Angewandte Chemie
Eine Zeitschrift der Gesellschaft Deutscher Chemiker

Supporting Information

A Stable Calcium Alumanyl

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Supporting Information

General

All manipulations were carried out using standard Schlenk line and glovebox techniques under an inert atmosphere of argon. NMR spectra were recorded on an Agilent ProPulse spectrometer at 298 K operating at 500 MHz (^{1}H), 126 MHz (^{13}C) and 160 MHz (^{11}B). The spectra were referenced relative to residual protio solvent resonances. Elemental analyses were performed at Elemental Microanalysis Ltd., Okehampton, Devon, UK. Solvents (toluene, hexane) were dried by passage through a commercially available solvent purification system, under nitrogen and stored in ampoules over 4 Å molecular sieves. C_6D_6 was purchased from Sigma-Aldrich, dried over a potassium mirror before vacuum distillation and storage under argon over molecular sieves. DippNH_2 and $\{CH_2SiMe_2Cl\}_2$ were purchased from Sigma-Aldrich and distilled prior to use. Cyclooctatetraene (COT),[1] [(^{Dipp}BDI)Mg(*n*Bu)],[2] [(^{Dipp}BDI)Ca(N$\{SiMe_3\}_2$)][3] and [$HNEt_3$][BPh_4][4] were synthesized by literature procedures. All other reagents were purchased from Sigma-Aldrich and used without further purification.

Synthetic Procedures

*Synthesis of {$CH_2SiMe_2N(Dipp)H$}$_2$ ({SiN^{Dipp}}H_2, **9**) and {CH_2SiMe_2}$_2$NDipp (**9**')*

A solution of *n*BuLi in hexane (23.4 mL of a 2.5M solution, 0.0584 mmol.) was added dropwise to a pre-cooled solution of $DippNH_2$ (9.4 g, 10 mL, 0.0531 mmol) in hexane (60 mL) at 0 °C. The resulting colorless suspension was stirred at room temperature for 1.5 hours followed by the dropwise addition of a solution of $\{CH_2SiMe_2Cl\}_2$ (5.7 g, 0.0266 mmol) in hexane (40 mL) at 0 °C. The resulting suspension was stirred for 12 hours at room temperature then allowed to settle for 3 hours and filtered to give a clear colorless solution. Removal of the volatiles *in vacuo* gave a colorless oil, which was 85 % **9** by ^{1}H NMR spectroscopy. Distillation of the oil at 100 °C at 2 x 10^{-2} mbar results in the isolation of the cyclic co-product **9**' as the distillate and clean **9** as the distilland. Yield **9**: 7.40 g, 56 %. NMR data for **9**: ^{1}H NMR (500 MHz, C_6D_6): δ 7.11 (m, 6H, C_6H_3), 3.49 (sept, J = 8.0 Hz, 4H, C*H*Me_2), 2.15 (s, 2H, N*H*), 1.23 (d, J = 8.0, 24H, CH*Me*$_2$), 0.62 (s, 4H, SiCH_2), 0.14 (s, 12H, Si*Me*$_2$). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6): δ 144.4, 139.9, 124.2, 123.4 (*C*$_6$H$_3$), 28.5, 23.9 (*C*HMe_2 and CH*Me*$_2$), 9.8 (Si*C*H$_2$), -1.5 (Si*Me*$_2$). NMR data for **9**': ^{1}H NMR (500 MHz, C_6D_6): δ 7.11 (m, 3H, C_6H_3), 3.41 (sept, J = 7.5 Hz, 2H, C*H*Me_2), 1.22 (d, J = 7.5, 12H, CH*Me*$_2$), 0.93 (s, 4H, SiCH_2), 0.11 (s, 12H, Si*Me*$_2$). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6): δ 147.7, 138.8, 124.9, 124.4 (*C*$_6$H$_3$), 27.4, 26.2 (*C*HMe_2 and CH*Me*$_2$), 9.1 (Si*C*H$_2$), 1.0 (Si*Me*$_2$).

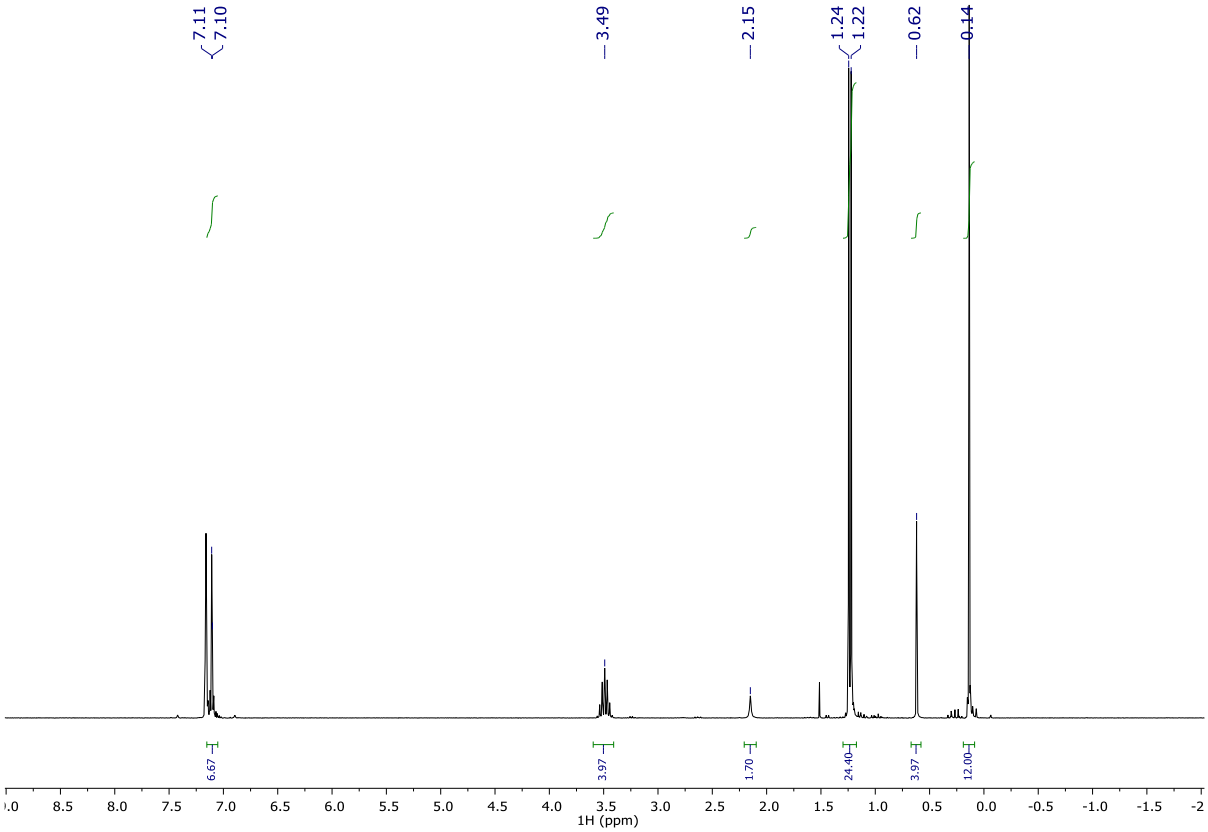


Figure S1. ^{1}H NMR spectrum of $\{SiN^{Dipp}\}H_2$ (**9**) in C_6D_6 (500 MHz).

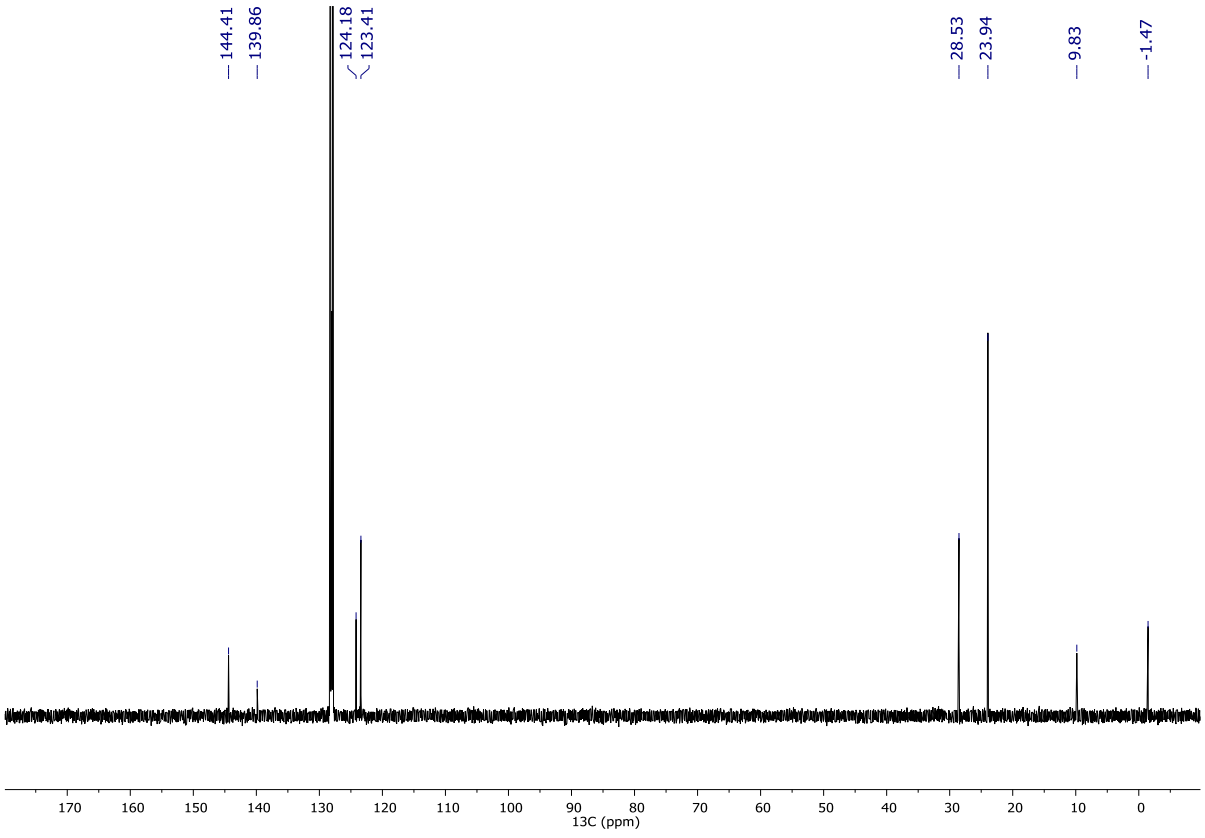


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of $\{SiN^{Dipp}\}H_2$ (**9**) in C_6D_6 (125 MHz).

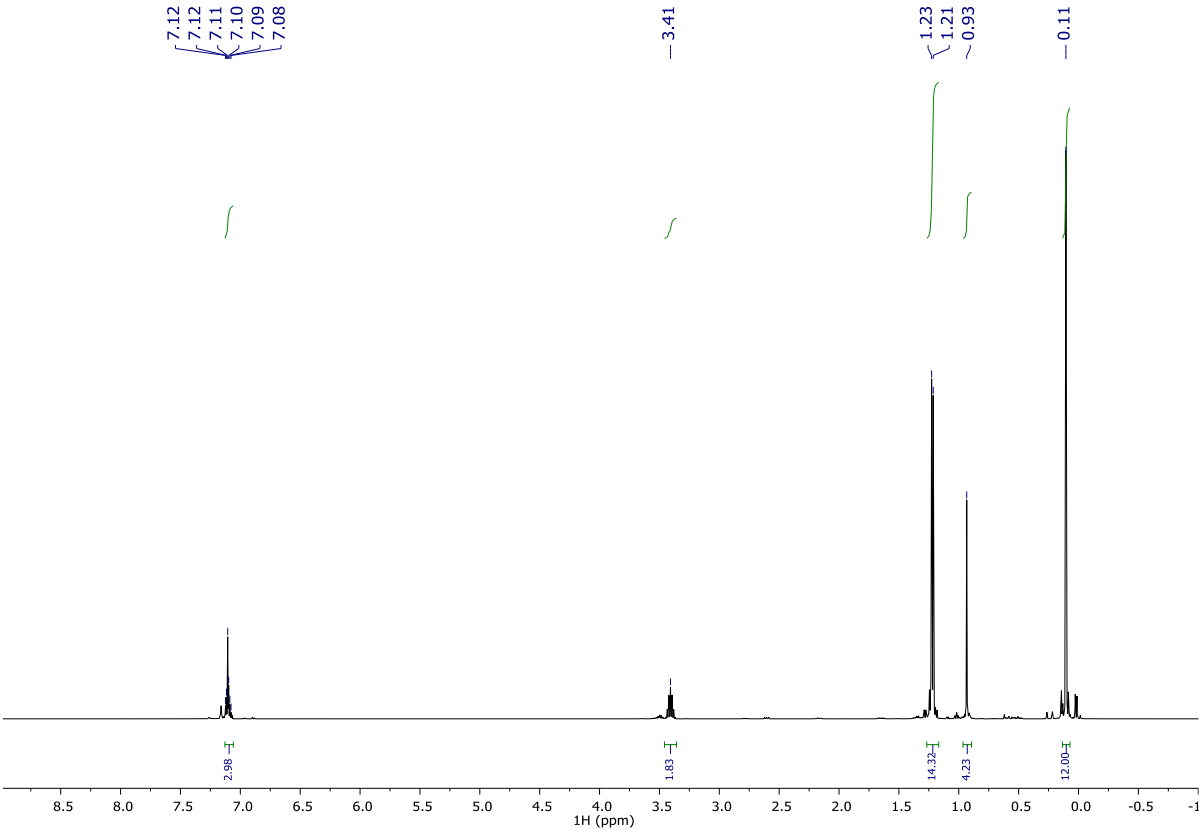


Figure S3. ^{1}H NMR spectrum of $\{CH_2SiMe_2\}_2NDipp$ (**9**') in C_6D_6 (500 MHz).

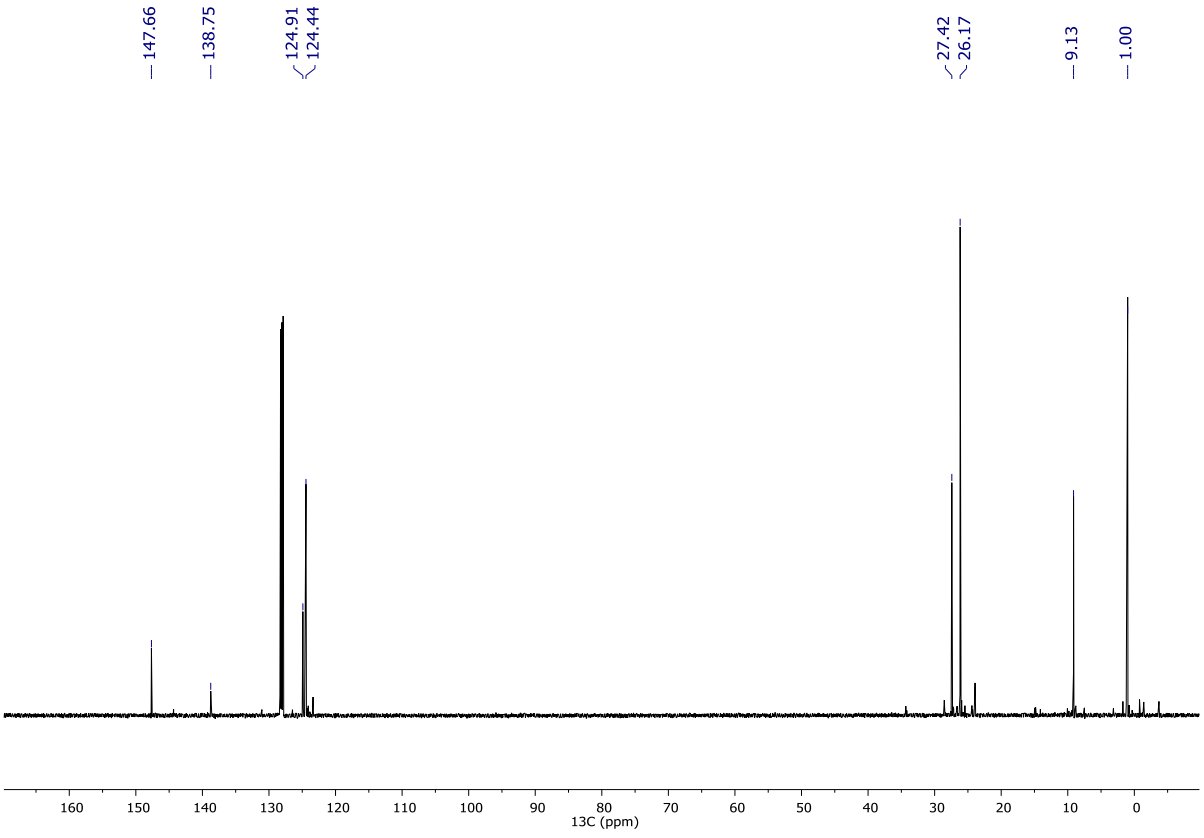


Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of $\{CH_2SiMe_2\}_2NDipp$ (**9**') in C_6D_6 (125 MHz).

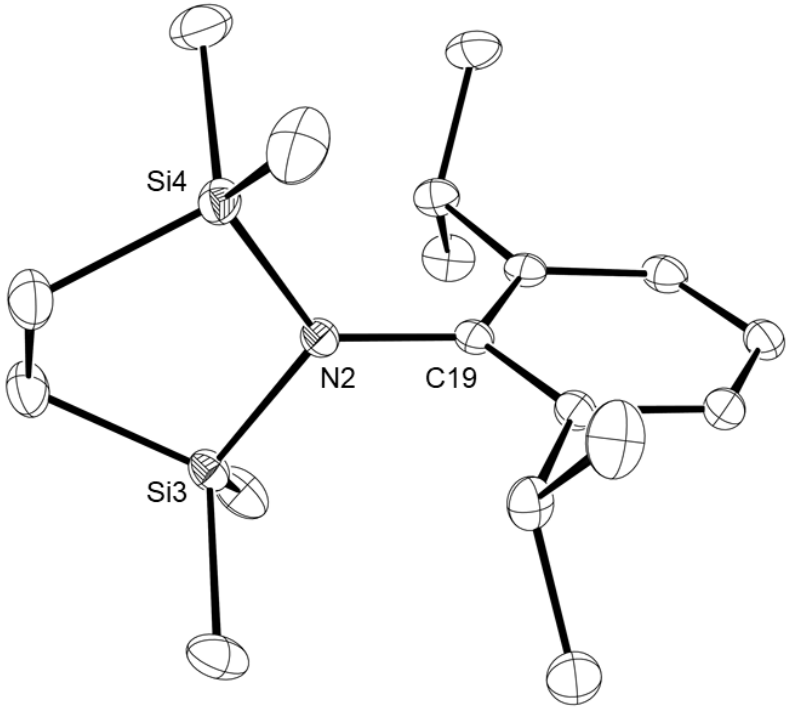


Figure S5. ORTEP representation of the N2-containing molecule of compound **9**' (30% probability ellipsoids). Hydrogen atoms removed for clarity.

*Synthesis of Al{SiN^{Dipp}}Me (**10**)*

A solution of $AlMe_3$ in hexane (1.51 mL of a 2 M solution, 3.02 mmol) was added dropwise to a stirring solution of **9** (1.50 g, 3.02 mmol) in toluene (30 mL) at room temperature. Upon addition, the solution bubbled and was stirred for 48 hours at room temperature under a weak flow of argon, followed by warming to 60 °C and stirring for 12 hours. The resulting colorless suspension was cooled to room temperature and the volatile components were removed *in vacuo* to give **10** as a colorless waxy solid. Yield: 1.52 g, 94 %. ^{1}H NMR (500 MHz, C_6D_6): δ 7.04 (m, 6H, C_6H_3), 3.75 (sept, J = 8.0 Hz, 4H, C*H*Me$_2$), 1.29, 1.20 (d, J = 8.0, 12H, CH*Me$_2$*), 1.05 (s, 4H, SiC*H$_2$*), 0.18 (s, 12H, Si*Me$_2$*), -1.08 (s, 3H, Al*Me*). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6): δ 145.7, 143.3, 124.5, 123.9 (*C*$_6$H$_3$), 28.4, 24.9, 24.4 (*C*HMe$_2$ and CH*Me$_2$*), 13.4 (Si*C*H$_2$), 0.0 (Si*Me$_2$*). ^{13}C NMR resonance for Al*Me* not observed.

