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Supporting Information

Magnesium(I) Reduction of Aluminum(III) Hydride Complexes: Generation of Mixed Valence Aluminum (Al^{I}/Al^{0}) Hydride Cluster Compounds, $[Al_6H_8(NR_3)_2\{Mg(\beta\text{-diketiminate})\}_4]$

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Supporting Information (83 pages)

Contents

1. Syntheses and Spectra

General considerations

All manipulations were carried out using standard Schlenk and glove box techniques under an atmosphere of high purity dinitrogen. Toluene, benzene, hexane and THF were dried over molten potassium. Benzene-d_6 was stored over a mirror of potassium and degassed three times *via* freeze-pump-thawing before use. ^{1}H, ^{13}C{^{1}H}, ^{29}Si and ^{27}Al NMR spectra were recorded on either Bruker Avance Neo or Bruker AvanceIII 400 spectrometers, and were referenced to the resonances of the solvent used, external $SiMe_4$ or external 1M $[Al(H_2O)_6]^{3+}$. FTIR spectra were recorded for solid samples using an Agilent Cary 630 attenuated total reflectance (ATR) spectrometer (Nujol mulls). Irradiations were carried out using a Kessil PR160L UV (λ = 370 nm, 43W) light LED lamp, with the reaction vessel placed approximately 2 cm from the light source, whilst being cooled by an external fan. Melting points were determined in sealed glass capillaries under dinitrogen and are uncorrected. Microanalyses were carried out using a PerkinElmer- 2400 CHNS/O Series II System, or were carried out at London Metropolitan University. The ICP analysis was carried out on a Perkin Elmer Avio 220 ICP-OES instrument. The starting materials $(BorO)_3SiCl$,[1] $[AlH_3(NMe_3)]$,[2] $[AlD_3(NMe_3)]$,[2] $[AlH_2\{N(SiMe_3)_2\}(NMe_3)]$,[3] $[AlH_3(NMP)]$,[4] $[\{(^{Mes}Nacnac)Mg\}_2]$,[5] $[\{(^{Dip}Nacnac)Mg\}_2]$,[5] $[\{(^{Xyl}Nacnac)Mg\}_2]$,[6] $[\{(^{Dip}Nacnac)Mg(\mu\text{-}H)\}_2]$,[7] $[(^{Mes}Nacnac)MgI(OEt_2)]$,[5] $[(^{Xyl}Nacnac)MgI(OEt_2)]$,[6] and TMC[8] were prepared by literature procedures. All other starting materials were used as received.

$(BorO)_3SiNH_2$.

$(BorO)_3SiCl$ (1.0 g, 1.91 mmol) was dissolved in THF (15 mL), then slowly added to a suspension of $LiNH_2$ (0.048 g, 2.1 mmol) in THF (10 mL) at -80 °C. The reaction mixture was slowly warmed to room temperature and stirred for 16 h. Volatiles were subsequently removed *in vacuo*, the residue extracted into toluene (30 mL), and the extract filtered. Volatiles were removed from the filtrate *in vacuo* to yield the title compound as an off-white solid (0.80 g, 84 %). M.p. 215-220 °C. ^{1}H NMR (400 MHz, C_6D_6, 298 K) δ = 0.84, 0.86, 0.99 (3 x s, 27H, OBor-C*H*$_3$), 1.21-1.31 (m, 6H, OBor-*H*), 1.34-1.44 (m, 3H, OBor-*H*), 1.57-1.62 (m, 3H, OBor-*H*), 1.69-1.80 (m, 3H, OBor-*H*), 2.26-2.42 (m, 6H , OBor-*H*), 4.35-4.40 (m, 3H, OBor-*H*), N*H* protons not observed; ^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K) δ = 14.0, 19.0, 20.2 (OBor-*C*H$_3$), 26.8, 28.9, 39.7, 45.7, 47.6 , 50.1, 77.9 (OBor-*C*); IR ν/cm^{-1}(Neat): 3505 (br.), 1536 (m), 1471 (m), 1166 (m), 1140 (m), 1113 (s), 1085 (s), 1066 (s), 1040 (m), 1027 (m), 997 (m), 981 (w), 927 (w), 907 (w); elemental analysis for $C_{30}H_{53}NO_3Si$ calcd.: C 71.52 %, H 10.60 %, N 2.78 %, found: C 72.47 %, H 10.97 %, N 2.29 %.

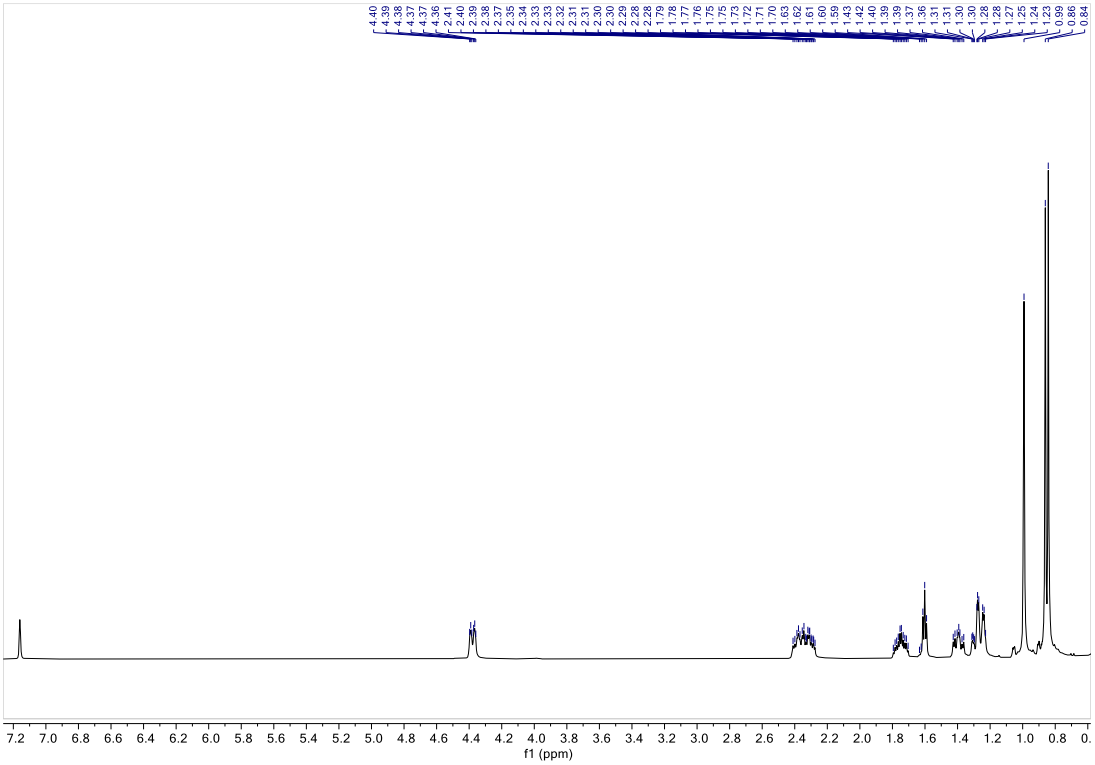

Figure S1. ^{1}H NMR spectrum (400 MHz, 298 K, C_6D_6) of $(BorO)_3SiNH_2$.

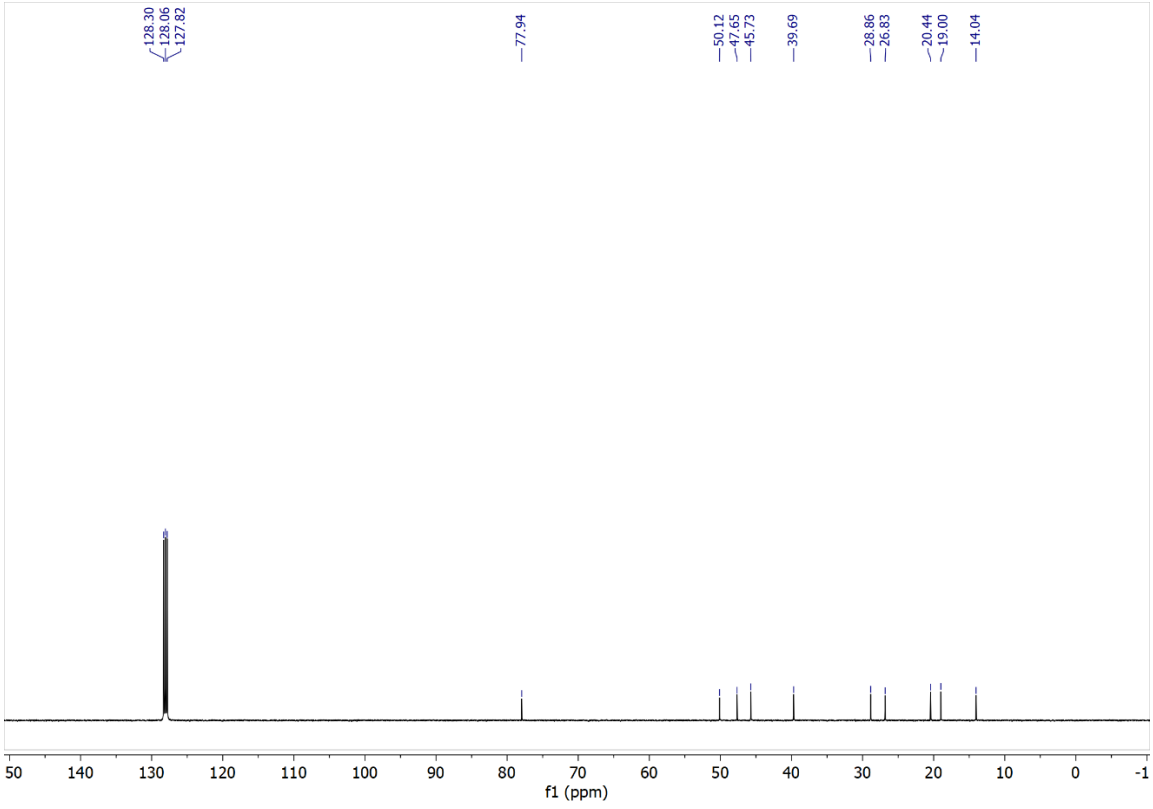

Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of $(BorO)_3SiNH_2$.

$(Me_2PhSi)\{(BorO)_3Si)\}NH$.

To a stirred solution of $(BorO)_3SiNH_2$ (0.5 g, 0.99 mmol) in THF (10 mL) cooled to -80 °C, was added Bu^nLi (0.68 mL, 1.6 M in hexane, 1.09 mmol) over 5 minutes. The resultant solution was warmed to room temperature and stirred for 3 h. To this solution at -80 °C, $PhMe_2SiCl$ (0.167 mL, 0.99 mmol) was added dropwise using a syringe. The reaction mixture was slowly warmed to room temperature, stirred for 16 h, then heated at 50 °C for 12 h . All volatiles were removed *in vacuo*, and the residue was extracted with hexane. Removal of volatiles from the filtrate under reduced pressure yielded the title compound as a viscous oil (0.54 g, 85%). ^{1}H NMR (400 MHz, C_6D_6, 298 K) δ = 0.50 (s, 6H, SiPh*Me*$_2$), 0.83, 0.85, 0.97 (s, 27H, OBor-C*H*$_3$), 1.19-1.28 (m, 6H, OBor-*H*), 1.30-1.39 (m, 3H, OBor-*H*), 1.56-1.60 (m, 3H, OBor-*H*), 1.68-1.79 (m, 3H, OBor-*H*), 2.24-2.34 (m, 6H, OBor-*H*), 4.35-4.40 (m, 3H, OBor-*H*), 7.19 – 7.74 (m, 5H, Ar-*H*), N*H* proton not observed. ^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K) δ = 1.3 (SiPh*Me*$_2$), 14.2, 19.0, 20.4 (OBor-*C*H$_3$), 26.9, 28.8, 39.6, 45.7, 47.6, 50.2, 78.1 (OBor-*C*), 129.3, 133.8, 141.3 (Ar-*C*); ^{29}Si{^{1}H} NMR (80 MHz, C_6D_6, 298 K) δ = -67.6 (*Si*(OBor)$_3$), -3.49 (*Si*PhMe$_2$); IR ν/cm^{-1}(neat): 3337 (m), 1453 (w), 1427 (vw), 1388 (w), 1249 (w), 1233 (w), 1166 (w), 1140 (w), 1112 (s), 1084 (m), 1069 (s), 1038 (m), 996 (w), 947 (m), 925 (w), 907 (m), 875 (w), 726 (w), 698 (w).

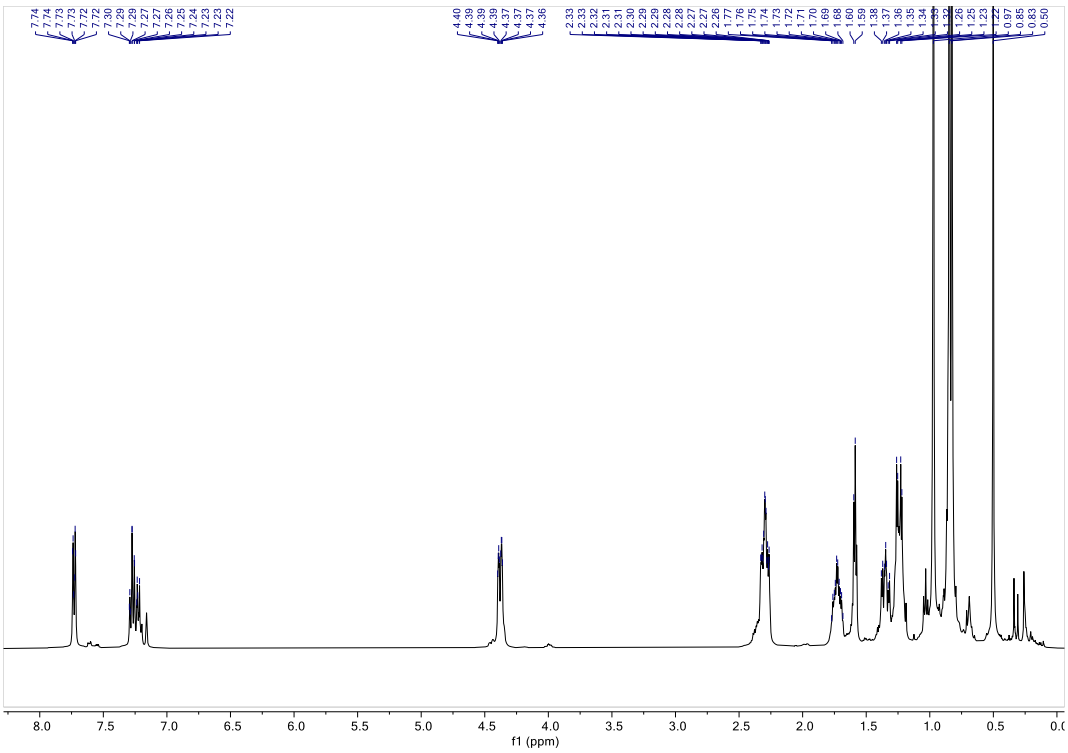

Figure S3. ^{1}H NMR spectrum (400 MHz, 298 K, C_6D_6) of $(Me_2PhSi)\{(BorO)_3Si)\}NH$.

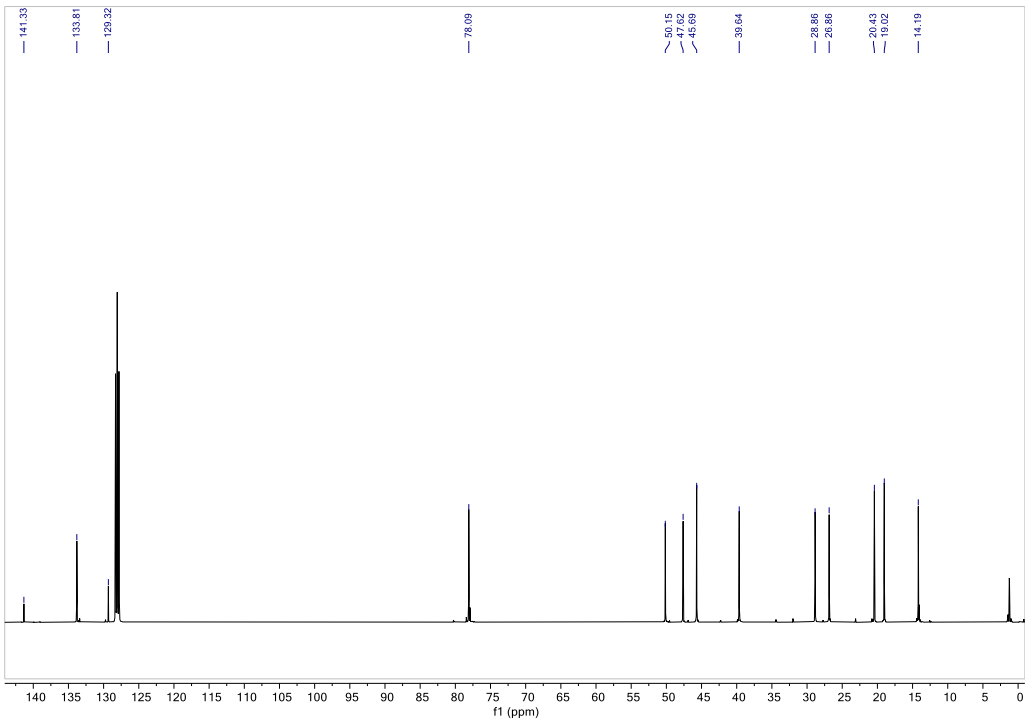

Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of $(Me_2PhSi)\{(BorO)_3Si)\}NH$.

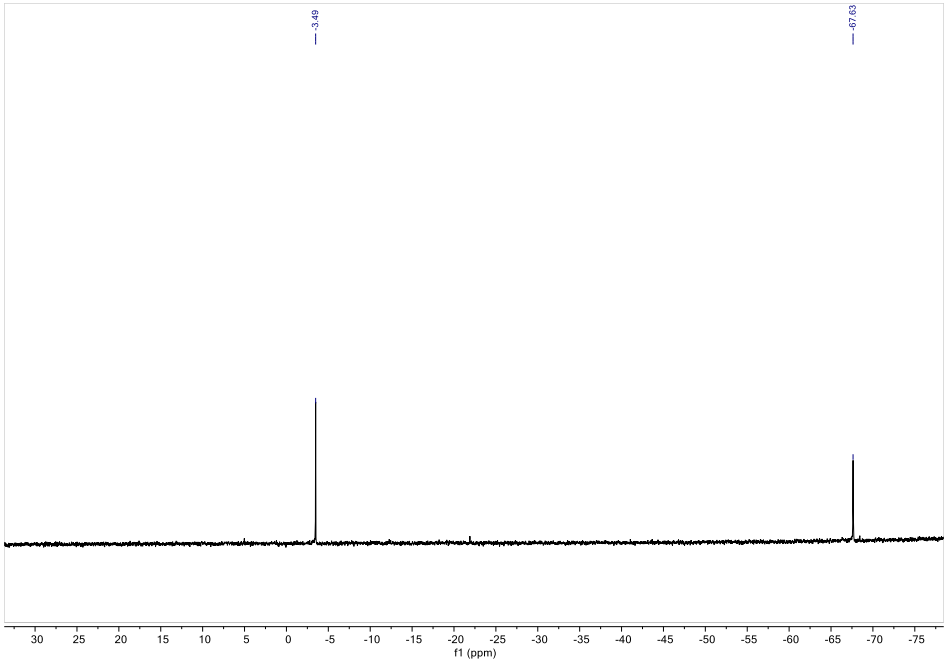

Figure S5.$^{29}Si\{^{1}H\}$ NMR spectrum (80 MHz, 298 K, C_6D_6) of $(Me_2PhSi)\{(BorO)_3Si)\}NH$.

[{(Me$_2$PhSi)[(BorO)$_3$Si)]N}AlH$_2$(NMe$_3$)].

[AlH$_3$(NMe$_3$)] (1.716 mL, 1M in toluene, 1.716 mmol) was added to a solution of (Me$_2$PhSi){(BorO)$_3$Si)}NH (1 g, 1.56 mmol) in toluene (20 mL) at -80 °C. The resultant mixture was stirred for 16 h, then all volatiles removed under reduced pressure to yield the title compound as a colourless solid (0.78 g, 69 %). M.p 80-84 °C; ^{1}H NMR (400 MHz, C$_6$D$_6$, 298 K) δ = 0.83 (s, 3H, SiPh*Me$_2$*), 0.86 (s, 9H, OBor-C*H$_3$*), 0.87 (s, 3H, SiPh*Me$_2$*), 0.95 (s, 9H, OBor-C*H$_3$*), 1.12 (s, 9H, OBor-C*H$_3$*), 1.22-1.32 (m, 3H, OBor-*H*), 1.38-1.45 (m, 3H, OBor-*H*), 1.48-1.54 (m, 3H, OBor-*H*), 1.63-1.66 (m, 3H, OBor-*H*), 1.71-1.81 (m, 3H, OBor-*H*), 1.92 (s, 9H, N*Me$_3$*), 2.37-2.48 (m, 6H, OBor-*H*), 4.2 (v. br., Al*H*), 4.57-4.62 (m, 3H, OBor-*H*), 7.18-8.00 (m, 5H, Ar-*H*); ^{13}C{^{1}H} NMR (101 MHz, C$_6$D$_6$, 298 K) δ = 4.4, 4.9 (SiPh*Me$_2$*), 14.7, 19.1, 20.4 (OBor-*C*H$_3$), 27.2, 28.9, 39.5, 45.6, 47.6 (OBor-*C*), 48.1 (N*Me$_3$*), 50.5 (OBor-*C*), 77.9 (OBor-*C*), 127.6, 128.4, 135.0, 145.0 (Ar-*C*); ^{29}Si{^{1}H} NMR (80 MHz, C$_6$D$_6$, 298 K) δ = -67.9 (*Si*(OBor)$_3$), -7.1 (*Si*PhMe$_2$); IR (Nujol) *ν* (cm^{-1}) : 1839 (m, Al-H str.), 1792 (s, Al-H str.), 1066 (s), 1039 (w), 1025 (w), 979 (s), 946 (vw), 924 (vw), 903 (w), 876 (w), 853 (w), 819 (w), 784 (w), 729 (s), 703 (vw); elemental analysis calculated for C$_{41}$H$_{73}$AlN$_2$O$_3$Si$_2$: C 67.91 %, H 10.15 % N 3.86 %; found C 67.51 %, H 9.92 %, N 3.75 %.

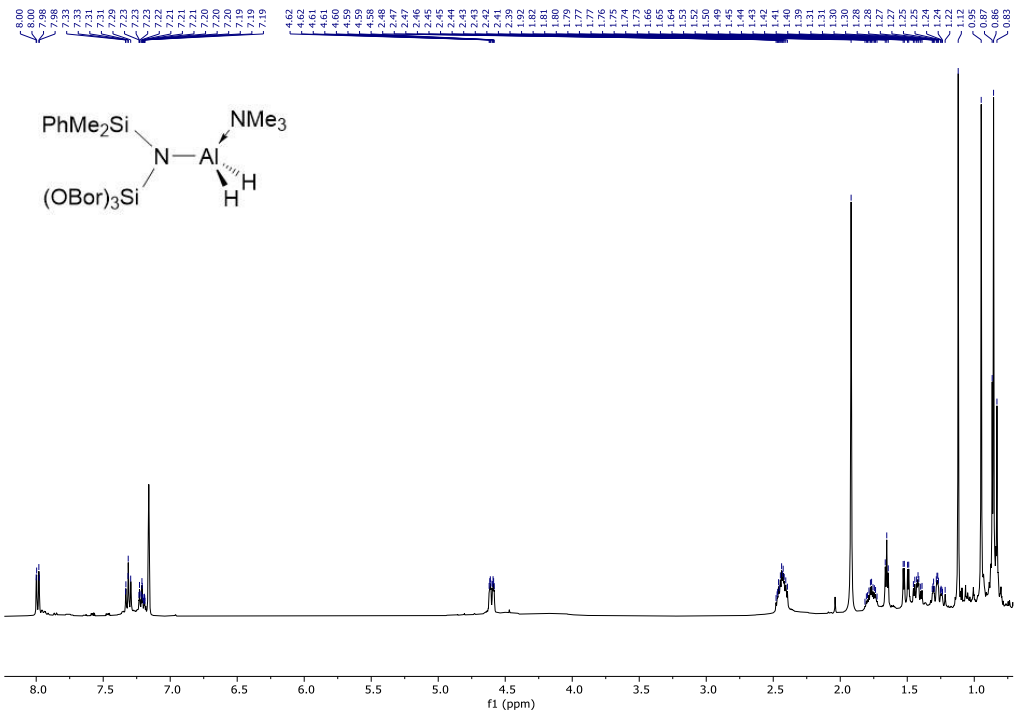

Figure S6. ^{1}H NMR spectrum (400 MHz, 298 K, C$_6$D$_6$) of [{(Me$_2$PhSi)[(BorO)$_3$Si)]N}AlH$_2$(NMe$_3$)].

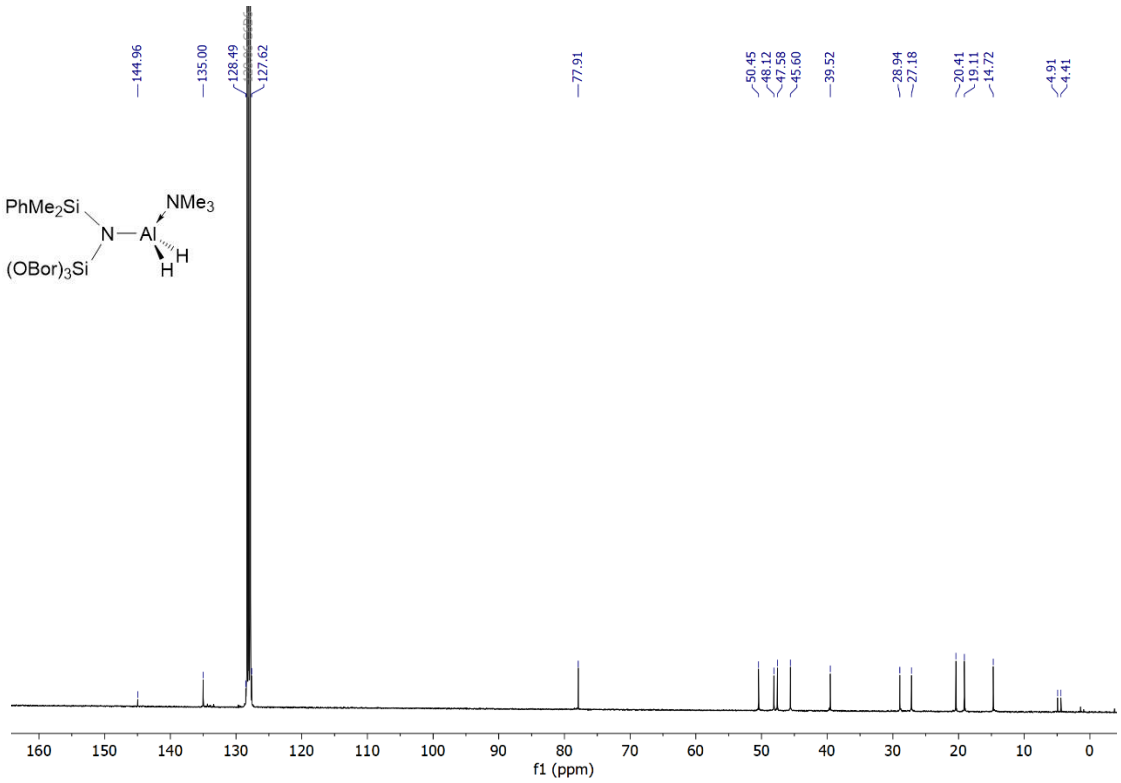

Figure S7. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of [{(Me_2PhSi)[($BorO)_3Si$)]N}$AlH_2(NMe_3)$].

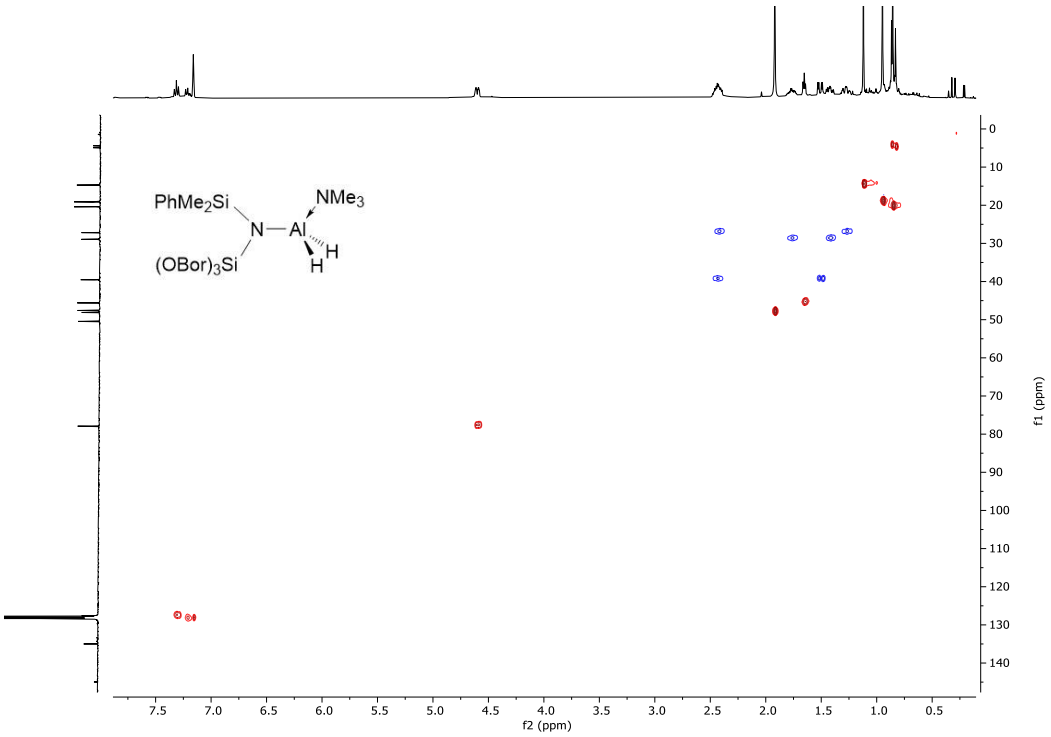

Figure S8. HMQC spectrum (^{1}H: 400 MHz; ^{13}C: 101 MHz, 298 K, C_6D_6) of [{(Me_2PhSi)[($BorO)_3Si$)]N}$AlH_2(NMe_3)$].

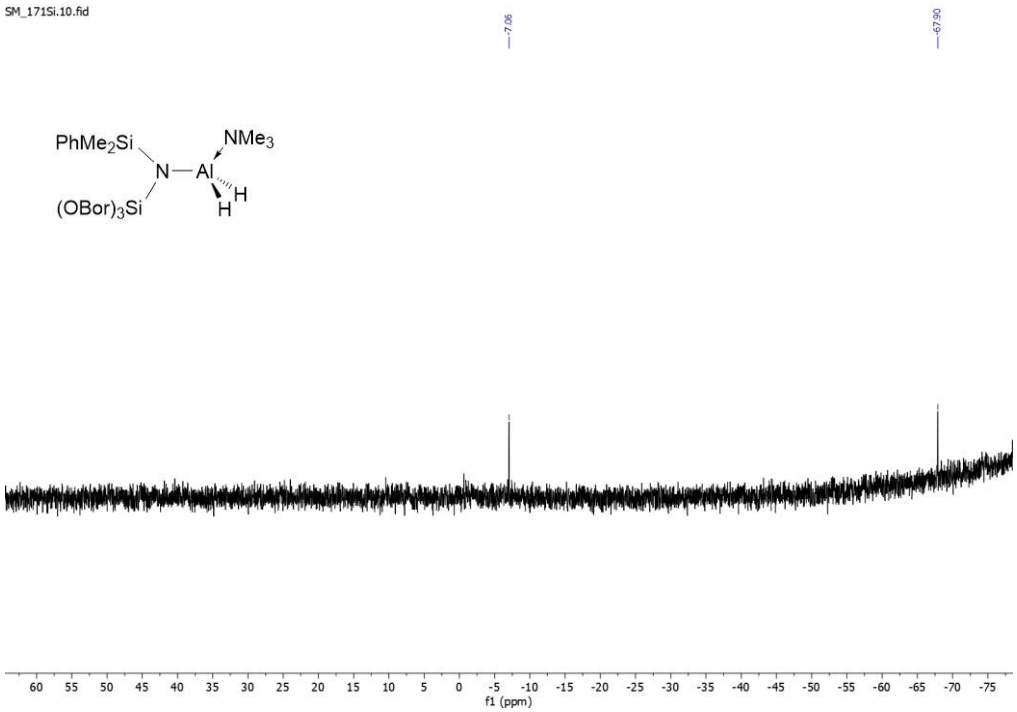

Figure S9. $^{29}Si\{^{1}H\}$ NMR spectrum (80 MHz, 298 K, C_6D_6) of [{(Me_2PhSi)[$(BorO)_3Si$)]N}$AlH_2(NMe_3)$].

[(2,6-Bu$^t_2$C$_6$H$_3$O)AlH$_2$(NMe$_3$)].

