Supporting Information for:

Isolating elusive 'Al(μ-O)M' intermediates in CO_2 reduction by bimetallic Al–M complexes (M = Zn, Mg)

Matthew J. Evans, George H. Iliffe, Samuel E. Neale, Claire L. McMullin, J. Robin Fulton, Mathew D. Anker and Martyn P. Coles

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General Experimental Procedures

All manipulations were performed under dry argon 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 Jeol JNM-ECZ500S 500 MHz spectrometer equipped with a ROYAL digital auto tune probe S, operating at 500.1 (^{1}H), 125.7 (^{13}C), 194.4 (^{7}Li) and 130.3 (^{27}Al) MHz. Spectra were recorded at 298 K (unless stated otherwise) and proton and carbon chemical shifts were referenced internally to residual solvent resonances. Elemental analyses were performed by the EA Services Team at the London Metropolitan University, UK. Coupling constants are quoted in Hz. Al(NON^{Dipp})I[S1] and Mg(BDI^{Mes})I(OEt$_2$)[S2] were prepared according to the literature procedures. [Li(THF)$_2$][Zn(BDI^{Mes})Cl$_2$] was made according to the procedure for [Li(Et$_2$O)$_2$][Zn(BDI^{Dipp})Cl$_2$][S3] using BDI^{Mes}H in THF solvent.

Synthesis of (NON^{Dipp})Al–Zn(BDI^{Mes}) (1-Zn)

A bright yellow toluene solution of [K{Al(NON^{Dipp})}]$_2$ (644 mg, 0.59 mmol) was added to [Li(THF)$_2$][Zn(BDI^{Mes})Cl$_2$] (729 mg, 1.17 mmol) in a Schlenk flask to give a dark brown/black suspension. The resulting solution was stirred for 18 hours after which time the volatiles were removed. The product was extracted in hexane and then filtered through celite to give a colourless solution. Crystallisation was achieved from the storage of the hexane solution at –30 °C for 18 hours. Yield 650 mg, 61 %.

Elemental Analysis for $C_{58}H_{83}AlN_4OSi_2Zn$ (*1000.78*)*. Calculated: C, 69.60; H, 8.36; N, 5.60. Found C, 69.92; H, 8.83; N, 5.09. * = toluene solvated sample

^{1}H NMR (500 MHz, C_7D_8, 293 K): δ 7.07-6.98* (m, 6H, C_6H_3), 6.68 (s, 2H, C_6H_2), 4.81 (s, 1H, BDI γ-C*H*), 3.69 (sept, *J* = 6.5, 4H, C*H*Me$_2$), 2.26 (s, 6H, *p*-Me), 1.96 (br s, 6H, *o*-Me), 1.31 (s, 6H, BDI-*Me*), 1.27 (br m, 12H, *o*-Me and CH*Me$_2$*), 1.24 (br d, 12H, CH*Me$_2$*), 0.68 (br s, 6H, CH*Me$_2$*), 0.46, –0.17 (br s, 6H, Si*Me$_2$*). *overlap with C_7D_8.

^{1}H NMR (500 MHz, C_7D_8, 213 K): δ 7.07-7.00* (m, 6H, C_6H_3), 6.69 (s, 2H, C_6H_2), 4.82 (s, 1H, BDI γ-C*H*), 3.79, 3.72 (br sept, 2H, C*H*Me$_2$), 2.29 (s, 6H, *p-Me*), 2.02 (br d, 6H, CH*Me$_2$*), 1.36 (s, 6H, BDI-*Me*), 1,34* (br m, 12H, *o*-Me and CH*Me$_2$*), 1.27 (br d, 12H, CH*Me$_2$*), 0.62 (br d CH*Me$_2$*), 0.57, –0.06 (s, 6H, Si*Me$_2$*).

$^{13}C\{^{1}H\}$ NMR (151 MHz, C_6D_6): δ 166.9 (s, 1H, BDI-*C*Me), 146.4, 142.8, 137.9, 133.5, 129.3, 128.6, 125.7, 124.0, 124.0 (*C*$_6$H$_3$, *C*$_6$H$_2$), 97.3 (BDI γ-*C*H), 27.7 (*C*HMe$_2$), 26.5, 23.5 (CH*Me*$_2$), 21.4 (*o*-*Me*), 20.9 (BDI-*Me*), 18.6 (*p*-*Me*), 4.2, 0.7 (Si*Me*$_2$).

Figure S1 ^{1}H NMR spectrum (500 MHz, C_7D_8, 293 K) of (NON^{Dipp})Al–Zn(BDI^{Mes}) (**1-Zn**).

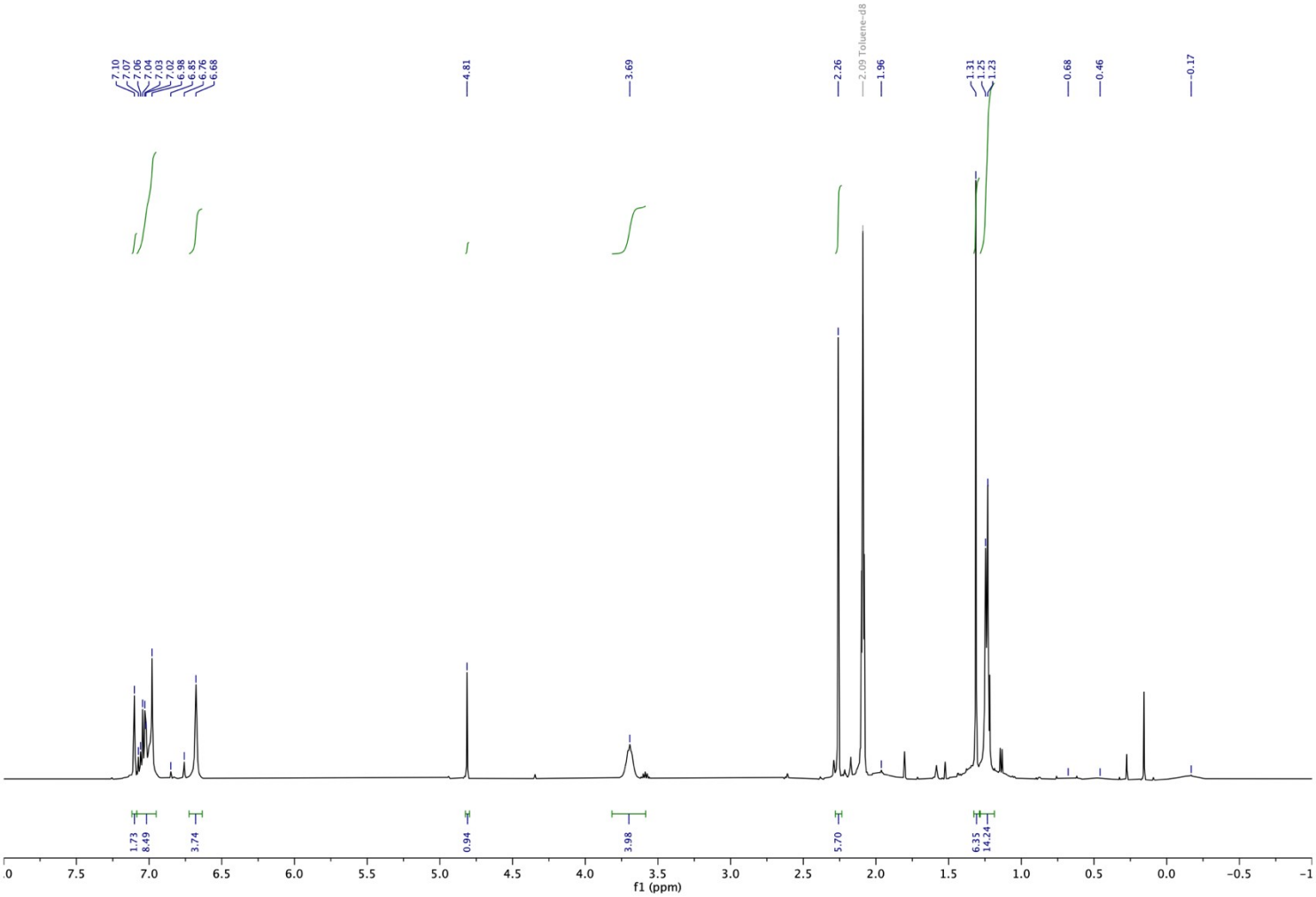


Figure S2 ^{1}H NMR spectrum (500 MHz, C_7D_8, 213 K) of (NON^{Dipp})Al–Zn(BDI^{Mes}) (**1-Zn**).

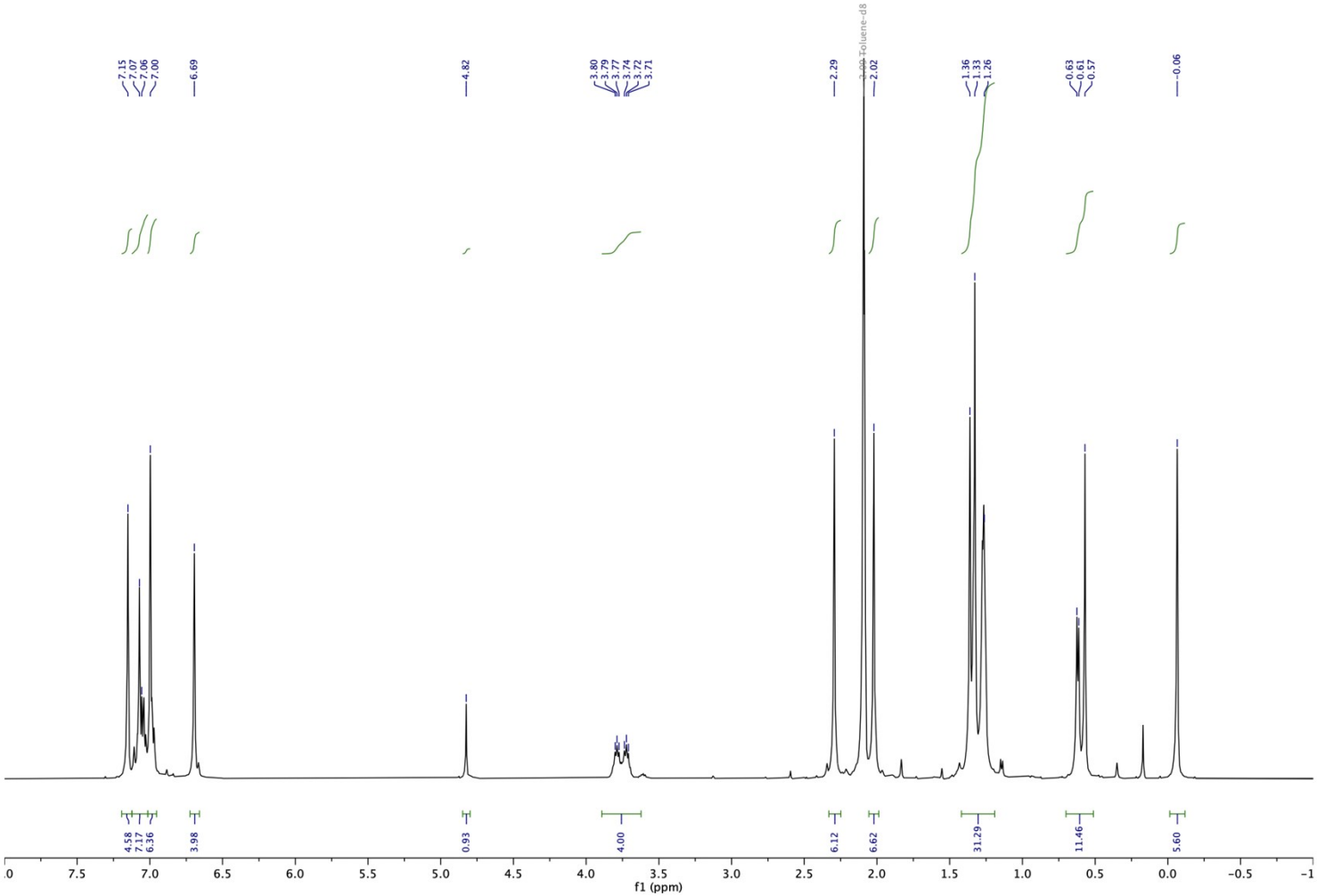


Figure S3 Stacked ^{1}H NMR spectra (500 MHz, C_7D_8) of (NON^{Dipp})Al–Zn(BDI^{Mes}) (**1-Zn**).

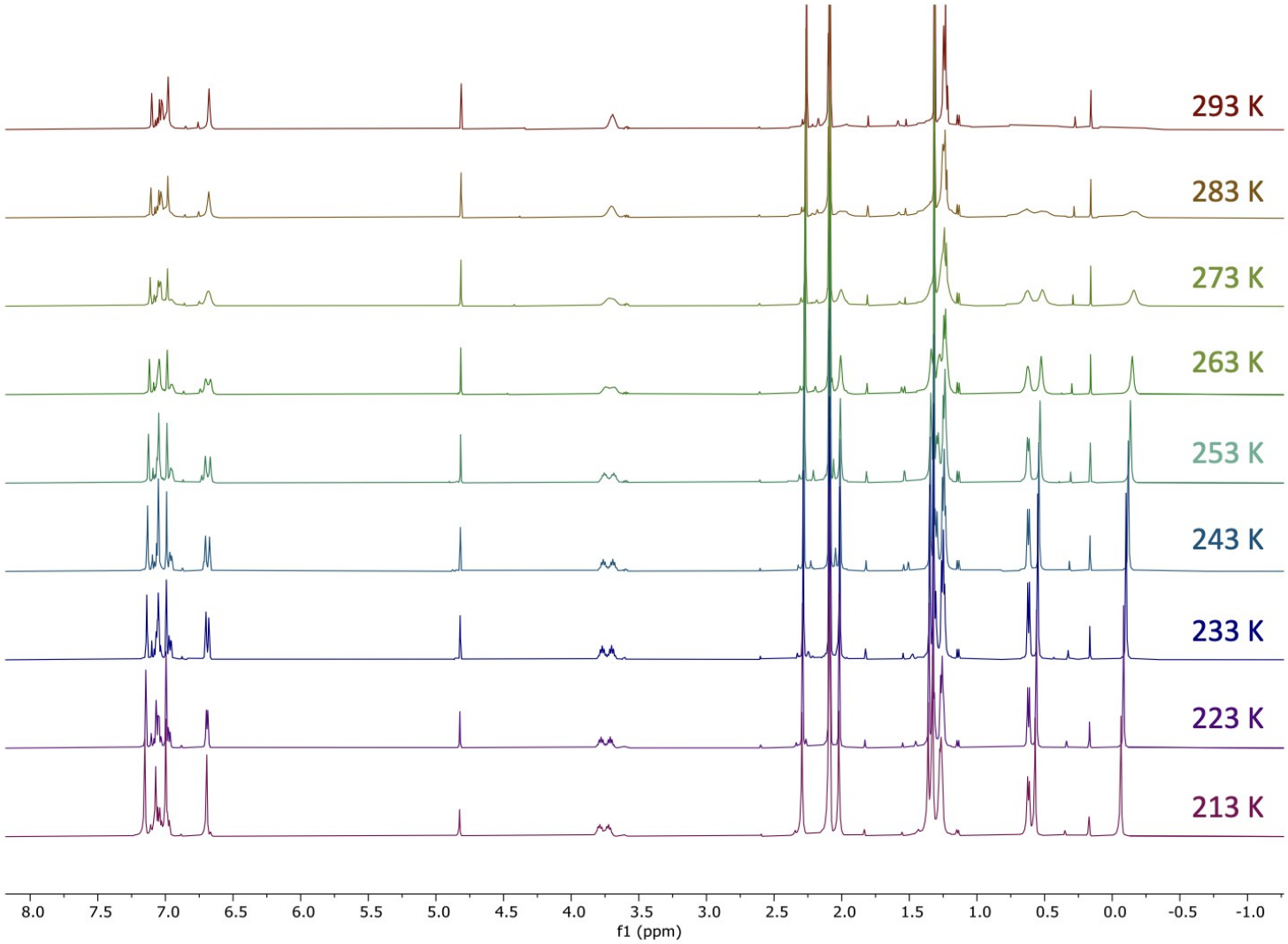


Figure S4 $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, C_6D_6) of (NON^{Dipp})Al–Zn(BDI^{Mes}) (**1-Zn**).

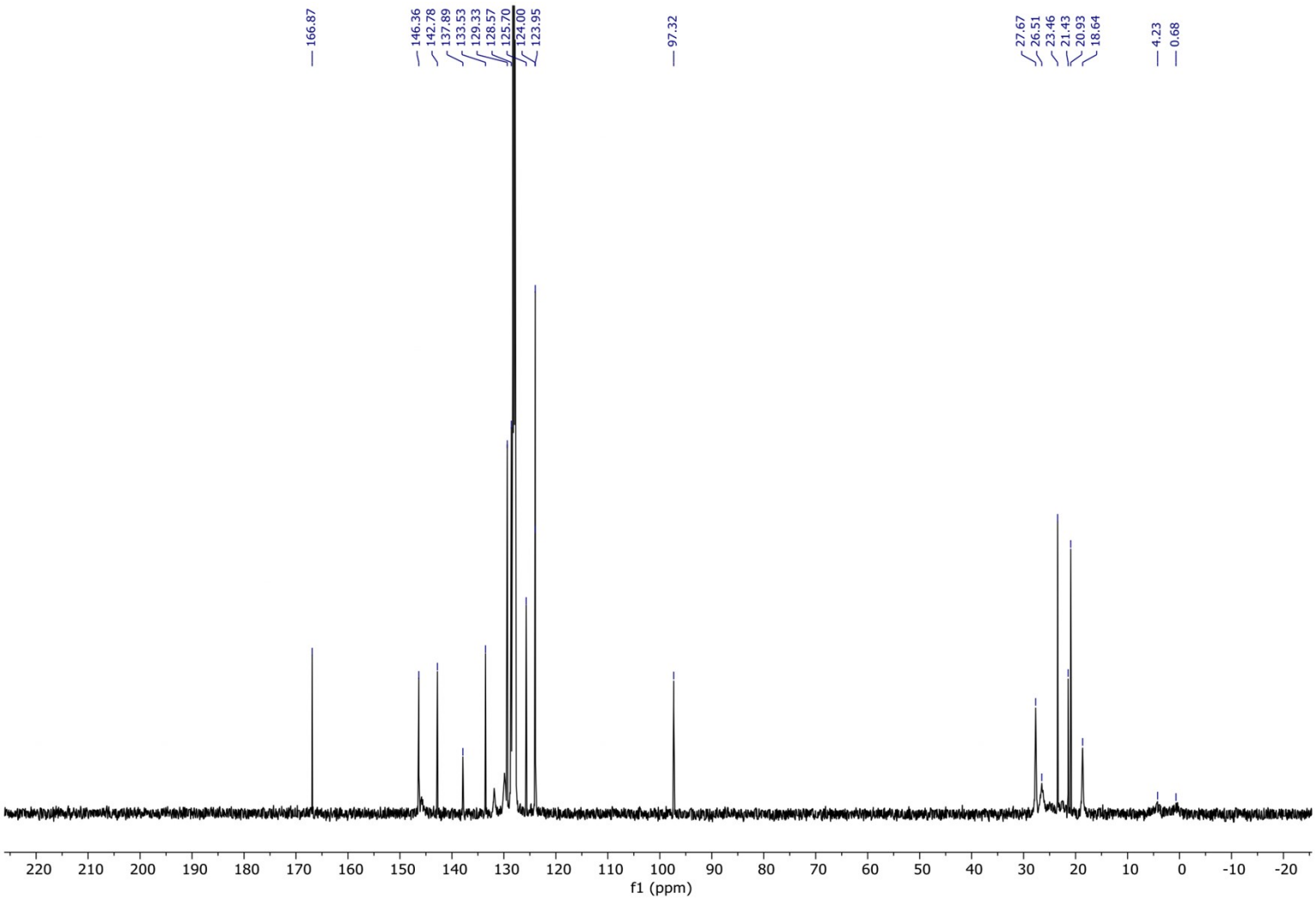
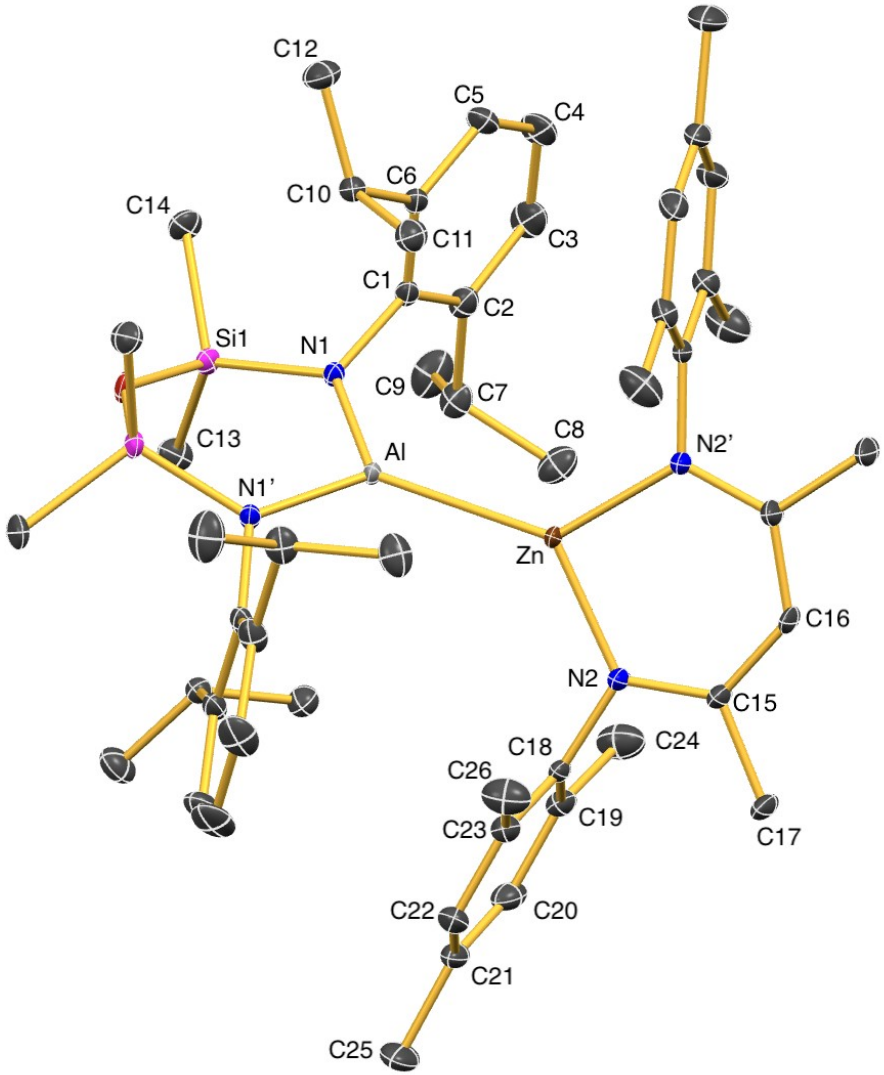


Figure S5 Thermal displacement plot (30 % probability) of (NON^{Dipp})Al–Zn(BDI^{Mes}) (**1-Zn**).



Synthesis of (NON^{Dipp})Al–Mg(BDI^{Mes}) (1-Mg)

A bright yellow toluene solution of [K{Al(NON^{Dipp})}]$_2$ (317 mg, 0.58 mmol) was added to a white suspension of Mg(BDI^{Mes})I(OEt$_2$) (323 mg, 0.58 mmol) in toluene (~ 5 mL) and stirred for 18 hours. The resulting suspension was filtered through celite to give a pale orange solution and the volatiles reduced *in vacuo* (~ 2 mL). The product separated from solution upon standing after ~ 0.5 hr as a white solid. The supernatant was decanted from the white powder and transferred to a scintillation vial. A second crop of the product was obtained as colourless crystals from the storage of the supernatant at –30 °C for 18 hours. Yield 298 mg, 59 %.

Elemental Analysis for $C_{51}H_{75}AlMgN_4OSi_2$ (867.55). Calculated: C, 70.60; H, 8.71; N, 6.46. Found C, 69.19; H, 9.09; N, 6.04.

^{1}H NMR (500 MHz, C_7D_8, 293 K): δ 7.02 – 6.98* (m, 6H, C_6H_3), 6.69 (s, 4H, C_6H_2), 4.72 (s, 1H, BDI γ-C*H*), 3.75 (sept, *J* = 6.8, 4H, C*H*Me$_2$), 2.26 (s, 6H, *p*-Me), 1.69 (s, 12H, *o*-Me), 1.31 (s, 6H, BDI-*Me*), 1.26, 0.93 (d, *J* = 6.8, 12H, CH*Me$_2$*), 0.19 (br s, 12H, Si*Me$_2$*). *overlap with C_7D_8.

^{1}H NMR (500 MHz, C_7D_8, 213 K): δ 7.07 – 7.00* (m, 6H, C_6H_3), 6.70 (s, 4H, C_6H_2), 4.73 (s, 1H, BDI γ-C*H*), 3.82 (br sept, 4H, C*H*Me$_2$), 2.29 (s, 6H, *p*-Me), 1.98, 1.43 (s, 6H, *o*-Me), 1.36 (br d, 6H, CH*Me$_2$*), 1.31 (s, 6H, BDI-*Me*), 1.27, 1.23, 0.68 (br d, 6H, CH*Me$_2$*), 0.59, 0.01 (br s, 6H, Si*Me$_2$*). *overlap with C_7D_8.

^{13}C{^{1}H} NMR (126 MHz, C_6D_6): δ 169.3 (BDI-*C*Me), 145.9, 144.6, 143.2, 133.4, 131.4, 130.0, 123.7, 123.6 (*C*$_6$H$_3$, *C*$_6$H$_2$), 96.5 (BDI γ-*C*H), 27.4 (*C*HMe$_2$), 26.6, 23.7 (CH*Me$_2$*), 23.3 (BDI-*Me*), 20.9 (*o*-*Me*), 18.5 (*p*-*Me*), 2.4 (Si*Me$_2$*).

Figure S6 ^{1}H NMR spectrum (500 MHz, C_7D_8, 273 K) of (NON^{Dipp})Al–Mg(BDI^{Mes}) (**1-Mg**).

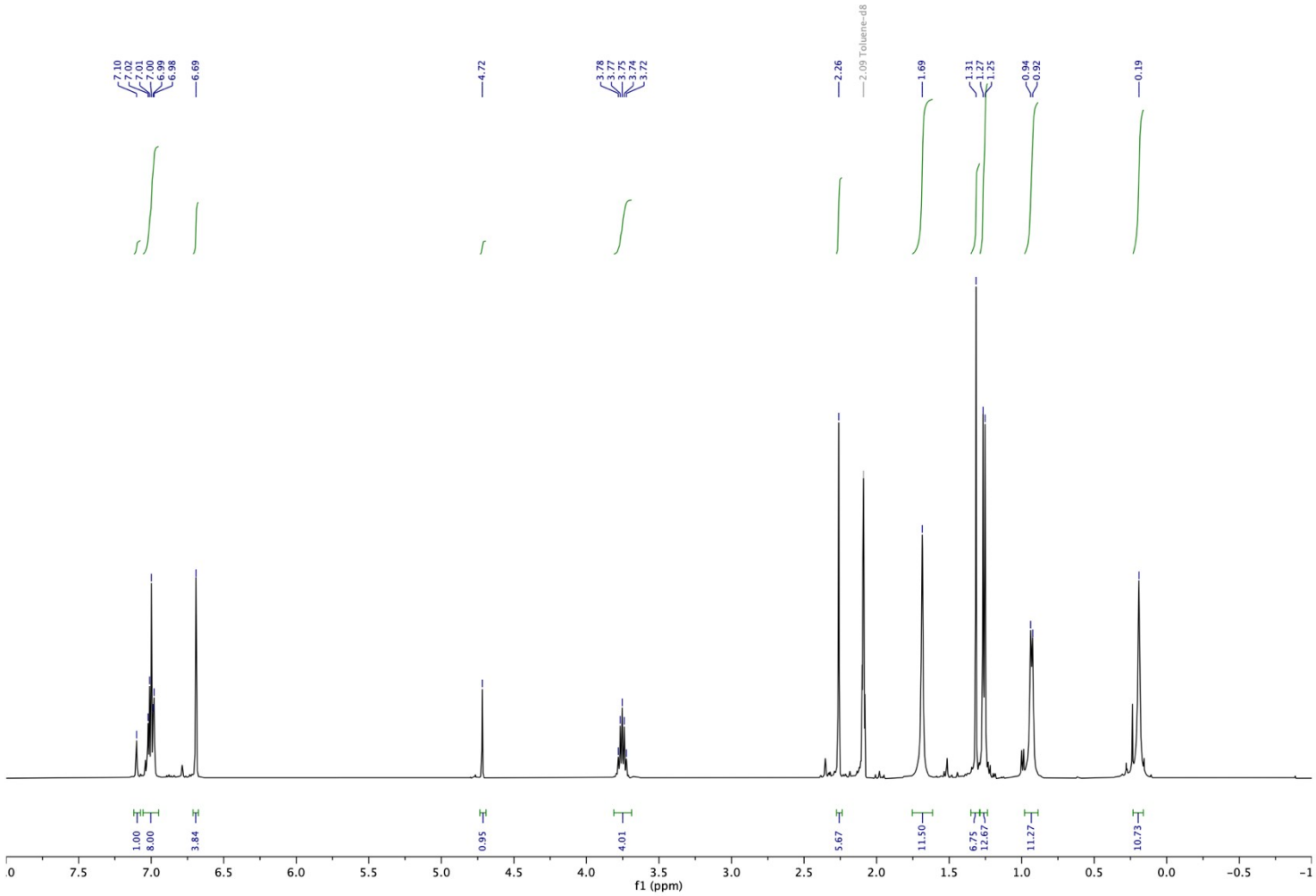


Figure S7 ^{1}H NMR spectrum (500 MHz, C_7D_8, 213 K) of (NON^{Dipp})Al–Mg(BDI^{Mes}) (**1-Mg**).