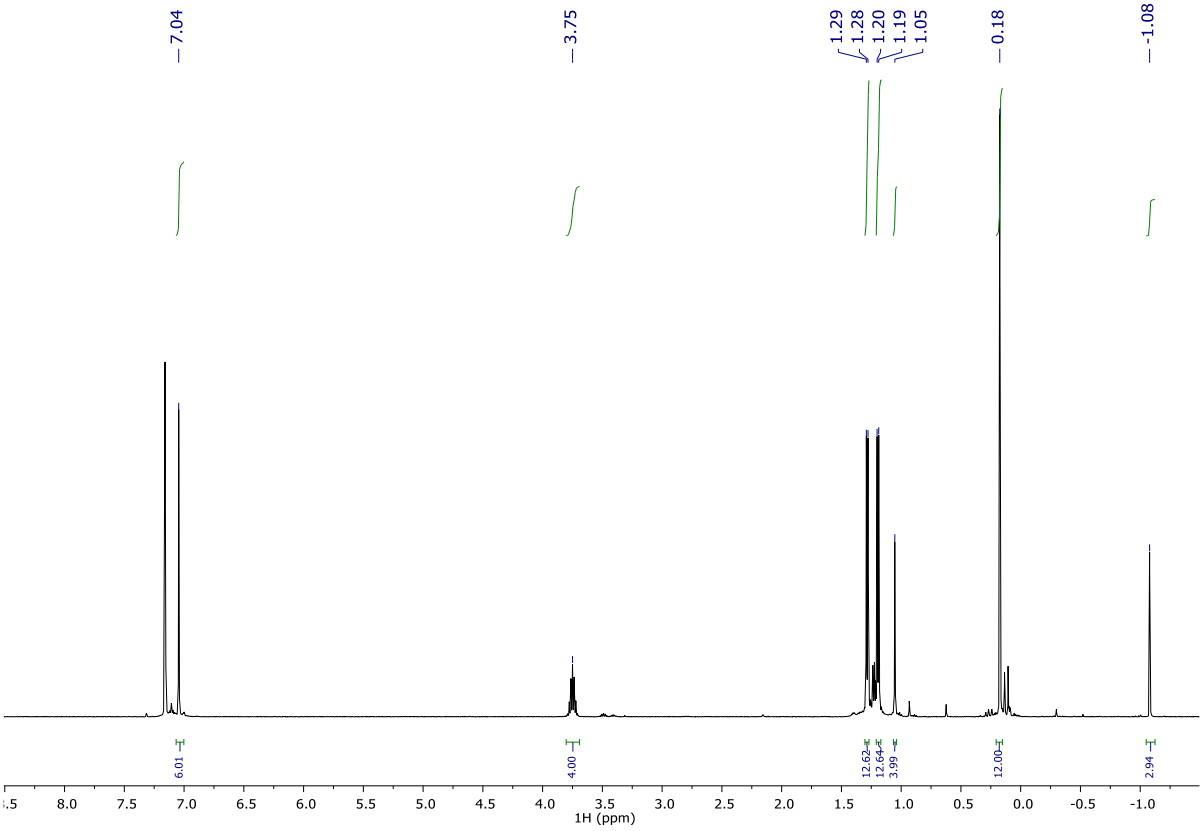


Figure S6. ^{1}H NMR spectrum of Al{SiN^{Dipp}}Me (**10**) in C_6D_6 (500 MHz).

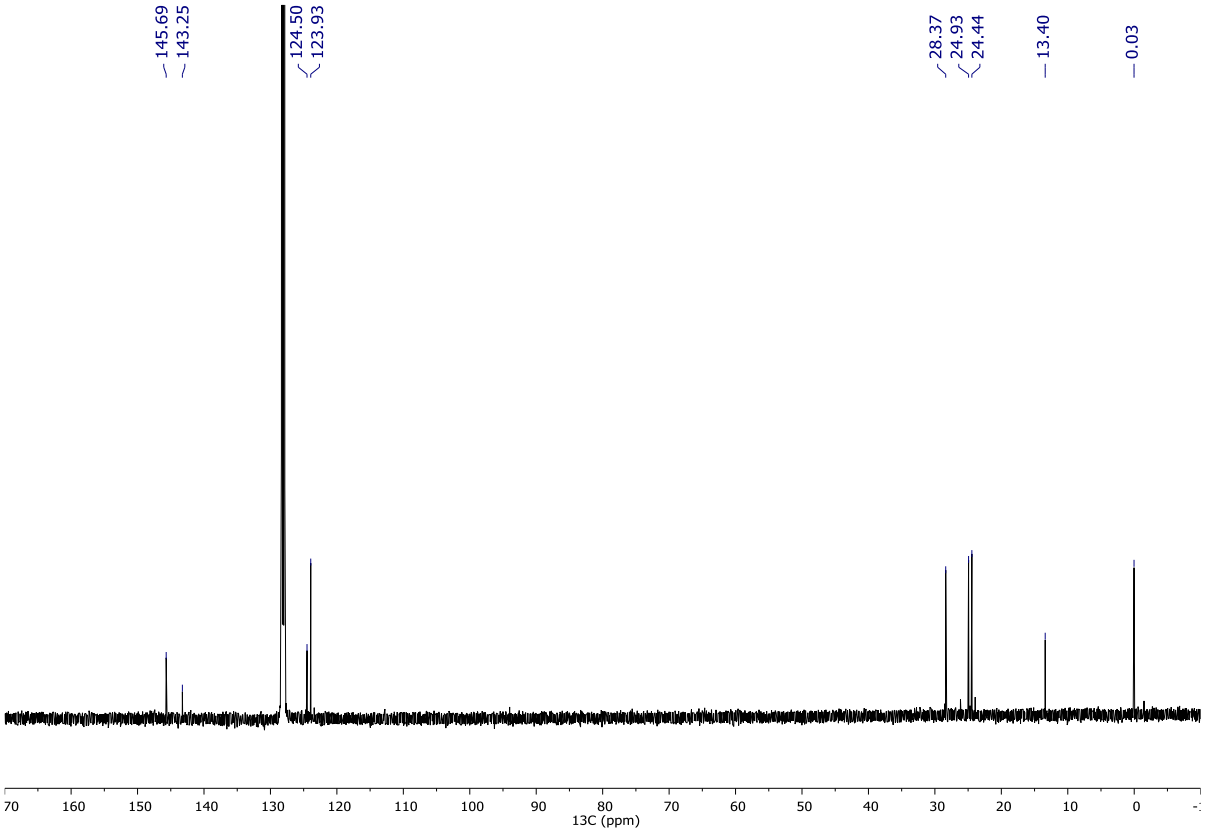


Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum of Al{SiN^{Dipp}}Me (**10**) in C_6D_6 (125 MHz).

*Synthesis of Al{SiN^{Dipp}}I (**11**)*

In a 250 mL Schlenk tube, iodine (2.08 g, 8.20 mmol) was added to a stirring solution of **10** (4.38 g, 8.20 mmol) in toluene (40 mL) resulting in the immediate formation of a red solution. The Schlenk tube was fitted with a cold-finger and the solution was refluxed for 4 days under a weak flow of argon. The resulting pale orange solution was allowed to cool to room temperature and the volatile components were removed *in vacuo* to give a waxy solid. Extraction into hexane and filtration gave a clear orange solution. Concentration of the orange solution followed by storage at -30 °C gave **11** as colorless crystals. Yield 4.45 g, 84 %. Anal. Calcd. for $C_{30}H_{50}AlIN_2Si_2$ (*648.79*): C, 55.54; H, 7.77; N, 4.32 %. Found: C, 54.98; H, 7.79, N, 4.38 %. ^{1}H NMR (500 MHz, C_6D_6): δ 7.07 (m, 6H, C_6H_3), 3.64 (sept, J = 8.0 Hz, 4H, C*H*Me$_2$), 1.38, 1.27 (d, J = 8.0, 12H, CH*Me$_2$*), 1.00 (s, 4H, SiC*H$_2$*), 0.17 (s, 12H, Si*Me$_2$*). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6): δ 145.5, 142.0, 125.2, 124.2 (*C*$_6$H$_3$), 28.9, 25.2, 24.6 (*C*HMe$_2$ and CH*Me$_2$*), 13.2 (Si*C*H$_2$), 0.15 (Si*Me$_2$*).

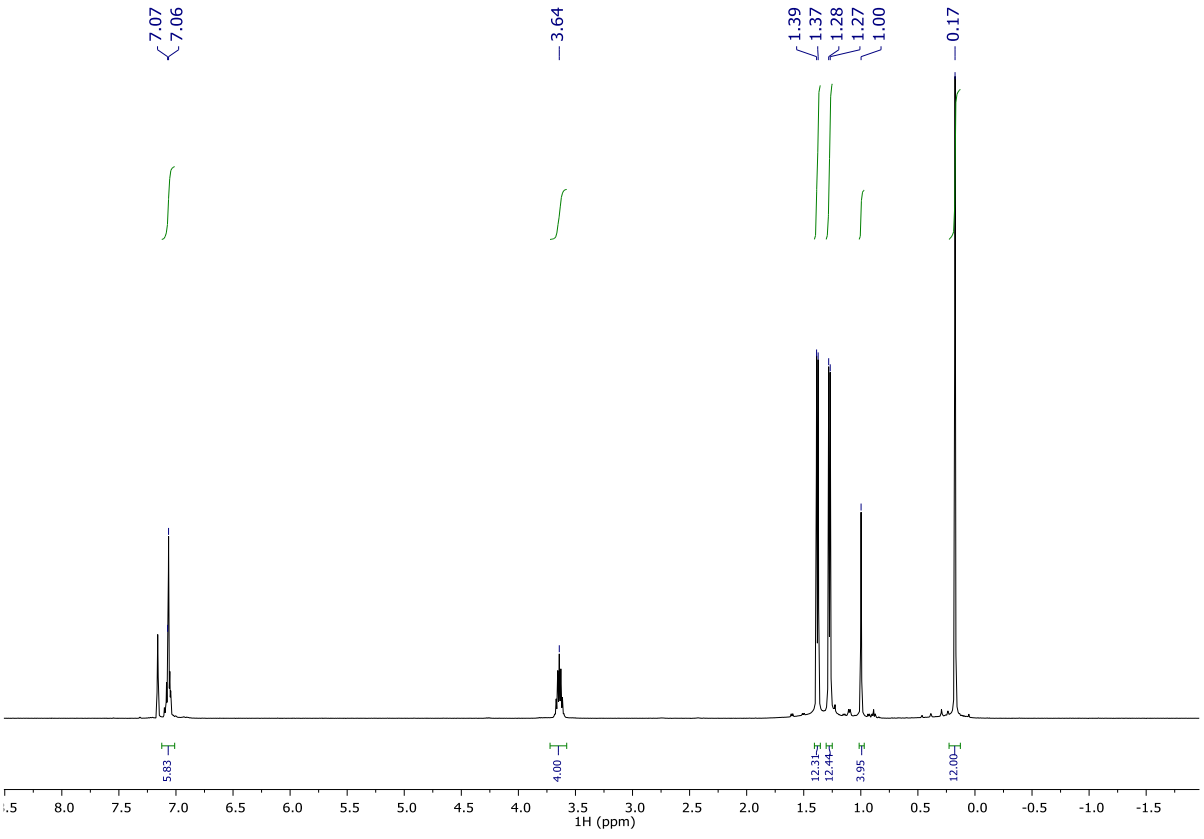


Figure S8. ^{1}H NMR spectrum of Al{SiN^{Dipp}}I (**11**) in C_6D_6 (500 MHz).

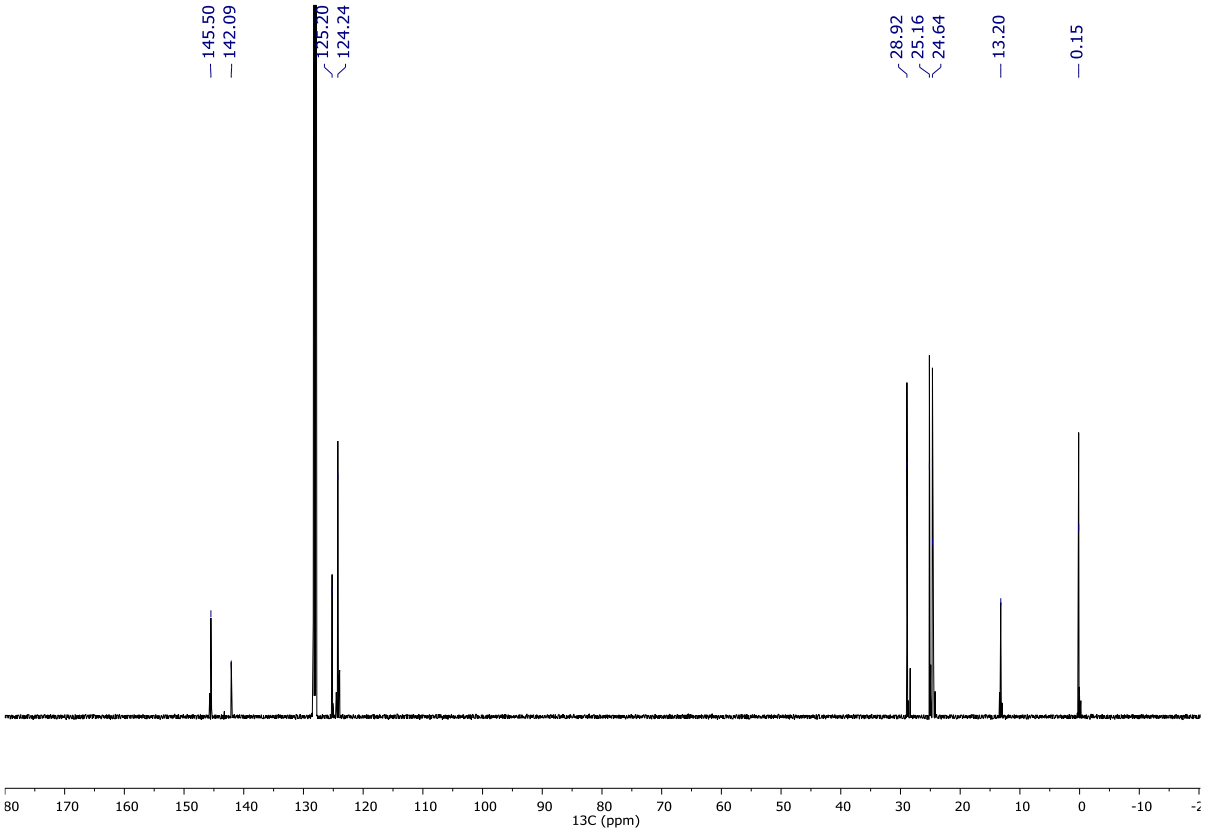


Figure S9. $^{13}C\{^{1}H\}$ NMR spectrum of Al{SiN^{Dipp}}I (**11**) in C_6D_6 (125 MHz).

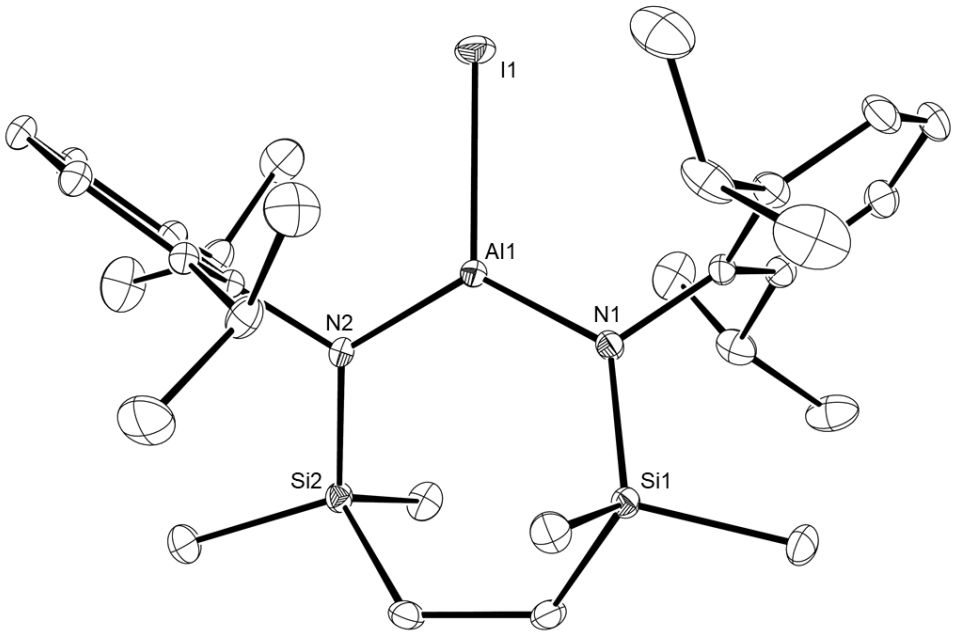


Figure S10. ORTEP representation of compound **11** (30% probability ellipsoids). Hydrogen atoms removed for clarity.

*Synthesis of [Al{SiN^{Dipp}}K]$_2$ (**12**)*

A solution of **11** (4.68 g, 7.24 mmol) in hexane (30 mL) was stirred on mirrored K (0.85 g, 0.0217 mmol) for 3 days at room temperature resulting in the gradual color change from colorless to yellow and the formation of a grey precipitate. The resulting clear dark yellow solution was filtered through a cannula filter, concentrated to *ca.* 15 mL and stored at -30 °C for 24 hours to give **12** as yellow blocks. A second crop of small yellow crystals was obtained by further concentration of the mother liquor and storage at -30 °C. Yield (combined): 3.2 g, 79 %. X-ray quality crystals were grown from a concentrated Et_2O solution at -30 °C. Anal. Calcd. for $C_{60}H_{100}Al_2K_2N_4Si_4$ (*1121.96*): C, 64.23; H, 8.98; N, 4.99 %. Found: C, 63.67; H, 9.02, N, 5.03 %. ^{1}H NMR (500 MHz, C_6D_6): δ 6.89 (d, J = 8.0 Hz, 4H, *m*-C_6H_3), 6.78 (t, J = 8.0 Hz, 2H, *p*-C_6H_3), 3.97 (sept, J = 8.0 Hz, 4H, C*H*Me$_2$), 1.29 (d, J = 8.0, 12H, CH*Me$_2$*), 1.12 (s, 4H, SiC*H$_2$*), 1.06 (d, J = 8.0, 12H, CH*Me$_2$*), 0.22 (s, 12H, Si*Me$_2$*). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6): δ 151.2, 149.0, 122.7, 122.6 (*C*$_6$H$_3$), 27.9, 25.1, 24.1 (*C*HMe$_2$ and CH*Me$_2$*), 14.4 (Si*C*H$_2$),* 1.7 (Si*Me$_2$*). *overlaps with hexane solvent impurity

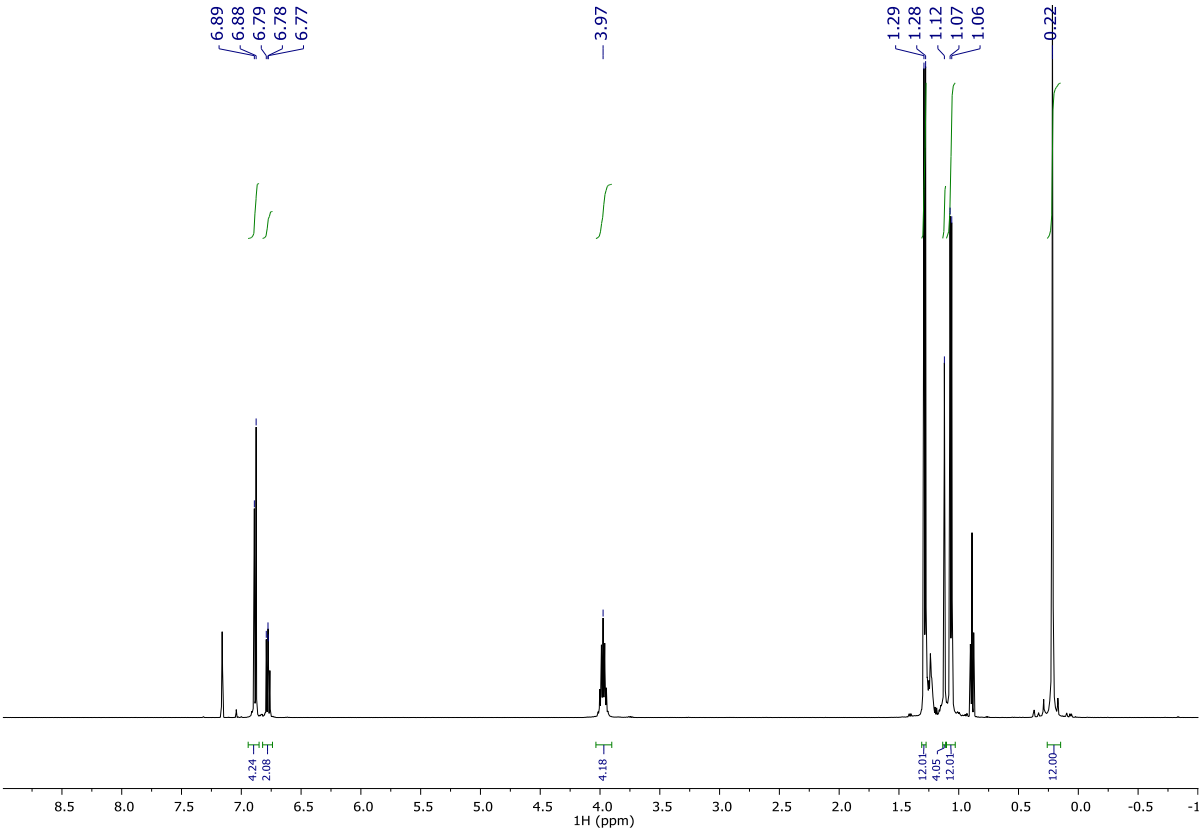


Figure S11. ^{1}H NMR spectrum of [Al{SiN^{Dipp}}K]$_2$ (**12**) in C_6D_6 (500 MHz).