2,6-di*tert*buytlphenol (1.0 g, 4.8 mmol) dissolved in hexane (5 mL) was added dropwise to a solution of $AlH_3(NMe_3)$ (5.1 mL, 1 M in toluene, 5.1 mmol), which had been diluted with 15 mL of hexane and cooled to −78 °C. The suspension was warmed to room temperature, then stirred overnight. The suspension was filtered to yield the title compound as a near spectroscopically pure colorless solid. The filtrate was stored at −30 °C to yield a further crop of needle like crystals of the title compound (1.17 g, 82 %). M.p. 152-154 °C; ^{1}H NMR (400 MHz, 298 K, C_6D_6) δ = 1.64 (s, 18H, ArC(CH_3)$_3$), 1.93 (s, 9H, N*Me*$_3$), 6.95 (t, $^{3}J_{HH}$ = 7.8 Hz ,1H, *p*-Ar*CH*), 7.41-7.43 (d, $^{3}J_{HH}$ = 7.8 Hz, 2H, *m*-Ar*CH*), Al*H* resonance not observed; $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6, 298 K): δ = 31.7 (ArC(*C*H$_3$)$_3$), 35.6 (Ar*C*(CH$_3$)$_3$), 47.5 (N(*C*H$_3$)$_3$), 118.5 (*p*-Ar*C*), 125.8 (*m*-Ar*C*), 139.2 (*o*-Ar*C*), 157.3 (Ar*C*O); IR ν/cm^{-1} (ATR): 2954 (s), 2909 (m), 2869 (m), 1838 (m, Al-H str.), 1806 (s, Al-H str.), 1460 (m), 1357 (w), 1253 (s), 1200 (w), 1124 (w), 1104 (w), 990 (m).

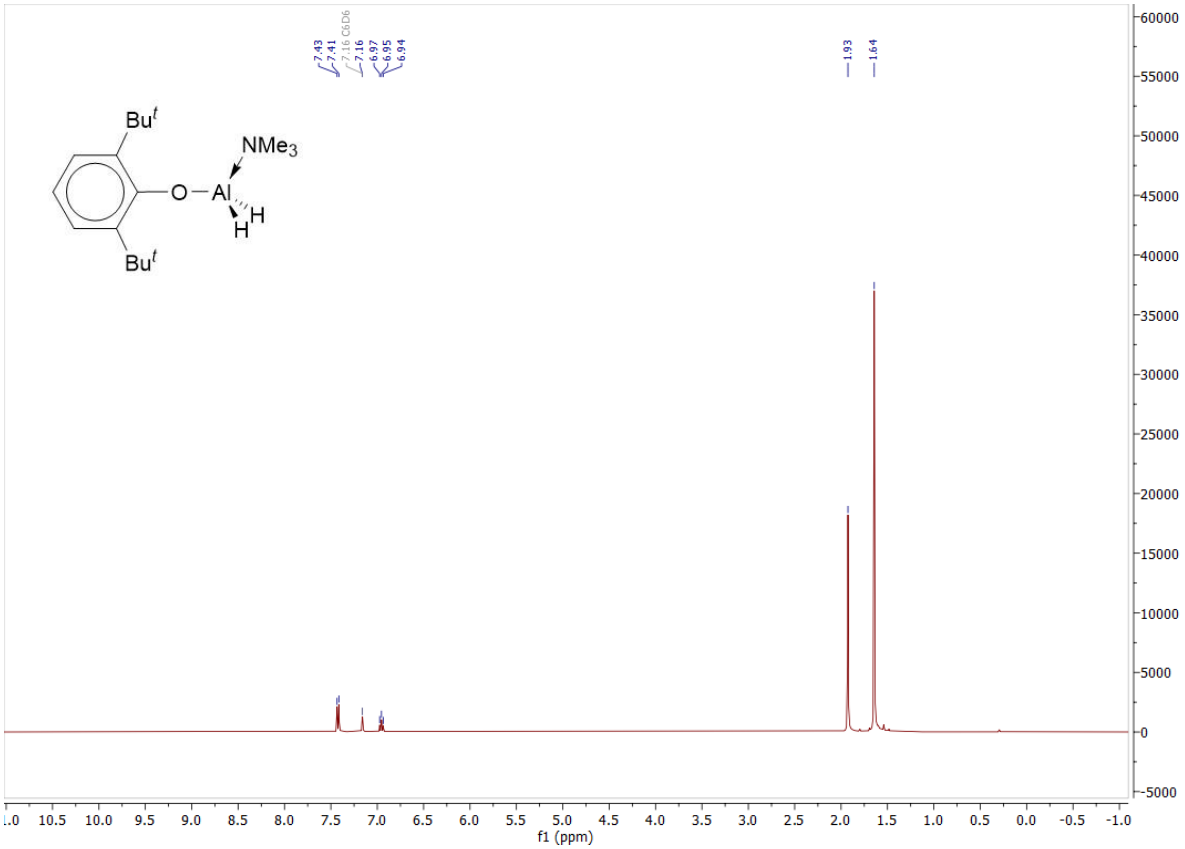

Figure S10. ^{1}H NMR spectrum (400 MHz, 298 K, C_6D_6) of [(2,6-Bu$^t_2$C$_6$H$_3$O)AlH$_2$(NMe$_3$)].

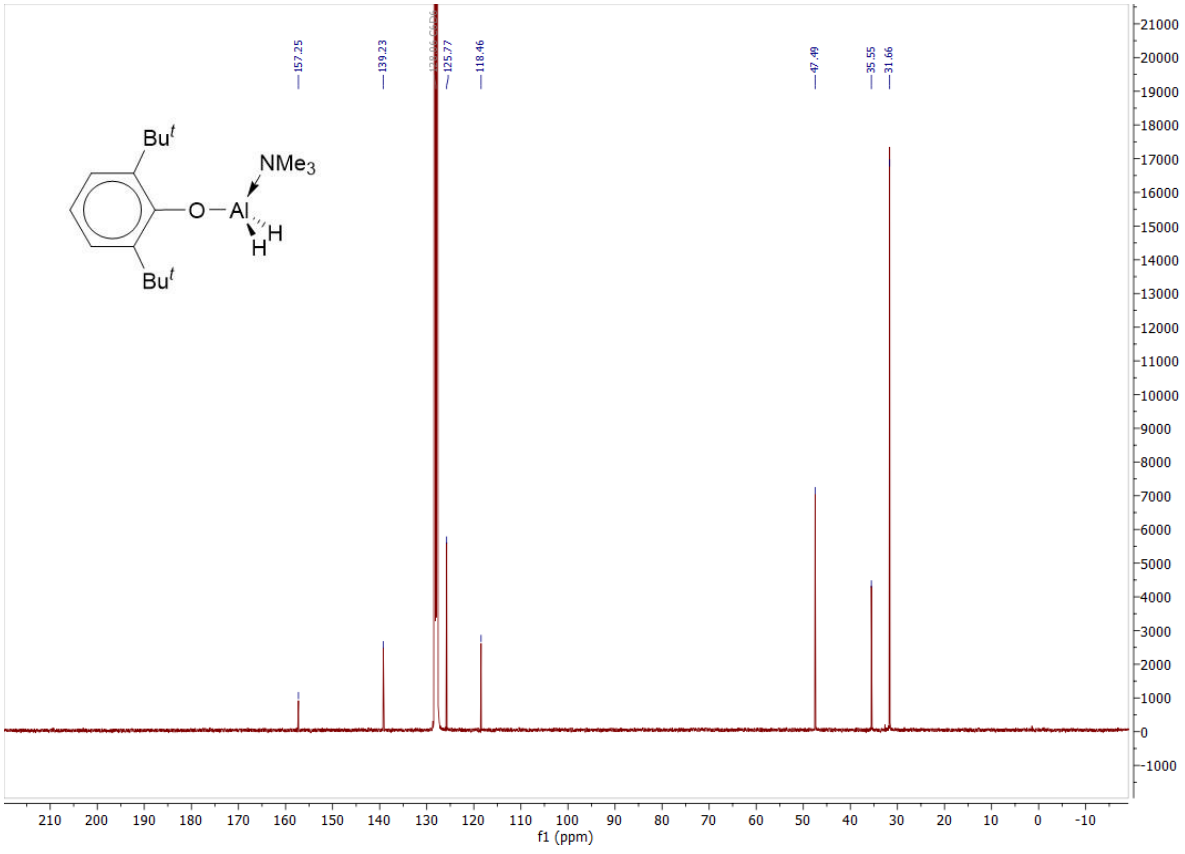

Figure S11. ^{13}C{^{1}H} NMR spectrum (101 MHz, 298 K, C_6D_6) of [(2,6-Bu$^t_2$C$_6$H$_3$O)AlH$_2$(NMe$_3$)].

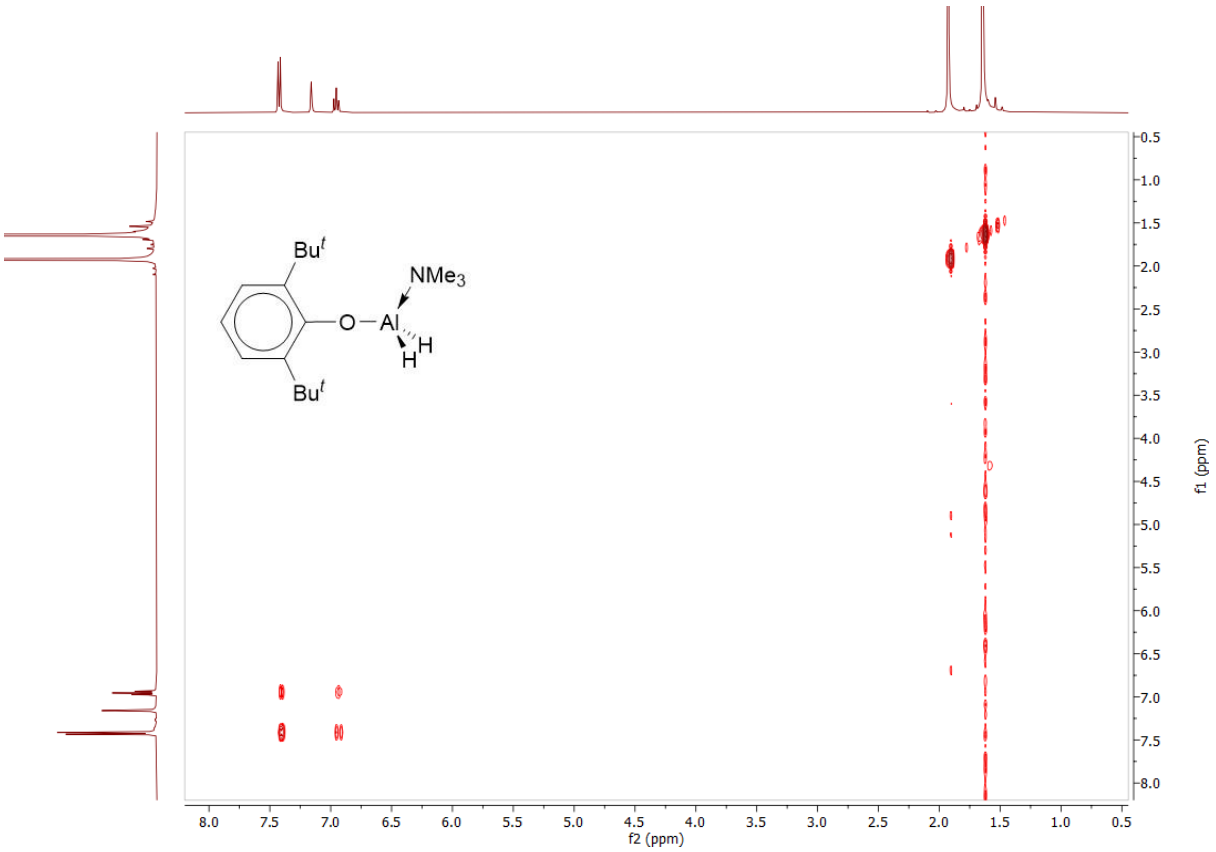

Figure S12. ^{1}H-COSY NMR spectrum (400 MHz, 298 K, C_6D_6) of [(2,6-Bu$^t_2$C$_6$H$_3$O)AlH$_2$(NMe$_3$)].

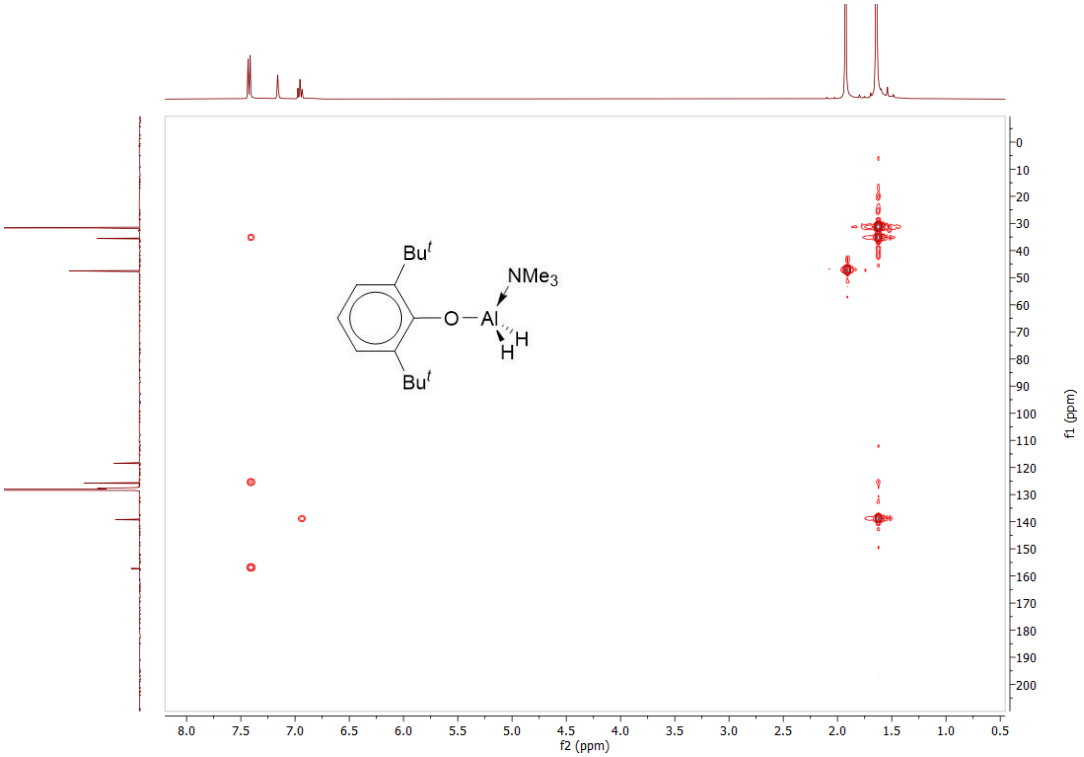

Figure S13. HMBC spectrum (^{1}H: 400 MHz; ^{13}C: 101 MHz, 298 K, C_6D_6) of [(2,6-Bu$^t_2$C$_6$H$_3$O)AlH$_2$(NMe$_3$)].

[AlD$_2${N(SiMe$_3$)$_2$)}(NMe$_3$)].

The title compound was synthesized by the procedure used to prepare [AlH$_2${N(SiMe$_3$)$_2$)}(NMe$_3$)],[3] but using the reagents HN(SiMe$_3$)$_2$ (0.23g, 1.43 mmol) and [AlD$_3$(NMe$_3$)] (3.14 mL, 1.57 mmol, 0.5 M in toluene) (0.33 g, 92 %). M.p. < 60 °C ; ^{1}H NMR (400 MHz, C$_6$D$_6$, 298 K) δ = 0.40 (s, 18H, Si*Me*$_3$), 1.80 (s, 9H, N*Me*$_3$); ^{13}C{^{1}H} NMR (101 MHz, C$_6$D$_6$, 298 K) δ = 6.0 (Si*Me*$_3$), 47.8 (N*Me*$_3$); ^{27}Al{^{1}H}NMR (104 MHz, C$_6$D$_6$, 298 K) δ = 136.7; ^{29}Si{^{1}H} NMR (80 MHz, 298 K, C$_6$D$_6$) δ = -0.8; IR (Nujol) ν (cm^{-1}) : 1478 (m), 1408 (w), 1298 (s), 1242 (s), 1102 (w), 996(m), 926(s), 884(s), 816(s), 756(w), 672(m).

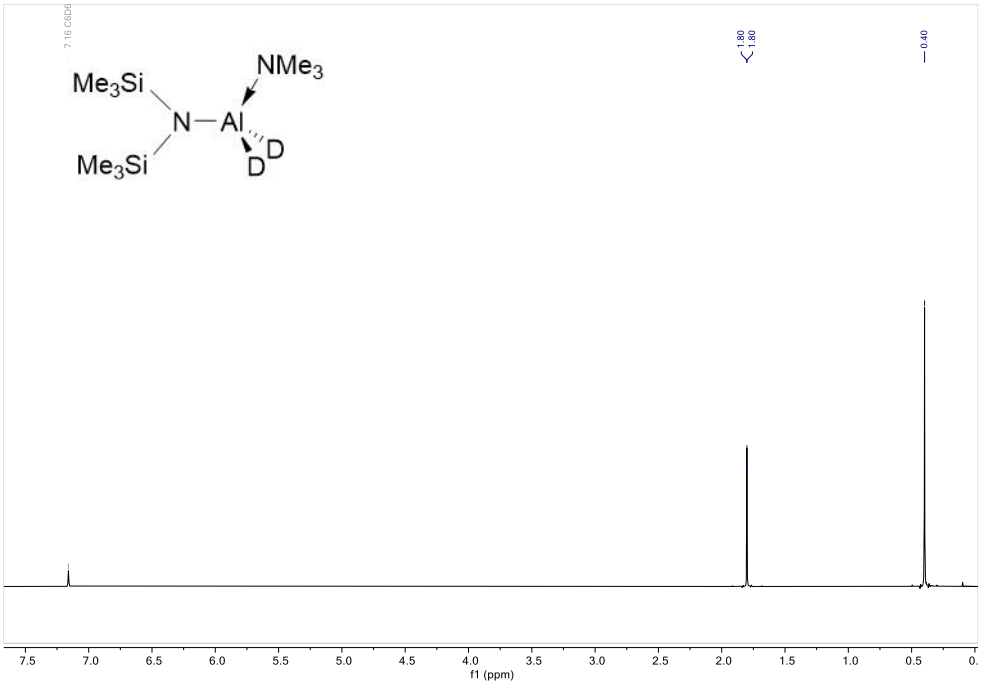

Figure S14. ^{1}H NMR spectrum (400 MHz, 298 K, C$_6$D$_6$) of [AlD$_2${N(SiMe$_3$)$_2$)}(NMe$_3$)].

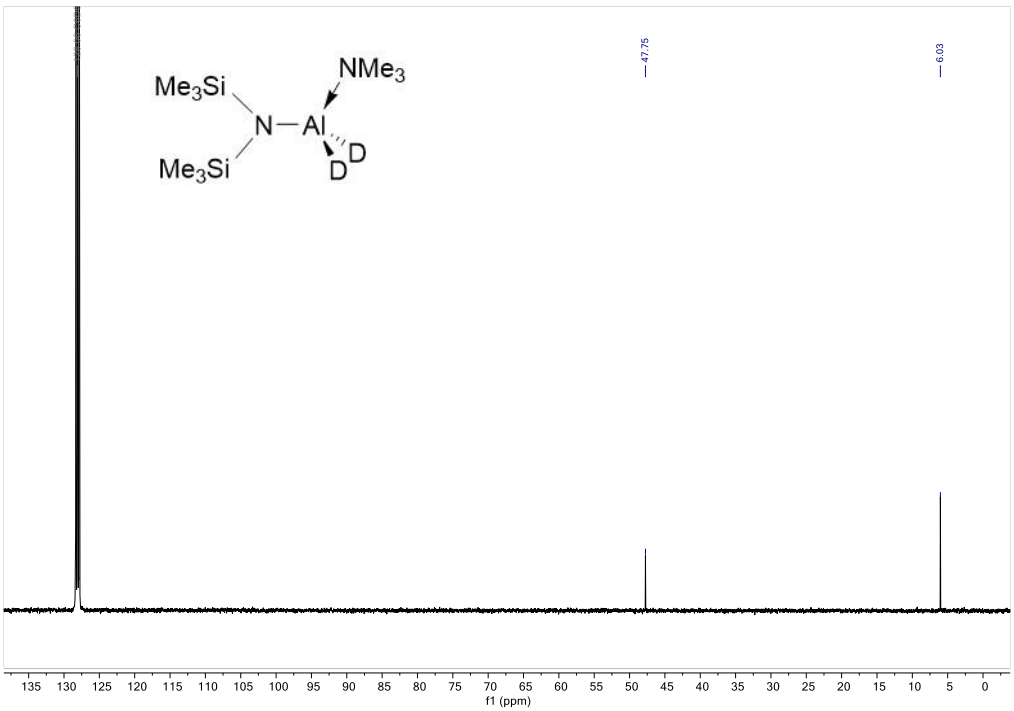

Figure S15. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of $[AlD_2\{N(SiMe_3)_2\}(NMe_3)]$.

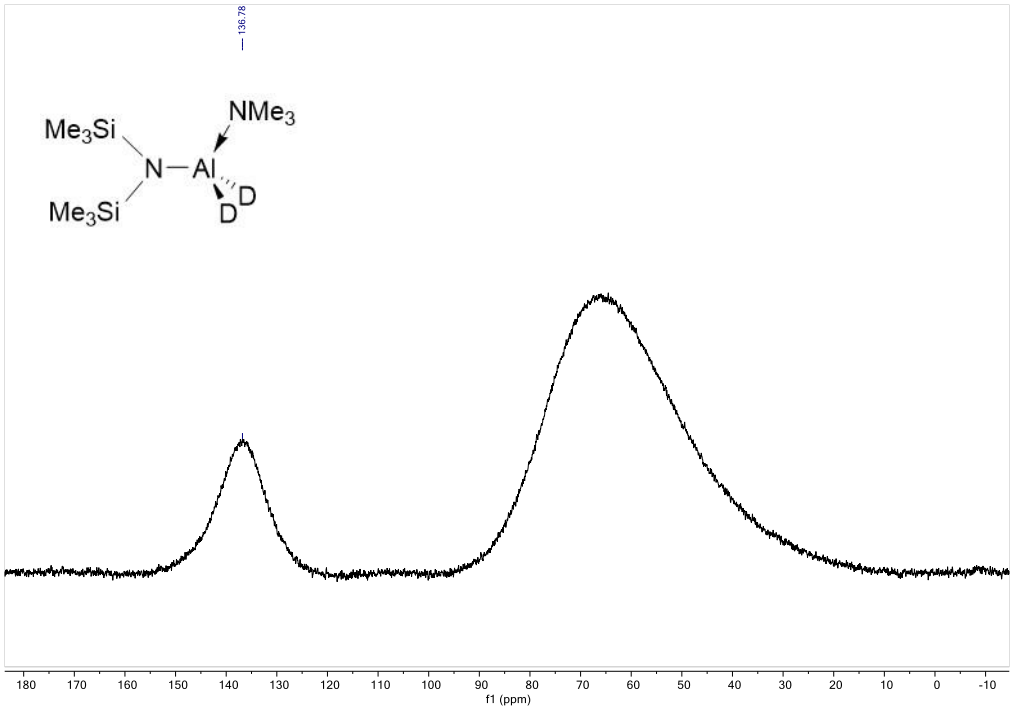

Figure S16. $^{27}Al\{^{1}H\}$ NMR spectrum (104 MHz, 298 K, C_6D_6) of $[AlD_2\{N(SiMe_3)_2\}(NMe_3)]$. N.B. the broad signal centred at *ca.* δ 65 ppm arises from the NMR probe.

$[\{(SiMe_3)_2N\}AlH_2(TMC)]$.

Compound $[\{(SiMe_3)_2N\}AlH_2(NMe_3)]$ (0.50 g, 2.01 mmol) and TMC (0.25 g, 2.01 mmol) were taken into a grease free Schlenk flask. Toluene (5 mL) was added to this solid mixture at room temperature. The resultant solution was stirred at room temperature overnight to form a clear yellow solution. The

solution was concentrated to approx. 3 mL *in vacuo*, and stored at -30 °C overnight, resulting in the deposition of colourless crystals of the product (0.56 g, 89 %). M.p. 80-83 °C; ^{1}H NMR (400 MHz, C_6D_6, 298 K) δ = 0.50 (s, 18H, Si*Me*$_3$), 1.15 (s, 6H, CC*H*$_3$), 3.30 (s, 6H, NC*H*$_3$), Al*H* resonance not observed; ^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K) δ 5.3 (Si*Me*$_3$), 7.7 (C*C*H$_3$), 33.2 (N*C*H$_3$), 125.1 (H$_3$C*C*=*C*CH$_3$), Al-*C* resonance was not observed; ^{29}Si{^{1}H} NMR (80 MHz, C_6D_6, 298 K) δ = -2.2; ^{27}Al{^{1}H} NMR (104 MHz, C_6D_6, 298 K) = 111.4; IR (Nujol) ν (cm^{-1}): 1749 (m, Al-H str.), 1709 (s, Al-H str.), 1649 (w), 1437 (w), 1393 (w), 1240 (s), 1384 (w), 962 (s), 889 (m), 830 (m), 780 (w), 752 (m), 717 (m), 669 (w); elemental analysis for $C_{13}H_{32}AlN_3Si_2$: C 49.80 %, H 10.29 % N 13.40 %; found C 49.31 %, 10.69 %, 13.17 %.

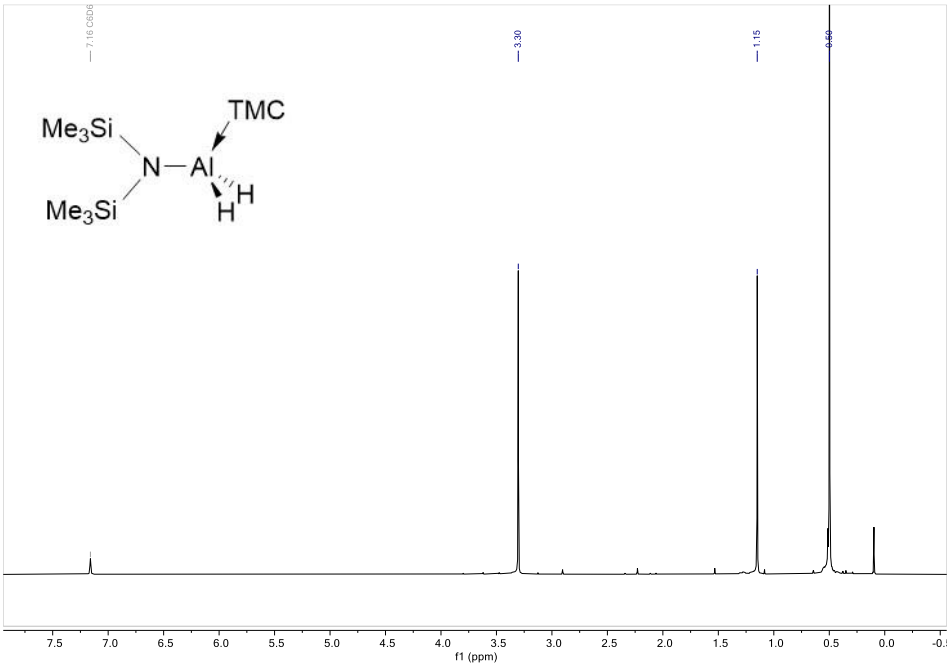

Figure S17. ^{1}H NMR spectrum (400 MHz, 298 K, C_6D_6) of [{(SiMe$_3$)$_2$N}AlH$_2$(TMC)].

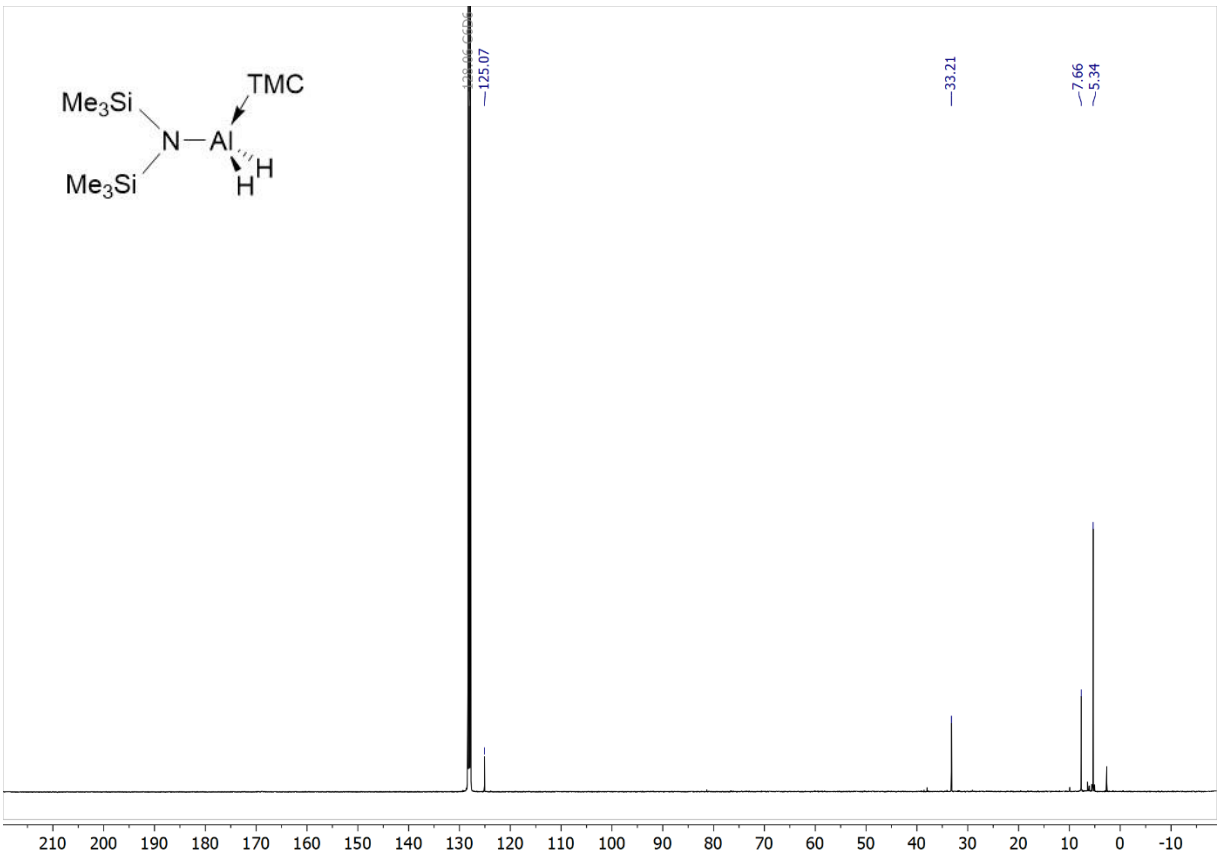

Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of [{$(SiMe_3)_2N$}AlH_2(TMC)].

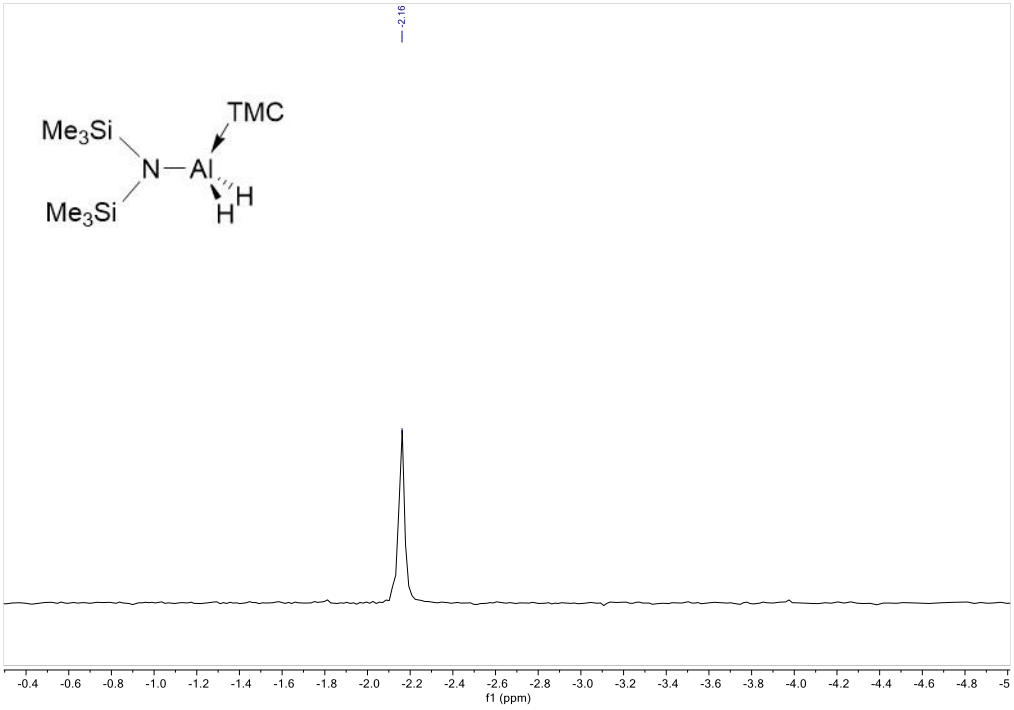

Figure S19. $^{29}Si\{^{1}H\}$ NMR spectrum (80 MHz, 298 K, C_6D_6) of [{$(SiMe_3)_2N$}AlH_2(TMC)].

