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**Supporting Information for:**

# Reactions of In–Zn Bonds with Organic Azides: Products that Result from Hetero- and Homo-bimetallic Behaviour

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**General Synthetic Procedures**

All manipulations were performed under dry nitrogen using standard Schlenk-line techniques, or in a conventional nitrogen-filled glovebox. Solvents were dried over appropriate drying agents and degassed prior to use. NMR spectra were recorded using a Bruker Avance DPX 300 MHz spectrometer at 300.1 ($^{1}$H) and 75.4 ($^{13}$C) MHz, a Varian DirectDrive 600 MHz spectrometer equipped with a triple-resonance HCN cryogenic probe, operating at 600.1 ($^{1}$H) and 150.9 ($^{13}$C) MHz or a Joel JNM-ECZ500S 500MHz spectrometer equipped with a ROYAL digital auto tune probe S, operating at 500 ($^{1}$H), 125.7 ($^{13}$C) MHz. Spectra were recorded at 298 K (unless stated otherwise) and proton and carbon chemical shifts were referenced internally to residual solvent resonances. Coupling constants are quoted in Hz. Elemental analyses were performed by S. Boyer at London Metropolitan University. K[In(NON$^{Dipp}$)],[S1] Zn(BDI$^{Mes}$)Cl,[S2] and Cd(BDI$^{Mes}$)Cl,[S3] were prepared according to a literature procedures. All other chemicals were purchased from Sigma-Aldrich and used without further purification.

**Preparation of (NON$^{Dipp}$)In–Zn(BDI$^{Mes}$) (1)**

The addition of solid 'BDI$^{Mes}$ZnCl' (20 mg, 0.032 mmol) to a bright yellow $C_6D_6$ solution of K[In(NON$^{Dipp}$)] (20.4 mg, 0.032 mmol) in a J. Youngs NMR tube resulted in immediate colour loss and precipitation of a fine white solid. The volatiles were removed *in vacuo* and the residue was re-dissolved in *n*-hexane, filtered and concentrated. Storage of the solution at –30 °C overnight resulted in the formation of large colourless blocks of **1**. Yield 31 mg (97%).

Anal. Calcd. For $C_{51}H_{75}InN_4OSi_2Zn$ (994.38): C, 61.47; H, 7.59; N, 5.62 % Found: C, 61.70; H, 7.70; N, 5.45.

$^{1}$H NMR (600 MHz, $C_6D_6$): $\delta$ 7.06 (s, 6H, $C_6H_3$-Dipp), 6.69 (s, 4H, $C_6H_2$-Mes), 4.81 (s, 1H, $\gamma$-C*H*), 3.95 (sept, *J* = 7.0, 4H, C*H*Me$_2$), 2.24 (s, 6H, NC*Me*), 1.67 (s, 12H, o-*Me*), 1.33 – 1.29 (m (br), 18H, p-*Me* and CH*Me$_2$*), 0.86 (d, *J* = 7.0, 12H, CH*Me$_2$*), 0.30 (s, 12H, Si*Me$_2$*).

$^{13}$C{$^{1}$H} NMR (151 MHz, $C_6D_6$): $\delta$ 168.5 (N*C*Me), 147.1, 145.1, 144.7, 134.3, 131.2, 130.1, 129.3, 125.7, 123.5, 122.7 (*C$_6$*H$_3$-Dipp and *C$_6$*H$_2$-Mes), 97.5 ($\gamma$-*C*H), 27.2, 26.3 (o-*Me* and p-*Me*), 23.8, 23.2 (*C*HMe$_2$), 21.0, 18.4, 14.3 (CH*Me$_2$* and NC*Me*), 2.8 (Si*Me$_2$*).

**Figure S1** $^{1}$H NMR spectrum (600 MHz, $C_6D_6$) of (NON$^{Dipp}$)In–Zn(BDI$^{Mes}$) (**1**)

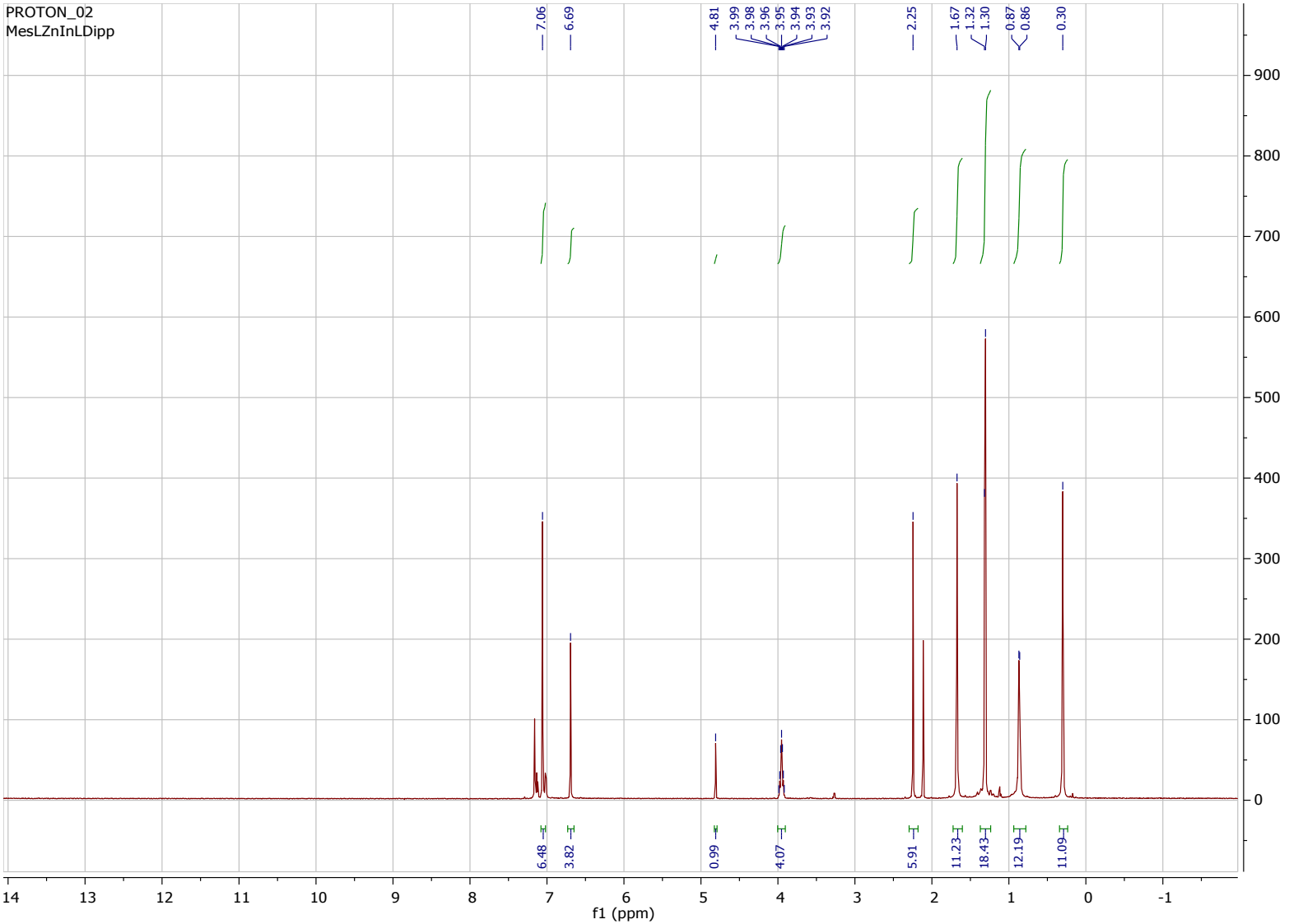


**Figure S2** $^{13}C\{^{1}H\}$ NMR spectrum (150 MHz, $C_6D_6$) of ($NON^{Dipp}$)In–Zn($BDI^{Mes}$) (**1**)

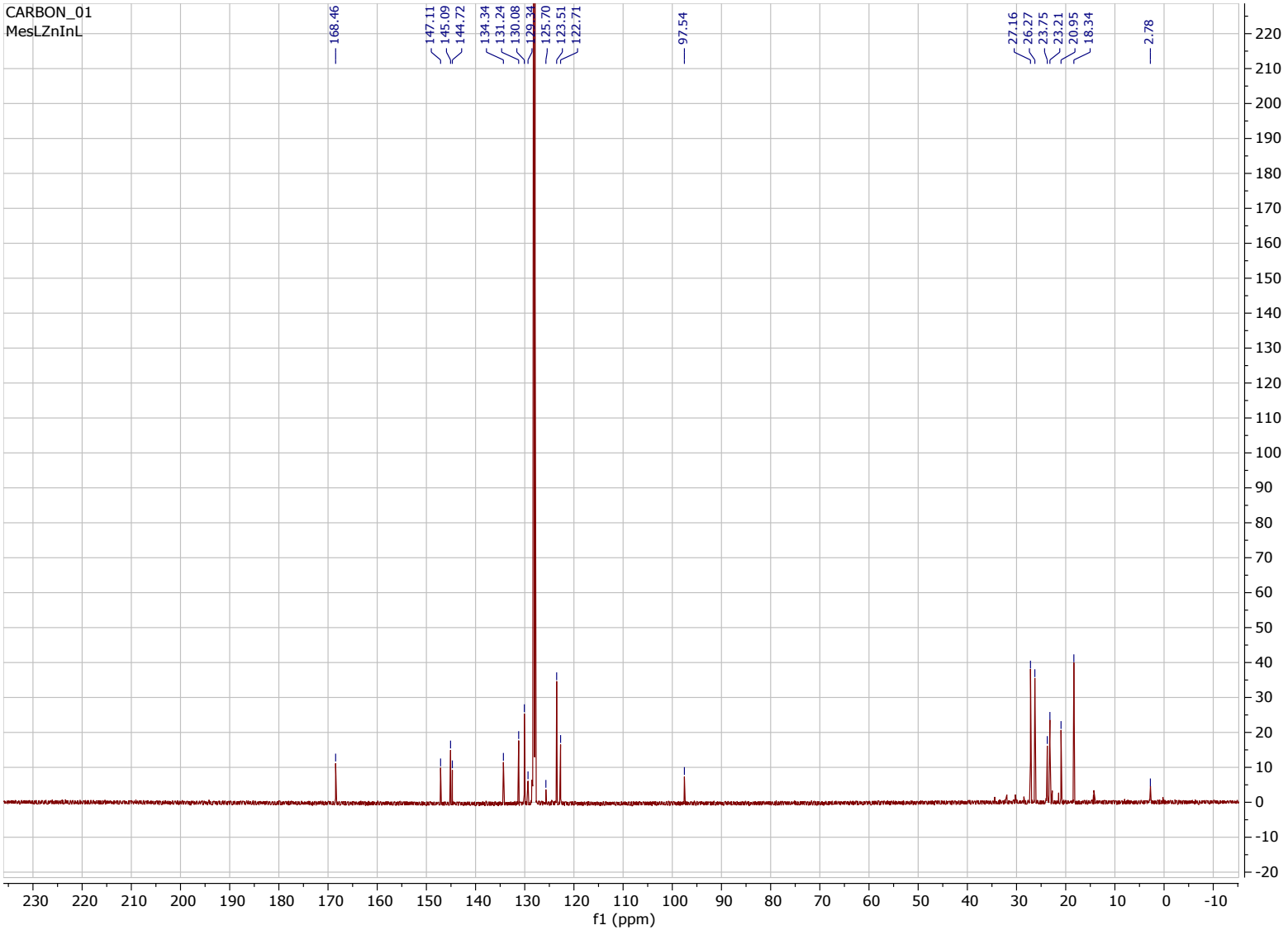
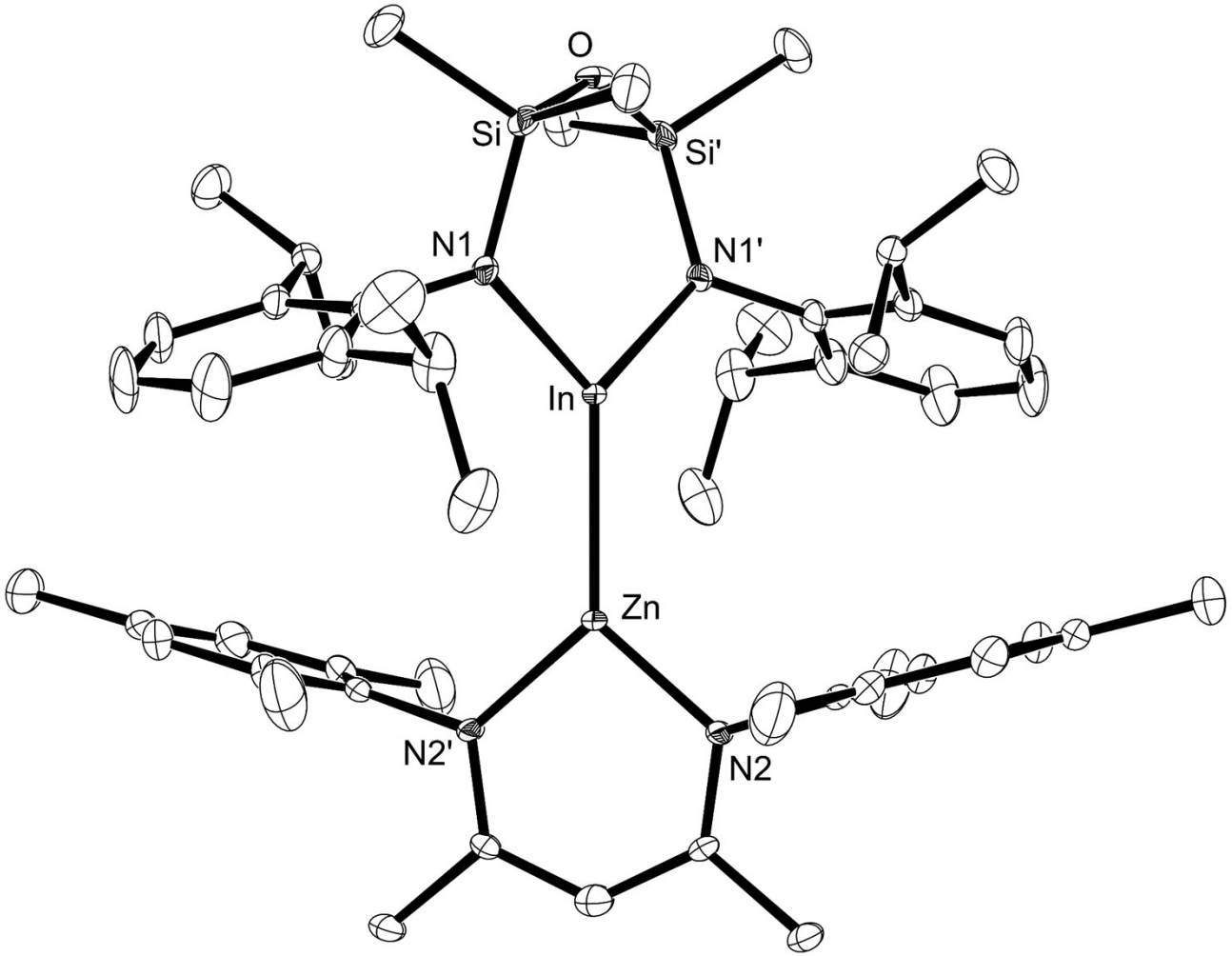


**Figure S3** ORTEP (ellipsoid 30% probability, H atoms omitted) of (NON$^{Dipp}$)In–Zn(BDI$^{Mes}$) (**1**, ' = –*x*, *y*, 1/2–*z*)



**Preparation of (NON$^{Dipp}$)In–Zn(BDI$^{Dipp}$) (2)**

Compound **2** was prepared using the method described for **1**, using K[In(NON$^{Dipp}$)] (20 mg, 0.028 mmol) and 'BDI$^{Dipp}$ZnCl' (20 mg, 0.028 mmol). The product **2** was isolated as colourless crystals. Yield 28 mg (92 %).

$^{1}$H NMR (600 MHz, $C_6D_6$): $\delta$ 7.13 – 7.09 (br m, 6H, $C_6H_3$), 7.03 – 6.99 (br m, 6H, $C_6H_3$), 4.77 (s, 1H, $\gamma$-C*H*), 4.04 (br sept, 2H, C*H*Me$_2$), 3.98 (br sept, 2H, C*H*Me$_2$), 3.09 (br sept, 2H, C*H*Me$_2$), 2.68 (br sept, 2H, C*H*Me$_2$), 1.39 (s, 6H, NC*Me*), 1.35, 1.31, 1.22, 1.13 (d, *J* = 6.7, 6H, CH*Me$_2$*), 1.04 (d, *J* = 6.8, 6H, CH*Me$_2$*), 0.84 (d, *J* = 6.9, 6H, CH*Me$_2$*), 0.74 (d, *J* = 6.8, 6H, CH*Me$_2$*), 0.65 (d, *J* = 6.9, 6H, CH*Me$_2$*), 0.47 (s, 6H, Si*Me$_2$*), 0.17 (s, 1H, Si*Me$_2$*), 0.12 (s, 5H, Si*Me$_2$*).

$^{13}$C{$^{1}$H} NMR (151 MHz, $C_6D_6$):$\delta$ 168.8 (N*C*Me), 146.2, 144.5, 129.3, 126.8, 125.7, 124.6, 123.8, 122.8 (*C$_6$*H$_3$), 97.9 ($\gamma$-*C*H), 31.6, 28.3, 27.2, 26.9, 26.5, 26.2, 25.6, 25.0, 24.3, 24.1, 23.5, 23.3, 22.6, 22.3, 21.0, 14.3 (*C*HMe$_2$ and CH*Me$_2$*), 5.4, 1.4, 0.3 (Si*Me$_2$*).