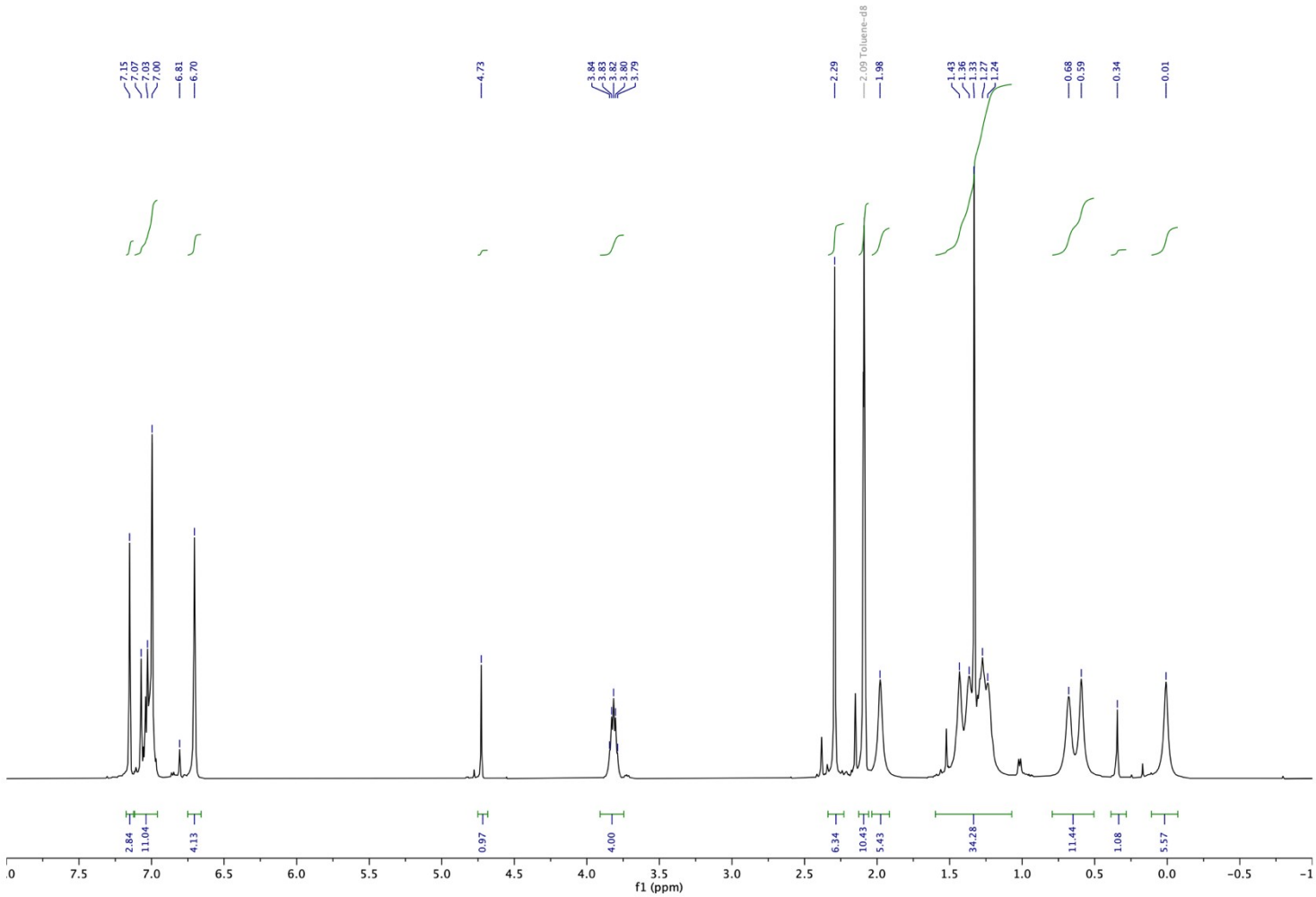


Figure S8 Stacked ^{1}H NMR spectra (500 MHz, C_7D_8) of (NON^{Dipp})Al–Mg(BDI^{Mes}) (**1-Mg**).

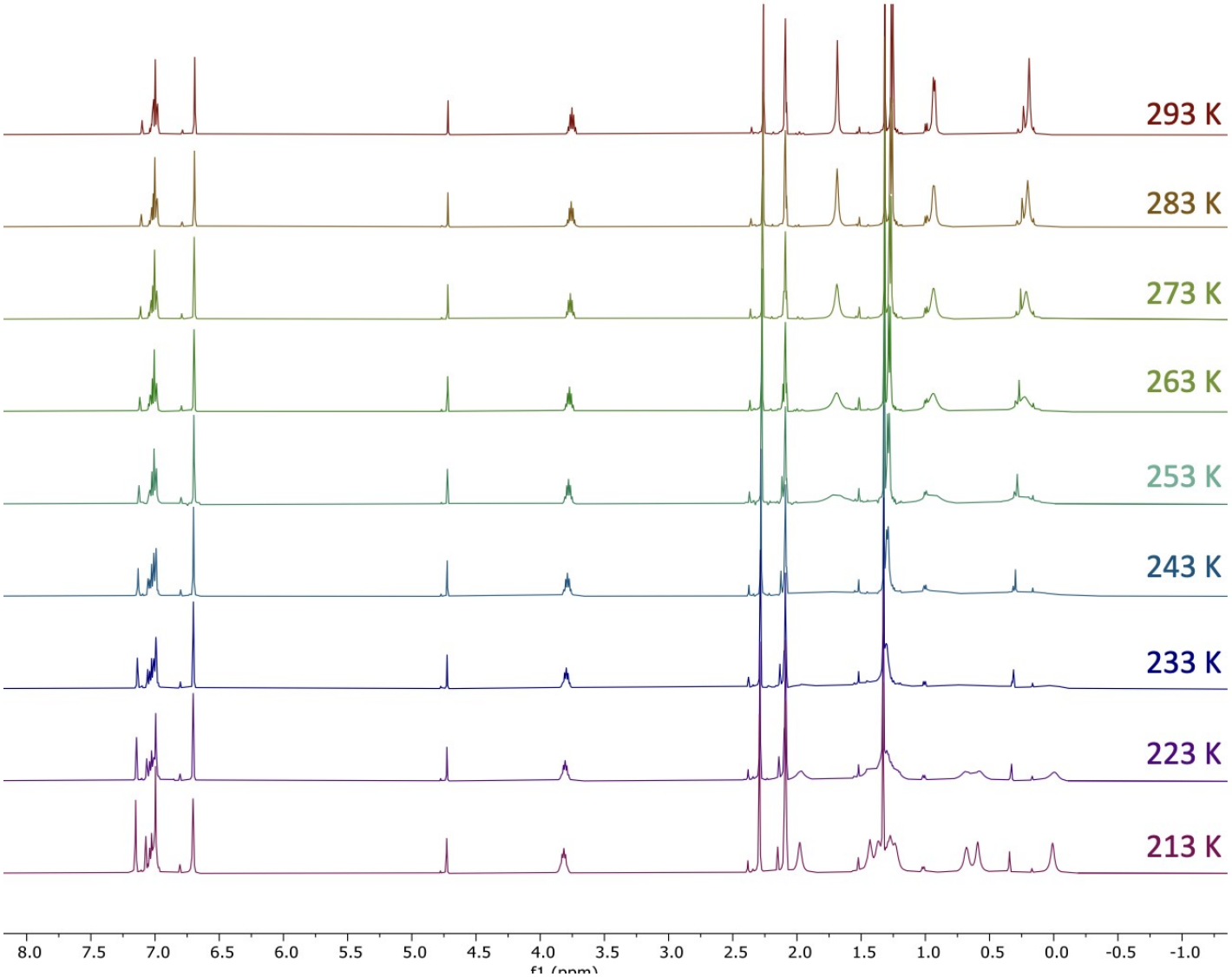


Figure S9 $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, C_6D_6) of (NON^{Dipp})Al–Mg(BDI^{Mes}) (**1-Mg**).

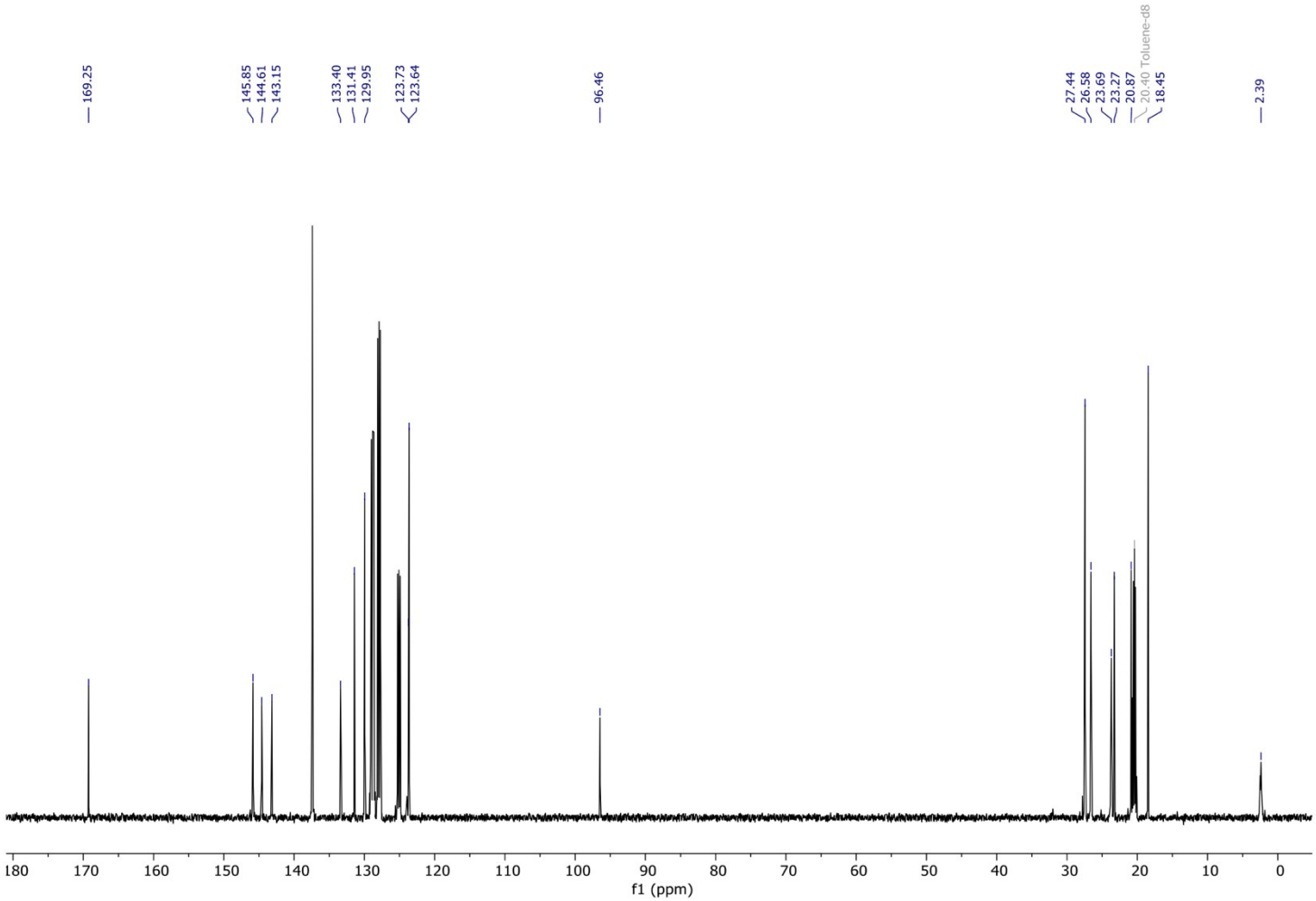
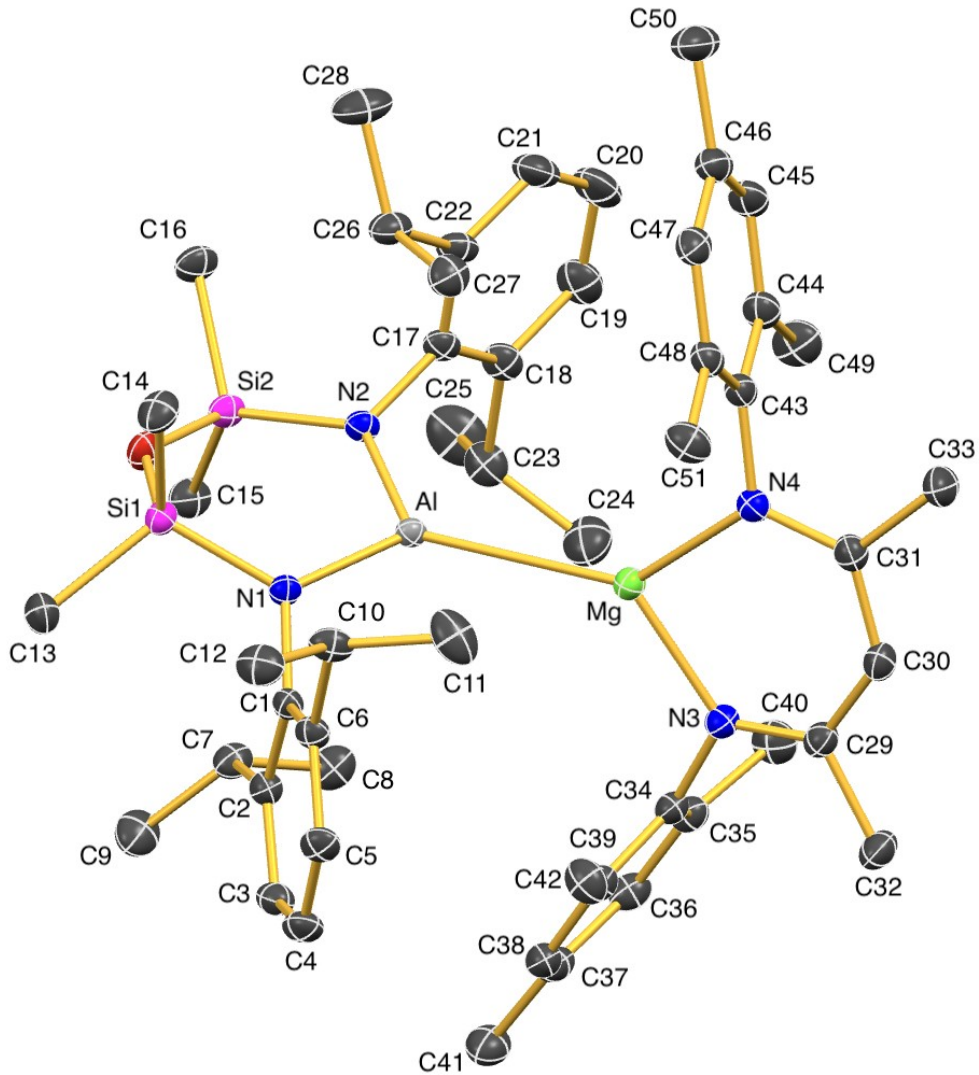


Figure S10 Thermal displacement plot (30 % probability) of (NON^{Dipp})Al–Mg(BDI^{Mes}) (**1-Mg**).



Synthesis of (NON^{Dipp})Al(μ-O$_2$C)Zn(BDI^{Mes}) (2)

A solution of (NON^{Dipp})Al–Zn(BDI^{Mes}) (**1-Zn**, 160 mg, 0.18 mmol) in C_6D_6 was transferred to a J. Youngs NMR tube. The solution was degassed and $^{13}CO_2$ (~1 atm.) was administered to the reaction vessel (condensed from lecture bottle at –196 °C). Reaction progress was monitored by ^{13}C NMR spectroscopy and shown to be complete after 2 days at room temperature. The solvent was removed *in vacuo* and the residue dissolved in toluene. Crystallisation was achieved from a toluene solution stored at –30 °C for 18 hours. Yield 100 mg, 60 %.

Elemental Analysis for $C_{52}H_{75}AlN_4O_3Si_2Zn$ (*952.66*). Calculated: C, 65.55; H, 7.93; N, 5.88. Found C, 64.60; H, 8.23; N, 5.59.

^{1}H NMR (600 MHz, C_6D_6) : δ 7.02 – 6.99 (m, 6H, C_6H_3), 6.73 (s, 4H, C_6H_2), 4.83 (s, 1H, BDI γ-C*H*), 3.84 (sept, *J* = 6.8, 4H, C*H*Me$_2$), 2.28 (s, 6H, *p*-Me), 1.81 (s, 12H, *o*-Me), 1.44 (s, 6H, BDI-*Me*), 1.34 (d, *J* = 6.8, 12H, CH*Me$_2$*), 1.09 (d, *J* = 6.8, 12H, CH*Me$_2$*), 0.38 (s, 12H, Si*Me$_2$*).

^{13}C{^{1}H} NMR (151 MHz, C_6D_6): 222.2 (^{13}*C*O$_2$), 169.1 (BDI–*C*Me), 146.2, 143.3, 140.6, 134.3, 130.2, 129.9, 123.7, 123.4 (*C$_6$*H$_3$, *C$_6$*H$_2$), 96.6 (BDI γ-*C*H), 27.7 (*C*HMe$_2$), 25.5, 24.8 (CH*Me$_2$*), 22.3 (BDI-*Me*), 21.2 (*p*-Me), 18.2 (*o*-Me), 2.3 (Si*Me$_2$*).

Figure S11 ^{1}H NMR spectrum (500 MHz, C_6D_6) of (NON^{Dipp})Al(μ-O_2C)Zn(BDI^{Mes}) (**2**).

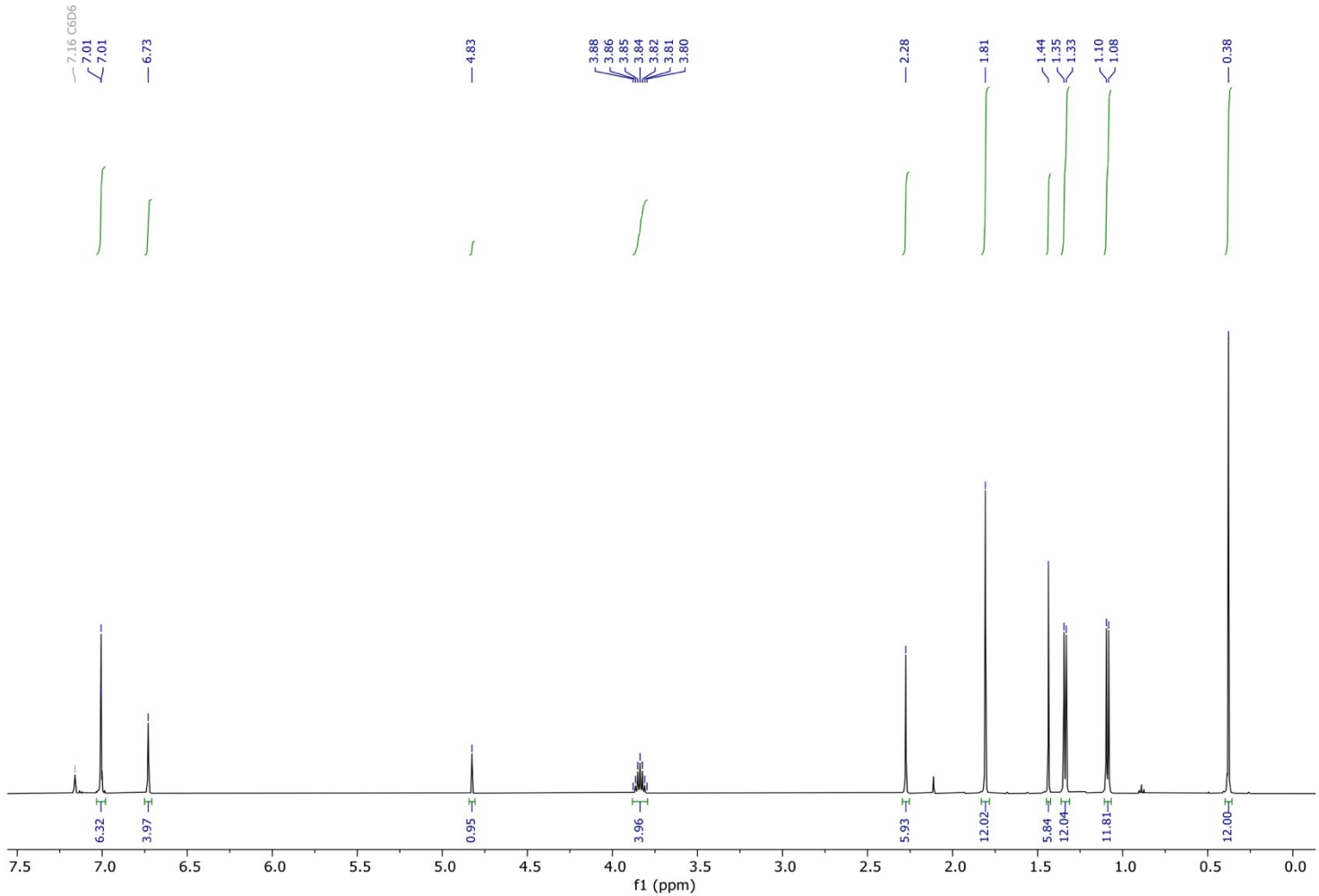


Figure S12 $^{13}C\{^{1}H\}$ NMR spectrum of (NON^{Dipp})Al(μ-O_2C)Zn(BDI^{Mes}) (**2**).

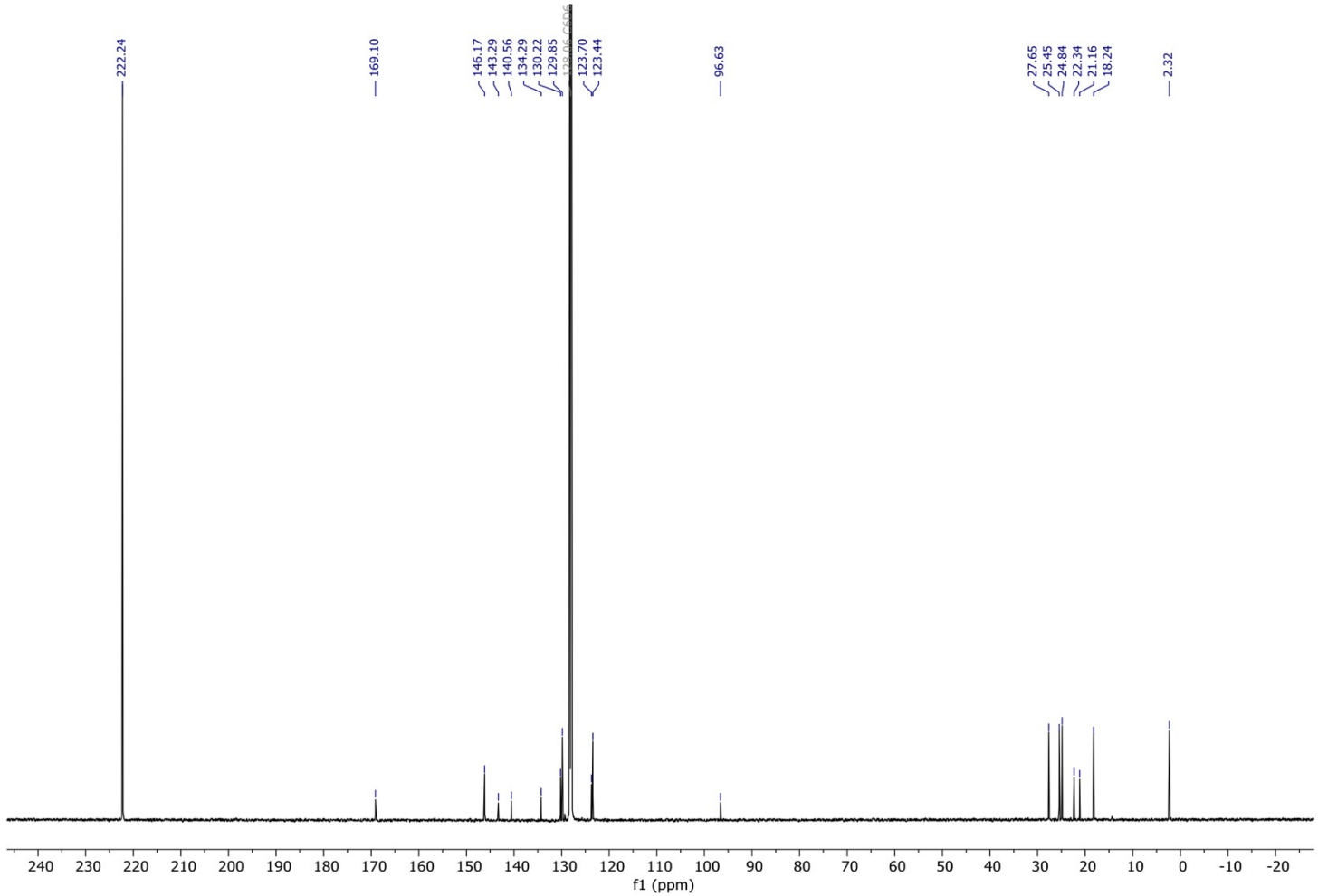
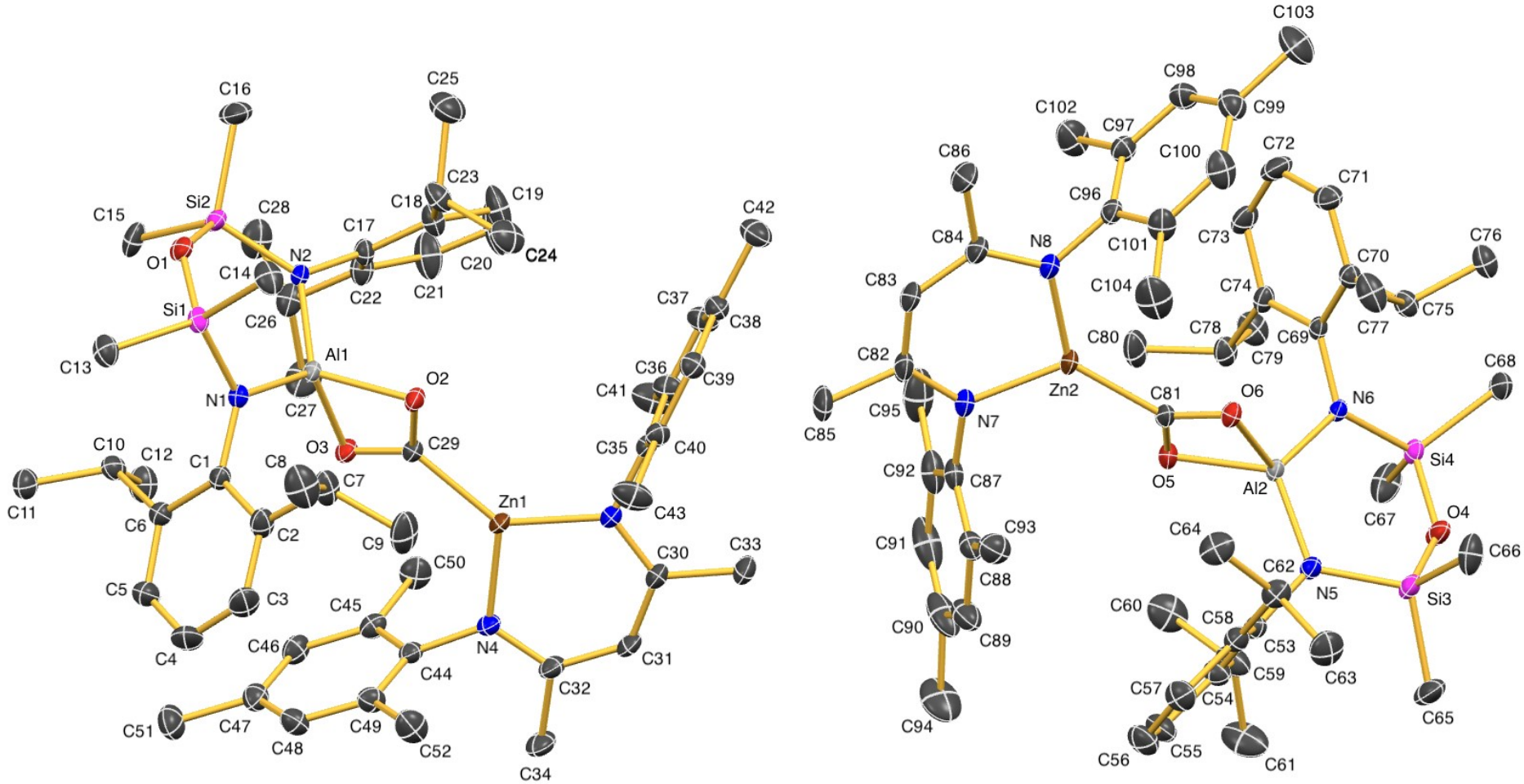


Figure S13 Thermal displacement plot (30 % probability) of (NON^{Dipp})Al–Zn(BDI^{Mes}) (**2**).



Synthesis of {(NON^{Dipp})Al(μ-CO$_3$)}$_2${Mg(THF)$_4$} (3)

A solution of (NON^{Dipp})Al–Mg(BDI^{Mes}) (107 mg, 0.12 mmol) was prepared in toluene-D$_8$ and transferred to a J. Youngs tap NMR tube. The solution was degassed and $^{13}CO_2$ (~1 atm) was administered to the reaction vessel (condensed from lecture bottle at –196 °C). An insoluble white precipitate formed upon warming the solution to room temperature. The solvent was removed *in vacuo* and the white powder dissolved in THF. Crystallisation was achieved from a THF solution stored at –30 °C for 18 hours. Yield 81 mg, 81%.

Elemental Analysis for $C_{74}H_{124}Al_2MgN_4O_{12}Si_4$ (*1452.28*). Calculated: C, 61.19; H, 8.61; N, 3.86. Found C, 60.60; H, 8.80; N, 3.73.

The observed data are a better fit for the formula calculated for loss of one equivalent of THF, $C_{70}H_{116}Al_2MgN_4O_{11}Si_4$ (*1380.81*). Calculated: C, 60.91; H, 8.47; N, 4.06. We therefore suggest the results indicate partial loss of THF during sample preparation and analysis.