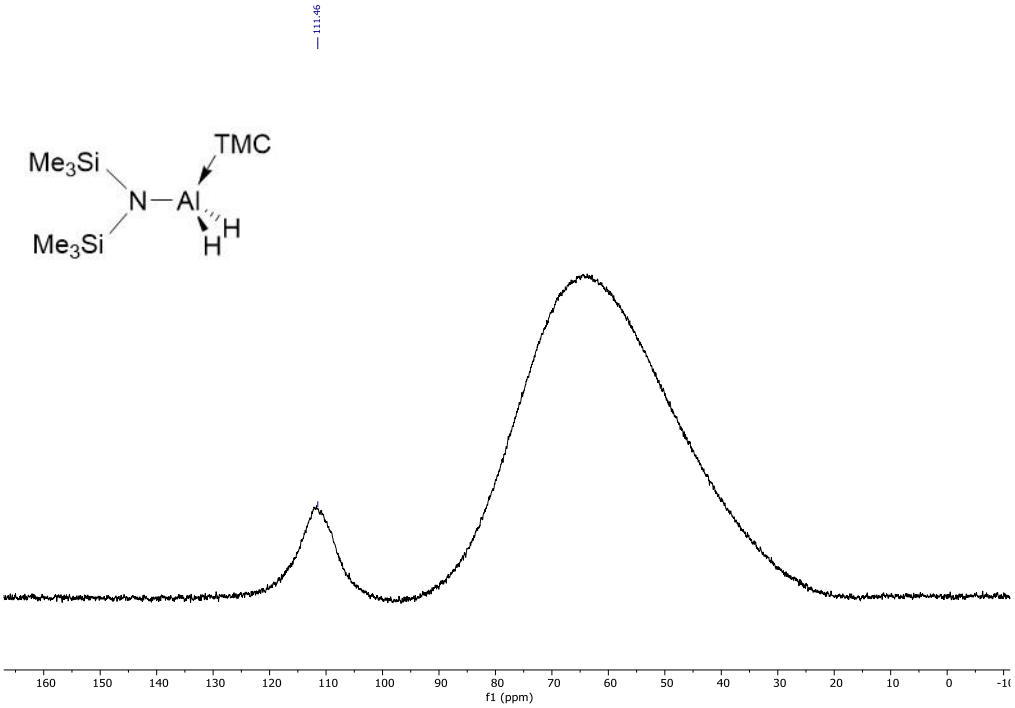

Figure S20. $^{27}Al\{^{1}H\}$ NMR spectrum (104 MHz, 298 K, C_6D_6) of [{$(SiMe_3)_2N$}AlH_2(TMC)].

[$Al_6H_8(NMe_3)_2${$Mg(^{Mes}Nacnac)$}$_4$] 1a and [(^{Mes}Nacnac)(Me_3N)Mg–Al(μ-H)$_3$[{$Mg(^{Mes}Nacnac)$}$_2$(μ-H)]] 3a.

[{$(SiMe_3)_2N$}$AlH_2(NMe_3)$] (100 mg, 0.403 mmol) and [{(^{Mes}Nacnac)Mg}$_2$] (289 mg, 0.403 mmol) were combined in a grease-free Schlenk flask. Benzene (3 mL) was added to these solids and the resultant mixture was heated at 40 °C for 10 mins, yielding a clear bright red solution. Allowing the solution to stand at room temperature for three days resulted in the deposition of red crystals of **1a** (49 mg, *ca.* 40 % based on Mg, assuming 7 molecules of [{(^{Mes}Nacnac)Mg}$_2$] are required to reduce 6 molecules of [{$(SiMe_3)_2N$}$AlH_2(NMe_3)$] from the +3 to avg. +0.66 oxidation state). After the isolation of compound **1a**, the mother liquor was stored at 5 °C for 2 days, affording colourless crystals of **3a** (20 mg, *ca.* 7 % based on Mg). N.B. compounds **1a** (39% yield) and **3a** (5% yield) were prepared in similar yields by irradiating benzene solutions of 1:1 mixtures of [{$(SiMe_3)_2N$}$AlH_2(NMe_3)$] and [{(^{Mes}Nacnac)Mg}$_2$] with a UV LED lamp (λ = 370 nm, 43 W) for 8 h at room temperature. Furthermore, **1a** was obtained from reactions of [{$(Me_2PhSi)[(BorO)_3Si)]N$}$AlH_2(NMe_3)$] or [(2,6-$Bu^t_2C_6H_3O$)$AlH_2(NMe_3)$] with [{(^{Mes}Nacnac)Mg}$_2$] in low (< 5%) and low-moderate yields (*ca.* 35%), respectively.

Data for **1a**: 150-155 °C (decomp.); Once crystallised, compound **1a** has negligible solubility in common coordinating and non-coordinating deuterated solvents. Therefore, solution state NMR spectroscopic data could not be obtained for the compound. IR (Nujol) ν (cm^{-1}): 1527 (s), 1396 (vs), 1378(m), 1261(s), 1200 (m), 1147 (w), 1012 (s), 1009 (s), 959(w), 926(w), 857(m), 825(w), 803(w),

771(w), 744(w), 685(w); ICP-OES analysis on HNO_3 digested crystalline sample gave an Al:Mg ratio of 1.6; elemental analysis calculated for $C_{98}H_{142}N_{10}Mg_4Al_6$: C 68.46 %, H 8.32 % N 8.15 %; found C 68.23 %, H 8.12 %, N 7.96 %.

Data for **3a**: M.p. 190-196 °C (decomp.); ^{1}H NMR (400 MHz, C_6D_6, 298 K) δ = 1.48 (s, 18H, NCC*H*$_3$), 1.55 (s, 9H, N*Me*$_3$), 1.95 (s, 24H, *ortho*-C*H*$_3$), 1.97 (s, 12H, *ortho*-C*H*$_3$), 2.25 (s, 6H, *para*-C*H*$_3$), 2.32 (s, 12H, *para*-C*H*$_3$), 2.94 (s, 1H, Mg-*H*-Mg), 3.74 (s, 3H, Al-*H*), 4.79 (s, 2H, β-C*H*), 4.87 (s, 1H, β-C*H*), 6.74 (s, 4H, Ar-*H*), 6.77 (s, 8H, Ar-*H*); IR (Nujol) ν (cm^{-1}): 1526 (s), 1393 (s), 1370 (m) 1261 (w), 1233 (w), 1199 (m), 1147 (m), 1011 (s), 958 (w), 927 (w), 901 (w), 853 (s), 736 (s), 681 (w); elemental analysis calculated for $C_{72}H_{100}N_7Mg_3Al$: C 74.32 %, H 8.66 % N 8.43 %; found C 75.22 %, H 8.72 %, N 7.45 %. N.B: Compound **3a** has low solubility in non-coordinating deuterated solvents, hence meaningful ^{13}C{^{1}H} and ^{27}Al NMR spectroscopic data could not be acquired.

N.B. The preparation of **1a** was attempted using either hexane or cyclohexane as a reaction solvent, in place of benzene. This proved problematic as the magnesium(I) starting material [{(^{Mes}Nacnac)Mg}$_2$] has low solubility in those solvents, even at elevated temperatures. It is important to have a homogeneous reaction solution, after heating, to obtain **1a** as a crystalline solid. No products could be crystallised or identified from the reactions in hexane and cyclohexane.

N.B. When the preparation of **1a** was carried out at a higher reaction temperature (70-100 °C), the cluster was formed in a much reduced isolated yield (*ca.* 5 %), from a complex mixture of unidentified by-products. Carrying out the reaction at room temperature led to the slow formation of a yellow-orange suspension after several hours. No cluster **1a** was isolated from the mixture, and the only identifiable product of the reaction was a few crystals of [{(^{Mes}Nacnac)Mg(μ-H)}$_2$]. The optimum temperature for the reaction was reproducibly found to be 40 °C.

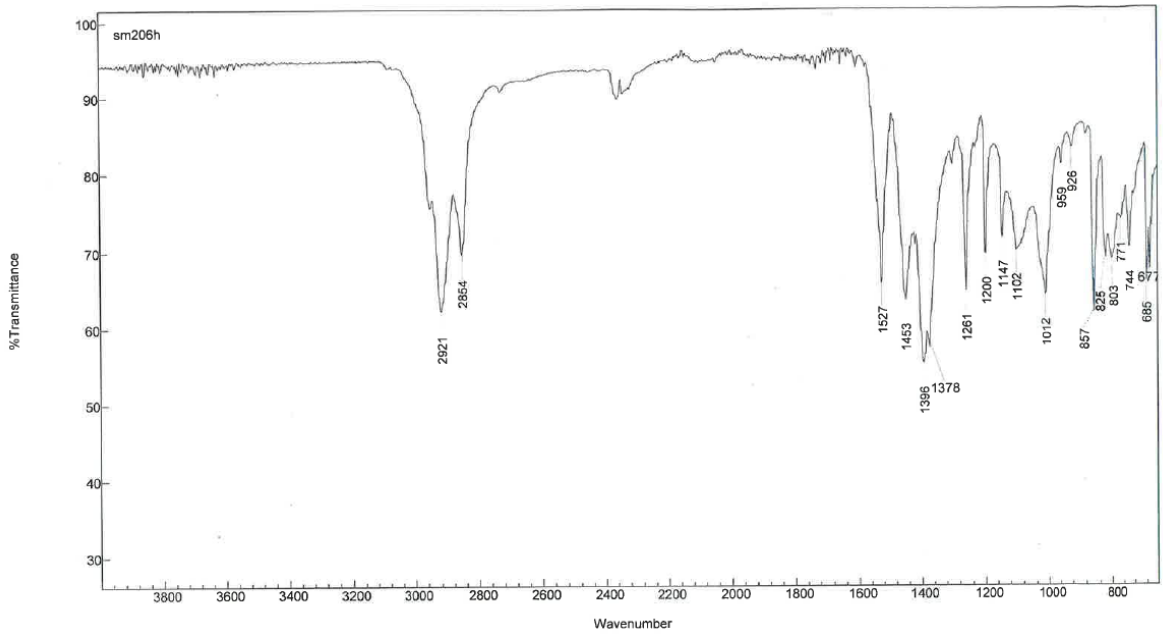

Figure S21. Infrared spectrum (Nujol mull) of **1a.**

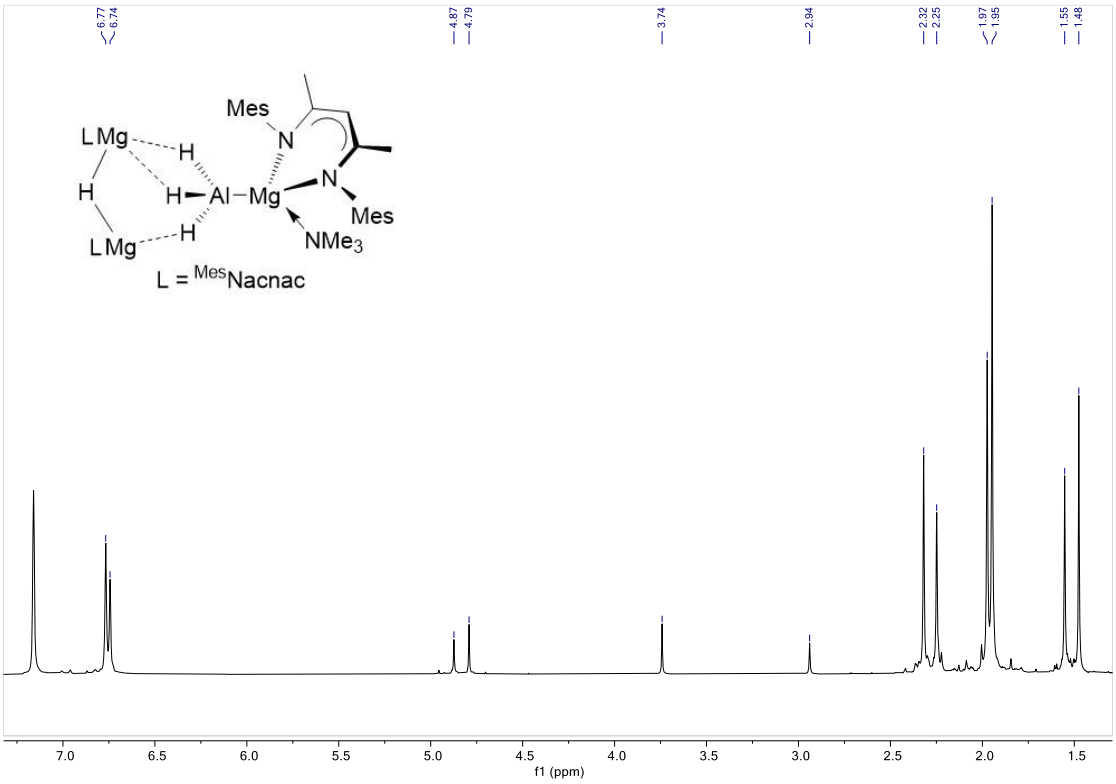

Figure S22. ^{1}H NMR spectrum (400 MHz, 298 K, C_6D_6) of **3a**.

[$Al_6D_8(NMe_3)_2${Mg(^{Mes}Nacnac)}$_4$] 1a-D.

1a-D was synthesised *via* a route similar to that for cluster **1a**, as described above, but using [{$(SiMe_3)_2N$}$AlD_2(NMe_3$}] (100 mg, 0.4 mmol) and [{(^{Mes}Nacnac)Mg}$_2$] (286 mg, 0.4 mmol). (50 mg, *ca.* 40 % based on Mg). M.p. 150 °C (decomp.); IR (Nujol) ν (cm^{-1}) =1526(s), 1388(s), 1375(s), 1303(w), 1261(m), 1147(w), 1080 (m), 1010(s), 959(w), 926(w), 880(w), 857(m), 824(m), 798(m), 744(w), 682(m); elemental analysis calculated for $C_{98}H_{134}D_8N_{10}Mg_4Al_6$: C 68.14 %, H 8.75 % N 8.11 %; found C 67.98 %, H 8.25 %, N 8.00 %.

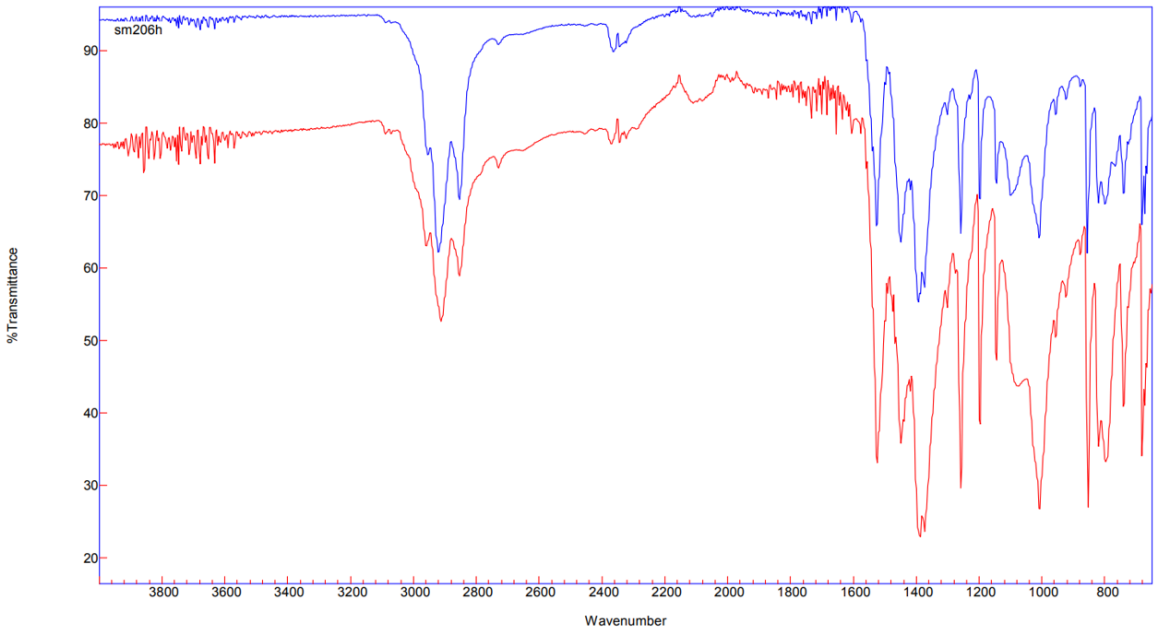

Figure S23. Infrared spectrum (Nujol mull) of **1a-D** (red trace) overlayed with that of **1a** (blue trace).

[$Al_6H_8(NMe_3)_2${$Mg(^{Xyl}Nacnac)$}$_4$] 1b and [(^{Xyl}Nacnac)(Me_3N)Mg–Al(μ-H)$_3$[{$Mg(^{Xyl}Nacnac)$}$_2$(μ-H)]] 3b.

[{$(SiMe_3)_2N$}$AlH_2(NMe_3$}] (150 mg, 0.605 mmol) and [{(^{Xyl}Nacnac)Mg}$_2$] (399 mg, 0.605 mmol) were combined in a grease free Schlenk flask. Benzene (4 mL) was added to these solids and the resultant mixture was heated at 40 °C for 15 mins until a clear bright red solution was formed. Allowing the solution to stand at room temperature overnight resulted in the deposition of colourless crystals of **3b** suitable for single crystal X-ray diffraction (25 mg, 6 % based on Mg). The mother liquor was filtered and concentrated under reduced pressure. Storing the solution at room temperature for 7 days resulted in the deposition of a few deep red crystals of **1b** (yield < 5%), M.p. > 160 °C. Solution state and solid-state spectroscopic data could not be obtained for **1b** due to its low yield, its negligible solubility in common deuterated solvents, and the fact that it consistently crystallised with a small amount of an insoluble colorless by-product, which could not be separated. Data for **3b**: M.p. >150 °C (decomp.); ^{1}H NMR (400 MHz, C_6D_6, 298 K) δ = 1.52 (s, 12H, NCC*H*$_3$), 1.56 (s, 6H, NCC*H*$_3$), 1.65 (s, 9H, N*Me*$_3$), 1.96 (s, 6H, *ortho*-C*H*$_3$), 2.10 (s, 24H, *ortho*-C*H*$_3$), 2.28 (br., s, 6H, *ortho*-C*H*$_3$), 4.82 (s, 2H, β-C*H*), 4.87 (s, 1H, β-C*H*), 6.92–7.06 (m, 18H, Ar-*H*), N.B. hydride resonances not observed; meaningful ^{13}C{^{1}H} and ^{27}Al NMR spectroscopic data could not be acquired due to the low solubility of the compound, and the fact that it slowly decomposes in C_6D_6 solutions at room temperature; IR (Nujol) ν (cm^{-1}): 1625 (w), 1547 (w), 1523 (w), 1264 (m), 1248 (m), 1184 (s), 1095 (w), 1018 (s), 932 (m), 884 (m), 839 (m), 819 (m), 763 (s); elemental analysis calculated for $C_{66}H_{88}N_7Mg_3Al$: C 73.44 %, H 8.22 % N 9.08 %; found C 74.22 %, H 8.18 %, N 8.94 %.

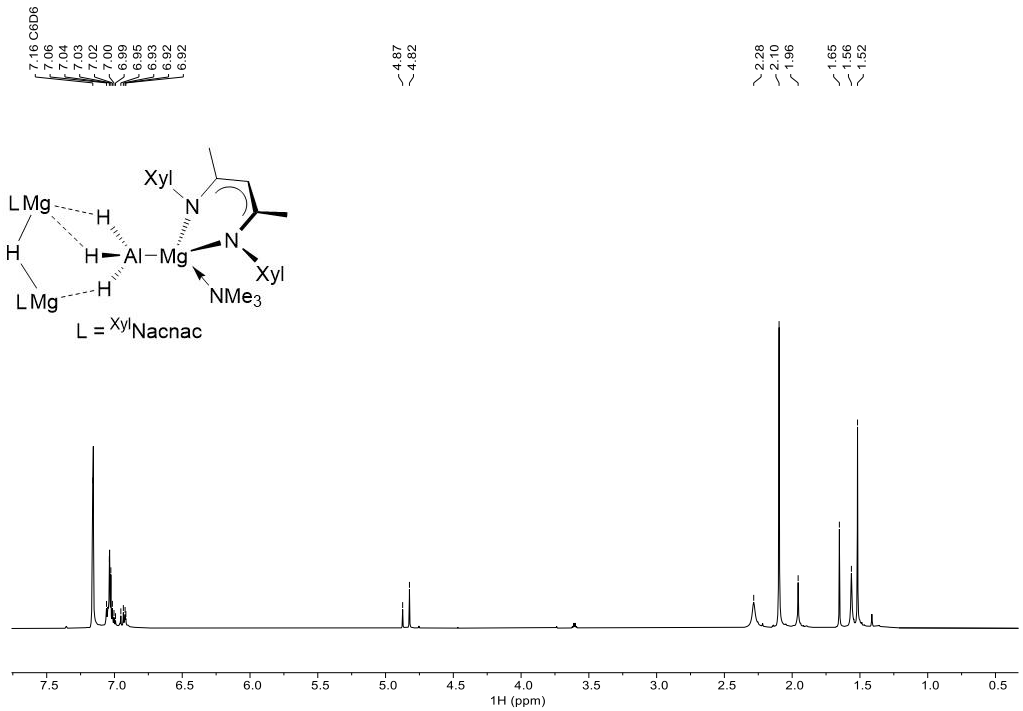

Figure S24. ^{1}H NMR spectrum (400 MHz, 298 K, C_6D_6) of **3b**.

[Al_6H_8(NMP)$_2${Mg(^{Mes}Nacnac)}$_4$] 1c.

[{($SiMe_3$)$_2$N}AlH_2(NMP)] (0.346 mmol, 0.12 M in benzene; prepared as a stock solution from reaction of [AlH_3(NMP)] and HN($SiMe_3$)$_2$, and used without purifying) and [{(^{Mes}Nacnac)Mg}$_2$] (248 mg, 0.346 mmol) were combined in a grease free Schlenk flask. Benzene (3 mL) was added to these solids and the resultant slurry was heated at 40 °C for 10 mins until a bright red solution was observed. Allowing the solution to stand at room temperature for five days resulted in the deposition of a few deep red crystals of **1c** (yield < 5%) suitable for single crystal X-ray diffraction analysis.

Solution state and solid state spectroscopic data could not be obtained for **1c** due to its low yield, its negligible solubility in common deuterated solvents, and the fact that it consistently crystallised with a small amount of an insoluble colorless by-product, which could not be separated.

[{(Me_3Si)$_2$N}Al(μ-H)$_3$[{Mg(^{Dip}Nacnac)}$_2$(μ-H)]] 2.

[{($SiMe_3$)$_2$N}AlH_2(NMe_3)] (150 mg, 0.605 mmol) and [{(^{Dip}Nacnac)Mg}$_2$] (533 mg, 0.605 mmol) were combined in a grease free Schlenk flask. Benzene (4 mL) was added to these solids and the resultant slurry was heated at 45 °C for 4 h until a yellowish green solution was observed. Allowing the solution to stand at room temperature overnight resulted in the deposition of colourless crystals of **2** (100 mg, 15 %).

Alternate method for the synthesis of [{(Me$_3$Si)$_2$N}Al(μ-H)$_3$[{Mg(^{Dip}Nacnac)}$_2$(μ-H)]] 2.

[{(SiMe$_3$)$_2$N}AlH$_2$(NMe$_3$)] (140 mg, 0.565 mmol) and [{^{Dip}NacnacMg(*μ*-H)}$_2$] (500 mg, 0.565 mmol) were combined in a Schlenk flask. Toluene (4 mL) was added to these solids and the resultant slurry was stirred overnight at room temperature. Volatiles were then removed *in vacuo*, and the residue extracted with hexane (5 mL). Storage of the extract at -30 °C overnight resulting in the formation of colourless crystals of **2** (400 mg, 61 %); M.p. 170-175 °C (decomp.). ^{1}H NMR (400 MHz, C$_6$D$_6$, 298 K) δ = -0.05 (s, 18H, Si*Me*$_3$), 0.44 (d, *J* = 6.8 Hz, 6H, CH(C*H*$_3$)$_2$), 1.14 (d, *J* = 6.8 Hz, 6H, CH(C*H*$_3$)$_2$), 1.17 (d, *J* = 6.8, 6H, CH(C*H*$_3$)$_2$), 1.20 (d, *J* = 6.8 Hz, 6H, CH(C*H*$_3$)$_2$), 1.31 (d, *J* = 7.4 Hz, 6H, CH(C*H*$_3$)$_2$), 1.34 (d, *J* = 7.3 Hz, 6H, CH(C*H*$_3$)$_2$), 1.37 (d, *J* = 6.3 Hz, 6H, CH(C*H*$_3$)$_2$), 1.46 (s, 6H, NCC*H*$_3$), 1.49 (s, 6H, NCC*H*$_3$), 1.52 (d, *J* = 6.8 Hz, 6H), 2.59 (br. s, 3H, Al-*H*), 2.81 (sept, *J* = 6.8 Hz, 2H, C*H*(CH$_3$)$_2$), 3.29–3.13 (sept, *J* = 6.9 Hz, 4H, C*H*(CH$_3$)$_2$), 3.51 (sept, *J* = 6.9 Hz, 2H, C*H*(CH$_3$)$_2$), 4.79 (s, 2H, β-C*H*), 7.01-7.20 (m, 12H, Ar-*H*), N.B. Mg-hydride resonance not observed; ^{13}C{^{1}H} NMR (101 MHz, C$_6$D$_6$, 298 K) δ = 5.2 (Si*Me*$_3$), 23.5, 23.8, 24.0, 24.4 (CH(*C*H$_3$)$_2$), 24.6, 24.7 (NC*C*H$_3$), 25.11, 25.16, 25.2, 26.9 (CH(*C*H$_3$)$_2$), 27.6, 28.5, 29.0, 29.1 (*C*H(CH$_3$)$_2$), 96.1 (β-C*H*), 123.9, 124.13, 124.16, 124.5, 125.9, 126.0, 141.6, 143.0, 143.3, 143.5, 145.8, 146.0 (Ar-*C*), 169.4, 170.0 (N*C*CH$_3$); ^{29}Si{^{1}H} NMR (80 MHz, C$_6$D$_6$, 298 K) δ = -0.30; ^{27}Al{^{1}H} NMR (104 MHz, C$_6$D$_6$, 298 K): no resonance signal was observed; IR (Nujol) ν (cm^{-1}): 1636 (w), 1519 (s), 1388 (s), 1311 (s), 1175 (m), 930 (m), 894 (s), 838 (m), 792 (w), 757 (w), 695 (w), 676 (w); elemental analysis calculated for C$_{64}$H$_{104}$AlMg$_2$N$_5$Si$_2$: C 71.49 %, H 9.75 % N 6.51%; found C 71.64 %, 9.57 %, 6.30 %.

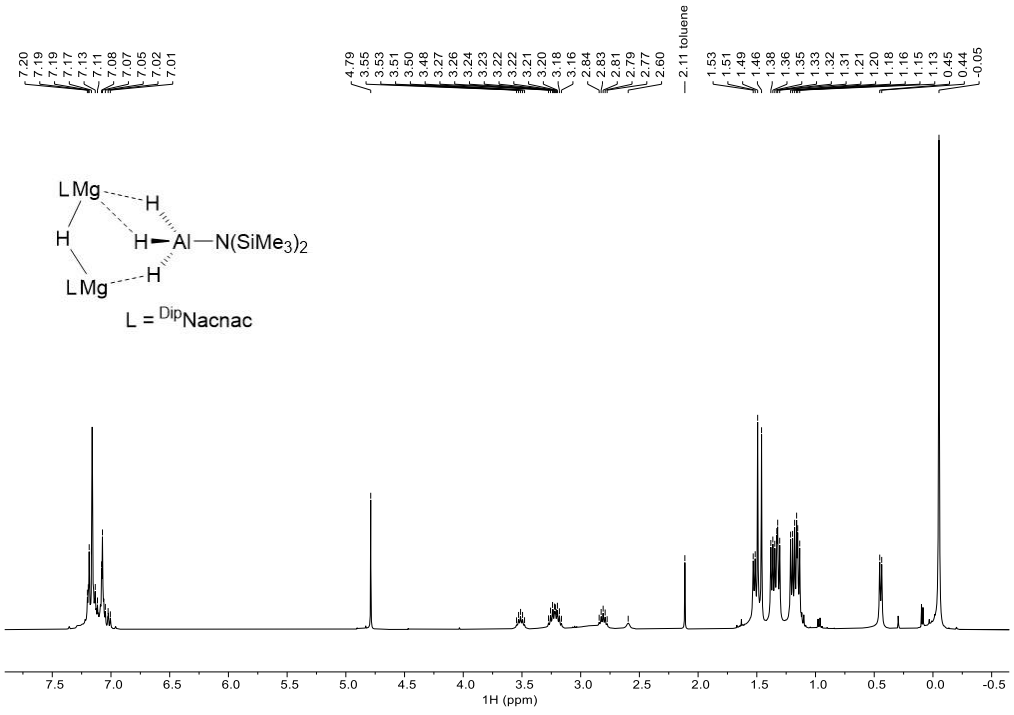

Figure S25. ^{1}H NMR spectrum (400 MHz, 298 K, C$_6$D$_6$) of **2**.

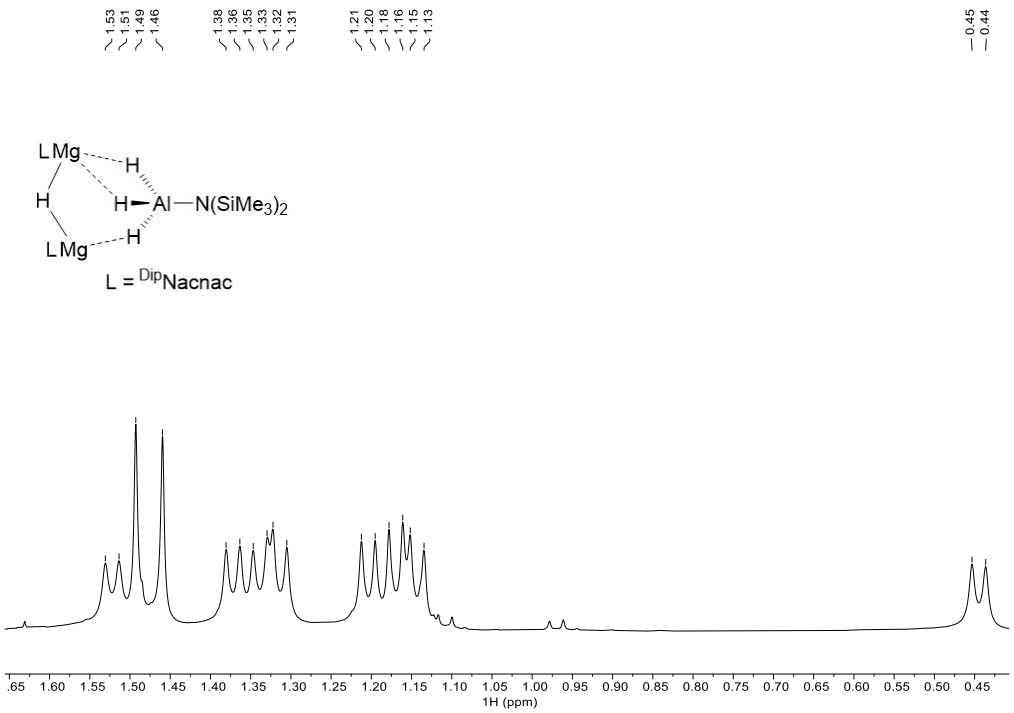

Figure S26. Expanded high field region of the ^{1}H NMR spectrum (400 MHz, 298 K, C_6D_6) of **2**.

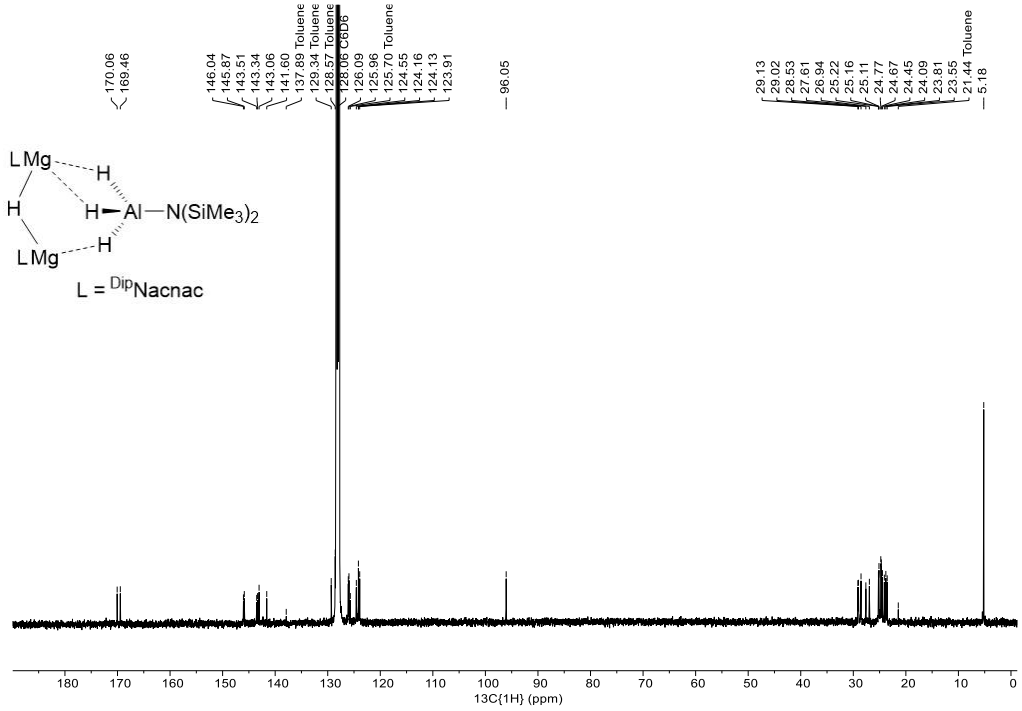

Figure S27. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of **2**.