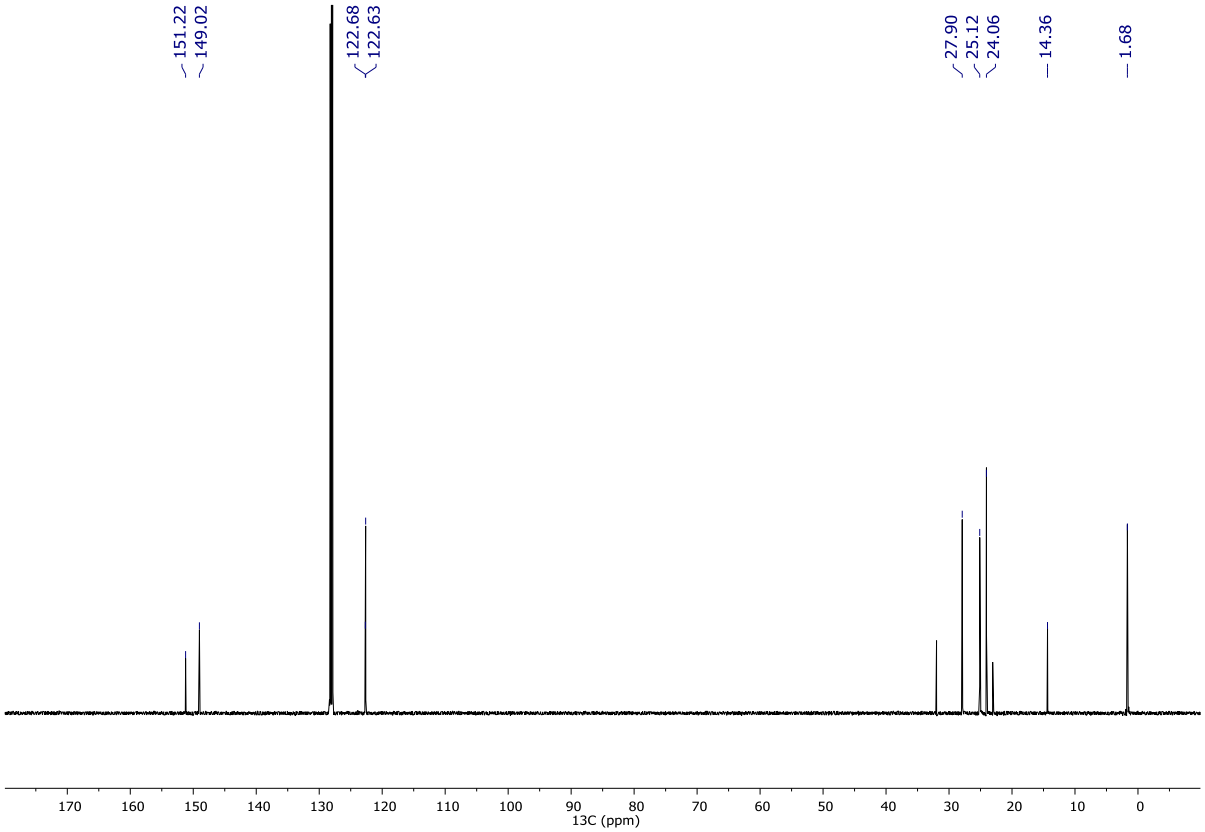


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum of $[Al\{SiN^{Dipp}\}K]_2$ (**12**) in C_6D_6 (125 MHz).

*Synthesis of (^{Dipp}BDI)Mg(μ-Ph)$_2$BPh$_2$ (**13**)*

A suspension of [HNEt$_3$][BPh$_4$] (1.05 g, 2.1 mmol) in toluene (40 mL) was added dropwise to a stirring solution of [(^{Dipp}BDI)Mg(*n*Bu)] (0.92 g, 2.2 mmol) in toluene (40 mL). The resulting colorless suspension was stirred at room temperature for 12 hours followed by the removal of the volatile components *in vacuo*. Extraction into hot toluene (approx. 60 °C) and filtration gave a colorless solution. Removal of the volatiles *in vacuo* gave **13** as a colorless solid. Colorless crystals suitable for characterization by X-ray diffraction were obtained by recrystallization from a concentrated toluene solution at -30 °C. Yield: 0.86 g, 53 %. ^{1}H NMR (500 MHz, C_6D_6): δ 7.70 (br, 8H, C_6H_5), 7.34 – 6.90 (m, 18H, C_6H_5 and C_6H_3), 4.54 (s, 1H, γ-C*H*), 2.71, 1.92 (br, 2H, C*H*Me$_2$), 1.30 (s, 6H, C*Me*), 1.25 – 0.92 (br, 12H, CH*Me$_2$*),* 0.90 (d, J = 8.0, 12 H, CH*Me$_2$*). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6): δ 170.5 (*C*Me), 163.0, 144.4, 144.2, 139.0, 126.6, 124.0 (*C*$_6$H$_5$ and *C*$_6$H$_3$), 95.8 (γ-*C*H), 30.9, 28.8, 25.3 (CH*Me$_2$*). ^{11}B{^{1}H} NMR (160 MHz, C_6D_6): δ -6.64. *overlapping with hexane solvent impurity

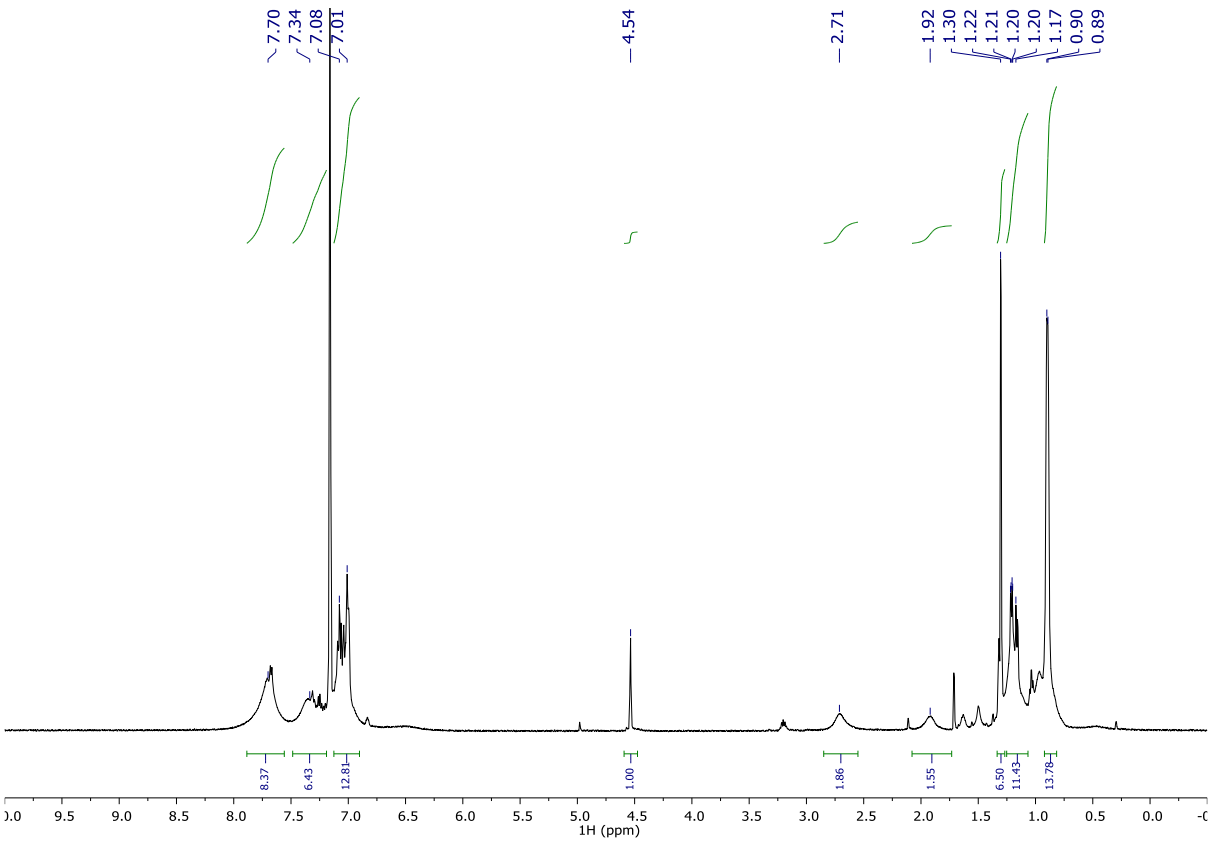


Figure S13. ^{1}H NMR spectrum of (^{Dipp}BDI)Mg(μ-Ph)$_2$BPh$_2$ (**13**) in C_6D_6 (500 MHz).

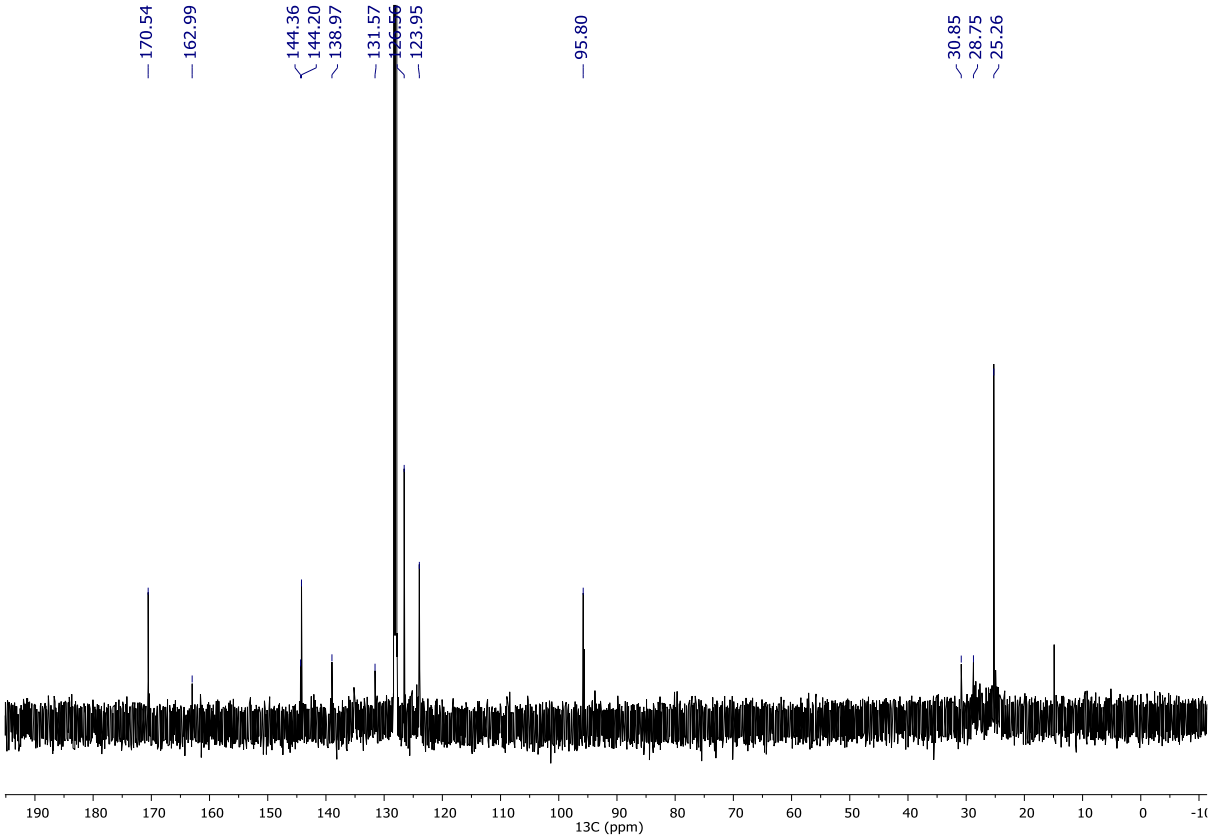


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of (^{Dipp}BDI)Mg(μ-Ph)$_2$BPh$_2$ (**13**) in C_6D_6 (125 MHz).

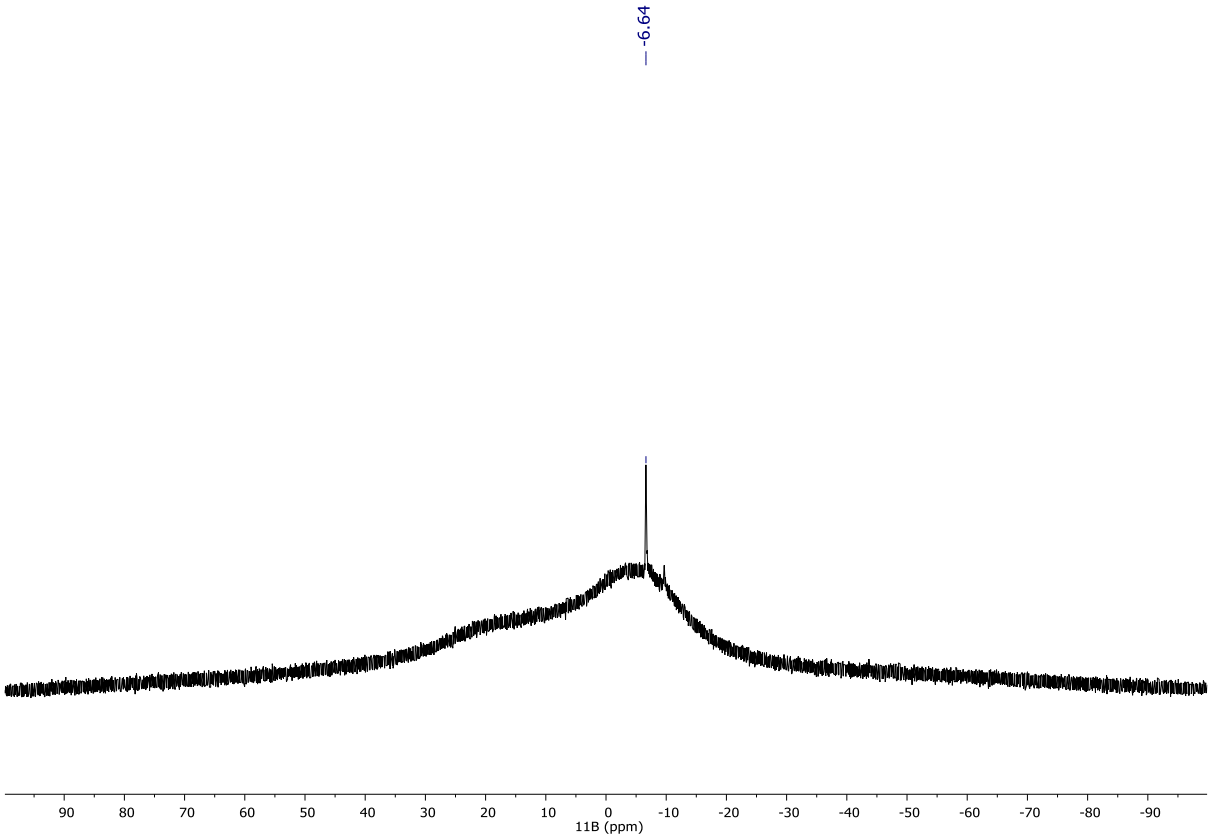


Figure S15. $^{11}B\{^{1}H\}$ NMR spectrum of (^{Dipp}BDI)Mg(μ-Ph)$_2$BPh$_2$ (**13**) in C_6D_6 (160 MHz).

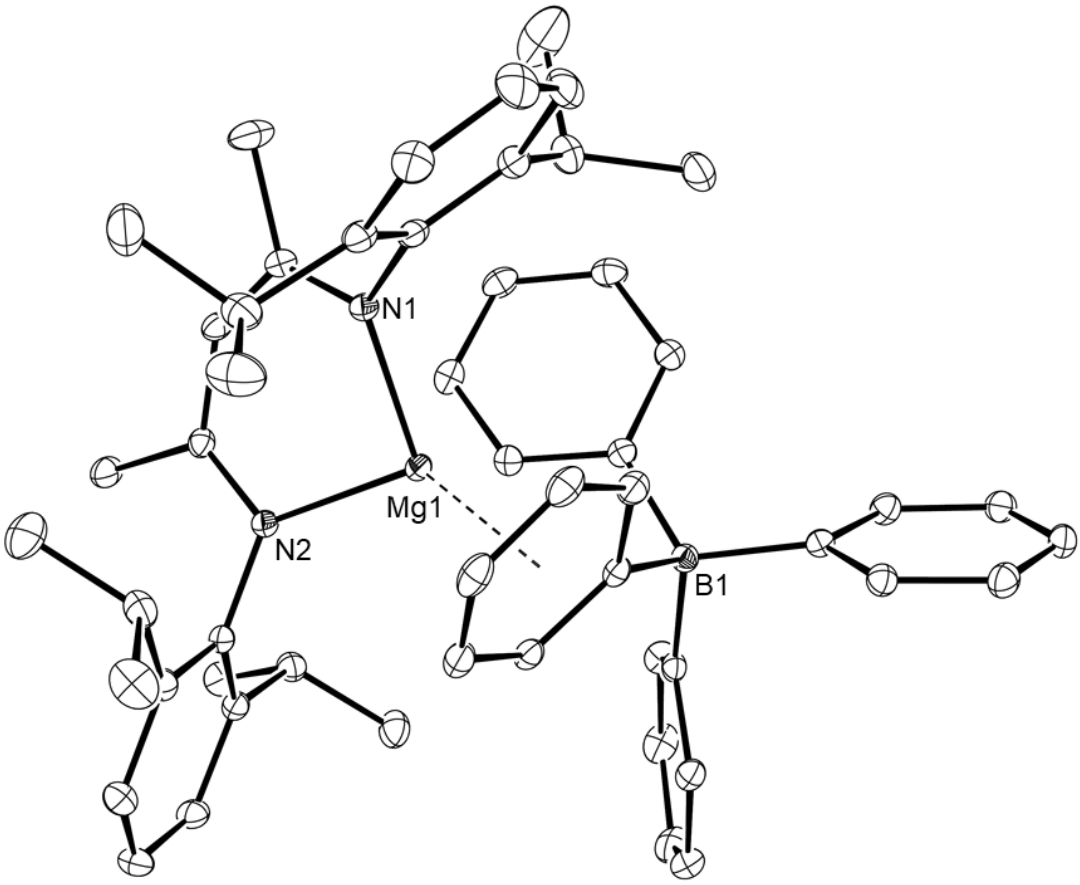


Figure S16. ORTEP representation of compound **13** (30% probability ellipsoids). Hydrogen atoms removed for clarity.

*Synthesis of (BDI^{Dipp})Ca(μ-Ph)$_2$BPh$_2$) (**14**)*

A suspension of [HNEt$_3$][BPh$_4$] (1.29 g, 3.06 mmol) in toluene (60 mL) was added dropwise to a stirring solution of [(^{Dipp}BDI)CaN{SiMe$_3$}$_2$] (1.90 g, 3.06 mmol) in toluene (60 mL). The resulting colorless suspension was stirred at room temperature for 12 hours followed by the removal of the volatile components *in vacuo*. Extraction into hot toluene (approx. 80 °C) and filtration gave a colorless solution. Upon cooling to room temperature, colorless crystals of **14** began to form which were isolated by filtration. A second crop of **14** was obtained by concentrating the mother liquor and cooling to -18 °C for 24 hours. Yield (combined): 1.95 g, 82 %. Anal. Calcd. for C$_{53}$H$_{61}$BCaN$_2$ (*776.95*): C, 81.93; H, 7.91; N, 3.61 %. Found: C, 81.87; H, 7.41, N, 3.71 %. ^{1}H NMR (500 MHz, C$_6$D$_6$): δ 8.02 (br, 8H, C$_6$*H*$_5$), 7.13 – 7.00 (m, 18H, C$_6$*H*$_5$ and C$_6$*H*$_3$), 4.25 (s, 1H, γ-C*H*), 2.78, 2.35 (br, 2H, C*H*Me$_2$), 1.33 (s, 6H, C*Me*), 1.25 – 1.10 (br, 12H, CH*Me*$_2$), 1.00 (d, J = 8.0, 12 H, CH*Me*$_2$). ^{13}C{^{1}H} NMR (125 MHz, C$_6$D$_6$): δ 166.6 (*C*Me), 146.6, 135.1 (br), 125.3, 124.2 (*C*$_6$H$_5$ and *C*$_6$H$_3$),* 88.4 (γ-*C*H), 25.7, 25.1, 25.0 (CH*Me*$_2$, br). ^{11}B NMR (160 MHz, C$_6$D$_6$): δ -4.90. *several resonances not observed due to the poor solubility of (^{Dipp}BDI)Ca(μ-Ph)$_2$BPh$_2$) in C$_6$D$_6$ and splitting of the ^{13}C resonances adjacent to the ^{11}B centre.