^{1}H NMR (600 MHz, THF-D$_8$): δ 6.90 (d, *J* = 7.8, 4H, C$_6$*H$_3$*), 6.83 (dd, *J* = 8.2, 6.8, 2H, C$_6$*H$_3$*), 3.77 (sept, *J* = 6.8, 4H, C*H*Me$_2$), 3.62 (s, 12H, THF), 1.78 (s, 12H, THF), 1.17 (d, *J* = 6.8, 6H, CH*Me$_2$*), 1.16 (d, *J* = 6.8, 6H, CH*Me$_2$*), 1.12 (d, *J* = 6.8, 12H, CH*Me$_2$*), 0.11 (s, 12H, Si*Me$_2$*).

^{13}C{^{1}H} NMR (126 MHz, THF-D$_8$): δ 164.1 ($^{13}CO_2$), 147.1, 142.5, 125.9, 123.8, 123.6, 123.5 (*C$_6$*H$_3$), 68.3 (THF), 28.3 (*C*HMe$_2$), 26.4 (THF), 25.9, 25.0, 24.2 (CH*Me$_2$*), 2.5 (Si*Me$_2$*).

NMR reactions were carried out in THF-D$_8$ to prevent precipitation of the product and to provide an insight into the reaction mechanism.

(NON^{Dipp})Al–Mg(BDI^{Mes}) + $^{13}CO_2$:

Using the general method detailed above. [(NON^{Dipp})Al–Mg(BDI^{Mes})] (38 mg, 0.04 mmol). Yield 28 mg, 79 %.

(NON^{Dipp})Al=O–Mg(BDI^{Mes}) + $^{13}CO_2$:

Using the general method detailed above. [(NON^{Dipp})Al=O–Mg(BDI^{Mes})] (62 mg, 0.07 mmol). Yield 55 mg, 97 %.

Figure S14 ^{1}H NMR spectrum (500 MHz, D_8-THF) of {(NON^{Dipp})Al(μ-CO_3)}$_2${Mg(THF)$_4$} (**3**).

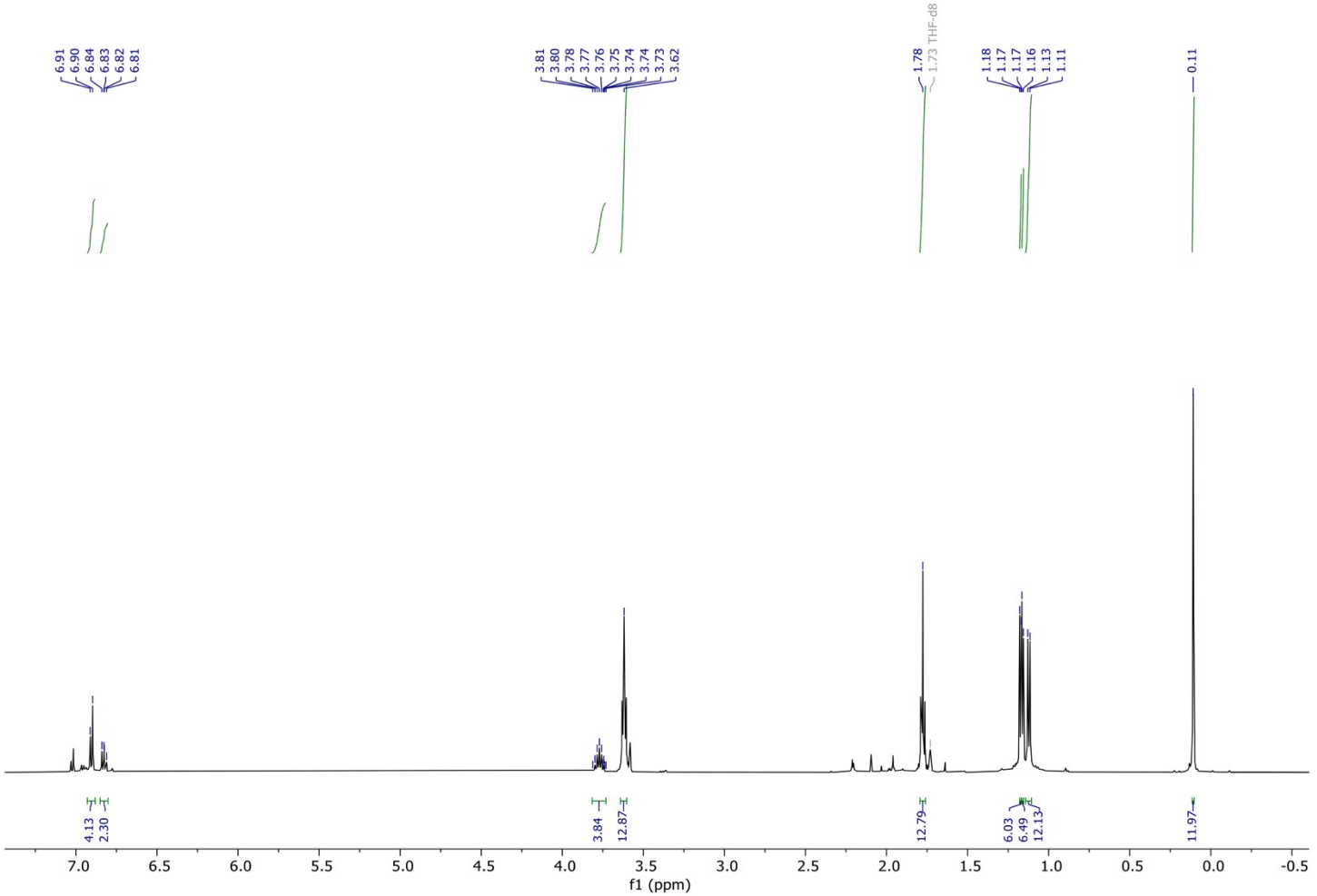


Figure S15 $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, D_8-THF) of $\{(NON^{Dipp})Al(\mu\text{-}CO_3)\}_2\{Mg(THF)_4\}$ (**3**).

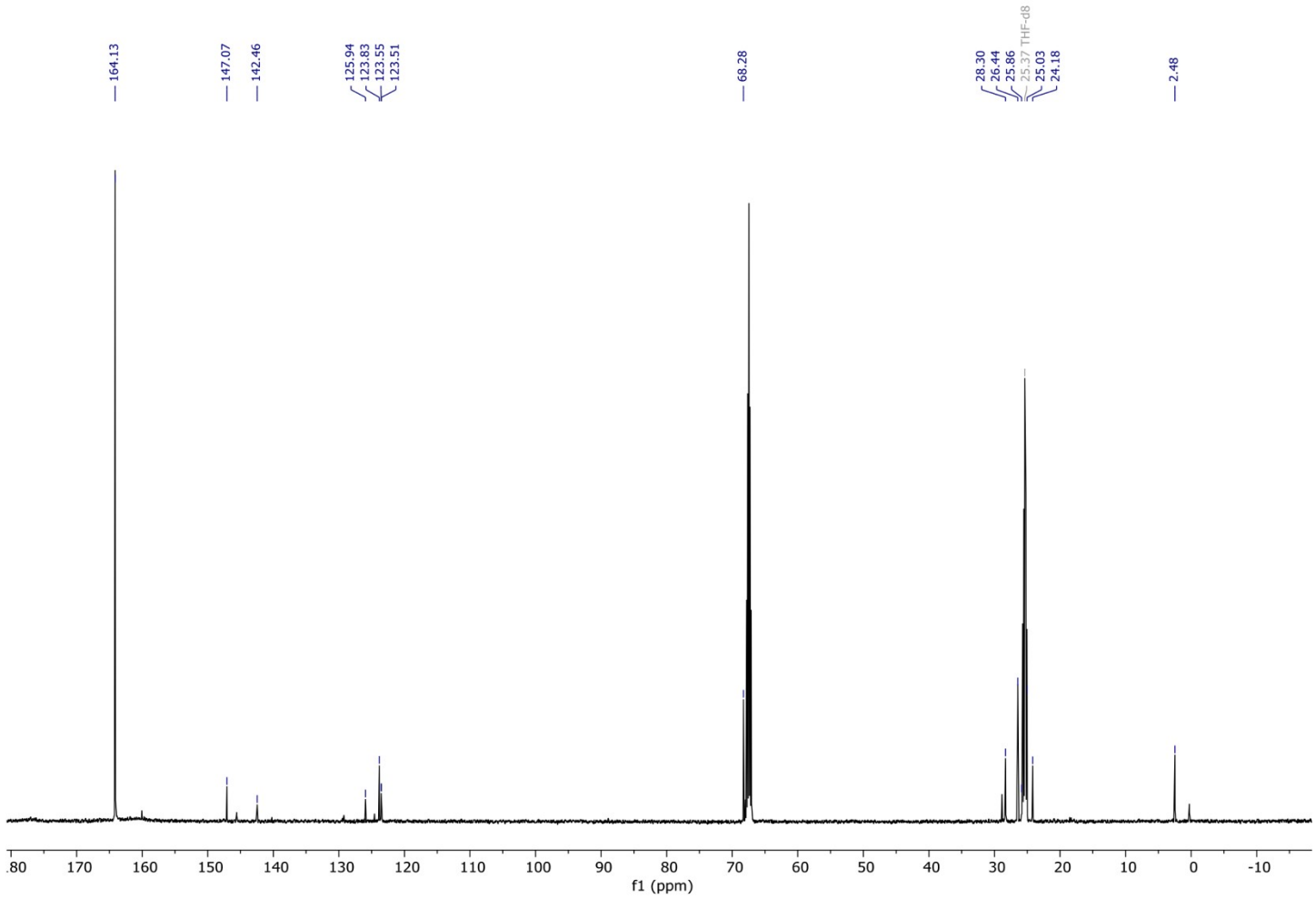


Figure S16 ^{1}H NMR spectra (500 MHz, D_8-THF) of (NON^{Dipp})Al–Mg(BDI^{Mes}) + $^{13}CO_2$.

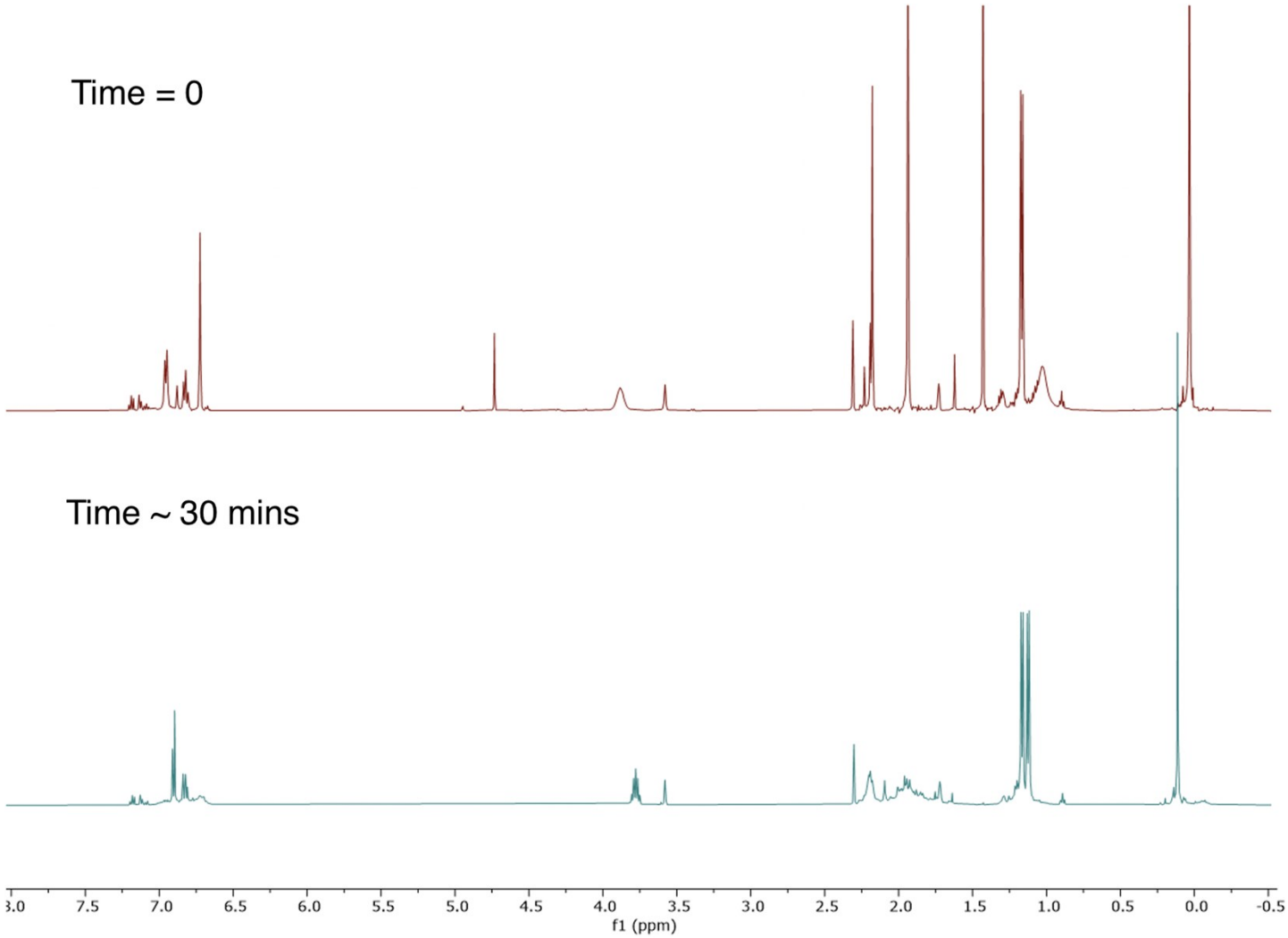


Figure S17 $^{13}C\{^{1}H\}$ NMR spectra (126 MHz, D_8-THF) of (NON^{Dipp})Al–Mg(BDI^{Mes}) + $^{13}CO_2$.

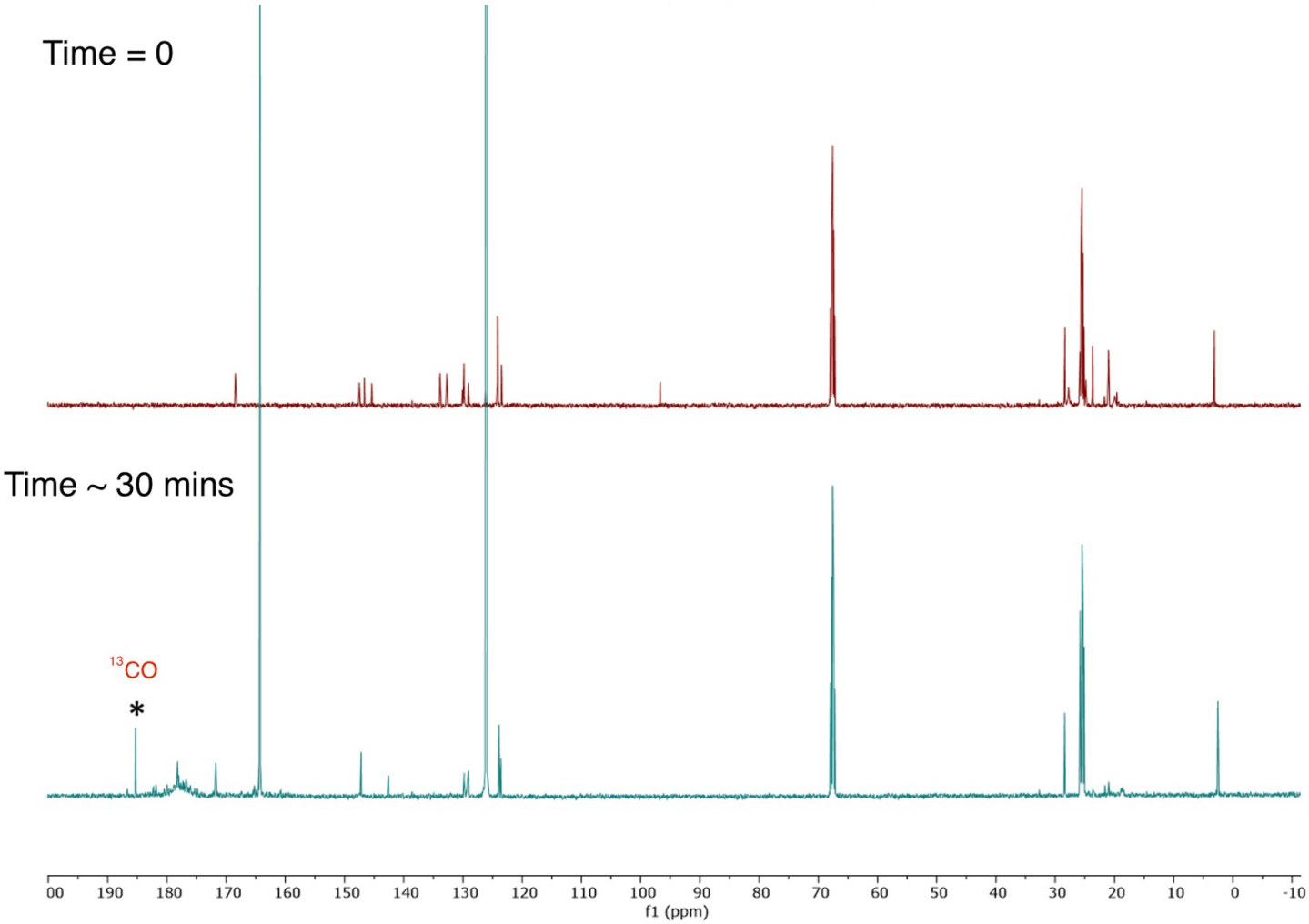


Figure S18 ^{1}H NMR spectra (500 MHz, D_8-THF) of (NON^{Dipp})Al–(μ-O)Mg(BDI^{Mes}) + $^{13}CO_2$.

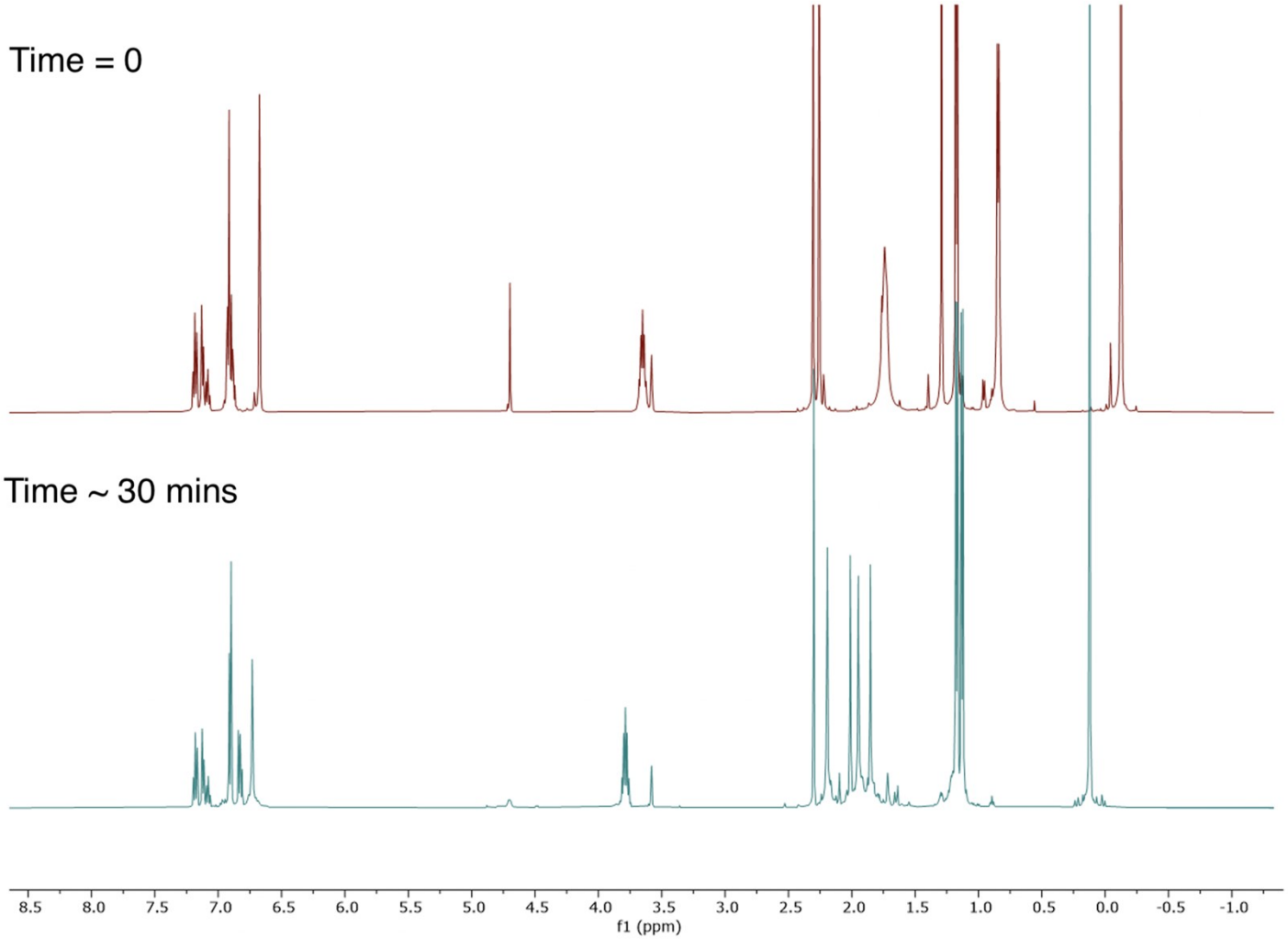


Figure S19 $^{13}C\{^{1}H\}$ NMR spectra (126 MHz, D_8-THF) of (NON^{Dipp})Al–(μ-O)Mg(BDI^{Mes}) + $^{13}CO_2$.

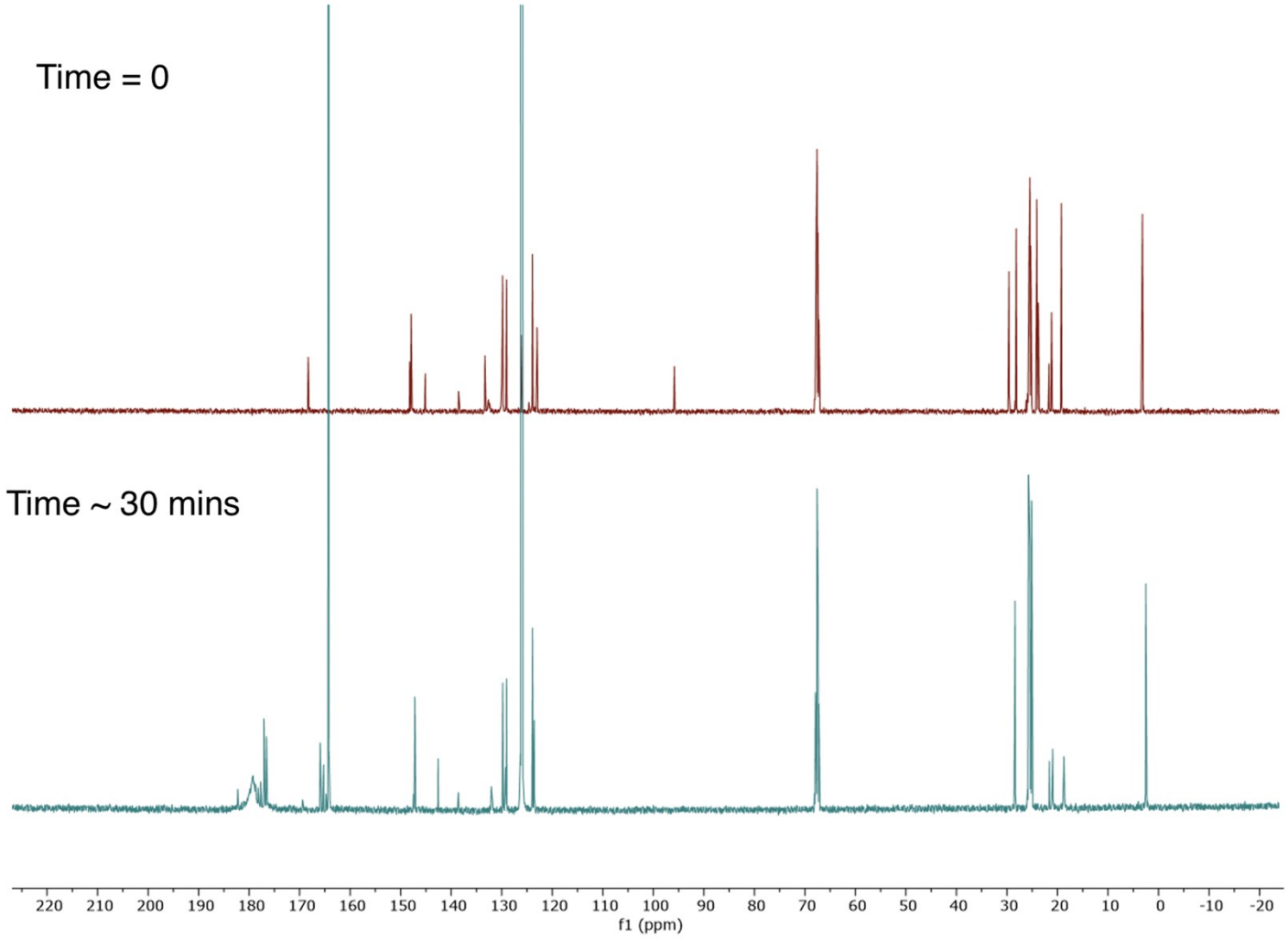
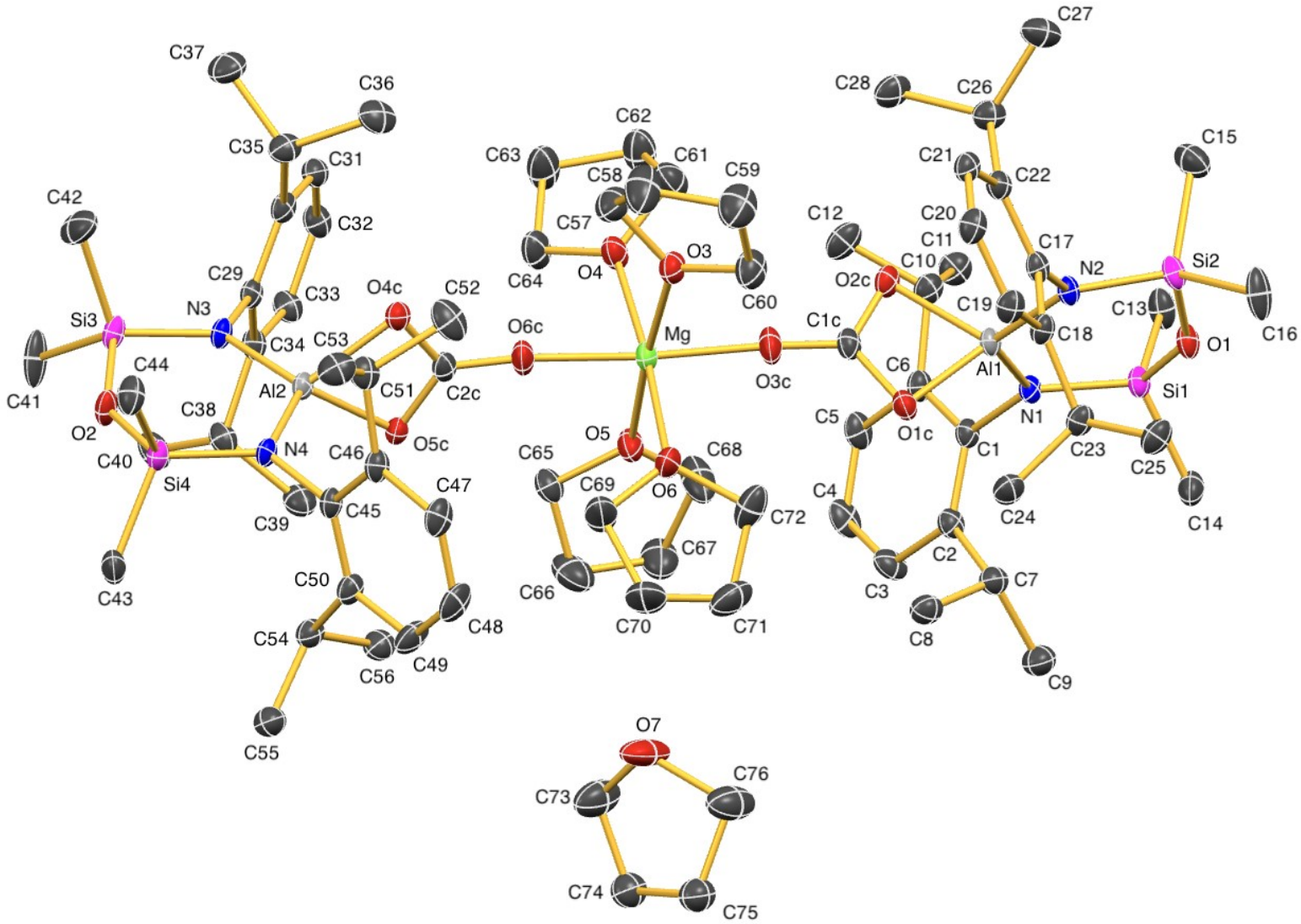


Figure S20 Thermal displacement plot (30 % probability) of {(NON^{Dipp})Al(μ-CO_3)}$_2${Mg(THF)$_4$} (**3**).



Synthesis of (NON^{Dipp})Al(μ-O)Zn(BDI^{Mes}) (4-Zn)

A solution of (NON^{Dipp})Al–Zn(BDI^{Mes}) (206 mg, 0.23 mmol) in toluene (ca. 5 mL) was transferred to an ampule. The solution was degassed and nitrous oxide (~1 atm.) was administered to the reaction vessel. The mixture was allowed to stir at room temperature for 72 hours to give a pale-yellow solution. The solvent was reduced *in vacuo* (ca. 2 mL) and transferred to a vial. Crystallisation was achieved from a toluene solution stored at –30 °C for 18 hours. Yield 87 mg, 42 %.