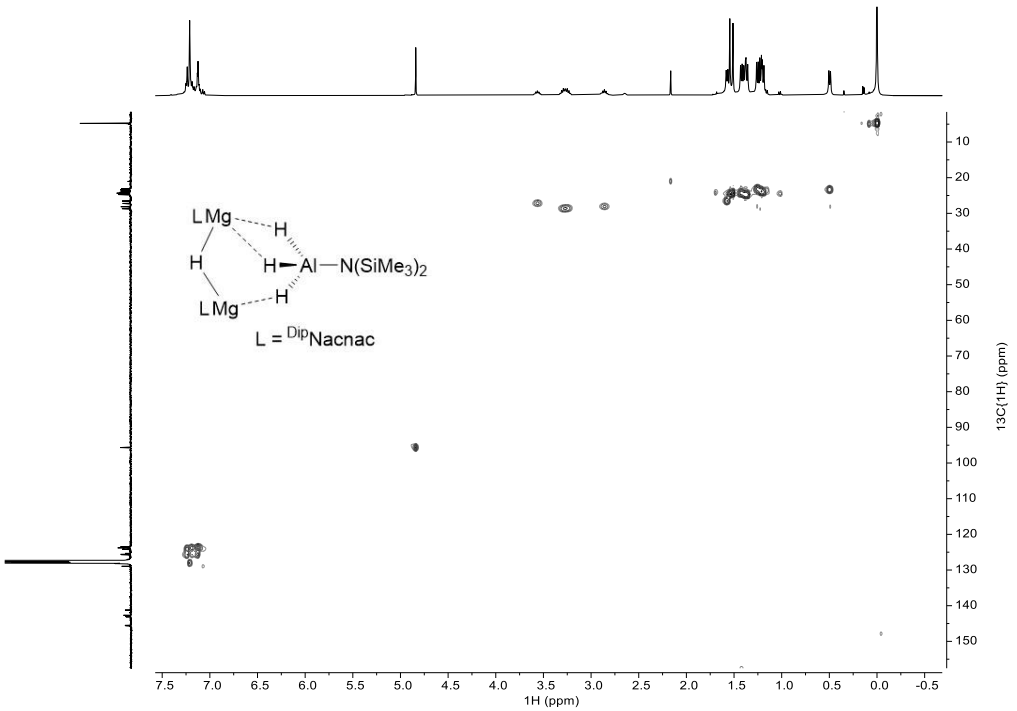

Figure S28. HMQC spectrum (^{1}H: 400 MHz; ^{13}C: 101 MHz, 298 K, C_6D_6) of **2**.

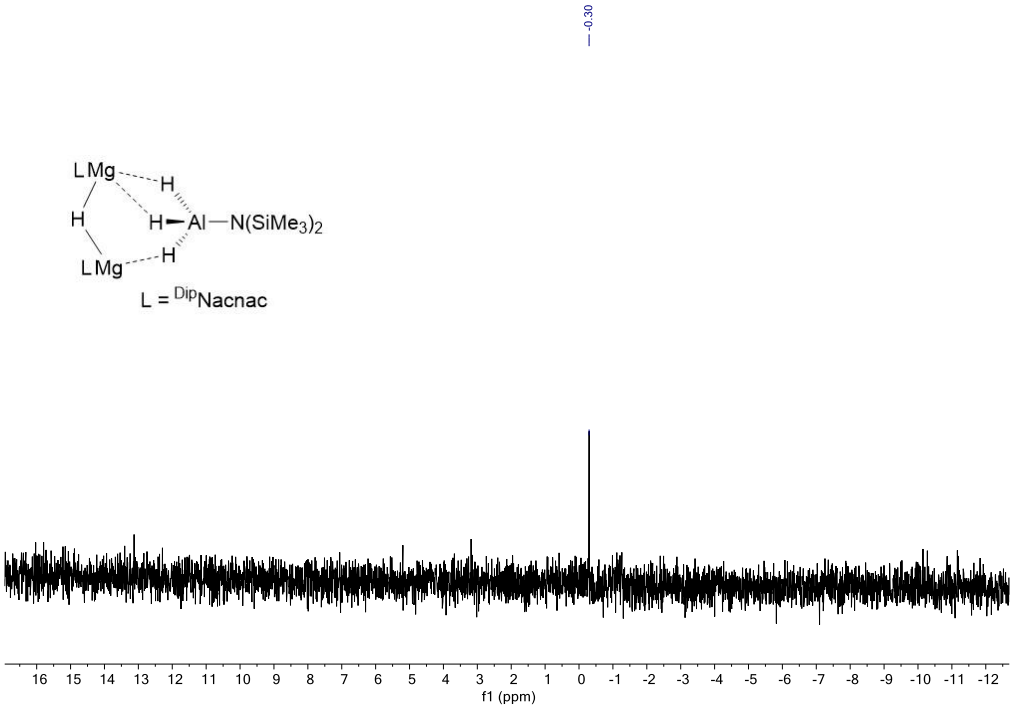

Figure S29. ^{29}Si{^{1}H} NMR spectrum (80 MHz, 298 K, C_6D_6) of **2**.

[(^{Mes}Nacnac)MgN(SiMe$_3$)$_2$].

[(^{Mes}Nanac)MgI(OEt$_2$)] (0.50 g, 0.89 mmol) and [KN(SiMe$_3$)$_2$] (0.18 g, 0.89 mmol) were added to a Schlenk flask. Toluene (8 mL) was added to these solids at room temperature. The resultant mixture was stirred at room temperature for 16 h. All volatiles were then removed *in vacuo*, the residue extracted into hexane (5 mL), filtered, and volatiles removed from the filtrate under reduced pressure

to yield the title compound as a colorless powder (0.39 g, 85 %). M.p. 110-115 °C; ^{1}H NMR (400 MHz, C_6D_6, 298 K) δ = 0.05 (s, 18H, Si*Me*$_3$), 1.60 (s, 6H, NCC*H*$_3$), 2.13 (s, 6H, *para*-CH_3), 2.23 (s, 12H, *ortho*-C*H*$_3$), 4.88 (s, 1H, β-C*H*), 6.82 (s, 4H, Ar*H*); ^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K) δ = 4.9 (Si*Me*$_3$), 19.1 (*ortho*- *C*H$_3$), 20.9 (*para*- *C*H$_3$), 23.4 (NC*C*H$_3$), 95.5 (β-C*H*), 129.7, 131.4, 134.1, 144.1 (Ar-*C*), 170.1 (N*C*CH$_3$); ^{29}Si{^{1}H} NMR (80 MHz, C_6D_6, 298 K) δ = -8.5; IR (Nujol) ν (cm^{-1}): 1610 (w), 1524 (s), 1096 (w), 1001 (s), 957 (w), 928 (w), 886 (m), 858 (m), 841 (w), 815 (s), 752 (s); elemental analysis calculated for $C_{29}H_{47}MgN_3Si_2$: C 67.22 %, H 9.14 % N 8.11 %; found C 67.96 %, 8.94 %, 8.24 %.

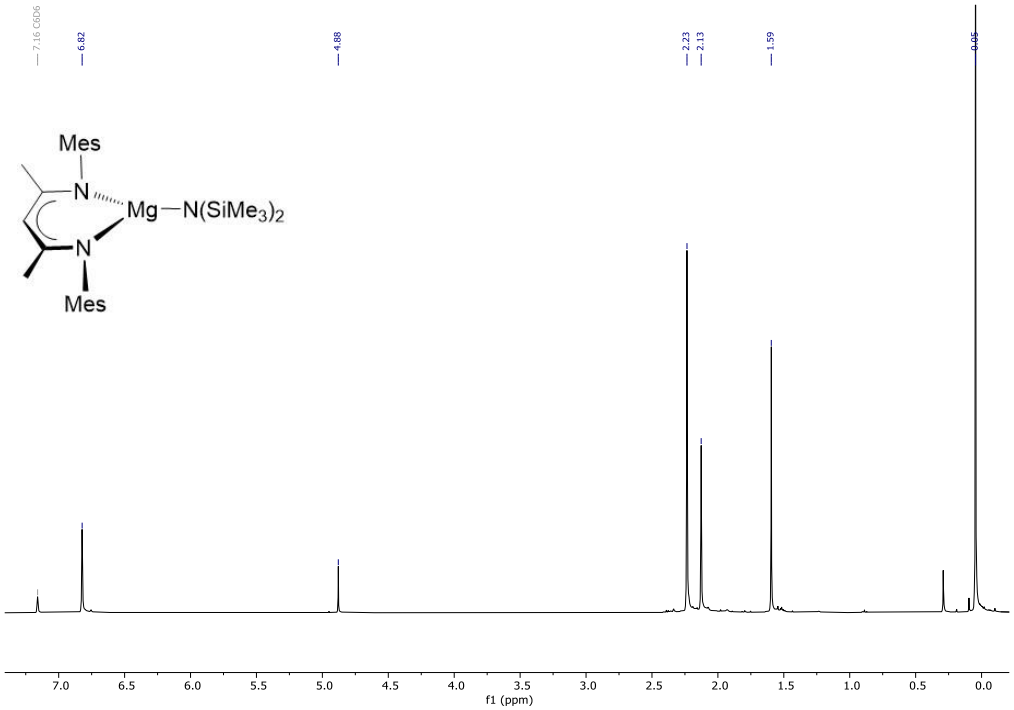

Figure S30. ^{1}H NMR spectrum (400 MHz, 298 K, C_6D_6) of [(^{Mes}Nacnac)MgN(SiMe$_3$)$_2$].

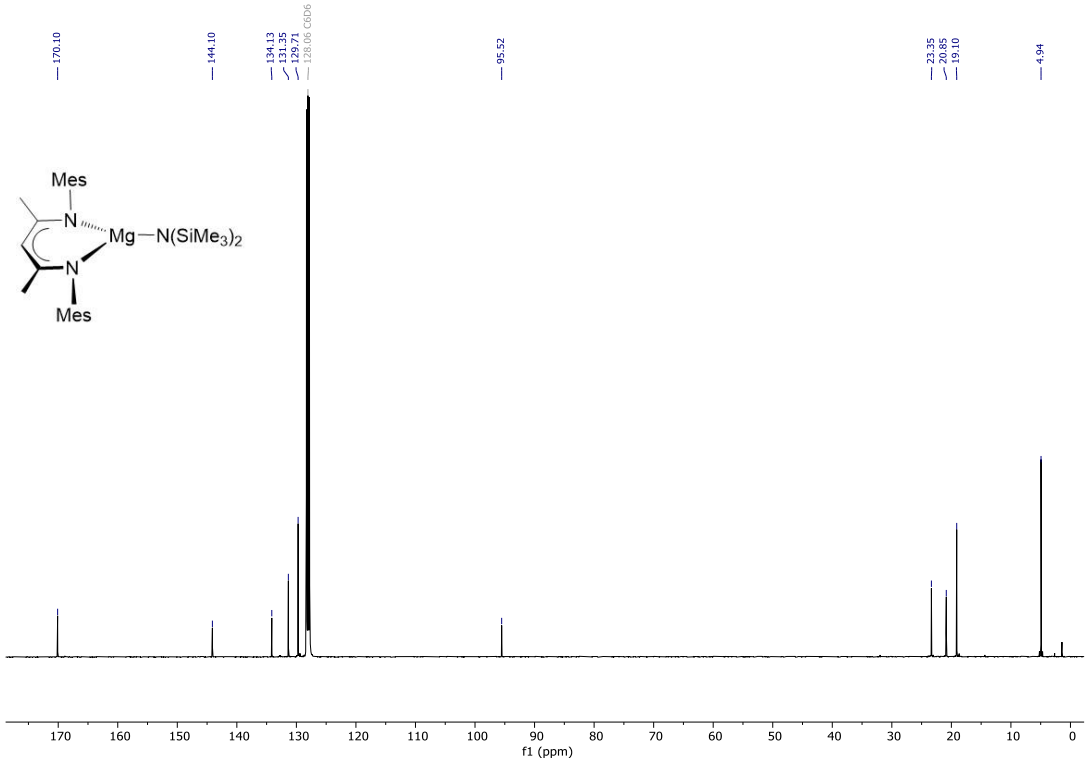

Figure S31. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of [(^{Mes}Nacnac)MgN(SiMe$_3$)$_2$].

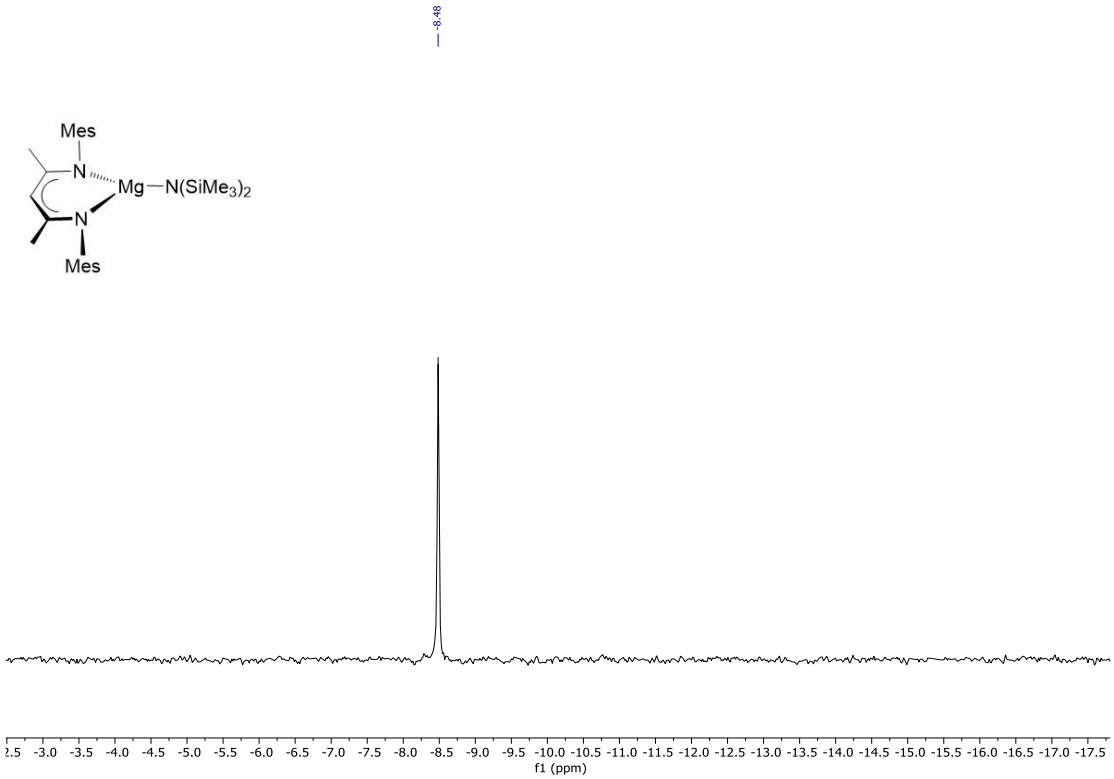

Figure S32. $^{29}Si\{^{1}H\}$ NMR spectrum (80 MHz, 298 K, C_6D_6) of [(^{Mes}Nacnac)MgN(SiMe$_3$)$_2$].

[(^{Xyl}Nacnac)MgN(SiMe$_3$)$_2$].

[(^{Xyl}Nacnac)MgN(SiMe$_3$)$_2$] was synthesised following the synthetic route as described for [(^{Mes}Nacnac)MgN(SiMe$_3$)$_2$] but using [(^{Xyl}Nanac)MgI(OEt$_2$)] (0.50 g, 0.94 mmol) and [KN(SiMe$_3$)$_2$] (0.18 g, 0.94 mmol) (0.37 g , 81%). M.p. 110-112 °C; ^{1}H NMR (400 MHz, C$_6$D$_6$, 298 K) δ 0.02 (s, 18H, Si*Me*$_3$), 1.55 (s, 6H, NCC*H*$_3$), 2.21 (s, 12H, *ortho*-C*H*$_3$), 4.84 (s, 1H, β-C*H*), 6.88–7.04 (m, 6H, Ar-*H*); ^{13}C NMR (101 MHz, C$_6$D$_6$, 298 K) δ 4.94 (Si*Me*$_3$), 19.1 (NC*C*H$_3$), 23.4 (*ortho*-*C*H$_3$), 95.5 (β-C*H*), 125.2, 128.6, 131.7, 146.6 (Ar-*C*), 169.9 (N*C*CH$_3$); ^{29}Si NMR (80 MHz, C$_6$D$_6$, 298K) δ -8.4; IR (Nujol) ν (cm^{-1}): 1515 (s), 1446 (m), 1018 (s), 932 (w), 883 (m), 841 (m), 825 (m), 813 (m), 765 (s), 704 (w); elemental analysis calculated for C$_{27}$H$_{43}$MgN$_3$Si$_2$: C 66.16 %, H 8.84 % N 8.57 %; found C 67.1 %, 8.98 %, 8.64 %.

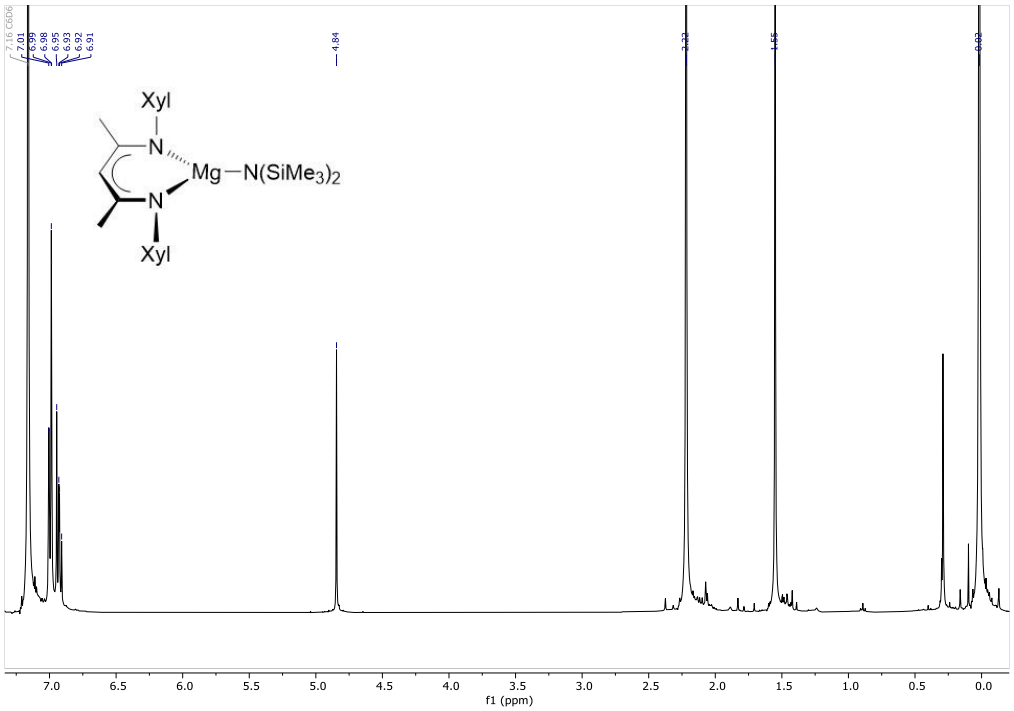

Figure S33. ^{1}H NMR spectrum (400 MHz, 298 K, C$_6$D$_6$) of [(^{Xyl}Nacnac)MgN(SiMe$_3$)$_2$].

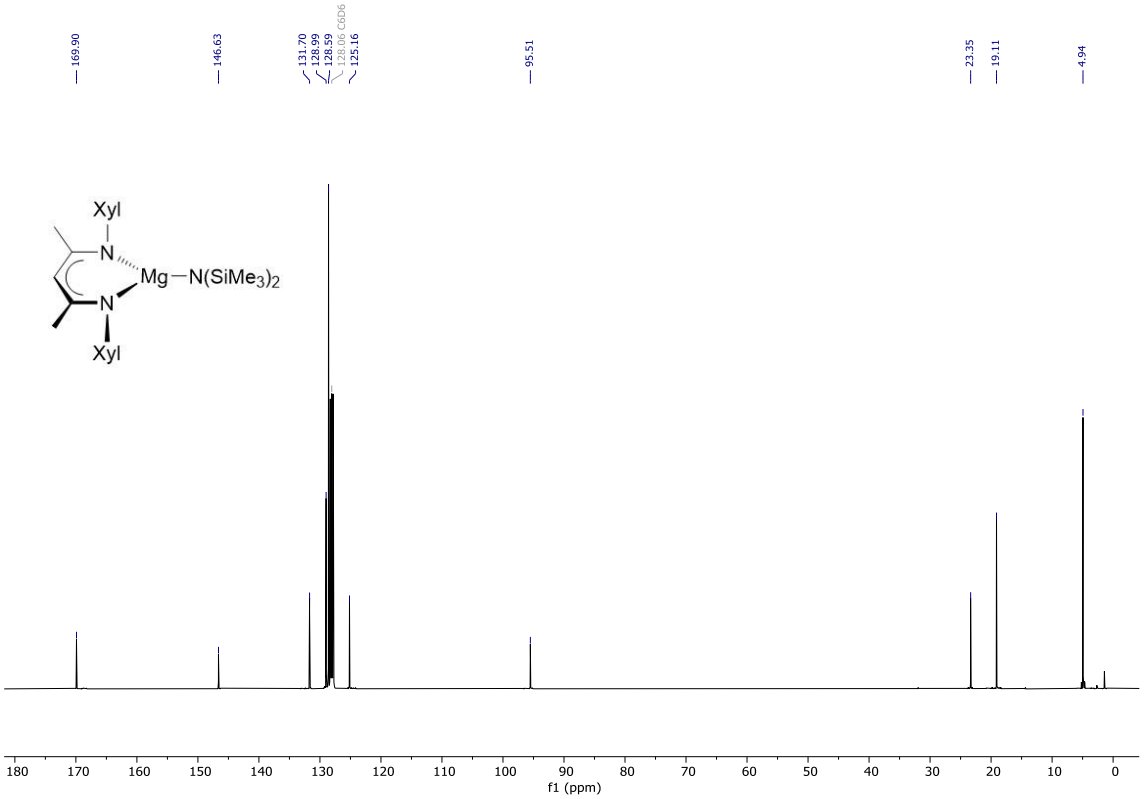

Figure S34. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of [(^{Xyl}Nacnac)MgN(SiMe$_3$)$_2$].

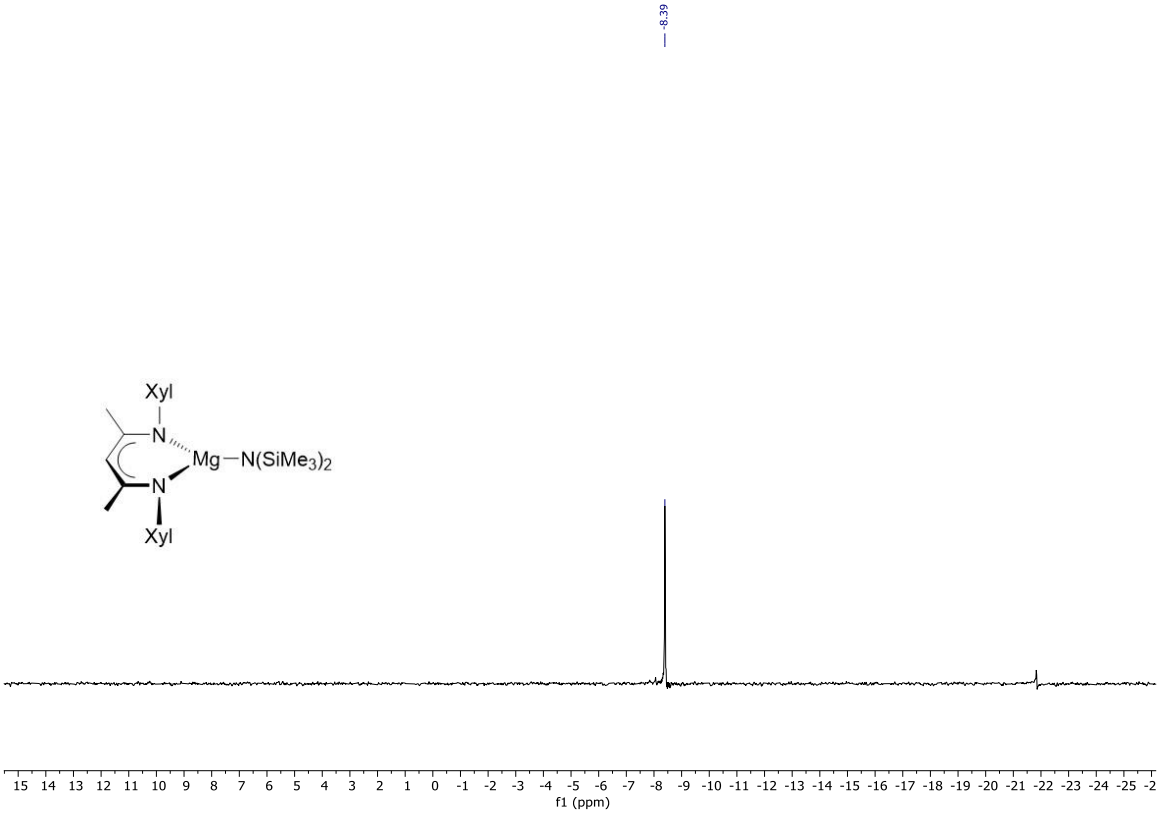

Figure S35. $^{29}Si\{^{1}H\}$ NMR spectrum (80 MHz, 298 K, C_6D_6) of [(^{Xyl}Nacnac)MgN(SiMe$_3$)$_2$].

2. Crystallographic Studies

X-ray Crystallography

Crystals suitable for X-ray structural determination were mounted in silicone oil. Crystallographic measurements were made using a Rigaku Xtalab Synergy Dualflex using a graphite monochromator with Mo Kα (0.71073 Å) or Cu Kα radiation (1.54180 Å), or the MX1 beamline of the Australian Synchrotron (λ = 0.71090 Å). The software package Blu-Ice[9] was used for synchrotron data acquisition, while the program XDS[10] was employed for synchrotron data reduction.. All structures were solved by direct methods and refined on F^2 by full matrix least squares (SHELX-16[11]) using all unique data. Hydrogen atoms are typically included in calculated positions (riding model). Crystal data, details of data collections and refinements can be found in their CIF files and are summarized in Table S1.

Table S1. Summary of Crystallographic Data for Compounds **1-3**, $[AlH_2(NMe_3)\{O(C_6H_3Bu^t_2\text{-}2,6)\}]$ **S1**, and $[AlH_2(TMC)\{N(SiMe_3)_2\}]$ **S2**.

	1a·(benzene)	**1b**	**1c**·(benzene)$_2$	**2**·(benzene)$_{0.5}$
empirical formula	$C_{104}H_{148}Al_6Mg_4N_{10}$	$C_{90}H_{126}Al_6Mg_4N_{10}$	$C_{116}H_{162}Al_6Mg_4N_{10}$	$C_{70}H_{110}AlMg_2N_5Si_2$
formula weight	1797.44	1607.12	1955.67	1153.40
crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	$P2_1/n$	$P2_1/c$	$P2_1/n$	$C2$
a (Å)	15.25460(10)	14.0194(3)	17.45180(10)	22.5941(2)
b (Å)	16.21290(10)	22.6927(5)	17.16630(10)	14.12550(10)
c (Å)	21.86480(10)	15.2771(3)	19.14810(10)	23.6499(3)
α (deg.)	90	90	90	90
β (deg)	101.1120(10)	105.503(2)	96.2910(10)	109.4820(10)
γ (deg.)	90	90	90	90
vol (Å^3)	5306.25(6)	4683.39(18)	5701.90(6)	7115.79(13)
Z	2	2	2	4
T (K)	120(2)	123(2)	123(2)	123(2)
ρ (calcd) (g.cm^{-3})	1.125	1.140	1.139	1.077
μ (mm^{-1})	1.166	1.267	1.123	1.046
F(000)	1936	1724	2108	2520
reflections collected	104657	46309	55919	48575
unique reflections	9653	8514	10362	12311
R_{int}	0.0276	0.0705	0.0342	0.0231
R1 indices [$I>2\sigma(I)$][a]	0.0577	0.1001	0.0380	0.0414
wR2 indices (all data)[b]	0.1501	0.2942	0.0998	0.1094
Largest peak and hole (e.A^{-3})	0.494, -0.808	1.738, -0.685	0.340, -0.451	1.716, -0.508
CCDC No.	2257647	2257642	2257645	2257643

Table S1 (contd.). Summary of Crystallographic Data for Compounds **1-3**, $[AlH_2(NMe_3)\{O(C_6H_3Bu^t_2\text{-}2,6)\}]$ **S1**, and $[AlH_2(TMC)\{N(SiMe_3)_2\}]$ **S2**.

	3a	**3b**·(benzene)	**S1**	**S2**
empirical formula	$C_{72}H_{100}AlMg_3N_7$	$C_{72}H_{94}AlMg_3N_7$	$C_{17}H_{32}AlNO$	$C_{13}H_{32}AlN_3Si_2$
formula weight	1163.49	1157.45	293.41	313.57
crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/c$
a (Å)	11.310(2)	13.4809(2)	6.800(14)	7.67040(10)
b (Å)	23.980(5)	39.0954(3)	14.750(3)	9.04860(10)
c (Å)	26.050(5)	14.0183(2)	18.090(4)	29.2255(3)
α (deg.)	90	90	90	90
β (deg)	90.53(3)	112.7290(10)	91.42(3)	94.0290(10)
γ (deg.)	90	90	90	90
vol ($Å^3$)	7065(2)	6814.47(16)	1813.9(6)	2023.42(4)
Z	4	4	4	4
T (K)	173(2)	123(2)	123(2)	123(2)
ρ (calcd) ($g.cm^{-3}$)	1.094	1.128	1.074	1.029
μ (mm^{-1})	0.099	0.868	0.110	1.951
F(000)	2520	2496	648	688
reflections collected	168609	66776	31012	19953
unique reflections	13039	12405	3302	3692
R_{int}	0.0686	0.0459	0.0300	0.0565
R1 indices $[I>2\sigma(I)]$[a]	0.0754	0.0381	0.0333	0.0458
*w*R2 indices (all data)[b]	0.2326	0.0979	0.0875	0.1309
Largest peak and hole ($e.A^{-3}$)	0.338, -0.237	0.312, -0.253	0.169, -0.276	0.608, -0.344
CCDC No.	2257648	2257646	2257644	2257641

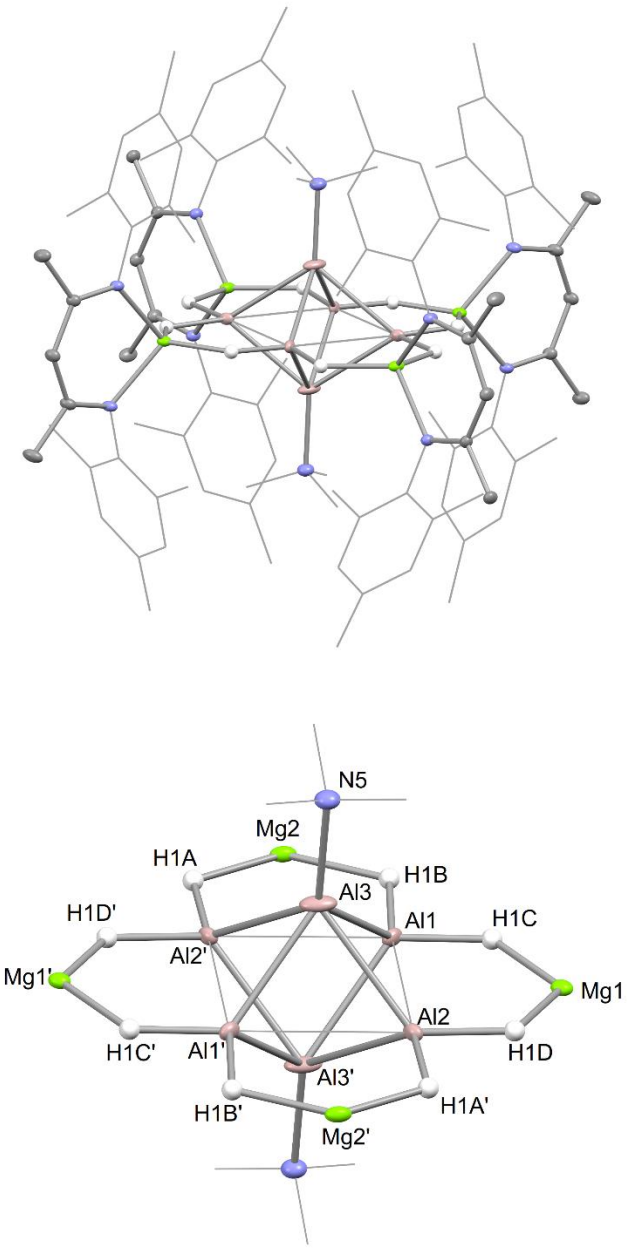

Figure S36. Molecular structure of **1a** (top, 20% displacement ellipsoids are shown; hydrogen atoms, except hydrides omitted; mesityl and NMe_3 groups shown as wireframe for clarity). Structure of the core of **1a**, with ^{Mes}Nacnac ligands deleted (bottom). Apparent positional disorder within the Al_6 core of the molecule could not be modelled. Accordingly, the freely refined hydride positions cannot be considered as accurate. Selected bond lengths (Å) and angles (°): Al(1)-Al(3)' 2.5741(13), Al(1)-Al(3) 2.5748(13), Al(1)-Mg(2) 2.8610(10), Al(1)-Al(2) 2.8904(10), Al(1)-Mg(1) 2.9732(10), Al(1)-Al(2)' 2.9834(10), Al(3)···Al(3)' 3.042(1), Al(1)'-Al(3)-Al(1) 107.56(3), Al(2)-Al(3)-Al(2)' 107.56(3), Al(3)'-Al(1)-Al(3) 72.43(3), Al(3)-Al(2)-Al(3)' 72.44(3).