**Figure S4** $^{1}$H NMR spectrum (600 MHz, $C_6D_6$) of (NON$^{Dipp}$)In–Zn(BDI$^{Dipp}$) (**2**)

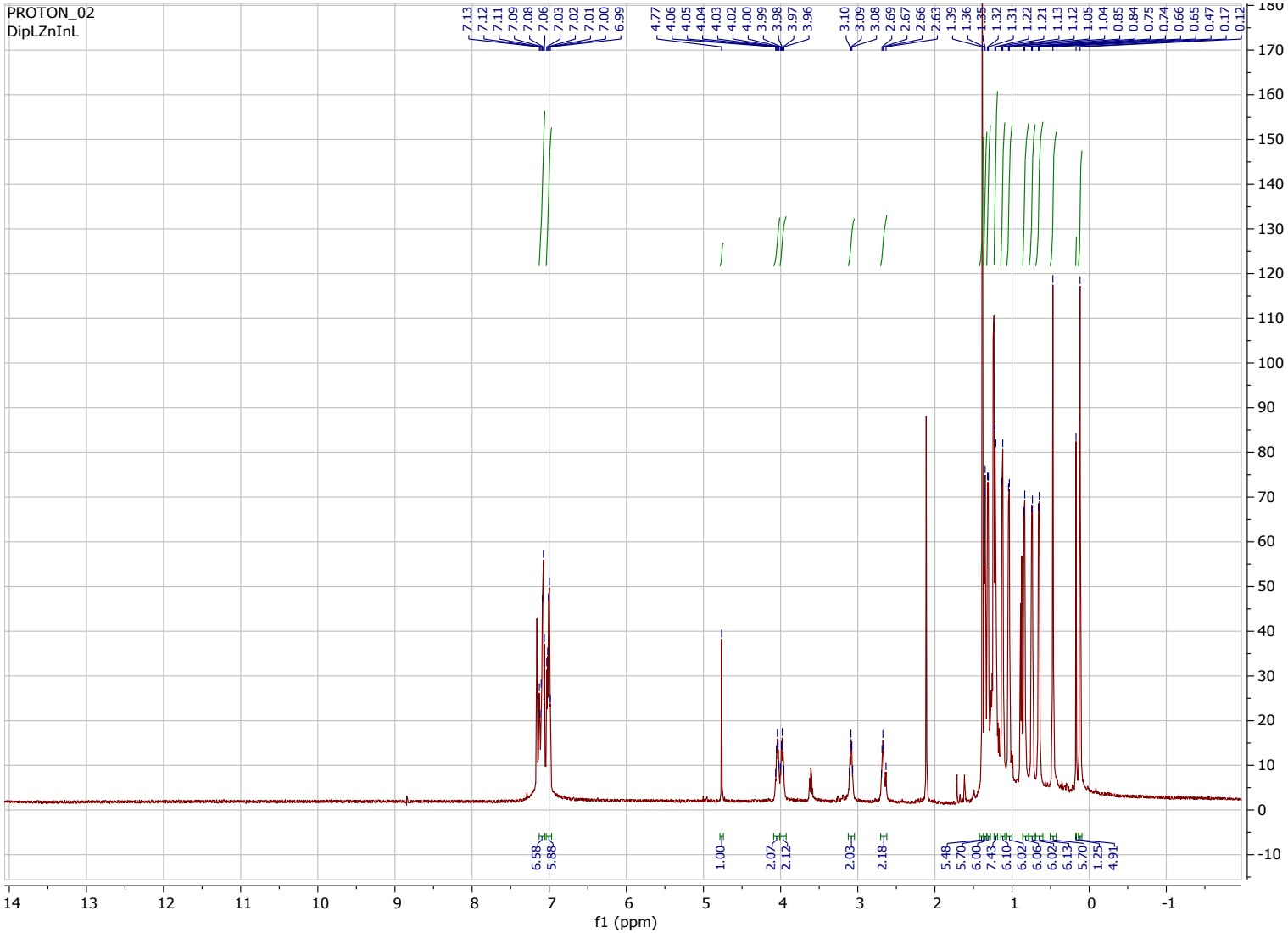


**Figure S5** $^{13}C\{^{1}H\}$ NMR spectrum (150 MHz, $C_6D_6$) of ($NON^{Dipp}$)In–Zn($BDI^{Dipp}$) (**2**)

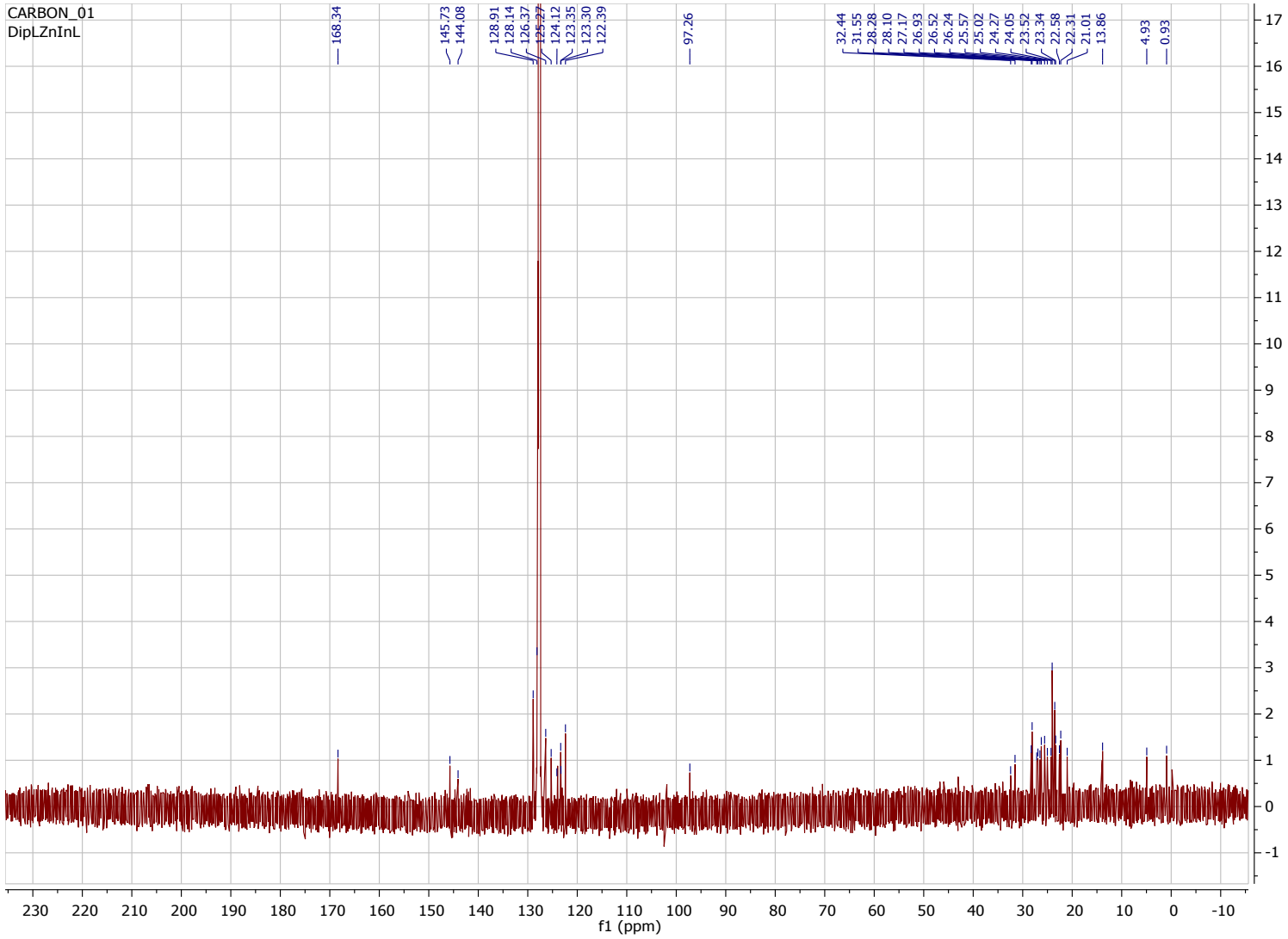
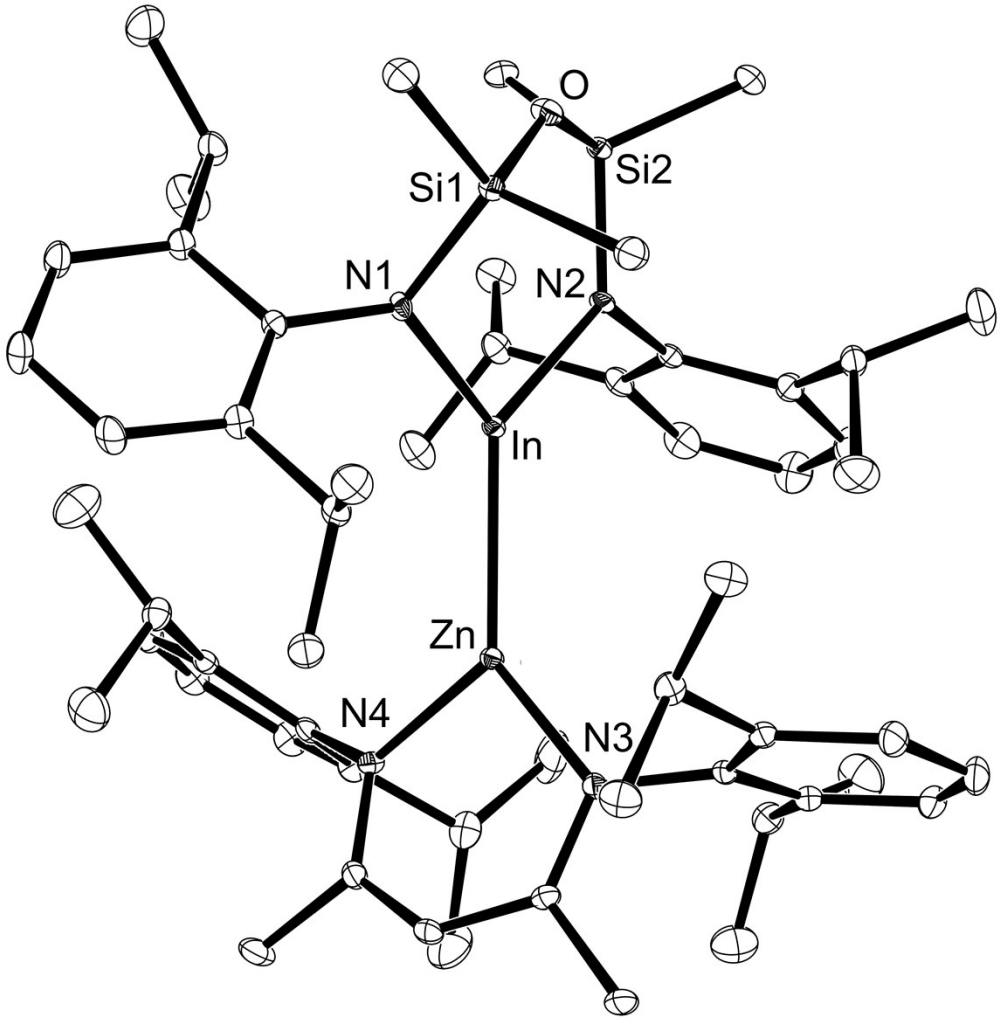


**Figure S6** ORTEP (ellipsoid 30% probability, H atoms and toluene solvate omitted) of ($NON^{Dipp}$)In–Zn($BDI^{Dipp}$) (**2**)



**Preparation of (NON$^{Dipp}$)In–Cd(BDI$^{Mes}$) (3)**

Compound **3** was prepared using the method described for **1**, using K[In(NON$^{Dipp}$)] (19 mg, 0.029 mmol) and 'BDI$^{Mes}$CdCl' (20 mg, 0.029 mmol). The product **3** was isolated as colourless crystals. Yield 25 mg (75 %).

$^{1}$H NMR (600 MHz, $C_6D_6$): $\delta$ 7.04 (s, 6H, $C_6H_3$-Dipp), 6.71 (s, 4H, $C_6H_2$-Mes), 4.69 (s, 1H, $\gamma$-C*H*), 3.90 (sept, *J* = 6.8, 4H, C*H*Me$_2$), 2.26 (s, 6H, NC*Me*), 1.73 (s, 12H, o-*Me*), 1.39 (s, 6H, p-*Me*), 1.29 (d, *J* = 6.8, 12H, CH*Me$_2$*), 0.84 (d, *J* = 6.8, 12H, CH*Me$_2$*), 0.29 (s, 12H, Si*Me$_2$*).

$^{13}$C{$^{1}$H} NMR (151 MHz, $C_6D_6$): $\delta$ 168.0 (N*C*Me), 146.7, 145.9, 145.1, 133.4, 130.2, 129.9, 123.5, 123.1 (*C$_6$*H$_3$-Dipp and *C$_6$*H$_2$-Mes), 95.4 ($\gamma$-*C*H), 27.2 (*C*HMe$_2$), 26.5, 23.6 (CH*Me$_2$*), 23.5 (o- / p-*Me*), 21.0 (NC*Me*), 18.4 (o- / p-*Me*), 2.6 (Si*Me$_2$*).

**Figure S7** $^{1}$H NMR spectrum (600 MHz, $C_6D_6$) of (NON$^{Dipp}$)In–Cd(BDI$^{Mes}$) (**3**)

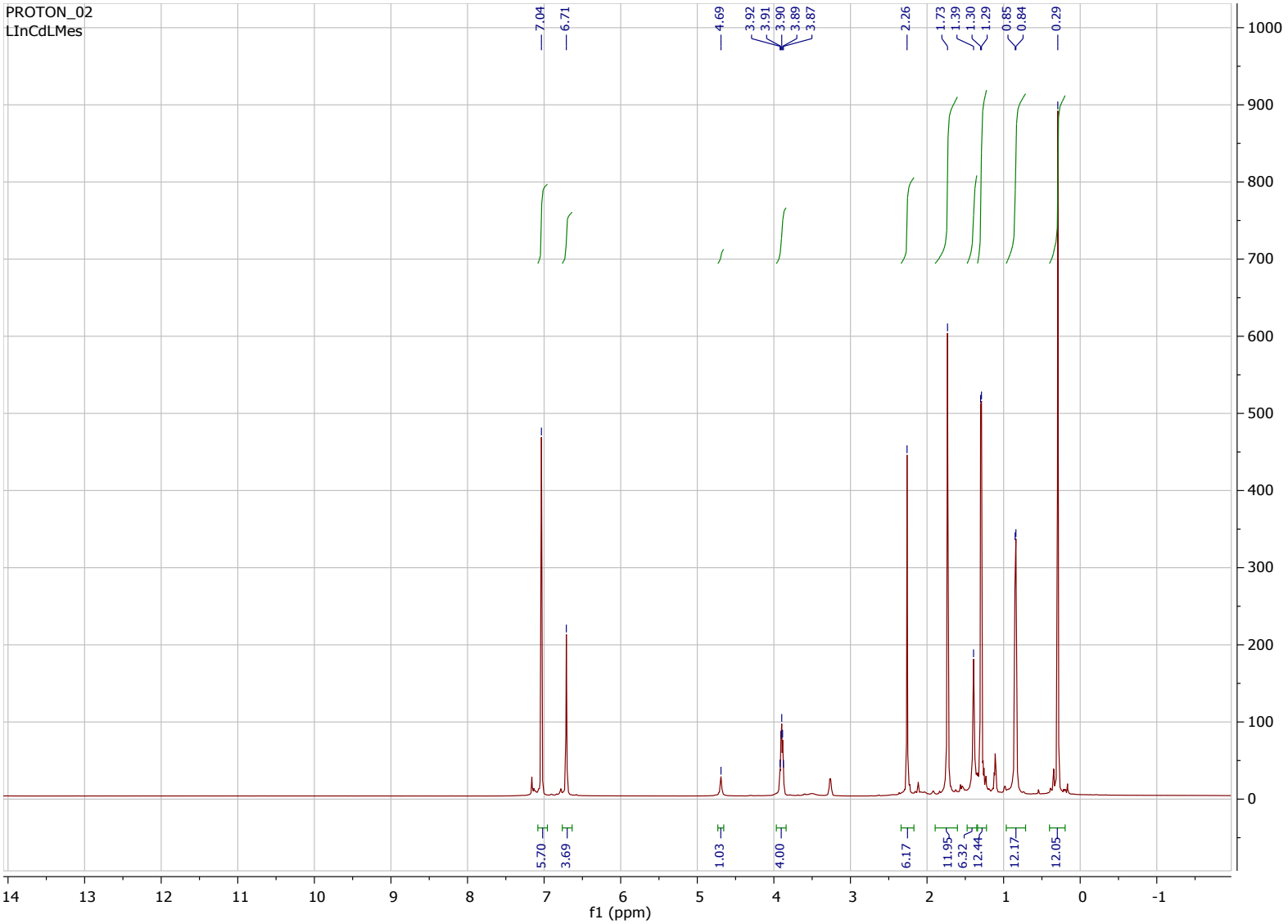


**Figure S8** $^{13}C\{^{1}H\}$ NMR spectrum (150 MHz, $C_6D_6$) of ($NON^{Dipp}$)In–Cd($BDI^{Mes}$) (**3**)

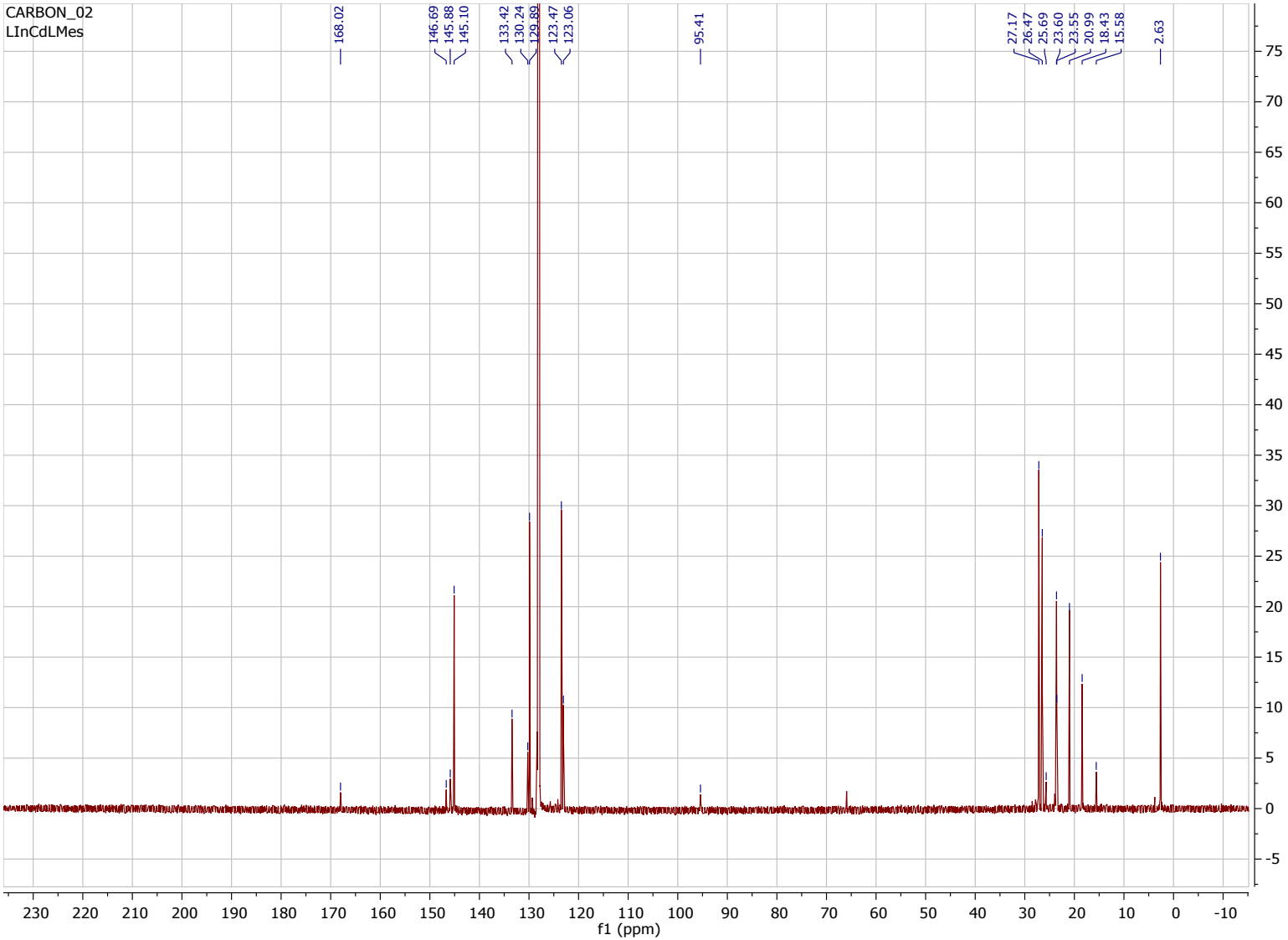
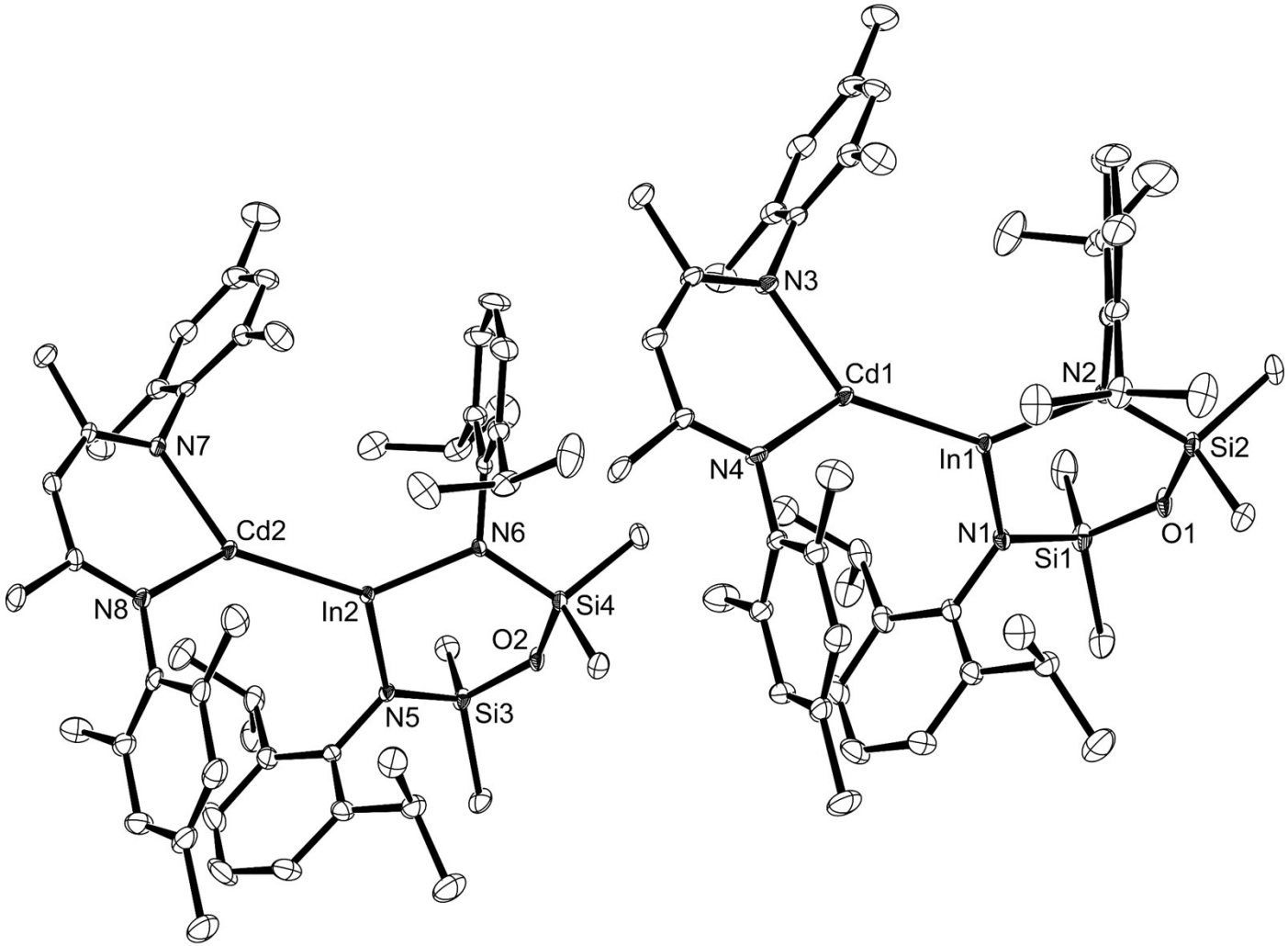


**Figure S9** ORTEP (ellipsoid 30% probability, H atoms and 4 x toluene solvate omitted; one component of disorder shown) of (NON$^{Dipp}$)In–Cd(BDI$^{Mes}$) (**3**)



**Preparation of (NON$^{Dipp}$)In–($\mu$-N$_3$Mes)–Zn(BDI$^{Mes}$) (4)**

Mesityl azide (3.2 mg, 0.02 mmol) was added to a colourless $C_6D_6$ solution of and **1** (20 mg, 0.02 mmol) in a J. Youngs NMR tube in a glovebox. Immediately after addition the mixture was stored at 6 °C. The reaction was monitored by *in situ* $^1$H NMR spectroscopy. Over the course of 2 days, all starting material had been consumed and only signals associated with a new intermediate compound **4** and the final product **5** were observed in solution. Removal of solvent *in situ* and addition of hexane followed by storage – 30 °C overnight gave a mixture of green and colourless crystals suitable for X-ray diffraction experiments. Mechanical separation and analysis by X-ray diffraction showed the colourless crystals to be compound **4** and the green crystals compound **5**. All attempts to isolate NMR pure samples of **4** failed, instead rapid nitrogen evolution gave samples of **5**. The $^1$H NMR of compound **4** is assigned from *in situ* measurements.