Accurate elemental analysis could not be obtained for this compound, likely due to high oxygen and moisture sensitivity and possible decomposition during sample preparation and analysis.

^{1}H NMR (500 MHz, C_6D_6): δ 7.09 – 7.03 (m, 6H, C_6H_3), 6.73 (s, 4H), 4.70 (s, 1H), 3.81 (sept, J = 6.9, 4H, C*H*Me$_2$), 2.29 (s, 6H, *p-Me*), 1.73 (s, 12H, *o-Me*), 1.37 (s, 6H, BDI-*Me*), 1.32 (d, J = 6.8, 12H, CHMe_2), 0.96 (d, J = 6.8, 12H, CHMe_2), 0.25 (s, 12H, SiMe_2).

^{13}C{^{1}H} NMR (126 MHz, C_6D_6): δ 169.3 (BDI-*C*Me), 145.2, 144.3, 142.4, 133.6, 131.2, 129.8, 129.3, 128.6, 123.8, 123.4 (C_6H_3, C_6H_2), 95.2 (BDI-*C*H), 28.1 (*C*HMe$_2$), 25.0, 23.0 (CHMe_2), 22.8 (BDI-C*Me*), 21.0 (*p-Me*), 18.2 (*o-Me*), 1.7 (SiMe_2).

Figure S21 ^{1}H NMR spectrum (500 MHz, C_6D_6) of (NON^{Dipp})Al(μ-O)Zn(BDI^{Mes}) (**4-Zn**).

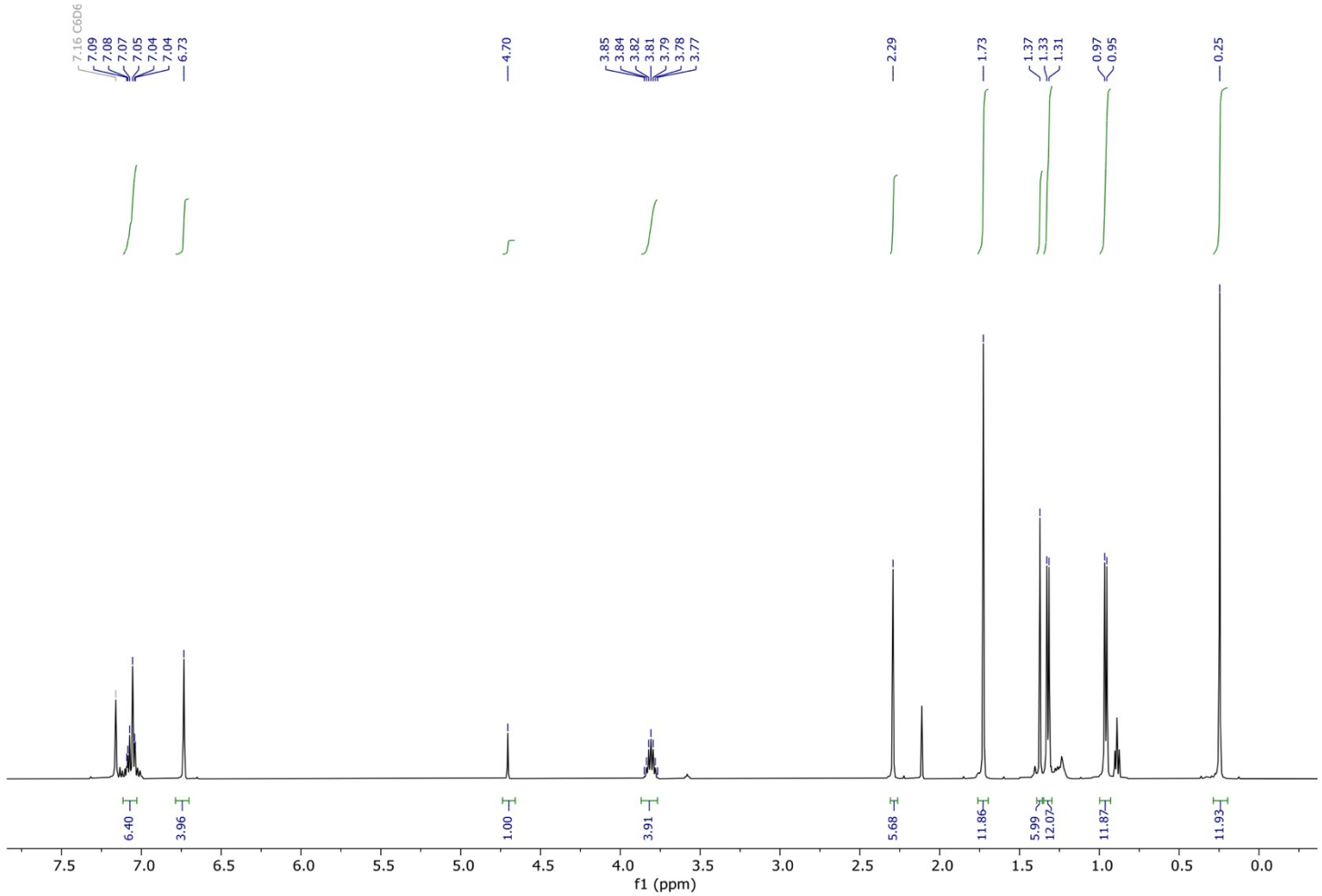


Figure S22 $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, C_6D_6) of (NON^{Dipp})Al(μ-O)Zn(BDI^{Mes}) (**4-Zn**).

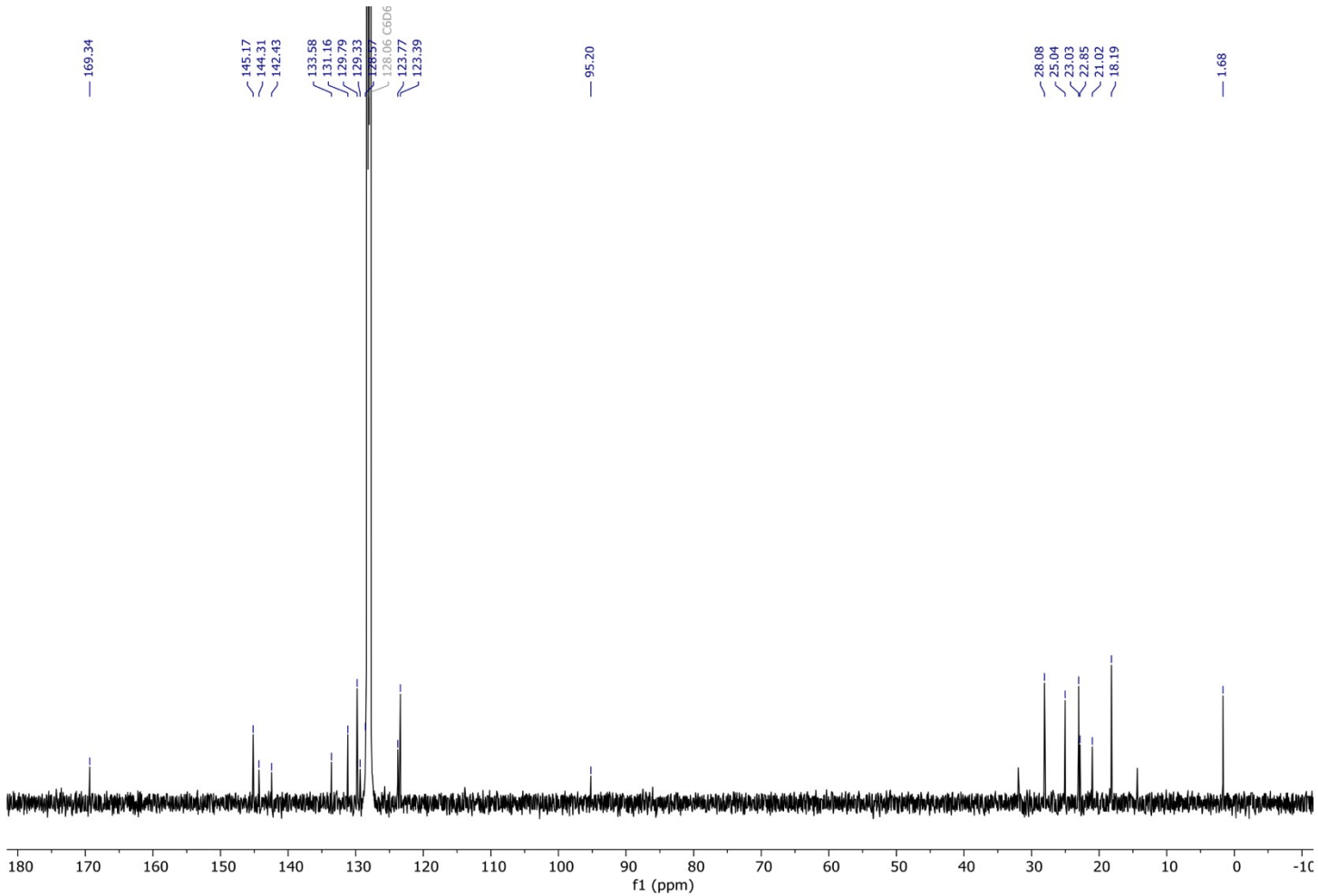
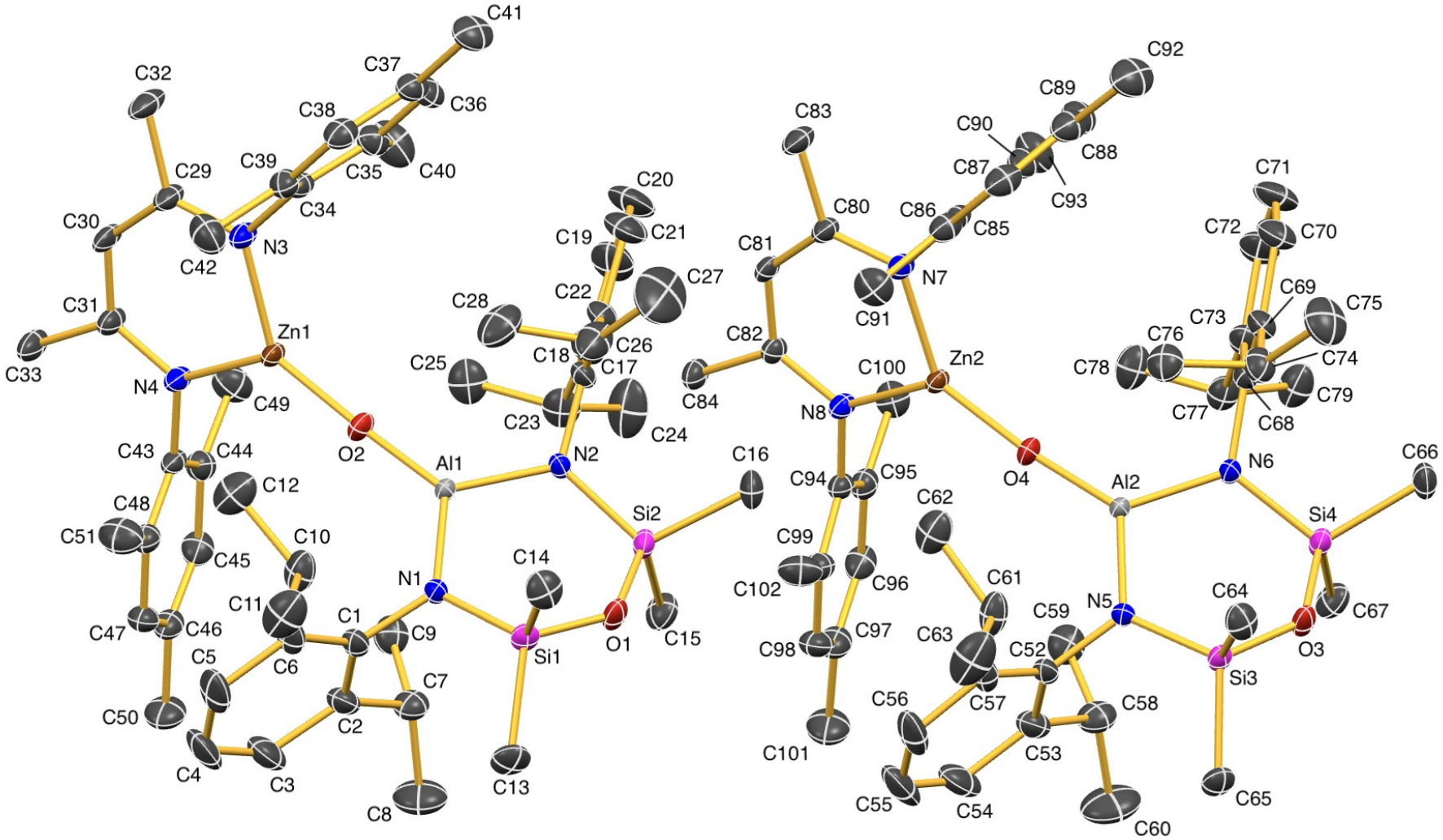


Figure S23 Thermal displacement plot (30 % probability) of (NON^{Dipp})Al(μ-O)Zn(BDI^{Mes}) (**4-Zn**).



Synthesis of (NON^{Dipp})Al(μ-O)Mg(BDI^{Mes}) (4-Mg)

A solution of (NON^{Dipp})Al–Mg(BDI^{Mes}) (222 mg, 0.26 mmol) in toluene (ca. 5 mL) was transferred to an ampule. The solution was degassed and nitrous oxide (~1 atm.) was administered to the reaction vessel. The mixture was allowed to stir at room temperature for 72 hours to give a yellow solution. The solvent was reduced *in vacuo* (ca. 2 mL) and transferred to a scintillation vial. Crystallisation was achieved from a toluene solution stored at –30 °C for 18 hours. Yield 103 mg, 46%.

Elemental Analysis for $C_{51}H_{75}AlMgN_4O_2Si_2$ (*883.55*). Calculated: C, 69.32; H, 8.55; N, 6.34. Found C, 68.61; H, 8.74; N, 5.88.

^{1}H NMR (500 MHz, C_7D_8): δ 7.04 – 6.97 (m, 6H, C_6H_3), 6.71 (s, 4H, C_6H_2), 4.68 (s, 1H, BDI-C*H*), 3.77 (sept, *J* = 6.8, 4H, C*H*Me$_2$), 2.28 (s, 6H, *p-Me*), 1.71 (s, 12H, *o-Me*), 1.38 (s, 6H, BDI-*Me*), 1.30 (d, *J* = 6.8, 12H, CH*Me$_2$*), 0.92 (d, *J* = 6.8, 12H, CH*Me$_2$*), 0.19 (s, 12H, Si*Me$_2$*).

^{13}C{^{1}H} NMR (126 MHz, C_7D_8): δ 170.1 (BDI-*C*Me), 145.2 (C_6H_3), 144.1 (C_6H_2), 142.3 (C_6H_3), 133.2, 130.9, 129.8 (C_6H_2), 123.8, 123.2 (C_6H_3), 95.3 (BDI-*C*H), 28.0 (*C*HMe$_2$), 25.1, 23.0 (CH*Me$_2$*), 22.9 (BDI-*Me*), 20.9 (*p-Me*), 18.2 (*o-Me*), 1.6 (Si*Me$_2$*).

Figure S24 ^{1}H NMR spectrum (500 MHz, C_7D_8) of (NON^{Dipp})Al(μ-O)Mg(BDI^{Mes}) (**4-Mg**).

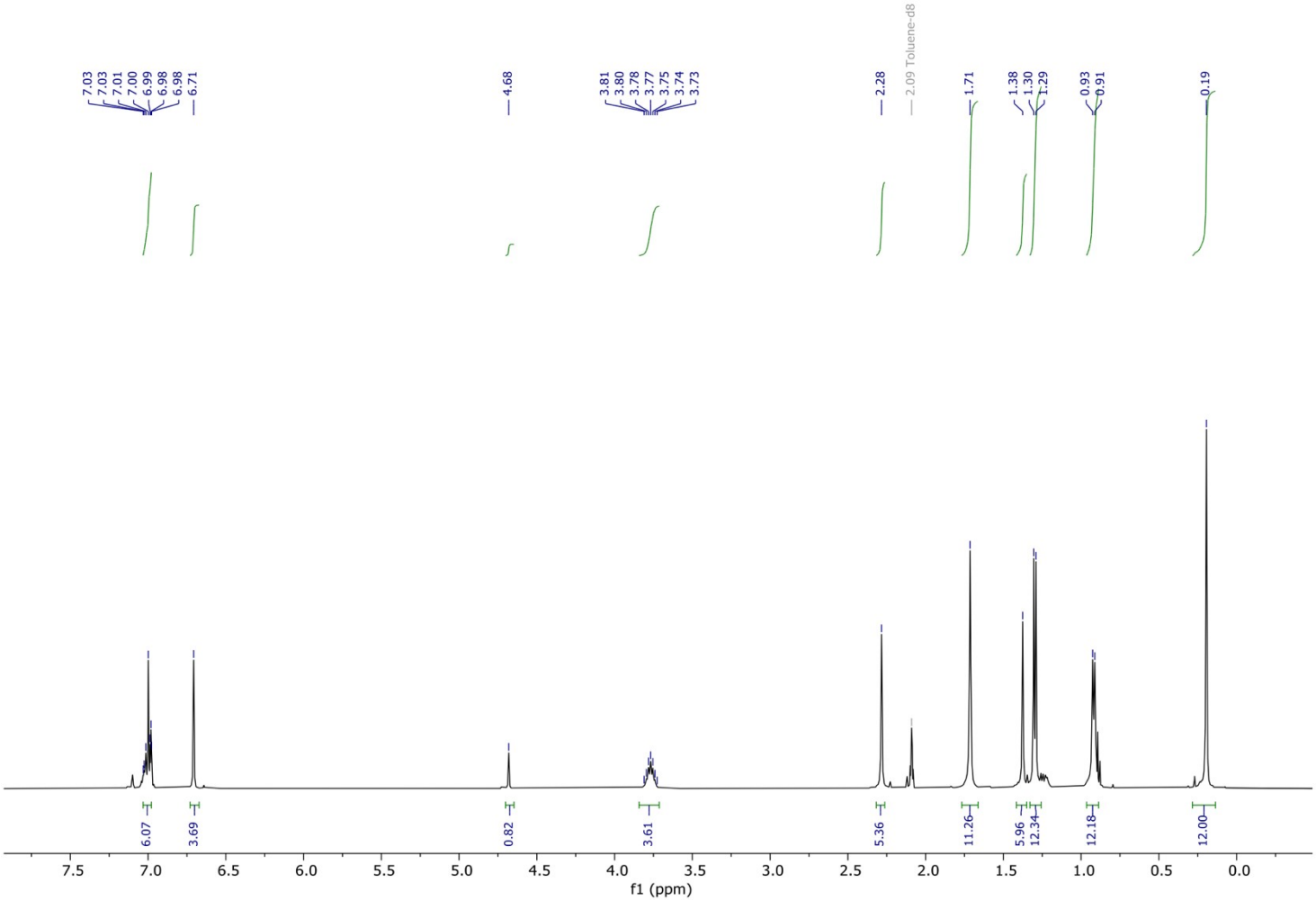


Figure S25 $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, C_7D_8) of (NON^{Dipp})Al(μ-O)Mg(BDI^{Mes}) (**4-Mg**).

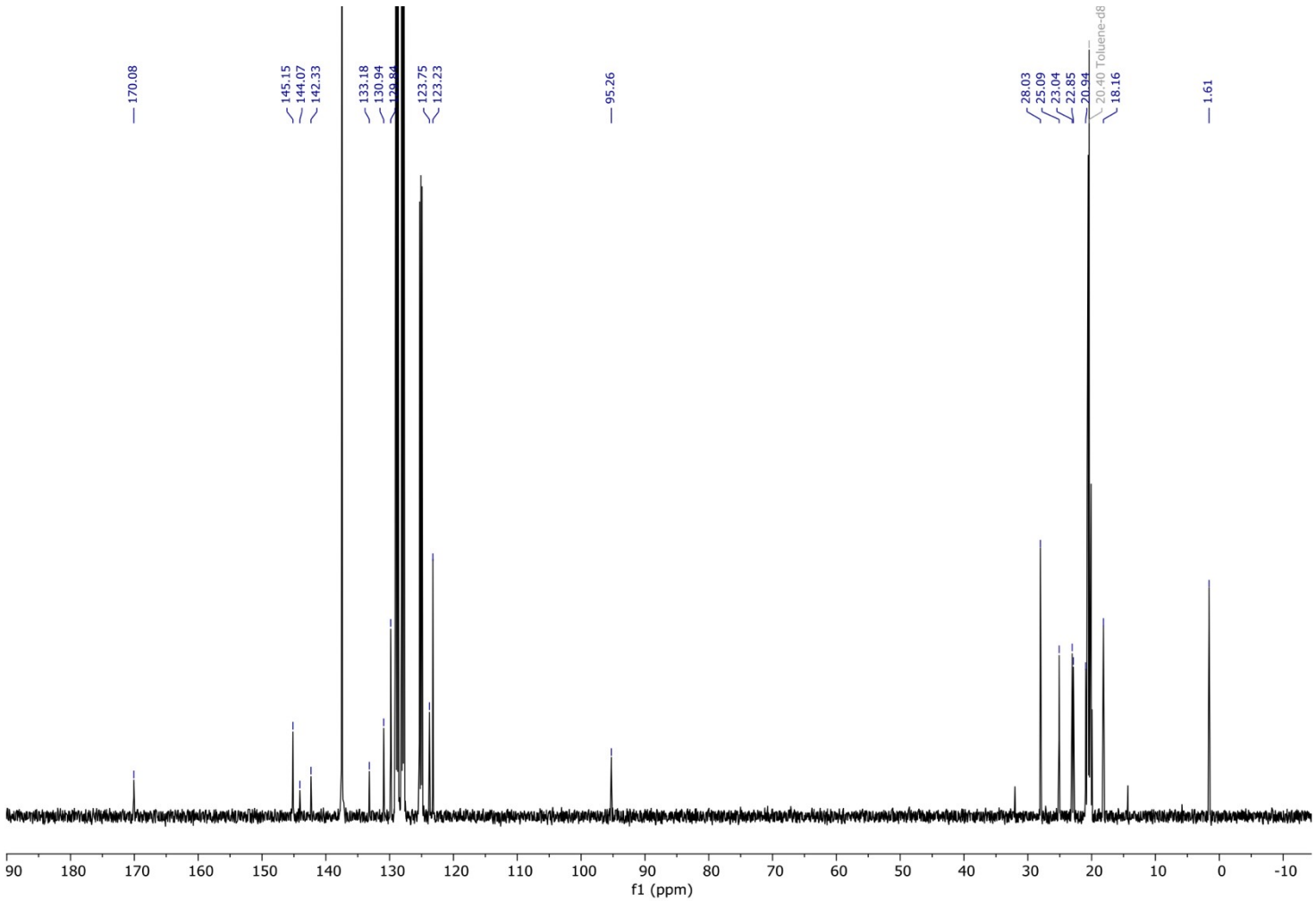
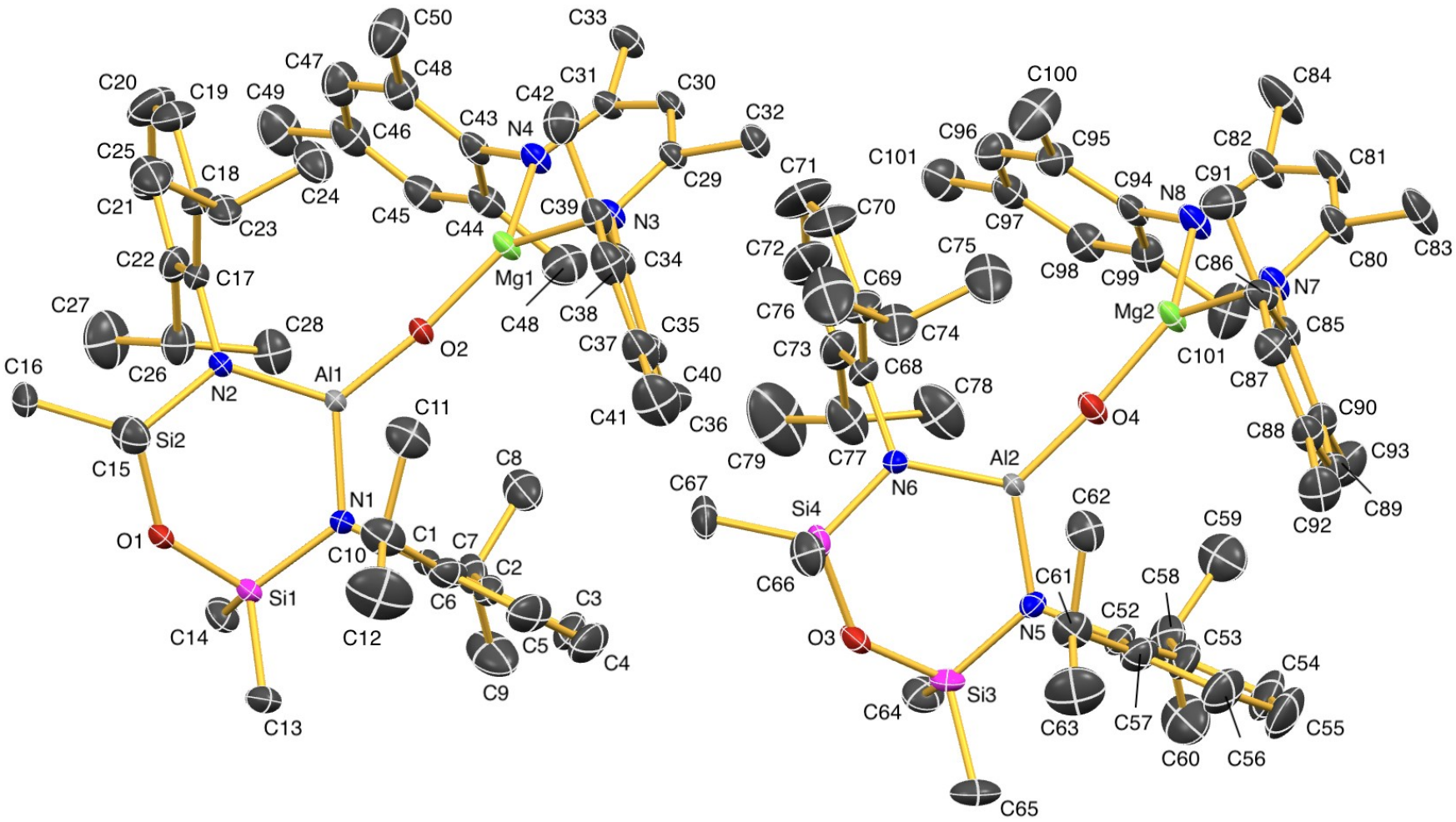


Figure S26 Thermal displacement plot (30 % probability) of (NON^{Dipp})Al(μ-O)Mg(BDI^{Mes}) (**4-Mg**).



Synthesis of (NON^{Dipp})Al(μ-CO_3)Zn(BDI^{Mes}) (5)

A solution of (NON^{Dipp})Al(μ-O)Zn(BDI^{Mes})] (56 mg, 0.06 mmol) in toluene-D_8 was transferred to a J. Youngs NMR tube. The solution was degassed and $^{13}CO_2$ (~1 atm.) was administered to the reaction vessel (condensed from lecture bottle at –196 °C). The solvent was removed *in vacuo* and the resulting white residue dissolved in hexane. Crystallisation was achieved by slow evaporation from a hexane solution stored at room temperature. Yield 52 mg, 89%.

Accurate elemental analysis could not be obtained for this compound, likely due to high oxygen and moisture sensitivity and possible decomposition during sample preparation and analysis.

^{1}H NMR (500 MHz, C_6D_6): δ 7.11 (s, 6H, C_6H_3), 6.73 (s, 4H, C_6H_2), 4.70 (s, 1H, BDI-C*H*), 4.01 (hept, J = 6.8 Hz, 4H, C*H*Me$_2$), 2.25 (s, 6H, *p*-*Me*), 1.75 (s, 12H, *o*-*Me*), 1.39 (d, J = 6.8 Hz, 12H, CH*Me$_2$*), 1.37 (s, 6H, BDI-*Me*), 1.10 (d, J = 6.8 Hz, 12H, CH*Me$_2$*), 0.38 (s, 12H, Si*Me$_2$*).

^{13}C{^{1}H} NMR (126 MHz, C_6D_6): δ 170.9 (BDI-*C*Me), 168.4 (*^{13}CO$_2$*), 167.0, 146.6, 142.5, 141.3, 134.9, 131.0, 129.9, 124.7, 123.8, 123.7 (C_6H_3, C_6H_2), 96.2 (BDI-*C*H), 27.9 (*C*HMe$_2$), 25.8, 24.8 (CH*Me$_2$*), 22.8 (BDI-*Me*), 21.0 (*p*-*Me*), 18.1 (*o*-*Me*), 2.2 (Si*Me$_2$*).

Figure S27 ^{1}H NMR spectrum (500 MHz, C_6D_6) of (NON^{Dipp})Al(μ-CO_3)Zn(BDI^{Mes}) (**5**).

