247616	4.016638344154	1.264448986524
H	-1.684489932332	4.399167814771	2.007689538903
H	0.033912030824	4.108235347917	1.717575162752
C	-1.013214887973	4.855742725067	-0.004305935124
H	-0.728141834643	5.895808996625	0.219154615802
H	-2.041446647198	4.904184027843	-0.398633367441
C	-0.073846101291	4.271726923635	-1.047385103933
H	0.962323673027	4.398090035078	-0.694323703979
H	-0.154153589566	4.825257715396	-1.997164610615
C	-0.297710261988	2.770953819789	-1.322999655219
C	-2.793110635312	2.408481596751	0.723536547106
H	-3.351946204393	2.281766197958	1.662938312362
H	-3.029329499064	1.560821814046	0.078732266394
H	-3.193885910857	3.306889233770	0.235084103773
C	-0.980324966719	1.770778860376	2.322355695082
H	-1.515041664188	2.254080462400	3.153221517012
H	0.093419988372	1.798556451170	2.560810794844
H	-1.309476811649	0.725495002543	2.267673712061
C	0.873204532911	2.305427068789	-2.198901320320
H	0.839632961157	2.855921790854	-3.150225155292
H	0.830257439235	1.231624517196	-2.432014168995
H	1.845508700185	2.506468758786	-1.732972728430
C	-1.575065080988	2.553393015058	-2.164596801730
H	-1.457713305813	2.998978358951	-3.164549278685
H	-2.468584454566	2.997204795737	-1.711727712670
H	-1.758351481844	1.474303572015	-2.286115991821

C	2.013284651197	0.717280060113	0.105626299532
N	2.602976938815	0.020924884215	-0.786592840519
C	4.059355154858	0.037163381291	-0.633235864903
C	4.334171353793	1.144242585090	0.409501622020
H	4.684722382108	2.055807176780	-0.099667724663
H	5.113396279594	0.859794059929	1.132533344544
C	2.973013345431	1.415897364399	1.090007309961
C	4.474633075571	-1.359715680219	-0.154835480533
H	5.569079925636	-1.429997112080	-0.056376828638
H	4.130744470967	-2.121985356429	-0.869570482567
H	4.018220206136	-1.597582548812	0.817410899665
C	4.706690744696	0.343029323350	-1.983874008765
H	5.799986844071	0.423925878053	-1.879313306539
H	4.327425484850	1.293856565219	-2.389139255054
H	4.488094473756	-0.451022426859	-2.713128100694
C	2.899875786808	0.748049824276	2.468814655178
H	3.633072279170	1.202973239858	3.153293943902
H	3.119413493880	-0.325180905390	2.399004789956
H	1.905274563748	0.856998363496	2.925616561172
C	2.708149265518	2.914636439238	1.233976152525
H	3.489523602572	3.378409543116	1.857166342967
H	1.737146351911	3.108422045641	1.706198716158
H	2.711742914691	3.418986247728	0.256413066768
C	0.502332984092	-1.806019509801	0.045244058754
C	0.868397089158	-2.444341646685	1.246851921036
C	1.550475058461	-3.663245553860	1.161840864063
H	1.859417270220	-4.172072129951	2.076219283376
C	1.829148759642	-4.248793882329	-0.066527339773
H	2.357895386129	-5.203636783796	-0.109596519429
C	1.424261704286	-3.621668707679	-1.238623517282
H	1.636547324630	-4.092435149045	-2.201325720217
C	0.761166711023	-2.393924953241	-1.209414485435
C	0.492777043879	-1.881833081167	2.610989473525
H	0.467509928768	-0.788028104664	2.518984478818
C	-0.915222443930	-2.341072628085	3.013584536433
H	-1.188609518415	-1.927773092352	3.997618535320
H	-0.957579833646	-3.440023675753	3.080041339951
H	-1.667699721592	-2.009261070618	2.287645278742
C	1.486060866031	-2.236956001235	3.720648195495
H	1.283089787253	-1.628686651343	4.615138436160
H	2.529171954970	-2.061805525028	3.421565118306
H	1.397909395058	-3.292527302252	4.022544566723
C	0.318178358500	-1.757066275651	-2.516347102223
H	-0.037016138248	-0.744462636652	-2.286881253166