**Figure S10** $^{1}$H NMR spectrum (600 MHz, $C_6D_6$) of a mixture of (NON$^{Dipp}$)In–($\mu$-N$_3$Mes)–Zn(BDI$^{Mes}$) (**4**) and (NON$^{Dipp}$)In–($\mu$-NMes)–Zn(BDI$^{Mes}$) (**5**)

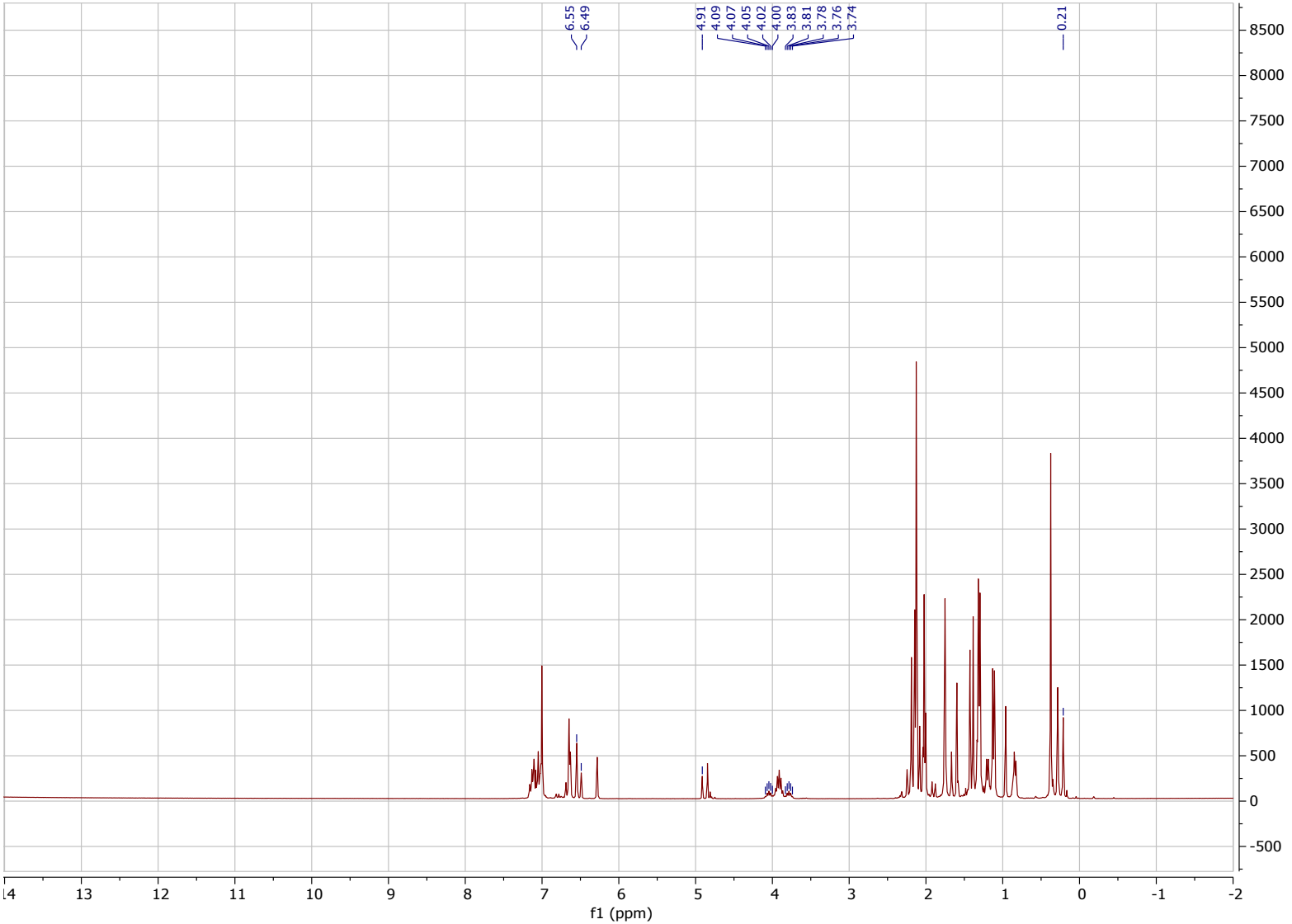


**Figure S11** [1] Stacked $^1$H NMR spectra of the reaction of **1** with$MesN_3$ at t = 0, 12 h, 24 h, 36 h and 48 h. ▼ = (NON$^{Dipp}$)In–Zn(BDI$^{Mes}$) (**1**), ✚ = '(NON$^{Dipp}$)In-($\mu$-$N_3$Mes)-Zn(BDI$^{Mes}$)' (**4**), ★ = (NON$^{Dipp}$)In–($\mu$-NMes)-Zn(BDI$^{Mes}$) (**5**).

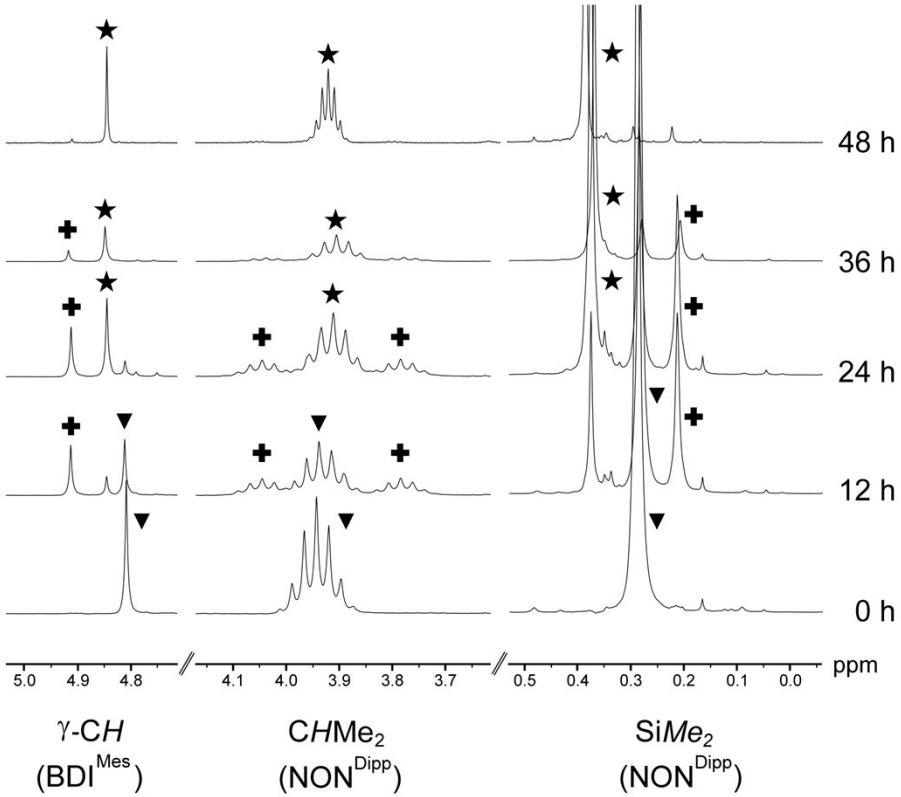
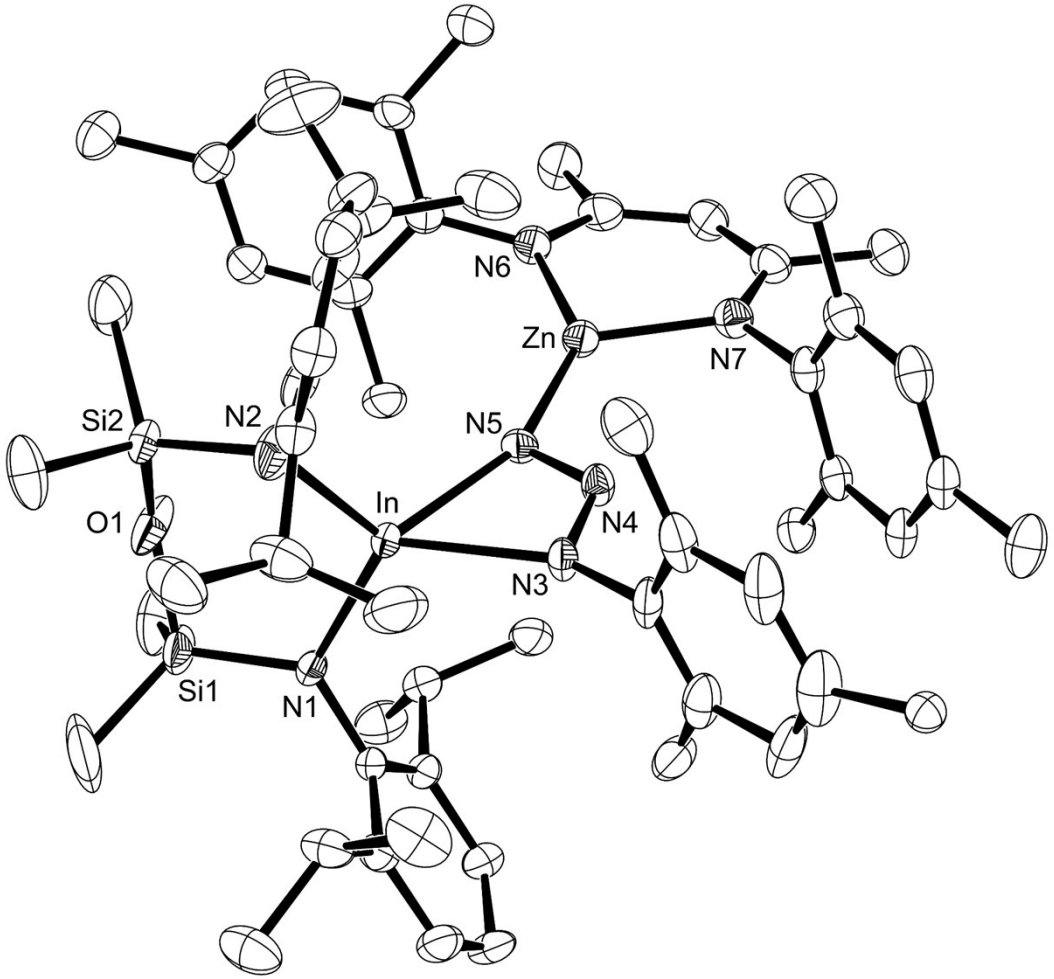


**Figure S12** ORTEP (ellipsoid 30% probability, H atoms omitted; one component of disorder shown) of ($NON^{Dipp}$)In–($\mu$-$N_3$Mes)–Zn($BDI^{Mes}$) (**4**)



**Preparation of (NON$^{Dipp}$)In–($\mu$-NMes)–Zn(BDI$^{Mes}$) (5)**

The addition of one equivalent of mesityl azide (3.2 mg, 0.02 mmol) to a colourless $C_6D_6$ solution of **1** (20 mg, 0.02 mmol) in a J. Youngs NMR tube resulted in the solution tuning yellow over two hours. The volatiles were removed *in vacuo* and the residue was re-dissolved in *n*-hexane, filtered and concentrated. Storage of the solution at –30 °C overnight resulted in the formation of large yellow blocks of **5**. Yield 18 mg (60 %).

$^1$H NMR (600 MHz, $C_6D_6$): $\delta$ 7.01 (s, 6H, $C_6H_3$-Dipp), 6.65 (s, 4H, $C_6H_2$-Mes), 6.29 (s, 2H, $C_6H_2$-Mes), 4.85 (s, 1H, $\gamma$-C*H*), 3.93 (sept, *J* = 6.8, 4H, C*H*Me$_2$), 2.19 (s, 6H, NC*Me*), 2.13 (s, 3H, o-*Me*), 2.09 (s, 3H, o-*Me*), 1.76 (s, 9H, o-*Me*), 1.44 (s, 6H, p-*Me*), 1.39 (s, 6H, p-*Me*), 1.31 (d, *J* = 6.8, 12H, CH*Me$_2$*), 1.13 (d, *J* = 6.8 Hz, 12H, CH*Me$_2$*), 0.39 (s, 12H, Si*Me$_2$*).

$^{13}$C{$^1$H} NMR (151 MHz, $C_6D_6$): $\delta$ 168.9 (N*C*Me), 153.2, 145.9, 145.5, 144.9, 135.2, 134.2, 132.2, 131.8, 129.7, 128.8, 127.1, 123.7 (*C*$_6$H$_3$-Dipp and *C*$_6$H$_2$-Mes), 96.7 ($\gamma$-*C*H), 32.0, 28.1, 26.1, 25.3, 23.3, 20.9, 20.7, 19.0, 18.0, 14.3 (*C*HMe$_2$, CH*Me$_2$*, NC*Me*, o-*Me* and p-*Me*), 3.0 (Si*Me$_2$*).

Extreme sensitivity to moisture and/or oxygen precluded the acquisition of accurate elemental analysis results for **5**.

**Figure S13** $^{1}$H NMR spectrum (600 MHz, $C_6D_6$) of ($NON^{Dipp}$)In–($\mu$-NMes)–Zn($BDI^{Mes}$) (**5**)

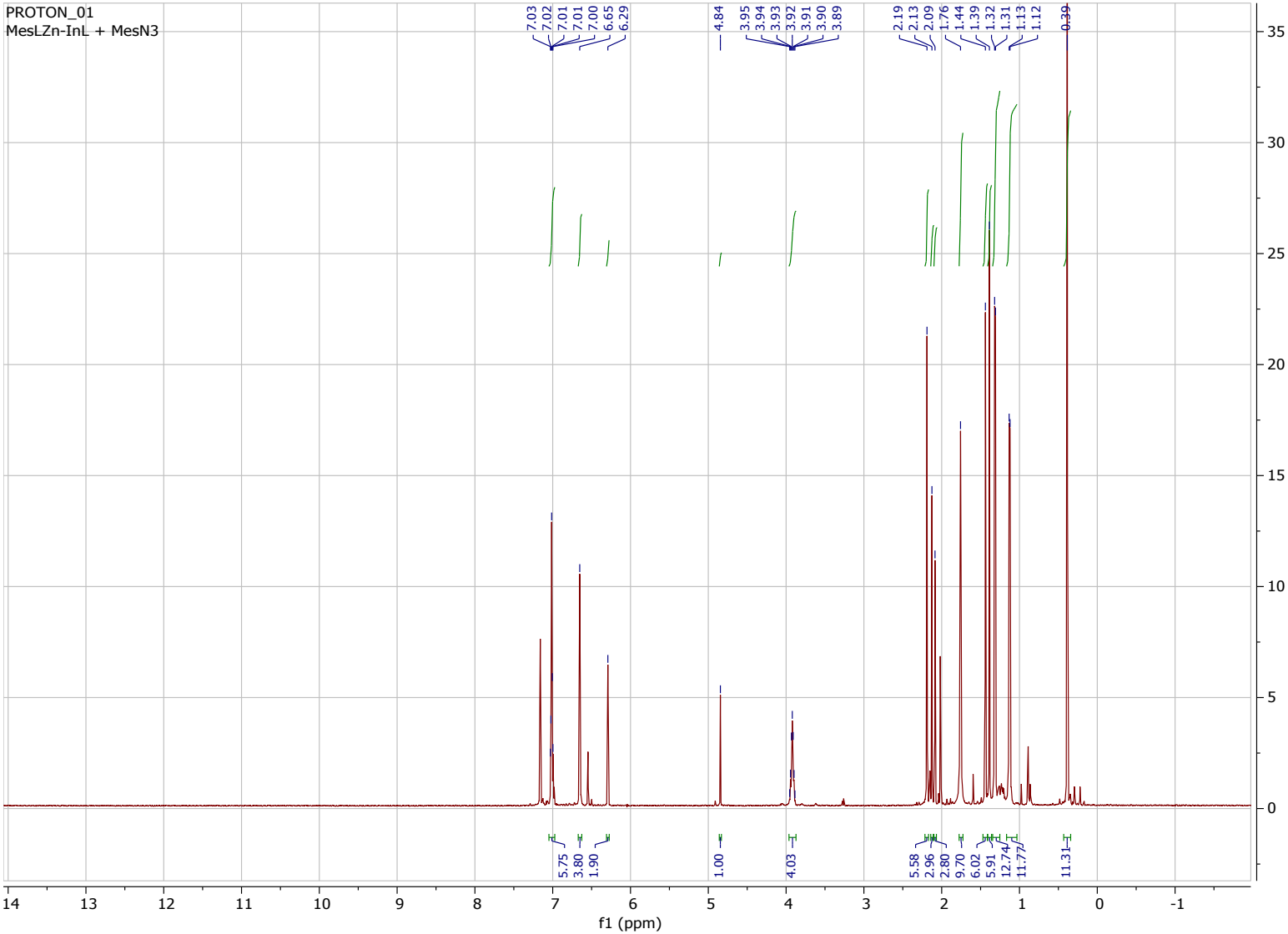


**Figure S14** $^{13}C\{^{1}H\}$ NMR spectrum (150 MHz, $C_6D_6$) of ($NON^{Dipp}$)In–($\mu$-NMes)–Zn($BDI^{Mes}$) (**5**)

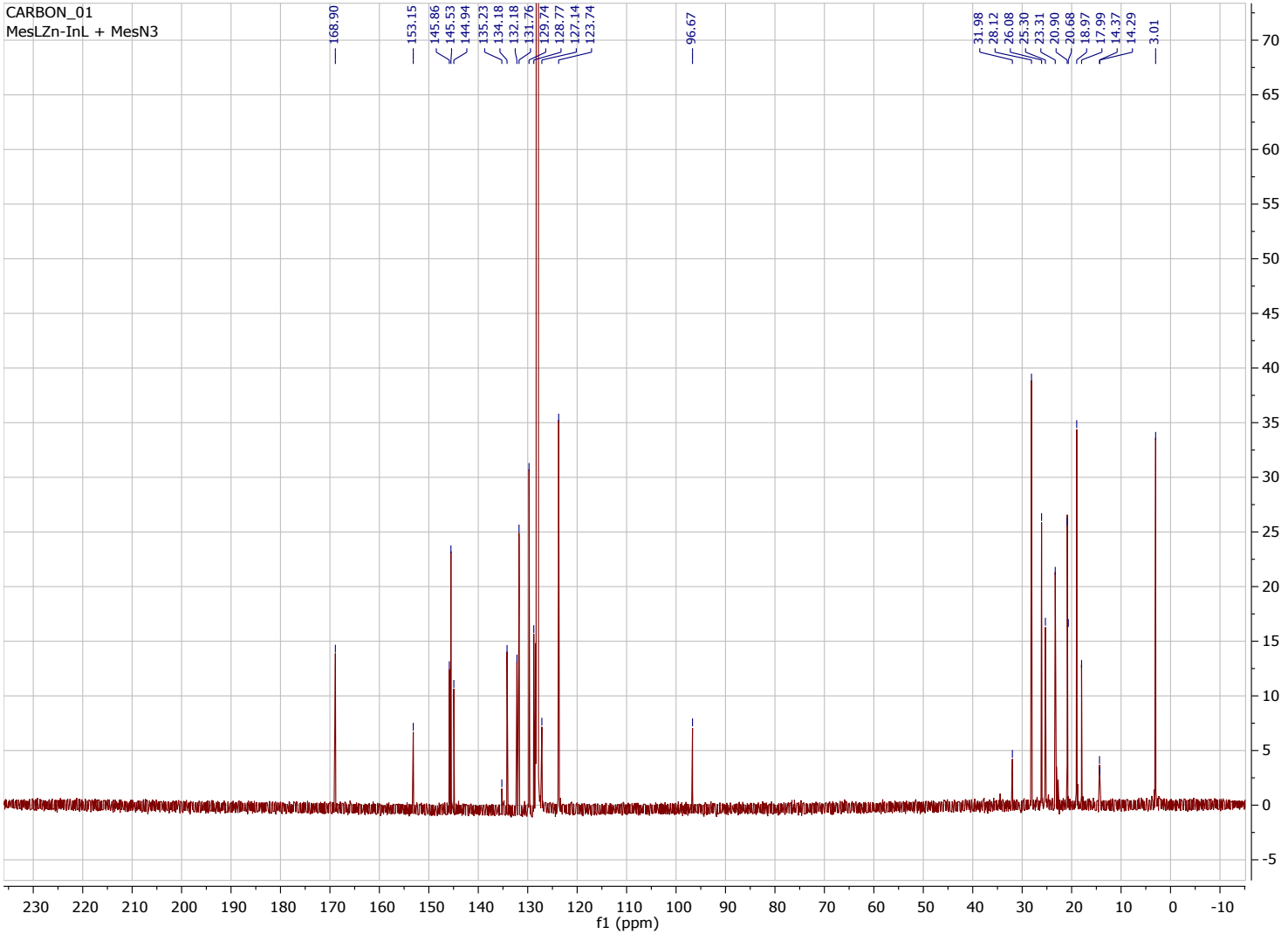
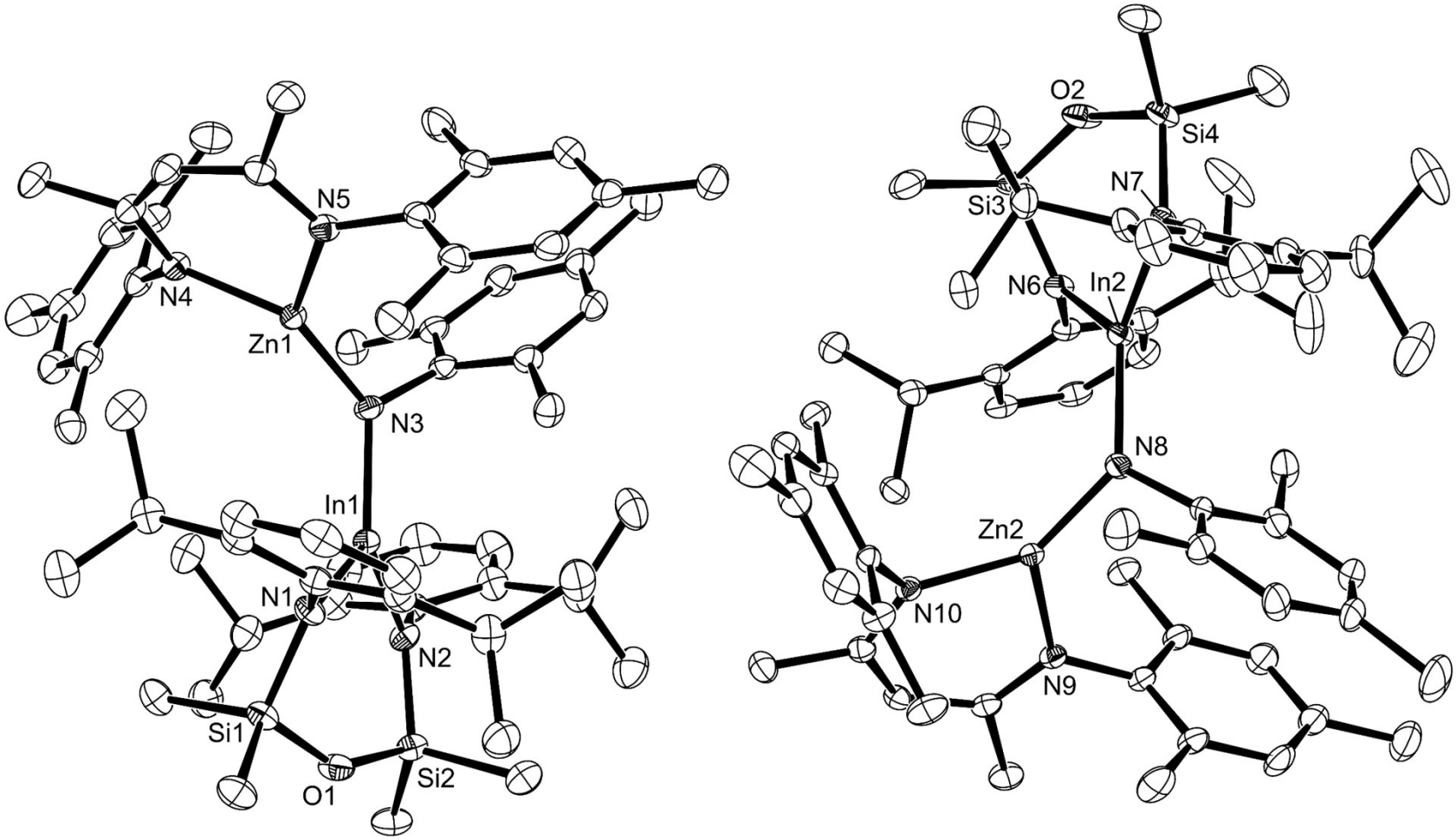


**Figure S15** ORTEP (ellipsoid 30% probability, hydrogen atoms omitted) of the asymmetric unit of(NON$^{Dipp}$)In–($\mu$-NMes)–Zn(BDI$^{Mes}$) (**5**)



**Preparation of (NON$^{Dipp}$)In–($\mu$-N$_4$Ph$_2$)–Zn(BDI$^{Mes}$) (6)**

The addition of two equivalents of phenyl azide (11.9 mg, 0.100 mmol) to a colourless $C_6D_6$ solution of **1** (50 mg, 0.050 mmol) in a J. Youngs NMR tube resulted in the solution immediately tuning bright yellow/orange with effervescence. A $^1$H NMR spectra recorded immediately after sample preparation showed complete consumption of starting material. The volatiles were removed *in vacuo* and the residue was re-dissolved in toluene, filtered and concentrated. Slow evaporation of the solution at room temperature resulted in the formation of bright yellow blocks of **6**. Yield 32 mg (53 %).