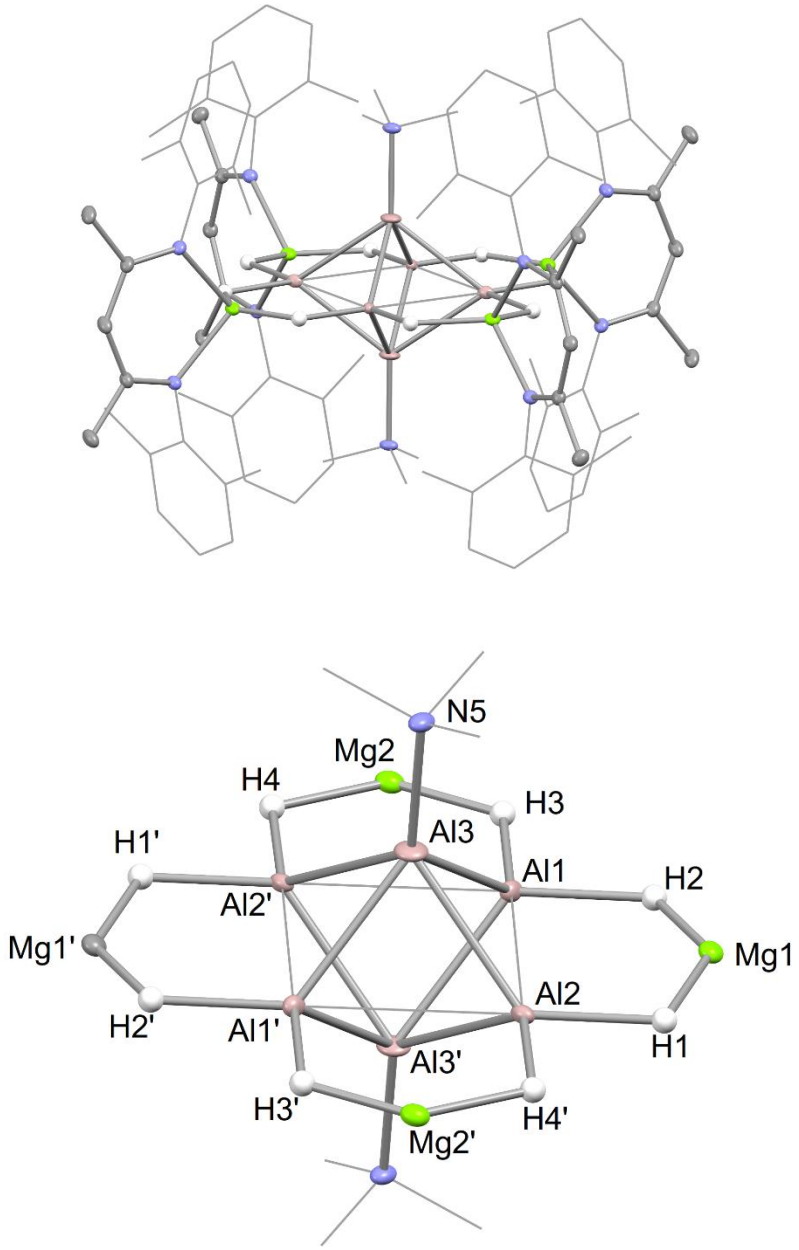

Figure S37. Molecular structure of **1b** (top, 20% displacement ellipsoids are shown; hydrogen atoms, except hydrides omitted; xylyl and NMe_3 groups shown as wireframe for clarity). Structure of the core of **1b**, with ^{Xyl}Nacnac ligands deleted (bottom). Apparent positional disorder within the Al_6 core of the molecule could not be modelled. Accordingly, the freely refined hydride positions cannot be considered as accurate. Selected bond lengths (Å) and angles (°): Al(1)-Al(3) 2.590(2), Al(1)-Al(3)' 2.595(2), Al(1)-Al(2) 2.9695(18), Al(2)-Al(3) 2.598(2), Al(2)-Al(3)' 2.600(2), Al(3)···Al(3)' 3.022(2), Al(2)-Al(3)-Al(2)' 108.91(6), Al(1)-Al(3)-Al(1)' 108.69(6), Al(3)-Al(1)-Al(3)' 71.31(6), Al(3)-Al(2)-Al(3)' 71.09(6).

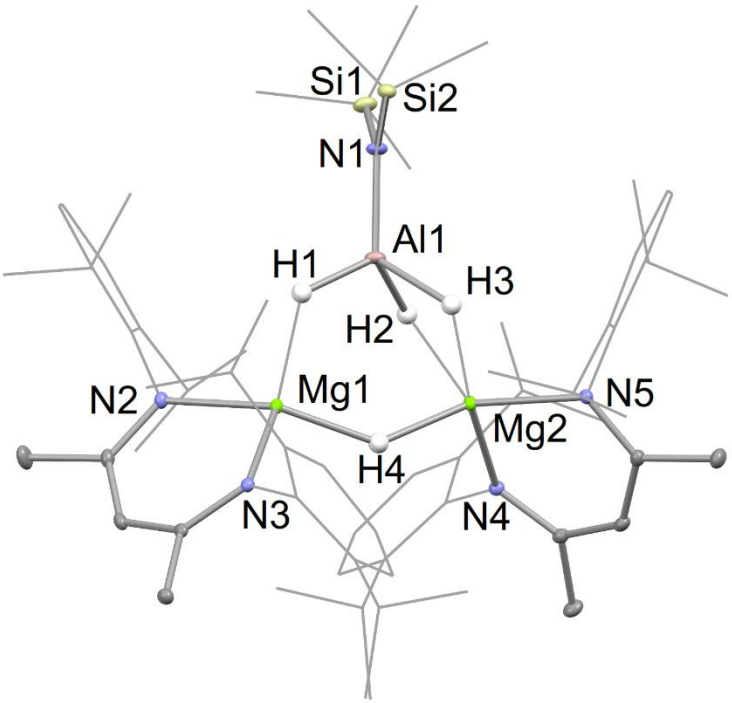

Figure S38. Molecular structure of **2** (20% displacement ellipsoids are shown; hydrogen atoms, except hydrides, omitted; Dip and $SiMe_3$ groups shown as wireframe for clarity). Selected bond lengths (Å) and angles (°):Al(1)-N(1) 1.811(3), Al(1)-H(2) 1.70(8), Al(1)-H(3) 1.67(5), Al(1)-H(1) 1.51(7), Mg(1)-H(4) 1.87(4), Mg(1)-H(1) 1.94(6), Mg(2)-H(2) 2.07(7), Mg(2)-H(4) 1.79(4), Mg(2)-H(3) 2.02(6), N(1)-Al(1)-H(2) 119(2), N(1)-Al(1)-H(3) 118.7(19), N(1)-Al(1)-H(1) 116(2).

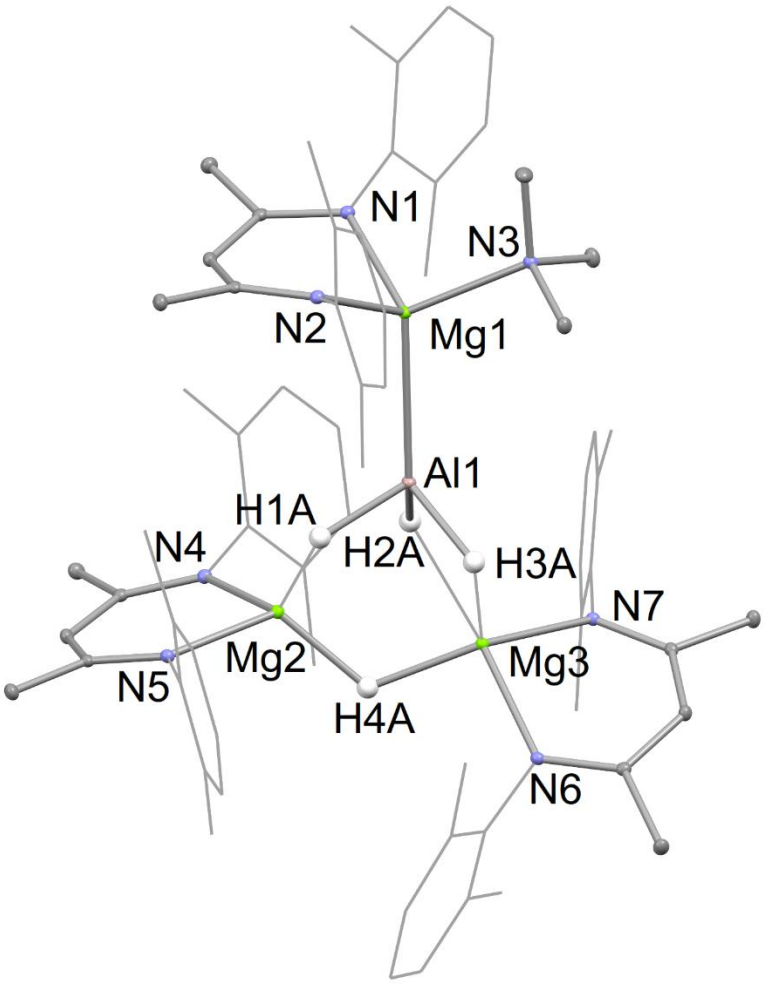

Figure S39. Molecular structure of **3b** (20% displacement ellipsoids are shown; hydrogen atoms, except hydrides, omitted; xylyl groups shown as wireframe for clarity). Selected bond lengths (Å) and angles (°): Al(1)-Mg(1) 2.7726(6), Al(1)-H(1A) 1.63(2), Al(1)-H(2A) 1.63(2), Al(1)-H(3A) 1.633(18), Mg(2)-H(1A) 1.92(2), Mg(2)-H(4A) 1.819(17), Mg(3)-H(2A) 2.22(2), Mg(3)-H(3A) 1.979(18), Mg(3)-H(4A) 1.891(17), Mg(1)-Al(1)-H(1A) 113.2(7), Mg(1)-Al(1)-H(2A) 132.2(7), Mg(1)-Al(1)-H(3A) 128.0(6).

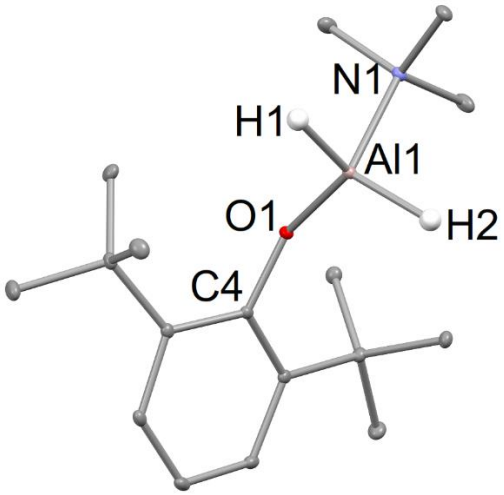

Figure S40. Molecular structure of [$AlH_2(NMe_3)\{O(C_6H_3Bu^t_2\text{-}2,6)\}$] **S1** (20% displacement ellipsoids are shown; hydrogen atoms, except hydrides, omitted). Selected bond lengths (Å) and angles (°): Al(1)-O(1) 1.7467(8), Al(1)-N(1) 1.9919(10), Al(1)-H(1) 1.506(14), Al(1)-H(2) 1.507(16), O(1)-Al(1)-N(1) 104.76(4), H(1)-Al(1)-H(2) 117.9(8).

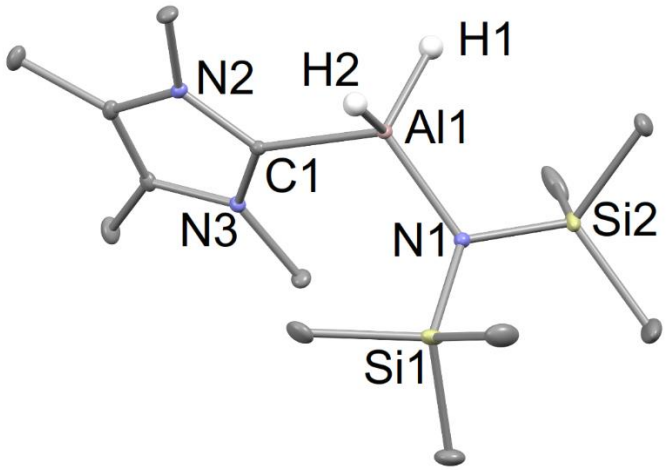

Figure S41. Molecular structure of [$AlH_2(TMC)\{N(SiMe_3)_2\}$] **S2** (20% displacement ellipsoids are shown; hydrogen atoms, except hydrides, omitted). Selected bond lengths (Å) and angles (°): Al(1)-N(1) 1.8531(14), Al(1)-C(1) 2.0545(17), Al(1)-H(1) 1.53(2), Al(1)-H(2) 1.55(2), N(1)-Al(1)-C(1) 111.88(6), H(1)-Al(1)-H(2) 112.7(11).

Neutron Single Crystal Diffraction Studies

Candidate crystals of compound **1a** were provided in various types of containers (sealed ampoules, Schlenk tubes etc), and media (e.g. reaction mother liquor, mineral oil) for examination by single-crystal neutron diffraction on the KOALA[12] instrument at ANSTO. Data amenable only to a limited difference analysis were found to be obtainable from two differently presented specimens. Details of the data collection, reduction and difference mapping can be found in Table S2. These data could not be optimally accessed by default or routine non-default methods and the two sets of images were subjected to careful examination, and individual parameterization of the data extraction for each image was chosen by the analyst prior to normalisation and merging.[13,14]

A low-resolution, limited completeness data set was derived for each set of images (a third possible data set which merged the two was also derived, but proved not to be suitable for use in analysis, perhaps due to some structural differences corresponding to the variable treatment post crystallisation).

The X-ray diffraction derived model presented in this paper was adjusted to provide a suitable starting point for a difference mapping exercise[15] against the neutron data in the following ways: all non-hydrogen atoms were set isotropic and refined against the X-ray data with hydrogen atoms riding on the atom of attachment. The hydrogen atoms of the ligands were then removed and replaced in geometrically calculated positions 1.08Å from the atoms of attachment. The NMe_3 disorder model of the X-ray study was retained.

For both data sets, this modified model was used as the starting point for assessment of the neutron data sets. In both cases, refinement of a scale factor resulted in an acceptable fit to the data, but only for the sample coated in mineral oil was subsequent refinement of the isotropic displacement parameters of all atoms possible. Cycles of refinement followed by difference mapping consistently yielded maps where the maximum negative peaks were well below the magnitude of a hydrogen atom and typically were found to lie in the vicinity of methyl groups, consistent with low occupancy of an alternative orientation for the hydrogens of the methyl group. This is consistent with the model accounting for all of the hydrogen atoms present in the structure based on the low-resolution neutron diffraction data available to us. It is important to note though that the contribution of hydrogen atoms to diffraction data lies predominantly in the low-resolution region, where occupancy dominates contribution to the scattering.

It was not possible to refine the positional parameters of the hydrides associated with the Al_6 core for either data set, and the displacement parameters of these atoms for the sample coated in mineral oil may reflect to some extent unresolved disorder which is evident in the X-ray studies of this and related structures. The much lower data recovery for the oil free crystal ("dry") was in all respects consistent with the X-ray derived model presented, but not suitable for a more detailed

analysis. This represents a pushing of the limits of this approach to modelling neutron diffraction data and without the data for the mineral oil coated sample, would on its own be significantly weaker evidence.

Table S2. Summary of neutron crystallographic data, and structure refinement details for two samples of compound **1a**, one sealed in an ampoule in the absence of mineral oil (dry), and one coated in mineral oil before being sealed in an ampoule (oil).

	Compound **1a** (dry)	Compound **1a** (oil)
Images	7	16
Time per image (s)	10000	8000
Integrated intensities		
R_{int} 4σ (number)	0.11(8)	0.17(12)
R_{int} all data	1.0(1.0)	1.0(1.0)
Refinement on *F*		
R	0.13	0.15
R_w	0.16	0.19
S	1.47	1.12
Data $I \geq 3\sigma I$	126	310
Data all	1267	1244
h min/max	0 10	0 10
k min/max	0 11	0 11
l min/max	-15 15	-15 15
Θ min/max (vs λ=0.85 Å)	3 18	3 18
Max shift/esd	1.6	0.0001
Residual density		
min	-0.38	-0.99
max	0.42	0.77
rms	0.09	0.17

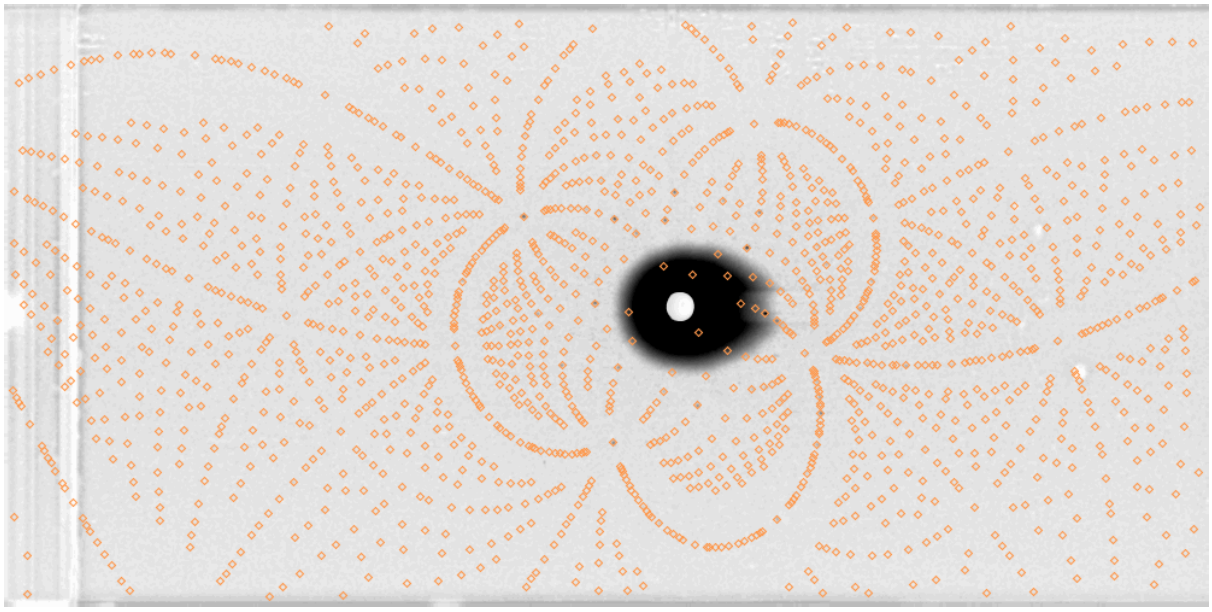

Figure S42. A 9000s Laue neutron single-crystal diffraction image captured from a crystal of compound **1a** (oil). The image is indexed to the known X-ray derived unit cell and the orange circles lie at all points on the image where a diffraction point corresponding to the known unit cell could occur with the calculated points corresponding to a d-spacing of 1.4 Å.

3. Computational Studies

All DFT calculations were performed with Gaussian 09.[16] Calculations were carried out at the DFT level of theory using the functionals B3PW91,[17] PBE0,[18]]BP86[19] and M06-L.[20] Dispersion corrections were treated with the D3 version of Grimme's dispersion with Becke-Johnson damping[21] for the B3PW91 functional or by using the wB97XD functional developed by Head-Gordon and co-workers including also empirical dispersion.[22] Geometry optimizations were typically achieved without any symmetry restriction. The geometry optimization of the **1c** was carried out in two steps. In a first step, the Al6 core was kept frozen and all the environment was optimized. Then in a second step, the optimized structure obtained in the first step was relaxed by allowing the Al6 core to optimize. Calculations of vibrational frequencies were systematically done to characterize the nature of stationary points. Hydrogen, nitrogen and carbon atoms were treated with 6-31G(d,p) double-ζ basis sets.[23] Aluminum and magnesium atoms were treated with 6-311++G(d,p) triple-ζ basis sets.[24] The electron density and partial charge distribution were examined in terms of localized electron-pair bonding units using the NBO program.[25]

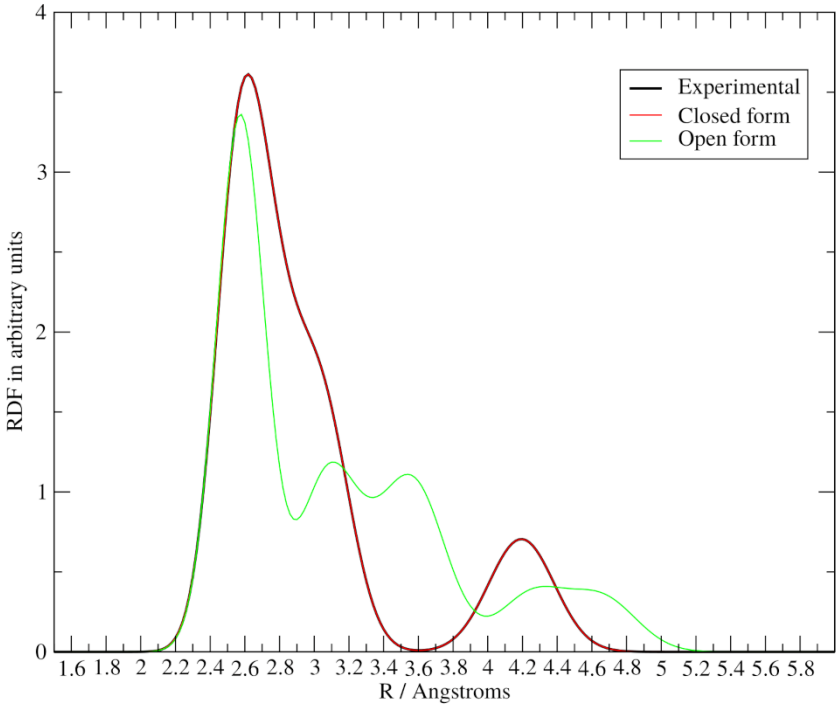

Figure S43. Radial distribution function plots of the experimental, and optimized (B3PW91-D3) distorted octahedral (closed) and open structures of **1c**.

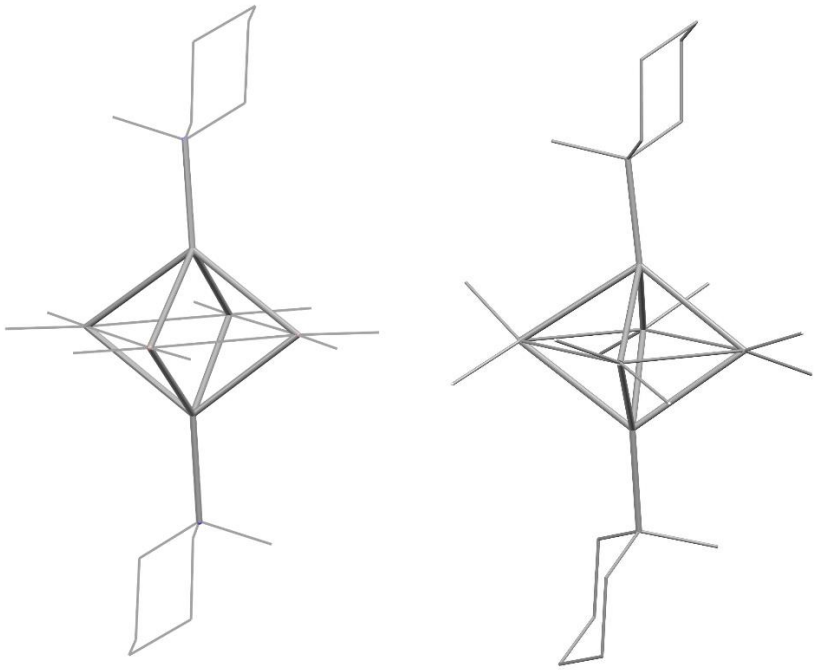

Figure S44. Comparison of the $Al_6H_8(NMP)_2$ cores of **1c**; crystal structure (left) and geometry optimised (B3PW91-D3) right. The geometries of the Al_6 cores are essentially identical. N.B. disorder of the hydride ligands over two sites in the crystal structure of **1c** has not been modelled, which gives rise to the observed differences in hydride positions. Selected distances (Å): experimental: Al-N_{NMP}: 2.022(3); $Al_{eq.}$-Al_{ax} range: 2.518(3)-2.717(3); $Al_{eq.}$-Al_{eq} range: 2.842(9)-3.100(3). Cald: Al-N_{NMP}: 1.994 and 1.993; $Al_{eq.}$-Al_{ax} range: 2.518-2.717; $Al_{eq.}$-Al_{eq} range: 2.841-3.100.

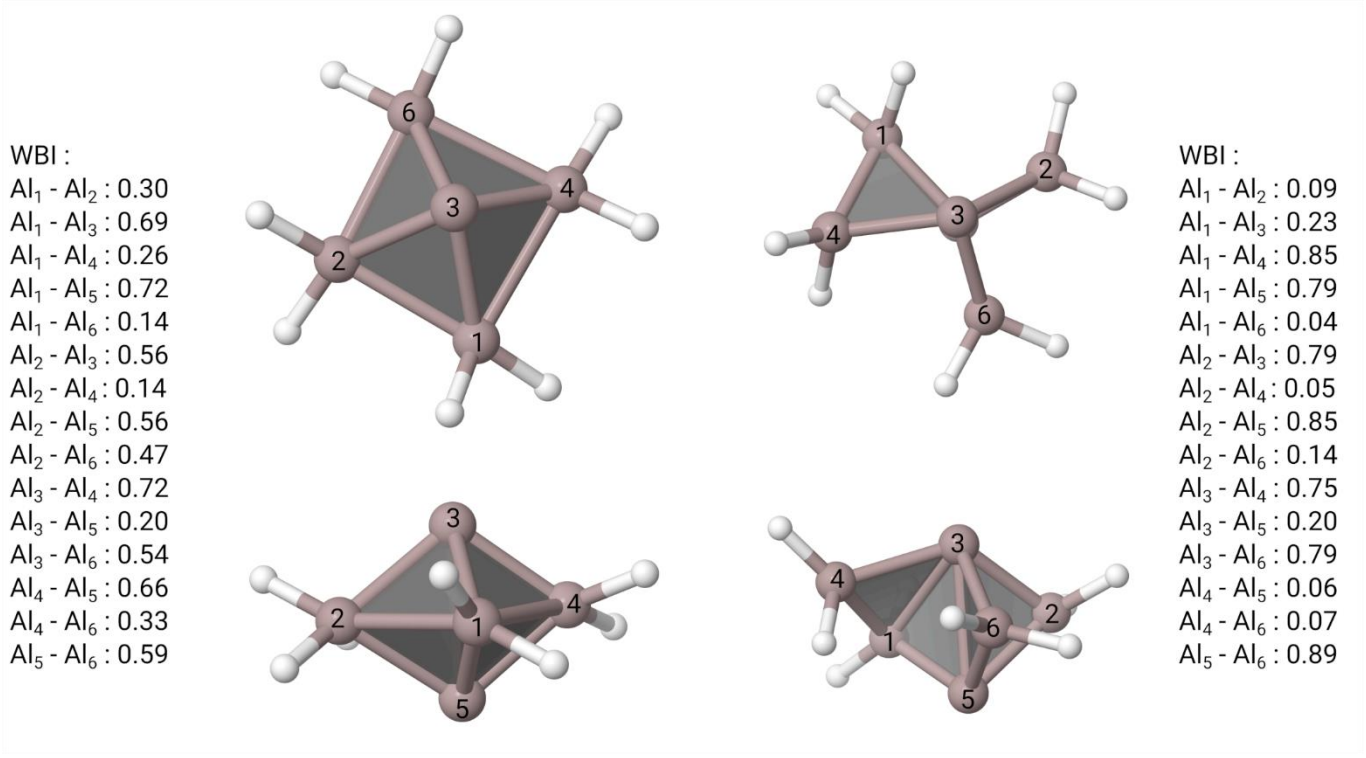

Figure S45. WIberg Bond Indexes obtained for the two optimized structures of **1c** (only the Al_6H_8 core of the molecules are shown).

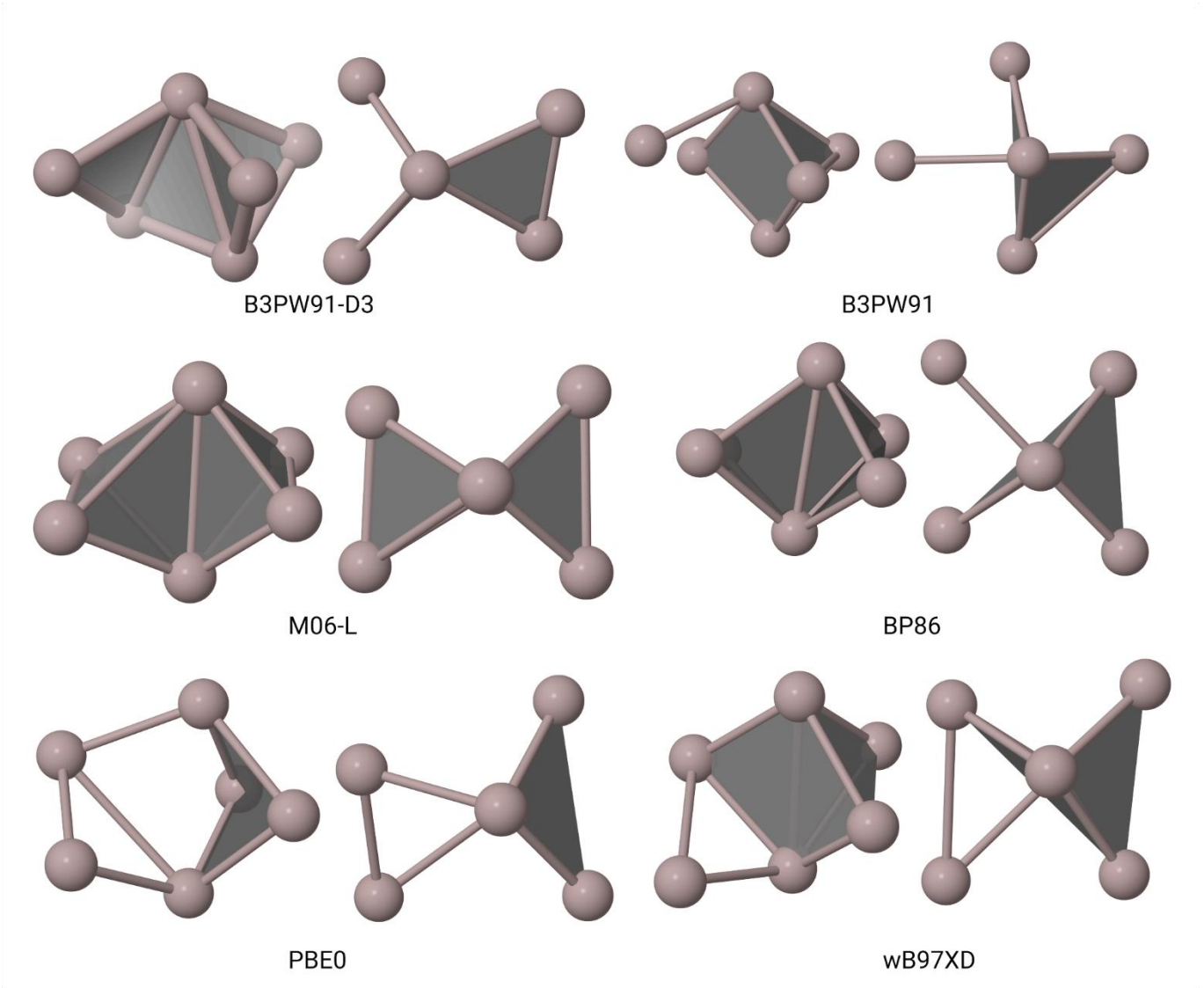

Figure S46. Optimized open structures of **1c** obtained with different functionals. Only the Al_6 cores have been depicted

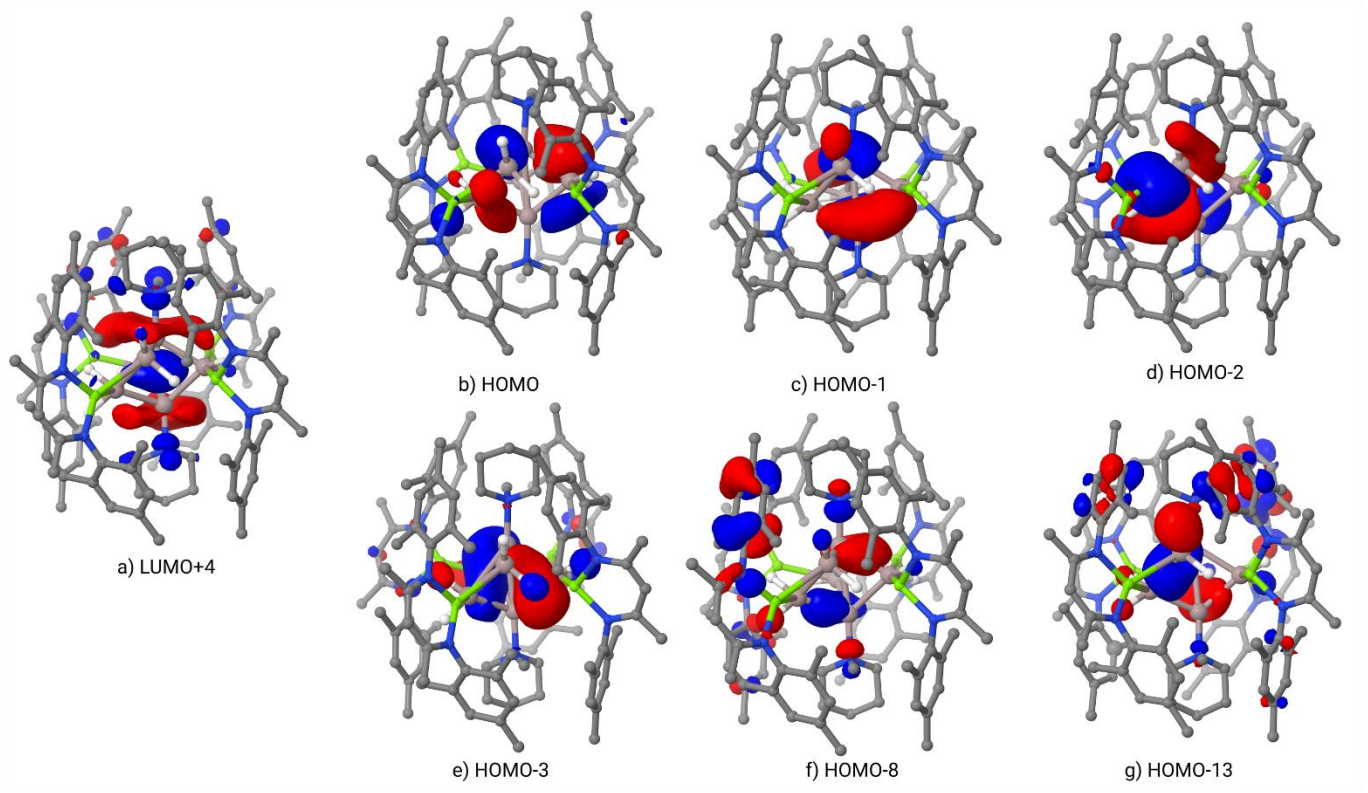

Figure S47. 3D-depiction of the seven skeletal orbitals of the Al_6 core for the optimized open fom of complex **1c** (B3PW91-D3). The iso-contour is set to 0.03.