C	-0.861264301020	-2.531139884929	-3.116806497446
H	-1.240243291961	-2.022737975197	-4.017881420241
H	-1.683787094343	-2.614747496912	-2.392385399351
H	-0.559750984755	-3.550019932040	-3.409573461813
C	1.465070596598	-1.612931661187	-3.518578214927
H	1.121741021253	-1.067147457586	-4.411618795950
H	1.843560202184	-2.590172115301	-3.858570955520
H	2.288022220833	-1.051788345990	-3.057780834796
N	-2.371730491655	-0.607970912292	0.547834582692
N	-1.529573928508	-0.785833059333	-0.325892034699
N	-0.200572452607	-0.544754402583	0.096623934619
C	-3.711419221742	-0.858805008871	0.140683519446
C	-4.642463000419	-0.991254761460	1.171772141760
H	-4.298372803639	-0.898232546249	2.203552670569
C	-5.979219956847	-1.240477611785	0.869879084871
H	-6.707840653168	-1.352591570816	1.675190593051
C	-6.384335702444	-1.337459922443	-0.460495289723
H	-7.433486965837	-1.524284389246	-0.699275566481
C	-5.452258189098	-1.184942712348	-1.490251140692
H	-5.774515239781	-1.249667985736	-2.531594088190
C	-4.114506759993	-0.944955015256	-1.197249439330
H	-3.375670832361	-0.814816785564	-1.988702821490

TS4 (Coordinates in Å), NEv = 1

E_{SCF} = –1663.19034424, ΔG = –1662.411937 Hartree



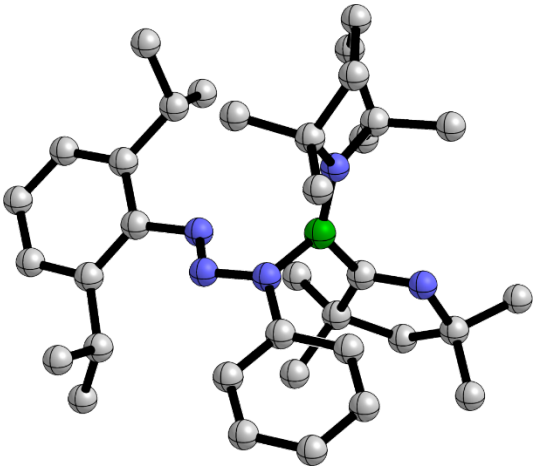
B	0.369713725533	0.553690531231	-0.116196485434
N	1.464320013226	1.536946036237	0.048773727300
C	2.668252784872	1.437097112813	-0.867922803509
C	3.212126023741	2.842654074841	-1.197070538792
H	4.086537381741	2.727541697676	-1.857163474687
H	2.445594820621	3.387192639249	-1.772755141117
C	3.575627654160	3.646546703945	0.034610603240
H	3.880970703416	4.667054095145	-0.244912657427
H	4.440468627199	3.202408017363	0.552883736084
C	2.367010967378	3.694491632512	0.943400027165
H	1.588516225473	4.300034818489	0.448211364249
H	2.608450157876	4.204659113597	1.889692716354
C	1.731125161494	2.327674342642	1.293246535542
C	3.821306516575	0.597185105676	-0.259516727052
H	4.498947252601	0.273427013623	-1.063001288266
H	3.450441283856	-0.301562898298	0.238818223587
H	4.434336232920	1.148831924534	0.459310953071
C	2.382508634197	0.776501171949	-2.221712460591
H	3.300198718148	0.843773687694	-2.823328651219
H	1.593466371710	1.284096020360	-2.785513046704
H	2.116355616145	-0.281480190116	-2.130121919080
C	0.433048444704	2.708990531956	1.987651982138
H	0.644642720538	3.429536652530	2.790693920920
H	-0.056649691330	1.842085708516	2.432193185072
H	-0.244062613162	3.197671715664	1.274867749059
C	2.581355466241	1.587257666711	2.352192839601
H	2.475146123549	2.090787709228	3.324955236158
H	3.650940452523	1.559658638574	2.123111696122