$^1$H NMR (500 MHz, $C_6D_6$): $\delta$ 7.13 (t, *J* = 7.6, 5H, C$_6$*H*$_5$-Ph), 7.00 – 6.94 (br m, 5H, C$_6$*H*$_5$-Ph), 6.85 – 6.79 (m, 6H, C$_6$*H*$_3$-Dipp), 6.67 (s, 4H, C$_6$*H*$_2$-Mes), 4.73 (s, 1H, $\gamma$-C*H*), 3.97 (sept, *J* = 6.7, 4H, C*H*Me$_2$), 2.26 (s, 6H, NC*Me*), 1.78 (s, 12H, *o*-*Me*), 1.35 (s, 6H, *p*-*Me*), 1.24 (d, *J* = 6.7, 12H, CH*Me$_2$*), 0.66 (d, *J* = 6.7, 12H, CH*Me$_2$*), 0.48 (s, 12H, Si*Me$_2$*).

$^{13}$C{$^1$H} NMR (125 MHz, $C_6D_6$):δ 170.4 (N*C*Me), 150.6, 146.8, 144.1, 142.8, 134.8, 131.0, 130.4, 129.9, 123.4, 122.6, 120.0 (*C*$_6$H$_5$-Ph, *C*$_6$H$_3$-Dipp and *C*$_6$H$_2$-Mes), 96.2 ($\gamma$-*C*H), 27.1 (CH*Me$_2$*), 25.8, 25.5 (*C*HMe$_2$), 23.1, 21.0 (*p*-Me), 18.4 (*o*-*Me*), 3.5 (Si*Me$_2$*).

**Figure S16** $^{1}$H NMR spectrum (500 MHz, $C_6D_6$) of ($NON^{Dipp}$)In–($\mu$-$N_4Ph_2$)–Zn($BDI^{Mes}$) (**6**)

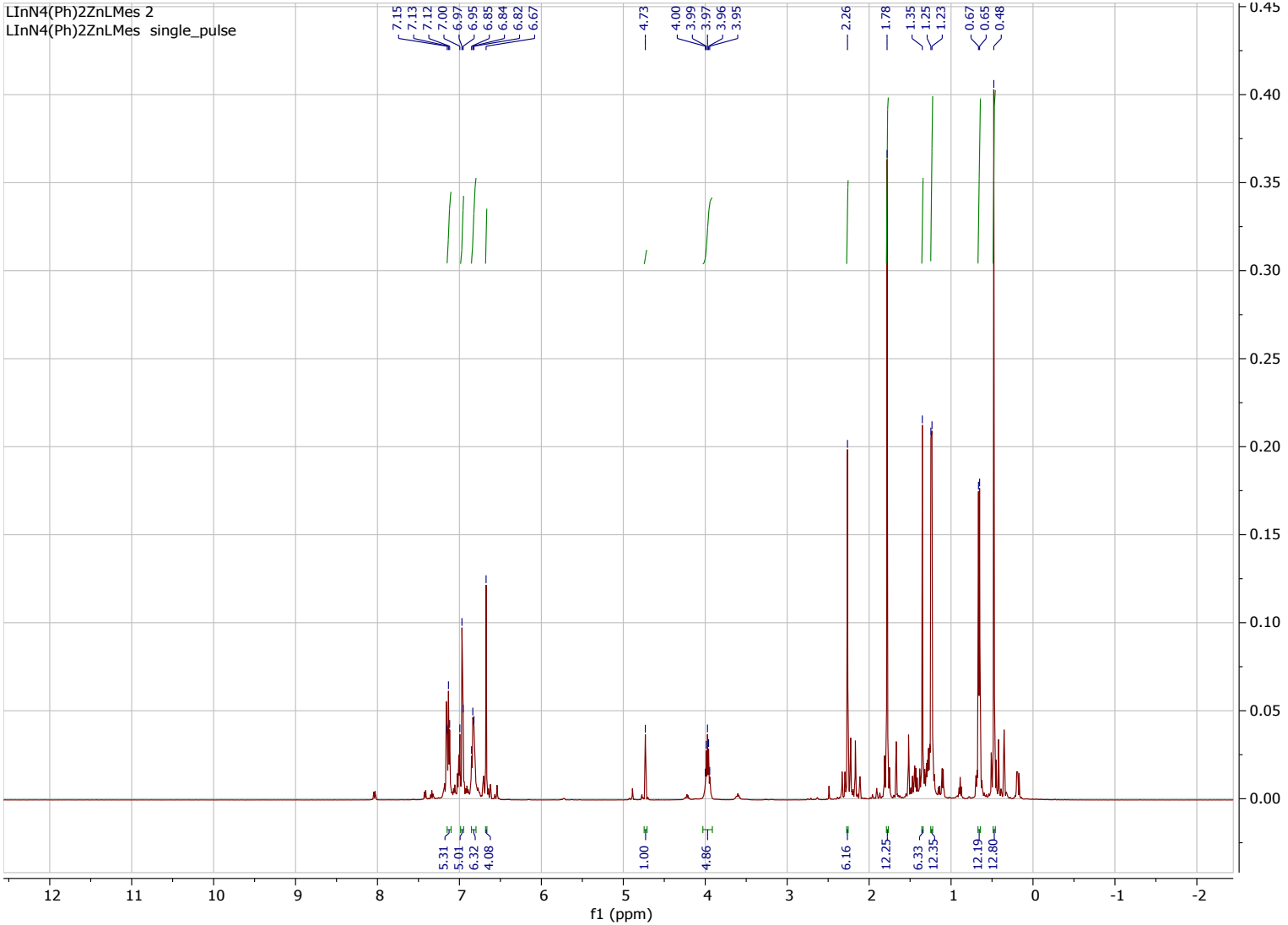


**Figure S17** $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, $C_6D_6$) of ($NON^{Dipp}$)In–($\mu$-$N_4Ph_2$)–Zn($BDI^{Mes}$) (**6**)

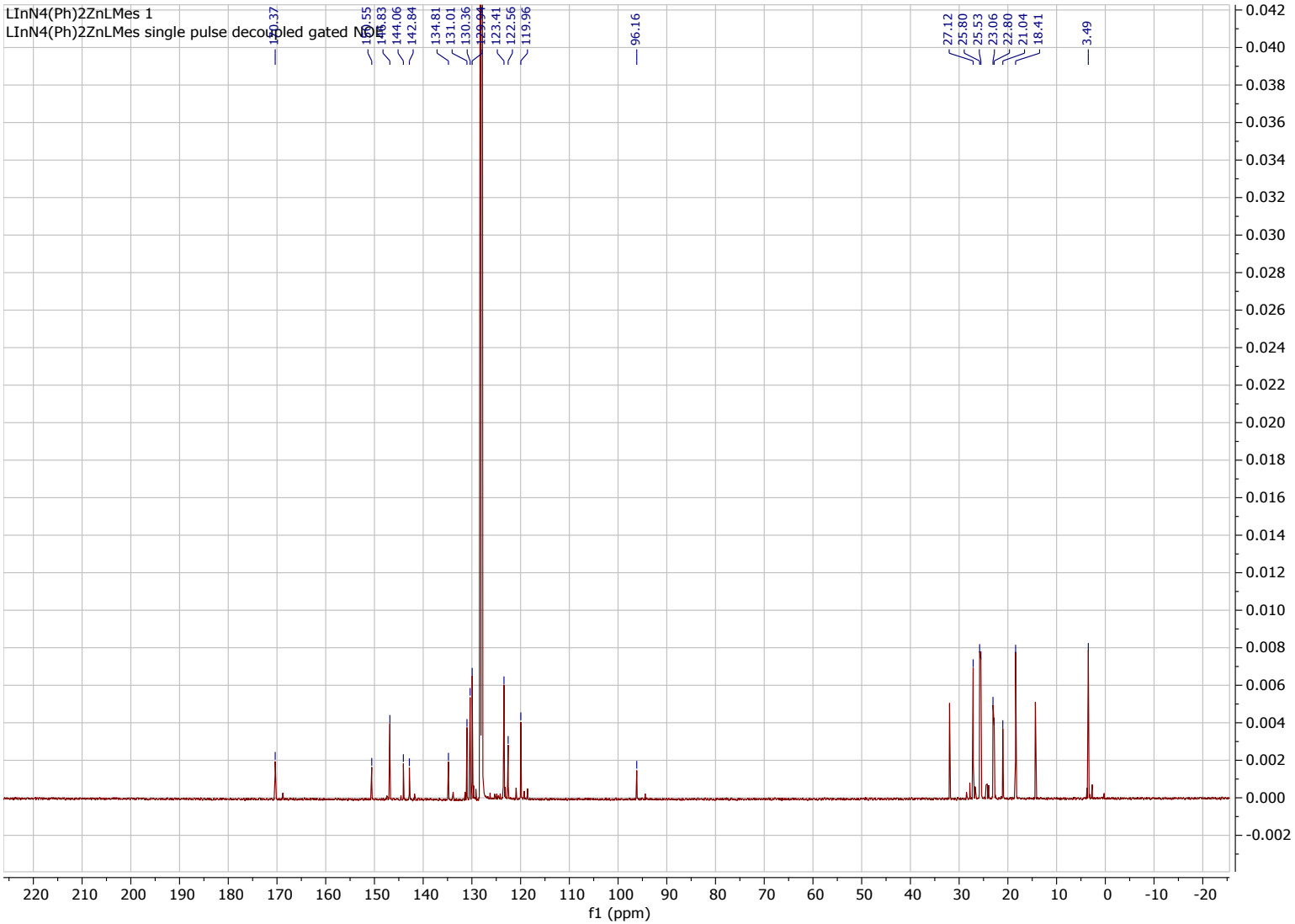
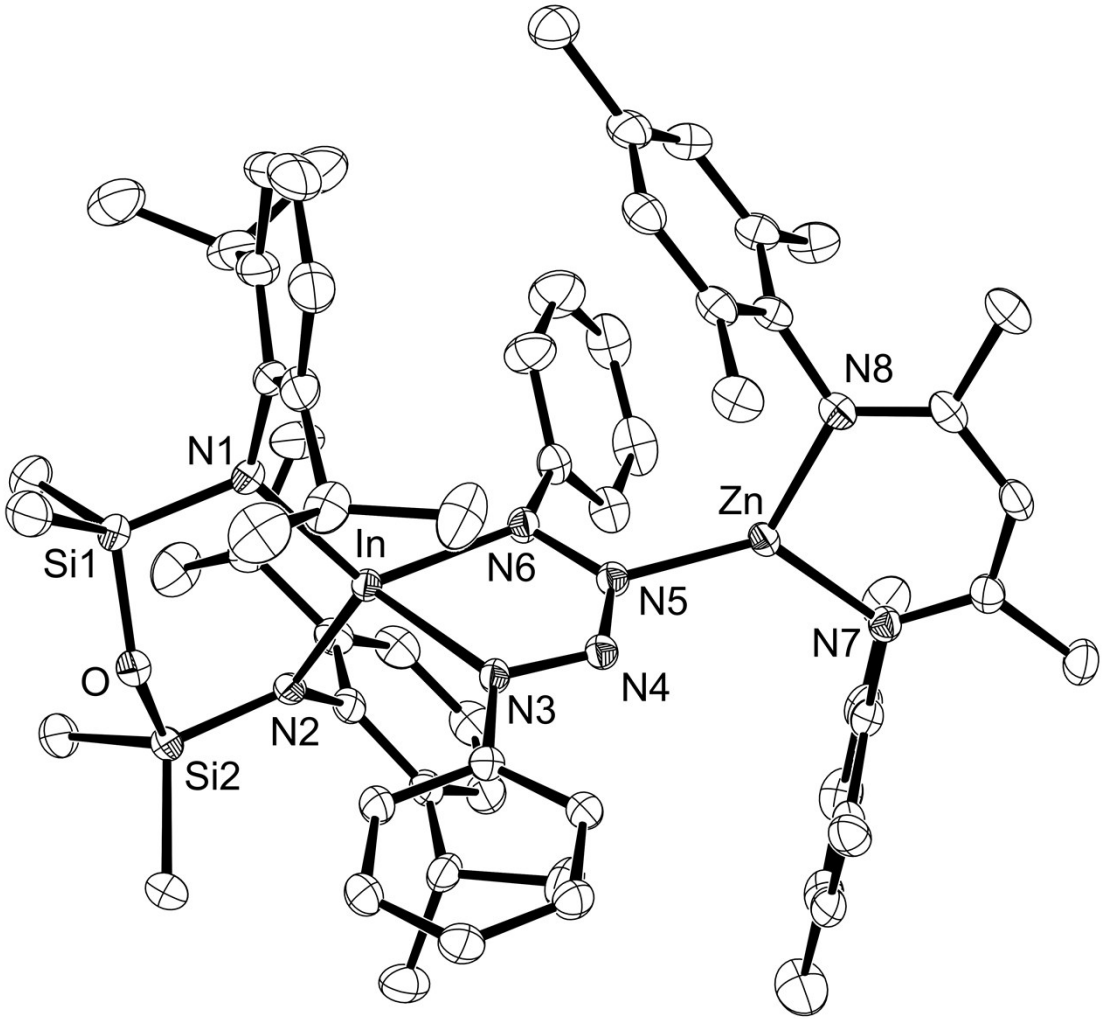


**Figure S18** ORTEP (ellipsoid 30% probability, hydrogen atoms omitted) of the asymmetric unit of(NON$^{Dipp}$)In–($\mu$-$N_4Ph_2$)–Zn(BDI$^{Mes}$) (**6**)



**Preparation of (NON$^{Dipp}$)In–($\mu$-$N_6Ph_2$)–Zn(BDI$^{Dipp}$) (7)**

The addition of two equivalents of phenyl azide (11 mg, 0.092 mmol) to a colourless $C_6D_6$ solution of **2** (50 mg, 0.046 mmol) in a J. Youngs NMR tube resulted in the solution immediately tuning bright yellow/orange. A $^1$H NMR spectra recorded immediately after sample preparation demonstrated complete consumption of starting material. The volatiles were removed *in vacuo* and the residue was re-dissolved in toluene, filtered and concentrated. Slow evaporation of the solution at room temperature resulted in the formation of bright yellow/orange blocks of **7**. Yield 38 mg (63 %).

$^1$H NMR (500 MHz, $C_6D_6$): $\delta$ 8.02 (d, *J* = 7.7, 2H, $C_6H_5$-Ph), 7.28 (t, *J* = 7.7, 2H, $C_6H_5$-Ph), 7.20 (t, *J* = 7.7, 2H, $C_6H_5$-Ph), 7.08 – 6.87 (m, 12H, $C_6H_3$-Dipp), 6.80 (dd, *J* = 17.1, 7.7, 4H, $C_6H_5$-Dipp), 4.83 (s, 1H, $\gamma$-C*H*), 3.40 (sept, *J* = 6.8, 2H, C*H*Me$_2$), 3.06 (sept, *J* = 7.1, 2H, C*H*Me$_2$), 2.71 (sept, *J* = 6.9, 2H, C*H*Me$_2$), 1.46 (s, 6H, NC*Me*), 1.18 (d, *J* = 6.9, 24H, CH*Me$_2$*), 0.95 (d, *J* = 6.7, 6H, CH*Me$_2$*), 0.75 (d, *J* = 6.8, 6H, CH*Me$_2$*), 0.35 (s, 6H, Si*Me$_2$*), 0.21 (s, 6H, Si*Me$_2$*), –0.07 (d, *J* = 6.8, 6H, CH*Me$_2$*), -–0.10 (d, *J* = 6.8, 6H, CH*Me$_2$*).

$^{13}$C{$^1$H} NMR (125 MHz, $C_6D_6$):δ 169.68 (N*C*Me), 146.9, 143.5, 143.0, 142.0, 141.6, 129.3, 129.0, 126.3, 125.7, 124.6, 124.2, 123.9, 123.8, 123.3, 118.9 (*C$_6$*H$_5$-Ph, *C$_6$*H$_3$-Dipp and *C$_6$*H$_2$-Mes), 94.3 ($\gamma$-*C*H), 28.6, 27.8, 27.5, 27.3, 26.8, 25.7, 25.6, 24.3, 24.0, 23.9, 23.8 (CH*Me$_2$* and *C*HMe$_2$), 2.8, 2.5 (Si*Me$_2$*).

**Figure S19** $^{1}$H NMR spectrum (500 MHz, $C_6D_6$) of ($NON^{Dipp}$)In–($\mu$-$N_6Ph_2$)–Zn($BDI^{Dipp}$) (**7**)

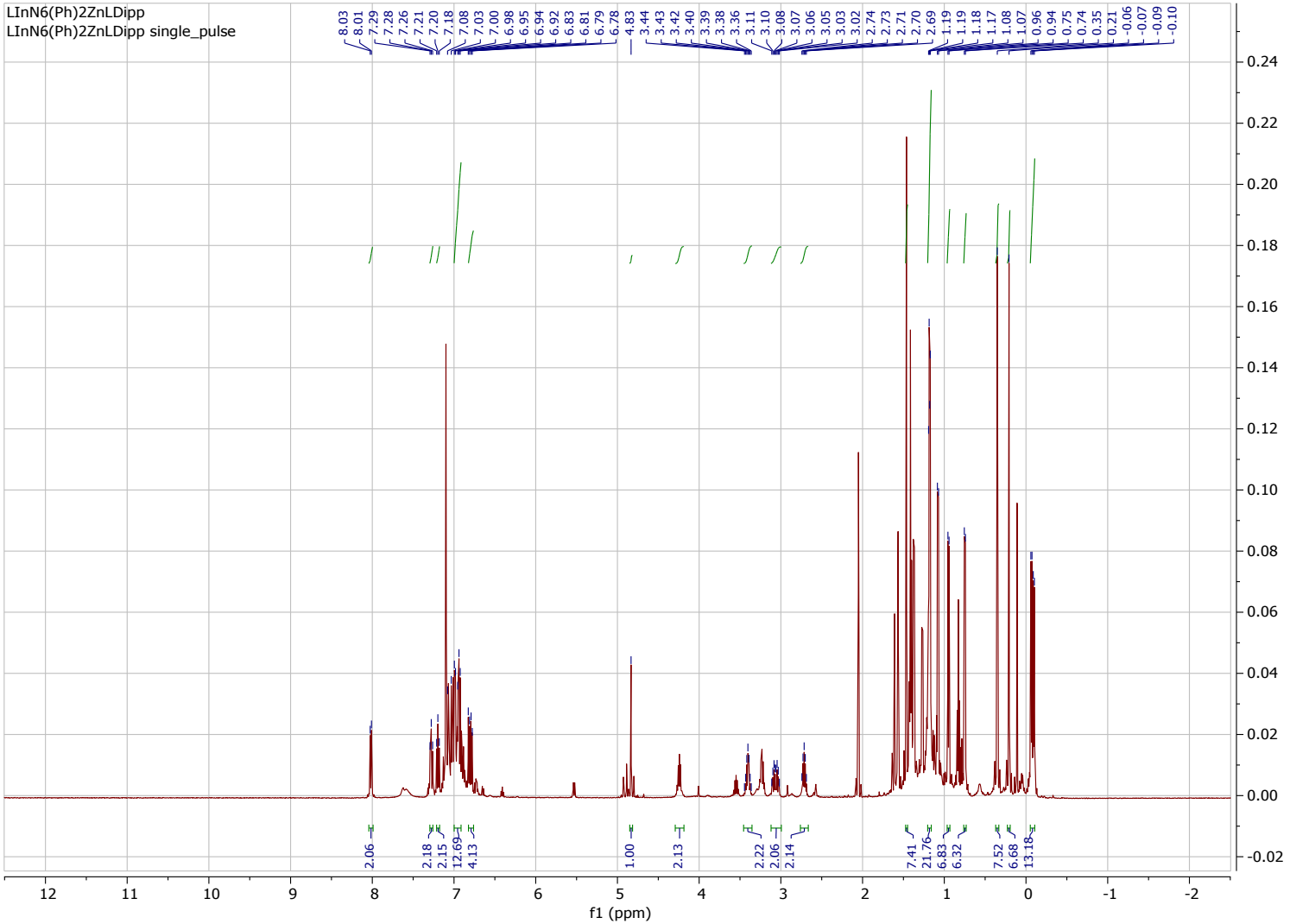


**Figure S20** $^{13}C\{^{1}H\}$ NMR spectrum (125 MHz, $C_6D_6$) of ($NON^{Dipp}$)In–($\mu$-$N_6Ph_2$)–Zn($BDI^{Dipp}$) (**7**)