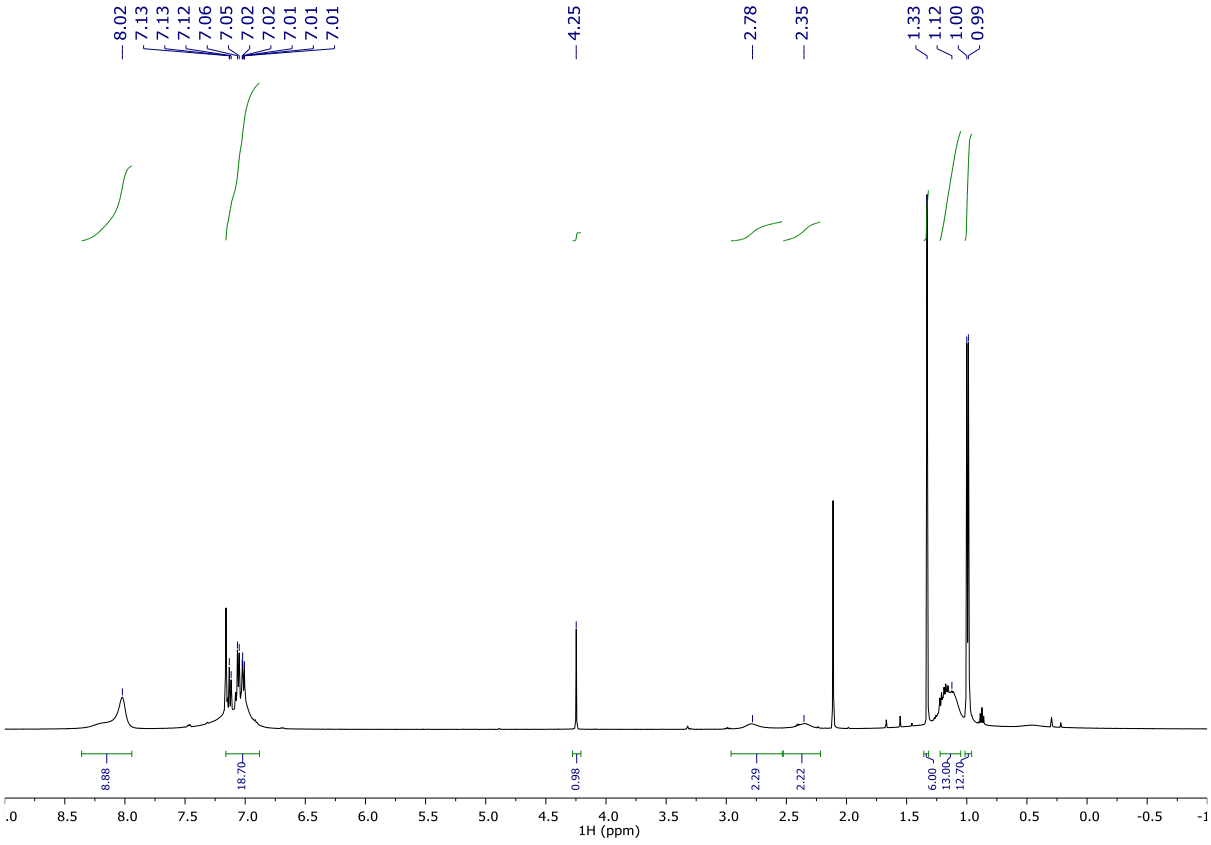


Figure S17. ^{1}H NMR spectrum of (^{Dipp}BDI)Ca(μ-Ph)$_2$BPh$_2$ (**14**) in C$_6$D$_6$ (500 MHz).

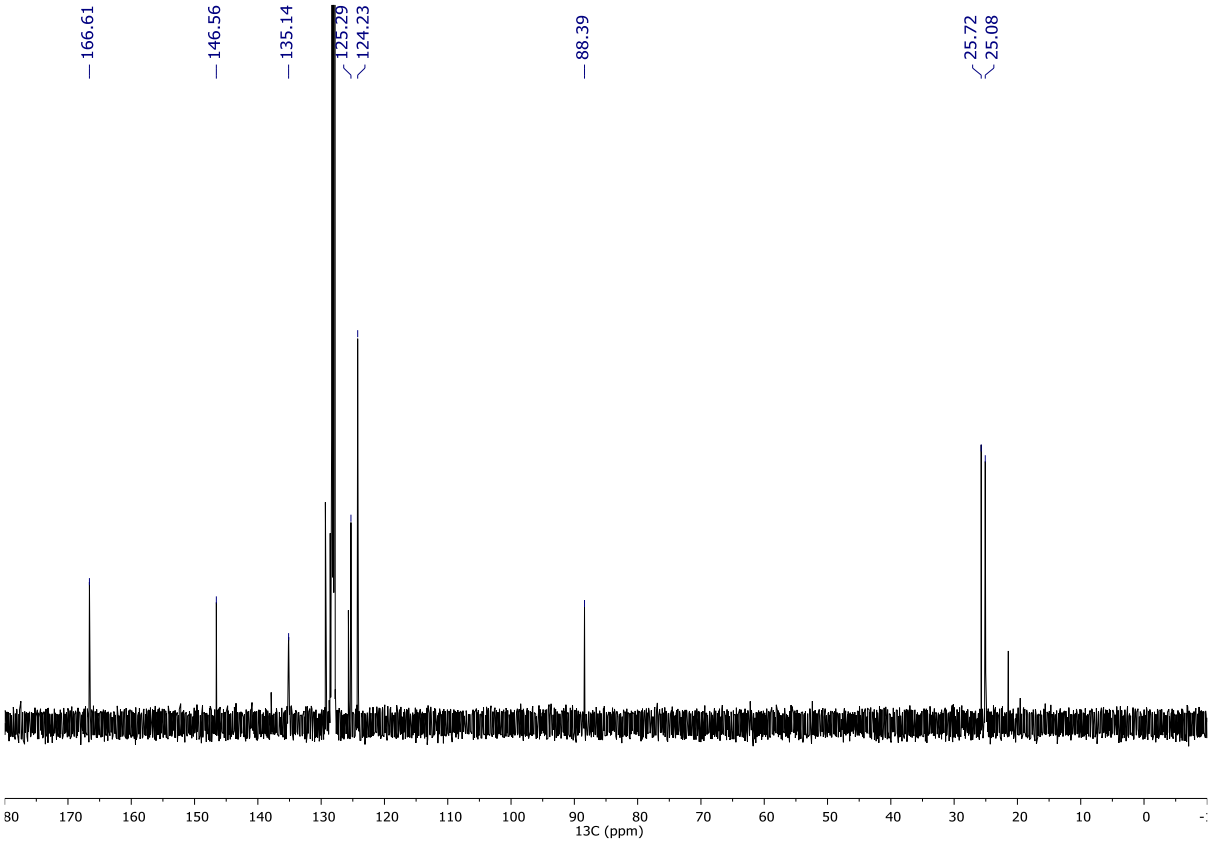


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of (^{Dipp}BDI)Ca(μ-Ph)$_2$BPh$_2$ (**14**) in C_6D_6 (125 MHz).

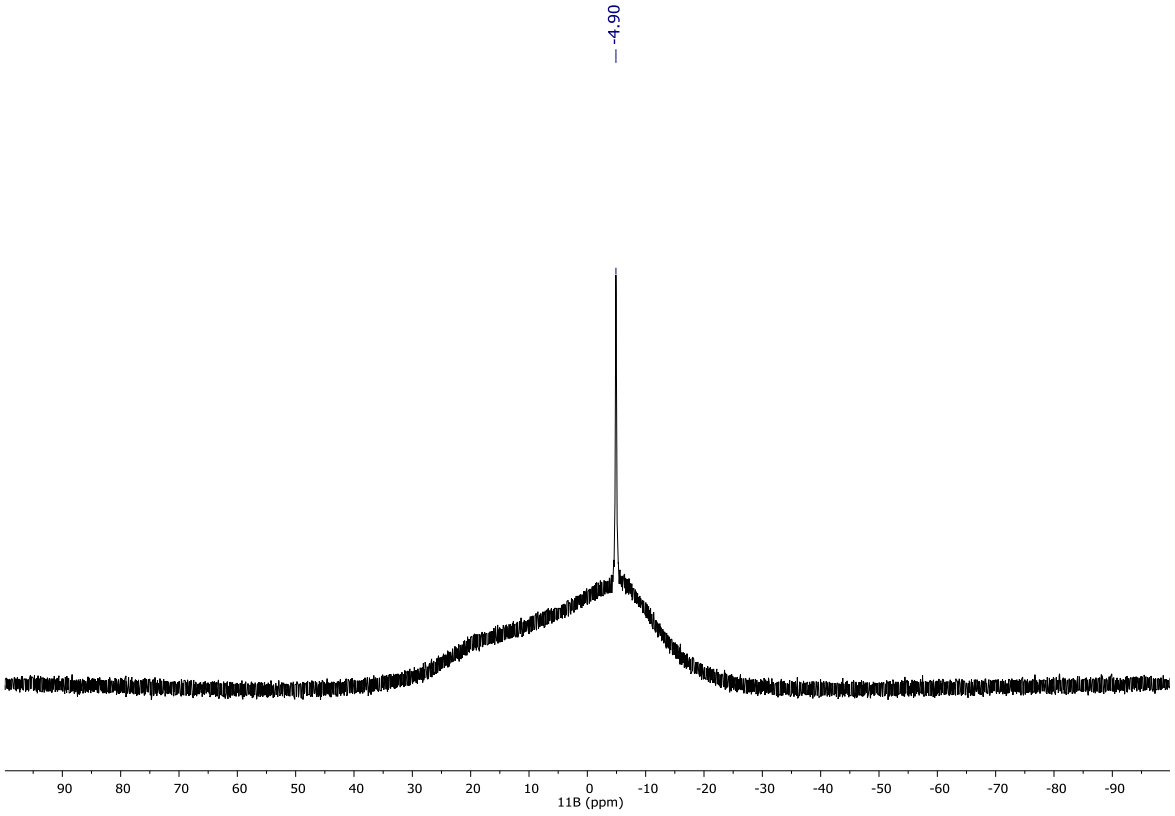


Figure S19. $^{11}B\{^{1}H\}$ NMR spectrum of (^{Dipp}BDI)Ca(μ-Ph)$_2$BPh$_2$ (**14**) in C_6D_6 (160 MHz).

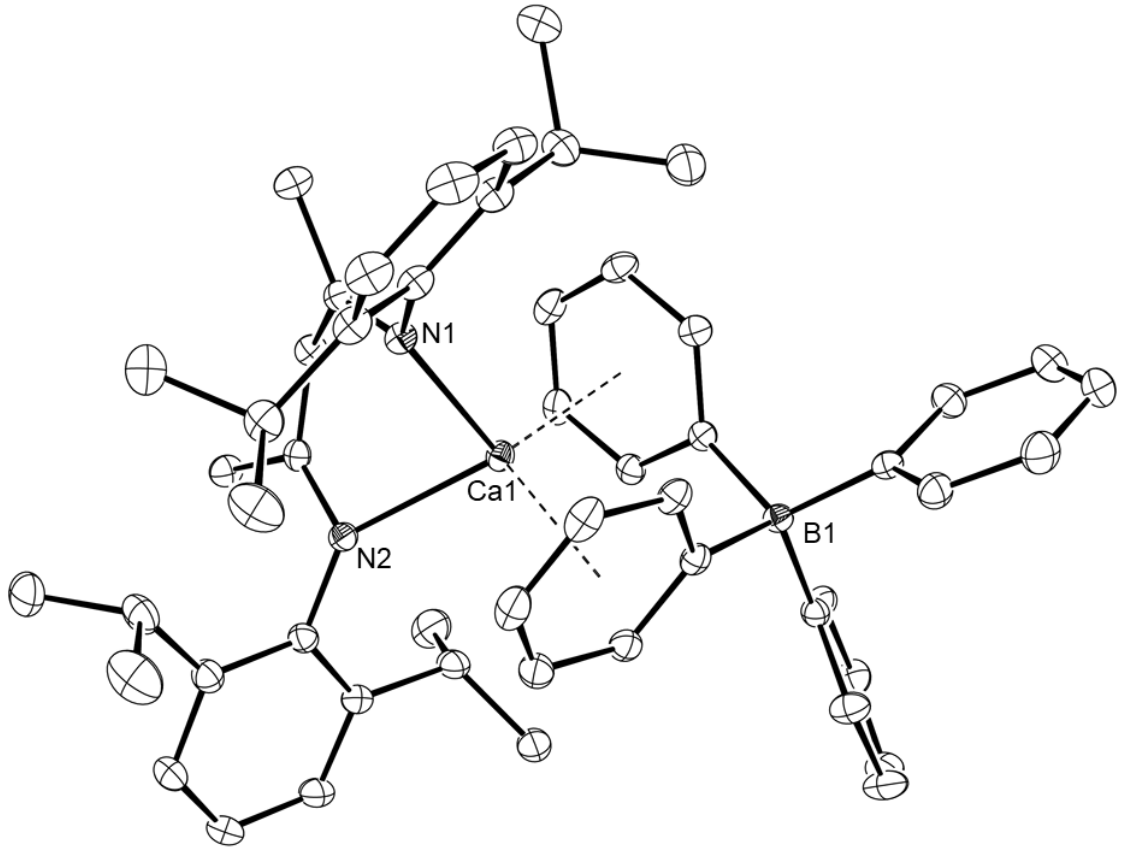


Figure S20. ORTEP representation of compound **14** (30% probability ellipsoids). Hydrogen atoms removed for clarity.

*Synthesis of {SiN^{Dipp}}Al-Mg(BDI^{Dipp}) (**15**)*

A solution of **13** (0.341 g, 0.45 mmol) in toluene (30 mL) was added dropwise to a stirring solution of **12** (0.250 g, 0.45 mmol) in toluene (10 mL). The resulting suspension was stirred at room temperature for 12 hours after which time a colorless precipitate had formed and the solution had become colorless. The suspension was filtered to give a clear colorless solution. Concentration of the solution to 20 mL and storage at room temperature resulted in the formation of colorless crystals of **15**. Yield 0.175 g, 40 %. ^{1}H NMR (500 MHz, C_6D_6): δ 7.13 – 7.01 (m, 12H, C_6H_3), 4.73 (s, 1H, γ-C*H*), 3.84 (br, 4H, C*H*Me$_2$), 3.05 (br, 2H, C*H*Me$_2$), 2.67 (br, 2H, C*H*Me$_2$), 1.38 (s, 6H, C*Me*), 1.35 – 0.71 (br m, 52H, CH*Me$_2$* and SiCH_2), 0.46, -0.24 (br s, 6H, Si*Me$_2$*). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6): δ* 169.8 (*C*Me), 126.2, 124.1, 124.0, 123.6 (C_6H_3),* 96.8 (γ-*C*H), 28.9, 28.6, 27.9 (br), 25.9, 25.3, 25.2, 24.6 (C*Me*, *C*HMe$_2$ and CH*Me$_2$*), 13.7 (Si*C*H$_2$), 3.3 (Si*Me$_2$*).*due to the poor solubility of **15** in C_6D_6 and fluxional processes in solution, several *C*$_6$H$_3$ resonances and one Si*Me$_2$* resonance are not observed.

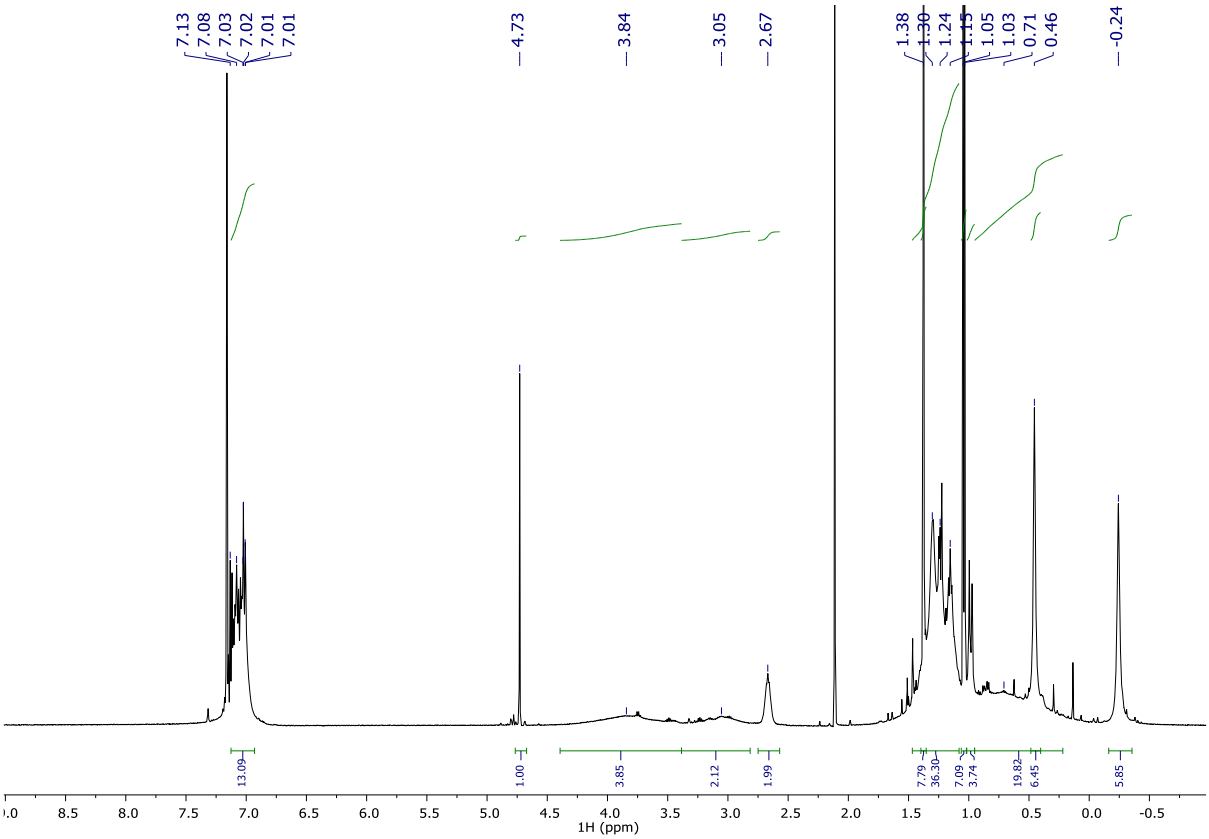


Figure S21. ^{1}H NMR spectrum of {SiN^{Dipp}}Al-Mg(^{Dipp}BDI) (**15**) in C_6D_6 (500 MHz).

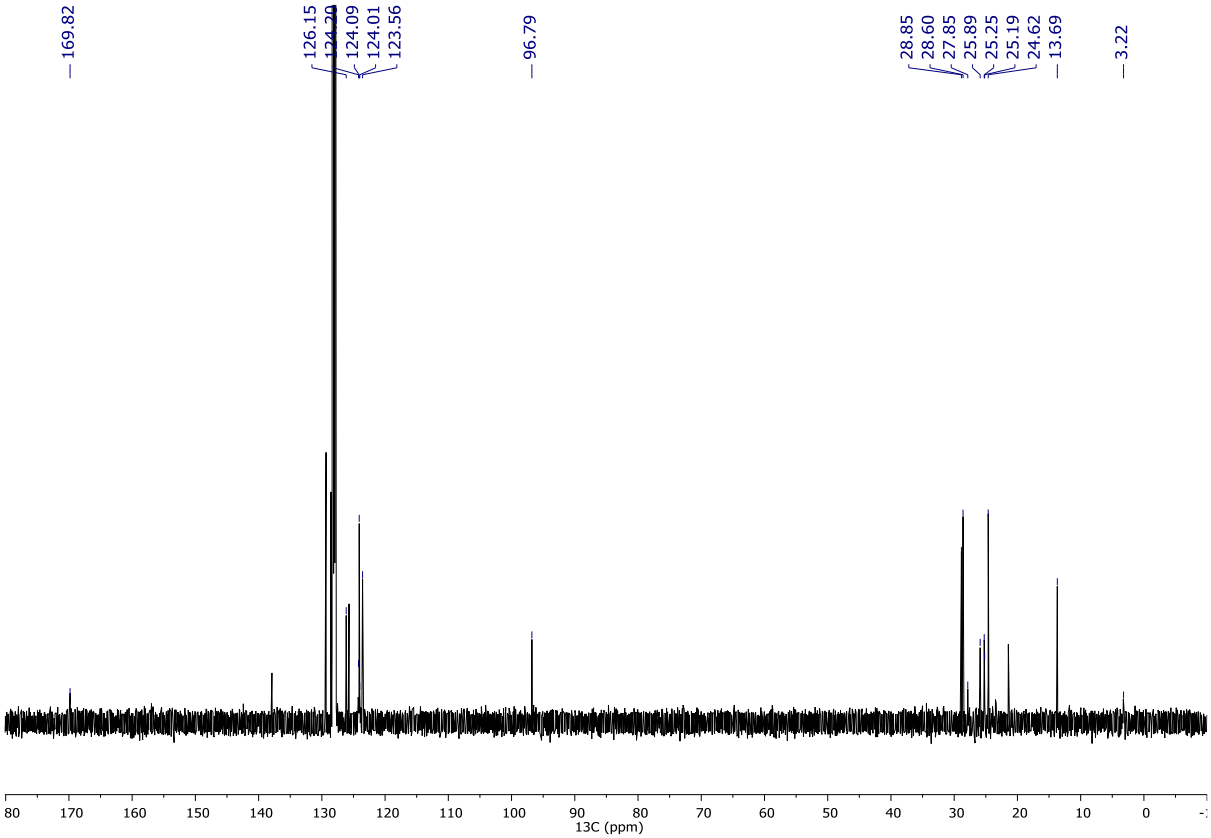


Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum of {SiN^{Dipp}}Al-Mg(^{Dipp}BDI) (**15**) in C_6D_6 (125 MHz).