H	2.236943866976	0.551854211143	2.473445896461
C	-0.309787957976	0.343228841756	-1.564909600477
N	-0.265577743922	-0.751583036961	-2.221351284322
C	-0.833197938423	-0.593231158995	-3.574163148415
C	-1.125661643649	0.920225685662	-3.709061848950
H	-2.072012557333	1.124869053922	-4.231798801676
H	-0.325335279301	1.406588411743	-4.289772235541
C	-1.121499777025	1.462290608627	-2.268194670279
C	0.223586039017	-1.062473650727	-4.578388677158
H	-0.139742690018	-0.932768243338	-5.610046891854
H	0.457532021015	-2.126006837694	-4.421500154514
H	1.154910152934	-0.487737403585	-4.468675551456
C	-2.090913821868	-1.447839369772	-3.739432269934
H	-2.499400508888	-1.327623467558	-4.754469019632
H	-2.871755000289	-1.159963318283	-3.020973209441
H	-1.856129565926	-2.510077114595	-3.587131588013
C	-0.547207262126	2.878243370141	-2.173595563702
H	-1.200760550212	3.578585187537	-2.717676071448
H	0.457361112707	2.952307091285	-2.610554789916
H	-0.476762033409	3.216646251728	-1.129956508436
C	-2.541671886151	1.493279588855	-1.676673884082
H	-3.189143801458	2.137786516781	-2.292130827782
H	-2.530239699604	1.908892867711	-0.661541187373
H	-2.996993353609	0.495146369628	-1.616158225859
C	-2.060621250214	-0.320243878103	1.081928095529
C	-2.472068422606	-1.632873524805	0.701822425672
C	-3.823780796653	-1.973371572448	0.843032920676
H	-4.141002894077	-2.981677129616	0.575950339258
C	-4.774064338585	-1.072729075070	1.291321781134
H	-5.821691685449	-1.368516453598	1.378326946606
C	-4.372340741877	0.210774011368	1.623315703646
H	-5.113115081008	0.928831376956	1.977022934069
C	-3.035064886123	0.600140571440	1.539664834309
C	-1.568708310227	-2.744591625653	0.153486608001
H	-0.707569689189	-2.279612861718	-0.336611767812
C	-1.092056761841	-3.692837663641	1.264114965530
H	-0.411604461025	-4.453194209709	0.849190535720
H	-1.952557802182	-4.216732562570	1.712020121296
H	-0.566690616832	-3.159463591316	2.064867776102
C	-2.250010539583	-3.578511813066	-0.940001827593
H	-1.485494346232	-4.138292480156	-1.499934648912
H	-2.800273979914	-2.952246869375	-1.651409551531
H	-2.951760698002	-4.319914583251	-0.526379985282
C	-2.683189989786	1.992362874701	2.016751482624

H	-1.773916870576	2.278834741180	1.489857737501
C	-2.381719363190	1.963524917748	3.520124405619
H	-2.006735033588	2.938605104487	3.868447216655
H	-1.632322369575	1.196675726716	3.764947653869
H	-3.296203100019	1.724370524515	4.086125866453
C	-3.727240329065	3.064770951644	1.695376484029
H	-3.311250557467	4.061100759899	1.910606450949
H	-4.638612829160	2.961323488269	2.304264849285
H	-4.024198517786	3.042589892980	0.636164779914
N	1.068366196542	-1.079730485886	0.718317284121
N	0.094492582034	-0.970677771106	1.505596874339
N	-0.643798203863	0.036437584446	1.038832508875
C	2.023207217219	-2.075256575211	0.990960544630
C	2.547440559470	-2.760807664934	-0.109675306366
H	2.195230263305	-2.490351535236	-1.107669114834
C	3.475304289603	-3.776464835263	0.094081279414
H	3.881349936317	-4.318726616381	-0.762343234646
C	3.883829699777	-4.104947648023	1.388385054575
H	4.616839953217	-4.898918432109	1.545169812773
C	3.356673720456	-3.417009435185	2.481262869456
H	3.676440708571	-3.672027064864	3.493834768396
C	2.426108295999	-2.398467137241	2.289069511384
H	2.007407145783	-1.848803160170	3.133798826581