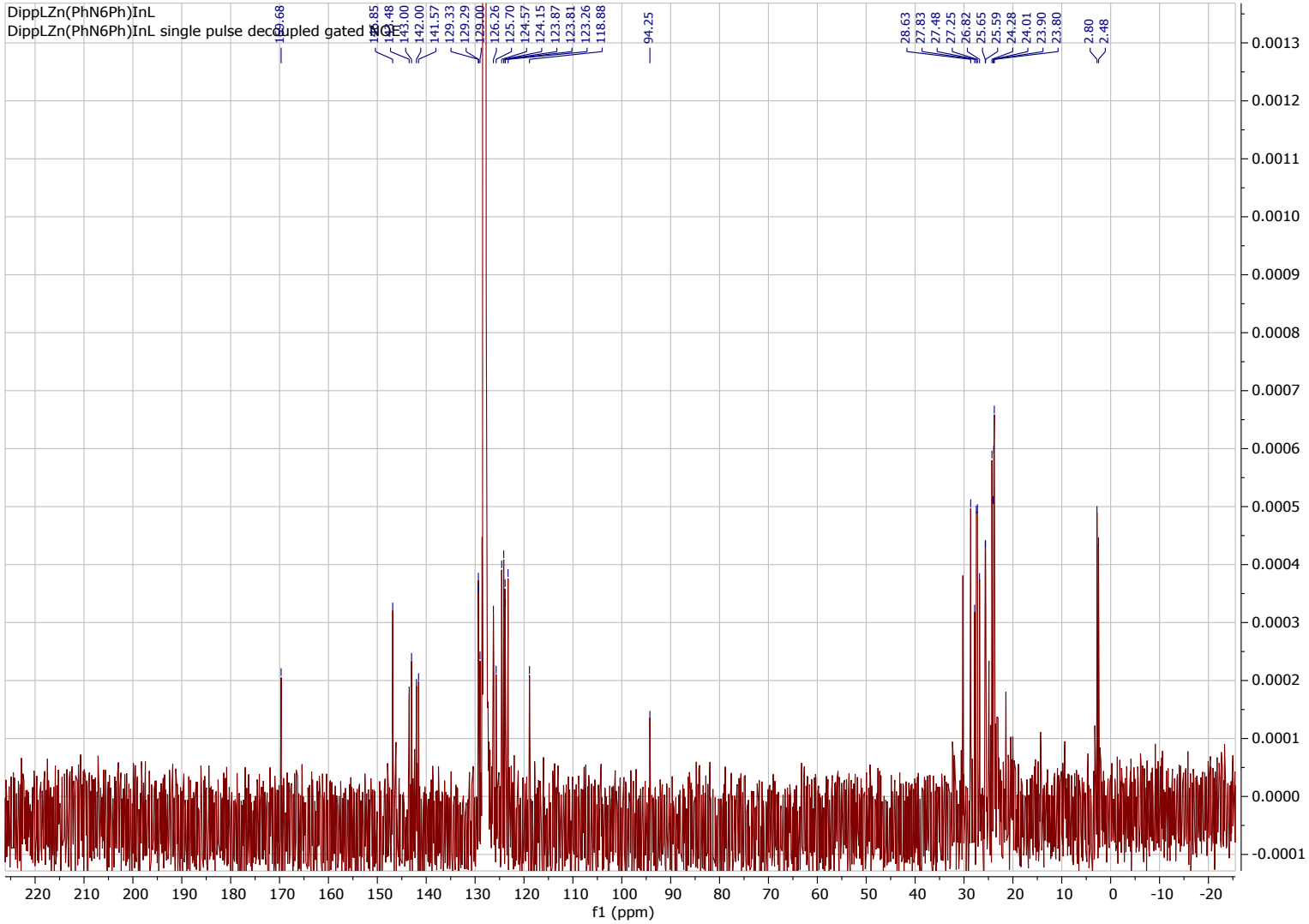
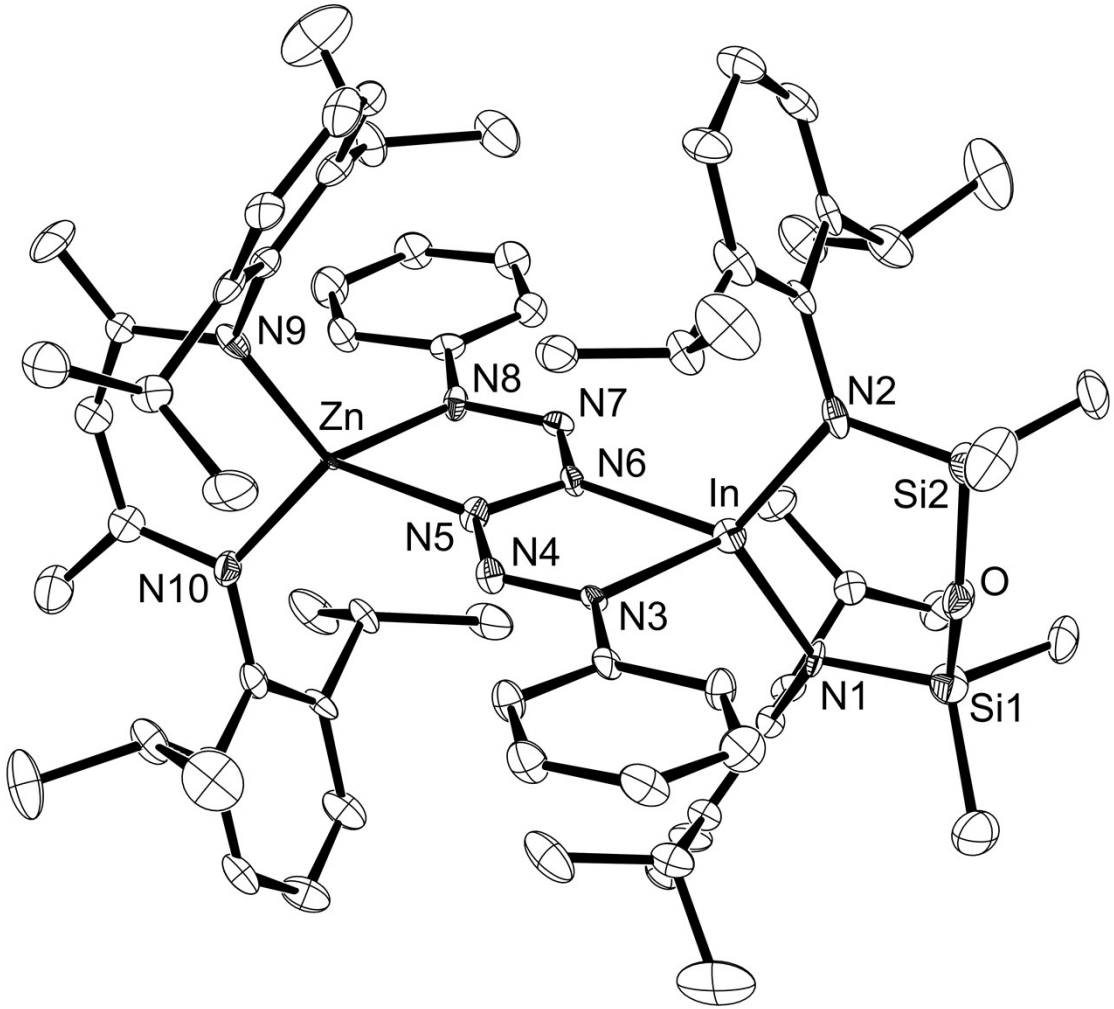


**Figure S21** ORTEP (ellipsoid 30% probability, hydrogen atoms and toluene solvate omitted) of the asymmetric unit of($NON^{Dipp}$)In–($\mu$-$N_6Ph_2$)–Zn($BDI^{Dipp}$) (**7**)



Isolation of [In($\mu$-1κ-$N^1$:2κ-$N^2$-NON$^{Dipp}$)]$_2$ (**A'**)

The addition of one equivalent of mesityl azide (3.2 mg, 0.02 mmol to a colourless $C_6D_6$ solution of [In(κ$^2$$N^{1,2}$-NON$^{Dipp}$)]$_2$ (**A**, 24 mg, 0.02 mmol) in a J Youngs NMR tube. The reaction was monitored by *in situ* $^1$H NMR spectroscopy. No reaction was evident after 2 days at room temperature. Increasing the temperature to 60 °C overnight led to complete consumption of starting material **A** with retention of signals corresponding to unreacted mesityl azide. Yellow block like crystals of **A'** formed at this temperature. Further heating to 100 °C for a further 7 days did not elicit any further changes. The crystals were isolated and analyzed by X-ray diffraction.

$^1$H NMR (600 MHz, $C_6D_6$): $\delta$ 7.15 (d, *J* = 9.5, 4H, $C_6H_3$), 7.12 (s, 4H, $C_6H_3$), 6.98 (t, *J* = 7.6, 2H, $C_6H_3$), 6.87 (t, *J* = 7.5 Hz, 2H, $C_6H_3$), 4.46 (sept, *J* = 6.8, 4H, C*H*Me$_2$), 4.33 (sept, *J* = 6.8, 4H, C*H*Me$_2$), 1.51 (d, *J* = 6.8, 12H, CH$Me_2$), 1.40 (d, *J* = 6.8, 24H, CH$Me_2$), 1.19 (d, *J* = 6.8, 12H, CH$Me_2$), 0.55 (s, 12H, Si$Me_2$), 0.53 (s, 12H, Si$Me_2$).

$^{13}$C{$^1$H} NMR (151 MHz, $C_6D_6$): $\delta$ 150.7, 147.4, 145.9, 145.0, 144.8, 124.2, 123.6, 122.94, 122.7, 119.3 ($C_6H_3$), 27.7, 27.3 (*C*HMe$_2$), 26.2, 25.81 (CH$Me_2$), 4.0, 3.1 (Si$Me_2$).

**Figure S22** $^{1}$H NMR spectrum (600 MHz, $C_6D_6$) of [In($\mu$-1κ-$N^1$:2κ-$N^2$-NON$^{Dipp}$)]$_2$ (**A'**)

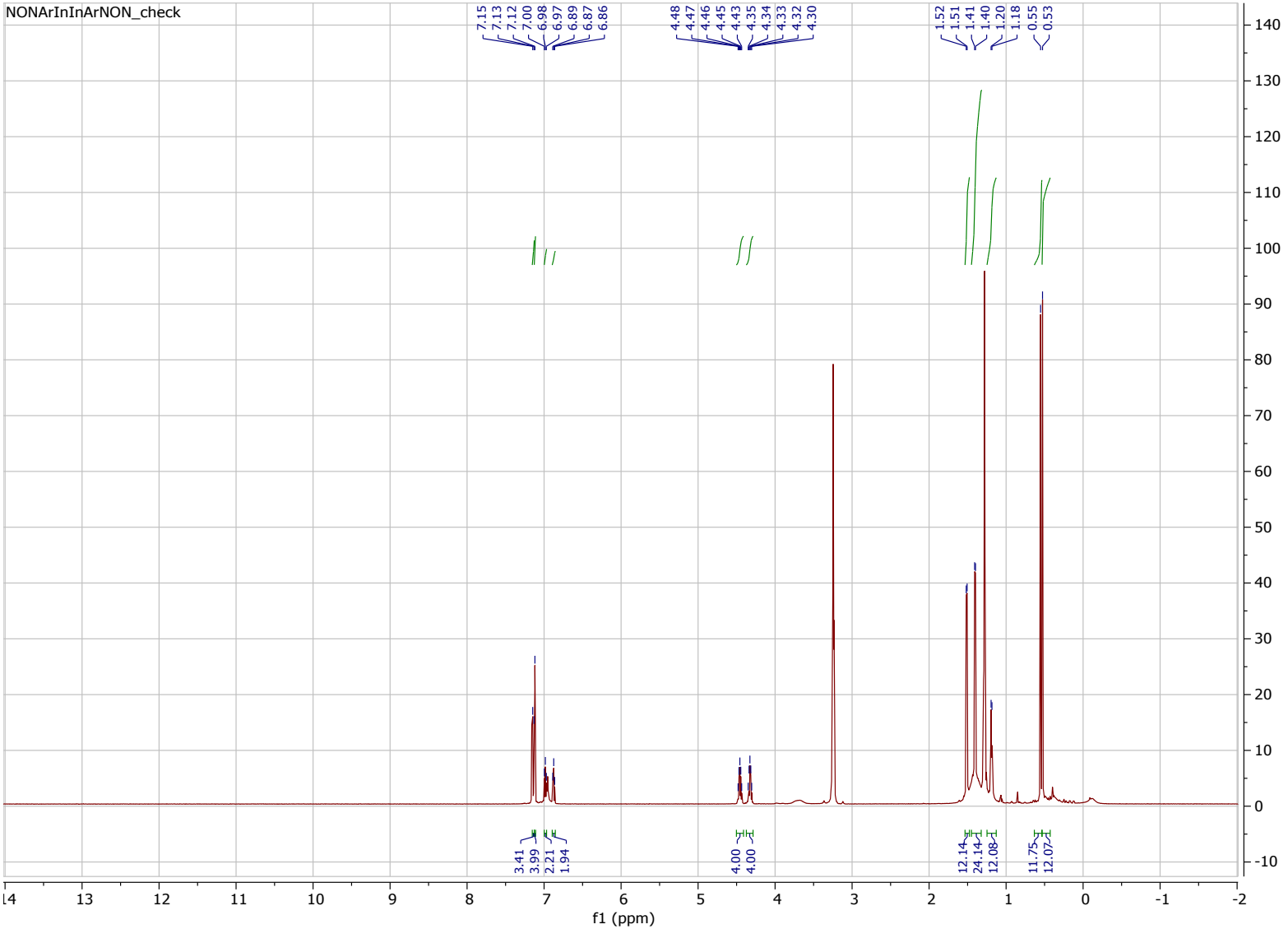


**Figure S23** $^{13}C\{^{1}H\}$ NMR spectrum (150 MHz, $C_6D_6$) of $[In(\mu\text{-}1\kappa\text{-}N^1\text{:}2\kappa\text{-}N^2\text{-}NON^{Dipp})]_2$ (**A'**)

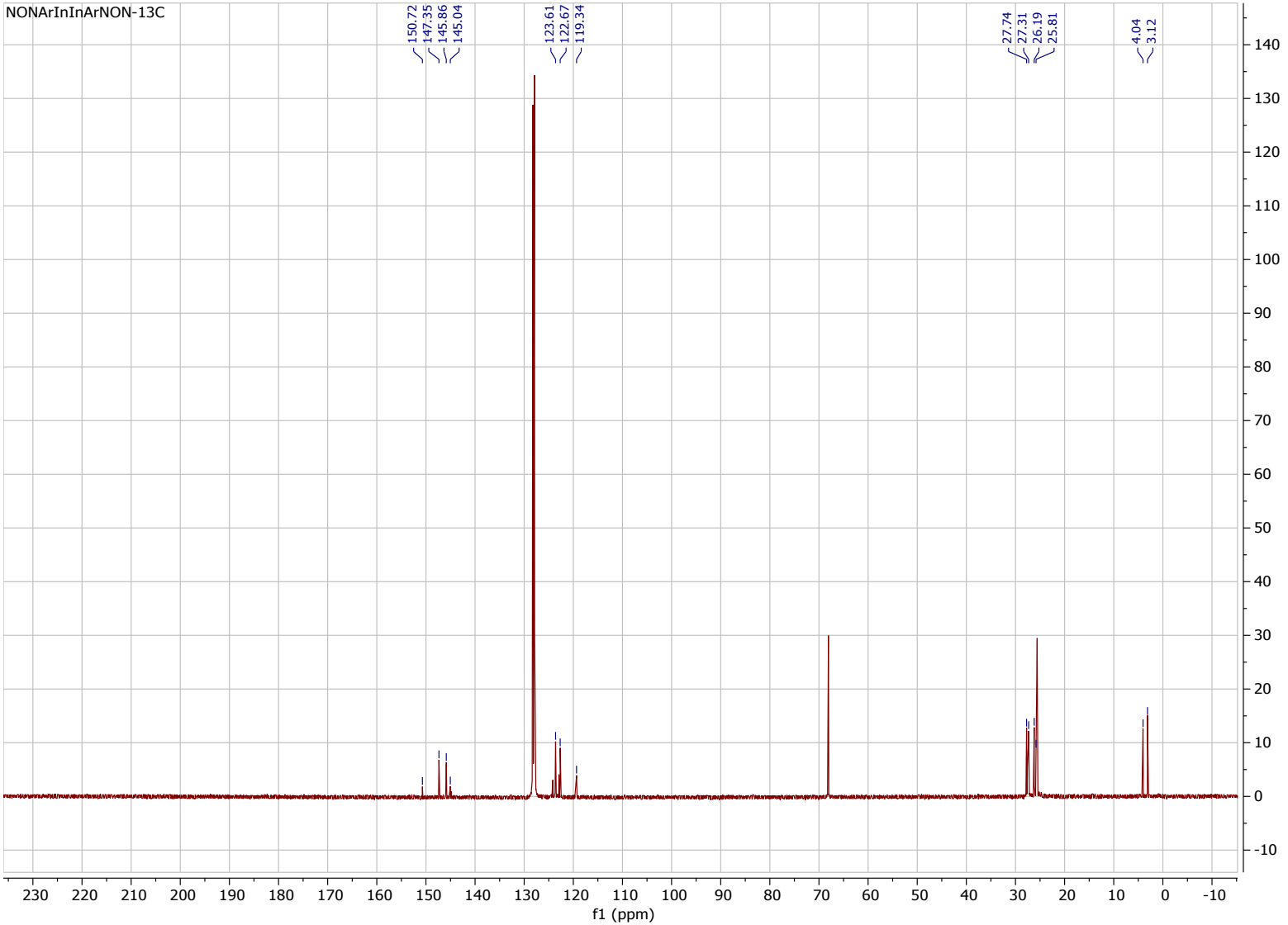
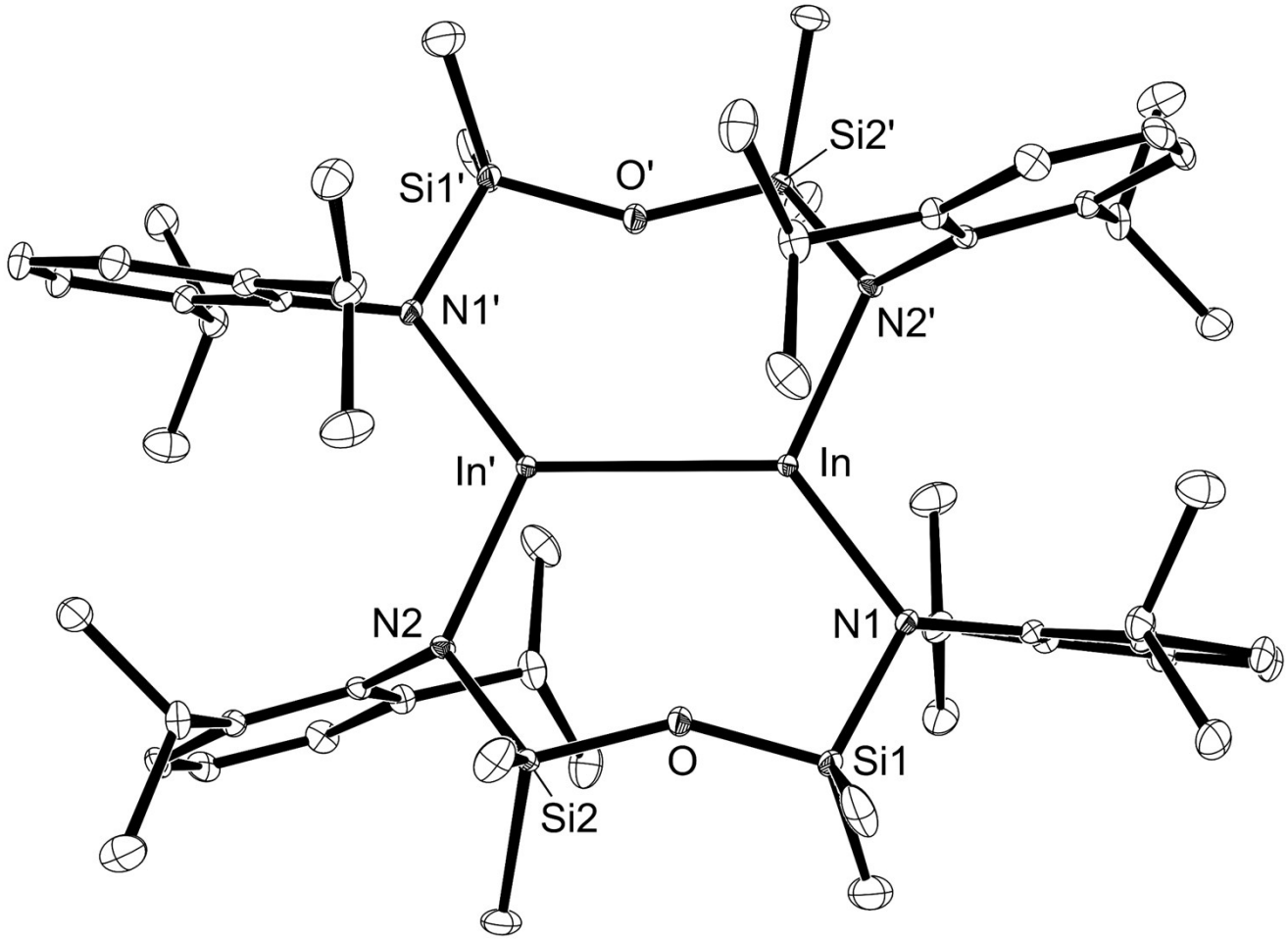


**Figure S24** ORTEP (ellipsoid 30% probability, hydrogen atoms omitted) of $[In(\mu\text{-}1\kappa\text{-}N^1\text{:}2\kappa\text{-}N^2\text{-}NON^{Dipp})]_2$ (**A**) (' 2–*x*, 1–*y*, –*z*)



**Crystallography**

Crystals were covered in inert oil and suitable single crystals were selected under a microscope and mounted on an Agilent SuperNova diffractometer fitted with an EOS S2 detector. Data were collected at the temperature indicated using focused microsource Cu Kα radiation at 1.54184 Å. Intensities were corrected for Lorentz and polarisation effects and for absorption using multi-scan methods.[S4] Space groups were determined from systematic absences and checked for higher symmetry. All structures were solved using direct methods with SHELXS,[S5] refined on $F^2$ using all data by full matrix least-squares procedures with SHELXL-2013,[S6] within the WinGX[S7] program. Non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were placed in calculated positions or manually assigned from residual electron density where appropriate, unless otherwise stated. The functions minimized were Σ*w*(*F2*o-*F2c),* with *w* = [σ2(F2o) + *a*P2 + *bP*]-1, where *P* = [max(Fo)2 + 2F2c]/3. The isotropic displacement parameters are 1.2 or 1.5 times the isotropic equivalent of their carrier atoms.