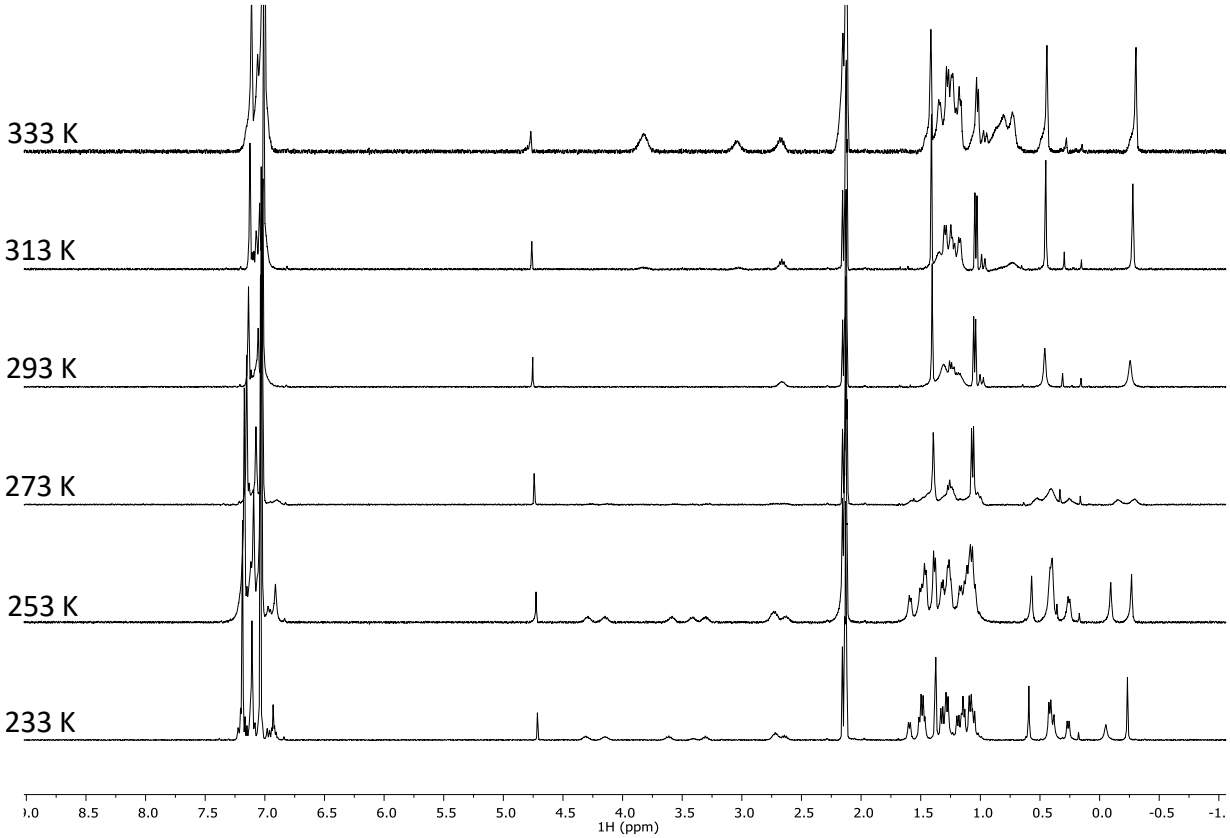


Figure S23. Stacked variable temperature ^{1}H NMR spectra of {SiN^{Dipp}}Al-Mg(^{Dipp}BDI) (**15**) in C_7D_8 (400 MHz).

*Synthesis of {SiN^{Dipp}}Al-Ca(^{Dipp}BDI) (**16**)*

A solution of **14** (0.69 g, 0.89 mmol) in toluene (30 mL) was added dropwise to a stirring solution of **12** (0.50 g, 0.89 mmol) in toluene (10 mL). The resulting suspension was stirred at room temperature for 12 hours after which a fine colorless precipitate had formed. The suspension was filtered to give a clear yellow solution. Removal of the volatiles gave **16** as a yellow powder which was washed with a small amount of cold hexane and dried under vacuum. Crystals (yellow blocks) suitable for single crystal X-ray diffraction were grown from a saturated hexane solution stored at -30 °C. Yield 0.61 g, 70 %. ^{1}H NMR (500 MHz, C_6D_6): δ 7.13 – 7.04 (m, 12H, C_6H_3), 4.59 (s, 1H, γ-C*H*), 3.86 (br, 4H, C*H*Me$_2$), 3.09 (br, 2H, C*H*Me$_2$), 2.90 (br, 2H, C*H*Me$_2$), 1.49 (s, 6H, C*Me*), 1.60 – 1.10 (br m, 52H, CH*Me$_2$* and SiC*H$_2$*),* 0.51, -0.04 (br s, 6H, Si*Me$_2$*). *overlaps with hexane solvent impurity. ^{13}C{^{1}H} NMR (125 MHz, C_6D_6): δ* 166.5 (*C*Me), 125.5, 123.9, 123.2 (*C*$_6$H$_3$),* 95.0 (γ-*C*H), 32.0, 28.3, 28.1, 25.2, 24.8 (br), 24.7, 24.4, 23.8, 23.1 (C*Me*, *C*HMe$_2$ and CH*Me$_2$*), 14.1 (Si*C*H$_2$), 2.3 (Si*Me$_2$*).*due to the poor solubility of **16** in C_6D_6 and fluxional processes in solution, several *C*$_6$H$_3$ resonances and one Si*Me$_2$* resonance are not observed.

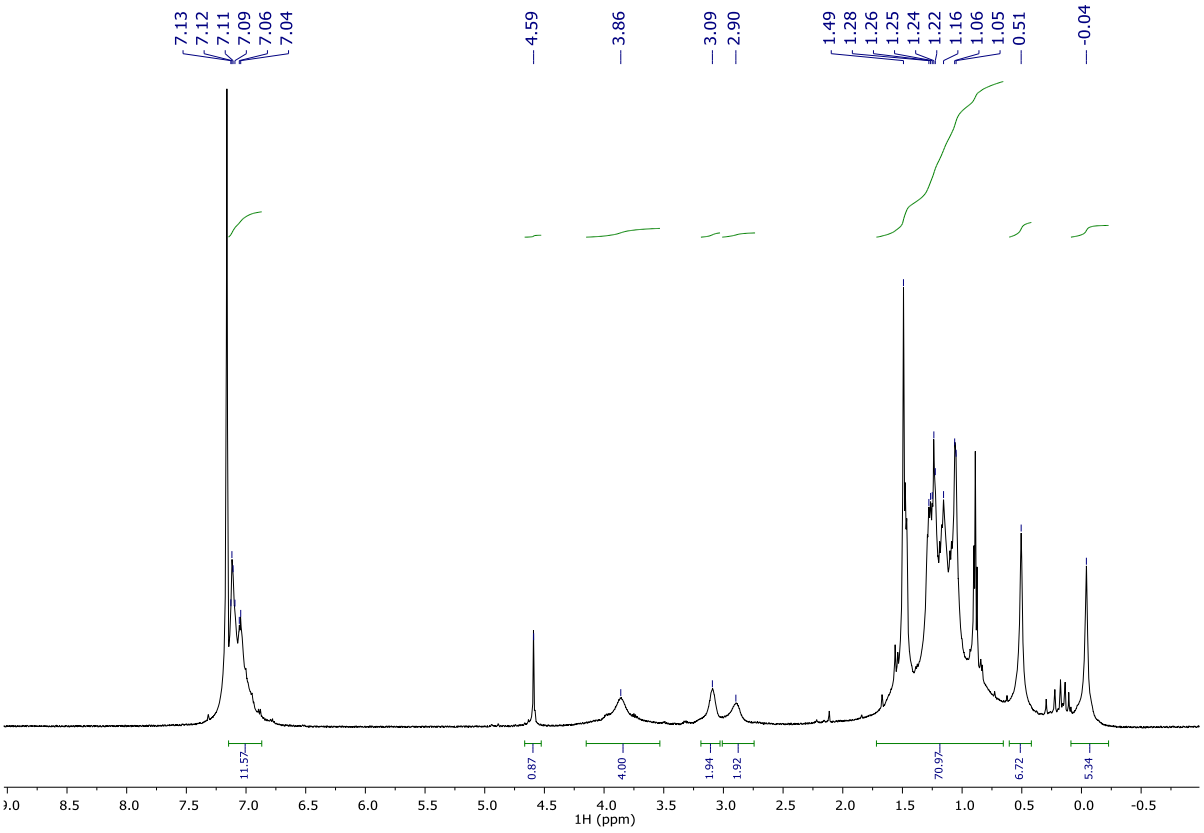


Figure S24. ^{1}H NMR spectrum of {SiN^{Dipp}}Al-Ca(^{Dipp}BDI) (**16**) in C_6D_6 (298K, 500 MHz).

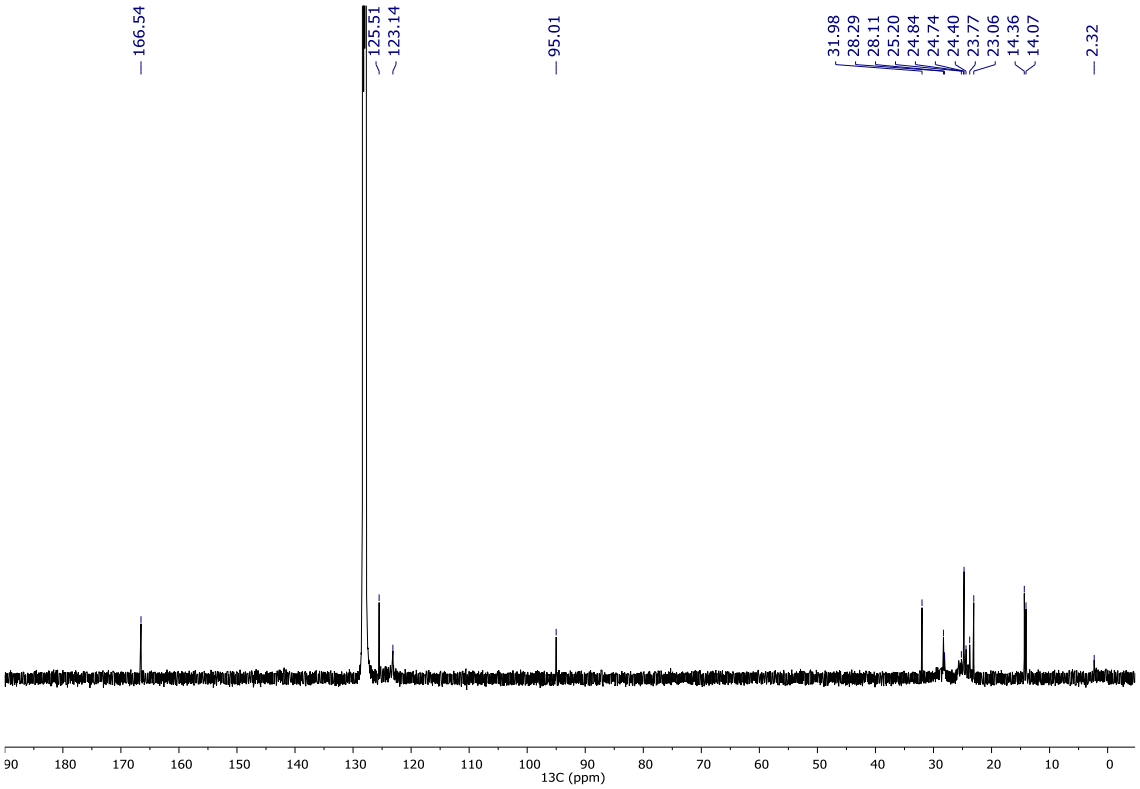


Figure S25. $^{13}C\{^{1}H\}$ NMR spectrum of {SiN^{Dipp}}Al-Ca(^{Dipp}BDI) (**16**) in C_6D_6 (298K, 125 MHz).

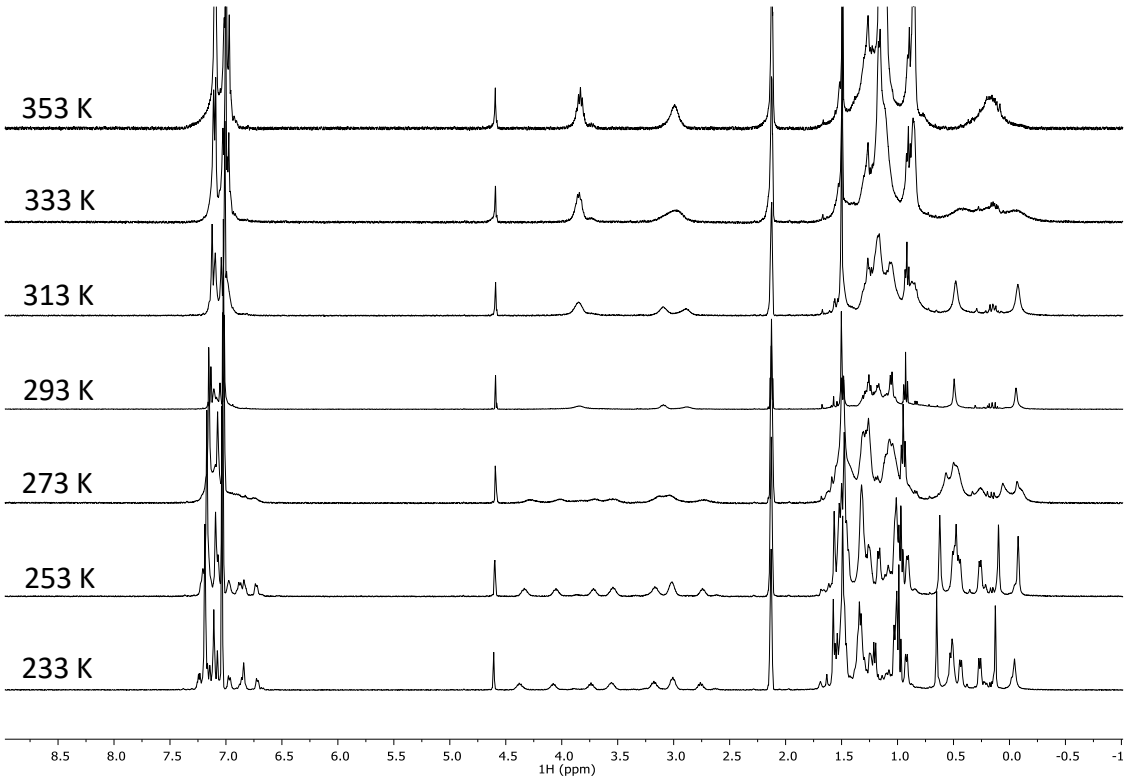


Figure S26. Stacked variable temperature ^{1}H NMR spectra of {SiN^{Dipp}}Al-Ca(^{Dipp}BDI) (**16**) in C_7D_8 (400 MHz).

*Synthesis of [{SiN^{Dipp}}Al-{κ^2-O(CH$_2$)$_4$}][(THF)$_3$Ca(^{Dipp}BDI)] (**17**)*

THF (0.05 mL, 0.62 mmol) was added dropwise to a solution of **16** (0.062 g, 0.063 mmol) in methylcyclohexane (3 mL) resulting in an immediate color change from yellow to colorless. The solution was allowed to sit at room temperature for 2 days after which colorless crystals of **17** had formed. Yield 0.049 g, 61 %. ^{1}H NMR (500 MHz, C_6D_6): δ 7.32 – 7.06 (m, 9H, C_6H_3), 6.88, 6.78 (dd, 1H, *m*-C_6H_3), 4.57 (s, 1H, γ-C*H*), 4.38 (t, J = 13.3 Hz, 1H, Al-OCH_2), 4.26,* 4.22,* 3.96, 3.82 (sept, J = 8.0 Hz, 1H, C*H*Me$_2$), 3.77 (m, 1H, Al-OCH_2), 3.57 (m, 8H, CH_2-THF), 3.32 (m, 2H, C*H*Me$_2$), 2.97, 2.89 (sept, J = 8.0 Hz, 1H, C*H*Me$_2$), 1.77 (br d, J = 13.3 Hz, 1H, OCH$_2$CH_2), 1.64 (s, 3H, C*Me*), 1.61 (d, J = 8.0 Hz, 3H, CH*Me$_2$*), 1.58 (s, 3H, C*Me*), 1.55 (d, J = 8.0 Hz, 3H, CH*Me$_2$*), 1.54 (d, J = 8.0 Hz, 6H, CH*Me$_2$*), 1.47, 1.45 (d, J = 8.0 Hz, 3H, CH*Me$_2$*), 1.42 (m, 8H, CH_2-THF), 1.38 (d, J = 8.0 Hz, 3H, CH*Me$_2$*), 1.26 (d, J = 8.0 Hz, 6H, CH*Me$_2$*), 1.17 (m, 2H, Al-CH$_2$CH_2), 1.11 (d, J = 8.0 Hz, 3H, CH*Me$_2$*), 1.01 (d, J = 8.0 Hz, 3H, CH*Me$_2$*), 0.98 (d, J = 8.0 Hz, 6H, CH*Me$_2$*), 0.86 (m, 6H, CH*Me$_2$*), 0.78 (m, 1H, Al-CH$_2$CH_2), 0.59, 0.54 (s, 3H, Si*Me$_2$*), 0.42 (dd, 6H, Si-CH_2), 0.36 (m, 1H, Al-CH_2CH$_2$), -0.04, -0.19 (s, 3H, Si*Me$_2$*), -0.43 (td, J = 13.3 Hz, 1H, Al-CH_2CH$_2$). *overlapping resonances ^{13}C{^{1}H} NMR (125 MHz, C_6D_6): δ 168.3 166.5 (*C*Me), 155.8, 154.0, 152.5, 149.4, 148.6, 147.6, 146.8, 146.1, 143.9, 141.0, 126.1, 125.9, 125.7, 125.5, 124.8, 124.4, 124.2, 123.1, 122.8, 122.6, 120.5 (*C$_6$*H$_3$), 93.8 (γ-*C*H), 67.9 (CH_2-THF), 63.6 (Al-O*C*H$_2$), 35.7, 33.0, 30.7, 30.3, 28.1, 28.0, 27.9, 27.6, 27.0, 26.9, 26.8, 26.8, 26.7, 26.4, 26.2, 25.8, 25.8, 25.7, 25.6, 25.4, 25.3, 25.1, 25.0, 24.3, 23.1, 22.6 (Al-OCH$_2$*C*H$_2$, AlCH$_2$*C*H$_2$, C*Me*, *C*HMe$_2$ and CH*Me$_2$*), 14.7, 13.6 (Si*C*H$_2$), 5.1, 4.3, 2.3, 1.6 (Si*Me$_2$*). * ^{13}C NMR resonance not observed for Al*C*H$_2$CH$_2$.

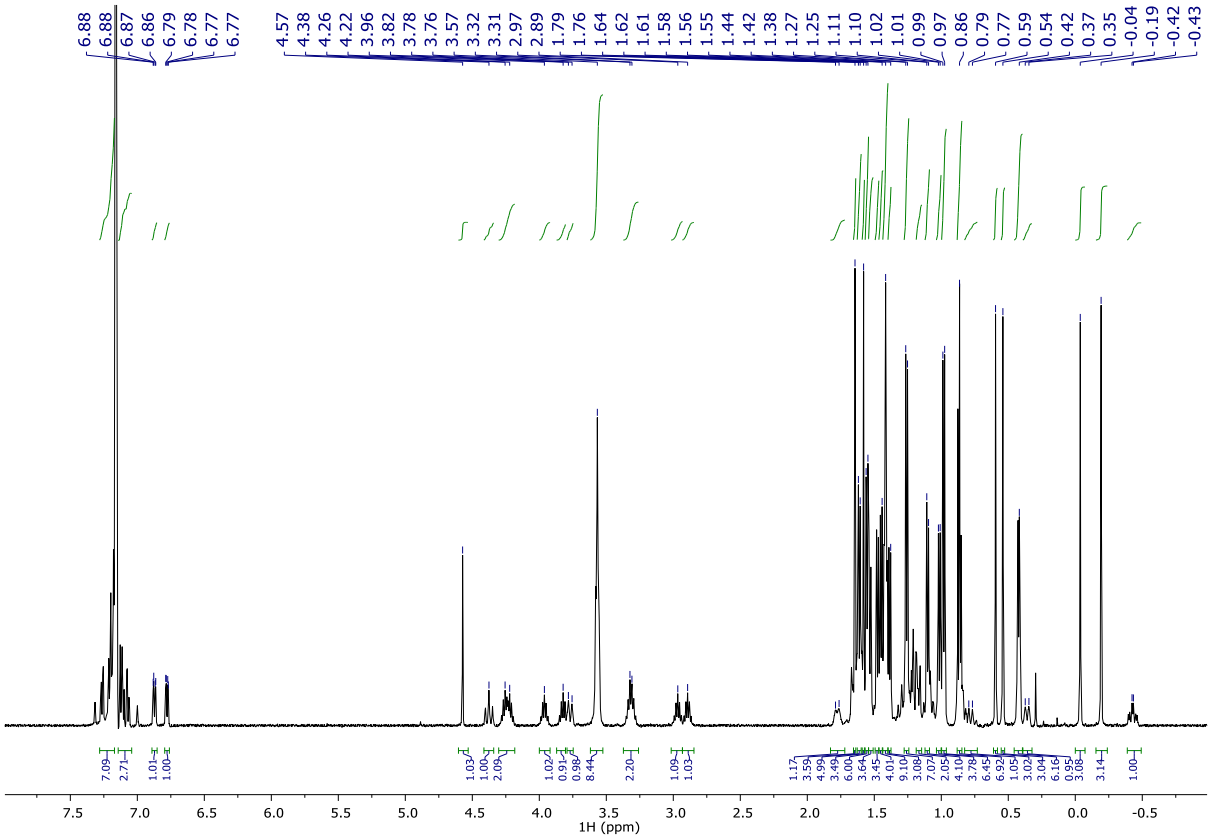


Figure S27. ^{1}H NMR spectrum of [{SiN^{Dipp}}Al-{κ^2-O(CH$_2$)$_4$}][(THF)$_3$Ca(^{Dipp}BDI)] (**17**) in C_6D_6 (500 MHz).