Table S3. NPA Charges on the Al centers, the hydride H atoms and of the NMP ligands.

	Atom Number	NPA Charge
H atoms		
H	136	-0,36
H	137	-0,36
H	138	-0,36
H	139	-0,37
H	270	-0,38
H	271	-0,35
H	272	-0,38
H	273	-0,33
SUM		**-2,9**
Al atoms		
Equatorail Al Atoms		
Al	1	-0,25
Al	2	-0,3
Al	4	-0,28
Al	6	-0,34
Axial Al atoms		
Al	3	0,48
Al	5	0,44
SUM		**-0,25**

	Atom Number	NPA Charge
NR3 ligands		
N	9	-0,64
C	15	-0,27
C	29	-0,27
C	32	-0,48
C	51	-0,49
C	54	-0,49
C	89	-0,49
H	33	0,26
H	34	0,26
H	35	0,23
H	30	0,27
	31	0,26
H	16	0,26
H	17	0,27
H	52	0,25
H	53	0,24
	55	0,26
H	56	0,24
H	90	0,25
H	91	0,24
SUM		**0,16**
N	143	-0,64
C	223	-0,48
C	185	-0,49
C	188	-0,49
C	149	-0,28
C	163	-0,27
C	166	-0,48
H	167	0,26
H	168	0,26
H	169	0,23
H	164	0,26
H	165	0,26
H	150	0,27
H	151	0,27
H	189	0,26
H	190	0,24
H	186	0,25
H	187	0,24
H	224	0,25
H	225	0,24
SUM		**0,17**

Table S4. NPA charges on the (^{Mes}Nacnac)Mg fragments.

	Atom Number	NPA Charge		Atom Number	NPA Charge		Atom Number	NPA Charge		Atom Number	NPA Charge
Mg	140	1,42	Mg	141	1,42	Mg	274	1,44	Mg	7	1,41
N	11	-0,75	N	142	-0,76	N	145	-0,76	N	8	-0,75
N	12	-0,75	N	144	-0,74	N	146	-0,75	N	10	-0,75
C	72	0,3	C	154	0,3	C	207	-0,44	C	14	0,15
C	73	-0,45	C	182	0,31	H	208	0,24	C	18	-0,25
C	94	0,3	C	200	-0,45	C	206	0,3	H	19	0,24
C	85	-0,75	H	201	0,24	C	228	0,3	C	20	0,31
H	86	0,26	C	209	-0,75	C	219	-0,75	C	21	-0,04
H	87	0,25	H	210	0,27	H	220	0,27	C	24	-0,03
H	88	0,26	H	211	0,25	H	221	0,25	C	25	-0,03
C	62	-0,75	H	212	0,26	H	222	0,26	C	28	0,15
H	63	0,26	C	245	-0,75	C	196	-0,75	C	37	-0,71
H	64	0,25	H	246	0,26	H	197	0,26	H	38	0,24
H	65	0,26	H	247	0,25	H	198	0,25	H	39	0,26
C	23	0,14	H	248	0,26	H	199	0,26	H	40	0,25
C	26	-0,25	C	155	-0,03	C	156	0,14	C	43	-0,71
C	13	-0,04	C	158	-0,03	C	170	-0,04	H	44	0,25
C	79	-0,04	C	162	0,14	C	175	-0,25	H	45	0,26
C	84	-0,03	C	183	-0,25	H	176	0,24	H	46	0,26
C	95	-0,24	H	184	0,24	C	195	-0,04	C	47	-0,03
C	57	-0,72	C	233	-0,25	C	226	-0,03	C	48	0,3
H	58	0,24	H	234	0,24	C	231	-0,24	C	49	-0,24
H	59	0,27	C	253	-0,04	H	232	0,24	H	50	0,24
H	60	0,25	C	258	-0,72	C	262	-0,71	C	66	-0,44
C	103	-0,72	H	259	0,25	H	263	0,25	H	67	0,24
H	104	0,25	H	260	0,25	H	264	0,26	C	68	-0,71
H	105	0,25	H	261	0,24	H	265	0,24	H	69	0,24
H	106	0,24	C	177	-0,71	C	241	-0,71	H	70	0,26
C	132	-0,71	H	178	0,24	H	242	0,24	H	71	0,26
H	133	0,27	H	179	0,25	H	243	0,27	C	75	-0,75
H	134	0,25	H	180	0,27	H	244	0,25	H	76	0,26
H	135	0,25	C	214	-0,71	C	147	-0,03	H	77	0,25
C	22	0,15	H	215	0,24	C	157	0,14	H	78	0,26
C	36	-0,03	H	216	0,27	C	218	-0,04	C	80	-0,72
C	41	-0,25	H	217	0,25	C	160	-0,25	H	81	0,24
C	61	-0,05	C	148	0,15	H	161	0,24	H	82	0,27
C	92	-0,03	C	152	-0,24	C	229	-0,25	H	83	0,25
C	97	-0,25	H	153	0,24	H	230	0,24	C	93	-0,04
H	27	0,24	C	235	-0,25	C	213	-0,04	C	99	-0,25
H	96	0,24	H	236	0,23	C	237	-0,72	H	100	0,24
H	42	0,24	C	227	-0,04	H	238	0,25	C	101	-0,25
H	98	0,24	C	254	-0,72	H	239	0,26	H	102	0,23
C	115	-0,72	H	255	0,24	H	240	0,24	C	111	-0,75
H	116	0,25	H	256	0,25	C	191	-0,71	H	112	0,26
H	117	0,25	H	257	0,25	H	192	0,25	H	113	0,25
H	118	0,26	C	171	-0,71	H	193	0,27	H	114	0,27
C	128	-0,71	H	172	0,25	H	194	0,25	C	119	-0,04
H	129	0,25	H	173	0,26	C	266	-0,71	C	120	-0,72
H	130	0,27	H	174	0,25	H	267	0,27	H	121	0,25
H	131	0,25	C	202	-0,71	H	268	0,24	H	122	0,24
C	107	-0,71	H	203	0,24	H	269	0,25	H	123	0,26
H	108	0,24	H	204	0,25	C	249	-0,72	C	124	-0,71
H	109	0,27	H	205	0,27	H	250	0,25	H	125	0,25
H	110	0,25	C	159	-0,03	H	251	0,25	H	126	0,24
H	74	0,24	C	181	-0,04	H	252	0,26	H	127	0,25
	SUM	**0,7**		**SUM**	**0,7**		**SUM**	**0,72**		**SUM**	**0,7**

Table S5. AIM properties of the geometry optimised structure of **1c**.

	ρ(r) Density of all electrons:	$\nabla^2\rho$(r) Laplacian	*G*(r)	*V*(r)	*H*(r)	ε *Ellipticity*
BCP						
Al - Al						
Al167-Al127	0.05	-0.02	0.02	-0.04	-0.02	0.21
Al167-Al128	0.04	-0.03	0.01	-0.02	-0.01	0.56
Al167-Al146	0.04	-0.03	0.01	-0.02	-0.01	0.72
Al167-Al147	0.05	-0.02	0.02	-0.04	-0.02	0.17
Al167-Al106	0.02	0.04	0.01	-0.01	0.00	-0.11
Al106-Al127	0.05	-0.01	0.02	-0.04	-0.02	0.30
Al106-Al128	0.04	-0.03	0.01	0.02	-0.01	0.45
Al106-Al146	0.04	-0.03	0.01	-0.02	-0.01	0.66
Al106-Al147	0.05	-0.02	0.02	-0.04	-0.02	0.48
Al127-Al128	0.03	0.01	0.01	-0.01	0.00	-2.46
Al127-Al147	0.03	0.01	0.01	-0.01	0.00	-2.51
Al128-Al146	0.03	-0.01	0.01	-0.02	-0.01	0.42
Al146-Al147	0.03	0.00	0.01	-0.01	-0.01	-4.69
Al - Mg						
Al146-Mg169	0.03	0.14	0.03	-0.03	0.00	0.15
Al147-Mg169	0.03	0.14	0.03	-0.03	0.00	0.14
Al127-Mg133	0.03	0.14	0.03	-0.03	0.00	0.15
Al147-Mg133	0.03	0.14	0.03	-0.03	0.00	0.22
Al127-Mg103	0.03	0.13	0.03	-0.03	0.00	0.21
Al128-Mg103	0.03	0.13	0.03	-0.03	0.00	0.24
Al128-Mg143	0.03	0.10	0.03	-0.02	0.00	0.57
Al146-Mg143	0.03	0.09	0.02	-0.02	0.00	0.88
Al - N						
Al106 - N74	0.06	0.33	0.09	-0.09	0.00	0.00
Al167 - N201	0.06	0.33	0.08	-0.09	0.00	0.00
RCP						
Al146/147-Mg169	0.02	0.02	0.01	-0.01	0.00	-1.55
Al127/147-Mg133	0.02	0.02	0.01	-0.01	0.00	-1.61
Al127/128-Mg103	0.02	0.02	0.01	-0.01	0.00	-1.67
Al128/146-Mg143	0.02	0.03	0.01	-0.01	0.00	-3.07

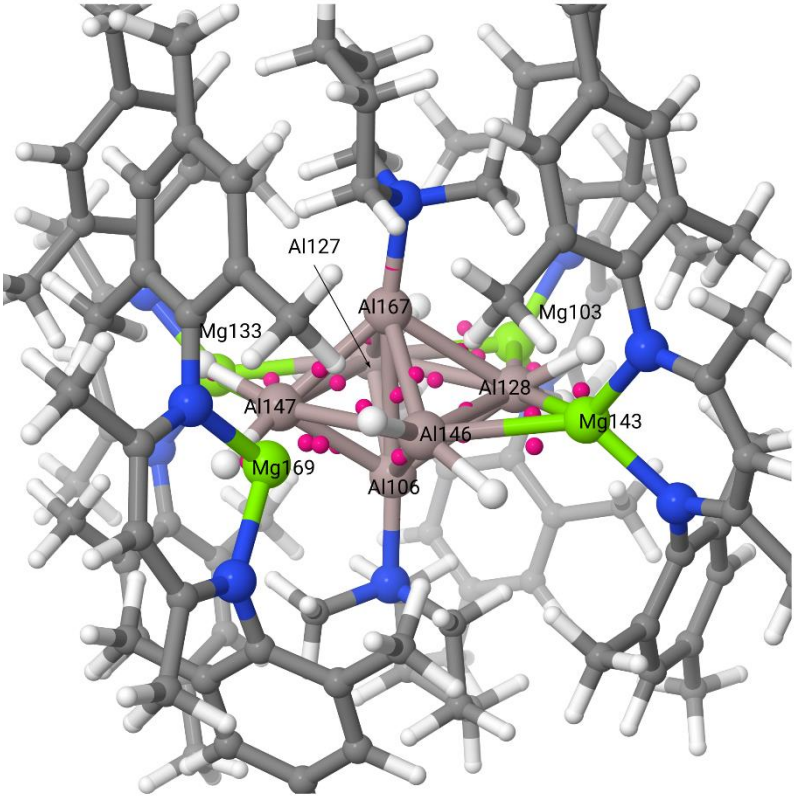

Figure S48. Geometry optimized structure of **1c** showing bond critical points between Al centers, and between Mg and hydride atoms.

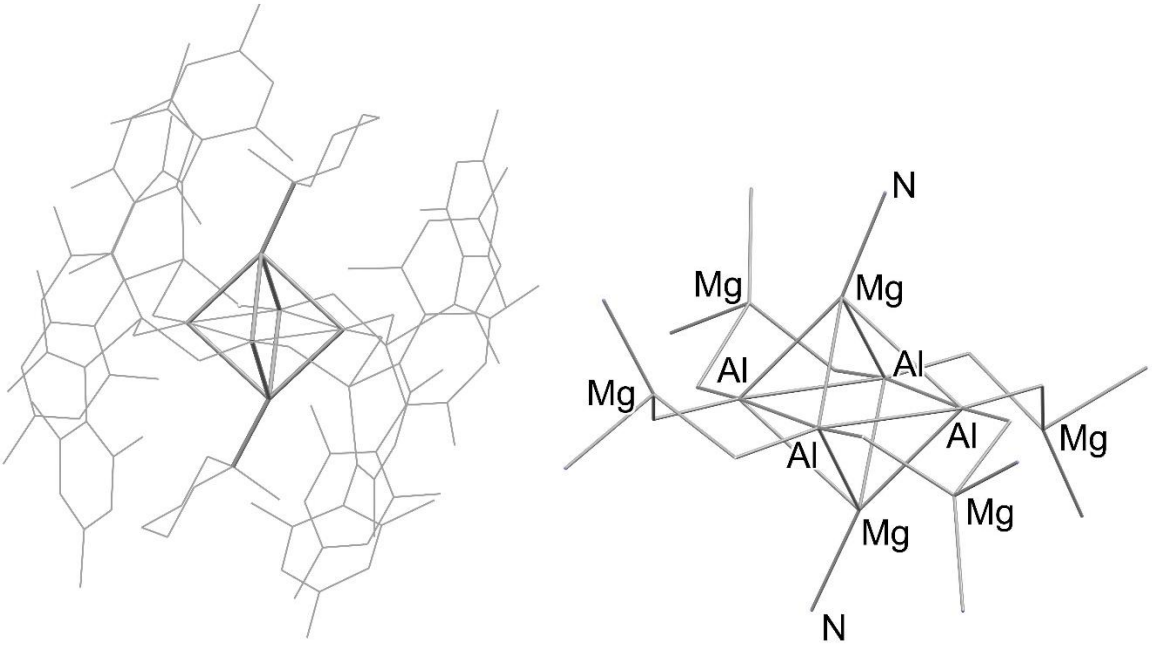

Figure S49. Geometry optimised (B3PW91-D3) structure of $[Mg_2Al_4H_8(NMP)_2\{Mg(^{Mes}Nacnac)\}_4]$, whole molecule with non-hydride hydrogens removed (left) and $Al_4Mg_6H_8N_{10}$ core (right). The geometrical features of this structure are markedly different to those of **1c**. Selected distances (Å): Mg-N_{NMP}: 2.101 and 2.105; $Al_{eq.}$-Mg_{ax} range: 2.662-2.843; $Al_{eq.}$-Al_{eq} range: 2.790-2.878; $Mg_{ax}\cdots Mg_{ax}$: 3.768.

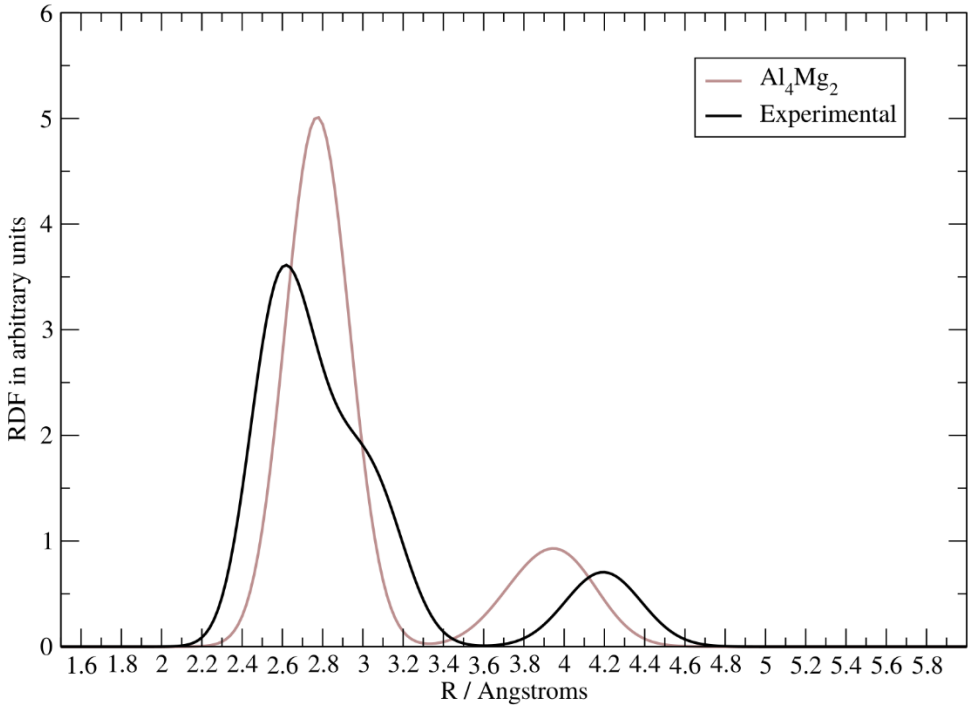

Figure S50. Radial distribution function plots of the experimental form of **1c** and geometry optimized (B3PW91-D3) $[Mg_2Al_4H_8(NMP)_2\{Mg(^{Mes}Nacnac)\}_4]$, highlighting the significant differences between the two structures.

Table S6. Cartesian coordinates of all optimized structures

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Al6 - B3PW91 - D3 : Closed Form

Al	9.97823	16.88190	1.83338
Al	6.94623	17.07174	1.21659
Al	8.96403	18.65666	0.32285
Al	10.40786	17.20833	-1.14560
Al	8.79580	15.60412	-0.00198
Al	7.54120	17.38775	-1.54355
Mg	12.55058	16.63599	0.59531
N	13.76328	14.98877	0.37494
N	8.78754	20.61219	0.66896
N	14.14684	17.84279	1.07454
N	7.47466	17.96417	5.30456
N	8.02162	15.02509	5.10336
C	8.31963	20.24159	4.99556
C	14.05066	19.23738	0.83069
C	9.89039	21.01721	1.58803
H	10.82636	20.67976	1.12929
H	9.75351	20.46276	2.52005
C	14.46829	21.11363	-0.63000
H	14.87233	21.50610	-1.56154
C	14.99186	14.92596	0.88676
C	12.64716	12.81367	0.43130
C	8.31536	13.72743	4.59982
C	7.25742	19.32328	4.95241
C	13.37876	13.75605	-1.69707
C	14.55635	19.74448	-0.38152
C	8.06064	21.58119	4.69381

H	8.87776	22.29733	4.75169
C	13.26405	13.84314	-0.29911
C	8.90058	21.34457	-0.62919
H	8.06639	21.02232	-1.25766
H	9.82537	21.01012	-1.11317
C	7.45970	20.82307	1.29438
H	7.40455	20.23739	2.21128
H	6.68729	20.47327	0.60952
H	7.28303	21.87473	1.51998
C	9.64548	13.27303	4.57941
C	15.17980	18.80653	-1.37563
H	15.49871	19.33921	-2.27483
H	14.46754	18.02651	-1.66514
H	16.05139	18.28954	-0.95998
C	9.89583	11.95322	4.20086
H	10.91794	11.58369	4.24027
C	13.98568	14.89481	-2.46591
H	14.12060	14.63405	-3.51807
H	14.95357	15.19222	-2.05084
H	13.33615	15.77816	-2.41584
C	13.43194	20.09010	1.75655
C	15.30551	17.36282	1.51965
C	12.92215	12.60242	-2.33783
H	13.02625	12.52559	-3.41698
C	9.94426	22.52030	1.81961
H	10.79585	22.73687	2.47290
H	9.04935	22.85194	2.35753
C	8.92242	22.85170	-0.43571
H	9.02040	23.31554	-1.41850
H	7.96601	23.18576	-0.02360
C	9.69742	19.78847	5.38767
H	10.40751	20.61877	5.34476
H	10.04934	18.99151	4.72362
H	9.71706	19.37602	6.40256
C	8.87010	11.08691	3.81601
C	6.93131	18.68819	7.58370
H	7.66579	19.49912	7.59266
H	6.85134	18.27409	8.58964
H	5.97328	19.14372	7.31308
C	15.65208	15.99972	1.51299
H	16.62575	15.76651	1.92718
C	12.84294	19.53321	3.02026
H	12.51049	20.33353	3.68651
H	13.55629	18.90329	3.56069
H	11.97445	18.89855	2.79566
C	7.78295	15.12450	6.41144
C	7.46818	16.31870	7.08402
H	7.30476	16.21572	8.14983
C	16.35588	18.32805	2.02079
H	16.74773	18.93449	1.19774
H	17.18848	17.79851	2.48644
H	15.92552	19.02679	2.74436
C	6.78755	22.02317	4.33164
C	12.46110	12.95139	1.91419
H	11.91836	12.09401	2.31539
H	11.89315	13.85762	2.15374
H	13.41489	13.03653	2.44625
C	5.97005	19.73694	4.56466
C	7.83381	13.87558	7.26374
H	7.09344	13.14514	6.92179
H	7.64093	14.10620	8.31215
H	8.80918	13.38648	7.18259

C	10.06720	23.25636	0.48800
H	10.08074	24.34135	0.64065
H	11.01957	22.97896	0.01781
C	7.27196	12.90068	4.15117
C	13.89599	21.99289	0.29389
C	7.31575	17.62281	6.58149
C	5.75704	21.08245	4.26425
H	4.76061	21.40219	3.97086
C	7.56915	11.59107	3.76510
H	6.75642	10.94117	3.44653
C	12.21349	11.67317	-0.24704
H	11.75590	10.86787	0.32360
C	13.37889	21.45842	1.47463
H	12.93461	22.12591	2.20940
C	6.54095	23.46055	3.96871
H	7.31908	24.11590	4.37021
H	5.57460	23.81084	4.34486
H	6.52552	23.59071	2.88045
C	5.86204	13.41469	4.12176
H	5.16153	12.61158	3.88558
H	5.74641	14.19874	3.36488
H	5.57326	13.85809	5.08028
C	15.78305	13.64457	0.74667
H	15.23656	12.78467	1.14331
H	16.74550	13.71823	1.25450
H	15.96386	13.43352	-0.31309
C	9.15873	9.64080	3.51217
H	10.10539	9.52194	2.97471
H	8.36561	9.19067	2.90776
H	9.23753	9.05447	4.43554
C	12.34666	11.54490	-1.63077
C	13.88353	23.47622	0.04028
H	13.12124	23.97951	0.64159
H	13.68697	23.70273	-1.01236
H	14.85047	23.92868	0.29147
C	11.82126	10.33190	-2.34700
H	12.39283	10.12119	-3.25576
H	10.77676	10.47883	-2.65053
H	11.85323	9.44253	-1.71102
C	10.76032	14.18874	4.99740
H	10.62056	14.55991	6.01841
H	10.80215	15.07085	4.34753
H	11.72614	13.68018	4.94401
C	4.85559	18.73323	4.49805
H	5.06042	17.98875	3.72005
H	3.90468	19.21653	4.26497
H	4.74546	18.18420	5.43876
H	6.56856	16.20368	2.59029
H	12.00479	17.64980	-0.91215
H	9.74883	17.24918	3.43524
H	11.50347	16.23328	2.11441
Mg	7.97788	16.63060	3.81970
Mg	4.96419	17.70106	-0.58606
N	3.81706	19.36900	-0.95822
N	8.65151	13.69715	-0.56186
N	3.32030	16.45868	-0.64212
N	9.22914	16.30338	-5.39327
N	10.05648	19.15490	-4.99467
C	7.64787	14.47671	-4.95733
C	3.42754	15.16790	-0.05726
C	7.25766	13.45067	-1.03963
H	6.57922	13.79605	-0.25092

H	7.10087	14.09536	-1.90862
C	3.27372	13.75041	1.88662
H	3.08069	13.63900	2.95091
C	2.58643	19.29777	-1.47095
C	5.11361	21.38208	-1.49448
C	10.28515	20.42618	-4.39878
C	8.96362	14.93098	-5.13345
C	3.96031	21.19539	0.64602
C	3.20185	15.02405	1.32182
C	7.43437	13.10890	-4.75236
H	6.41322	12.75208	-4.63483
C	4.30167	20.65755	-0.60743
C	8.95474	12.82704	0.61171
H	9.98014	13.03820	0.91815
H	8.29631	13.14355	1.42806
C	9.62781	13.50932	-1.65983
H	9.35719	14.17633	-2.47896
H	10.62360	13.77166	-1.30258
H	9.63255	12.48332	-2.02841
C	9.30627	21.42695	-4.54368
C	2.87862	16.22816	2.15877
H	2.71986	15.94909	3.20352
H	3.69976	16.95264	2.11936
H	1.98510	16.74838	1.79699
C	9.55261	22.69307	-4.01172
H	8.80919	23.47611	-4.15046
C	3.13221	20.38459	1.60003
H	2.92392	20.94520	2.51480
H	2.17638	20.08245	1.15933
H	3.65916	19.46222	1.86637
C	3.76601	14.05633	-0.84627
C	2.14774	16.81889	-1.15309
C	4.39236	22.48283	0.96968
H	4.10710	22.90688	1.92992
C	7.01010	11.98617	-1.36247
H	5.97302	11.87744	-1.68705
H	7.63146	11.68334	-2.20957
C	8.73846	11.35095	0.31769
H	8.95804	10.79260	1.22889
H	9.44822	11.00840	-0.44425
C	6.49850	15.43970	-5.03013
H	5.54339	14.90905	-5.05114
H	6.48928	16.10699	-4.15828
H	6.56571	16.07502	-5.91889
C	10.73523	22.98442	-3.32624
C	9.28850	15.61754	-7.74957
H	8.28157	15.19385	-7.68373
H	9.42151	16.06478	-8.73556
H	9.98435	14.77886	-7.65037
C	1.85712	18.10915	-1.63903
H	0.87619	18.22664	-2.08381
C	4.06303	14.23581	-2.30823
H	4.36056	13.28978	-2.76844
H	3.19986	14.62346	-2.86072
H	4.87033	14.96260	-2.44857
C	10.29697	19.03285	-6.29913
C	9.99468	17.89115	-7.06301
H	10.20034	17.97979	-8.12291
C	1.01065	15.82240	-1.17048
H	0.71239	15.58133	-0.14429
H	0.14356	16.22196	-1.69823
H	1.30841	14.87860	-1.63458

C	8.48440	12.19058	-4.73363
C	5.51042	20.78507	-2.81063
H	6.04867	21.51465	-3.41691
H	6.16596	19.91575	-2.66405
H	4.64336	20.43018	-3.37696
C	10.04756	14.03344	-5.05242
C	10.96139	20.17476	-7.03545
H	11.93580	20.38804	-6.58309
H	11.10923	19.93201	-8.08847
H	10.38024	21.09795	-6.96358
C	7.30746	11.10589	-0.15245
H	7.15174	10.04814	-0.39230
H	6.61311	11.36112	0.65914
C	11.46074	20.67806	-3.67340
C	3.57034	12.62173	1.12097
C	9.50040	16.64078	-6.65543
C	9.78858	12.67668	-4.86988
H	10.62607	11.98331	-4.82851
C	11.65982	21.95518	-3.14115
H	12.57564	22.14826	-2.58753
C	5.52107	22.66888	-1.13522
H	6.12399	23.24051	-1.83803
C	3.81041	12.79787	-0.24315
H	4.02657	11.92725	-0.85796
C	8.22744	10.71437	-4.58747
H	7.16314	10.50731	-4.44776
H	8.56137	10.16542	-5.47506
H	8.76376	10.28976	-3.73081
C	12.49784	19.60897	-3.49429
H	13.48087	20.05051	-3.32211
H	12.26471	18.98336	-2.62342
H	12.54958	18.94918	-4.36411
C	1.87941	20.57863	-1.85465
H	2.51082	21.19812	-2.49850
H	0.94086	20.37023	-2.37017
H	1.66071	21.17820	-0.96478
C	11.02587	24.37754	-2.83577
H	10.12597	24.99942	-2.83680
H	11.43087	24.37223	-1.81978
H	11.76520	24.87185	-3.47710
C	5.15810	23.24522	0.08464
C	3.65763	11.25713	1.74830
H	4.68917	11.01843	2.03570
H	3.04466	11.19145	2.65194
H	3.32743	10.47601	1.05680
C	5.58714	24.64521	0.43381
H	5.53729	25.30434	-0.43835
H	4.95413	25.07129	1.21695
H	6.62200	24.67770	0.79796
C	8.04286	21.12894	-5.29987
H	8.24144	20.89374	-6.35123
H	7.53501	20.25515	-4.87949
H	7.35877	21.98085	-5.27249
C	11.45470	14.54935	-5.14936
H	11.67017	15.21684	-4.30765
H	12.17228	13.72668	-5.13092
H	11.62416	15.13171	-6.06029
H	10.68223	16.82230	-2.75198
H	5.57577	18.04584	1.28901
H	7.82181	18.29036	-2.95249
H	6.06250	16.83306	-2.08863
Mg	9.35307	17.62179	-3.81779

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Al6 - B3PW91 - D3 : Open Form
Al 10.02817 16.21502 1.11683
Al 6.58397 16.71668 1.27219
Al 8.22235 18.51119 0.30711
Al 10.62112 18.03403 -0.65591
Al 8.08934 15.53895 -0.39301
Al 7.20565 17.44375 -1.79771
Mg 12.62393 16.33548 0.57276
N 13.90697 14.79828 0.12518
N 8.22002 20.53380 0.53270
N 14.11643 17.49497 1.35663
N 7.73184 18.48183 5.00048
N 8.52337 15.58980 4.88187
C 8.19320 20.86065 4.66477
C 13.85082 18.88325 1.52494
C 9.38870 20.87656 1.39260
H 10.27281 20.41677 0.93595
H 9.22243 20.39862 2.35946
C 14.00581 21.13531 0.67200
H 14.33941 21.82322 -0.10133
C 15.17285 14.75001 0.53399
C 12.84001 12.59637 0.12110
C 8.88310 14.29142 4.41686
C 7.28227 19.79108 4.67220
C 13.31006 13.72852 -1.98829
C 14.26281 19.77610 0.51728
C 7.72088 22.15023 4.41323
H 8.42557 22.97892 4.42759
C 13.36452 13.69419 -0.58489
C 8.36819 21.17992 -0.79881
H 7.48622 20.91289 -1.38515
H 9.24108 20.72238 -1.27840
C 6.94588 20.90953 1.17100
H 6.85136 20.36722 2.10969
H 6.12917 20.62510 0.50789
H 6.87761 21.98022 1.36962
C 10.24509 13.93048 4.38974
C 14.92689 19.24985 -0.72082
H 15.32683 20.06556 -1.32789
H 14.19004 18.70463 -1.32245
H 15.74025 18.55266 -0.50177
C 10.58926 12.62109 4.06564
H 11.63658 12.33478 4.10158
C 13.85742 14.91967 -2.72266
H 13.93675 14.72425 -3.79412
H 14.84322 15.20817 -2.34650
H 13.20591 15.79257 -2.58620
C 13.13871 19.34946 2.63852
C 15.33819 17.04129 1.62990
C 12.75399 12.64270 -2.66846
H 12.73182 12.65841 -3.75374
C 9.60643 22.37449 1.53558
H 10.49371 22.52593 2.15613
H 8.76498 22.83113 2.06861
C 8.55337 22.68679 -0.69878
H 8.66141 23.08903 -1.70875
H 7.65322 23.14687 -0.27908
C 9.64464 20.61305 4.96519
H 10.23561 21.51763 4.80074
H 10.05274 19.81552 4.33621
H 9.79627 20.29002 6.00153