Additional Details:

*(NON$^{Dipp}$)In–Zn(BDI$^{Mes}$) (**1**)*: The molecule is located on a C2-axis that passes through the In-Zn bond. The metallacycle of the BDI unit is disordered and was modelled over two positions. The disorder in the gamma carbon could not be adequately modelled and so the ISOR restraint was applied to obtain a more satisfactory and realistic displacement ellipsoid. The unit cell also contains poorly defined hexane solvate molecules that have been treated as a diffuse contribution to the overall scattering without specific atom positions by SQUEEZE/PLATON. Full details are provided in the .cif file.

*(NON$^{Dipp}$)In–Zn(BDI$^{Dipp}$) (**2**)*:The molecule is a racemic twin and was refined with the TWIN command, giving a BASF of 0.48. The carbon atoms of the aromatic component of the toluene solvate were refined with SIMU and DELU restraints.

*(NON$^{Dipp}$)In–Cd(BDI$^{Mes}$) (**3**)*: One of the Dipp groups of the NON-ligand is disordered and was modelled over two positions. The lower occupancy orientation was refined with isotropic carbon atoms. The 4 toluene solvate molecules were poorly resolved. Two of them were modelled over two orientations. All but one of the aromatic rings were refined as fixed bodies using the AFIX66 command and the carbon atoms of all four were refined isotropically.

*(NON$^{Dipp}$)In–(μ-N$_3$Mes)–Zn(BDI$^{Mes}$) (**4**)*: There is poorly defined disorder in the NON-backbone. This was modelled over 2 positions (for 1 x $SiMe_2$, the O-atom and 1 x Me) with the minor component refined with isotropic atoms.

*(NON$^{Dipp}$)In–(μ-NMes)–Zn(BDI$^{Mes}$)* (***5***): One of the Mes-groups of the bridging imide ligand is disordered and was modelled over two positions. Both components were contained as rigid bodies using AFIX66 and the atoms of the lower occupancy part were left isotropic. The unit cell also contains a poorly defined toluene solvate molecule that has been treated as a diffuse contribution to the overall scattering Details provided in the .cif file.

*(NON$^{Dipp}$)In–(μ-N$_6$Ph$_2$)–Zn(BDI$^{Dipp}$)* (***7***): The two halves of the molecule are very similar as dictated by the large Dipp groups. The exception is the ligand backbone (Me2Si-O-SiMe vs. MeC-C(H)-CMe). As such there is a minor component to the structure in which the orientation of the Zn(BDI) and In(NON) ligands are reversed, which cannot be adequately described with a disordered model. As such the TWIN command was employed and the structure was solved and refined in the Cc (not C2/c) space group. As a consequence of this model, the C-C-C backbone of the BDI ligand was refined with isotropic C-atoms to prevent them from going NPD. The toluene solvate was also modelled with isotropic C-atoms.

*In$_2$(μ-1κ-N$^1$:2κ-N$^2$-NON$^{Dipp}$)$_2$* (***A'***): The asymmetric unit consists of half a molecule located on an inversion centre. The methyl groups of one of the $SiMe_2$ units are disordered and were modelled over two positions.

**Computational Methods**

All structural optimisations were carried out with the Gaussian 09 suite of programs (Revision D.01),[S8] using the density functional method (DFT) with the the PBE0 hybrid functional,[S9] and the split valence, polarised def2-SVP basis-set,[S10] of double-ζ quality. Grimme's empirical dispersion correction[S11] along with Becke-Johnson damping[S12] (D3BJ) was applied. We refer to the resulting computational model as PBE0-D3BJ/def2-SVP. Frequency calculations at the same level of theory were employed to ensure that the obtained structures are minima on the potential energy surface.

The bonding was analysed using the Natural Bond Orbital (NBO) approach[S13-S19] using the NBO 6.0 program.[S20-S21] and Wiberg Bond Indices (WBI) were computed.[S22] Additional analysis was carried out with the Quantum Theory of Atoms in Molecules (QTAIM) approach using the AIMAll programme package.

**Table S1** Calculated bond distances (PBE0-D3/def2-SVP)

| | **1** (Zn,In) / Å | **5** (Zn,N) / Å | **5** (In,N) / Å |
|---|---|---|---|
| **r(A,B)** | 2.56 | 1.90 | 2.02 |
| **X-ray values** | 2.5486(4) | 1.890(3)<br>1.878(3) | 2.005(3)<br>2.020(3) |

**Table S2** Results from NBO analysis.

| | **1** (Zn–In) | **1** Zn | **1** In | **5** (In–N) | **5** (Zn–N) | **5** In | **5** Zn | **5** N |
|---|---|---|---|---|---|---|---|---|
| WBI | 0.64 | - | - | 0.61 | 0.23 | - | - | - |
| NPA charge | - | 1.30 | 0.86 | - | - | 1.83 | 1.65 | –1.45 |
| NBO | 74 % In (77 % *s*-; 23 % *p*-)<br>26 % Zn (95 % *s*-; 5 % *p*-) | - | - | - | - | | - | - |

**Table S3** Results from QTAIM analysis.

| | $\rho(r_{BCP})$ | $\nabla^2\rho(r_{BCP})$ | $G(r_{BCP})/\rho(r_{BCP})$ | $H(r_{BCP})$ | **Verdict*** |
|---|---|---|---|---|---|
| **1** BCP (Zn,In) | 0.0575 | +0.0153 | 0.4443 | +0.0217 | donor/acceptor |
| **5** BCP (In,N) | 0.1082 | +0.4533 | 1.2843 | +0.0257 | polar covalent |
| **5** BCP (Zn,N) | 0.1066 | +0.5345 | 1.4242 | +0.0182 | polar covalent |

* Comparison with Table 8.1 in P. Popelier "The QTAIM Perspective of Chemical Bonding". The Chemical Bond: Fundamental Aspects of Chemical Bonding, First Edition. Edited by Gernot Frenking, Sason Shaik, Wiley 2014

**Figure S25** Molecular graph of (NON$^{Dipp}$)In–Zn(BDI$^{Mes}$) (**1**). Solid lines between the atoms are bond paths (very long bond paths are shown with dotted lines). Small green spheres are bond critical points (note the bond critical point between Zn and In).

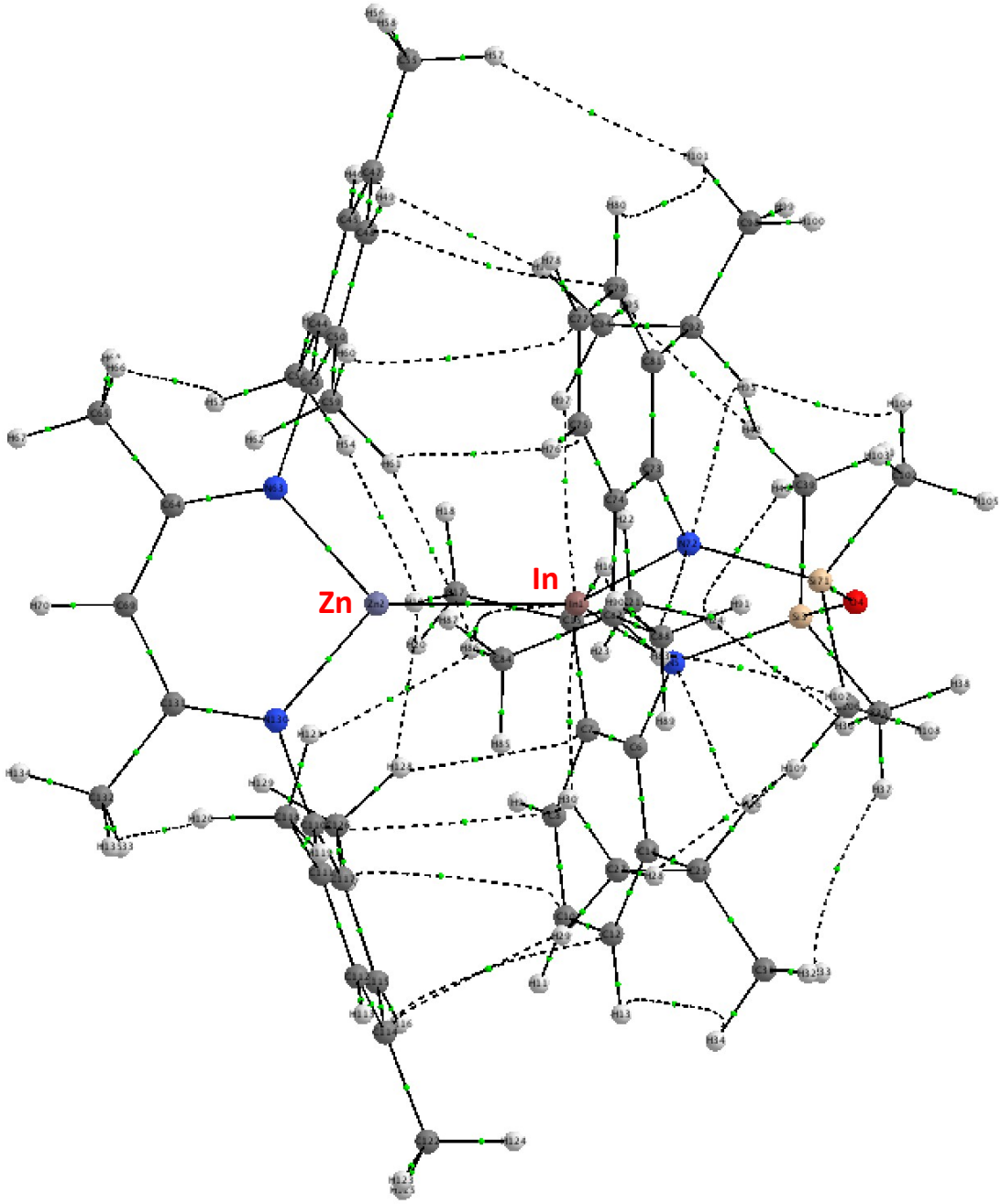


**Figure S26** Laplacian of the electron density of compound **1** (shown in the plane of Zn, In and the ring system connected to Zn)

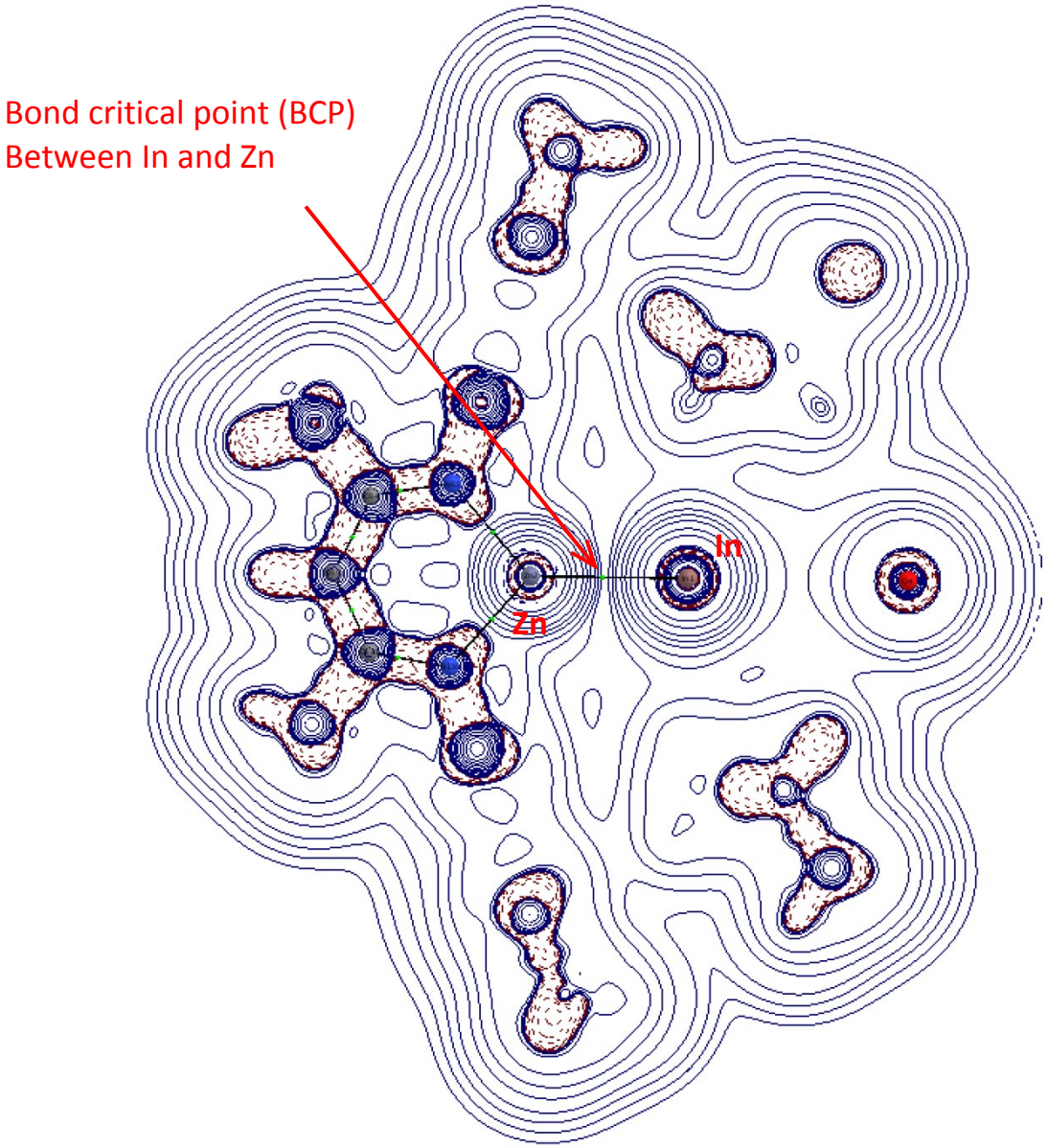


**Figure S27** Molecular graph of (NON$^{Dipp}$)In–($\mu$-NMes)–Zn(BDI$^{Mes}$) (**5**). Solid lines between the atoms are bond paths (very long bond paths are shown with dotted lines). Small green spheres are bond critical points.

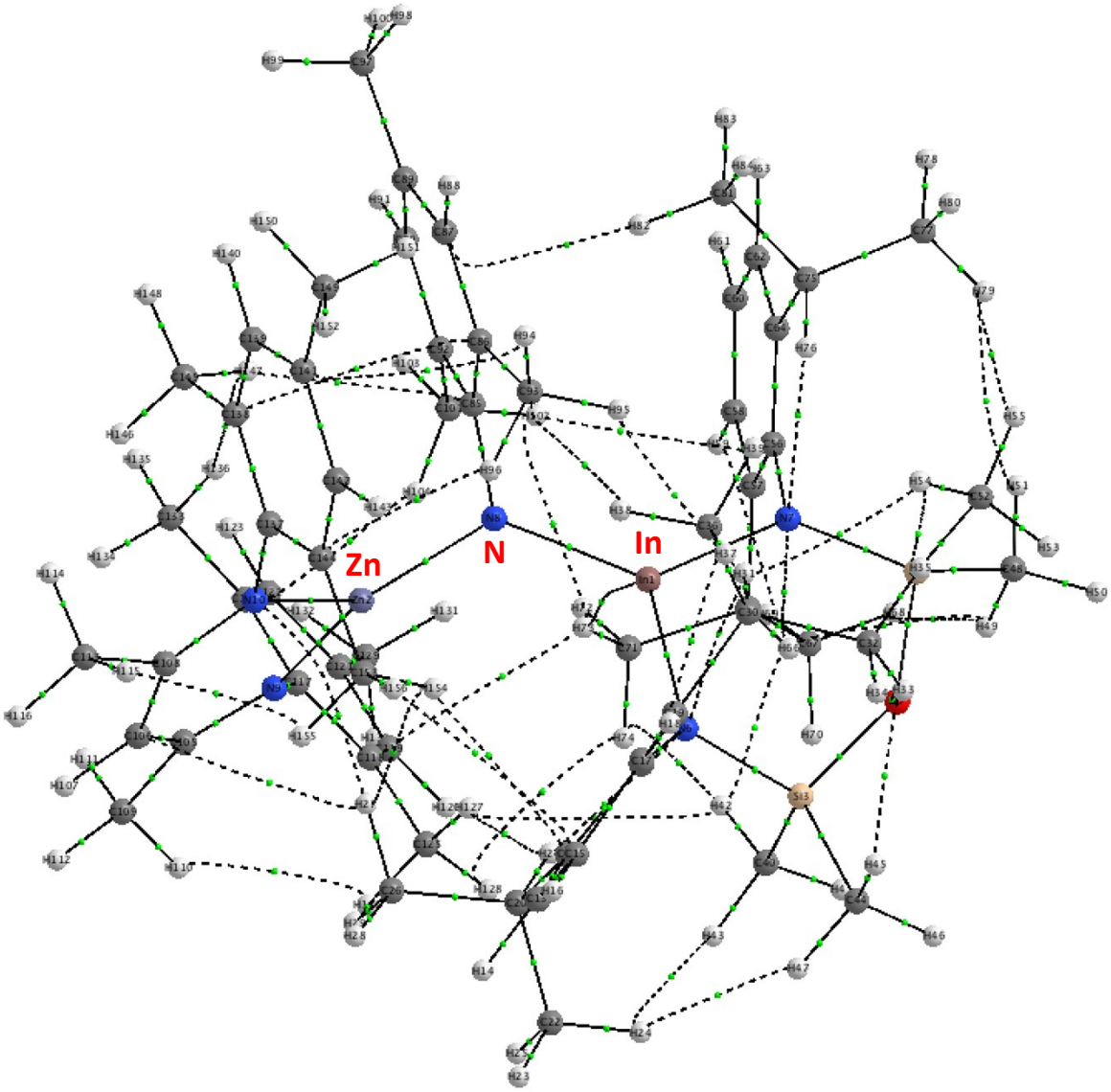


**Figure S28** Top: Laplacian of the electron density of compound **5** (shown in the plane of Zn, N and In). Bottom: expansion of Zn-N-In area.