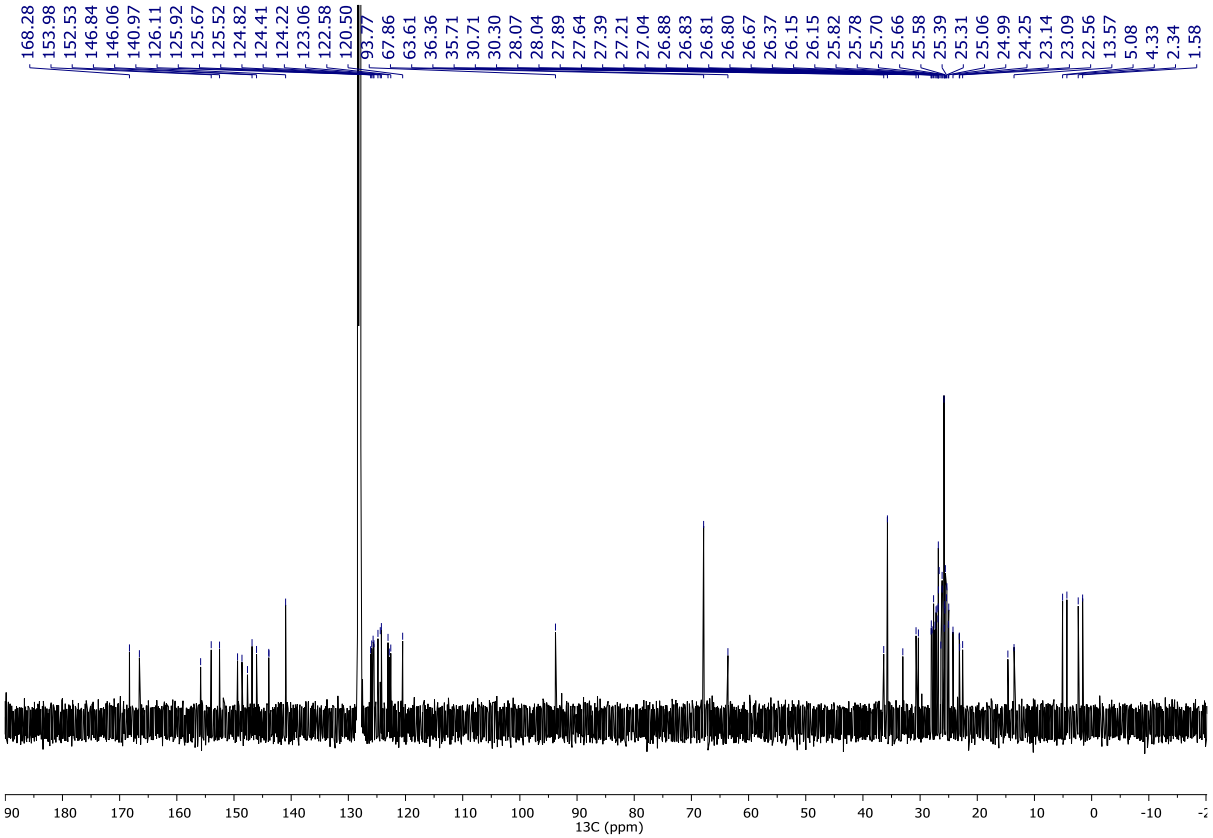


Figure S28. $^{13}C\{^{1}H\}$ NMR spectrum of [{SiN^{Dipp}}Al-{κ^2-O$(CH_2)_4$}][$(THF)_3$Ca(^{Dipp}BDI)] (**17**) in C_6D_6 (125 MHz).

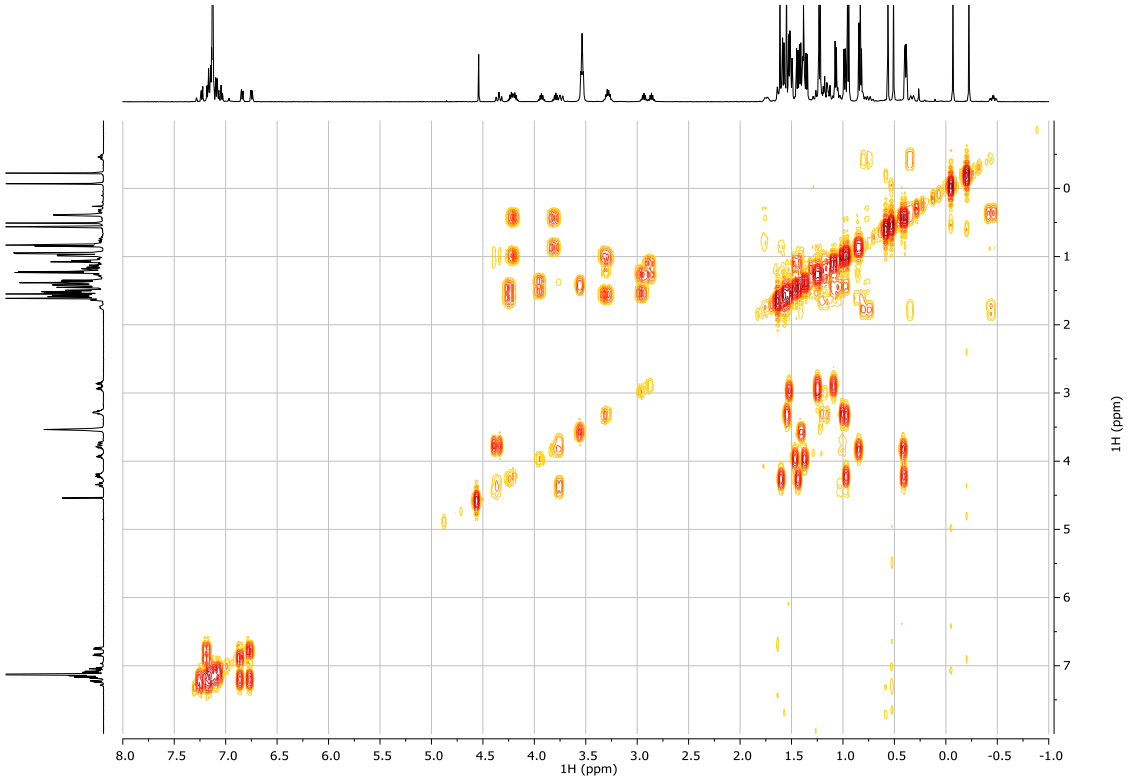


Figure S29. ^{1}H-^{1}H COSY NMR spectrum of [{SiN^{Dipp}}Al-{κ^2-O$(CH_2)_4$}][$(THF)_3$Ca(^{Dipp}BDI)] (**17**) in C_6D_6.

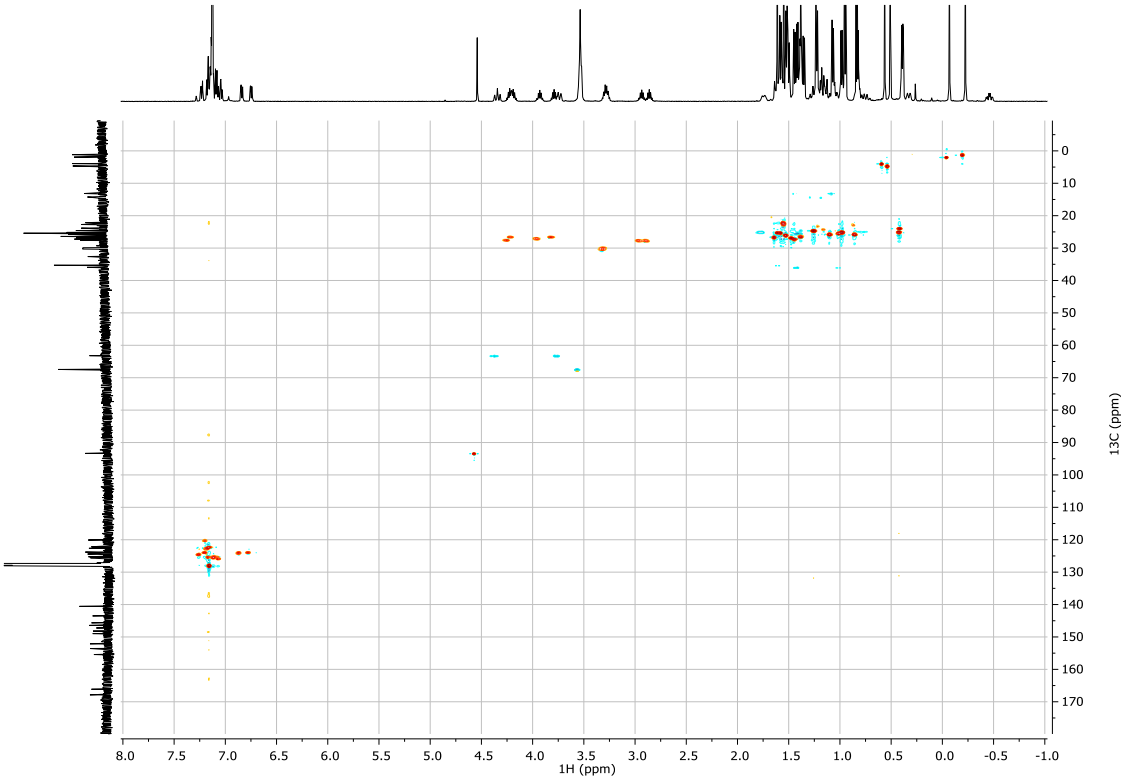


Figure S30. ^{1}H-^{13}C HSQC NMR spectrum of [{SiN^{Dipp}}Al-{κ^2-O$(CH_2)_4$}][$(THF)_3$Ca(^{Dipp}BDI)] (**17**) in C_6D_6.

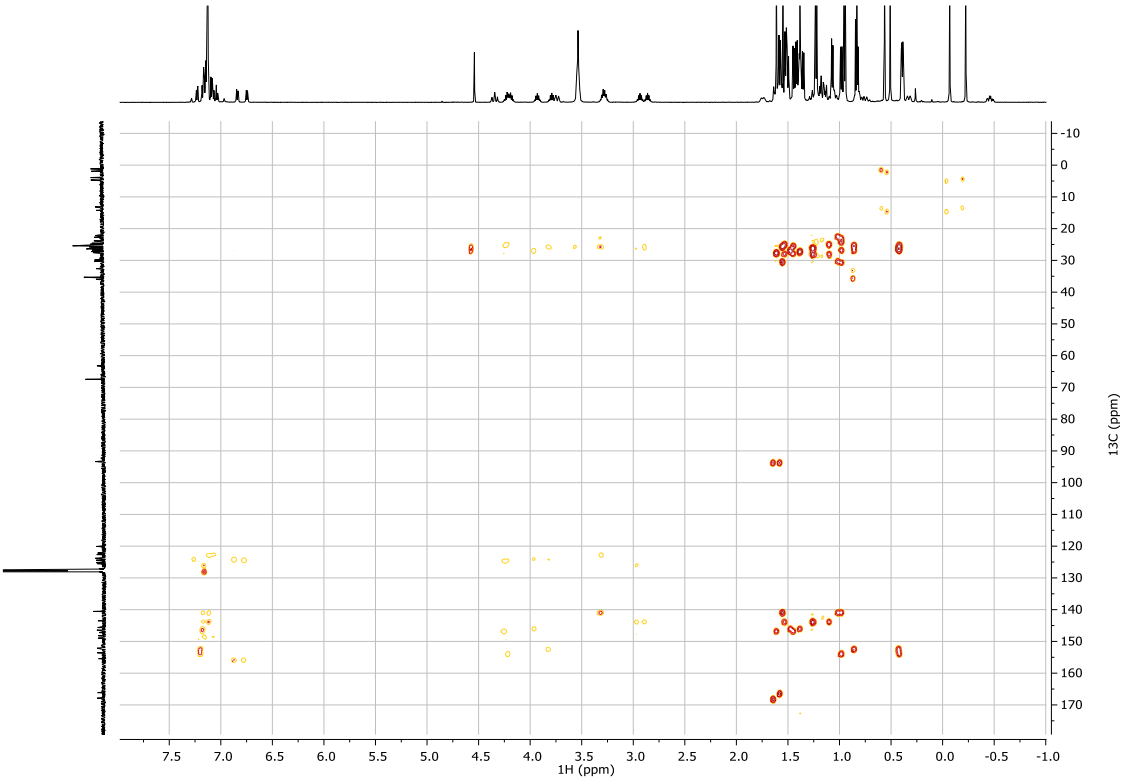


Figure S31. ^{1}H-^{13}C HMBC NMR spectrum of [{SiN^{Dipp}}Al-{κ^2-O$(CH_2)_4$}][$(THF)_3$Ca(^{Dipp}BDIp)] (**17**) in C_6D_6.

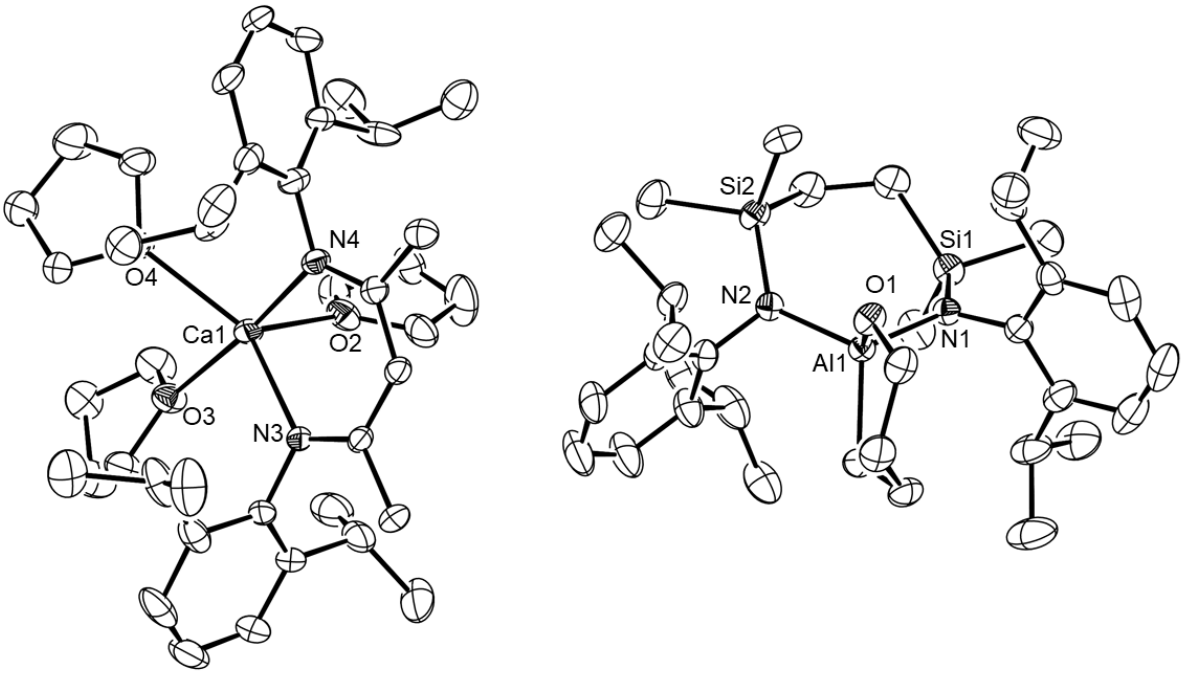


Figure S32. ORTEP representation (30% probability ellipsoids) of the ion paired structure of compound **17** Hydrogen atoms omitted for clarity.

*Synthesis of {SiN^{Dipp}}Al-COT-Ca(^{Dipp}BDI) (**18**)*

1,3,5,7-cyclooctatetraene (2.9 μL, 0.025 mmol) was added to a J. Youngs NMR tube charged with **16** (0.025 g, 0.025 mmol) in C_6D_6 (0.5 mL). The resulting solution was warmed to 40 °C was stirred at room temperature for 12 hours. Upon cooling to room temperature, colorless crystals of **18** began to form which were isolated by decanting the mother liquor and drying *in vacuo*. Yield 0.018 g, 67 %. ^{1}H NMR (500 MHz, C_6D_6): δ 7.13 – 7.04 (m, 12H, C_6H_3), 5.71 (s, 8H, C_8H_8), 4.42 (s, 1H, γ-C*H*), 3.55 (br, 4H, C*H*Me$_2$), 2.58 (br, 4H, C*H*Me$_2$), 1.46 (s, 6H, C*Me*), 1.33, 1.23 (d, J = 8.0 Hz, 12H, CH*Me$_2$*), 1.10 (br m, 12H, CH*Me$_2$*), 1.06 (d, J = 8.0 Hz, 12H, CH*Me$_2$*), 0.98 (s, 4H, SiC*H$_2$*), 0.09 (br s, 12H, Si*Me$_2$*). ^{13}C{^{1}H} NMR (125 MHz, C_6D_6): δ 165.5 (*C*Me), 147.3, 144.9, 144.6, 141.5, 124.7, 124.4, 123.9, 123.4 (C_6H_3), 94.2 (γ-*C*H), 93.6 (C_8H_8) 29.1, 28.3, 25.7, 25.1, 24.8, 24.6, 24.4 (C*Me*, *C*HMe$_2$ and CH*Me$_2$*), 13.9 (Si*C*H$_2$), 1.1 (Si*Me$_2$*).

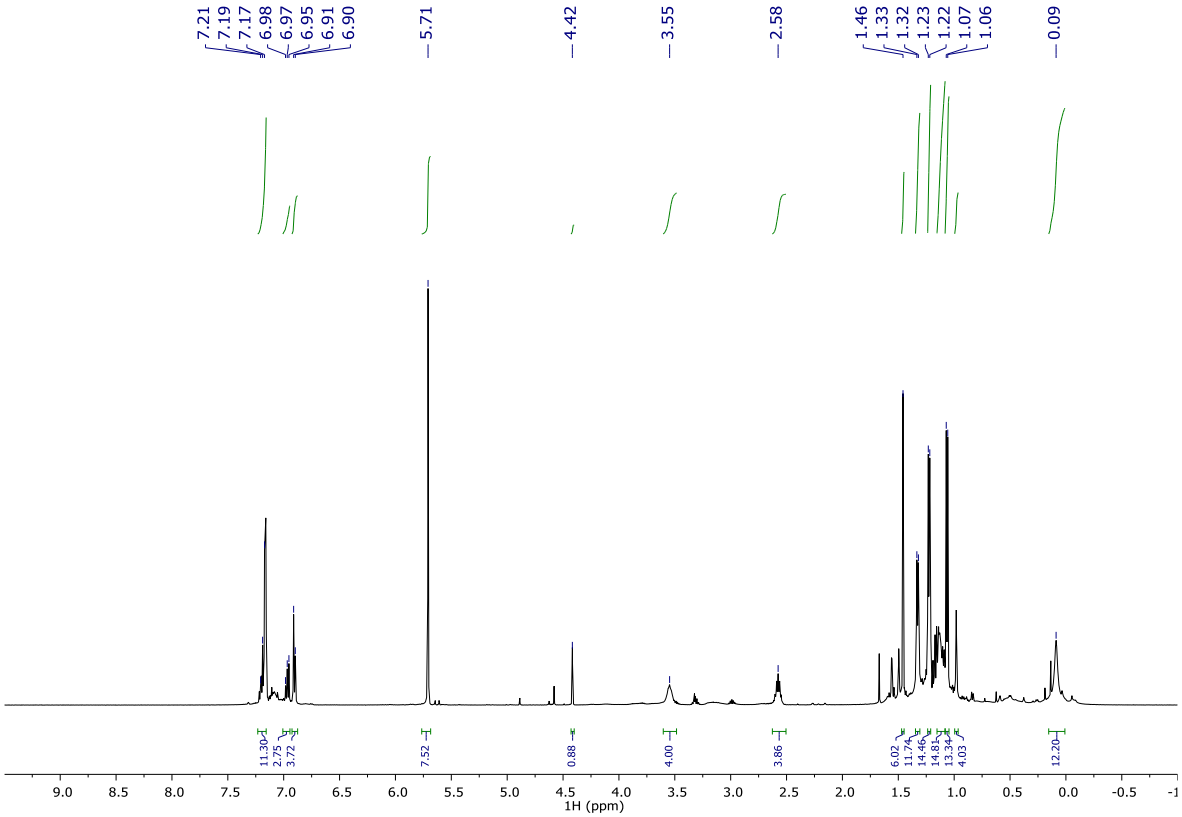


Figure S33. ^{1}H NMR spectrum of {SiN^{Dipp}}Al-COT-Ca(^{Dipp}BDI) (**18**) in C_6D_6 (500 MHz).