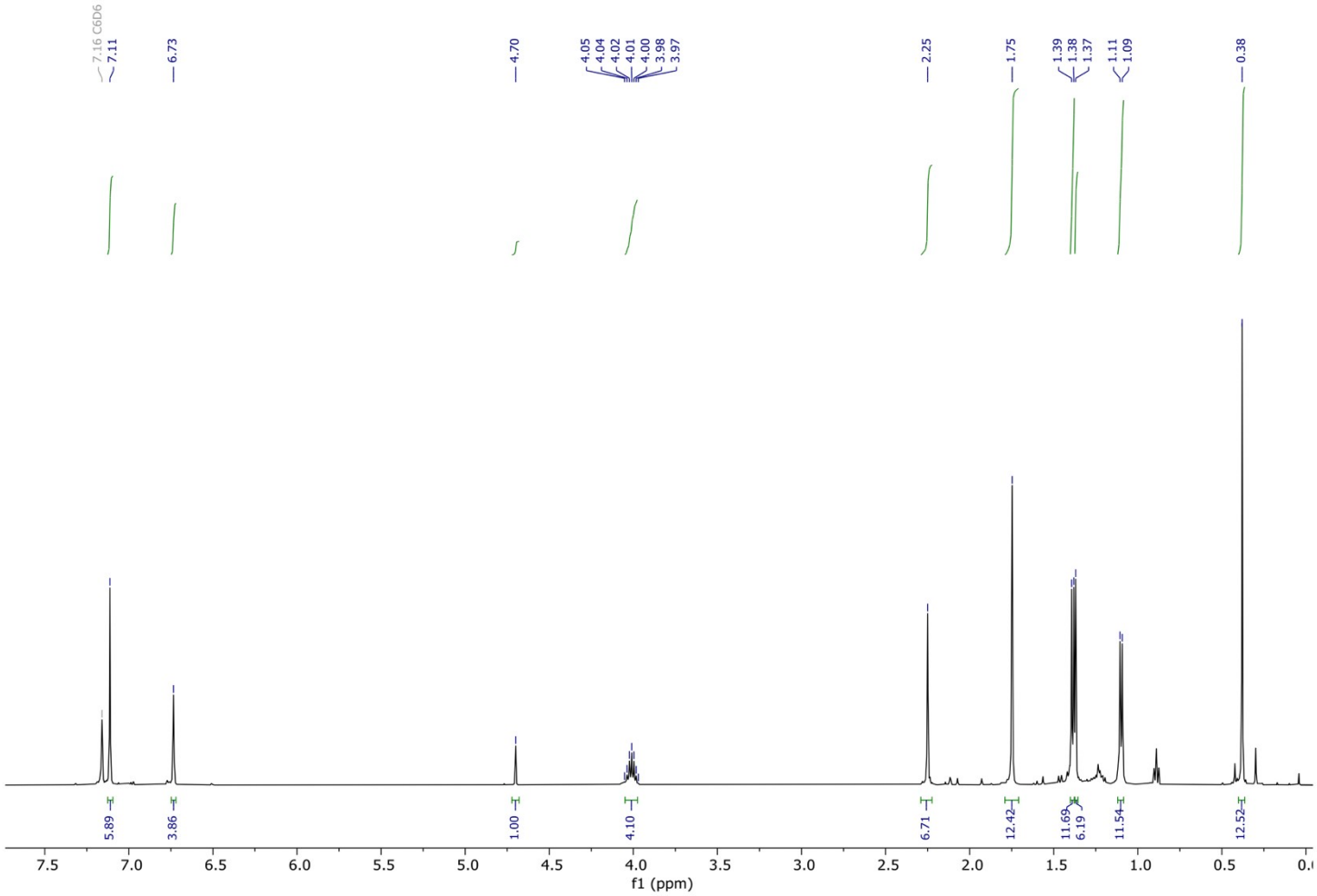


Figure S28 $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, C_6D_6) of (NON^{Dipp})Al(μ-CO_3)Zn(BDI^{Mes}) (**5**).

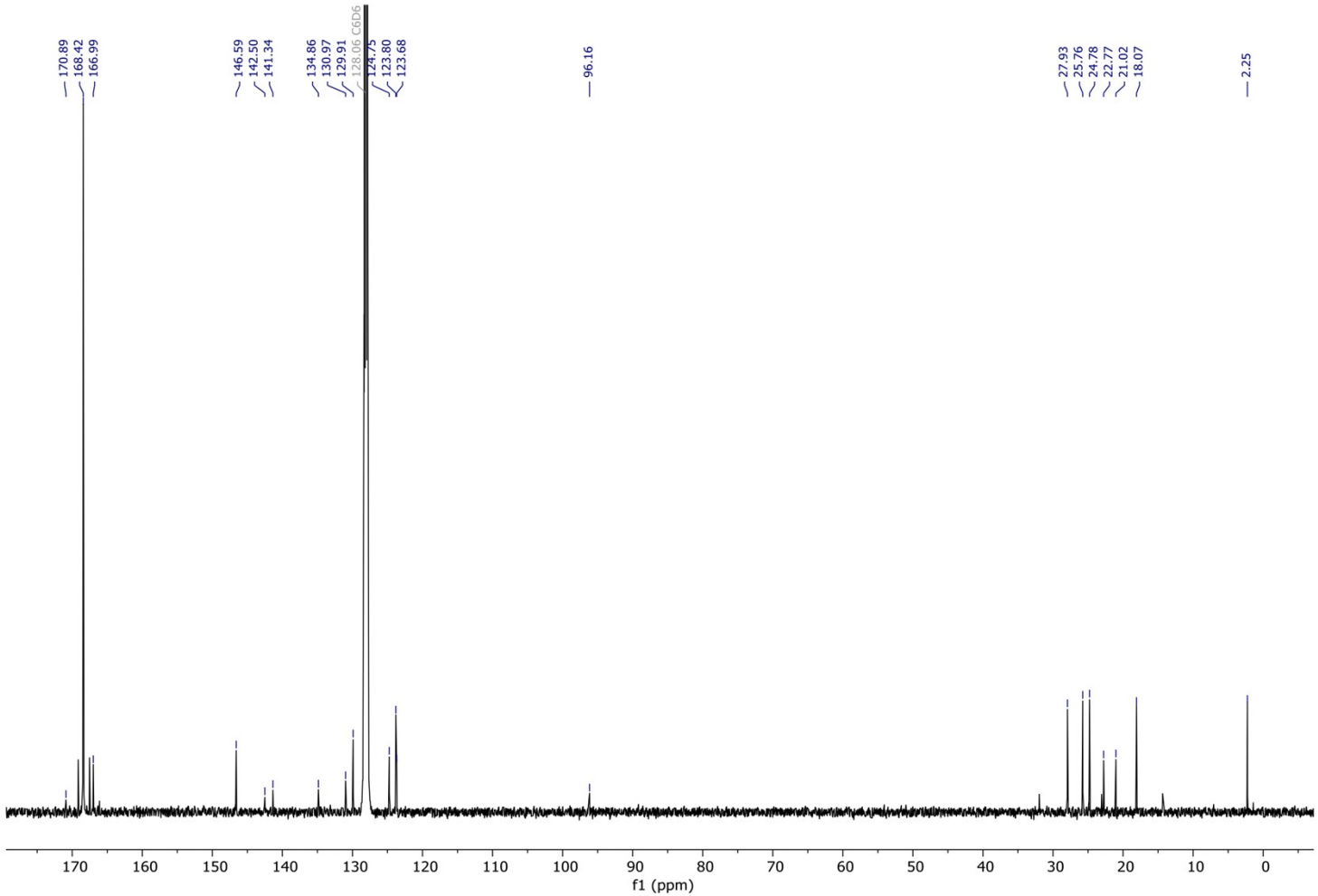
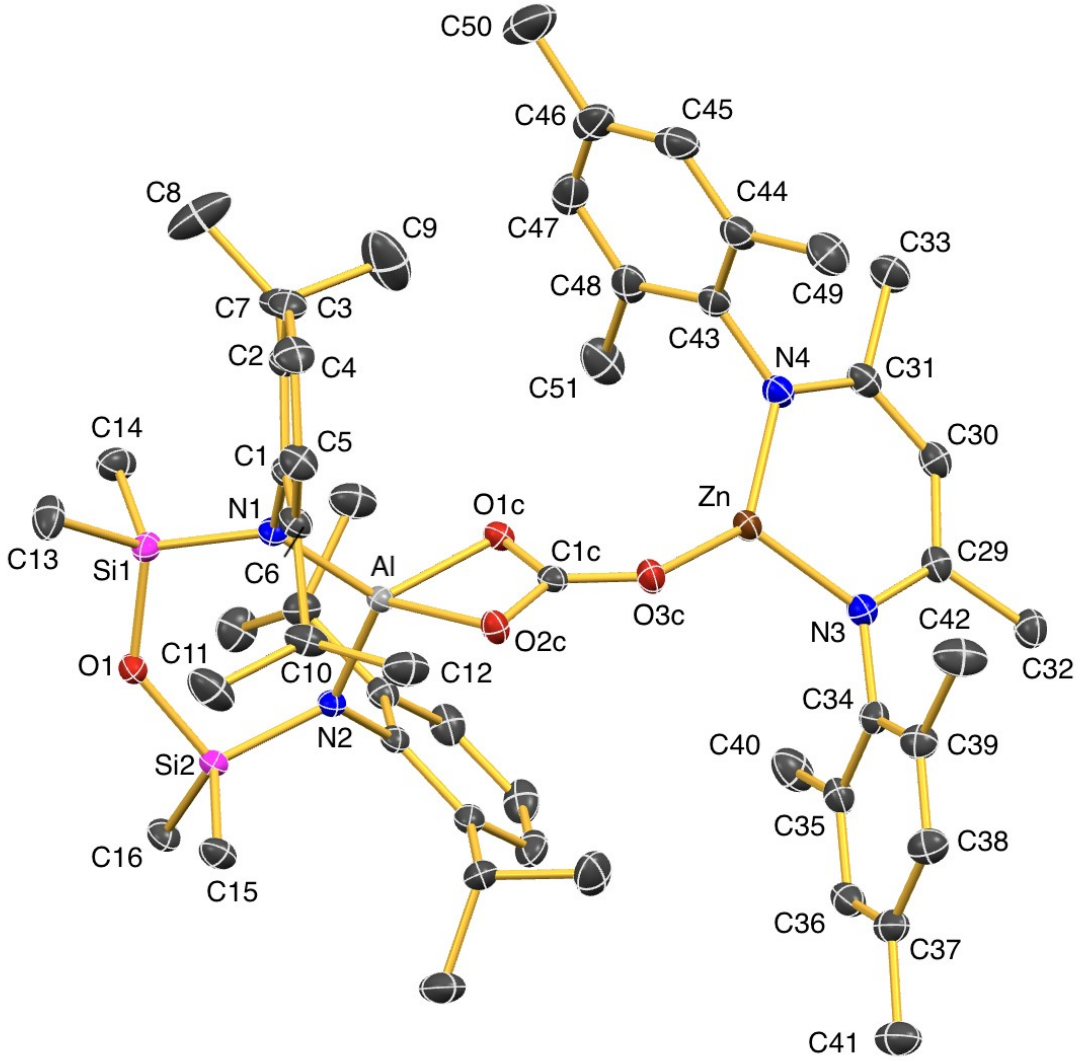


Figure S29 Thermal displacement plot (30 % probability) of(NON^{Dipp})Al(μ-CO_3)Zn(BDI^{Mes}) (**5**).



Computational Details

DFT calculations were run with Gaussian 16 (C.01).[S4] The Al, Si, P, Mg and Zn centres were described with the Stuttgart RECPs and associated basis sets,[S5] and the 6-31G** basis set was used for all other atoms (BS1).[S6] A polarization function was also added to Al (ζd = 0.190), Si (ζd = 0.284) and P (ζd = 0.387).[S7] Initial BP86 optimizations[S8] were performed using the 'grid = ultrafine' option, with all stationary points being fully characterized via analytical frequency calculations as minima or transition states (all positive eigenvalues or one imaginary eigenvalue respectively). All energies were recomputed with a larger basis set featuring 6-311++G** basis sets on all atoms. Corrections for the effect of benzene (ε = 2.2706) solvent were employed using the polarizable continuum model and BS1.[S9] Single-point dispersion corrections to the BP86 results employed Grimme's D3 parameter set with Becke-Johnson damping as implemented in Gaussian.[S10]

The Quantum Theory of Atoms in Molecules (QTAIM, AIMALL program)[S11] and Natural Bonding Orbital (NBO7[S12]) analyses were performed on the BP86-optmised geometries of **1-Mg**, **4-Mg, 1-Zn**, **4-Zn, [Al(NC$_2$N^{Dipp})]-Mg**, **[Al($_{Xanth}$NON^{Dipp})]-Mg**, **[Al($_{Xanth}$NON^{Dipp})]-Zn** and **[Al($_{Xanth}$NON^{Dipp})]-Li**. The QTAIM topological analyses used wavefunction files obtained at the BP86/6-311++G** level, whilst NBO analyses were carried out with NBO 7 within Gaussian 16 (C.01) at the same methodology level as the QTAIM calculations. Contour plots were generated in the AIMStudio package, using critical point (CP) visualisation threshold values of 0.025 *e* bohr^{-3} (solid line BCP = strong) and 0.02 *e* bohr^{-3} (dashed line BCP = weak).

Table S1 Computed QTAIM BCP data, interatomic distances (in Å) and WBIs for **1-Mg**, **1-Zn**, **4-Mg**, **4-Zn**, **[Al(NC$_2$N^{Dipp})]–Mg**, **[Al($_{xanth}$NON^{Dipp})]–Mg**, **[Al($_{xanth}$NON^{Dipp})]–Zn** and **[Al($_{xanth}$NON^{Dipp})]–Li**.

Asterisk denotes BCP is under the threshold of 0.02 for visualization in the corresponding Laplacian contour plot.

Complex	BCP	ρ(r)	∇²ρ(r)	ε	G(r)	V(r)	H(r)	DI(A|B)	R_{AB}	WBI
1-Mg	Al3 - Mg81	0.03083	0.028309	0.04386	0.013605	-0.02013	-0.00653	0.381463	2.80	0.6015
4-Mg	Al3 - O6	0.104281	0.874522	0.023981	0.218567	-0.2185	0.000064	0.428464	1.69	0.4255
	Mg4 - O6	0.065697	0.560808	0.009136	0.125653	-0.1111	0.014549	0.270464	1.84	0.0749
[Al(NC$_2$N^{Dipp})]–Mg	Al1 - Mg86	0.029404	0.023232	0.003636	0.012067	-0.01833	-0.00626	0.377625	2.85	0.6589
[Al($_{xanth}$NON^{Dipp})]–Mg	Al1 - Mg114	0.032735	0.033421	0.003409	0.015283	-0.02221	-0.00693	0.386029	2.76	0.6268
1-Zn	Zn1 - Al3	0.054633	-0.06299	0.120399	0.008707	-0.03316	-0.02446	0.705544	2.52	0.7401
4-Zn	Al4 - O6	0.101311	0.858249	0.027501	0.213088	-0.21161	0.001475	0.403974	1.70	0.3715
	Zn1 - O6	0.115768	0.659099	0.017047	0.184404	-0.20403	-0.01963	0.71041	1.82	0.1988
[Al($_{xanth}$NON^{Dipp})]–Zn	Zn1 - Al2	0.05736	-0.05187	0.119682	0.014576	-0.04212	-0.02755	0.637282	2.48	0.7442
[Al($_{xanth}$NON^{Dipp})]–Li	Al1 - Li144*	0.017811	0.032456	0.045272	-0.01102	0.009567	-0.00145	0.109863	2.78	0.3097

Table S2 Selected QTAIM and NBO atomic data for **1-Mg**, **1-Zn**, **4-Mg**, **4-Zn**, **[Al(NC$_2$N^{Dipp})]–Mg**, **[Al(**$_{Xanth}$**NON^{Dipp})]–Mg**, **[Al(**$_{Xanth}$**NON^{Dipp})]–Zn** and **[Al(**$_{Xanth}$**NON^{Dipp})]–Li**.

Complex	Atom	Vol(r)	Loc(r)	q(A)$_{AIM}$	q(A)$_{NBO7}$	q(A)$_{NBO7}$[†]
1-Mg	Al3	182.3954	92.29855	0.989647	0.98503	
	Mg81	77.70651	95.4012	1.513973	1.38126	
4-Mg	Al3	40.303809	94.014683	2.387243	2.21056	
	O6	187.46068	93.238026	-1.63577	-1.69546	
	Mg4	53.42904	96.38614	1.699277	1.81141	
[Al(NC$_2$N^{Dipp})]–Mg	Al1	181.83053	92.216446	1.001614	1.13864	
	Mg86	79.430356	95.476229	1.517331	1.27820	
[Al($_{Xanth}$**NON^{Dipp})]–Mg**	Al1	175.28208	92.398796	1.055461	0.99398	0.78822
	Mg114	71.942566	95.396063	1.513374	1.35405	1.48422
1-Zn	Al3	85.203333	91.765124	1.812006	1.28794	
	Zn1	185.05725	96.114087	0.331426	1.00385	
4-Zn	Al4	39.965208	94.026105	2.388986	2.23603	
	O6	162.67005	91.140775	-1.46555	-1.64700	
	Zn1	114.48646	96.31231	1.176645	1.64002	
[Al($_{Xanth}$**NON^{Dipp})]–Zn**	Al2	73.27507	92.407916	1.987558	1.26191	0.95981
	Zn1	177.25782	96.152346	0.226972	1.00110	1.26128
[Al($_{Xanth}$**NON^{Dipp})]–Li**	Al1	208.35093	93.204108	0.929222	0.79477	0.68705
	Li144	30.512036	92.875442	0.878518	0.71647	0.72517

[†] Data taken from reference 11: M. M. D. Roy, J. Hicks, P. Vasko, A. Heilmann, A.-M. Baston, J. M. Goicoechea and S. Aldridge, *Angew. Chem. Int. Ed.*, 2021, **60**, 22301-22306.

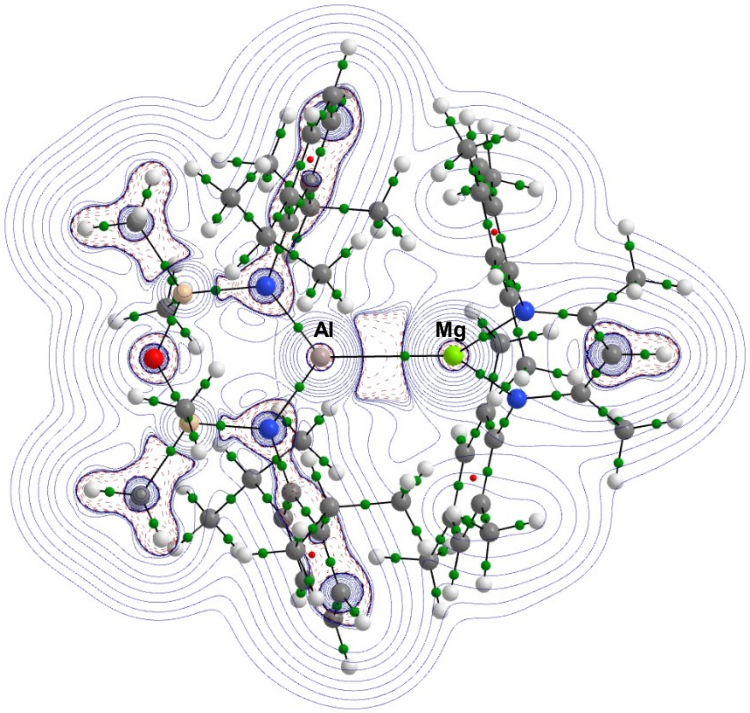
Table S3 NBO atomic charges for **[Al(**$_{Xanth}$**NON^{Dipp})]–Mg**, **[Al(**$_{Xanth}$**NON^{Dipp})]–Zn** and **[Al(**$_{Xanth}$**NON^{Dipp})]–Li** at different levels of theory.

Complex	Atom	q(A)$_{NBO7}$		
OPT METHOD =		**BP86/BS1**		**PBE0/SVP[†]**
SP METHOD =		**BP86/BS2**	**BP86/6-31G****	**PBE0/SVP[†]**
[Al($_{Xanth}$**NON^{Dipp})]–Mg**	Al1	0.99398	0.80498	0.78822
	Mg114	1.35405	1.40365	1.48422
[Al($_{Xanth}$**NON^{Dipp})]–Zn**	Al2	1.26191	0.97654	0.95981
	Zn1	1.00110	1.17592	1.26128
[Al($_{Xanth}$**NON^{Dipp})]–Li**	Al1	0.79477	0.65654	0.68705
	Li144	0.71647	0.73735	0.72517

[†] Data taken from reference 11: M. M. D. Roy, J. Hicks, P. Vasko, A. Heilmann, A.-M. Baston, J. M. Goicoechea and S. Aldridge, *Angew. Chem. Int. Ed.*, 2021, **60**, 22301-22306.

Figure S30 QTAIM contour plot of the Laplacian ($\nabla^2\rho(r)$) of **1-Mg**. (a) complete molecule; (b) focus on the Al-Mg motif. Bond critical points (BCPs) shown as small green spheres.

(a)



(b)

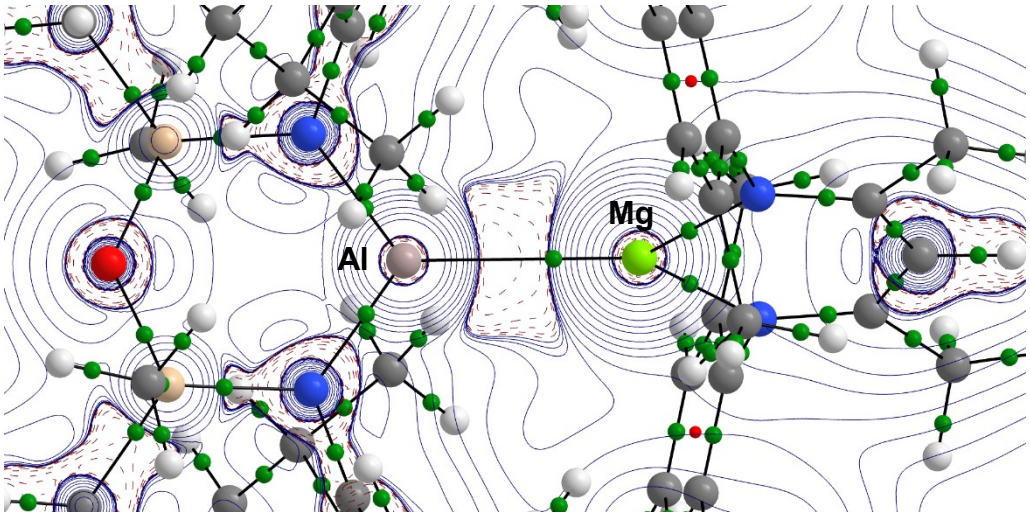
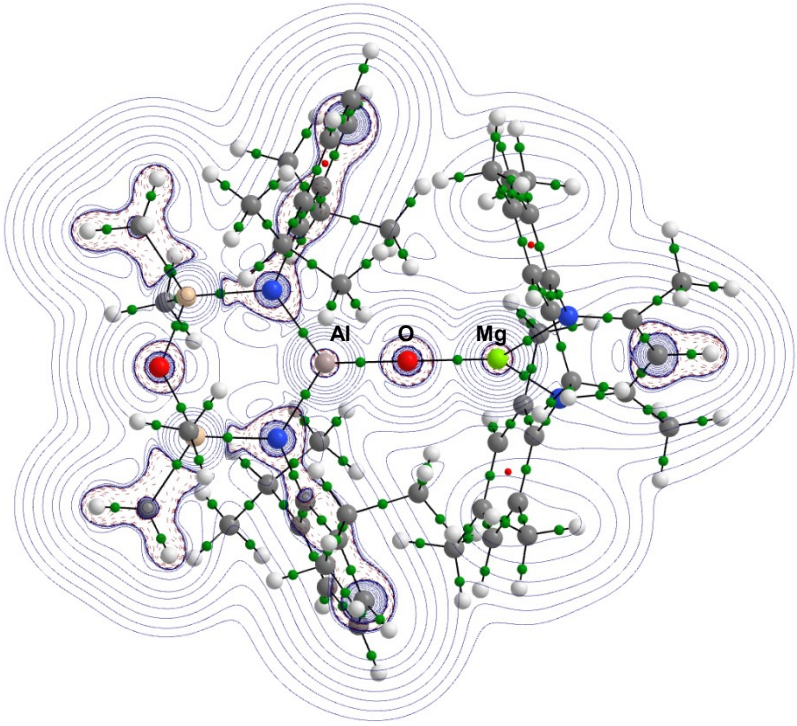


Figure S31 QTAIM contour plot of the Laplacian ($\nabla^2\rho(r)$) of **4-Mg**. (a) complete molecule; (b) focus on the Al-O-Mg motif. Bond critical points (BCPs) shown as small green spheres.

(a)



(b)

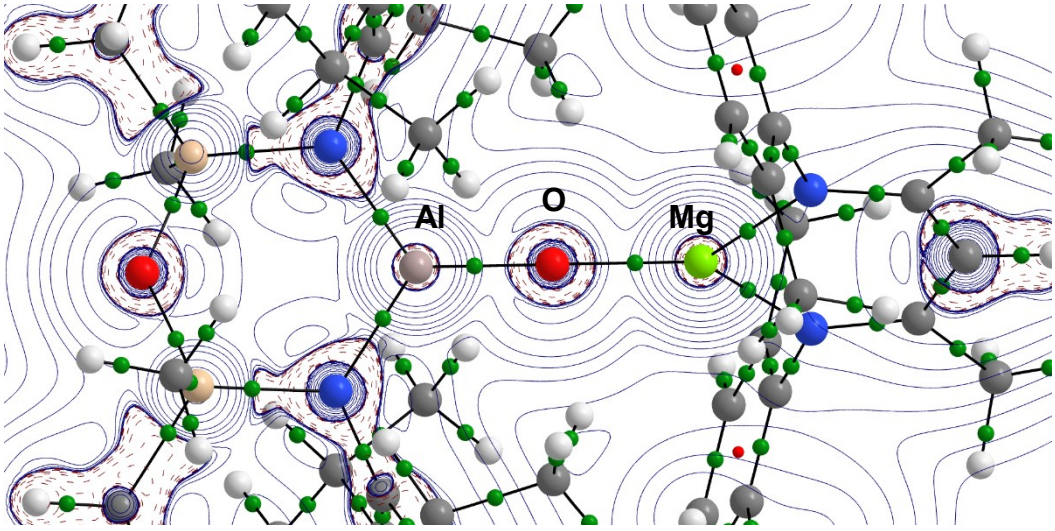
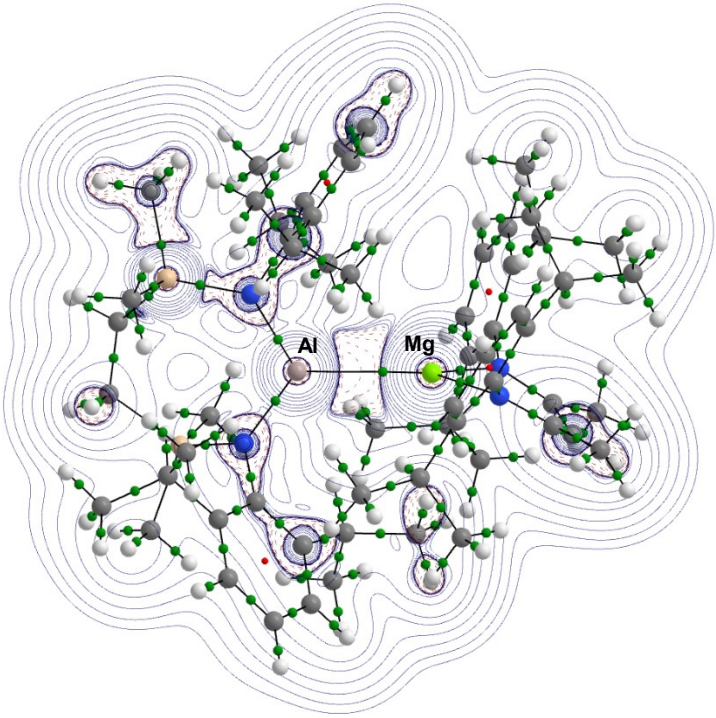


Figure S32 QTAIM contour plot of the Laplacian ($\nabla^2\rho(r)$) of **[Al(NC$_2$N^{Dipp})]–Mg**. (a) complete molecule; (b) the Al-Mg motif. Bond critical points (BCPs) shown as small green spheres.

(a)



(b)

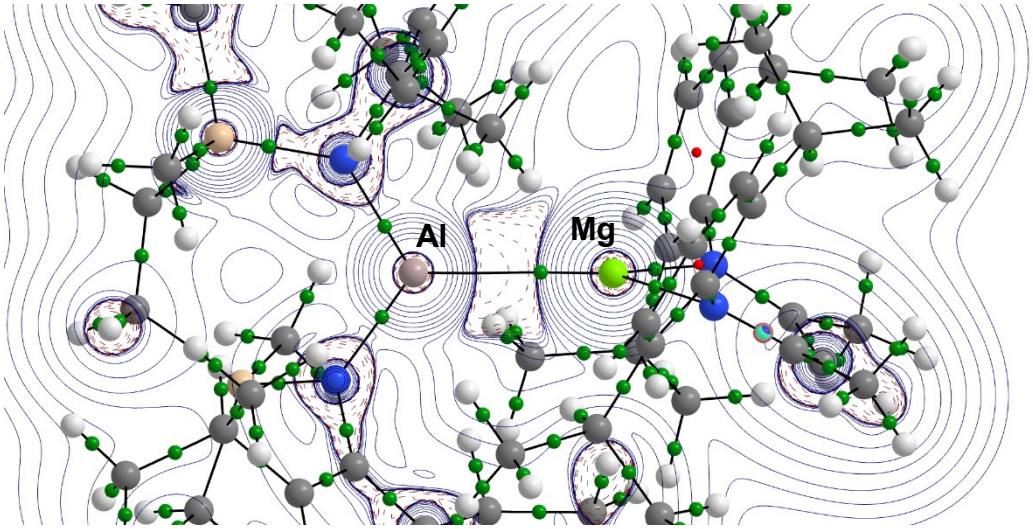
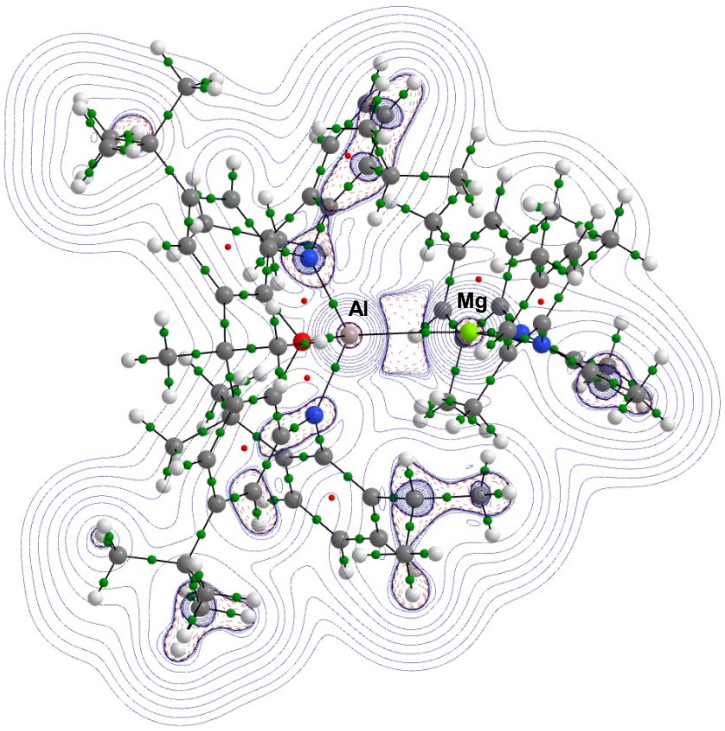


Figure S33 QTAIM contour plot of the Laplacian ($\nabla^2\rho(r)$) of **[Al($_{Xanth}$NON^{Dipp})]–Mg**. (a) complete molecule; (b) focus on the Al-Mg motif). Bond critical points (BCPs) shown as small green spheres.