7a (Coordinates in Å), NEv = 0

E_{SCF} = –1663.24706802, ΔG = –1662.470318 Hartree



B	0.561577521251	-0.184082838164	0.862287799130
N	0.321146657431	-1.448740964327	1.429301320190
C	1.179433427657	-2.629551525059	1.044512901629
C	0.313865512480	-3.903545580909	1.036628271393
H	0.945466693423	-4.736247428504	0.693880033159
H	-0.459430866551	-3.773067186207	0.263590882108
C	-0.323771163179	-4.244967903461	2.380217955251
H	0.307618165990	-4.951893867367	2.939671416900
H	-1.280892058358	-4.761836736921	2.211156661558
C	-0.533540731587	-2.988241351707	3.218042835799
H	0.335850924494	-2.804852273155	3.865403259307
H	-1.385176700111	-3.126930442545	3.900012708135
C	-0.805625232298	-1.705931698854	2.407636906919
C	1.708873881223	-2.497458027366	-0.392733098250
H	2.018557837160	-3.488501698274	-0.755088674622
H	0.931730770587	-2.117278384996	-1.067277021482
H	2.585238236596	-1.845736677654	-0.461198205504
C	2.386311434883	-2.782505385991	1.985124965522
H	3.038167089997	-3.591744968286	1.619673081738
H	2.956149388729	-1.843793944365	2.001585384421
H	2.098952087849	-3.027648754181	3.015091113635
C	-0.912765303783	-0.591008084010	3.459622931182
H	-1.532377441609	-0.946230973848	4.295970136998
H	0.077722509784	-0.333918275897	3.860680895352
H	-1.383425482597	0.319249451742	3.077848969020
C	-2.155385342107	-1.851130665428	1.691500362089
H	-2.951717095704	-2.004783106513	2.435769529545
H	-2.405978379438	-0.956240358275	1.110989357974
H	-2.167234822451	-2.708684057375	1.007938686616

C	1.952184497102	0.315493301998	0.241375453745
N	2.937723093479	0.310234974396	1.056754806119
C	4.127047279714	0.953457259602	0.483364756903
C	3.771878658303	1.173174928927	-1.005027692679
H	4.239867837834	0.386297224962	-1.617482150154
H	4.133945325283	2.138718056817	-1.388108819407
C	2.233668129855	1.046852363100	-1.087193678572
C	4.374595831884	2.262340609077	1.241649285106
H	5.282789647260	2.759925274368	0.868311155970
H	3.528683312686	2.955785134203	1.130549820515
H	4.504758274440	2.059834210485	2.315332316636
C	5.319219639794	0.013027235738	0.664471618816
H	6.224799913391	0.441660875534	0.207490124942
H	5.516505937454	-0.162503621562	1.732492258425
H	5.121728419603	-0.960512064220	0.189742975769
C	1.558549482118	2.431328141247	-1.072282775826
H	1.927930053345	3.031673573977	-1.918144564187
H	0.470463843265	2.346295552126	-1.181742308494
H	1.759579258086	2.984231299705	-0.143587444826
C	1.780650002223	0.293430467406	-2.342041369327
H	1.990020924363	0.899743642713	-3.237459033409
H	2.308709117755	-0.663784941109	-2.458220516084
H	0.700576700369	0.090295937928	-2.311287510677
C	-2.173672854778	0.199612264182	-1.938272972790
C	-2.691940110850	1.385454100220	-2.519798434302
C	-3.548218066588	1.252689573537	-3.618211337168
H	-3.967363950588	2.152385852136	-4.073470967347
C	-3.880511844650	0.013246934106	-4.149387913562
H	-4.557001769595	-0.053905645585	-5.004089275313
C	-3.334180649985	-1.136889388220	-3.593716940240
H	-3.578304868527	-2.111881587756	-4.022361546382
C	-2.474369776067	-1.065683812518	-2.498086790753
C	-2.379947161843	2.793354356121	-2.028477073428
H	-1.514821238925	2.739414283449	-1.359205908875
C	-1.999039023368	3.750805815998	-3.161657757292
H	-1.655663300022	4.708780553296	-2.741586713502
H	-1.183996136821	3.336729770654	-3.774160739002
H	-2.844913196730	3.974971662046	-3.829866557164
C	-3.545659269529	3.337887890991	-1.196528008692
H	-3.305428966349	4.332034368028	-0.787074539967
H	-4.456532455299	3.434666781311	-1.808940193611
H	-3.774523593156	2.661295707447	-0.359890818594
C	-1.867501602042	-2.345685572410	-1.944924597677
H	-1.309654461107	-2.071220035310	-1.040437002027