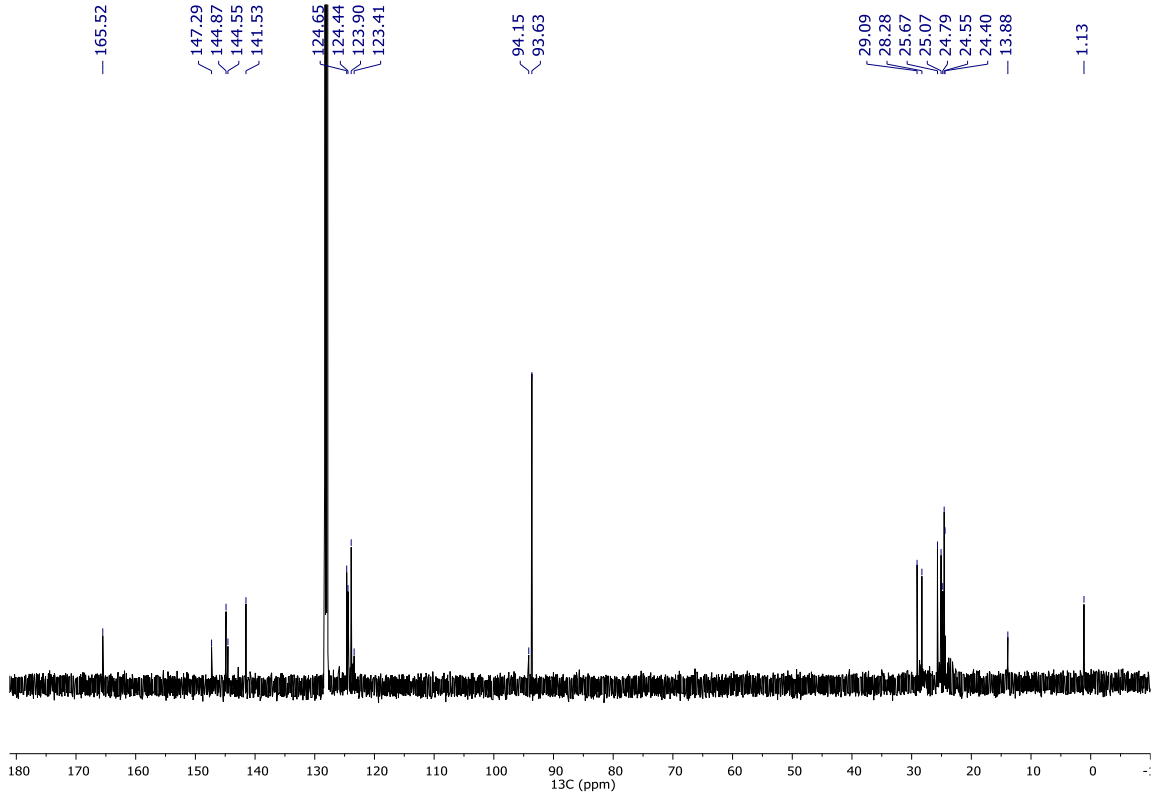


Figure S34. ^{13}C{^{1}H} NMR spectrum of {SiN^{Dipp}}Al-COT-Ca(^{Dipp}BDI) (**18**) in C_6D_6 (125 MHz).

Single Crystal X-ray Diffraction analysis.

Single Crystal X-ray diffraction data for compounds **9'** and **11 - 18** were collected using Cu*K*α (λ = 1.54184 Å) on a SuperNova, Dual Cu at zero, EosS2 diffractometer. The crystals were maintained at 150 K during data collections. All structures were solved using Olex2,[5] and refined with ShelXL[6] using Least Squares minimisation.

Two molecules of the complex are present in the asymmetric unit of **9'**.. The entity based on N2 is entirely ordered. However, in the molecule based on N1, atoms Si1, Si2 and C13-C18 were treated for 50:50 disorder. Chemically comparable distances were restrained to being similar in the disordered components.

The asymmetric unit in **12** includes one molecule of the aluminum/potassium containing complex and one molecule of diethyl ether. The latter was disordered in an 85:15 ratio, but successfully modelled with the inclusion of some distance and ADP restraints. The hydrogens attached to C21, C35, C44 and C59 in the main feature were located and each refined at a distance of 0.98Å from the relevant parent atom.

In **13**, the asymmetric unit contains one molecule of the organometallic complex and a molecule of toluene with half site occupancy. The latter is disordered with itself about a crystallographic inversion centre – and was ultimately modelled using the FragmentDB plugin for Olex2 (a GUI-specific implementation of the invaluable DSR refinement package by Kratzert *et al*.[7]). The hydrogen atoms attached to the coordinated phenyl ring were located and refined at a distance of 0.98 Å from the relevant parent atoms.

Compound **14** also contains one, guest, benzene molecule in the asymmetric unit.

In addition to one molecule of the target compound, the asymmetric unit in the structure of **15** is host to 2 regions of solvent, each of which approximates to half of a molecule of toluene. The latter moieties both straddle space group symmetry elements and are (necessarily) disordered. Symmetry related disorder normally lends itself to being well resolved with careful modelling, but the situation here was complicated by more extensive disorder, as there are extended channels in the gross structure in which the solvent resides. Ultimately, the guest toluene has been addressed *via* the solvent mask algorithm available in Olex-2, and an allowance for same made in the formula as presented. C41 and C42 in the main feature were treated for 50:50 disorder and associated C-C distance restraints were employed in this isopropyl group.

The crystal of compound **16** selected was deliberately large for good reason. In particular, several previous data collections led us to conclude that the crystals used were reacting over the duration of these experiments. The choice of a larger sample, in this instance, facilitated a speedy data collection and the added bulk of the larger sample was expected to confine reaction to the surface. This strategy appears to have been successful, given that there is no evidence of unassigned electron density in the Ca-Al region. Refinement was unremarkable and the asymmetric unit was seen to host half of one molecule of benzene as well as one molecule of the compound under study.

The asymmetric unit in **17** contains one cation and one anion. Disorder was prevalent in both moieties, but more extensive in the former. In the latter, disorder was limited to the two isopropyl groups containing C7 and C25 (each disordered in a 60:40 ratio). In the cation, however, all atoms in the THF ligands based on O2 and O4, the isopropyl methyl groups containing C42 and C43, and the *Dipp* functionality based on C52 were also modelled as being split over two sites in a component ratio of 60:40. Lastly, C69 in the THF ligand based on O3 was found to be disordered in a 65:35 split. Similarity distance restraints and ADP restraints were used in disordered regions to assist convergence. Furthermore, the minor component of the phenyl ring based on C52 was treated as a rigid hexagon.

One molecule of the complex and one molecule of benzene comprise the asymmetric unit in the structure of **18**. Atoms Si1, C13, C14, C15 and C16 were modelled to take account of 55:45 disorder, while the isopropyl group based on C62 was treated for 50:50 disorder. Distance and ADP restraints were employed in disordered regions to assist convergence. The hydrogen atoms attached to C32 and C33 were located and refined at a distance of 0.93 Å from the relevant parent carbon atoms. Unfortunately, the solvent was disordered to a large extent. Ultimately, this was treated via the solvent-mask algorithm available in Olex,[5] and allowance for same was made in the unit cell contents as presented.

Table S1: Single Crystal X-ray Data Parameters for compounds **9'** and **11 - 14**.

Compound	**9'**	**11**	**12**	**13**	**14**
Empirical formula	$C_{36}H_{66}N_2Si_4$	$C_{30}H_{50}AlIN_2Si_2$	$C_{64}H_{110}Al_2K_2N_4OSi_4$	$C_{56.5}H_{65}BMgN_2$	$C_{59}H_{67}BCaN_2$
Formula weight	639.26	648.78	1196.07	807.22	855.03
Temperature/K	150.00(10)	150.00(10)	150.00(10)	150.01(10)	150.01(10)
Crystal system	triclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	*P*-1	$P2_1/c$	$P2_1$	$P2_1/n$	$P2_1/n$
a/Å	9.9684(4)	8.96893(5)	10.66086(9)	11.6955(2)	15.1700(2)
b/Å	13.5669(6)	19.60916(13)	17.75185(14)	15.0628(2)	16.9006(2)
c/Å	15.8961(7)	19.34132(12)	19.60288(13)	26.6703(4)	19.1592(2)
α/°	71.271(4)	90	90	90	90
β/°	89.165(3)	99.6605(6)	94.6395(7)	101.833(1)	92.3230(10)
γ/°	75.145(4)	90	90	90	90
Volume/Å^3	1962.51(16)	3353.38(4)	3697.69(5)	4598.58(12)	4908.04(10)
Z	2	4	2	4	4
ρ_{calc} g/cm^3	1.082	1.285	1.074	1.166	1.157
μ/mm^{-1}	1.580	8.581	2.269	0.619	1.388
F(000)	704.0	1352.0	1300.0	1740.0	1840.0
Crystal size/mm^3	0.364 × 0.165 × 0.122	0.189 × 0.166 × 0.126	0.139 × 0.105 × 0.09	0.386 × 0.156 × 0.117	0.213 × 0.140 × 0.105
2θ range /°	5.886 to 146.768	6.466 to 146.284	6.728 to 146.274	6.772 to 146.644	6.976 to 146.412
Reflections collected	22962	42839	27636	68240	67682
Independent reflections	7869, 0.0361	6694 0.0352	12920 0.0276	9195 0.0406	9813 0.0562
Data/restraints/parameters	7869/35/471	6694/0/337	12920/154/809	9195/110/608	9813/0/578
Goodness-of-fit on F^2	1.036	1.056	1.047	1.027	1.023
Final *R* indexes [I>=2σ (I)]	0.0372, 0.0979	0.0236, 0.0576	0.0314, 0.0796	0.0406, 0.1040	0.0424, 0.1023
Final *R* indexes [all data]	0.0419, 0.1020	0.0245, 0.0580	0.0328, 0.0807	0.0432, 0.1065	0.0509, 0.1071
Largest diff. peak/hole/e Å^{-3}	0.31/–0.26	0.63/–0.88	0.38/–0.15	0.33/–0.33	0.38/–0.36

Table S2: Single Crystal X-ray Data Parameters for compounds **15 - 18**.

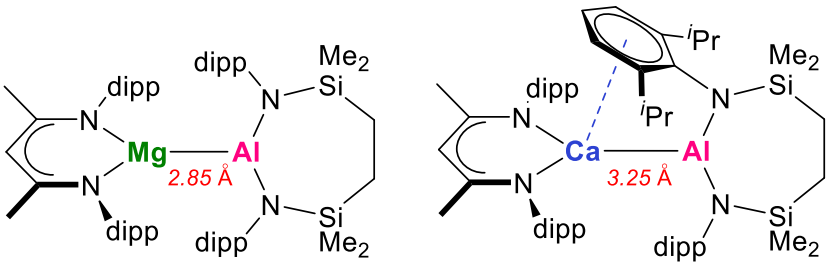
Compound	**15**	**16**	**17**	**18**
Empirical formula	$C_{66}H_{99}AlMgN_4Si_2$	$C_{62}H_{94}AlCaN_4Si_2$	$C_{75}H_{123}AlCaN_4O_4Si_2$	$C_{73}H_{105}AlCaN_4Si_2$
Formula weight	1055.96	1018.65	1268.01	1161.84
Temperature/K	150.00(10)	150.00(10)	150.00(10)	150.00(10)
Crystal system	monoclinic	monoclinic	orthorhombic	triclinic
Space group	*I*2/a	$P2_1/n$	*Pbca*	*P*-1
a/Å	22.7811(2)	15.3502(1)	24.6044(3)	12.6087(3)
b/Å	23.4456(2)	18.4658(1)	24.3835(2)	13.0722(3)
c/Å	24.3950(2)	21.5635(1)	25.4954(3)	23.4013(5)
α/°	90	90	90	97.692(2)
β/°	99.224(1)	93.130(1)	90	98.162(2)
γ/°	90	90	90	111.553(2)
Volume/Å^3	12861.29(19)	6103.14(6)	15295.7(3)	3477.82(15)
Z	8	4	8	2
ρ_{calc} g/cm^3	1.091	1.109	1.101	1.109
μ/mm^{-1}	1.024	1.690	1.474	1.540
F(000)	4608.0	2220.0	5552.0	1264.0
Crystal size/mm^3	0.234 × 0.221 × 0.187	0.57 × 0.372 × 0.209	0.218 × 0.164 × 0.152	0.392 × 0.3 × 0.205
2θ range /°	5.446 to 158.636	6.306 to 146.086	6.17 to 146.17	7.424 to 146.324
Reflections collected	65665	42390	80501	46933
Independent reflections	12814 0.0254	12081 0.0415	14675 0.0512	13842 0.0537
Data/restraints/parameters	12814/6/646	12081/0/653	14675/876/1074	13842/15/782
Goodness-of-fit on F^2	1.056	1.029	1.031	1.049
Final *R*1, *w*2 indexes [$I>=2\sigma(I)$]	0.0444, 0.1238	0.0481, 0.1310	0.0619, 0.1685	0.0855, 0.2228
Final *R*1, *w*2 indexes [all data]	0.0502, 0.1299	0.0513, 0.1355	0.0725, 0.1800	0.0884, 0.2305
Largest diff. peak/hole/e Å^{-3}	0.76/–0.65	0.47/–0.41	0.42/–0.32	1.41/–0.86

Computational Details / Methodology

DFT calculations were run with Gaussian 09 (Revision D.01).[8] The Mg, Al, Si and Ca centres were described with the Stuttgart RECPs and associated basis sets,[9] and 6-31G** basis sets were used for all other atoms (BS1).[10] A polarization function was also added to Al (ζd = 0.180) and Si (ζd = 0.284). Initial BP86[11] optimizations were performed using the 'grid = ultrafine' option, with all stationary points being fully characterized via analytical frequency calculations as minima (all positive eigenvalues).

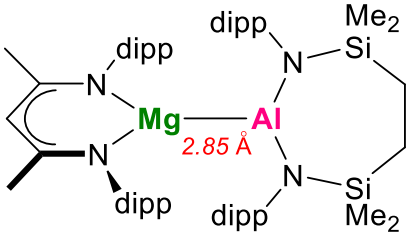
The Quantum Theory of Atoms in Molecules (QTAIM, AIMAll program[12]), Natural Bonding Orbital (NBO6.0[13]) and Non-Covalent Interactions Plot (NCI, NCIPLOT[14]) analyses were performed on the BP86-optmised geometries of **1** and **2**. The Pipek-Mezey localized orbitals[15] were also computed with ORCA[16] (Version 4.1.1) using the def2-TZVP[17] basis set for all atoms.

Orbital Calculations and Results

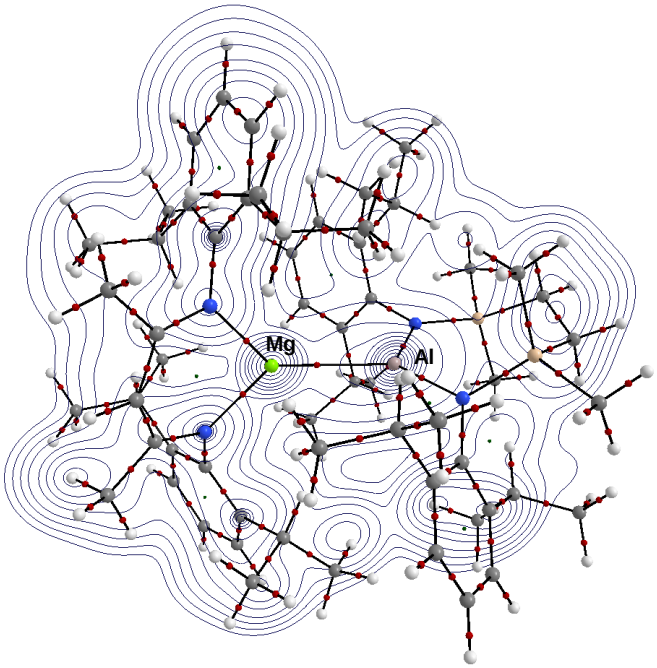


15 **16**

Quantum Theory of Atoms in Molecules (QTAIM, Figures S35 and S36), Natural Bonding Orbital (NBO, Figure S37), Pipek–Mezey localised orbitals (Figure S38) and a Non-Covalent Interaction (NCI) (Figure S39) plot were used to characterize the nature of the interaction between the s-block metal (Ca or Mg) and Al centres in the BP86-optimised geometries of **15** and **16**.



15



BCP	ρ(r)	$\nabla^2\rho(r)$	ε	H(r)
Mg-Al	**0.028**	+0.033	0.049	-0.008

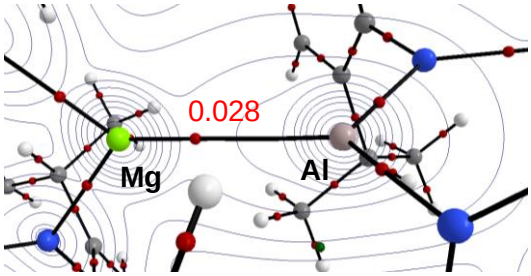
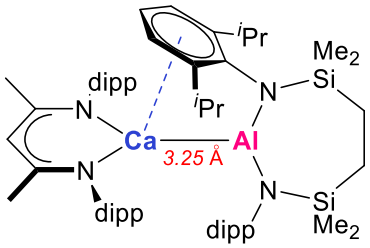
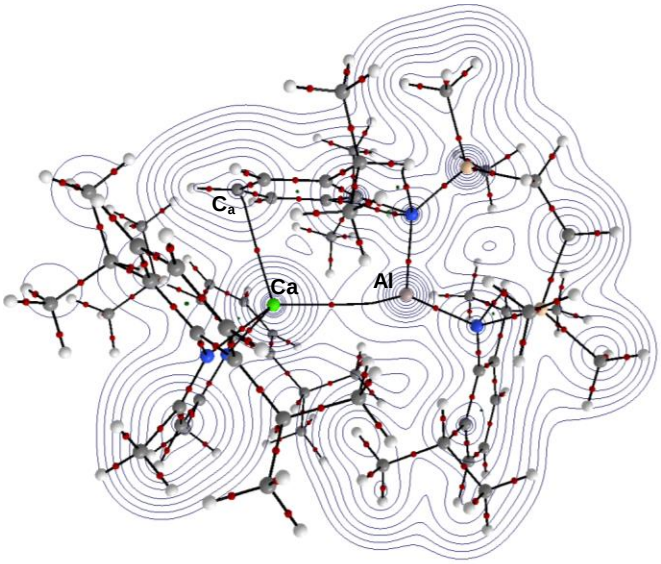


Figure S35. QTAIM molecular graph of **15**. The electron density contours are computed in the {Mg/Al/Si} planes with bond critical points (BCPs) shown as small red spheres. BCP electron densities (ρ(r) in eÅ^{-3}), values of the Laplacian of the electron density [$\nabla^2\rho(r)$ in eÅ^{-5}), ellipticities (ε) and total energy densities (H(r) in a.u.].



1



BCP	ρ(r)	$\nabla^2\rho(r)$	ε	H(r)
Ca-Al	**0.020**	+0.020	0.052	-0.002
Ca-C_a	**0.014**	+0.051	1.125	+0.015

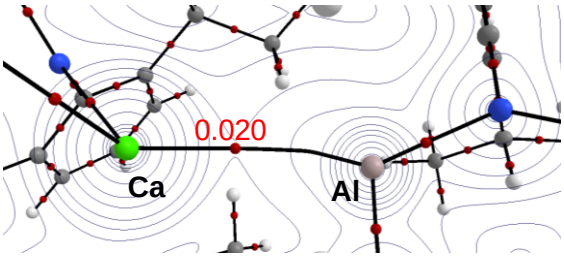


Figure S36. QTAIM molecular graph of **16**. The electron density contours are computed in the {Ca/Al/Si} planes with bond critical points (BCPs) shown as small red spheres. BCP electron densities (ρ(r) in eÅ^{-3}), values of the Laplacian of the electron density ($\nabla^2\rho(r)$ in eÅ^{-5}), ellipticities (ε) and total energy densities (H(r) in a.u.).