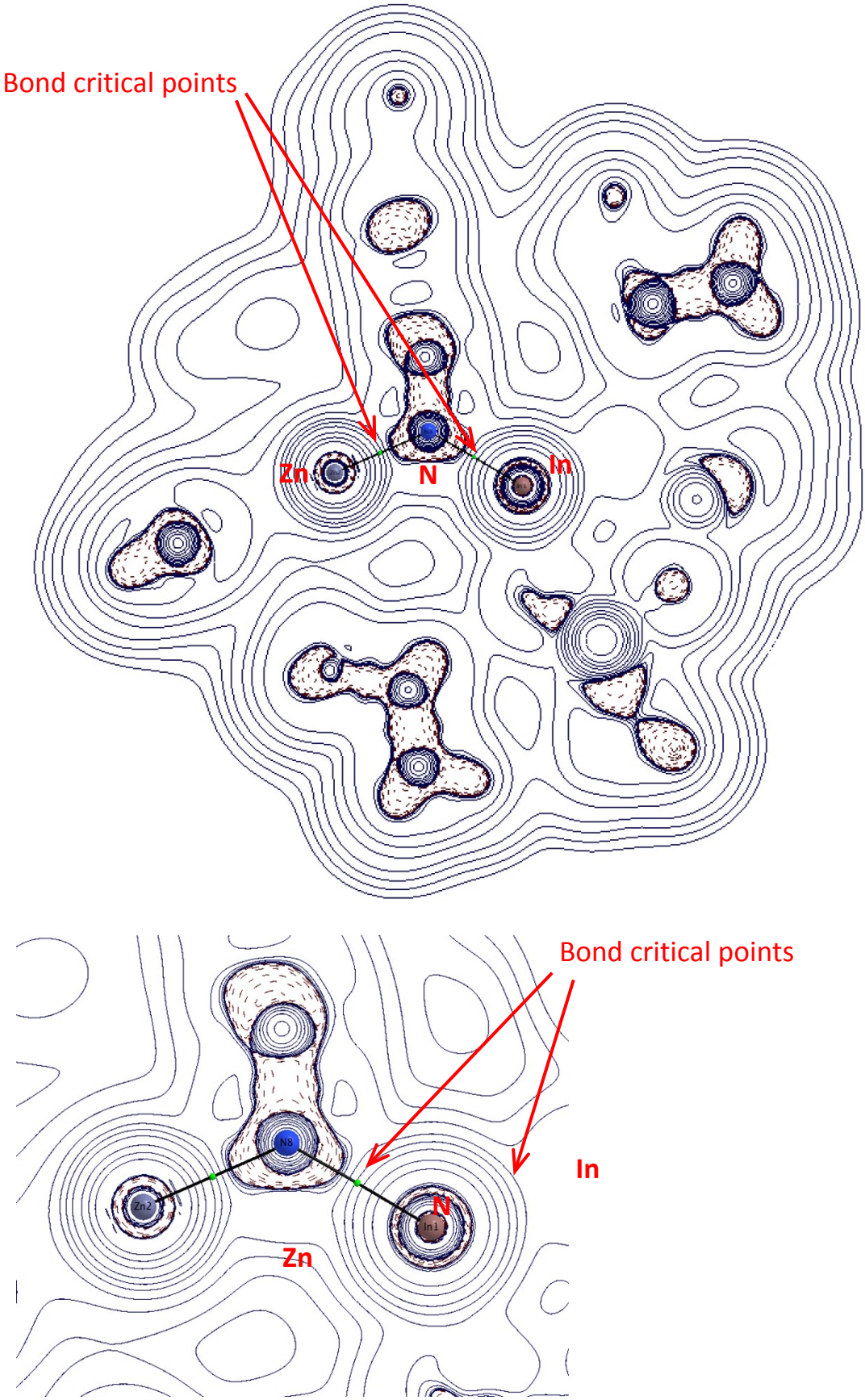


**Figure S29** HOMO of (NON$^{Dipp}$)In–($\mu$-NMes)–Zn(BDI$^{Mes}$) (**5**).

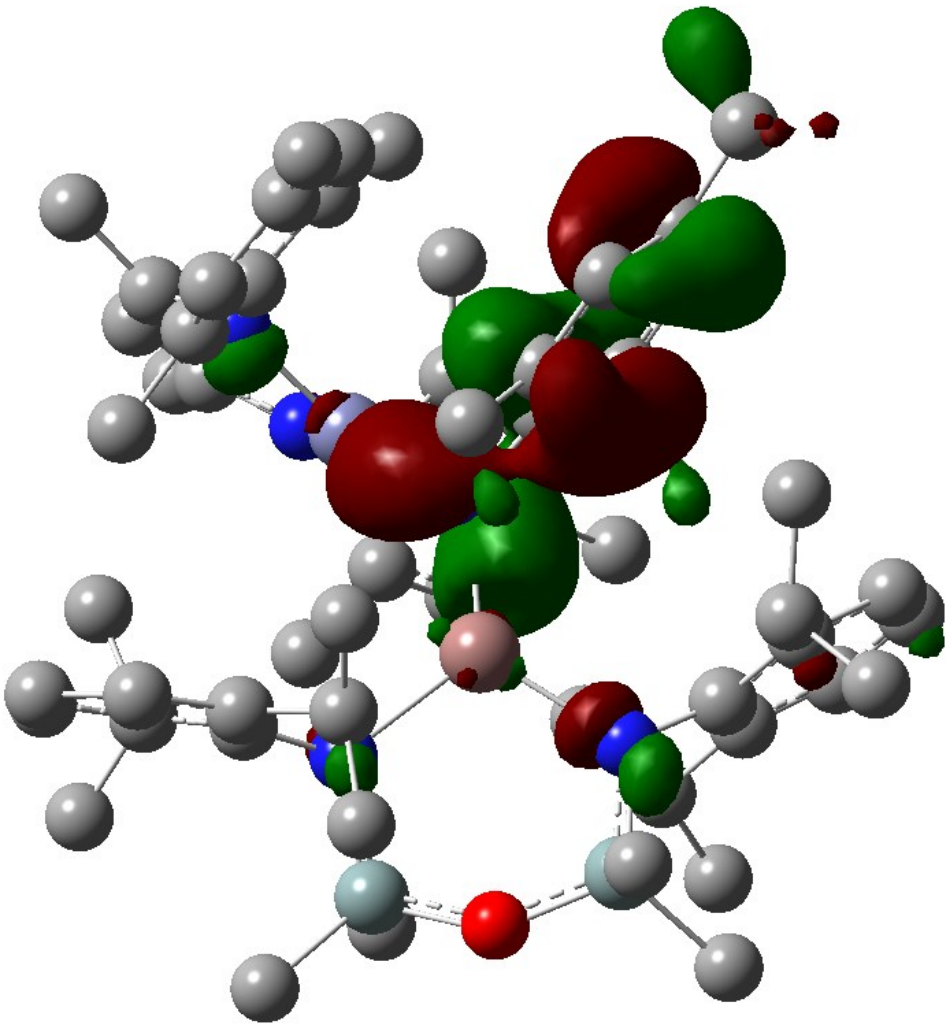
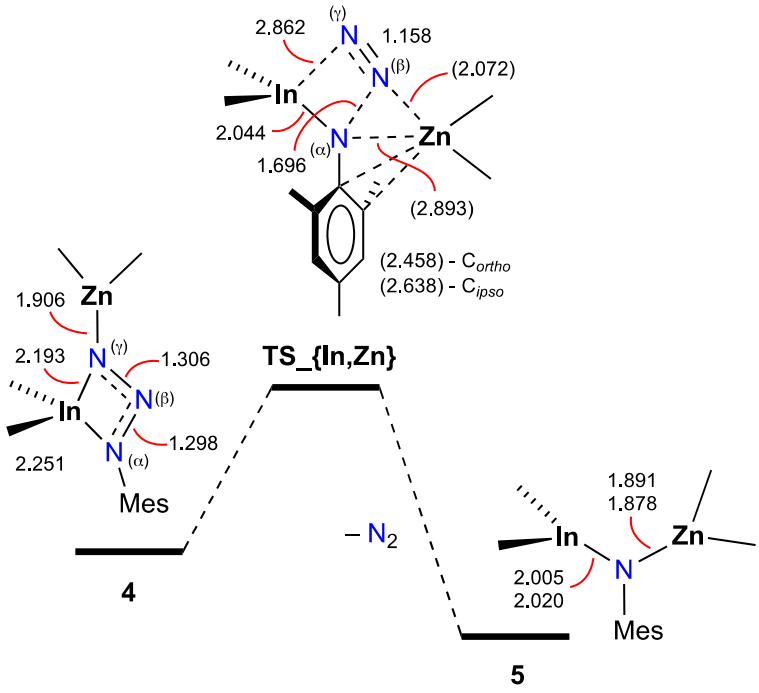


**Figure S30** Parameters associated with **TS_{In,Zn}**




Values (Å) listed for compounds **4** and **5** (2 molecules in asymmetric unit) taken from X-ray diffraction data. Values (Å) listed for **TS_{In,Zn}** from DFT calculation.

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**Cartesian (*x*, *y*, *z*) coordinates**

**(NON$^{Dipp}$)In–Zn(BDI$^{Mes}$) (1)**

| | | | |
|---|---|---|---|
| In | -0.045000 | -0.703000 | -0.041000 |
| Zn | 0.131000 | 1.846000 | -0.107000 |
| Si | -0.895000 | -3.664000 | -1.372000 |
| O | -0.279000 | -4.267000 | 0.054000 |
| N | -1.307000 | -1.986000 | -1.133000 |
| C | -2.547000 | -1.482000 | -1.569000 |
| C | -2.710000 | -0.978000 | -2.883000 |
| C | -3.966000 | -0.522000 | -3.294000 |
| H | -4.091000 | -0.141000 | -4.312000 |
| C | -5.057000 | -0.540000 | -2.434000 |
| H | -6.033000 | -0.184000 | -2.771000 |
| C | -4.896000 | -1.020000 | -1.136000 |
| H | -5.754000 | -1.037000 | -0.461000 |
| C | -3.663000 | -1.496000 | -0.688000 |
| C | -1.540000 | -0.922000 | -3.843000 |
| H | -0.677000 | -1.335000 | -3.300000 |
| C | -1.195000 | 0.516000 | -4.228000 |
| H | -0.312000 | 0.548000 | -4.885000 |
| H | -0.975000 | 1.123000 | -3.335000 |
| H | -2.026000 | 1.006000 | -4.760000 |
| C | -1.774000 | -1.788000 | -5.080000 |
| H | -0.882000 | -1.799000 | -5.727000 |
| H | -2.617000 | -1.414000 | -5.682000 |
| H | -2.004000 | -2.827000 | -4.799000 |
| C | -3.499000 | -2.030000 | 0.722000 |
| H | -2.672000 | -2.754000 | 0.680000 |
| C | -3.089000 | -0.921000 | 1.689000 |
| H | -2.869000 | -1.318000 | 2.693000 |
| H | -3.879000 | -0.162000 | 1.782000 |
| H | -2.196000 | -0.369000 | 1.347000 |

| | | | |
|---|---|---|---|
| C | -4.725000 | -2.766000 | 1.250000 |
| H | -4.494000 | -3.248000 | 2.213000 |
| H | -5.059000 | -3.547000 | 0.550000 |
| H | -5.575000 | -2.086000 | 1.425000 |
| C | -2.423000 | -4.640000 | -1.824000 |
| H | -2.876000 | -4.264000 | -2.755000 |
| H | -3.183000 | -4.572000 | -1.031000 |
| H | -2.168000 | -5.702000 | -1.966000 |
| C | 0.440000 | -3.902000 | -2.669000 |
| H | 0.072000 | -3.670000 | -3.680000 |
| H | 0.797000 | -4.944000 | -2.662000 |
| H | 1.301000 | -3.249000 | -2.464000 |
| C | 2.870000 | 2.475000 | -0.999000 |
| C | 3.187000 | 2.228000 | -2.346000 |
| C | 4.464000 | 1.756000 | -2.656000 |
| H | 4.715000 | 1.569000 | -3.705000 |
| C | 5.417000 | 1.500000 | -1.667000 |
| C | 5.058000 | 1.719000 | -0.335000 |
| H | 5.777000 | 1.503000 | 0.459000 |
| C | 3.795000 | 2.198000 | 0.021000 |
| C | 2.166000 | 2.467000 | -3.418000 |
| H | 2.547000 | 2.166000 | -4.403000 |
| H | 1.864000 | 3.525000 | -3.480000 |
| H | 1.245000 | 1.897000 | -3.220000 |
| C | 6.762000 | 0.935000 | -2.018000 |
| H | 7.091000 | 1.258000 | -3.017000 |
| H | 6.733000 | -0.168000 | -2.026000 |
| H | 7.530000 | 1.235000 | -1.290000 |
| C | 3.423000 | 2.413000 | 1.456000 |
| H | 4.279000 | 2.233000 | 2.118000 |
| H | 2.629000 | 1.711000 | 1.761000 |
| H | 3.042000 | 3.430000 | 1.637000 |

| | | | |
|---|---|---|---|
| N | 1.603000 | 3.025000 | -0.661000 |
| C | 1.469000 | 4.350000 | -0.679000 |
| C | 2.660000 | 5.196000 | -1.046000 |
| H | 3.490000 | 5.008000 | -0.348000 |
| H | 2.411000 | 6.263000 | -1.023000 |
| H | 3.040000 | 4.938000 | -2.045000 |
| C | 0.283000 | 5.035000 | -0.366000 |
| H | 0.328000 | 6.117000 | -0.477000 |
| Si | 0.502000 | -3.724000 | 1.418000 |
| N | 1.035000 | -2.087000 | 1.125000 |
| C | 2.256000 | -1.631000 | 1.666000 |
| C | 2.309000 | -1.044000 | 2.955000 |
| C | 3.534000 | -0.596000 | 3.456000 |
| H | 3.573000 | -0.141000 | 4.450000 |
| C | 4.704000 | -0.721000 | 2.716000 |
| H | 5.655000 | -0.371000 | 3.125000 |
| C | 4.655000 | -1.304000 | 1.453000 |
| H | 5.576000 | -1.406000 | 0.875000 |
| C | 3.453000 | -1.767000 | 0.914000 |
| C | 1.044000 | -0.875000 | 3.771000 |
| H | 0.277000 | -1.489000 | 3.280000 |
| C | 0.548000 | 0.568000 | 3.723000 |
| H | -0.402000 | 0.682000 | 4.269000 |
| H | 0.369000 | 0.884000 | 2.682000 |
| H | 1.281000 | 1.265000 | 4.160000 |
| C | 1.189000 | -1.369000 | 5.207000 |
| H | 0.220000 | -1.328000 | 5.730000 |
| H | 1.899000 | -0.757000 | 5.786000 |
| H | 1.548000 | -2.409000 | 5.235000 |
| C | 3.410000 | -2.391000 | -0.466000 |
| H | 2.540000 | -3.063000 | -0.474000 |
| C | 3.175000 | -1.328000 | -1.535000 |

| | | | |
|---|---|---|---|
| H | 3.089000 | -1.774000 | -2.539000 |
| H | 3.994000 | -0.597000 | -1.550000 |
| H | 2.256000 | -0.746000 | -1.350000 |
| C | 4.642000 | -3.224000 | -0.803000 |
| H | 4.489000 | -3.762000 | -1.752000 |
| H | 4.853000 | -3.967000 | -0.019000 |
| H | 5.542000 | -2.601000 | -0.926000 |
| C | 1.963000 | -4.834000 | 1.787000 |
| H | 2.539000 | -4.453000 | 2.645000 |
| H | 2.646000 | -4.910000 | 0.928000 |
| H | 1.610000 | -5.847000 | 2.033000 |
| C | -0.734000 | -3.887000 | 2.823000 |
| H | -0.267000 | -3.708000 | 3.804000 |
| H | -1.153000 | -4.906000 | 2.825000 |
| H | -1.570000 | -3.180000 | 2.709000 |
| C | -2.441000 | 2.876000 | 0.891000 |
| C | -2.633000 | 2.921000 | 2.283000 |
| C | -3.882000 | 2.563000 | 2.797000 |
| H | -4.033000 | 2.592000 | 3.880000 |
| C | -4.940000 | 2.177000 | 1.970000 |
| C | -4.717000 | 2.144000 | 0.591000 |
| H | -5.524000 | 1.834000 | -0.078000 |
| C | -3.482000 | 2.477000 | 0.034000 |
| C | -1.534000 | 3.388000 | 3.191000 |
| H | -1.709000 | 3.062000 | 4.226000 |
| H | -1.460000 | 4.489000 | 3.200000 |
| H | -0.554000 | 3.015000 | 2.867000 |
| C | -6.259000 | 1.750000 | 2.544000 |
| H | -6.426000 | 2.179000 | 3.542000 |
| H | -6.305000 | 0.652000 | 2.647000 |
| H | -7.097000 | 2.049000 | 1.896000 |
| C | -3.258000 | 2.403000 | -1.445000 |

| | | | |
|---|---|---|---|
| H | -4.205000 | 2.270000 | -1.983000 |
| H | -2.630000 | 1.533000 | -1.697000 |
| H | -2.749000 | 3.297000 | -1.835000 |
| N | -1.182000 | 3.242000 | 0.340000 |
| C | -0.941000 | 4.530000 | 0.104000 |
| C | -2.040000 | 5.531000 | 0.344000 |
| H | -2.929000 | 5.270000 | -0.250000 |
| H | -1.718000 | 6.544000 | 0.080000 |
| H | -2.363000 | 5.522000 | 1.395000 |

**(NON$^{Dipp}$)In–($\mu$-N$_3$Mes)–Zn(BDI$^{Mes}$) (4)**

| | | | |
|---|---|---|---|
| In | 1.22103400 | -0.58886900 | -0.36365000 |
| Zn | -2.57463900 | 0.94496100 | -0.24333800 |
| Si | 2.24765600 | -3.63871900 | -1.15114600 |
| O | 3.18710700 | -2.69957600 | -2.15138900 |
| N | 1.65396600 | -2.58699500 | 0.10680600 |
| C | 1.38270500 | -3.05682200 | 1.41374100 |
| C | 0.11345000 | -3.59175900 | 1.74687800 |
| C | -0.13763200 | -4.00702600 | 3.05818000 |
| H | -1.12302600 | -4.40908000 | 3.31023200 |
| C | 0.83683000 | -3.91308000 | 4.04370600 |
| H | 0.62264000 | -4.23228800 | 5.06652500 |
| C | 2.09353800 | -3.41831200 | 3.71089400 |
| H | 2.86700800 | -3.35950300 | 4.48055700 |
| C | 2.39256900 | -3.00484500 | 2.41070300 |
| C | -0.98108000 | -3.71257200 | 0.71013800 |
| H | -0.54710000 | -3.38320700 | -0.24357600 |
| C | -2.15442200 | -2.79040500 | 1.01501200 |
| H | -2.90942800 | -2.85332800 | 0.21868100 |
| H | -1.82496800 | -1.74436000 | 1.08983500 |
| H | -2.64733900 | -3.06117000 | 1.96226700 |
| C | -1.45149100 | -5.15554600 | 0.53609100 |
| H | -2.17687500 | -5.22851900 | -0.29029500 |
| H | -1.94752300 | -5.53055600 | 1.44606400 |
| H | -0.61099300 | -5.83192500 | 0.31755000 |
| C | 3.78458000 | -2.50349700 | 2.08238200 |
| H | 3.87713800 | -2.54729800 | 0.98777400 |
| C | 3.95174100 | -1.04258700 | 2.48920400 |
| H | 4.95681400 | -0.66807500 | 2.23666200 |
| H | 3.79560400 | -0.90363500 | 3.57075900 |
| H | 3.21471100 | -0.40551700 | 1.98304600 |
| C | 4.88940000 | -3.37169300 | 2.67723400 |

| | | | |
|---|---|---|---|
| H | 5.87178800 | -3.05288100 | 2.29462800 |
| H | 4.74982200 | -4.43276400 | 2.42121400 |
| H | 4.92980200 | -3.29453600 | 3.77538700 |
| C | 3.25512000 | -5.03775700 | -0.42818600 |
| H | 2.68827500 | -5.56138200 | 0.35777100 |
| H | 4.19106400 | -4.66898500 | 0.01592500 |
| H | 3.51162800 | -5.76688900 | -1.21225000 |
| C | 0.91092600 | -4.35437600 | -2.26078900 |
| H | 0.31434200 | -5.12347900 | -1.74819200 |
| H | 1.37837100 | -4.81601700 | -3.14515000 |
| H | 0.22206500 | -3.57222400 | -2.61583600 |
| C | -4.85332500 | -0.89299600 | -0.32717500 |
| C | -5.13688800 | -1.39246700 | 0.95809600 |
| C | -5.53157000 | -2.72329600 | 1.08862900 |
| H | -5.74922500 | -3.11216800 | 2.08788400 |
| C | -5.61636400 | -3.58022900 | -0.01236700 |
| C | -5.31876500 | -3.05922000 | -1.27271700 |
| H | -5.37961700 | -3.71115300 | -2.14940200 |
| C | -4.94876000 | -1.72293800 | -1.45505300 |
| C | -4.96680200 | -0.51504300 | 2.16271900 |
| H | -5.27279400 | -1.03803200 | 3.07865400 |
| H | -5.54435700 | 0.41947300 | 2.08847100 |
| H | -3.91075500 | -0.21866800 | 2.28535200 |
| C | -5.95719200 | -5.03066800 | 0.16708600 |
| H | -6.68376900 | -5.17813000 | 0.97955300 |
| H | -5.05569300 | -5.61165400 | 0.42584300 |
| H | -6.37579600 | -5.46602800 | -0.75155500 |
| C | -4.69333800 | -1.17750000 | -2.82759500 |
| H | -4.42128600 | -1.97584000 | -3.53152800 |
| H | -3.89168200 | -0.42810700 | -2.81899100 |
| H | -5.58892500 | -0.67392800 | -3.23015500 |
| N | -4.44167400 | 0.46183100 | -0.45572300 |

| | | | |
|---|---|---|---|
| C | -5.37968500 | 1.40931500 | -0.57271400 |
| C | -6.81252300 | 0.97489700 | -0.73105100 |
| H | -6.92356500 | 0.26820600 | -1.56580100 |
| H | -7.46956500 | 1.83597500 | -0.89927400 |
| H | -7.15412300 | 0.44168300 | 0.16945000 |
| C | -5.14193800 | 2.78950000 | -0.52574000 |
| H | -6.01995500 | 3.41723900 | -0.67016900 |
| Si | 3.69989600 | -1.13633100 | -2.41471400 |
| N | 2.39335600 | -0.04240400 | -2.01847200 |
| C | 1.92088000 | 0.91255300 | -2.94631500 |
| C | 2.53281900 | 2.19041500 | -3.04370800 |
| C | 2.05291100 | 3.11125400 | -3.97926600 |
| H | 2.53224800 | 4.09079900 | -4.05600000 |
| C | 0.98302600 | 2.81014300 | -4.81420900 |
| H | 0.61867700 | 3.54666700 | -5.53437400 |
| C | 0.39143600 | 1.55531200 | -4.73033800 |
| H | -0.43559400 | 1.30522300 | -5.40089600 |
| C | 0.85214100 | 0.59444100 | -3.82650500 |
| C | 3.73309000 | 2.55172900 | -2.19099900 |
| H | 3.77692900 | 1.79882500 | -1.38964900 |
| C | 3.61262600 | 3.92810400 | -1.54433000 |
| H | 4.44698200 | 4.09927200 | -0.84631200 |
| H | 2.67473200 | 4.02363700 | -0.98331300 |
| H | 3.64459300 | 4.73656700 | -2.29244400 |
| C | 5.03119400 | 2.46530400 | -2.99642700 |
| H | 5.90258800 | 2.68561700 | -2.35884200 |
| H | 5.02646200 | 3.19454200 | -3.82282000 |
| H | 5.17895700 | 1.47055400 | -3.43783700 |
| C | 0.22489600 | -0.78553200 | -3.83287400 |
| H | 0.83967900 | -1.41332100 | -3.17127500 |
| C | -1.19923000 | -0.76680100 | -3.28263000 |
| H | -1.62445000 | -1.78219600 | -3.23840100 |

| | | | |
|---|---|---|---|
| H | -1.85602000 | -0.15519300 | -3.92170200 |
| H | -1.23333400 | -0.34632100 | -2.26603500 |
| C | 0.26016600 | -1.43434800 | -5.21536400 |
| H | -0.09051800 | -2.47709200 | -5.16063000 |
| H | 1.27957500 | -1.43872100 | -5.62727400 |
| H | -0.38676100 | -0.90338800 | -5.93181500 |
| C | 4.12820500 | -1.02351900 | -4.23181500 |
| H | 4.12676800 | 0.00733700 | -4.61297700 |
| H | 3.38437000 | -1.59709500 | -4.80470700 |
| H | 5.11681700 | -1.46859700 | -4.42287500 |
| C | 5.17811300 | -0.86214800 | -1.29635600 |
| H | 5.67990800 | 0.09465500 | -1.50274400 |
| H | 5.91284200 | -1.67311600 | -1.41995100 |
| H | 4.86069100 | -0.85399800 | -0.24208000 |
| C | -1.65952200 | 3.64395000 | 0.39324200 |
| C | -0.79278400 | 4.18243400 | -0.56953000 |
| C | 0.30698300 | 4.92465300 | -0.13116700 |
| H | 0.96624900 | 5.37092500 | -0.88014700 |
| C | 0.59282400 | 5.09547200 | 1.22547400 |
| C | -0.26167400 | 4.50122300 | 2.15760000 |
| H | -0.03561300 | 4.58593300 | 3.22435300 |
| C | -1.39455400 | 3.78688600 | 1.76694900 |
| C | -1.01883700 | 3.92206100 | -2.02826000 |
| H | -0.32889000 | 4.50747600 | -2.64888400 |
| H | -2.04969800 | 4.14676400 | -2.34205500 |
| H | -0.83476800 | 2.86022600 | -2.26738400 |
| C | 1.78465800 | 5.88943500 | 1.67539500 |
| H | 2.56914000 | 5.91135000 | 0.90501400 |
| H | 2.21722900 | 5.46643300 | 2.59434600 |
| H | 1.50797300 | 6.93449900 | 1.89393700 |
| C | -2.29044300 | 3.14320600 | 2.78058000 |
| H | -1.92859200 | 3.32897500 | 3.80061200 |

| | | | |
|---|---|---|---|
| H | -2.31066700 | 2.05316000 | 2.62347600 |
| H | -3.32944300 | 3.50268800 | 2.70863000 |
| N | -2.78550100 | 2.88508200 | -0.02155800 |
| C | -3.95293800 | 3.48009300 | -0.20762600 |
| C | -4.04306600 | 4.97305800 | -0.04972800 |
| H | -3.77104200 | 5.26488600 | 0.97609400 |
| H | -5.05287300 | 5.33942700 | -0.26849200 |
| H | -3.32262100 | 5.47734800 | -0.71066800 |
| N | -0.78940200 | 0.29513200 | 0.07638000 |
| N | 0.79067900 | 0.64438600 | 1.50159400 |
| N | -0.44547900 | 0.80822300 | 1.19446500 |
| C | 2.78333200 | 2.46207000 | 4.01332900 |
| C | 2.21413000 | 2.03811400 | 5.21757900 |
| C | 2.31158400 | 2.01358400 | 2.77997900 |
| C | 1.15880300 | 1.12466500 | 5.15917300 |
| C | 1.23408400 | 1.11151100 | 2.75544200 |
| C | 0.65774400 | 0.63948600 | 3.94843300 |
| H | 0.71789700 | 0.75741900 | 6.09095200 |
| C | 2.71220500 | 2.56235000 | 6.53344300 |
| H | 3.79268500 | 2.76651100 | 6.50391000 |
| H | 2.20967800 | 3.50772400 | 6.79977400 |
| H | 2.52086600 | 1.85065000 | 7.34965200 |
| C | 2.92687100 | 2.47259000 | 1.49669000 |
| H | 3.41332200 | 1.64116000 | 0.95954800 |
| H | 3.68630000 | 3.24615400 | 1.67163300 |
| C | -0.43216700 | -0.38951800 | 3.92904200 |
| H | -0.59492600 | -0.80322000 | 4.93325100 |
| H | -1.38504700 | 0.03072800 | 3.57191100 |
| H | -0.17626700 | -1.22242200 | 3.25662100 |
| H | 3.62221800 | 3.16468400 | 4.03176100 |
| H | 2.16083000 | 2.88105200 | 0.82364300 |