(a)



(b)

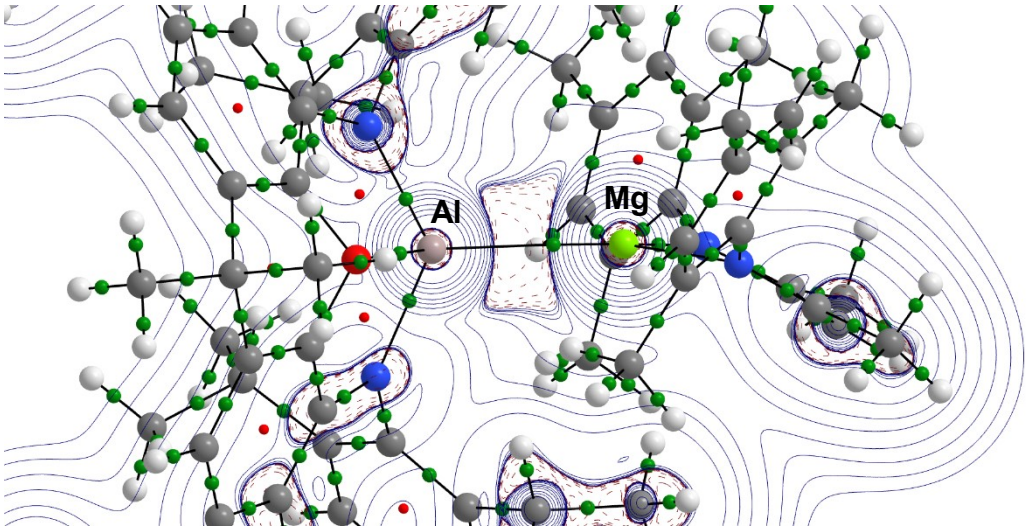
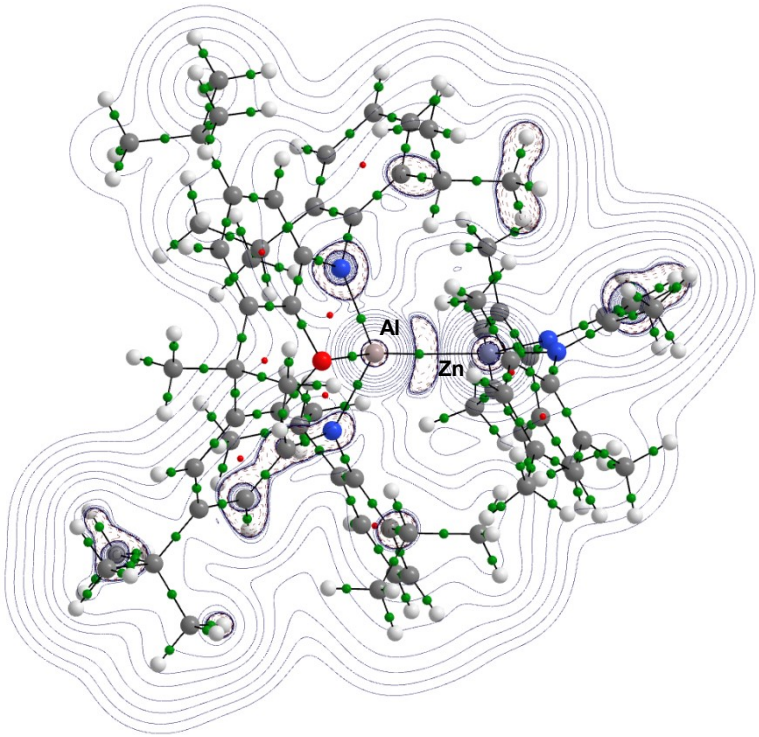


Figure S34 QTAIM contour plot of the Laplacian ($\nabla^2\rho(r)$) of **1-Zn**. (a) complete molecule; (b) focus on the Al-Zn motif. Bond critical points (BCPs) shown as small green spheres.

(a)



(b)

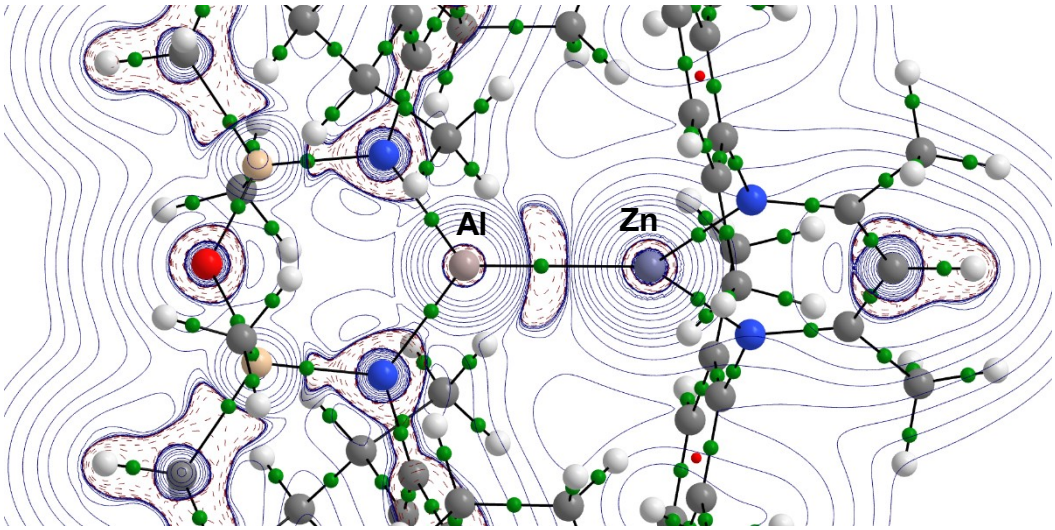
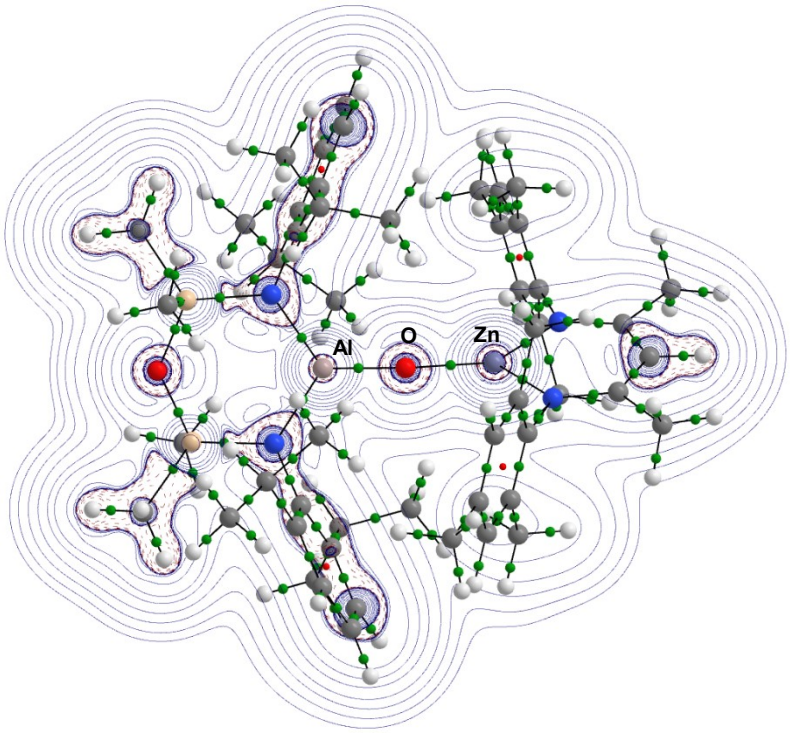


Figure S35 QTAIM contour plot of the Laplacian ($\nabla^2\rho(r)$) of **4-Zn**. (a) complete molecule; (b) focus on the Al-O-Zn motif. Bond critical points (BCPs) shown as small green spheres.

(a)



(b)

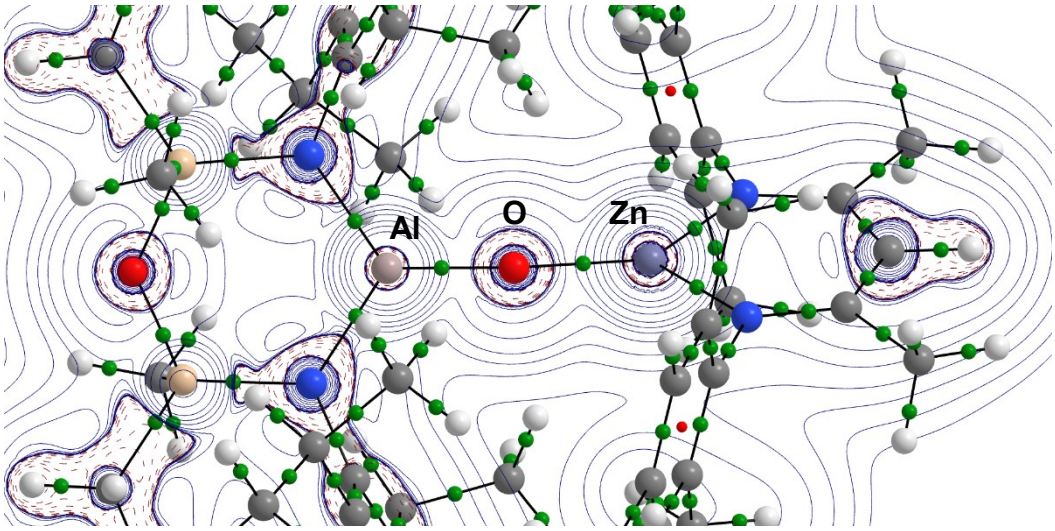
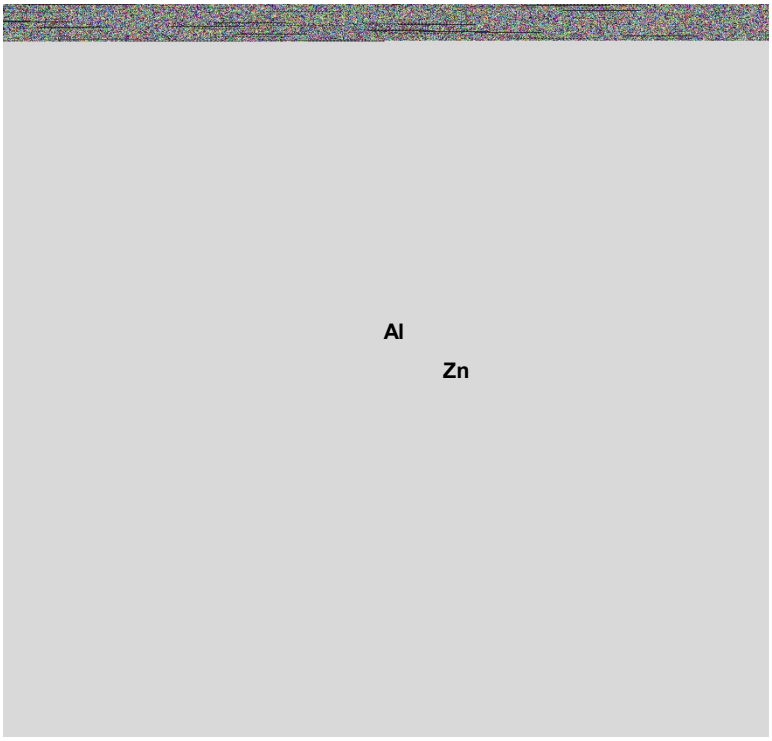


Figure S36 QTAIM contour plot of the Laplacian ($\nabla^2\rho(r)$) of **[Al($_{xanth}$NON^{Dipp})]–Zn**. (a) complete molecule; (b) focus on the Al-Zn motif. Bond critical points (BCPs) shown as small green spheres.

(a)



(b)

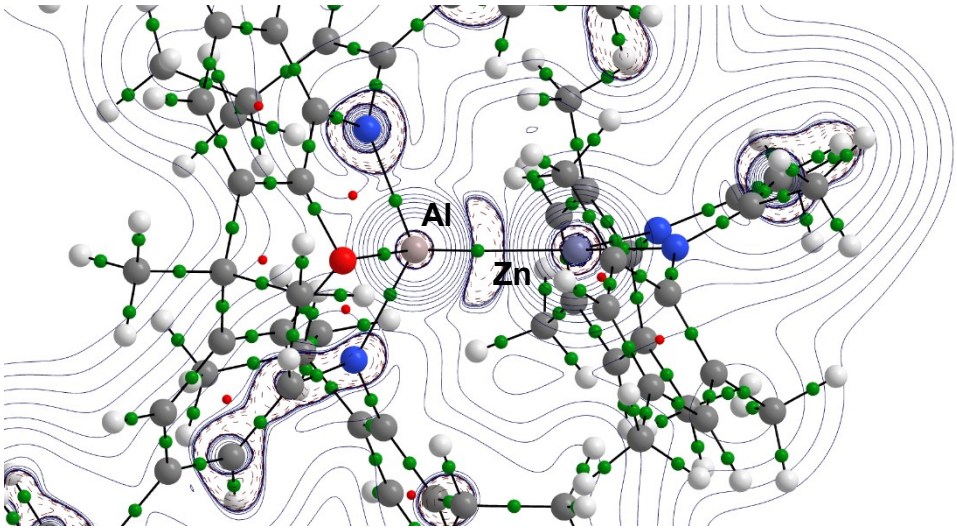
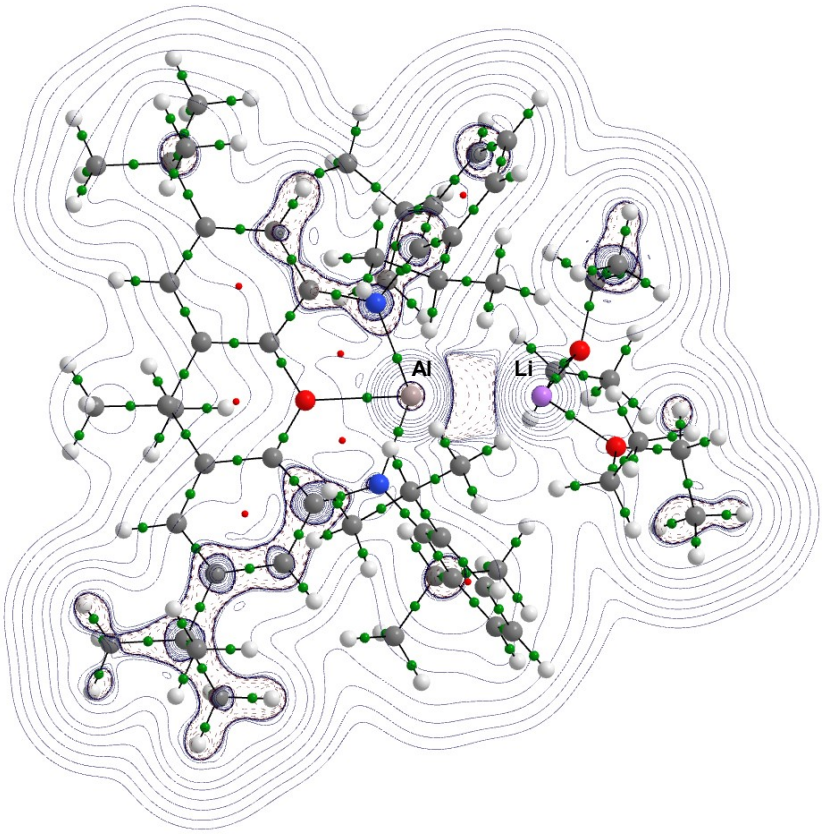


Figure S37 QTAIM contour plot of the Laplacian ($\nabla^2\rho(r)$) of **[Al($_{xanth}$NON^{Dipp})]–Li**. (a) complete molecule; (b) focus on the Al-Li motif. Bond critical points (BCPs) shown as small green spheres.

(a)



(b)

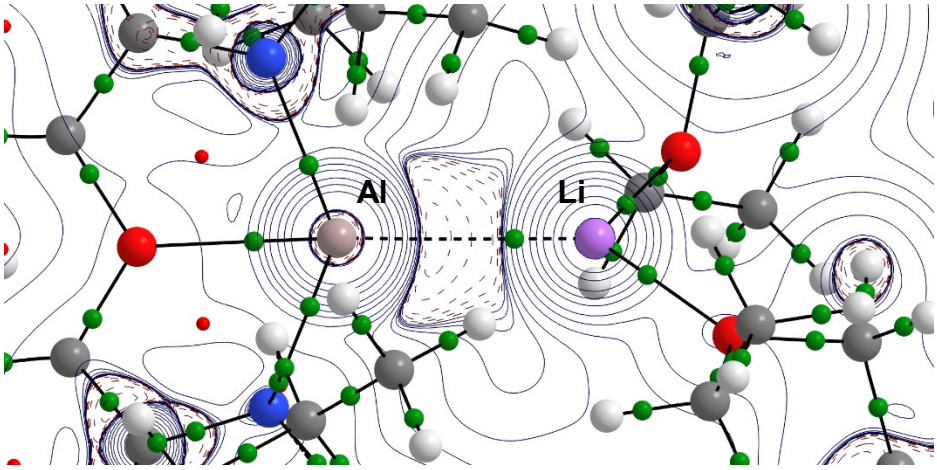


Table S4 Central bonding NLMO compositions in **1-Mg**, **1-Zn**, **[Al(NC$_2$N^{Dipp})]–Mg**, **[Al(**$_{Xanth}$**NON^{Dipp})]–Mg**, **[Al(**$_{Xanth}$**NON^{Dipp})]–Zn** and **[Al(**$_{Xanth}$**NON^{Dipp})]–Li**.

Complex	**Bond**	**Atom**	**Contribution to NLMO in % (*s, p, d* character)**			
			overall	***s orbital***	***p orbital***	***d* orbital**
1-Mg	Al-Mg	Al	75.84	78.24	21.69	0.07
		Mg	24.16	94.18	4.89	0.93
[Al(NC$_2$N^{Dipp})]–Mg	Al-Mg	Al	70.09	85.42	14.51	0.07
		Mg	29.91	93.73	5.42	0.85
[Al($_{Xanth}$**NON^{Dipp})]–Mg**	Al-Mg	Al	73.63	76.33	23.59	0.09
		Mg	26.37	96.42	3.16	0.41
1-Zn	Al-Zn	Al	57.27	81.90	18.02	0.09
		Zn	42.73	95.52	3.40	1.08
[Al($_{Xanth}$**NON^{Dipp})]–Zn**	Al-Zn	Al	56.61	77.49	22.41	0.10
		Zn	43.39	96.41	2.57	1.02
[Al($_{Xanth}$**NON^{Dipp})]–Li**	Al-Li	Al	n/a	n/a	n/a	n/a
		Li	n/a	n/a	n/a	n/a

Note: for **[Al(**$_{Xanth}$**NON^{Dipp})]–Li**, no formal Al-Li bond was identified in the NBO search, only a strong donor-acceptor interaction in the second-order perturbation energy analysis, where $\Delta E[LP_{Al} \rightarrow n\text{Li}^*] = 42.1$ kcal/mol.

Table S5 Selected donor acceptor interaction energies (in kcal mol^{-1}), $\Delta E^{(2)}$, for **4-Mg** and **4-Zn** resulting from second-order perturbation energy analysis of the Fock matrix in NBO basis.

4-Mg				**4-Zn**		
Donor NBO (Unit)	**Acceptor NBO (Unit)**	**$\Delta E^{(2)}$ (kcal/mol)**		**Donor NBO (Unit)**	**Acceptor NBO (Unit)**	**$\Delta E^{(2)}$ (kcal/mol)**
LP_{O6} (1)	n_{Al4}* (2)	37.7		LP_{O6} (1)	n_{Al3}* (2)	50.9
LP_{O6} (1)	n_{Al4}* (2)	20.8		LP_{O6} (1)	n_{Al3}* (2)	26.1
LP_{O6} (1)	n_{Al4}* (2)	8.1		LP_{O6} (1)	n_{Al3}* (2)	8.3
LP_{O6} (1)	n_{Al4}* (2)	6.0		LP_{O6} (1)	n_{Al3}* (2)	7.6
LP_{O6} (1)	n_{Al3}* (2)	5.4		LP_{O6} (1)	n_{Al3}* (2)	6.7
LP_{O6} (1)	n_{Zn1}* (3)	49.3		LP_{O6} (1)	n_{Mg4}* (3)	16.2
LP_{O6} (1)	n_{Zn1}* (3)	9.0				

Figure S38 NBOs of **4-Mg** involved in the donor acceptor interactions as out lined in Table S5. Arene substituents on both the [Al] and [Mg] complexes, and all hydrogen atoms have been removed for clarity. Al = pink, Mg = orange.

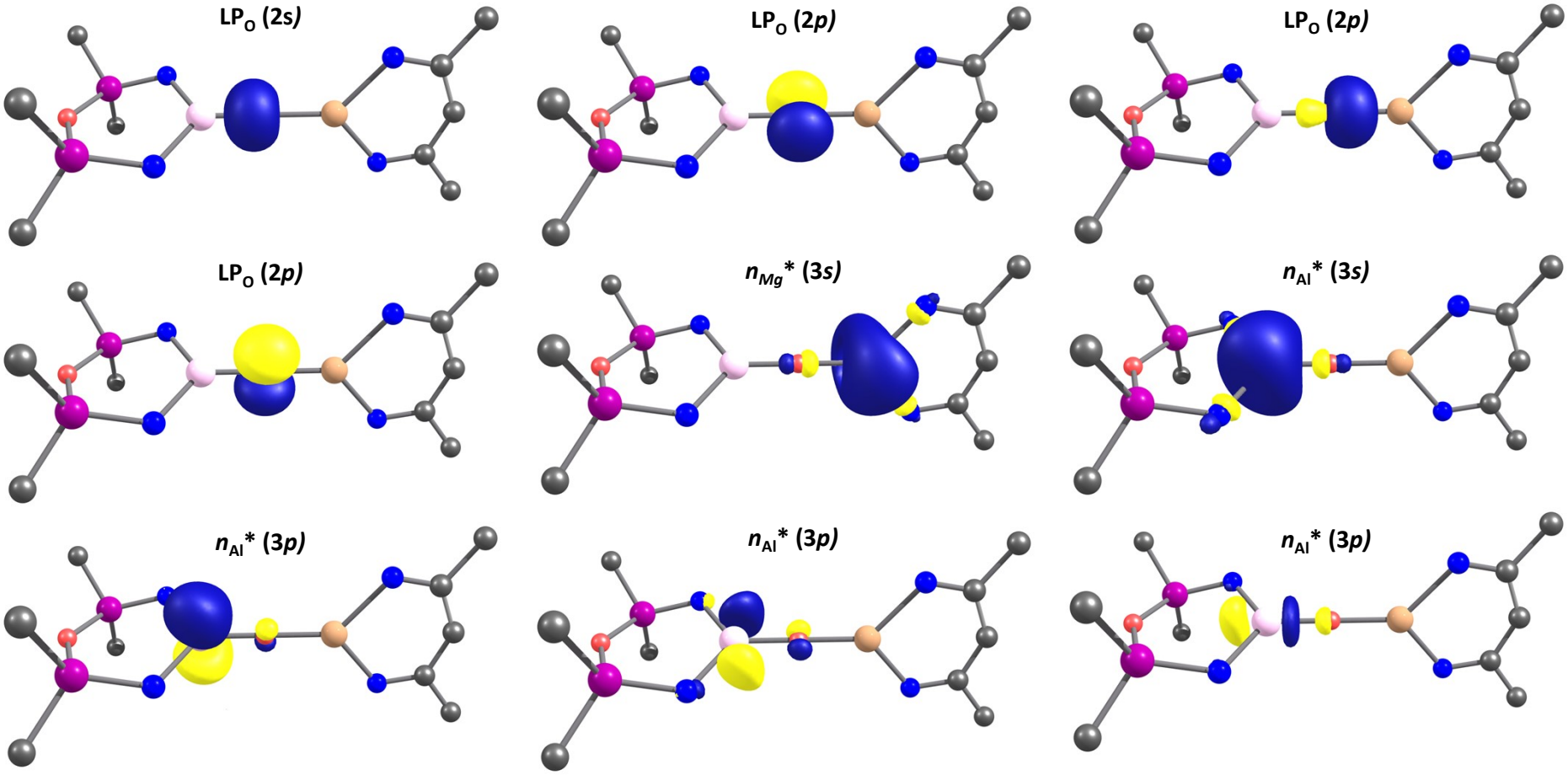
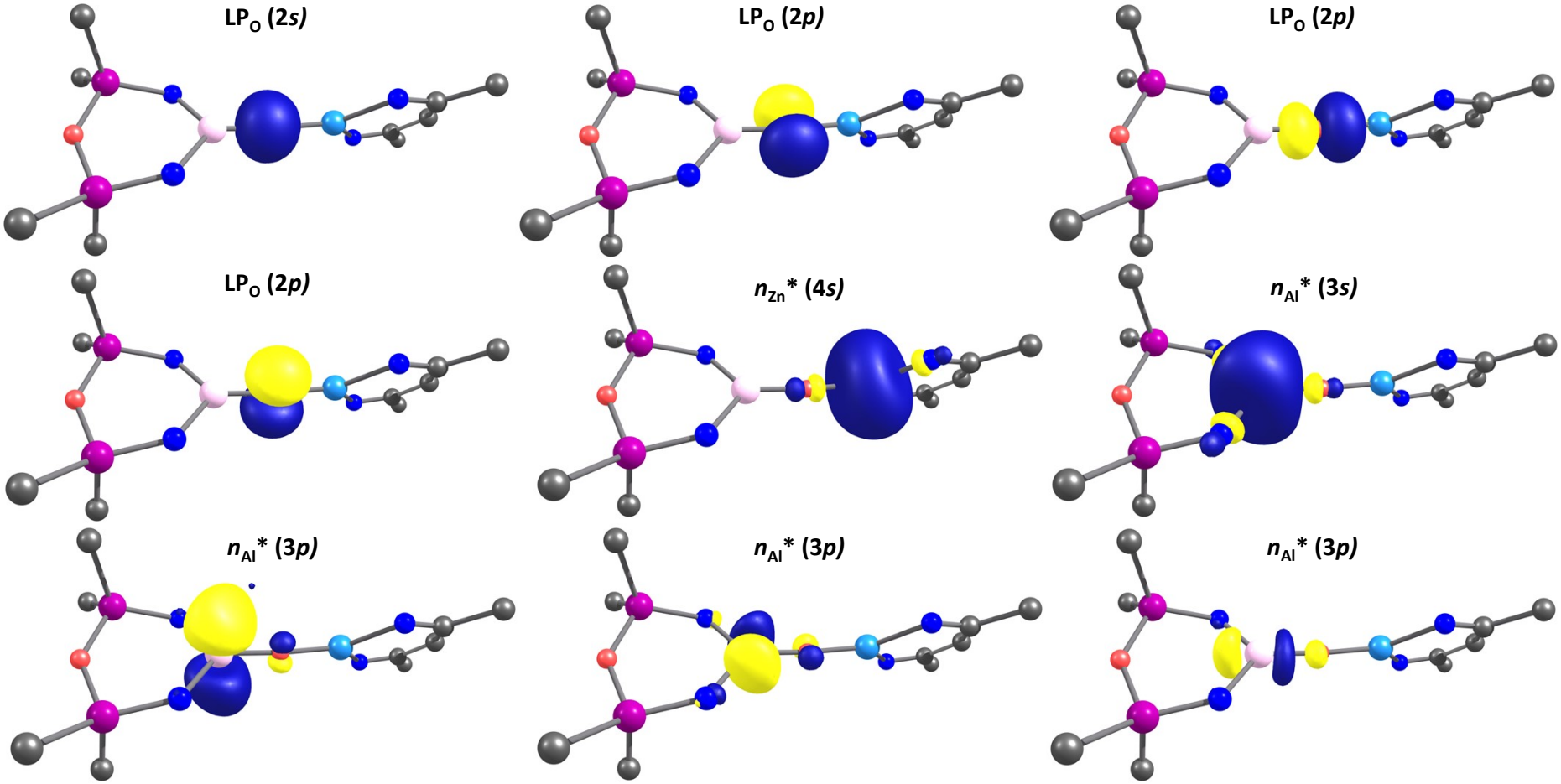


Figure S39 NBOs of **4-Zn** involved in the donor acceptor interactions as out lined in Table S5. Arene substituents on both the [Al] and [Zn] complexes, and all hydrogen atoms have been removed for clarity. Al = pink, Zn = blue.



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Crystallographic Details

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 120 K or 150 K 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.[S13] Space groups were determined from systematic absences and checked for higher symmetry. All structures were solved using direct methods with SHELXS,[S14] refined on F^2 using all data by full matrix least-squares procedures with SHELXL-97,[S15] within the WinGX[S16] 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*(*F2o-F2c),* with *w* = [σ2(*F2o*) + *a*P2 + *bP*]–1, where *P* = [max(*Fo*)2 + 2*F2c*]/3. The isotropic displacement parameters are 1.2 or 1.5 times the isotropic equivalent of their carrier atoms.