C	9.62750	11.66450	3.73006
C	7.23743	19.21281	7.29798
H	7.83406	20.12603	7.21999
H	7.30571	18.83421	8.31842
H	6.20060	19.50595	7.10370
C	15.80717	15.76083	1.28034
H	16.82835	15.54754	1.57296
C	12.64630	18.38576	3.67921
H	12.35437	18.90453	4.59613
H	13.40173	17.63521	3.92870
H	11.76684	17.84189	3.31005
C	8.36625	15.71710	6.19458
C	8.00894	16.91504	6.84253
H	7.92501	16.84573	7.92004
C	16.31408	17.95244	2.33829
H	16.59171	18.79830	1.70137
H	17.22191	17.41709	2.62051
H	15.85461	18.37824	3.23569
C	6.37259	22.40171	4.15491
C	12.88442	12.56924	1.61850
H	12.45764	11.63876	1.99808
H	12.31115	13.40712	2.02858
H	13.90522	12.66100	2.00462
C	5.91929	20.01588	4.40304
C	8.53974	14.50948	7.08994
H	7.81008	13.73644	6.82821
H	8.40743	14.77582	8.13936
H	9.52705	14.05686	6.96081
C	9.76943	23.01827	0.16173
H	9.90206	24.10265	0.25060
H	10.66719	22.61365	-0.32317
C	7.89584	13.35774	4.06120
C	13.33860	21.63360	1.79513
C	7.69152	18.16657	6.30152
C	5.48952	21.32045	4.15329
H	4.43572	21.49451	3.95081
C	8.29128	12.05901	3.72021
H	7.52193	11.32848	3.47480
C	12.28629	11.53589	-0.59724
H	11.89251	10.68246	-0.04860
C	12.89959	20.72312	2.75616
H	12.37580	21.08853	3.63660
C	5.89754	23.79021	3.82923
H	6.48813	24.55066	4.34855
H	4.84753	23.92942	4.10275
H	5.98156	23.98811	2.75373
C	6.43517	13.71018	4.07534
H	5.82890	12.84061	4.34512
H	6.10710	14.05566	3.08842
H	6.21986	14.52165	4.77332
C	16.01578	13.55352	0.15630
H	15.55747	12.61924	0.49227
H	17.01980	13.62628	0.57622
H	16.09613	13.48299	-0.93396
C	10.03682	10.25449	3.40071
H	10.55456	10.20253	2.43512
H	9.17124	9.58768	3.34735
H	10.72311	9.85324	4.15380
C	12.23751	11.53623	-1.99202
C	13.12850	23.11452	1.96465
H	12.69313	23.34612	2.94110
H	12.45925	23.52032	1.19784

H	14.07516	23.66002	1.88564
C	11.60519	10.39408	-2.73792
H	12.05990	10.25593	-3.72333
H	10.53491	10.57508	-2.89919
H	11.69808	9.45435	-2.18581
C	11.30205	14.93087	4.75726
H	11.17579	15.30699	5.77852
H	11.24820	15.79599	4.09083
H	12.29997	14.49353	4.67058
C	4.95110	18.86833	4.39528
H	5.17991	18.17409	3.57892
H	3.92593	19.22325	4.26419
H	5.00206	18.28581	5.32087
H	6.56349	16.33650	2.87269
H	11.64599	19.25722	-0.86614
H	9.89795	16.84425	2.65086
H	11.32013	15.20919	1.56826
Mg	8.21650	17.12756	3.49372
Mg	4.64868	17.78726	-0.61997
N	3.43170	19.39698	-1.00118
N	8.29090	13.57669	-0.82328
N	3.02613	16.50944	-0.49508
N	9.18014	16.22166	-5.25130
N	10.25773	18.96023	-4.72809
C	7.63748	14.32151	-4.96468
C	3.25063	15.25702	0.13452
C	7.03979	13.13152	-1.49237
H	6.22078	13.41848	-0.82681
H	6.94430	13.70599	-2.41599
C	3.41038	13.92741	2.13988
H	3.31509	13.84555	3.22038
C	2.17454	19.26462	-1.43865
C	4.70981	21.35008	-1.76012
C	10.89549	20.05108	-4.07265
C	8.93738	14.82532	-5.13174
C	3.62167	21.36258	0.42462
C	3.11092	15.14677	1.52907
C	7.45926	12.93518	-4.92247
H	6.44925	12.54316	-4.81869
C	3.91727	20.71503	-0.79059
C	8.50072	12.81001	0.43837
H	9.43814	13.15112	0.88673
H	7.69656	13.10119	1.12374
C	9.46125	13.47523	-1.72384
H	9.28006	14.09679	-2.60242
H	10.34681	13.84105	-1.19947
H	9.63875	12.45067	-2.05056
C	10.16847	21.22407	-3.81124
C	2.63100	16.31892	2.33607
H	2.69278	16.10792	3.40660
H	3.23197	17.20771	2.12233
H	1.59196	16.57461	2.09702
C	10.83372	22.30800	-3.23634
H	10.28844	23.23453	-3.07274
C	2.83879	20.63825	1.48252
H	2.65351	21.28507	2.34355
H	1.87490	20.27716	1.11006
H	3.38781	19.75407	1.82587
C	3.67309	14.15699	-0.63036
C	1.81663	16.80070	-0.95107
C	4.08483	22.66152	0.62941
H	3.84441	23.16397	1.56359

C	6.99847	11.63455	-1.75857
H	6.03177	11.39196	-2.21538
H	7.76270	11.36636	-2.49498
C	8.49802	11.30402	0.21734
H	8.61066	10.82194	1.19086
H	9.37064	11.01311	-0.38000
C	6.46243	15.24961	-4.86708
H	5.52072	14.70417	-4.96930
H	6.45007	15.76429	-3.89751
H	6.50023	16.03360	-5.62879
C	12.18271	22.24217	-2.88262
C	8.83323	15.79493	-7.64915
H	7.83909	15.36770	-7.48864
H	8.83450	16.34119	-8.59322
H	9.52263	14.94895	-7.73624
C	1.46065	18.05743	-1.48253
H	0.45460	18.12697	-1.87858
C	3.86482	14.30343	-2.11265
H	4.17693	13.35747	-2.56375
H	2.95256	14.63843	-2.61742
H	4.63117	15.05799	-2.32392
C	10.22055	18.99343	-6.05583
C	9.65736	17.98418	-6.85937
H	9.64393	18.19467	-7.92170
C	0.72479	15.75941	-0.86888
H	0.48436	15.55037	0.17897
H	-0.18338	16.09483	-1.37179
H	1.04808	14.81104	-1.30707
C	8.52695	12.04377	-5.03581
C	5.06272	20.63712	-3.03307
H	5.55165	21.31123	-3.74054
H	5.75022	19.80462	-2.83227
H	4.18157	20.20166	-3.51386
C	10.03399	13.94814	-5.22885
C	10.86111	20.14943	-6.79141
H	11.93990	20.15659	-6.60154
H	10.69769	20.07031	-7.86695
H	10.48255	21.11330	-6.44230
C	7.21122	10.84930	-0.46805
H	7.23855	9.77251	-0.66840
H	6.36506	11.02890	0.20744
C	12.24858	19.95258	-3.71554
C	3.81756	12.81389	1.40291
C	9.22668	16.69979	-6.50094
C	9.81357	12.57270	-5.17218
H	10.66233	11.89910	-5.26431
C	12.86912	21.05242	-3.12458
H	13.91881	20.97954	-2.85511
C	5.15955	22.65011	-1.51230
H	5.76113	23.14770	-2.27018
C	3.92541	12.94633	0.01685
H	4.21951	12.08420	-0.57873
C	8.29285	10.55730	-5.07999
H	7.31134	10.29460	-4.67618
H	8.33395	10.18636	-6.11101
H	9.05071	10.00831	-4.51255
C	12.99992	18.67941	-3.97369
H	14.06744	18.80287	-3.77645
H	12.62186	17.88577	-3.31796
H	12.87280	18.32980	-5.00315
C	1.43089	20.50133	-1.89138
H	2.01455	21.05651	-2.63218

H	0.46295	20.24260	-2.32291
H	1.26560	21.18434	-1.05185
C	12.86900	23.41450	-2.23741
H	12.44521	24.36470	-2.57608
H	12.76315	23.38093	-1.14696
H	13.94030	23.42222	-2.45965
C	4.84975	23.32796	-0.33214
C	4.16311	11.51722	2.08207
H	5.23830	11.45952	2.29203
H	3.64108	11.41316	3.03753
H	3.90551	10.65599	1.45795
C	5.34880	24.72613	-0.08650
H	5.59453	25.23188	-1.02443
H	4.60356	25.32967	0.44035
H	6.25811	24.72780	0.52829
C	8.71356	21.30108	-4.18186
H	8.56127	21.23933	-5.26534
H	8.15596	20.46539	-3.74677
H	8.26776	22.23640	-3.83350
C	11.41035	14.51412	-5.42837
H	11.71271	15.12054	-4.56877
H	12.14657	13.71934	-5.56811
H	11.45403	15.17424	-6.30049
H	10.58918	17.23547	-2.15865
H	5.13840	17.54444	1.18979
H	7.67853	18.12193	-3.24042
H	5.59458	17.17703	-2.16840
Mg	9.41338	17.44779	-3.59103

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Al6 - B3PW91

Al	9.75492	16.67571	1.59566
Al	6.53105	17.40017	1.46397
Mg	12.93977	16.85876	0.57433
Al	8.67988	18.53093	0.15781
N	14.23986	15.25162	0.27106
N	8.79014	20.58951	0.39419
N	14.46264	18.12054	1.26769
N	7.75935	18.43422	5.57221
N	7.52254	15.42779	5.36841
C	9.15972	20.38426	5.08611
C	14.18105	19.43689	1.74620
C	10.08274	20.94613	1.05516
H	10.87934	20.48521	0.45962
H	10.09279	20.46587	2.03742
C	14.01567	21.81731	1.37411
H	14.04793	22.66232	0.68807
C	15.55879	15.34066	0.47997
C	13.37226	12.99512	0.69893
C	7.55470	14.07842	4.90460
C	7.88350	19.82037	5.26228
C	13.75927	13.73299	-1.59580
C	14.18806	20.52934	0.85846
C	9.26766	21.75580	4.83171
H	10.26000	22.18811	4.71459
C	13.77442	13.98996	-0.21019
C	8.71471	21.24871	-0.94496
H	7.75198	20.97729	-1.38722
H	9.49782	20.79836	-1.56616
C	7.63375	20.97551	1.24193
H	7.68995	20.43960	2.19070
H	6.70962	20.69502	0.73238
H	7.61549	22.04941	1.44262

C	8.76759	13.35954	4.93111
C	14.42090	20.32136	-0.61422
H	14.38310	21.27331	-1.15096
H	13.66651	19.65532	-1.04774
H	15.39538	19.86029	-0.81256
C	8.76095	12.00884	4.57456
H	9.69446	11.45011	4.62813
C	14.15814	14.80385	-2.57469
H	14.11484	14.42972	-3.60074
H	15.17341	15.17250	-2.39091
H	13.49137	15.67096	-2.49932
C	13.93868	19.63903	3.11855
C	15.74562	17.75249	1.30265
C	13.39665	12.46052	-2.04178
H	13.40816	12.25938	-3.11166
C	10.31571	22.45047	1.16655
H	11.30667	22.59856	1.60628
H	9.59459	22.89434	1.86298
C	8.90162	22.76284	-0.88708
H	8.88392	23.14039	-1.91418
H	8.05848	23.23109	-0.36517
C	10.39165	19.52978	5.20915
H	11.29016	20.11133	4.98987
H	10.36272	18.68029	4.51754
H	10.49344	19.10653	6.21552
C	7.59059	11.35040	4.18657
C	7.73747	19.21260	7.91331
H	8.69116	19.74469	7.83465
H	7.65523	18.79626	8.91859
H	6.95304	19.96425	7.78334
C	16.23355	16.48615	0.93276
H	17.30593	16.36946	1.03014
C	13.89994	18.47200	4.06848
H	13.67840	18.80440	5.08607
H	14.85218	17.92970	4.09113
H	13.13309	17.74751	3.77283
C	7.39202	15.58807	6.68772
C	7.45130	16.82057	7.36198
H	7.34682	16.75621	8.43849
C	16.79775	18.73482	1.78039
H	16.78145	19.65260	1.18451
H	17.79555	18.29806	1.71908
H	16.61423	19.03612	2.81649
C	8.14579	22.58156	4.74183
C	13.34964	13.27232	2.17844
H	13.02995	12.38735	2.73548
H	12.65951	14.08947	2.41915
H	14.33369	13.57255	2.55521
C	6.73155	20.62552	5.13841
C	7.16346	14.37770	7.57380
H	6.28545	13.81418	7.24224
H	7.01278	14.67731	8.61216
H	8.00894	13.68400	7.53317
C	10.21872	23.12623	-0.20118
H	10.31569	24.21388	-0.10232
H	11.05283	22.78890	-0.83159
C	6.37723	13.45715	4.45073
C	13.82746	22.05155	2.73851
C	7.64705	18.12092	6.86382
C	6.88750	21.98966	4.88283
H	5.99577	22.60968	4.80436
C	6.41711	12.10272	4.10424

H	5.49553	11.61944	3.78412
C	13.01880	11.73368	0.20647
H	12.73195	10.95798	0.91445
C	13.77118	20.94446	3.58837
H	13.61616	21.10004	4.65477
C	8.28245	24.06874	4.53825
H	8.15788	24.61179	5.48345
H	7.52516	24.45382	3.84717
H	9.26732	24.33157	4.14083
C	5.08858	14.22804	4.37430
H	4.26583	13.57968	4.06239
H	5.16546	15.04351	3.64499
H	4.82442	14.68130	5.33611
C	16.44047	14.13269	0.22705
H	16.12250	13.28039	0.83569
H	17.48262	14.35558	0.45998
H	16.37997	13.80652	-0.81590
C	7.58755	9.86696	3.91979
H	8.49958	9.54327	3.40762
H	6.73256	9.56951	3.30572
H	7.52779	9.29915	4.85684
C	13.04005	11.43788	-1.15732
C	13.72744	23.45396	3.28121
H	13.11784	23.49268	4.18914
H	13.28904	24.14026	2.55004
H	14.71801	23.84825	3.54033
C	12.71519	10.05679	-1.66520
H	13.61979	9.53419	-1.99927
H	12.03184	10.09201	-2.52044
H	12.25095	9.44264	-0.88832
C	10.04383	14.02377	5.37446
H	9.98655	14.37485	6.41132
H	10.26200	14.90335	4.75936
H	10.88780	13.33181	5.30134
C	5.35855	20.03200	5.29648
H	5.18876	19.25586	4.54232
H	4.58827	20.79995	5.18321
H	5.22301	19.55907	6.27551
H	7.15372	16.08380	2.32470
H	12.17900	17.68025	-0.96828
H	9.50553	16.59461	3.24196
H	11.48911	16.83221	1.75822
Mg	7.68641	17.02380	4.00117
Al	10.57600	17.29938	-1.38009
Mg	4.46298	17.38050	-0.36813
N	3.27443	19.07861	-0.78622
N	8.86087	13.42799	-0.75205
N	2.84444	16.08948	-0.78283
N	9.28687	16.13420	-5.85353
N	9.96095	19.08939	-5.59812
C	7.65744	14.32741	-5.49774
C	2.96314	14.70473	-0.46602
C	7.40221	13.10051	-0.83693
H	6.92168	13.57676	0.02533
H	7.00933	13.58788	-1.73325
C	2.71166	12.89051	1.11147
H	2.43655	12.54724	2.10750
C	2.04091	19.01893	-1.28975
C	4.46271	21.11996	-1.46178
C	10.30180	20.37862	-5.08599
C	8.99385	14.75721	-5.60667
C	3.58121	20.91707	0.80549

C	2.63383	14.25596	0.82827
C	7.40049	12.96136	-5.34330
H	6.36538	12.63056	-5.27776
C	3.77946	20.37647	-0.48224
C	9.44648	12.76911	0.45620
H	10.50948	13.02251	0.48284
H	8.97666	13.23752	1.32811
C	9.56730	13.02676	-1.98989
H	9.16952	13.60349	-2.82652
H	10.63062	13.24545	-1.88195
H	9.44364	11.96199	-2.20713
C	9.30327	21.36289	-4.95733
C	2.18649	15.23396	1.88013
H	1.94734	14.72115	2.81583
H	2.97336	15.97049	2.08640
H	1.30260	15.79950	1.56528
C	9.66769	22.64380	-4.53426
H	8.89726	23.41074	-4.46897
C	2.87233	20.11779	1.86489
H	2.77685	20.69341	2.78944
H	1.86896	19.81489	1.54555
H	3.42230	19.19667	2.09347
C	3.40226	13.78869	-1.43977
C	1.67616	16.49433	-1.28430
C	4.03055	22.21165	1.07251
H	3.85776	22.62951	2.06301
C	7.11620	11.60119	-0.83468
H	6.02907	11.47521	-0.83566
H	7.48419	11.13853	-1.75922
C	9.22609	11.25877	0.48941
H	9.64275	10.88046	1.42961
H	9.78769	10.77154	-0.31749
C	6.52402	15.31261	-5.59742
H	5.55894	14.80496	-5.52446
H	6.57333	16.06317	-4.80069
H	6.54683	15.86143	-6.54582
C	10.98767	22.97144	-4.21426
C	9.18811	15.42965	-8.21857
H	8.19894	14.97067	-8.12786
H	9.27705	15.86950	-9.21289
H	9.91513	14.61588	-8.13334
C	1.34000	17.83052	-1.56654
H	0.35212	17.97211	-1.98832
C	3.78534	14.26309	-2.81539
H	4.15150	13.43123	-3.42390
H	2.94182	14.72130	-3.34474
H	4.56976	15.02641	-2.76580
C	10.01713	18.94750	-6.92369
C	9.73180	17.75780	-7.61771
H	9.79531	17.83749	-8.69605
C	0.57970	15.47930	-1.54733
H	0.25096	15.01618	-0.61064
H	-0.28447	15.95006	-2.01888
H	0.92887	14.66494	-2.18863
C	8.42456	12.01205	-5.30297
C	4.70040	20.54399	-2.83143
H	5.21568	21.26471	-3.47169
H	5.30899	19.63408	-2.77682
H	3.76482	20.26082	-3.32631
C	10.04696	13.82672	-5.51661
C	10.42235	20.12384	-7.79023
H	11.42717	20.47121	-7.52952

H	10.41340	19.85232	-8.84686
H	9.75332	20.97714	-7.64329
C	7.73869	10.92200	0.38457
H	7.58964	9.83687	0.34004
H	7.23296	11.27976	1.29039
C	11.63445	20.67164	-4.73812
C	3.10815	11.95560	0.15229
C	9.40540	16.47687	-7.14270
C	9.74216	12.47015	-5.37835
H	10.55984	11.75252	-5.33185
C	11.94936	21.96286	-4.30493
H	12.98403	22.19002	-4.05339
C	4.89255	22.41496	-1.14995
H	5.39786	22.99643	-1.91963
C	3.45232	12.42963	-1.11574
H	3.75654	11.72127	-1.88533
C	8.11653	10.53962	-5.21385
H	7.18803	10.35509	-4.66500
H	7.99504	10.09946	-6.21149
H	8.92022	9.98940	-4.71474
C	12.71084	19.62734	-4.86202
H	13.68574	20.03923	-4.58698
H	12.50498	18.77351	-4.20705
H	12.78441	19.23446	-5.88231
C	1.27860	20.30143	-1.56460
H	1.83742	20.96722	-2.22892
H	0.30843	20.09076	-2.01743
H	1.11260	20.85863	-0.63637
C	11.36850	24.37655	-3.82542
H	10.55133	24.88788	-3.30738
H	12.24369	24.38838	-3.16896
H	11.61733	24.97751	-4.70905
C	4.67582	22.98708	0.10460
C	3.18503	10.48780	0.48417
H	3.05571	9.86733	-0.40803
H	4.15577	10.22665	0.92442
H	2.41548	10.20034	1.20748
C	5.10882	24.39801	0.40978
H	4.24889	25.03906	0.63693
H	5.77368	24.43675	1.28037
H	5.63888	24.84539	-0.43599
C	7.87185	21.05051	-5.30326
H	7.75837	20.74029	-6.34814
H	7.48283	20.22865	-4.69188
H	7.23424	21.92425	-5.14277
C	11.47757	14.28803	-5.58551
H	11.70457	14.98437	-4.76992
H	12.16351	13.44003	-5.50837
H	11.69724	14.81810	-6.51878
H	10.71355	17.91246	-2.95078
H	6.46139	18.25700	2.94665
H	7.85311	17.61161	-3.29442
H	5.78922	17.24556	-1.93197
Al	9.04114	15.47940	-0.55668
Al	7.43094	17.21038	-1.65193
Mg	9.42413	17.53338	-4.30203

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Al6 - BP86

Al	10.06460	16.73468	1.89101
Al	6.98396	17.22868	1.16130
Mg	13.00417	16.64183	0.63102
Al	9.06361	18.74110	0.74089

N	14.22821	14.98400	1.02837
N	8.98995	20.80968	0.93980
N	14.60172	17.98473	0.60853
N	8.52325	18.02333	5.85945
N	7.35612	15.22203	5.46826
C	10.34542	19.65802	5.48206
C	14.39531	19.35414	0.22033
C	10.35070	21.34810	1.31107
H	11.06622	20.92982	0.58016
H	10.60307	20.93999	2.30392
C	14.31560	21.07417	-1.49712
H	14.38514	21.35449	-2.55572
C	15.54711	15.09579	1.28805
C	13.11251	13.15626	2.27938
C	6.77027	14.04988	4.87822
C	8.96636	19.37717	5.66289
C	13.63052	12.88081	-0.11207
C	14.46306	19.71734	-1.14862
C	10.75380	20.99983	5.35147
H	11.82385	21.21273	5.23227
C	13.65754	13.66533	1.07030
C	8.56854	21.37573	-0.39926
H	7.55954	20.98883	-0.61547
H	9.25362	20.94359	-1.15075
C	7.97743	21.11788	1.99598
H	8.29251	20.64394	2.93790
H	7.00725	20.69972	1.68793
H	7.86733	22.20301	2.15751
C	7.56780	12.89841	4.65168
C	14.71264	18.67313	-2.21455
H	14.77744	19.13801	-3.21157
H	13.89563	17.92923	-2.23873
H	15.64690	18.11186	-2.03498
C	6.95621	11.74341	4.12778
H	7.56894	10.84337	3.98643
C	14.20938	13.42062	-1.40159
H	14.16374	12.66131	-2.19878
H	15.26250	13.73160	-1.28521
H	13.65796	14.31294	-1.74958
C	14.13233	20.33754	1.20965
C	15.86987	17.62061	0.89887
C	13.07311	11.58907	-0.06100
H	13.07057	10.98010	-0.97406
C	10.42826	22.88314	1.29480
H	11.46910	23.17082	1.52729
H	9.80025	23.31011	2.09894
C	8.60719	22.90888	-0.45683
H	8.34158	23.20521	-1.48622
H	7.83276	23.33837	0.20589
C	11.36159	18.53871	5.45768
H	12.38691	18.93846	5.39979
H	11.20289	17.88085	4.58145
H	11.29170	17.89558	6.35254
C	5.58810	11.70290	3.80101
C	8.81784	18.56405	8.26916
H	9.86420	18.89056	8.14281
H	8.71875	18.07525	9.24935
H	8.20569	19.48233	8.27512
C	16.27581	16.30892	1.24311
H	17.33802	16.20933	1.47780
C	14.00070	19.94431	2.66451
H	13.84526	20.83255	3.29863

H	14.89166	19.40900	3.03741
H	13.14038	19.26555	2.81371
C	7.36873	15.28423	6.81323
C	7.88955	16.36902	7.56161
H	7.85657	16.22990	8.64460
C	16.97961	18.66449	0.84473
H	17.07435	19.08446	-0.17168
H	17.94695	18.22722	1.13207
H	16.76560	19.51659	1.51191
C	9.83996	22.06945	5.39784
C	13.15788	13.96876	3.55498
H	12.71584	13.40644	4.39335
H	12.60257	14.91710	3.44477
H	14.19237	14.23885	3.83378
C	8.01780	20.43447	5.67025
C	6.77487	14.14002	7.62733
H	5.70280	14.01324	7.39656
H	6.87884	14.32692	8.70614
H	7.25863	13.17836	7.38730
C	9.99684	23.44574	-0.07111
H	9.99962	24.55071	-0.05680
H	10.73096	23.13135	-0.83876
C	5.39540	14.04926	4.52569
C	14.10656	22.07671	-0.53382
C	8.39820	17.62084	7.14589
C	8.47503	21.75993	5.54515
H	7.73952	22.57441	5.56965
C	4.83268	12.87458	3.99319
H	3.76546	12.87335	3.73742
C	12.55576	11.86319	2.27720
H	12.14376	11.47027	3.21552
C	14.00651	21.68135	0.81458
H	13.84142	22.44212	1.58872
C	10.31245	23.50781	5.33540
H	11.26190	23.59994	4.78235
H	10.48480	23.91785	6.34810
H	9.56859	24.15966	4.84662
C	4.54494	15.28194	4.74022
H	3.50245	15.09810	4.43396
H	4.93040	16.13447	4.15212
H	4.54077	15.60310	5.79732
C	16.34936	13.84827	1.64044
H	15.92178	13.33346	2.51750
H	17.39736	14.10057	1.85853
H	16.33078	13.11832	0.81259
C	4.93993	10.43057	3.29471
H	5.66939	9.77568	2.78920
H	4.12539	10.64647	2.58298
H	4.49840	9.84624	4.12359
C	12.53295	11.05655	1.12356
C	14.01990	23.53743	-0.92690
H	13.14573	24.03356	-0.46972
H	13.94055	23.65530	-2.01999
H	14.91491	24.09703	-0.59819
C	11.98543	9.64435	1.16980
H	12.73257	8.93576	1.57339
H	11.70677	9.28509	0.16516
H	11.09409	9.57418	1.81619
C	9.04313	12.90163	4.99044
H	9.22315	13.05115	6.07066
H	9.57050	13.72179	4.47046
H	9.51261	11.94779	4.69896

C	6.54006	20.14400	5.82410
H	6.17504	19.47912	5.02082
H	5.95285	21.07605	5.79037
H	6.31233	19.63296	6.77655
H	6.87623	17.01511	2.89031
H	11.92966	16.91695	-0.86069
H	9.66132	15.95088	3.35734
H	11.71382	16.34443	1.98666
Mg	8.14420	16.73673	4.24281
Al	10.30963	17.53013	-1.16778
Mg	4.66304	17.70142	-0.92670
N	3.32026	19.27589	-0.45993
N	8.65220	13.72591	-0.53494
N	3.06139	16.42760	-1.48527
N	9.84775	16.15622	-5.54335
N	9.10476	19.11357	-5.46214
C	9.05195	13.82358	-5.33211
C	3.34216	15.06324	-1.83204
C	7.65106	13.38308	-1.61598
H	6.68568	13.82215	-1.30658
H	7.97233	13.90194	-2.53408
C	3.52019	12.71978	-1.19498
H	3.45674	11.94489	-0.41972
C	2.00222	19.24803	-0.74526
C	4.36204	21.51036	-0.60479
C	8.69894	20.42564	-5.04081
C	10.08603	14.78588	-5.18886
C	3.76633	20.57744	1.59344
C	3.29889	14.06029	-0.82780
C	9.32882	12.47821	-5.01767
H	8.53311	11.73385	-5.15015
C	3.81793	20.46002	0.17792
C	8.27376	13.01552	0.74391
H	9.03837	13.26919	1.49721
H	7.32132	13.46352	1.08094
C	10.03905	13.36191	-0.95922
H	10.26824	13.87159	-1.90767
H	10.74783	13.69571	-0.18587
H	10.15608	12.27497	-1.10189
C	7.33787	20.81393	-5.14412
C	2.98976	14.42870	0.60663
H	3.00303	13.53593	1.25269
H	3.72785	15.14891	1.00379
H	2.00013	14.91032	0.70394
C	6.98206	22.13442	-4.81378
H	5.93393	22.43938	-4.92745
C	3.21563	19.44863	2.43715
H	3.28209	19.69153	3.51041
H	2.15754	19.23351	2.20203
H	3.77186	18.51195	2.25404
C	3.66648	14.71951	-3.17090
C	1.78233	16.83404	-1.60389
C	4.21345	21.76952	2.19266
H	4.15435	21.86224	3.28489
C	7.48978	11.87323	-1.84259
H	6.70380	11.73409	-2.60466
H	8.41748	11.44657	-2.26742
C	8.11950	11.49546	0.57959
H	7.78455	11.08988	1.55002
H	9.10037	11.03010	0.36577
C	7.69209	14.22818	-5.85663
H	7.00991	13.36278	-5.88791

H	7.24013	15.01040	-5.22026
H	7.75454	14.64956	-6.87651
C	7.92863	23.07489	-4.36524
C	10.62339	15.44746	-7.79673
H	9.90885	14.61245	-7.89893
H	10.79406	15.88301	-8.79231
H	11.56941	15.00372	-7.44178
C	1.31941	18.13633	-1.29354
H	0.25358	18.29734	-1.47207
C	3.76113	15.78535	-4.24049
H	3.96652	15.33577	-5.22570
H	2.83384	16.38007	-4.31977
H	4.57649	16.49805	-4.01261
C	9.48497	18.99667	-6.75159
C	9.93485	17.79929	-7.35703
H	10.19572	17.89349	-8.41369
C	0.72189	15.85194	-2.09187
H	0.64656	14.98358	-1.41430
H	-0.26542	16.33328	-2.15102
H	0.97641	15.44766	-3.08636
C	10.59324	12.05886	-4.56686
C	4.43816	21.38010	-2.10925
H	4.92054	22.26297	-2.55775
H	5.02132	20.48912	-2.40811
H	3.43733	21.26412	-2.56362
C	11.36680	14.39324	-4.71503
C	9.44111	20.21890	-7.66412
H	10.09202	21.02482	-7.28363
H	9.76403	19.96127	-8.68353
H	8.42298	20.64148	-7.71399
C	7.11457	11.15364	-0.53521
H	7.06473	10.06060	-0.69071
H	6.10364	11.48219	-0.22490
C	9.66431	21.33523	-4.53854
C	3.78879	12.34403	-2.52542
C	10.10643	16.50103	-6.82108
C	11.59555	13.03655	-4.42035
H	12.59479	12.73500	-4.08167
C	9.25973	22.64436	-4.21238
H	10.01515	23.35296	-3.84769
C	4.79619	22.68533	0.04006
H	5.19354	23.50461	-0.57292
C	3.87893	13.36430	-3.49003
H	4.10304	13.10008	-4.53155
C	10.86711	10.60618	-4.23520
H	10.12164	9.93862	-4.69827
H	11.86592	10.29180	-4.58428
H	10.83660	10.42459	-3.14397
C	11.11012	20.91439	-4.38896
H	11.70872	21.72153	-3.93591
H	11.20380	20.01683	-3.75141
H	11.56724	20.65451	-5.36135
C	1.14550	20.47893	-0.46443
H	1.55628	21.37257	-0.96477
H	0.11204	20.32701	-0.80938
H	1.12104	20.71126	0.61437
C	7.53211	24.51301	-4.09648
H	6.52305	24.58320	-3.65515
H	8.23918	25.00862	-3.40999
H	7.51631	25.10659	-5.02969
C	4.71522	22.84548	1.43535
C	3.92590	10.88494	-2.91143

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H 13.40455 14.93397 -4.21849
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H 5.33047 17.30475 0.93115
H 8.25003 18.47201 -2.54649
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Al 8.60300 15.79422 -0.21574
Al 7.17265 17.26627 -2.03092
Mg 9.08557 17.50463 -4.09150
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Al6 - PBE0
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C 14.39484 20.75902 -2.01636
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C 11.14445 20.28075 5.57318
H 12.21286 20.19274 5.76321
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H 8.30763 21.24446 -1.29559
H 10.06908 21.21538 -1.29357
C 7.94742 21.11969 1.32101
H 7.98382 20.54555 2.24854
H 7.09659 20.77739 0.72745
H 7.81120 22.17838 1.56046
C 7.37765 13.06545 4.59592
C 14.92634 18.30865 -2.22557
H 15.05707 18.57688 -3.27751
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C 6.96351 11.82435 4.11041