**(NON$^{Dipp}$)In–($\mu$-NMes)–Zn(BDI$^{Mes}$) (5)**

| | | | |
|---|---|---|---|
| In | 0.000000 | 0.000000 | 0.000000 |
| Zn | -3.240151 | 1.255596 | -0.262623 |
| Si | 1.494384 | -1.284068 | -2.549458 |
| Si | 3.232334 | -0.653115 | 0.019343 |
| O | 2.755058 | -1.257942 | -1.459995 |
| N | -0.000170 | -1.299577 | -1.637198 |
| N | 1.958121 | 0.404635 | 0.582167 |
| N | -1.634234 | 0.954356 | 0.697964 |
| N | -3.844800 | 2.650471 | -1.508196 |
| N | -4.965085 | 0.330163 | -0.035337 |
| C | -0.950278 | -2.318487 | -1.871711 |
| C | -1.865811 | -2.207291 | -2.950508 |
| C | -2.661937 | -3.301671 | -3.299006 |
| H | -3.342497 | -3.215886 | -4.150585 |
| C | -2.611425 | -4.488936 | -2.581292 |
| H | -3.229992 | -5.340910 | -2.872948 |
| C | -1.784974 | -4.567946 | -1.466859 |
| H | -1.768939 | -5.488364 | -0.878399 |
| C | -0.961183 | -3.504220 | -1.088391 |
| C | -2.031874 | -0.911813 | -3.717053 |
| H | -1.343013 | -0.189281 | -3.254372 |
| C | -1.650371 | -1.040941 | -5.190136 |
| H | -2.318123 | -1.740625 | -5.717947 |
| H | -0.622320 | -1.411913 | -5.311285 |
| H | -1.721726 | -0.066190 | -5.698757 |
| C | -3.458359 | -0.382379 | -3.568884 |
| H | -3.729859 | -0.224074 | -2.514391 |
| H | -4.194292 | -1.087937 | -3.984981 |
| H | -3.586955 | 0.575183 | -4.093384 |
| C | -0.077034 | -3.673564 | 0.130980 |
| H | 0.246121 | -2.664915 | 0.443963 |

| | | | |
|---|---|---|---|
| C | 1.189423 | -4.464456 | -0.199357 |
| H | 1.838252 | -3.915988 | -0.895257 |
| H | 0.928015 | -5.431362 | -0.657988 |
| H | 1.775120 | -4.668859 | 0.709907 |
| C | -0.819201 | -4.303959 | 1.308466 |
| H | -1.012178 | -5.374982 | 1.139741 |
| H | -1.785912 | -3.812531 | 1.490249 |
| H | -0.215915 | -4.226619 | 2.226353 |
| C | 1.625604 | 0.266800 | -3.595876 |
| H | 2.646290 | 0.385420 | -3.992043 |
| H | 1.386896 | 1.165241 | -3.008234 |
| H | 0.926996 | 0.230743 | -4.445626 |
| C | 1.649710 | -2.803324 | -3.622738 |
| H | 1.540580 | -3.727729 | -3.038654 |
| H | 2.639300 | -2.811560 | -4.105410 |
| H | 0.880549 | -2.816975 | -4.408938 |
| C | 4.831980 | 0.294048 | -0.169838 |
| H | 4.765655 | 1.031440 | -0.982959 |
| H | 5.657050 | -0.397442 | -0.400721 |
| H | 5.081994 | 0.832543 | 0.757805 |
| C | 3.501430 | -2.138979 | 1.128018 |
| H | 4.082698 | -2.908233 | 0.596361 |
| H | 2.543698 | -2.586550 | 1.430808 |
| H | 4.047424 | -1.865372 | 2.041885 |
| C | 2.208309 | 1.595968 | 1.311518 |
| C | 2.410745 | 2.818309 | 0.619256 |
| C | 2.609013 | 3.996529 | 1.342374 |
| H | 2.752993 | 4.936496 | 0.803976 |
| C | 2.619126 | 3.996076 | 2.732465 |
| H | 2.765532 | 4.927361 | 3.284682 |
| C | 2.450962 | 2.795751 | 3.410600 |
| H | 2.474092 | 2.788239 | 4.503259 |

| | | | |
|---|---|---|---|
| C | 2.258911 | 1.591380 | 2.727273 |
| C | 2.367697 | 2.869094 | -0.892342 |
| H | 2.510986 | 1.837997 | -1.244685 |
| C | 3.474191 | 3.721510 | -1.505663 |
| H | 4.465152 | 3.426030 | -1.129767 |
| H | 3.339582 | 4.792794 | -1.287015 |
| H | 3.476321 | 3.612210 | -2.601712 |
| C | 0.996268 | 3.335897 | -1.371243 |
| H | 0.781378 | 4.357718 | -1.022960 |
| H | 0.177586 | 2.705759 | -0.985268 |
| H | 0.936523 | 3.337189 | -2.470215 |
| C | 2.164509 | 0.304967 | 3.518700 |
| H | 1.867870 | -0.480822 | 2.807528 |
| C | 3.535434 | -0.064278 | 4.089412 |
| H | 3.852576 | 0.671708 | 4.845758 |
| H | 4.310053 | -0.081940 | 3.308293 |
| H | 3.510256 | -1.054044 | 4.572946 |
| C | 1.114434 | 0.365860 | 4.623469 |
| H | 0.136160 | 0.676641 | 4.234559 |
| H | 1.399408 | 1.076198 | 5.415865 |
| H | 0.995587 | -0.620842 | 5.099183 |
| C | -1.804533 | 1.239665 | 2.065320 |
| C | -2.094515 | 0.214658 | 2.998693 |
| C | -2.430055 | 0.542680 | 4.313510 |
| H | -2.675194 | -0.267210 | 5.007595 |
| C | -2.451231 | 1.862731 | 4.765584 |
| C | -2.064518 | 2.858091 | 3.863759 |
| H | -2.012315 | 3.897245 | 4.204330 |
| C | -1.724406 | 2.574950 | 2.539230 |
| C | -1.982860 | -1.214396 | 2.580718 |
| H | -2.302886 | -1.896616 | 3.379286 |
| H | -0.931658 | -1.468853 | 2.340809 |

| | | | |
|---|---|---|---|
| H | -2.577057 | -1.428127 | 1.682214 |
| C | -2.872046 | 2.200980 | 6.166225 |
| H | -2.678746 | 1.367762 | 6.857991 |
| H | -3.951989 | 2.423617 | 6.217607 |
| H | -2.341293 | 3.087338 | 6.544756 |
| C | -1.211562 | 3.654565 | 1.639828 |
| H | -0.122598 | 3.544398 | 1.506286 |
| H | -1.399794 | 4.653377 | 2.057878 |
| H | -1.649059 | 3.606957 | 0.634634 |
| C | -5.042357 | 2.575351 | -2.090225 |
| C | -6.002367 | 1.587674 | -1.820027 |
| H | -6.922608 | 1.664017 | -2.397343 |
| C | -6.012161 | 0.617261 | -0.798664 |
| C | -5.433972 | 3.647283 | -3.072947 |
| H | -4.647984 | 3.799964 | -3.826431 |
| H | -5.558386 | 4.613320 | -2.559673 |
| H | -6.374662 | 3.396182 | -3.577049 |
| C | -7.315239 | -0.091278 | -0.544832 |
| H | -7.679217 | 0.147411 | 0.466591 |
| H | -7.189697 | -1.182927 | -0.574277 |
| H | -8.078051 | 0.204960 | -1.274281 |
| C | -3.101018 | 3.852684 | -1.651571 |
| C | -2.106723 | 3.974709 | -2.635731 |
| C | -1.408143 | 5.179124 | -2.737537 |
| H | -0.637918 | 5.274689 | -3.508614 |
| C | -1.649632 | 6.251814 | -1.877187 |
| C | -2.633177 | 6.096596 | -0.897946 |
| H | -2.834907 | 6.919293 | -0.205508 |
| C | -3.366016 | 4.915615 | -0.767741 |
| C | -1.805533 | 2.830787 | -3.553541 |
| H | -2.654142 | 2.604311 | -4.218352 |
| H | -1.605028 | 1.909641 | -2.986221 |

| | | | |
|---|---|---|---|
| H | -0.930926 | 3.042013 | -4.183191 |
| C | -0.840032 | 7.512156 | -1.974383 |
| H | -0.621539 | 7.772590 | -3.020668 |
| H | 0.128898 | 7.396895 | -1.459607 |
| H | -1.358432 | 8.363323 | -1.510396 |
| C | -4.394124 | 4.761008 | 0.313572 |
| H | -5.386789 | 4.502213 | -0.087265 |
| H | -4.490806 | 5.684623 | 0.899830 |
| H | -4.119402 | 3.950378 | 1.008979 |
| C | -5.115803 | -0.588478 | 1.038940 |
| C | -5.376422 | -0.096781 | 2.329439 |
| C | -5.492152 | -1.009011 | 3.380593 |
| H | -5.688336 | -0.625141 | 4.386052 |
| C | -5.352155 | -2.384355 | 3.187202 |
| C | -5.090326 | -2.841548 | 1.893405 |
| H | -4.968024 | -3.914418 | 1.716056 |
| C | -4.960101 | -1.967438 | 0.812287 |
| C | -5.483317 | 1.377700 | 2.578762 |
| H | -6.122250 | 1.880757 | 1.837425 |
| H | -4.486652 | 1.850562 | 2.531294 |
| H | -5.885185 | 1.579100 | 3.580772 |
| C | -5.429152 | -3.338848 | 4.343420 |
| H | -6.090671 | -2.961271 | 5.136666 |
| H | -4.433674 | -3.491628 | 4.794460 |
| H | -5.798211 | -4.326192 | 4.029677 |
| C | -4.604466 | -2.481663 | -0.547440 |
| H | -3.583572 | -2.177812 | -0.830313 |
| H | -5.268145 | -2.097085 | -1.336013 |
| H | -4.632586 | -3.577848 | -0.578693 |

**TS_{In,Zn}**

| | | | |
|---|---|---|---|
| In | -1.887000 | 0.263000 | -0.048000 |
| Zn | 2.781000 | -0.491000 | 0.400000 |
| Si | -4.708000 | -0.162000 | 1.445000 |
| Si | -4.542000 | 2.033000 | -0.848000 |
| O | -5.111000 | 0.877000 | 0.206000 |
| N | -3.237000 | -0.962000 | 0.940000 |
| N | -2.800000 | 2.022000 | -0.704000 |
| N | 0.075000 | -0.053000 | -0.525000 |
| N | 4.294000 | 0.209000 | 1.434000 |
| N | 3.319000 | -2.375000 | 0.308000 |
| C | -2.985000 | -2.339000 | 1.100000 |
| C | -2.703000 | -2.887000 | 2.379000 |
| C | -2.569000 | -4.273000 | 2.515000 |
| H | -2.374000 | -4.691000 | 3.506000 |
| C | -2.662000 | -5.121000 | 1.422000 |
| H | -2.559000 | -6.202000 | 1.548000 |
| C | -2.867000 | -4.578000 | 0.157000 |
| H | -2.918000 | -5.247000 | -0.704000 |
| C | -3.025000 | -3.203000 | -0.031000 |
| C | -2.532000 | -2.015000 | 3.607000 |
| H | -2.561000 | -0.972000 | 3.260000 |
| C | -3.660000 | -2.228000 | 4.617000 |
| H | -3.650000 | -3.258000 | 5.009000 |
| H | -4.651000 | -2.057000 | 4.173000 |
| H | -3.550000 | -1.546000 | 5.475000 |
| C | -1.173000 | -2.229000 | 4.272000 |
| H | -0.353000 | -2.026000 | 3.571000 |
| H | -1.063000 | -3.256000 | 4.656000 |
| H | -1.056000 | -1.543000 | 5.127000 |
| C | -3.253000 | -2.657000 | -1.430000 |
| H | -2.661000 | -1.722000 | -1.513000 |

| | | | |
|---|---|---|---|
| C | -4.714000 | -2.284000 | -1.682000 |
| H | -5.046000 | -1.466000 | -1.031000 |
| H | -5.365000 | -3.155000 | -1.508000 |
| H | -4.856000 | -1.959000 | -2.725000 |
| C | -2.751000 | -3.578000 | -2.537000 |
| H | -3.387000 | -4.471000 | -2.638000 |
| H | -1.719000 | -3.911000 | -2.358000 |
| H | -2.777000 | -3.053000 | -3.504000 |
| C | -4.503000 | 0.912000 | 2.970000 |
| H | -5.343000 | 1.622000 | 3.034000 |
| H | -3.570000 | 1.495000 | 2.922000 |
| H | -4.482000 | 0.322000 | 3.898000 |
| C | -6.094000 | -1.393000 | 1.675000 |
| H | -6.417000 | -1.805000 | 0.709000 |
| H | -6.960000 | -0.905000 | 2.149000 |
| H | -5.781000 | -2.235000 | 2.310000 |
| C | -5.221000 | 3.719000 | -0.413000 |
| H | -5.051000 | 3.953000 | 0.649000 |
| H | -6.304000 | 3.762000 | -0.605000 |
| H | -4.733000 | 4.503000 | -1.014000 |
| C | -5.174000 | 1.494000 | -2.528000 |
| H | -6.261000 | 1.328000 | -2.474000 |
| H | -4.706000 | 0.545000 | -2.831000 |
| H | -4.978000 | 2.239000 | -3.312000 |
| C | -1.987000 | 3.160000 | -0.924000 |
| C | -1.646000 | 4.006000 | 0.165000 |
| C | -0.815000 | 5.108000 | -0.051000 |
| H | -0.550000 | 5.750000 | 0.792000 |
| C | -0.319000 | 5.402000 | -1.317000 |
| H | 0.332000 | 6.267000 | -1.468000 |
| C | -0.661000 | 4.583000 | -2.385000 |
| H | -0.275000 | 4.812000 | -3.382000 |

| | | | |
|---|---|---|---|
| C | -1.488000 | 3.468000 | -2.215000 |
| C | -2.137000 | 3.707000 | 1.566000 |
| H | -2.980000 | 3.011000 | 1.455000 |
| C | -2.652000 | 4.939000 | 2.303000 |
| H | -3.401000 | 5.480000 | 1.705000 |
| H | -1.842000 | 5.645000 | 2.545000 |
| H | -3.121000 | 4.645000 | 3.255000 |
| C | -1.057000 | 2.993000 | 2.378000 |
| H | -0.156000 | 3.621000 | 2.475000 |
| H | -0.738000 | 2.049000 | 1.909000 |
| H | -1.413000 | 2.746000 | 3.391000 |
| C | -1.845000 | 2.633000 | -3.427000 |
| H | -2.439000 | 1.784000 | -3.058000 |
| C | -2.711000 | 3.430000 | -4.403000 |
| H | -2.142000 | 4.264000 | -4.845000 |
| H | -3.589000 | 3.865000 | -3.902000 |
| H | -3.066000 | 2.793000 | -5.228000 |
| C | -0.609000 | 2.072000 | -4.127000 |
| H | 0.025000 | 1.506000 | -3.431000 |
| H | 0.010000 | 2.873000 | -4.561000 |
| H | -0.899000 | 1.398000 | -4.949000 |
| C | 1.036000 | 0.160000 | -1.468000 |
| C | 1.184000 | -0.681000 | -2.613000 |
| C | 2.269000 | -0.504000 | -3.458000 |
| H | 2.357000 | -1.151000 | -4.337000 |
| C | 3.269000 | 0.455000 | -3.216000 |
| C | 3.118000 | 1.283000 | -2.110000 |
| H | 3.839000 | 2.086000 | -1.935000 |
| C | 2.017000 | 1.180000 | -1.232000 |
| C | 0.125000 | -1.692000 | -2.896000 |
| H | 0.412000 | -2.361000 | -3.717000 |
| H | -0.823000 | -1.198000 | -3.169000 |

| | | | |
|---|---|---|---|
| H | -0.073000 | -2.293000 | -1.998000 |
| C | 4.452000 | 0.575000 | -4.130000 |
| H | 5.049000 | 1.468000 | -3.898000 |
| H | 4.141000 | 0.637000 | -5.184000 |
| H | 5.114000 | -0.302000 | -4.041000 |
| C | 1.706000 | 2.331000 | -0.310000 |
| H | 0.833000 | 2.873000 | -0.709000 |
| H | 2.552000 | 3.029000 | -0.256000 |
| H | 1.449000 | 2.041000 | 0.714000 |
| C | 5.150000 | -0.618000 | 2.024000 |
| C | 5.122000 | -2.018000 | 1.891000 |
| H | 5.870000 | -2.554000 | 2.472000 |
| C | 4.300000 | -2.827000 | 1.081000 |
| C | 6.225000 | -0.030000 | 2.898000 |
| H | 5.784000 | 0.623000 | 3.665000 |
| H | 6.905000 | 0.603000 | 2.308000 |
| H | 6.814000 | -0.814000 | 3.390000 |
| C | 4.555000 | -4.310000 | 1.120000 |
| H | 4.747000 | -4.704000 | 0.111000 |
| H | 3.662000 | -4.837000 | 1.490000 |
| H | 5.406000 | -4.552000 | 1.767000 |
| C | 4.450000 | 1.615000 | 1.521000 |
| C | 3.697000 | 2.341000 | 2.463000 |
| C | 3.761000 | 3.734000 | 2.436000 |
| H | 3.169000 | 4.300000 | 3.162000 |
| C | 4.543000 | 4.424000 | 1.504000 |
| C | 5.301000 | 3.675000 | 0.603000 |
| H | 5.931000 | 4.193000 | -0.127000 |
| C | 5.275000 | 2.277000 | 0.595000 |
| C | 2.838000 | 1.625000 | 3.463000 |
| H | 3.430000 | 0.935000 | 4.085000 |
| H | 2.059000 | 1.012000 | 2.983000 |

| | | | |
|---|---|---|---|
| H | 2.336000 | 2.339000 | 4.130000 |
| C | 4.538000 | 5.924000 | 1.460000 |
| H | 4.558000 | 6.358000 | 2.471000 |
| H | 3.626000 | 6.299000 | 0.965000 |
| H | 5.401000 | 6.316000 | 0.903000 |
| C | 6.110000 | 1.496000 | -0.377000 |
| H | 7.003000 | 1.068000 | 0.109000 |
| H | 6.460000 | 2.133000 | -1.202000 |
| H | 5.550000 | 0.649000 | -0.800000 |
| C | 2.600000 | -3.275000 | -0.524000 |
| C | 3.094000 | -3.529000 | -1.821000 |
| C | 2.383000 | -4.387000 | -2.656000 |
| H | 2.766000 | -4.580000 | -3.663000 |
| C | 1.195000 | -5.002000 | -2.243000 |
| C | 0.731000 | -4.732000 | -0.957000 |
| H | -0.197000 | -5.193000 | -0.608000 |
| C | 1.410000 | -3.873000 | -0.083000 |
| C | 4.372000 | -2.887000 | -2.271000 |
| H | 5.243000 | -3.282000 | -1.723000 |
| H | 4.353000 | -1.802000 | -2.088000 |
| H | 4.544000 | -3.057000 | -3.343000 |
| C | 0.425000 | -5.889000 | -3.178000 |
| H | -0.105000 | -5.294000 | -3.941000 |
| H | -0.330000 | -6.480000 | -2.641000 |
| H | 1.088000 | -6.585000 | -3.714000 |
| C | 0.851000 | -3.630000 | 1.287000 |
| H | -0.174000 | -3.237000 | 1.226000 |
| H | 1.456000 | -2.918000 | 1.862000 |
| H | 0.790000 | -4.569000 | 1.859000 |
| N | 0.807000 | -0.270000 | 0.989000 |
| N | 0.125000 | -0.238000 | 1.924000 |