Additional Information:

(NON^{Dipp})Al–Zn(BDI^{Mes}) (***1-Zn***): The molecule is located on a C2-axis that passes through the Al-Zn bond. The unit cell contains poorly defined toluene solvate molecules that have been treated as a diffuse contribution to the overall scattering without specific atom positions by SQUEEZE/PLATON. Details are given in the .cif.

(NON^{Dipp})Al(μ-O$_2$C)Zn(BDI^{Mes}) (***2***): The toluene solvate is on an inversion centre and was modelled as a full molecule at 50% occupancy. One of the ortho-Me groups of a Mes substituent is disordered and was modelled over two positions with SADI restraints applied.

{(NON^{Dipp})Al(μ-CO$_3$)}$_2${Mg(THF)$_4$} (***3***): One of the methylene groups of a coordinated THF is disordered and was modelled over two positions. The oxygen atom of the THF solvate is also disordered and was modelled over two positions.

(NON^{Dipp})Al(μ-O)Zn(BDI^{Mes}) (***4-Zn***): The aromatic group of one of the NON-ligands is disordered and the C6-ring and one of the iPr substituents were modelled over two positions. In addition, the asymmetric unit contains 4 poorly defined toluene solvate molecules. These were treated as a diffuse contribution to the overall scattering without specific atom positions by SQUEEZE/PLATON. Details are given in the .cif.

(NON^{Dipp})Al(μ-O)Mg(BDI^{Mes}) (***4-Mg***): The asymmetric unit contains 4 poorly defined toluene solvate molecules. These were treated as a diffuse contribution to the overall scattering without specific atom positions by SQUEEZE/PLATON. Details are given in the .cif.

Table S6 Crystal structure and refinement data for **1-Zn**, **1-Mg** and **2**

	1-Zn	**1-Mg**	**2**
Empirical formula	$C_{58}H_{85}AlN_4OSi_2Zn$	$C_{51}H_{75}AlMgN_4OSi_2$	$C_{215}H_{308}Al_4N_{16}O_{12}Si_8Zn_4$
CCDC Number	2183690	2183691	2183692
M_r	1000.81	867.62	3902.97
T [K]	120.0(1)	150(2)	150.0(1)
Crystal size [mm]	0.48 × 0.13 × 0.11	0.22 × 0.13 × 0.08	0.20 × 0.14 × 0.11
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	C2/c (No.15)	$P2_1/n$ (alternative No.14)	$P\bar{1}$ (No. 2)
a [Å]	19.79296(16)	11.5558(2)	14.3252(2)
b [Å]	12.46075(9)	18.8726(3)	19.0153(3)
c [Å]	26.05702(19)	24.3018(4)	22.8866(3)
α [°]	90	90	73.2612(13)
β [°]	97.9035(7)	90.5318(13)	86.3624(13)
γ [°]	90	90	71.2352(15)
V [Å^3]	6365.53(8)	5299.69(15)	5649.87(16)
Z	4	4	1
$D_{calc.}$ [mg m^{-3}]	1.044	1.088	1.147
Absorption coefficient [mm^{-1}]	1.302	1.162	1.482
θ range for data collection [°]	4.2039 to 72.176	3.6378 to 73.4215	3.6679 to 73.6941
Reflections collected	20014	34093	78880
Independent reflections	6202 [R_{int} 0.015]	10464 [R_{int} 0.034]	22585 [R_{int} 0.031]
Reflections with $I > 2\sigma(I)$	5876	8804	20053
Data/restraints/parameters	6202 / 0 / 283	10464 / 0 / 561	22585 / 3 / 1250
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.031, wR_2 = 0.088	R_1 = 0.040, wR_2 = 0.102	R_1 = 0.035, wR_2 = 0.092
Final R indices (all data)	R_1 = 0.033, wR_2 = 0.089	R_1 = 0.049, wR_2 = 0.109	R_1 = 0.040, wR_2 = 0.096
GOOF on F^2	1.02	1.04	1.018
Largest diff. peak/hole [e.Å^{-3}]	0.27 and –0.26	0.26 and –0.21	0.57 and –0.39

Table S7 Crystal structure and refinement data for **3**, **4-Zn**, **4-Mg** and **5**

	3	**4-Zn**	**4-Mg**	**5**
Empirical formula	$C_{78}H_{132}Al_2MgN_4O_{13}Si_4$	$C_{130}H_{182}Al_2N_8O_4Si_4Zn_2$	$C_{130}H_{182}Al_2Mg_2N_8O_4Si_4$	$C_{52}H_{75}AlN_4O_4Si_2Zn$
CCDC Number	2183693	2183694	2183695	2183696
M_r	1524.5	2217.89	2135.77	968.69
T [K]	120.0(1)	150.0(1)	150.0(1)	150.0(1)
Crystal size [mm]	0.18 × 0.12 × 0.08	0.48 × 0.37 × 0.12	0.40 × 0.24 × 0.12	0.31 × 0.13 × 0.08
Crystal system	Triclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P\bar{1}$ (No. 2)	$P2_1/c$ (No. 14)	$P2_1/c$ (No. 14)	$P2_1/c$ (No. 14)
a [Å]	16.8558(7)	19.0790(2)	19.0122(4)	14.56239(17)
b [Å]	17.0958(8)	26.4548(3)	26.6902(5)	15.0196(2)
c [Å]	19.1000(6)	26.1164(3)	26.0942(6)	25.1167(3)
α [°]	115.826(4)	90	90	90
β [°]	93.517(3)	96.4642(10)	96.081(2)	97.8850(10)
γ [°]	114.756(4)	90	90	90
V [Å^3]	4294.2(3)	13098.0(2)	13166.0(5)	5441.60(11)
Z	2	4	4	4
$D_{calc.}$ [mg m^{-3}]	1.179	1.133	1.078	1.182
Absorption coefficient [mm^{-1}]	1.382	1.331	1.031	1.55
θ range for data collection [°]	3.6353 to 73.3746	3.4672 to 73.3138	3.4573 to 73.4317	3.747 to 73.24
Reflections collected	62418	91143	87564	40320
Independent reflections	17097 [R_{int} 0.055]	26101 [R_{int} 0.031]	26221 [R_{int} 0.043]	10851 [R_{int} 0.027]
Reflections with $I > 2\sigma(I)$	13500	20965	18454	9420
Data/restraints/parameters	17097 / 28 / 963	26101 / 0 / 1162	26221 / 0 / 1139	10851 / 0 / 597
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.078, wR_2 = 0.210	R_1 = 0.051, wR_2 = 0.154	R_1 = 0.068, wR_2 = 0.193	R_1 = 0.034, wR_2 = 0.088
Final R indices (all data)	R_1 = 0.095, wR_2 = 0.223	R_1 = 0.063, wR_2 = 0.162	R_1 = 0.089, wR_2 = 0.211	R_1 = 0.041, wR_2 = 0.093
GOOF on F^2	1.059	1.082	0.947	1.012
Largest diff. peak/hole [e.Å^{-3}]	1.24 and –0.53	0.36 and –0.47	0.37 and –0.67	0.36 and –043

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Cartesian Coordinates and Computed Energies (in Hartrees) for Calculated Structures

1-Mg

SCF (BP86) Energy = -2293.85429396
Enthalpy 0K = -2292.736029
Enthalpy 298K = -2292.660484
Free Energy 298K = -2292.848804
Lowest Frequency = 11.4634 cm^{-1}
Second Frequency = 18.7712 cm^{-1}

Si	0.61978	-3.80684	1.40893
Si	-0.70238	-3.79769	-1.40324
Al	-0.01121	-0.97725	-0.00204
O	-0.04683	-4.48180	0.00324
N	1.05273	-2.10294	1.07072
N	-1.09964	-2.08379	-1.07028
C	2.29674	-1.63447	1.62820
C	3.49874	-1.72713	0.85364
C	4.71237	-1.28065	1.40769
H	5.62925	-1.35375	0.81362
C	4.77703	-0.76192	2.70728
H	5.73434	-0.43204	3.12551
C	3.60668	-0.68234	3.46796
H	3.65311	-0.28303	4.48819
C	2.36412	-1.10929	2.95618
C	3.47492	-2.30560	-0.56142
H	2.60323	-2.98161	-0.61090
C	3.25421	-1.19355	-1.61063
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H	4.06452	-0.44594	-1.57574
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H	5.62910	-2.50487	-1.01525
H	4.58077	-3.64249	-1.88505
H	4.93533	-3.90404	-0.15402
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H	0.35539	-1.75811	5.75602
H	2.09562	-1.38143	5.79308
C	2.14468	-4.82474	1.87765
H	1.83663	-5.86697	2.06902
H	2.62848	-4.43623	2.78882
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H	0.20731	-3.78944	-3.75942
H	0.93683	-5.08232	-2.76975
C	-2.24906	-4.78545	-1.86533
H	-1.96289	-5.83432	-2.05442
H	-2.72739	-4.38980	-2.77630
H	-2.99565	-4.77546	-1.05543
C	-2.33298	-1.59129	-1.63099
C	-2.38770	-1.06824	-2.96042
C	-3.62059	-0.61774	-3.47538
H	-3.65727	-0.22024	-4.49670
C	-4.79354	-0.67161	-2.71654
H	-5.74334	-0.32361	-3.13719
C	-4.74144	-1.18799	-1.41545
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C	-1.32116	-1.77726	-5.16547
H	-1.58598	-2.83006	-4.96975
H	-0.38797	-1.76173	-5.75603
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H	-2.67035	-2.92584	0.61103
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H	-2.33123	-0.59500	1.42539
H	-3.25539	-1.54011	2.62850
H	-4.08230	-0.35888	1.56572
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H	-5.68712	-2.38877	1.00749
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H	0.05699	6.24557	-0.01832
C	-1.19248	4.57875	0.35026
C	2.43106	5.51713	-0.63999
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H	2.11338	6.56125	-0.50602
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H	-1.99385	6.59820	0.46964
H	-2.72026	5.45820	1.64097
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C	4.41969	2.33238	-2.64411
H	4.65866	2.26735	-3.71330
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H	5.82737	1.88178	0.42518
C	3.78527	2.49545	0.09151
C	2.08635	3.04467	-3.32157
H	1.75484	4.09739	-3.26668
H	1.17747	2.42917	-3.20786
H	2.48843	2.87112	-4.33265
C	6.82243	1.67589	-2.13038
H	6.81638	1.02237	-3.01934
H	7.37149	1.15494	-1.32891
H	7.40698	2.57639	-2.39609
C	3.46206	2.57715	1.56661
H	4.37076	2.44976	2.17484
H	2.76170	1.77750	1.87123
H	2.99382	3.53994	1.83560
C	-2.74377	2.85800	0.88731
C	-3.73233	2.55742	-0.08301
C	-5.02472	2.20730	0.35165
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C	-5.36284	2.13888	1.71470
C	-4.35767	2.42741	2.65633
H	-4.59557	2.38245	3.72678
C	-3.05265	2.78417	2.27108
C	-3.41555	2.63026	-1.55990
H	-2.72416	1.82259	-1.86387
H	-2.93901	3.58710	-1.83566

H -4.32817 2.50865 -2.16335
C -6.75533 1.74045 2.15793
H -6.81658 0.65673 2.37012
H -7.50560 1.96330 1.38122
H -7.05299 2.26693 3.08054
C -2.01162 3.11213 3.31876
H -1.11425 2.47845 3.21352
H -2.41501 2.96129 4.33296
H -1.66120 4.15764 3.24710

1-Zn
SCF (BP86) Energy = -2520.22693586
Enthalpy 0K = -2519.108200
Enthalpy 298K = -2519.032787
Free Energy 298K = -2519.219363
Lowest Frequency = 12.6603 cm^{-1}
Second Frequency = 20.1429 cm^{-1}

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Si 0.65362 -3.70457 1.40855
Al -0.00002 -0.89320 -0.00000
O -0.00001 -4.38685 0.00005
N 1.07669 -1.99228 1.07130
N -1.42951 3.00129 0.48245
C 2.34854 -1.56198 1.60538
C 2.46475 -1.06861 2.94139
C 3.73501 -0.70243 3.43250
H 3.81988 -0.32776 4.45944
C 4.88391 -0.81109 2.64412
H 5.86230 -0.52641 3.04640
C 4.77104 -1.30400 1.33790
H 5.67170 -1.40526 0.72396
C 3.52925 -1.69388 0.80454
C 1.26139 -0.93468 3.87418
H 0.37539 -1.28283 3.31615
C 1.01918 0.53583 4.27655
H 1.87150 0.94382 4.84864
H 0.11785 0.62777 4.90780
H 0.88365 1.17399 3.38651
C 1.41293 -1.81243 5.13784
H 1.59624 -2.86954 4.88173
H 0.50165 -1.76226 5.75994
H 2.25949 -1.47453 5.76168
C 3.45408 -2.26848 -0.61023
H 2.58021 -2.94315 -0.63039
C 3.20199 -1.15606 -1.64998
H 2.26796 -0.59978 -1.43904
H 3.12212 -1.57211 -2.67062
H 4.01620 -0.41311 -1.64093
C 4.68877 -3.10077 -1.01250
H 5.58735 -2.47336 -1.15024
H 4.50195 -3.61114 -1.97318
H 4.92732 -3.86934 -0.25772
C -0.65547 -3.91601 2.76559
H -1.53010 -3.26756 2.59930
H -0.24691 -3.68783 3.76348
H -1.00403 -4.96325 2.77199
C 2.18355 -4.71322 1.87951
H 1.87498 -5.75642 2.06537
H 2.66222 -4.32775 2.79447
H 2.93652 -4.71742 1.07581
C -1.22132 4.33356 0.38251
C 0.00005 4.92646 -0.00008
H 0.00006 6.01852 -0.00010
C -2.36028 5.29764 0.69164
H -3.22796 5.10620 0.03767
H -2.03799 6.33944 0.54991
H -2.72274 5.17989 1.72649
C -2.74426 2.60079 0.92009
C -3.03124 2.51524 2.30722
C -4.34164 2.19926 2.70952
H -4.56309 2.14662 3.78315
C -5.37183 1.96141 1.78055
C -5.05338 2.03744 0.41302
H -5.83644 1.85415 -0.33266
C -3.75743 2.35161 -0.03852
C -1.96220 2.79635 3.33846
H -2.34190 2.61683 4.35719
H -1.60187 3.84021 3.29176
H -1.07649 2.15817 3.18435
C -6.77021 1.60608 2.24139
H -7.52261 1.84954 1.47302
H -7.04088 2.14357 3.16606
H -6.86157 0.52529 2.45778
C -3.46345 2.45505 -1.51697
H -3.03053 3.43500 -1.78520
H -4.37746 2.30340 -2.11109
H -2.73732 1.68547 -1.83277
Si -0.65370 -3.70463 -1.40846
N -1.07674 -1.99232 -1.07124
C -2.34859 -1.56201 -1.60535
C -2.46479 -1.06869 -2.94137
C -3.73504 -0.70248 -3.43249
H -3.81989 -0.32786 -4.45945
C -4.88394 -0.81107 -2.64410
H -5.86232 -0.52637 -3.04639
C -4.77107 -1.30392 -1.33786
H -5.67174 -1.40512 -0.72391
C -3.52930 -1.69383 -0.80449
C -1.26143 -0.93483 -3.87418
H -0.37544 -1.28301 -3.31615
C -1.01914 0.53567 -4.27657
H -1.87145 0.94369 -4.84865
H -0.11782 0.62755 -4.90784
H -0.88356 1.17383 -3.38654
C -1.41302 -1.81259 -5.13782
H -1.59639 -2.86969 -4.88170
H -0.50173 -1.76248 -5.75992
H -2.25955 -1.47464 -5.76167
C -3.45415 -2.26837 0.61030
H -2.58032 -2.94309 0.63049
C -3.20199 -1.15593 1.65000
H -2.26792 -0.59972 1.43903
H -3.12214 -1.57194 2.67065
H -4.01615 -0.41292 1.64092
C -4.68889 -3.10058 1.01260
H -5.58744 -2.47311 1.15031
H -4.50210 -3.61091 1.97330
H -4.92747 -3.86917 0.25785
C 0.65534 -3.91613 -2.76554
H 1.52996 -3.26765 -2.59929
H 0.24675 -3.68800 -3.76342
H 1.00391 -4.96337 -2.77189
C -2.18366 -4.71327 -1.87931
H -1.87512 -5.75647 -2.06521
H -2.66239 -4.32779 -2.79423
H -2.93658 -4.71748 -1.07557
N 1.42959 3.00126 -0.48253
C 1.22142 4.33353 -0.38265
C 2.36040 5.29758 -0.69180
H 3.22807 5.10614 -0.03782
H 2.03812 6.33940 -0.55009
H 2.72286 5.17980 -1.72664
C 2.74434 2.60072 -0.92015
C 3.03132 2.51511 -2.30728
C 4.34172 2.19910 -2.70955

H	4.56317	2.14640	-3.78318
C	5.37190	1.96125	-1.78057
C	5.05344	2.03734	-0.41305
H	5.83650	1.85406	0.33265
C	3.75749	2.35155	0.03848
C	1.96229	2.79617	-3.33853
H	2.34199	2.61662	-4.35725
H	1.60194	3.84003	-3.29187
H	1.07658	2.15799	-3.18440
C	6.77027	1.60587	-2.24139
H	7.52268	1.84941	-1.47305
H	7.04094	2.14326	-3.16612
H	6.86163	0.52506	-2.45767
C	3.46351	2.45505	1.51692
H	3.03063	3.43503	1.78512
H	4.37751	2.30338	2.11105
H	2.73735	1.68551	1.83274

4-Mg

SCF (BP86) Energy = -2369.18621984
Enthalpy 0K = -2368.064569
Enthalpy 298K = -2367.987402
Free Energy 298K = -2368.183272
Lowest Frequency = 7.4342 cm^{-1}
Second Frequency = 11.7140 cm^{-1}

Si	0.71052	-4.09718	1.41074
Si	-0.66462	-4.10404	-1.40983
Al	0.00784	-1.34683	0.00054
Mg	-0.01310	2.19201	0.00024
O	0.02315	-4.74411	0.00192
O	-0.00177	0.34769	0.00181
N	1.06476	-2.37150	1.11106
N	-1.03693	-2.38199	-1.11172
N	-1.47629	3.54758	0.44354
N	1.43434	3.56429	-0.44340
C	2.24200	-1.79917	1.71886
C	3.47880	-1.79979	1.00007
C	4.62431	-1.25139	1.60600
H	5.57283	-1.25473	1.05882
C	4.57855	-0.70814	2.89648
H	5.48379	-0.29584	3.35563
C	3.36582	-0.70135	3.59370
H	3.32557	-0.27016	4.60079
C	2.19114	-1.24007	3.03094
C	3.55246	-2.34482	-0.42647
H	2.73970	-3.08566	-0.52792
C	3.27693	-1.21755	-1.44960
H	2.31015	-0.71357	-1.26089
H	3.26169	-1.61190	-2.48165
H	4.05109	-0.43285	-1.38897
C	4.87841	-3.05877	-0.75626
H	5.73091	-2.35728	-0.79222
H	4.81456	-3.53872	-1.74830
H	5.11614	-3.83887	-0.01317
C	0.88537	-1.16609	3.82109
H	0.14940	-1.78826	3.28600
C	0.33688	0.27932	3.82940
H	1.04666	0.97202	4.31670
H	-0.62266	0.33526	4.37372
H	0.16746	0.62433	2.79394
C	1.01735	-1.71380	5.25795
H	1.41199	-2.74427	5.26396
H	0.03397	-1.72006	5.76027
H	1.69506	-1.09663	5.87421
C	2.29069	-5.05612	1.80933
H	2.03716	-6.11250	2.00205
H	2.78874	-4.65301	2.70639
H	3.00840	-5.02308	0.97439
C	-0.56130	-4.38219	2.78996
H	-1.47398	-3.78516	2.62434
H	-0.15689	-4.12150	3.78234
H	-0.85194	-5.44678	2.80979
C	0.61472	-4.37596	-2.78473
H	1.52060	-3.76942	-2.61637
H	0.21068	-4.11938	-3.77835
H	0.91649	-5.43746	-2.80376
C	-2.23373	-5.07868	-1.81385
H	-1.96915	-6.13277	-2.00428
H	-2.73189	-4.68140	-2.71344
H	-2.95522	-5.05163	-0.98196
C	-2.22025	-1.82277	-1.71978
C	-3.45707	-1.83656	-1.00118
C	-4.60840	-1.30108	-1.60764
H	-5.55692	-1.31445	-1.06063
C	-4.56837	-0.75824	-2.89849
H	-5.47801	-0.35622	-3.35807
C	-3.35567	-0.73858	-3.59554
H	-3.32000	-0.30768	-4.60292
C	-2.17525	-1.26392	-3.03216
C	-3.52492	-2.38187	0.42557
H	-2.70507	-3.11485	0.52701
C	-3.25990	-1.25171	1.44830
H	-2.29819	-0.73827	1.25902
H	-3.24034	-1.64565	2.48042
H	-4.04176	-0.47465	1.38783
C	-4.84378	-3.10847	0.75613
H	-5.70297	-2.41520	0.79240
H	-4.77481	-3.58760	1.74821
H	-5.07439	-3.89098	0.01332
C	-0.87008	-1.17592	-3.82187
H	-0.12732	-1.78912	-3.28581
C	-0.33807	0.27563	-3.83140
H	-1.05534	0.95976	-4.31982
H	0.62113	0.34192	-4.37514
H	-0.17320	0.62372	-2.79624
C	-0.99520	-1.72653	-5.25825
H	-1.37762	-2.76160	-5.26334
H	-0.01168	-1.72168	-5.76032
H	-1.68000	-1.11801	-5.87526
C	-1.27163	4.87915	0.33998
C	-0.03202	5.47514	-0.00001
H	-0.03829	6.56746	-0.00003
C	1.21439	4.89342	-0.33989
C	-2.43297	5.83098	0.58988
H	-3.26586	5.61460	-0.10128
H	-2.12584	6.87785	0.45325
H	-2.84012	5.71288	1.60812
C	2.36478	5.85854	-0.58953
H	3.20002	5.65161	0.10169
H	2.04564	6.90180	-0.45275
H	2.77336	5.74532	-1.60776
C	-2.78133	3.09020	0.84726
C	-3.72664	2.70522	-0.13583
C	-4.99276	2.25442	0.28285
H	-5.72508	1.96632	-0.48115
C	-5.34188	2.16227	1.64179
C	-4.37475	2.52912	2.59632
H	-4.62038	2.46013	3.66372
C	-3.09716	2.98666	2.22748
C	-3.38571	2.77465	-1.60842
H	-2.97039	3.75667	-1.89410
H	-4.27619	2.58092	-2.22645
H	-2.63579	2.00990	-1.88502
C	-6.70427	1.65581	2.06856
H	-7.45238	1.78738	1.26940

H	-7.06916	2.18238	2.96675
H	-6.67479	0.57823	2.31549
C	-2.08301	3.36304	3.28624
H	-1.76887	4.41948	3.21196
H	-1.16248	2.75863	3.19765
H	-2.49365	3.20364	4.29613
C	2.74457	3.12182	-0.84693
C	3.69382	2.74710	0.13640
C	4.96500	2.31060	-0.28192
H	5.70018	2.03039	0.48227
C	5.31562	2.22283	-1.64080
C	4.34484	2.57923	-2.59552
H	4.59169	2.51342	-3.66285
C	3.06204	3.02232	-2.22702
C	3.35155	2.81246	1.60886
H	2.92640	3.79023	1.89475
H	4.24359	2.62727	2.22724
H	2.60906	2.04025	1.88477
C	6.68369	1.73149	-2.06707
H	7.03857	2.25487	-2.97108
H	6.66853	0.65136	-2.30400
H	7.43224	1.88063	-1.27139
C	2.04412	3.38753	-3.28609
H	1.13067	2.77235	-3.19832
H	2.45709	3.23352	-4.29586
H	1.71763	4.44018	-3.21135

4-Zn

SCF (BP86) Energy = -2595.52413223
Enthalpy 0K = -2594.402860
Enthalpy 298K = -2594.325484
Free Energy 298K = -2594.520986
Lowest Frequency = 9.2236 cm^{-1}
Second Frequency = 12.3800 cm^{-1}

Zn	0.22167	2.14119	0.01983
Si	-1.09935	-4.05732	1.36480
Si	0.27434	-4.12834	-1.45170
Al	-0.14386	-1.35757	0.00611
O	-0.42439	-4.74116	-0.03300
O	0.02163	0.32965	0.07333
N	-1.30300	-2.30284	1.08154
N	0.80845	-2.45225	-1.12780
N	1.78621	3.25650	0.45576
N	-1.08488	3.54522	-0.43471
C	-2.44611	-1.65208	1.67835
C	-3.66246	-1.54314	0.93338
C	-4.77831	-0.92728	1.52936
H	-5.71239	-0.84836	0.96355
C	-4.72197	-0.42158	2.83475
H	-5.60503	0.04419	3.28603
C	-3.52859	-0.52251	3.55732
H	-3.47987	-0.12109	4.57621
C	-2.38383	-1.13269	3.00574
C	-3.74158	-2.05175	-0.50620
H	-3.00742	-2.87208	-0.59498
C	-5.12069	-2.61815	-0.89765
H	-5.89379	-1.83093	-0.95078
H	-5.46621	-3.38122	-0.17957
H	-5.06893	-3.08596	-1.89614
C	-3.31415	-0.94360	-1.49685
H	-2.31234	-0.53604	-1.26102
H	-4.00911	-0.08739	-1.45384
H	-3.29284	-1.32294	-2.53438
C	-1.09619	-1.17819	3.82720
H	-0.39594	-1.84082	3.29271
C	-1.30588	-1.75178	5.24472
H	-1.77923	-2.74821	5.21396
H	-1.94851	-1.09950	5.86239
H	-0.33853	-1.84743	5.76866
C	-0.44131	0.22062	3.88800
H	-1.10846	0.95114	4.38018
H	-0.22188	0.58243	2.86852
H	0.50557	0.18749	4.45608
C	-2.76458	-4.88538	1.70797
H	-2.60408	-5.96263	1.88470
H	-3.45769	-4.77706	0.85871
H	-3.24805	-4.45866	2.60204
C	0.10518	-4.47005	2.77156
H	1.06889	-3.94920	2.64262
H	0.30505	-5.55555	2.77666
H	-0.30392	-4.19484	3.75793
C	-1.05532	-4.24883	-2.79995
H	-1.89489	-3.56183	-2.60120
H	-1.45780	-5.27600	-2.83243
H	-0.64818	-4.01093	-3.79695
C	1.74136	-5.22618	-1.91508
H	1.38233	-6.25311	-2.09906
H	2.49181	-5.26398	-1.10966
H	2.23901	-4.86606	-2.83036
C	3.23263	-2.72550	0.48364
H	2.34423	-3.37841	0.55151
C	4.46239	-3.57572	0.85966
H	5.38174	-2.96775	0.93290
H	4.64592	-4.37560	0.12217
H	4.30940	-4.04795	1.84557
C	3.03989	-1.57801	1.50301
H	2.14754	-0.96285	1.27831
H	3.89962	-0.88609	1.48309
H	2.93468	-1.97186	2.52998
C	1.71427	4.60161	0.35590
C	0.54275	5.31454	0.01184
H	0.65134	6.40131	0.01453
C	-0.74780	4.84912	-0.33027
C	2.96338	5.42694	0.62416
H	3.78380	5.12060	-0.04716
H	3.33327	5.27747	1.65246
H	2.76654	6.49824	0.47393
C	-1.81156	5.90707	-0.58121
H	-2.67106	5.76062	0.09524
H	-2.21159	5.84551	-1.60709
H	-1.40642	6.91688	-0.42261
C	3.02832	2.66237	0.87689
C	3.94793	2.19952	-0.09557
C	5.16347	1.64013	0.34111
H	5.87899	1.29013	-0.41271
C	5.48247	1.51648	1.70521
C	4.53589	1.96172	2.64703
H	4.75800	1.86832	3.71766
C	3.30801	2.52860	2.26122
C	3.63365	2.30676	-1.57048
H	2.76758	1.67538	-1.83989
H	4.48502	1.96492	-2.17884
H	3.38405	3.34028	-1.86896
C	6.78934	0.89326	2.15041
H	6.66415	-0.18009	2.38563
H	7.18077	1.37907	3.06028
H	7.56029	0.96788	1.36576
C	2.31251	2.98892	3.30360
H	1.34418	2.47023	3.19092
H	2.09678	4.07004	3.23148
H	2.68895	2.78791	4.31936
C	-2.42350	3.21016	-0.84551
C	-2.74541	3.16573	-2.22640
C	-4.06574	2.85539	-2.59894
H	-4.31854	2.83241	-3.66659

C	-5.06539	2.57761	-1.64797
C	-4.70667	2.60269	-0.28821
H	-5.46348	2.37662	0.47260
C	-3.39952	2.90717	0.13525
C	-1.69699	3.44887	-3.28012
H	-0.83799	2.76167	-3.18663
H	-1.28627	4.47163	-3.20299
H	-2.11794	3.33165	-4.29154
C	-6.47476	2.22808	-2.07917
H	-6.57134	1.14947	-2.30378
H	-6.76672	2.77516	-2.99148
H	-7.20859	2.46379	-1.29069
C	-3.04631	2.91337	1.60522
H	-2.60259	3.87366	1.92234
H	-2.30942	2.12379	1.84000
H	-3.93621	2.71970	2.22357
C	2.06389	-2.02497	-1.69772
C	2.12035	-1.47764	-3.01388
C	3.36894	-1.09579	-3.54503
H	3.41167	-0.67408	-4.55608
C	4.55048	-1.24661	-2.81172
H	5.51319	-0.95598	-3.24658
C	4.49118	-1.77912	-1.51715
H	5.41608	-1.89774	-0.94325
C	3.26955	-2.17541	-0.94254
C	0.85881	-1.25721	-3.84731
H	0.02988	-1.75126	-3.31415
C	0.95631	-1.87795	-5.25737
H	-0.00065	-1.76448	-5.79676
H	1.73653	-1.39013	-5.86834
H	1.19818	-2.95366	-5.21091
C	0.51536	0.24723	-3.92919
H	-0.41398	0.40891	-4.50394
H	0.37143	0.66190	-2.91632
H	1.32417	0.81571	-4.42254