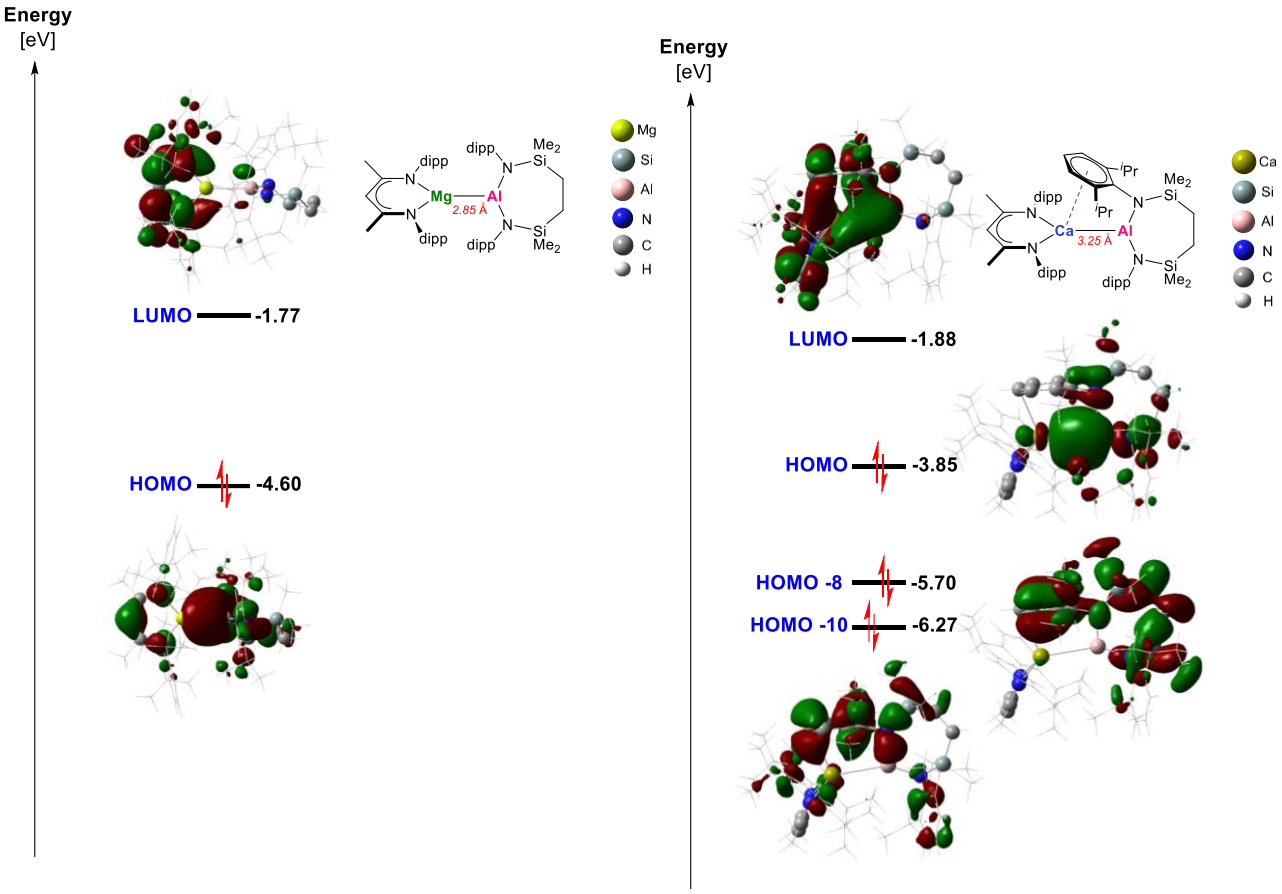
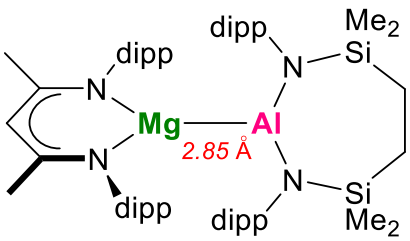
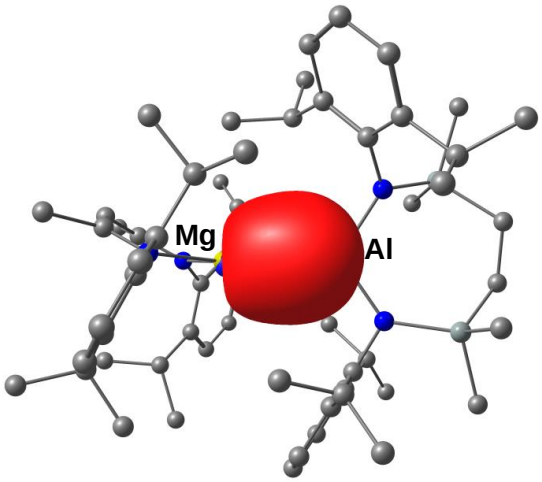


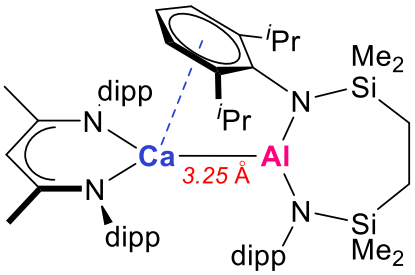
Figure S37. Natural Bond Orbitals and energies (eV) of the Frontier Molecular Orbitals computed for **15** (left) and **16** (right).



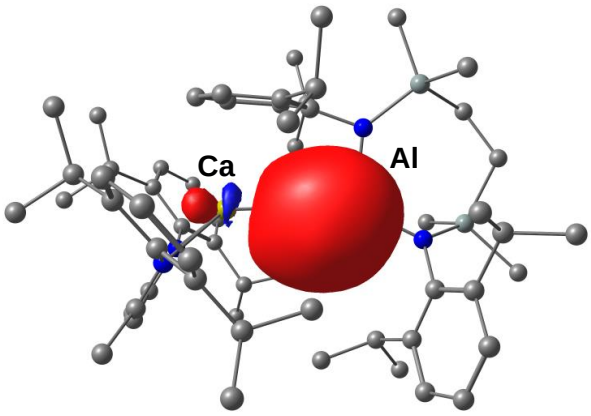
15



$\sigma_{Al—Mg}$ = 0.35**Mg** + 0.64**Al**

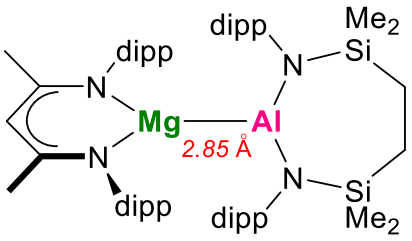


16

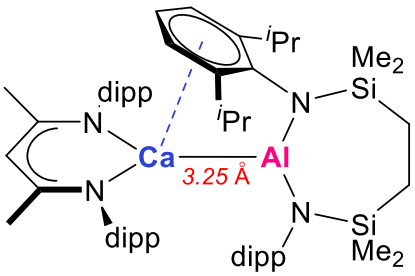


$\sigma_{Al—Ca}$ = 0.17**Ca** + 0.87**Al**

Figure S38. Localised Pipek–Mezey orbitals of **15** and **16** showing Al—Ca and Al—Mg σ-bonding orbitals, respectively.



15



16

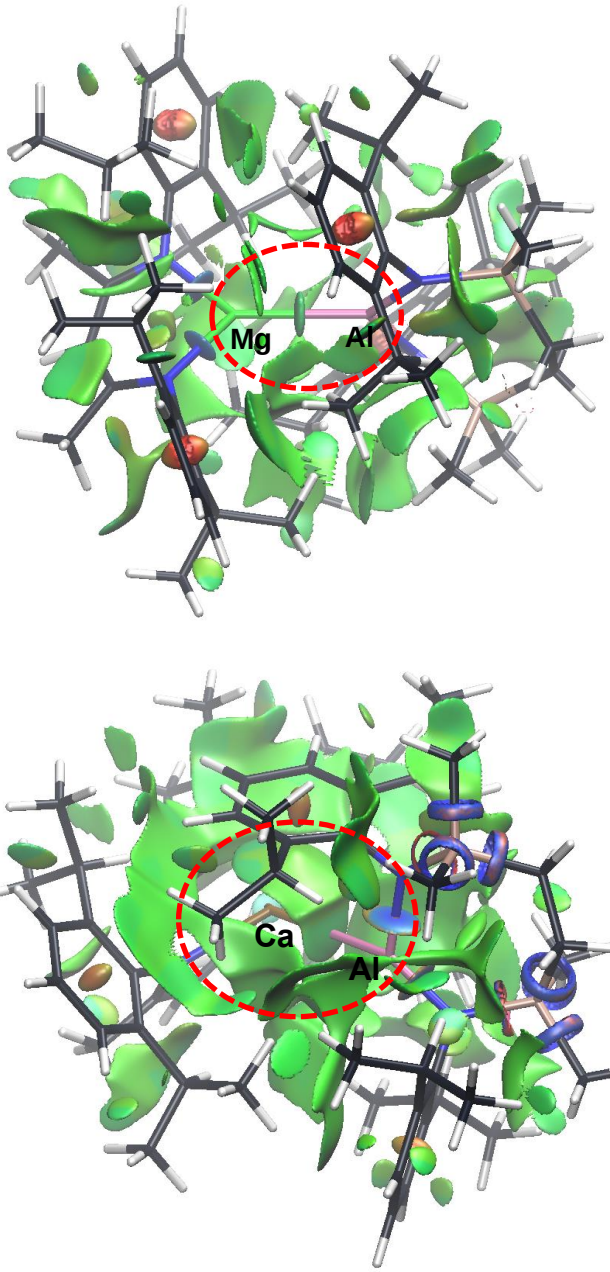
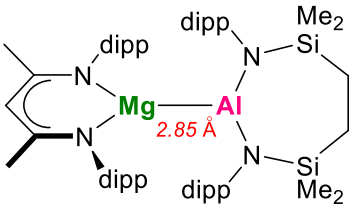


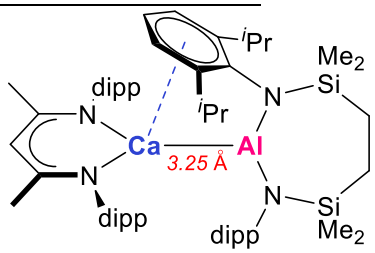
Figure S39. NCI plots computed for the BP86-optimised geometries of **15** and **16**. Isosurfaces generated for s = 0.3 au and −0.07 < ρ < 0.07 au. Regions of weak interactions are color coded, with stronger stabilising interactions in blue, weaker stabilising interactions in green and stronger destabilising areas in red.

Table S3. NBO Charges (a.u.) of selected atoms in the Mg-Al species **15** and the Ca-Al species **16**.

Species	Mg	Ca	Al
15	+1.45	–	+0.83
16	–	+1.65	+0.72



15



16

Cartesian Coordinates and Computed Energies (in Hartrees)

15
SCF (BP86) Energy = -2532.99685666
Enthalpy 0K = -2531.660674
Enthalpy 298K = -2531.577133
Free Energy 298K = -2531.777441
Lowest Frequency = 17.3298 cm^{-1}
Second Frequency = 21.0370 cm^{-1}

Al	1.38177	-0.40164	0.17016
Si	4.01202	-1.61813	-1.31791
Si	3.29959	-1.90722	2.50942
N	1.74457	-1.33647	1.77334
N	2.91470	-0.23667	-0.94353
C	0.58749	-1.55898	2.61597
C	0.16008	-0.56580	3.55349
C	-0.12190	-2.80170	2.54580
C	0.94016	0.72843	3.79018
H	1.81355	0.70855	3.11623
C	3.19737	0.98836	-1.65851
C	2.52503	1.31404	-2.88236
C	-0.98693	-0.80723	4.33834
H	-1.31264	-0.04158	5.05218
C	1.44000	0.42867	-3.49693
H	1.27272	-0.41395	-2.80274
C	0.33456	-3.92111	1.60936
H	1.40135	-3.73696	1.39070
C	-1.25351	-2.99734	3.35959
H	-1.78985	-3.95114	3.30835
C	0.10810	1.19351	-3.66090
H	-0.22054	1.65604	-2.71165
H	0.19930	2.01867	-4.38925
H	-0.69425	0.52612	-4.02040
C	4.20884	1.88881	-1.18209
C	-1.69765	-2.00775	4.24650
H	-2.57943	-2.18035	4.87272
C	1.46204	0.80732	5.24449
H	0.62913	0.88572	5.96576
H	2.05099	-0.08437	5.51816
H	2.10181	1.69755	5.37917
C	1.87679	-0.15428	-4.86084
H	2.11285	0.64830	-5.58172
H	2.77298	-0.78891	-4.76435
H	1.07106	-0.76829	-5.30069
C	2.99003	-3.14170	-1.83669
H	2.20176	-3.38496	-1.10387
H	2.50575	-2.98051	-2.81332
H	3.64321	-4.02843	-1.92428
C	0.11588	1.98739	3.45579
H	-0.21360	1.99304	2.40325
H	-0.78766	2.06112	4.08583
H	0.71130	2.90157	3.62446
C	5.10648	-2.17154	0.15044
H	5.86948	-2.83756	-0.30445
H	5.67258	-1.30452	0.53788
C	2.87953	2.48493	-3.58392
H	2.36521	2.71418	-4.52481
C	4.36541	-0.49287	3.22179
H	4.51273	0.33512	2.51321
H	3.91547	-0.07699	4.13769
H	5.36160	-0.88916	3.48992
C	4.38831	-2.91233	1.29964
H	5.13958	-3.38686	1.96544
H	3.78661	-3.75249	0.90334
C	4.96416	1.65011	0.12494
H	4.61537	0.68045	0.51503
C	-0.42171	-3.85976	0.26726
H	-1.50496	-4.01422	0.40916
H	-0.29387	-2.87274	-0.21374
H	-0.05538	-4.63066	-0.43368
C	4.53373	3.03801	-1.92810
H	5.31762	3.70742	-1.55461
C	3.88266	3.34496	-3.12747
H	4.15256	4.24042	-3.69728
C	2.93699	-3.07050	3.97661
H	2.26328	-2.60975	4.71673
H	2.48556	-4.02383	3.65848
H	3.89049	-3.30229	4.48384
C	5.17936	-1.16730	-2.75318
H	4.62744	-0.84478	-3.65029
H	5.87414	-0.35454	-2.48803
H	5.77899	-2.05490	-3.02155
C	4.63003	2.73157	1.17749
H	4.90502	3.73919	0.81861
H	3.55294	2.74426	1.41311
H	5.18222	2.54884	2.11659
C	0.21513	-5.33148	2.22427
H	0.70127	-5.39238	3.21275
H	-0.83773	-5.64057	2.34932
H	0.69120	-6.07461	1.56104
C	6.49372	1.56121	-0.07564
H	6.76797	0.77706	-0.80072
H	6.91212	2.51509	-0.44299
H	6.99445	1.32874	0.88104
Mg	-1.26003	0.39984	-0.53475
N	-2.83369	-0.54566	-1.59613
N	-2.22752	2.27415	-0.48475
C	-3.11602	2.56801	-1.45930
C	-2.03222	3.28415	0.53298
C	-3.15504	-1.95721	-1.53362
C	-3.60556	0.22209	-2.40314
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C	-2.65851	-2.87999	-2.49977
C	-3.61409	1.63734	-2.40589
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C	-1.75497	-2.46376	-3.66162
H	-1.70158	-1.36089	-3.66509
C	-3.00827	-4.24051	-2.38374
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H	0.09626	5.82605	1.40632
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H	-3.50419	4.52473	3.37382
C	-3.83660	-4.69825	-1.35583
H	-4.10231	-5.75853	-1.28841
C	0.15795	4.00958	-0.63020

H	0.26026	2.92659	-0.84604
C	-4.32235	-3.78631	-0.41146
H	-4.97226	-4.14472	0.39255
C	-2.29755	-2.92390	-5.03509
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H	-3.94156	2.19365	3.91841
H	-4.88434	0.91214	3.11758
C	-4.76860	-2.08817	1.95222
H	-5.55701	-2.86162	1.95790
H	-3.83149	-2.54093	2.31328
H	-5.07322	-1.31656	2.67883
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H	-5.57878	3.86505	2.73829
H	-5.66079	3.91405	0.96215
H	-6.36547	2.53749	1.85300
C	1.54517	4.52031	-0.19812
H	1.57317	5.62360	-0.13977
H	1.83777	4.12246	0.78734
H	2.30419	4.21092	-0.93340
C	-0.25027	4.70187	-1.95210
H	-1.15768	4.26128	-2.39255
H	-0.43490	5.77839	-1.78548
H	0.56407	4.60520	-2.69068

16

SCF (BP86) Energy = -2532.99685666
Enthalpy 0K = -2531.660674
Enthalpy 298K = -2531.577133
Free Energy 298K = -2531.777441
Lowest Frequency = 17.3298 cm^{-1}
Second Frequency = 21.0370 cm^{-1}

Al	1.38177	-0.40164	0.17016
Si	4.01202	-1.61813	-1.31791
Si	3.29959	-1.90722	2.50942
N	1.74457	-1.33647	1.77334
N	2.91470	-0.23667	-0.94353
C	0.58749	-1.55898	2.61597
C	0.16008	-0.56580	3.55349
C	-0.12190	-2.80170	2.54580
C	0.94016	0.72843	3.79018
H	1.81355	0.70855	3.11623
C	3.19737	0.98836	-1.65851
C	2.52503	1.31404	-2.88236
C	-0.98693	-0.80723	4.33834
H	-1.31264	-0.04158	5.05218
C	1.44000	0.42867	-3.49693
H	1.27272	-0.41395	-2.80274
C	0.33456	-3.92111	1.60936
H	1.40135	-3.73696	1.39070
C	-1.25351	-2.99734	3.35959
H	-1.78985	-3.95114	3.30835
C	0.10810	1.19351	-3.66090
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H	0.19930	2.01867	-4.38925
H	-0.69425	0.52612	-4.02040
C	4.20884	1.88881	-1.18209
C	-1.69765	-2.00775	4.24650
H	-2.57943	-2.18035	4.87272
C	1.46204	0.80732	5.24449
H	0.62913	0.88572	5.96576
H	2.05099	-0.08437	5.51816
H	2.10181	1.69755	5.37917
C	1.87679	-0.15428	-4.86084
H	2.11285	0.64830	-5.58172
H	2.77298	-0.78891	-4.76435
H	1.07106	-0.76829	-5.30069
C	2.99003	-3.14170	-1.83669
H	2.20176	-3.38496	-1.10387
H	2.50575	-2.98051	-2.81332
H	3.64321	-4.02843	-1.92428
C	0.11588	1.98739	3.45579
H	-0.21360	1.99304	2.40325
H	-0.78766	2.06112	4.08583
H	0.71130	2.90157	3.62446
C	5.10648	-2.17154	0.15044
H	5.86948	-2.83756	-0.30445
H	5.67258	-1.30452	0.53788
C	2.87953	2.48493	-3.58392
H	2.36521	2.71418	-4.52481
C	4.36541	-0.49287	3.22179
H	4.51273	0.33512	2.51321
H	3.91547	-0.07699	4.13769
H	5.36160	-0.88916	3.48992
C	4.38831	-2.91233	1.29964
H	5.13958	-3.38686	1.96544
H	3.78661	-3.75249	0.90334
C	4.96416	1.65011	0.12494
H	4.61537	0.68045	0.51503
C	-0.42171	-3.85976	0.26726
H	-1.50496	-4.01422	0.40916
H	-0.29387	-2.87274	-0.21374
H	-0.05538	-4.63066	-0.43368
C	4.53373	3.03801	-1.92810
H	5.31762	3.70742	-1.55461
C	3.88266	3.34496	-3.12747
H	4.15256	4.24042	-3.69728
C	2.93699	-3.07050	3.97661
H	2.26328	-2.60975	4.71673
H	2.48556	-4.02383	3.65848
H	3.89049	-3.30229	4.48384
C	5.17936	-1.16730	-2.75318
H	4.62744	-0.84478	-3.65029
H	5.87414	-0.35454	-2.48803
H	5.77899	-2.05490	-3.02155
C	4.63003	2.73157	1.17749
H	4.90502	3.73919	0.81861
H	3.55294	2.74426	1.41311
H	5.18222	2.54884	2.11659

C	0.21513	-5.33148	2.22427
H	0.70127	-5.39238	3.21275
H	-0.83773	-5.64057	2.34932
H	0.69120	-6.07461	1.56104
C	6.49372	1.56121	-0.07564
H	6.76797	0.77706	-0.80072
H	6.91212	2.51509	-0.44299
H	6.99445	1.32874	0.88104
Mg	-1.26003	0.39984	-0.53475
N	-2.83369	-0.54566	-1.59613
N	-2.22752	2.27415	-0.48475
C	-3.11602	2.56801	-1.45930
C	-2.03222	3.28415	0.53298
C	-3.15504	-1.95721	-1.53362
C	-3.60556	0.22209	-2.40314
C	-2.97602	3.41085	1.59408
C	-2.65851	-2.87999	-2.49977
C	-3.61409	1.63734	-2.40589
H	-4.26337	2.08018	-3.16514
C	-0.89816	4.14769	0.46930
C	-1.75497	-2.46376	-3.66162
H	-1.70158	-1.36089	-3.66509
C	-3.00827	-4.24051	-2.38374
H	-2.62480	-4.95215	-3.12339
C	-3.99595	-2.41740	-0.47307
C	-0.76269	5.15041	1.44967
H	0.09626	5.82605	1.40632
C	-4.17818	2.47658	1.75207
H	-4.21791	1.81758	0.86754
C	-4.56945	-0.43005	-3.38840
H	-4.01777	-0.87160	-4.23576
H	-5.13613	-1.24910	-2.91893
H	-5.27906	0.30677	-3.79174
C	-1.69630	5.29861	2.48227
H	-1.56889	6.08690	3.23182
C	-2.78281	4.42284	2.55515
H	-3.50419	4.52473	3.37382
C	-3.83660	-4.69825	-1.35583
H	-4.10231	-5.75853	-1.28841
C	0.15795	4.00958	-0.63020
H	0.26026	2.92659	-0.84604
C	-4.32235	-3.78631	-0.41146
H	-4.97226	-4.14472	0.39255
C	-2.29755	-2.92390	-5.03509
H	-2.26772	-4.02327	-5.13180
H	-3.34121	-2.60866	-5.20136
H	-1.67978	-2.50744	-5.84974
C	-4.59368	-1.45515	0.55754
H	-3.89411	-0.60355	0.65832
C	-3.72792	3.96161	-1.56079
H	-4.64677	4.01720	-0.95092
H	-3.05131	4.74892	-1.20030
H	-4.01401	4.17658	-2.60231
C	-0.32294	-3.00318	-3.46140
H	0.12016	-2.62679	-2.52634
H	-0.31935	-4.10621	-3.41016
H	0.33110	-2.70309	-4.29839
C	-5.94404	-0.87639	0.06940
H	-5.83465	-0.30305	-0.86458
H	-6.67177	-1.68818	-0.10883
H	-6.37176	-0.20035	0.83101
C	-4.01371	1.58138	3.00197
H	-3.10628	0.95694	2.94697
H	-3.94156	2.19365	3.91841
H	-4.88434	0.91214	3.11758
C	-4.76860	-2.08817	1.95222
H	-5.55701	-2.86162	1.95790
H	-3.83149	-2.54093	2.31328
H	-5.07322	-1.31656	2.67883
C	-5.51806	3.24461	1.82690
H	-5.57878	3.86505	2.73829
H	-5.66079	3.91405	0.96215
H	-6.36547	2.53749	1.85300
C	1.54517	4.52031	-0.19812
H	1.57317	5.62360	-0.13977
H	1.83777	4.12246	0.78734
H	2.30419	4.21092	-0.93340
C	-0.25027	4.70187	-1.95210
H	-1.15768	4.26128	-2.39255
H	-0.43490	5.77839	-1.78548
H	0.56407	4.60520	-2.69068

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