C	-0.869813523335	-2.948156530313	-2.939749106329
H	-0.375664452240	-3.832754650483	-2.507714098441
H	-1.370036521432	-3.261647756600	-3.870119663061
H	-0.089787980226	-2.220045643685	-3.208480473433
C	-2.936391204322	-3.365491195636	-1.541900919690
H	-2.472941784474	-4.231517761795	-1.041946261533
H	-3.669375111768	-2.923838785276	-0.850743060497
H	-3.487579275937	-3.749620392256	-2.414850460066
N	-1.259120989178	0.166735086869	-0.859080786493
N	-1.371519651883	1.050082442848	0.018962735803
N	-0.450595017394	0.959512726490	0.974915383921
C	-0.291363957675	2.098346281586	1.793162878036
C	-1.188487451472	3.174066437078	1.731969475859
H	-2.030381233271	3.134158009202	1.044827656637
C	-0.999356751154	4.286026653060	2.547468629798
H	-1.709779608855	5.113712312065	2.486422487999
C	0.077429771525	4.353520290901	3.430304261830
H	0.221217793513	5.230559837205	4.064114716532
C	0.966479867998	3.282320829747	3.490475664291
H	1.818746221553	3.313020136661	4.173033885485
C	0.788301893066	2.160879582897	2.685276891339
H	1.508046564412	1.342373488190	2.736996174685

References

1. M. Rang, F. Fantuzzi, M. Arrowsmith, I. Krummenacher, E. Beck, R. Witte, A. Matler, A. Rempel, T. Bischof, K. Radacki, B. Engels and H. Braunschweig, *Angew. Chem. Int. Ed.*, 2021, **60**, 2963-2968.
2. M.-A. Légaré, M. Rang, G. Bélanger-Chabot, J. I. Schweizer, I. Krummenacher, R. Bertermann, M. Arrowsmith, M. C. Holthausen and H. Braunschweig, *Science*, 2019, **363**, 1329-1332.
3. R. Witte, M. Arrowsmith, A. Lamprecht, F. Schorr, I. Krummenacher and H. Braunschweig, *Chem. Eur. J.*, 2023, **29**, e202203663.
4. L.-M. Jin, H. Lu, Y. Cui, C. L. Lizardi, T. N. Arzua, L. Wojtas, X. Cui and X. P. Zhang, *Chem. Sci.*, 2014, **5**, 2422-2427.
5. P. Awolade, N. Cele, N. Kerru and P. Singh, *Mol. Diversity*, 2021, **25**, 2201-2218.
6. F. Kloss, U. Köhn, B. O. Jahn, M. D. Hager, H. Görls and U. S. Schubert, *Chem. Asian J.*, 2011, **6**, 2816-2824.
7. G. M. Sheldrick, *Acta Crystallogr. A* 2015, **71**, 3-8.
8. G. M. Sheldrick, *Acta Crystallogr. A*, 2008, **64**, 112-122.
9. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, Williams, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Journal*, 2016.
10. J.-D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, 2008, **10**, 6615-6620.
11. A. E. Reed, L. A. Curtiss and F. Weinhold, *Chem. Rev.*, 1988, **88**, 899-926.
12. F. Weinhold and C. R. Landis, *Valency and Bonding: A Natural Bond Orbital Donor-Acceptor Perspective*, Cambridge University Press, Cambridge, 2005.
13. E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales, C. R. Landis and F. Weinhold, *NBO 6.0*, Theoretical Chemistry Institute, University of Wisconsin, Madison, WI, USA, 2013.
14. K. B. Wiberg, *Tetrahedron*, 1968, **24**, 1083-1096.
15. R. F. W. Bader, *Atoms in Molecules: A Quantum Theory*, Oxford University Press, Oxford, U. K., 1990.
16. R. F. W. Bader, *J. Phys. Chem. A.*, 1998, **102**, 7314-7323.
17. T. Lu and F. Chen, *J. Comput. Chem*, 2012, **33**, 580-592.
18. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297-3305.