[Al($_{xanth}$NON^{Dipp})]-Mg

SCF (BP86) Energy = -3019.54944840
Enthalpy 0K = -3018.142253
Enthalpy 298K = -3018.054531
Free Energy 298K = -3018.268668
Lowest Frequency = 10.9818 cm^{-1}
Second Frequency = 15.6475 cm^{-1}

Al	-0.15293	-0.11342	-0.21954
O	-1.93190	0.29661	0.75727
N	-0.55448	1.66111	-0.96845
N	-1.12585	-1.82172	-0.50368
C	-2.54431	1.50467	0.33612
C	-2.85110	-0.78308	0.76997
C	-1.77829	2.23028	-0.59465
C	-2.38200	-1.92540	0.10069
C	-2.35906	3.44381	-1.03497
H	-1.79695	4.05984	-1.74298
C	-3.82130	1.81942	0.78243
C	-3.64702	3.84451	-0.60424
C	-0.63718	-3.01002	-1.15387
C	-3.26777	-3.03659	0.10868
H	-2.94013	-3.96025	-0.37222
C	0.42211	2.55937	-1.52709
C	-4.36998	3.02481	0.29071
H	-5.37421	3.31417	0.60314
C	1.05731	3.52391	-0.68436
C	-4.13672	-0.58940	1.26593
C	-4.55756	-2.94000	0.67397
C	-4.50410	0.82953	1.75453
C	0.06440	-4.00222	-0.40316
C	0.75586	2.49795	-2.91306
C	-5.53017	-4.14351	0.68287
C	-0.88947	-3.21811	-2.54501
C	-4.24193	5.16052	-1.16117
C	-4.99112	-1.70852	1.22336
H	-6.01067	-1.61745	1.60664
C	0.79187	3.60910	0.81989
H	0.10974	2.78526	1.08978
C	1.97542	4.42823	-1.25317
H	2.45416	5.17664	-0.61094
C	0.33663	-3.85101	1.09298
H	0.05851	-2.81819	1.36744
C	0.07666	1.50044	-3.85275
H	-0.15985	0.59775	-3.25848
C	-3.92198	1.04625	3.18445
H	-4.14451	2.06860	3.53563
H	-2.82918	0.90893	3.19822
H	-4.36961	0.32585	3.89084
C	0.49438	-5.17574	-1.05434
H	1.02580	-5.94169	-0.47818
C	-1.68082	-2.21174	-3.38200
H	-1.62801	-1.23950	-2.85927
C	1.69084	3.41775	-3.42778
H	1.94936	3.38063	-4.49014
C	-0.43404	-4.40741	-3.14787
H	-0.62828	-4.57514	-4.21237
C	-6.02959	1.03678	1.80204
H	-6.49259	0.89299	0.81209
H	-6.27115	2.05233	2.15699
H	-6.49388	0.33086	2.51048
C	-3.30947	6.34887	-0.80812
H	-3.71886	7.29221	-1.21247
H	-2.29826	6.21622	-1.22710
H	-3.21009	6.46112	0.28542
C	-5.91021	-4.48311	2.14881
H	-6.39241	-3.62992	2.65451
H	-5.01565	-4.75781	2.73385
H	-6.61385	-5.33465	2.17750
C	1.82821	-4.05125	1.43670
H	2.15809	-5.08671	1.23965
H	2.01251	-3.84902	2.50568
H	2.48379	-3.38695	0.84632
C	2.29159	4.38510	-2.61435
H	3.00729	5.09688	-3.03996
C	-5.64239	5.46582	-0.58453
H	-6.01665	6.41561	-1.00419
H	-5.61992	5.57295	0.51393
H	-6.37374	4.67991	-0.84101
C	0.25052	-5.38408	-2.41548
H	0.58849	-6.30471	-2.90360
C	0.10788	4.93655	1.21777
H	0.74927	5.80366	0.97798
H	-0.09193	4.95762	2.30360
H	-0.85074	5.06266	0.69034
C	-3.17504	-2.60594	-3.47434
H	-3.28640	-3.58532	-3.97437
H	-3.73556	-1.85866	-4.06360
H	-3.63842	-2.67459	-2.47769
C	2.09128	3.41635	1.62933
H	2.59270	2.46846	1.35865
H	1.88274	3.38638	2.71181
H	2.81397	4.23054	1.44349
C	-4.91666	-5.40776	0.04154
H	-5.64582	-6.23543	0.08369
H	-4.00704	-5.73843	0.57185
H	-4.65732	-5.24748	-1.01901
C	-1.10071	-2.02941	-4.79969
H	-0.01826	-1.82316	-4.77518
H	-1.60266	-1.18859	-5.30875

H	-1.26036	-2.92409	-5.42761
C	-1.26701	2.06612	-4.37187
H	-1.95180	2.30488	-3.54245
H	-1.76955	1.33721	-5.03257
H	-1.09730	2.98981	-4.95431
C	-6.81463	-3.77895	-0.10828
H	-7.52255	-4.62733	-0.10400
H	-6.57496	-3.53750	-1.15797
H	-7.33256	-2.90790	0.32643
C	-4.37068	5.05314	-2.70426
H	-5.03704	4.21988	-2.98626
H	-3.39377	4.87915	-3.18479
H	-4.79112	5.98585	-3.12182
C	-0.54101	-4.81098	1.92946
H	-1.61268	-4.63379	1.74395
H	-0.35215	-4.66991	3.00855
H	-0.31870	-5.86514	1.68397
C	0.97029	1.06879	-5.03239
H	0.47482	0.27064	-5.60879
H	1.94685	0.69000	-4.68559
H	1.15295	1.90098	-5.73560
Mg	2.37658	-0.42995	0.82780
N	4.17610	-1.00900	-0.02484
N	3.12008	-0.55509	2.77125
C	4.47493	-0.67259	-1.39378
C	2.58674	0.22847	3.85357
C	5.17941	0.52655	-1.67827
C	4.14464	-1.39607	3.04437
C	4.02917	-1.50745	-2.45075
C	5.08129	-1.72248	0.67436
C	4.97732	-1.98931	2.06506
H	5.73643	-2.66920	2.45954
C	1.31618	-0.07447	4.40906
C	3.31268	1.35790	4.32387
C	4.31730	-1.13176	-3.77666
H	3.98406	-1.78837	-4.59032
C	5.02316	0.04466	-4.08685
C	5.44326	0.85793	-3.01947
H	5.99502	1.78195	-3.23338
C	6.31545	-2.26625	-0.03126
H	6.04609	-2.81745	-0.94740
H	6.89168	-2.92963	0.63028
H	6.97424	-1.43917	-0.34956
C	4.46003	-1.74066	4.49511
H	4.92501	-0.89032	5.02275
H	5.15071	-2.59503	4.55405
H	3.53863	-1.98584	5.04941
C	4.65168	1.73290	3.72556
H	4.96504	2.73279	4.06619
H	4.61319	1.73683	2.62294
H	5.45213	1.02262	4.00244
C	3.27106	-2.78423	-2.16815
H	2.30807	-2.58862	-1.66228
H	3.83482	-3.46678	-1.50778
H	3.04516	-3.32515	-3.10030
C	2.75676	2.14765	5.34743
H	3.32090	3.02017	5.70119
C	0.80200	0.74684	5.42954
H	-0.17874	0.50038	5.85573
C	5.63866	1.44201	-0.56375
H	6.24692	2.26949	-0.96288
H	6.23725	0.91099	0.19662
H	4.77935	1.89041	-0.03139
C	0.52350	-1.26836	3.92907
H	-0.38530	-1.41029	4.53544
H	1.11519	-2.19929	3.97044
H	0.20357	-1.14659	2.87638
C	5.29868	0.43579	-5.52383
H	6.21763	1.03958	-5.60962
H	4.47157	1.03941	-5.94136
H	5.41134	-0.45081	-6.17023
C	1.50474	1.86124	5.92028
C	0.94420	2.70822	7.04349
H	-0.15781	2.74181	7.01416
H	1.31792	3.74458	6.99396
H	1.23059	2.30590	8.03328

[Al(NC$_2$N^{Dipp})]-Mg

SCF (BP86) Energy = -2532.99685646
Enthalpy 0K = -2531.660673
Enthalpy 298K = -2531.577132
Free Energy 298K = -2531.777438
Lowest Frequency = 17.3343 cm^{-1}
Second Frequency = 21.0452 cm^{-1}

Al	1.38182	-0.40161	0.17023
Si	4.01193	-1.61817	-1.31803
Si	3.29954	-1.90735	2.50937
N	1.74449	-1.33647	1.77342
N	2.91473	-0.23664	-0.94345
C	0.58742	-1.55912	2.61598
C	0.15985	-0.56603	3.55354
C	-0.12187	-2.80190	2.54571
C	0.93976	0.72831	3.79027
H	1.81315	0.70857	3.11632
C	3.19740	0.98833	-1.65853
C	2.52518	1.31389	-2.88248
C	-0.98714	-0.80763	4.33834
H	-1.31297	-0.04204	5.05220
C	1.44017	0.42850	-3.49704
H	1.27294	-0.41416	-2.80288
C	0.33468	-3.92118	1.60917
H	1.40145	-3.73688	1.39047
C	-1.25349	-2.99771	3.35946
H	-1.78973	-3.95155	3.30814
C	0.10823	1.19333	-3.66086
H	-0.22028	1.65583	-2.71155
H	0.19938	2.01853	-4.38916
H	-0.69415	0.52596	-4.02030
C	4.20879	1.88884	-1.18208
C	-1.69774	-2.00822	4.24642
H	-2.57951	-2.18094	4.87263
C	1.46161	0.80723	5.24460
H	0.62866	0.88549	5.96585
H	2.05066	-0.08439	5.51826
H	2.10124	1.69755	5.37931
C	1.87684	-0.15436	-4.86102
H	2.11259	0.64827	-5.58196
H	2.77318	-0.78879	-4.76471
H	1.07115	-0.76853	-5.30073
C	2.98986	-3.14161	-1.83704
H	2.20117	-3.38457	-1.10458
H	2.50608	-2.98043	-2.81393
H	3.64285	-4.02851	-1.92419
C	0.11529	1.98717	3.45592
H	-0.21416	1.99281	2.40338
H	-0.78825	2.06072	4.08598
H	0.71058	2.90142	3.62464
C	5.10633	-2.17169	0.15030
H	5.86930	-2.83774	-0.30462
H	5.67246	-1.30469	0.53773
C	2.87971	2.48474	-3.58410
H	2.36546	2.71391	-4.52504
C	4.36539	-0.49308	3.22185
H	4.51319	0.33470	2.51312
H	3.91509	-0.07687	4.13742

H	5.36137	-0.88950	3.49053
C	4.38813	-2.91246	1.29948
H	5.13937	-3.38710	1.96524
H	3.78632	-3.75254	0.90318
C	4.96392	1.65024	0.12507
H	4.61510	0.68058	0.51513
C	-0.42168	-3.85985	0.26713
H	-1.50490	-4.01446	0.40909
H	-0.29401	-2.87277	-0.21381
H	-0.05530	-4.63064	-0.43391
C	4.53374	3.03799	-1.92814
H	5.31757	3.70745	-1.55463
C	3.88278	3.34482	-3.12761
H	4.15271	4.24026	-3.69746
C	2.93693	-3.07082	3.97642
H	2.26348	-2.61009	4.71678
H	2.48520	-4.02394	3.65814
H	3.89047	-3.30299	4.48340
C	5.17935	-1.16725	-2.75320
H	4.62751	-0.84434	-3.65022
H	5.87436	-0.35478	-2.48784
H	5.77871	-2.05496	-3.02182
C	4.62960	2.73174	1.17751
H	4.90479	3.73934	0.81870
H	3.55244	2.74455	1.41282
H	5.18151	2.54898	2.11677
C	0.21550	-5.33163	2.22398
H	0.70168	-5.39254	3.21243
H	-0.83732	-5.64088	2.34905
H	0.69164	-6.07462	1.56067
C	6.49352	1.56136	-0.07526
H	6.76788	0.77719	-0.80028
H	6.91195	2.51524	-0.44258
H	6.99410	1.32894	0.88150
Mg	-1.25997	0.39997	-0.53463
N	-2.83368	-0.54564	-1.59589
N	-2.22733	2.27427	-0.48480
C	-3.11587	2.56810	-1.45935
C	-2.03198	3.28431	0.53285
C	-3.15508	-1.95717	-1.53337
C	-3.60563	0.22207	-2.40284
C	-2.97581	3.41112	1.59391
C	-2.65860	-2.87992	-2.49959
C	-3.61410	1.63734	-2.40576
H	-4.26342	2.08011	-3.16500
C	-0.89784	4.14778	0.46919
C	-1.75501	-2.46367	-3.66139
H	-1.70160	-1.36079	-3.66482
C	-3.00847	-4.24041	-2.38362
H	-2.62506	-4.95206	-3.12331
C	-3.99600	-2.41735	-0.47285
C	-0.76233	5.15047	1.44958
H	0.09666	5.82606	1.40630
C	-4.17802	2.47691	1.75189
H	-4.21783	1.81794	0.86734
C	-4.56979	-0.43013	-3.38782
H	-4.01835	-0.87256	-4.23485
H	-5.13699	-1.24856	-2.91785
H	-5.27898	0.30684	-3.79162
C	-1.69597	5.29875	2.48216
H	-1.56849	6.08703	3.23171
C	-2.78256	4.42309	2.55499
H	-3.50395	4.52505	3.37363
C	-3.83684	-4.69815	-1.35574
H	-4.10261	-5.75841	-1.28839
C	0.15832	4.00959	-0.63027
H	0.26090	2.92653	-0.84574
C	-4.32252	-3.78624	-0.41131
H	-4.97244	-4.14465	0.39269
C	-2.29754	-2.92370	-5.03493
H	-2.26782	-4.02306	-5.13167
H	-3.34113	-2.60833	-5.20127
H	-1.67965	-2.50726	-5.84950
C	-4.59359	-1.45507	0.55784
H	-3.89375	-0.60372	0.65884
C	-3.72758	3.96175	-1.56099
H	-4.64620	4.01769	-0.95081
H	-3.05069	4.74904	-1.20092
H	-4.01398	4.17653	-2.60246
C	-0.32302	-3.00316	-3.46111
H	0.12001	-2.62693	-2.52596
H	-0.31948	-4.10619	-3.41003
H	0.33112	-2.70297	-4.29800
C	-5.94371	-0.87578	0.06966
H	-5.83403	-0.30207	-0.86405
H	-6.67161	-1.68732	-0.10899
H	-6.37140	-0.19995	0.83148
C	-4.01355	1.58165	3.00174
H	-3.10606	0.95731	2.94677
H	-3.94153	2.19386	3.91823
H	-4.88413	0.91231	3.11724
C	-4.76887	-2.08825	1.95239
H	-5.55758	-2.86140	1.95787
H	-3.83198	-2.54141	2.31346
H	-5.07327	-1.31665	2.67911
C	-5.51785	3.24500	1.82680
H	-5.57855	3.86535	2.73826
H	-5.66055	3.91456	0.96212
H	-6.36530	2.53794	1.85282
C	1.54539	4.52082	-0.19838
H	1.57304	5.62414	-0.14029
H	1.83815	4.12332	0.78718
H	2.30451	4.21148	-0.93359
C	-0.25004	4.70132	-1.95243
H	-1.15732	4.26037	-2.39275
H	-0.43491	5.77786	-1.78618
H	0.56435	4.60458	-2.69094

[Al($_{xanth}$NON^{Dipp})]-Zn

SCF (BP86) Energy = -3245.92561827
Enthalpy 0K = -3244.517730
Enthalpy 298K = -3244.430191
Free Energy 298K = -3244.642189
Lowest Frequency = 12.4975 cm^{-1}
Second Frequency = 19.3366 cm^{-1}

Zn	-2.09530	-0.45945	0.87180
Al	0.08788	-0.07035	-0.23009
O	1.89298	0.24744	0.67807
N	0.43709	1.73504	-0.88043
N	0.98747	-1.76430	-0.69544
N	-3.93878	-0.92798	0.15103
N	-2.62420	-0.75286	2.82614
C	2.50114	1.47159	0.28998
C	1.69676	2.25856	-0.55287
C	2.27648	3.48200	-0.96519
H	1.68621	4.14515	-1.60417
C	3.59633	3.83507	-0.59362
C	4.35191	2.95785	0.21601
H	5.37850	3.21227	0.48281
C	3.80776	1.73899	0.67729
C	4.52499	0.68341	1.55032
C	4.11139	-0.69516	0.98922
C	4.94964	-1.81154	0.80582
H	5.99106	-1.75721	1.13295
C	4.47238	-2.99060	0.18234

C	3.15093	-3.03331	-0.31104
H	2.78828	-3.91007	-0.85049
C	2.27591	-1.92258	-0.17119
C	2.79579	-0.84272	0.55974
C	5.43223	-4.19491	0.03170
C	6.67762	-3.76760	-0.79012
H	7.22740	-2.94274	-0.30713
H	6.38651	-3.43130	-1.79994
H	7.37545	-4.61724	-0.89911
C	5.88401	-4.66590	1.43984
H	6.58026	-5.51977	1.35580
H	5.01832	-4.98783	2.04388
H	6.39949	-3.86341	1.99349
C	4.77416	-5.39303	-0.68745
H	4.45887	-5.13527	-1.71302
H	3.89230	-5.76866	-0.14046
H	5.49780	-6.22328	-0.76101
C	6.05362	0.86971	1.53053
H	6.54318	0.11473	2.16778
H	6.32753	1.85782	1.93581
H	6.46311	0.78421	0.51069
C	4.02098	0.81551	3.01966
H	2.92861	0.69026	3.08525
H	4.27743	1.81070	3.42181
H	4.49575	0.04712	3.65404
C	4.18925	5.16294	-1.12403
C	4.23065	5.12094	-2.67516
H	3.22509	4.98759	-3.10714
H	4.86190	4.28801	-3.02957
H	4.64802	6.06269	-3.07499
C	3.30543	6.35365	-0.66916
H	3.26721	6.41939	0.43192
H	2.27042	6.26248	-1.03811
H	3.71534	7.30482	-1.05401
C	5.62579	5.41335	-0.61341
H	5.99735	6.37382	-1.01041
H	6.32448	4.62603	-0.94547
H	5.66613	5.47052	0.48827
C	-0.55341	2.69196	-1.31013
C	-1.08347	3.62631	-0.36745
C	-2.02040	4.58152	-0.80836
H	-2.42221	5.30427	-0.08886
C	-2.45031	4.62101	-2.13776
H	-3.18050	5.37042	-2.46226
C	-1.94042	3.69198	-3.05128
H	-2.28252	3.72371	-4.08962
C	-0.99042	2.72485	-2.66773
C	-0.40150	1.78319	-3.71930
H	-0.17290	0.82572	-3.21465
C	-1.36766	1.48268	-4.88180
H	-2.33987	1.11287	-4.51504
H	-0.93381	0.71618	-5.54414
H	-1.54810	2.37611	-5.50608
C	0.93514	2.34323	-4.26258
H	0.77100	3.31961	-4.75339
H	1.37161	1.65837	-5.01135
H	1.67331	2.48444	-3.45716
C	-0.68527	3.63460	1.10983
H	0.00680	2.79344	1.28176
C	-1.91125	3.41150	2.01807
H	-2.64793	4.22825	1.91698
H	-1.60811	3.35426	3.07689
H	-2.42118	2.46589	1.76518
C	0.04700	4.93643	1.50626
H	0.95429	5.08521	0.89994
H	0.34606	4.90088	2.56867
H	-0.60474	5.81833	1.37177
C	0.46821	-2.89771	-1.42291
C	0.61727	-2.96100	-2.84287
C	0.13637	-4.09555	-3.52626
H	0.24710	-4.15101	-4.61388
C	-0.46666	-5.15971	-2.84625
H	-0.82620	-6.03493	-3.39830
C	-0.59777	-5.09790	-1.45599
H	-1.06142	-5.93356	-0.91962
C	-0.14079	-3.98398	-0.72330
C	-0.28818	-4.00343	0.79744
H	0.03505	-3.01663	1.16728
C	0.62558	-5.07143	1.44284
H	0.35310	-6.08677	1.10274
H	0.52777	-5.04955	2.54280
H	1.68441	-4.89768	1.19186
C	-1.75279	-4.21621	1.23621
H	-2.42416	-3.44691	0.81993
H	-1.83599	-4.17496	2.33606
H	-2.13481	-5.20197	0.91575
C	1.33517	-1.86444	-3.63171
H	1.26722	-0.93405	-3.03888
C	0.69851	-1.60409	-5.01199
H	0.87412	-2.44199	-5.70995
H	1.14807	-0.70776	-5.47238
H	-0.39006	-1.44735	-4.93840
C	2.83915	-2.19000	-3.80428
H	3.34308	-2.31537	-2.83326
H	3.34843	-1.37920	-4.35476
H	2.96704	-3.12433	-4.38062
C	-4.31936	-0.49108	-1.16720
C	-4.93382	0.77708	-1.33223
C	-5.31313	1.18346	-2.62437
H	-5.79821	2.16004	-2.74563
C	-5.09407	0.37844	-3.75627
C	-4.46335	-0.86449	-3.56510
H	-4.28136	-1.51352	-4.43112
C	-4.06561	-1.31674	-2.29277
C	-3.40100	-2.66431	-2.13490
H	-3.27251	-3.15855	-3.11044
H	-3.98282	-3.34309	-1.48566
H	-2.40281	-2.57557	-1.67215
C	-5.50193	0.84455	-5.13864
H	-6.37001	1.52355	-5.09614
H	-5.76514	-0.00526	-5.79069
H	-4.68202	1.39457	-5.63702
C	-5.18069	1.68347	-0.14651
H	-5.79306	2.55168	-0.43851
H	-4.22938	2.07189	0.26051
H	-5.69281	1.16169	0.68026
C	-6.16380	-2.01860	0.25069
H	-6.77428	-1.11909	0.05666
H	-6.73216	-2.68294	0.91819
H	-6.02896	-2.51793	-0.72276
C	-4.83085	-1.63115	0.87463
C	-4.62141	-2.02413	2.21949
H	-5.38511	-2.68601	2.63495
C	-3.65724	-1.56531	3.14318
C	-3.82693	-2.02522	4.58609
H	-2.85996	-2.33625	5.01516
H	-4.53034	-2.86967	4.64214
H	-4.21317	-1.21886	5.23256
C	-1.95484	-0.06756	3.89800
C	-2.60327	1.02351	4.54120
C	-1.92677	1.70823	5.56820
H	-2.43438	2.54808	6.05994
C	-0.62925	1.35537	5.97831
C	-0.01169	0.27231	5.32819
H	0.99450	-0.03712	5.63826
C	-0.64579	-0.44482	4.29729

C	0.05432	-1.61756	3.65367
H	-0.56365	-2.53170	3.68180
H	1.01255	-1.83117	4.15340
H	0.26759	-1.42039	2.58751
C	0.08873	2.13028	7.06318
H	-0.62160	2.58279	7.77519
H	0.69287	2.95350	6.63815
H	0.77774	1.48439	7.63309
C	-3.99759	1.45917	4.14272
H	-4.77822	0.78298	4.53804
H	-4.12089	1.46822	3.04751
H	-4.21430	2.46877	4.52726

[Al($_{xanth}$NON^{Dipp})]-Li

SCF (BP86) Energy = -2490.06405633
Enthalpy 0K = -2488.838766
Enthalpy 298K = -2488.763651
Free Energy 298K = -2488.953241
Lowest Frequency = 10.0289 cm^{-1}
Second Frequency = 11.5685 cm^{-1}

Al	0.56100	-0.29901	0.20918
O	-1.34336	0.52827	0.97064
N	0.63424	1.70127	-0.17997
N	-0.87311	-1.68938	-0.24116
C	-1.51465	1.91516	0.80559
C	-0.40666	2.54369	0.19979
C	-0.51085	3.94961	0.05119
H	0.33494	4.48924	-0.38587
C	-1.68747	4.64692	0.41737
C	-2.78682	3.92838	0.93247
H	-3.71215	4.45091	1.17851
C	-2.71713	2.53034	1.13222
C	-3.85318	1.64097	1.67812
C	-3.76452	0.29100	0.93455
C	-4.86235	-0.49850	0.52292
H	-5.87334	-0.13503	0.71127
C	-4.66887	-1.73090	-0.13767
C	-3.35254	-2.18468	-0.39226
H	-3.18782	-3.13139	-0.91600
C	-2.21742	-1.42242	-0.01558
C	-2.49851	-0.21330	0.65662
C	-5.86224	-2.58722	-0.62666
C	-7.22697	-1.96767	-0.25152
H	-7.36668	-0.97300	-0.70901
H	-7.34423	-1.86493	0.84132
H	-8.04204	-2.61751	-0.61501
C	-5.80144	-2.71375	-2.17249
H	-6.64294	-3.32652	-2.54411
H	-4.86411	-3.18919	-2.50564
H	-5.86228	-1.72078	-2.65023
C	-5.79128	-4.00285	0.00292
H	-6.63260	-4.62526	-0.35250
H	-5.84798	-3.94820	1.10388
H	-4.85507	-4.52217	-0.26007
C	-5.23316	2.30345	1.50086
H	-5.45538	2.50577	0.44024
H	-5.28084	3.25542	2.05508
H	-6.02866	1.65724	1.90763
C	-3.60946	1.38962	3.19771
H	-4.38933	0.72333	3.60595
H	-3.63442	2.34414	3.75185
H	-2.62881	0.91777	3.37062
C	-1.74008	6.18103	0.21869
C	-0.60883	6.85022	1.04300
H	-0.62943	7.94719	0.90920
H	0.38750	6.49305	0.73367
H	-0.72555	6.63430	2.11914
C	-1.54521	6.52099	-1.28269
H	-2.34090	6.06369	-1.89567
H	-0.57649	6.15616	-1.66246
H	-1.57745	7.61473	-1.43886
C	-3.08520	6.78960	0.67422
H	-3.93496	6.38741	0.09587
H	-3.06843	7.88300	0.52276
H	-3.27761	6.60383	1.74516
C	1.84326	2.33302	-0.60888
C	2.79794	2.77917	0.35915
C	3.97778	3.40950	-0.08350
H	4.70404	3.76528	0.65712
C	4.23629	3.59868	-1.44684
H	5.15452	4.10095	-1.77143
C	3.30688	3.14675	-2.39240
H	3.50794	3.30142	-3.45841
C	2.10976	2.51232	-2.00183
C	1.09862	2.08171	-3.06539
H	0.41672	1.35980	-2.58164
C	1.75534	1.38657	-4.27536
H	2.39133	2.07818	-4.85666
H	0.97862	1.01114	-4.96436
H	2.37978	0.53189	-3.96526
C	0.24262	3.28085	-3.53822
H	-0.29869	3.74109	-2.69658
H	-0.50194	2.95544	-4.28647
H	0.87722	4.05570	-4.00589
C	2.55711	2.61816	1.86112
H	1.64844	2.00243	1.97653
C	3.71418	1.87153	2.55919
H	3.89351	0.89122	2.08314
H	3.47789	1.70546	3.62565
H	4.65921	2.44261	2.51636
C	2.30182	3.98050	2.54550
H	3.18005	4.64508	2.45306
H	2.09641	3.84250	3.62208
H	1.43564	4.49164	2.09611
C	-0.51063	-3.02191	-0.60316
C	-0.07540	-3.28394	-1.94525
C	0.28159	-4.59361	-2.31786
H	0.60082	-4.79286	-3.34566
C	0.22487	-5.65067	-1.40158
H	0.49512	-6.66728	-1.70795
C	-0.16585	-5.38644	-0.08647
H	-0.19185	-6.20707	0.64252
C	-0.52541	-4.09124	0.35149
C	-0.92038	-4.02132	1.84230
H	-0.27536	-4.78756	2.32100
C	-0.65684	-2.71260	2.61112
H	0.33206	-2.28378	2.36961
H	-0.69604	-2.91818	3.69706
H	-1.41440	-1.94326	2.39636
C	-2.37602	-4.49596	2.07387
H	-2.58154	-4.58437	3.15593
H	-2.55635	-5.48056	1.60982
H	-3.09413	-3.77851	1.64581
C	-0.06072	-2.16741	-2.99246
H	0.20814	-1.23289	-2.46300
C	0.97445	-2.38481	-4.11263
H	1.98221	-2.58414	-3.70782
H	1.03358	-1.48758	-4.75062
H	0.70263	-3.22941	-4.77112
C	-1.46789	-1.95825	-3.60067
H	-1.79779	-2.86987	-4.13138
H	-1.45832	-1.12686	-4.32800
H	-2.21267	-1.72547	-2.82365
O	4.79925	-0.98169	-0.10405
O	3.48466	-2.86208	1.99389

C	5.02147	-0.83543	-2.57161
H	5.95016	-1.42850	-2.62934
H	5.04033	-0.10861	-3.40137
H	4.16445	-1.51130	-2.72932
C	4.88277	-0.08473	-1.24960
H	3.94603	0.49491	-1.22141
H	5.71520	0.62469	-1.09608
C	6.06456	-1.53554	0.33024
H	6.61628	-1.92878	-0.54511
H	5.78617	-2.38863	0.96981
C	6.91998	-0.53834	1.11300
H	7.21873	0.32768	0.50012
H	7.84387	-1.03449	1.45781
H	6.37671	-0.16267	1.99522
C	3.39667	-4.49667	0.21203
H	2.68808	-3.89998	-0.38845
H	3.19426	-5.55471	-0.01857
H	4.42940	-4.26623	-0.09849
C	3.19866	-4.25372	1.70060
H	2.15327	-4.47130	1.99488
H	3.87142	-4.89826	2.29852
C	3.27994	-2.50713	3.38545
H	2.31202	-2.92586	3.72278
H	3.18358	-1.40758	3.39043
C	4.42684	-2.95314	4.29213
H	4.53094	-4.05023	4.32377
H	4.23690	-2.60938	5.32332
H	5.38461	-2.52108	3.95848
Li	3.04533	-1.45362	0.64391