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C	14.68193	13.83027	-1.21849
H	14.83210	13.14195	-2.05481
H	15.66318	14.19981	-0.90042
H	14.12559	14.70078	-1.58480
C	13.98921	20.52854	0.73369
C	15.68034	17.83910	1.11357
C	13.55502	11.82028	-0.20400
H	13.80608	11.27342	-1.11172
C	10.49181	22.80335	1.54554
H	11.42473	23.01555	2.08003
H	9.68251	23.16000	2.19543
C	9.24239	23.09292	-0.61064
H	9.27996	23.51358	-1.61949
H	8.31765	23.46816	-0.15321
C	10.96502	17.82137	6.06200
H	12.04125	17.92755	6.22239
H	10.80822	17.07086	5.28021
H	10.52171	17.41954	6.98038
C	5.69387	11.63010	3.56464
C	7.91195	18.84193	7.91044
H	8.98435	18.88465	8.12778
H	7.38728	18.54893	8.82083
H	7.61093	19.85892	7.64200
C	16.02207	16.60100	1.68937
H	17.02043	16.55090	2.10697
C	13.75689	20.41044	2.21417
H	13.46973	21.37619	2.64002
H	14.64927	20.06118	2.74608
H	12.96226	19.68869	2.43605
C	6.55012	15.59499	6.39339
C	6.87158	16.74148	7.14021
H	6.53118	16.72545	8.16832
C	16.79660	18.85721	1.03980
H	17.06574	19.04603	-0.00526
H	17.68511	18.50380	1.56489
H	16.49593	19.82092	1.45962
C	10.60870	21.53081	5.25840
C	12.56216	13.99689	3.36173
H	12.07538	13.34129	4.08916
H	11.87759	14.82594	3.14101
H	13.44603	14.43849	3.83449
C	8.40930	20.48718	5.09226
C	5.81508	14.51248	7.15335
H	4.86575	14.26263	6.67057
H	5.61590	14.82245	8.17998
H	6.40210	13.58846	7.17543
C	10.45418	23.53335	0.20555
H	10.44758	24.61909	0.35545
H	11.36695	23.29344	-0.35579
C	5.20381	13.98410	3.98610
C	14.06824	21.90179	-1.28489
C	7.63301	17.86706	6.78713
C	9.23860	21.60819	5.01056
H	8.79399	22.57074	4.76166
C	4.83822	12.72913	3.49803
H	3.84870	12.60832	3.06126
C	12.54081	11.90381	1.95897
H	11.99381	11.42020	2.76678
C	13.87385	21.76284	0.08916
H	13.63219	22.64216	0.68445
C	11.47793	22.75811	5.23439

H	12.45941	22.54633	4.79791
H	11.65306	23.13784	6.24825
H	11.01710	23.56587	4.65879
C	4.24538	15.13742	3.92122
H	3.29642	14.82898	3.47477
H	4.65886	15.94576	3.30832
H	4.03710	15.55701	4.91194
C	16.10018	14.18613	2.18333
H	15.52268	13.62569	2.92448
H	17.04425	14.49703	2.63314
H	16.32050	13.48779	1.36878
C	5.25072	10.27083	3.09703
H	4.82375	9.68724	3.92179
H	6.08648	9.69350	2.68975
H	4.48341	10.34610	2.32086
C	12.86236	11.16880	0.81855
C	13.91490	23.23424	-1.96584
H	12.94463	23.31355	-2.47241
H	14.68750	23.38653	-2.72614
H	13.97931	24.05949	-1.25080
C	12.49881	9.71399	0.69869
H	13.36930	9.07143	0.87710
H	12.12312	9.47331	-0.30160
H	11.72989	9.43274	1.42376
C	8.75355	13.23918	5.17617
H	8.72016	13.56698	6.22140
H	9.32412	13.99960	4.62936
H	9.31313	12.30032	5.13324
C	6.93268	20.61093	4.85019
H	6.58618	19.91581	4.07709
H	6.67565	21.62355	4.52959
H	6.35100	20.38266	5.75132
H	6.79584	17.10323	2.37219
H	12.22791	16.76412	-1.09454
H	9.63503	16.56636	3.45197
H	11.76365	17.34971	2.22494
Mg	7.82789	16.82961	3.94253
Al	10.63616	17.32717	-1.26942
Mg	4.57128	17.73637	-0.61670
N	3.24707	19.23529	-0.05620
N	9.11748	13.61011	-0.26049
N	3.08093	16.58655	-1.50182
N	9.48126	15.95895	-5.27468
N	8.77827	18.91231	-5.22374
C	9.02812	13.61317	-4.73755
C	3.40648	15.32047	-2.06982
C	7.91977	13.25594	-1.07552
H	7.05423	13.71125	-0.57881
H	8.03638	13.73728	-2.05043
C	3.55949	12.91928	-1.89965
H	3.43277	12.01270	-1.30993
C	1.94338	19.19659	-0.32564
C	4.13057	21.51999	-0.11317
C	8.56150	20.26112	-4.81443
C	9.94553	14.66232	-4.90845
C	3.82915	20.38555	2.02467
C	3.26802	14.14842	-1.30479
C	9.50888	12.33447	-4.44276
H	8.79456	11.52004	-4.33472
C	3.73837	20.38561	0.62216
C	9.01627	12.95424	1.07293
H	9.91775	13.21557	1.63386

H	8.15981	13.41004	1.58504
C	10.36971	13.24030	-0.94868
H	10.42117	13.77018	-1.90171
H	11.21530	13.54249	-0.32790
H	10.43786	12.16422	-1.13283
C	7.24948	20.74258	-4.64640
C	2.80309	14.21211	0.12164
H	2.63943	13.20594	0.51824
H	3.55935	14.70202	0.74687
H	1.87220	14.77875	0.22983
C	7.06067	22.08729	-4.32979
H	6.04323	22.46005	-4.22467
C	3.44140	19.16640	2.81230
H	3.51871	19.35429	3.88676
H	2.41825	18.84269	2.59271
H	4.09621	18.31954	2.57090
C	3.86346	15.24840	-3.39709
C	1.80949	16.97556	-1.57497
C	4.26670	21.54214	2.67214
H	4.30030	21.54911	3.75979
C	7.69374	11.75465	-1.21454
H	6.76554	11.61026	-1.77917
H	8.49704	11.29617	-1.80515
C	8.82759	11.44362	0.99305
H	8.72026	11.06613	2.01545
H	9.72400	10.96787	0.57585
C	7.55584	13.85778	-4.90311
H	6.98535	12.94443	-4.71758
H	7.19071	14.62471	-4.21048
H	7.31093	14.21183	-5.91132
C	8.13235	22.96849	-4.17322
C	9.73819	15.11900	-7.57274
H	9.13343	14.22431	-7.39746
H	9.57583	15.45736	-8.59687
H	10.78364	14.80936	-7.47168
C	1.29623	18.16542	-1.02803
H	0.23212	18.30971	-1.17059
C	4.03265	16.49950	-4.21069
H	4.38119	16.26518	-5.22028
H	3.09827	17.06617	-4.29414
H	4.76520	17.17212	-3.74990
C	8.81014	18.69430	-6.53755
C	9.05790	17.45113	-7.14658
H	9.03282	17.46425	-8.22929
C	0.80653	16.09919	-2.29182
H	0.72505	15.11909	-1.81170
H	-0.18056	16.56327	-2.30731
H	1.12392	15.91229	-3.32271
C	10.86984	12.07335	-4.29463
C	4.04466	21.52423	-1.61271
H	4.38850	22.48043	-2.01697
H	4.66198	20.72602	-2.04011
H	3.02038	21.35533	-1.96436
C	11.32507	14.43013	-4.74631
C	8.59292	19.84938	-7.49061
H	9.36528	20.61364	-7.35419
H	8.61886	19.51114	-8.52724
H	7.63441	20.34347	-7.30576
C	7.60103	11.09158	0.15676
H	7.49662	10.00491	0.05600
H	6.70303	11.45633	0.67325
C	9.65958	21.11338	-4.61232

C	3.98386	12.81760	-3.22443
C	9.40537	16.21304	-6.58159
C	11.75893	13.13961	-4.44356
H	12.82733	12.96228	-4.33094
C	9.42231	22.45541	-4.30222
H	10.27556	23.12096	-4.17804
C	4.57748	22.64828	0.57611
H	4.86570	23.52912	0.00410
C	4.13393	13.99783	-3.95323
H	4.45968	13.94763	-4.99081
C	11.37057	10.69566	-3.95926
H	10.58164	9.94601	-4.06700
H	12.20317	10.40277	-4.60736
H	11.73590	10.64844	-2.92568
C	11.06419	20.60116	-4.76370
H	11.78991	21.40326	-4.60244
H	11.27534	19.80406	-4.04137
H	11.23847	20.17785	-5.75946
C	1.05602	20.32925	0.14141
H	1.37361	21.28425	-0.28893
H	0.01563	20.15165	-0.13402
H	1.11549	20.44550	1.22845
C	7.89108	24.42662	-3.89127
H	7.31171	24.56966	-2.97205
H	8.83170	24.97409	-3.78244
H	7.32612	24.89846	-4.70298
C	4.64522	22.68600	1.96936
C	4.28268	11.48019	-3.84488
H	4.02956	11.46783	-4.90944
H	5.34733	11.22626	-3.76364
H	3.72160	10.67867	-3.35554
C	5.13394	23.91332	2.68868
H	4.71569	23.97870	3.69748
H	6.22717	23.91159	2.79002
H	4.86255	24.82721	2.15163
C	6.07246	19.82990	-4.83391
H	6.08887	19.33028	-5.80851
H	6.06963	19.04468	-4.06976
H	5.13337	20.38332	-4.74833
C	12.31646	15.54358	-4.93065
H	12.13132	16.35706	-4.22096
H	13.33721	15.18231	-4.77869
H	12.25587	15.98118	-5.93372
H	10.67379	17.65159	-2.91971
H	5.70813	15.06318	1.12903
H	7.54408	17.31654	-2.67611
H	5.88865	18.81276	-1.69491
Al	9.11884	15.67246	-0.00436
Al	7.26685	17.96557	-1.11143
Mg	9.04953	17.39145	-3.82655

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Al6 - wB97XD

Al	9.77015	17.15732	1.67439
Al	6.63130	16.71755	1.32922
Mg	12.75725	16.64315	0.70316
Al	9.18129	18.85153	-0.17387
N	13.94299	14.97738	0.67105
N	8.99399	20.80328	0.32015
N	14.33791	17.89466	1.03293
N	7.64519	18.07105	5.38375
N	7.49155	15.10951	5.26003
C	9.04749	20.04675	5.01077

C	14.17212	19.28052	0.74595
C	10.26932	21.26272	0.94463
H	11.07627	21.02019	0.24363
H	10.42429	20.66512	1.84766
C	14.26978	21.09583	-0.83428
H	14.48215	21.45664	-1.83877
C	15.18643	14.96886	1.14374
C	12.71092	12.86184	0.80138
C	7.43977	13.78521	4.73805
C	7.78273	19.43977	5.00860
C	13.65659	13.59552	-1.32123
C	14.44510	19.74296	-0.55268
C	9.14162	21.40965	4.71308
H	10.12057	21.88514	4.73723
C	13.44380	13.79490	0.05329
C	8.69800	21.60943	-0.89848
H	7.74543	21.25462	-1.30083
H	9.47566	21.38158	-1.63643
C	7.86648	20.84637	1.28760
H	8.12085	20.23101	2.15229
H	6.97231	20.43358	0.81487
H	7.65201	21.86325	1.62078
C	8.63279	13.08102	4.52477
C	14.92696	18.78257	-1.60832
H	15.13883	19.30243	-2.54558
H	14.17194	18.01360	-1.80696
H	15.83556	18.25835	-1.29422
C	8.56661	11.77694	4.03014
H	9.49315	11.22154	3.89278
C	14.39892	14.62530	-2.13180
H	14.52972	14.29012	-3.16359
H	15.38673	14.83816	-1.71026
H	13.84894	15.57255	-2.14704
C	13.70000	20.15878	1.73006
C	15.52341	17.46713	1.45291
C	13.17200	12.42999	-1.91355
H	13.33862	12.27436	-2.97747
C	10.28076	22.75587	1.25236
H	11.25878	23.01182	1.66709
H	9.54435	22.98317	2.02839
C	8.67118	23.10967	-0.62482
H	8.47252	23.62228	-1.57012
H	7.84334	23.35465	0.04878
C	10.27380	19.25080	5.37485
H	11.17009	19.87530	5.33741
H	10.40775	18.40784	4.68954
H	10.19580	18.82624	6.38156
C	7.35081	11.16765	3.72477
C	7.40660	18.95515	7.66739
H	8.32425	19.55078	7.65561
H	7.24235	18.58892	8.68118
H	6.59030	19.63382	7.40176
C	15.87545	16.11021	1.59486
H	16.86779	15.92806	1.98831
C	13.32188	19.64543	3.09430
H	13.01380	20.46633	3.74740
H	14.14701	19.11309	3.57863
H	12.48761	18.93754	3.02339
C	7.38829	15.26994	6.57474
C	7.37835	16.51627	7.22556
H	7.26712	16.47584	8.30199
C	16.60831	18.48044	1.75621

H	16.90031	19.00513	0.84065
H	17.49244	17.99992	2.17612
H	16.25292	19.24229	2.45554
C	8.01706	22.17705	4.41878
C	12.41442	13.11885	2.25486
H	11.78640	12.32469	2.66740
H	11.88576	14.07010	2.38721
H	13.32794	13.18164	2.85606
C	6.64434	20.17639	4.63992
C	7.26435	14.04737	7.46316
H	6.35905	13.48157	7.22225
H	7.23017	14.32551	8.51703
H	8.10796	13.36873	7.30537
C	9.99145	23.56893	-0.00806
H	9.96590	24.64101	0.21396
H	10.79902	23.40451	-0.73251
C	6.20170	13.20577	4.41216
C	13.85169	22.00264	0.14061
C	7.48714	17.80780	6.67769
C	6.77935	21.53511	4.36823
H	5.89244	22.10658	4.10287
C	6.18188	11.90764	3.90779
H	5.22111	11.45149	3.67607
C	12.26324	11.69944	0.17419
H	11.71311	10.96747	0.76161
C	13.57729	21.51256	1.41559
H	13.24907	22.19976	2.19222
C	8.11841	23.65741	4.14879
H	9.13885	24.02247	4.29410
H	7.46090	24.22680	4.81395
H	7.82079	23.89920	3.12157
C	4.92177	13.97168	4.61081
H	4.05396	13.31996	4.47857
H	4.85761	14.78543	3.88002
H	4.86168	14.42381	5.60536
C	15.96013	13.66601	1.16043
H	15.39343	12.87587	1.66102
H	16.92171	13.78410	1.66071
H	16.14175	13.32213	0.13692
C	7.28144	9.74452	3.22890
H	8.27777	9.30321	3.13493
H	6.79578	9.68631	2.24877
H	6.70325	9.11676	3.91484
C	12.49000	11.46012	-1.18032
C	13.72284	23.46981	-0.18364
H	13.14376	24.00150	0.57637
H	13.22491	23.61737	-1.14762
H	14.70566	23.94928	-0.24810
C	12.01764	10.18682	-1.83429
H	12.75388	9.38433	-1.71385
H	11.85838	10.32841	-2.90698
H	11.07851	9.83357	-1.39598
C	9.95594	13.72432	4.84966
H	9.97817	14.10870	5.87431
H	10.14970	14.58025	4.19185
H	10.77616	13.01155	4.73425
C	5.30253	19.50254	4.55601
H	5.29752	18.76619	3.74249
H	4.51637	20.23228	4.35198
H	5.05303	18.96994	5.47924
H	7.29483	17.83622	2.40641
H	12.21893	16.80142	-1.05812

H	9.50882	16.86972	3.28116
H	11.43157	16.77845	1.93329
Mg	7.66819	16.63696	3.88332
Al	10.63859	17.21636	-1.35517
Mg	4.65495	17.53993	-0.31713
N	3.44484	19.19196	-0.62166
N	8.68784	13.77887	-0.59832
N	3.07634	16.26076	-0.72477
N	9.55164	16.31128	-5.52709
N	9.94252	19.27054	-5.18083
C	8.18816	14.33080	-5.05135
C	3.27561	14.89389	-0.38186
C	7.36834	13.41746	-1.20122
H	6.58915	13.77700	-0.51938
H	7.27081	13.97613	-2.13615
C	3.29719	13.14259	1.27545
H	3.15185	12.82510	2.30566
C	2.22732	19.14959	-1.15407
C	4.70954	21.28246	-0.90647
C	10.09932	20.56743	-4.60657
C	9.44842	14.92365	-5.21632
C	3.62558	20.77278	1.21544
C	3.07727	14.47885	0.94643
C	8.11854	12.96101	-4.78286
H	7.13970	12.49885	-4.66962
C	3.92168	20.43304	-0.11566
C	8.89006	13.01506	0.66987
H	9.87245	13.28724	1.06398
H	8.13962	13.36587	1.38869
C	9.79160	13.53566	-1.55770
H	9.61447	14.12565	-2.45796
H	10.73486	13.84836	-1.10640
H	9.87274	12.48350	-1.83878
C	9.00584	21.44951	-4.57412
C	2.63682	15.47174	1.98852
H	2.45458	14.97987	2.94732
H	3.41319	16.23366	2.13851
H	1.72480	15.99754	1.68755
C	9.20646	22.75041	-4.11599
H	8.36975	23.44684	-4.12812
C	2.77954	19.85068	2.05398
H	2.59077	20.28055	3.04066
H	1.81371	19.64707	1.58043
H	3.27269	18.88117	2.19057
C	3.71966	13.98190	-1.34912
C	1.89978	16.63322	-1.20942
C	4.10742	21.97522	1.72862
H	3.86924	22.24015	2.75716
C	7.20618	11.91808	-1.42383
H	6.21354	11.74267	-1.84216
H	7.92504	11.56697	-2.17000
C	8.75856	11.50653	0.48269
H	8.90089	11.03167	1.45557
H	9.55440	11.13570	-0.17238
C	6.93347	15.15307	-5.18903
H	6.04342	14.52404	-5.10944
H	6.87739	15.92153	-4.40979
H	6.89908	15.67605	-6.15044
C	10.45100	23.18629	-3.65573
C	9.62945	15.59469	-7.87439
H	8.67763	15.05849	-7.81085
H	9.72164	16.03095	-8.86933

H	10.41890	14.84828	-7.74541
C	1.54431	17.96783	-1.49129
H	0.56247	18.10593	-1.92720
C	4.04790	14.44814	-2.74366
H	4.40415	13.61518	-3.35702
H	3.18663	14.89949	-3.24720
H	4.83061	15.21520	-2.71611
C	10.09222	19.16400	-6.50168
C	9.94427	17.97625	-7.24019
H	10.06509	18.08580	-8.31053
C	0.82589	15.58756	-1.43878
H	0.56266	15.10849	-0.49011
H	-0.07399	16.03066	-1.86667
H	1.17893	14.79392	-2.10305
C	9.26162	12.17286	-4.67229
C	5.05256	20.90834	-2.32430
H	5.69188	21.66800	-2.78265
H	5.57875	19.94854	-2.36184
H	4.15670	20.79693	-2.94465
C	10.62013	14.16077	-5.05384
C	10.46362	20.39749	-7.30286
H	11.39395	20.83074	-6.92283
H	10.59493	20.15824	-8.35826
H	9.69827	21.17378	-7.21276
C	7.39543	11.15893	-0.11204
H	7.30237	10.07881	-0.26953
H	6.60891	11.45725	0.59426
C	11.33935	20.95543	-4.08086
C	3.67597	12.20159	0.31783
C	9.70460	16.65995	-6.79853
C	10.50329	12.79647	-4.79888
H	11.41038	12.20448	-4.69267
C	11.49187	22.26097	-3.60927
H	12.46232	22.56708	-3.22328
C	5.15589	22.48621	-0.35903
H	5.74809	23.15426	-0.98118
C	3.87178	12.64305	-0.98850
H	4.15353	11.92445	-1.75430
C	9.17302	10.69367	-4.39430
H	8.15313	10.32242	-4.52525
H	9.82849	10.12385	-5.06031
H	9.47949	10.46300	-3.36697
C	12.49075	19.98680	-4.05247
H	13.42158	20.49775	-3.79645
H	12.32045	19.20733	-3.29942
H	12.62266	19.48488	-5.01565
C	1.47392	20.44732	-1.37490
H	2.07196	21.15387	-1.95721
H	0.52999	20.27367	-1.89269
H	1.25930	20.93198	-0.41687
C	10.67298	24.62602	-3.26520
H	9.80330	25.04652	-2.75134
H	11.53727	24.73419	-2.60385
H	10.85776	25.24251	-4.15178
C	4.86534	22.85286	0.95415
C	3.84660	10.74861	0.68481
H	4.39262	10.20357	-0.09077
H	4.40042	10.64012	1.62297
H	2.87716	10.25595	0.81858
C	5.32081	24.17588	1.51666
H	4.57232	24.95701	1.34207
H	5.48139	24.11355	2.59702

H 6.25389 24.51347 1.05469
C 7.65121 20.98951 -5.04657
H 7.66897 20.66762 -6.09310
H 7.30807 20.12990 -4.45951
H 6.91065 21.78761 -4.95005
C 11.97591 14.80761 -5.16149
H 12.09029 15.58510 -4.39847
H 12.76824 14.06774 -5.01996
H 12.12707 15.28923 -6.13325
H 10.80140 16.80645 -2.95984
H 6.47409 15.61022 2.60127
H 7.83149 17.71659 -3.22010
H 5.83544 17.53833 -1.92135
Al 8.68151 15.78829 -0.19640
Al 7.44525 17.56373 -1.55811
Mg 9.48509 17.67350 -3.98542
274
Al6 - M06-L
Al 10.21286 17.26321 1.60860
Al 6.75288 17.44931 0.99871
Mg 12.88710 16.64319 0.53752
Al 9.23725 18.82764 -0.13671
N 14.03594 14.93936 0.58313
N 9.16506 20.82226 0.40552
N 14.50351 17.84363 0.89005
N 7.80352 18.40077 5.14985
N 7.66096 15.43741 4.80265
C 9.06939 20.48648 4.90211
C 14.39969 19.23484 0.61433
C 10.46202 21.23257 1.02677
H 11.24801 20.99937 0.29393
H 10.62364 20.58196 1.89631
C 14.65003 21.06953 -0.93219
H 14.93592 21.43265 -1.92048
C 15.27879 14.89197 1.05771
C 12.71068 12.88065 0.73288
C 7.59440 14.11494 4.27262
C 7.84453 19.79460 4.86419
C 13.69323 13.55387 -1.39759
C 14.74838 19.70243 -0.66403
C 9.07776 21.85555 4.62688
H 10.02791 22.39024 4.66970
C 13.49085 13.77419 -0.02137
C 8.88700 21.68230 -0.78489
H 7.93742 21.33976 -1.21775
H 9.67925 21.47588 -1.51552
C 8.05226 20.91007 1.38072
H 8.27878 20.27435 2.24105
H 7.13303 20.55051 0.90584
H 7.89206 21.93265 1.73304
C 8.72956 13.28779 4.32291
C 15.22678 18.73766 -1.70527
H 15.53246 19.25521 -2.61869
H 14.44104 18.01885 -1.97470
H 16.07342 18.13625 -1.35354
C 8.59851 11.94603 3.95641
H 9.46946 11.29288 4.03058
C 14.50711 14.51792 -2.20341
H 14.64921 14.15846 -3.22608
H 15.49533 14.69513 -1.76272
H 14.01391 15.49761 -2.25302
C 13.93150 20.12743 1.59543

C	15.67379	17.38357	1.34678
C	13.12558	12.42369	-1.98804
H	13.28356	12.25519	-3.05392
C	10.50018	22.70491	1.39665
H	11.49259	22.93345	1.80186
H	9.78743	22.90204	2.20710
C	8.86912	23.16556	-0.44932
H	8.68530	23.72568	-1.37310
H	8.03171	23.39982	0.22224
C	10.33448	19.77785	5.27486
H	11.17459	20.47597	5.32532
H	10.58442	18.98990	4.55437
H	10.25108	19.27768	6.24678
C	7.38275	11.41497	3.51767
C	7.45577	19.12468	7.47250
H	8.33686	19.77460	7.49320
H	7.31893	18.69363	8.46502
H	6.60489	19.78130	7.26056
C	15.99292	16.02310	1.49595
H	16.97872	15.82096	1.90120
C	13.50425	19.61943	2.93678
H	13.19302	20.44003	3.58997
H	14.29705	19.05830	3.44464
H	12.65813	18.92391	2.84453
C	7.44411	15.53278	6.12342
C	7.44743	16.72768	6.85904
H	7.26993	16.61224	7.92259
C	16.76407	18.36640	1.68743
H	17.08720	18.91481	0.79539
H	17.63438	17.86503	2.11302
H	16.41492	19.12393	2.39675
C	7.91038	22.55957	4.32448
C	12.44733	13.14737	2.18240
H	11.78179	12.38853	2.60689
H	11.97661	14.12906	2.32855
H	13.36689	13.16447	2.77988
C	6.65087	20.47982	4.56361
C	7.14209	14.28540	6.91784
H	6.24291	13.78899	6.53657
H	6.98611	14.51693	7.97214
H	7.94664	13.54710	6.83989
C	10.19168	23.57670	0.18749
H	10.18437	24.63841	0.46110
H	10.99020	23.44428	-0.55713
C	6.37448	13.62497	3.77457
C	14.22516	21.98312	0.03279
C	7.58821	18.05413	6.41900
C	6.70794	21.85006	4.30047
H	5.78006	22.38069	4.08249
C	6.29353	12.28295	3.39629
H	5.33897	11.90353	3.02801
C	12.18452	11.74959	0.10531
H	11.59923	11.04822	0.70090
C	13.87294	21.48690	1.29069
H	13.54477	22.17995	2.06593
C	7.95205	24.02259	4.00010
H	8.76755	24.53209	4.52188
H	7.01493	24.52404	4.26051
H	8.11095	24.19703	2.92505
C	5.17300	14.51413	3.71958
H	4.27225	13.93903	3.49490
H	5.26893	15.28112	2.93651

H	5.02028	15.05360	4.66129
C	16.00726	13.57436	1.09015
H	15.41618	12.80241	1.59379
H	16.97366	13.66029	1.58919
H	16.17926	13.20591	0.07222
C	7.24061	9.95517	3.20454
H	8.18535	9.42105	3.34330
H	6.91192	9.78319	2.17281
H	6.49536	9.47788	3.85071
C	12.38200	11.49824	-1.25371
C	14.15808	23.45156	-0.26055
H	13.15649	23.85945	-0.07505
H	14.41350	23.66535	-1.30305
H	14.84831	24.02461	0.36869
C	11.83146	10.26517	-1.90360
H	12.51219	9.41208	-1.79718
H	11.67060	10.41385	-2.97613
H	10.87684	9.96051	-1.45938
C	10.03029	13.84085	4.81772
H	9.95990	14.18964	5.85532
H	10.33990	14.71578	4.23019
H	10.82840	13.09564	4.76670
C	5.34131	19.75412	4.56640
H	5.26891	19.05647	3.72219
H	4.50415	20.45375	4.49428
H	5.20618	19.15218	5.47196
H	6.89764	18.15233	2.46781
H	12.19015	16.34949	-1.16642
H	9.88925	17.43897	3.23920
H	11.73580	16.63150	1.99233
Mg	8.08465	17.05276	3.57503
Al	10.61464	17.04422	-1.15740
Mg	4.59525	16.93240	-0.62388
N	3.37969	18.58462	-0.82529
N	8.60300	13.89172	-0.35818
N	2.98038	15.66212	-0.82699
N	9.24571	16.61191	-5.16615
N	9.84255	19.50294	-4.74613
C	7.89851	14.60074	-4.76969
C	3.11731	14.32508	-0.36225
C	7.25029	13.59716	-0.93382
H	6.51157	13.87522	-0.16395
H	7.10825	14.27667	-1.78399
C	2.95317	12.71655	1.43091
H	2.69801	12.48728	2.46655
C	2.13724	18.54752	-1.30847
C	4.60227	20.68519	-1.17496
C	10.18829	20.76083	-4.17704
C	9.15537	15.21372	-4.91288
C	3.63965	20.16958	1.00775
C	2.78572	14.02451	0.97185
C	7.84584	13.21886	-4.56127
H	6.86897	12.74304	-4.46423
C	3.87150	19.82627	-0.33761
C	8.85966	12.98434	0.80283
H	9.86672	13.21020	1.17293
H	8.14783	13.26624	1.58994
C	9.65377	13.73341	-1.39307
H	9.42047	14.38971	-2.23685
H	10.62361	14.01932	-0.96968
H	9.72802	12.70343	-1.75760
C	9.24480	21.80561	-4.16581

C	2.26845	15.10411	1.87089
H	2.00984	14.71136	2.85832
H	3.01991	15.89499	2.00258
H	1.38027	15.59668	1.45679
C	9.64554	23.07040	-3.74050
H	8.92238	23.88658	-3.76945
C	2.87408	19.23755	1.89637
H	2.73550	19.66320	2.89378
H	1.88522	18.99453	1.48878
H	3.39920	18.27816	2.00512
C	3.61193	13.32090	-1.21341
C	1.79530	16.03538	-1.31572
C	4.12603	21.38680	1.48449
H	3.92855	21.65910	2.52186
C	7.08201	12.14188	-1.32297
H	6.07831	12.00914	-1.73456
H	7.77846	11.89234	-2.13075
C	8.70060	11.51290	0.45541
H	8.88836	10.92458	1.36034
H	9.47087	11.21325	-0.26818
C	6.63997	15.40142	-4.90203
H	5.76333	14.75001	-4.95909
H	6.49321	16.07638	-4.04855
H	6.65401	16.03541	-5.79538
C	10.93925	23.31881	-3.27333
C	9.21611	15.95571	-7.53497
H	8.28235	15.39249	-7.43470
H	9.23939	16.42013	-8.52201
H	10.02124	15.21450	-7.48661
C	1.44930	17.36230	-1.62597
H	0.45976	17.49800	-2.04943
C	3.99604	13.65653	-2.62162
H	4.31913	12.76627	-3.17053
H	3.17011	14.11627	-3.17721
H	4.81270	14.39266	-2.64719
C	9.90889	19.43765	-6.08604
C	9.62009	18.30072	-6.85352
H	9.69122	18.44013	-7.92672
C	0.72032	14.99714	-1.50943
H	0.38510	14.60403	-0.54263
H	-0.14675	15.41015	-2.02730
H	1.09207	14.13453	-2.07222
C	8.99556	12.43046	-4.50828
C	4.84607	20.30659	-2.60042
H	5.33305	21.11643	-3.14889
H	5.48930	19.41682	-2.67163
H	3.91860	20.04788	-3.12359
C	10.33647	14.44451	-4.83770
C	10.36774	20.64583	-6.86689
H	11.35145	20.97967	-6.51899
H	10.43479	20.42265	-7.93229
H	9.69987	21.50303	-6.73691
C	7.31902	11.23750	-0.12251
H	7.21430	10.18072	-0.39886
H	6.55243	11.44985	0.64003
C	11.48001	20.96719	-3.66421
C	3.42372	11.69609	0.60323
C	9.35105	16.98332	-6.43992
C	10.23175	13.06711	-4.64493
H	11.14642	12.47349	-4.60474
C	11.82649	22.24295	-3.20625
H	12.83229	22.40303	-2.81580

C	5.07322	21.89411	-0.65461
H	5.62603	22.56905	-1.31170
C	3.73821	12.02224	-0.71743
H	4.09539	11.23750	-1.38520
C	8.91361	10.94901	-4.29280
H	7.89730	10.57502	-4.44740
H	9.58051	10.40190	-4.96745
H	9.20762	10.66792	-3.27164
C	12.47722	19.85096	-3.66418
H	13.46592	20.20798	-3.36633
H	12.19340	19.05427	-2.95904
H	12.55821	19.37504	-4.64840
C	1.37465	19.83514	-1.48260
H	1.96530	20.58182	-2.02310
H	0.43400	19.67489	-2.01193
H	1.14430	20.28151	-0.50817
C	11.35803	24.70409	-2.88178
H	10.57332	25.22468	-2.32158
H	12.25981	24.69508	-2.26210
H	11.57681	25.31933	-3.76232
C	4.83991	22.26915	0.66996
C	3.56413	10.28944	1.10272
H	4.46411	9.80722	0.70559
H	3.61924	10.25052	2.19521
H	2.71391	9.66531	0.80314
C	5.35730	23.56446	1.21713
H	4.62788	24.05092	1.87367
H	6.26111	23.41080	1.82271
H	5.61489	24.26898	0.42041
C	7.83828	21.54943	-4.60927
H	7.75930	21.37380	-5.68941
H	7.43580	20.64808	-4.13219
H	7.18689	22.39318	-4.36093
C	11.67694	15.09244	-5.00068
H	11.83594	15.86940	-4.24214
H	12.48126	14.35727	-4.90944
H	11.78128	15.58873	-5.97339
H	10.54053	16.70765	-2.76987
H	5.14686	16.74085	1.21727
H	7.49502	17.95801	-2.95336
H	5.90698	16.44002	-1.92798
Al	8.62178	15.86383	0.25809
Al	7.31639	17.41152	-1.38852
Mg	9.30282	17.91520	-3.52964

Alternative $[Al_4H_8Mg_6(NMP)_2(^{Mes}Nacnac)_4]$ cluster
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scf done: -6770.677973

C	5.022341	23.320057	0.439922
C	4.263019	22.511923	1.289836
C	3.879102	21.220413	0.925926
C	4.264732	20.720254	-0.331953
C	5.062646	21.497858	-1.187023
C	5.417154	22.790578	-0.789408
C	5.510805	20.947626	-2.506763
C	3.037917	20.372244	1.834846
N	3.797489	19.439419	-0.736846
C	2.583006	19.416889	-1.305002
C	1.912143	20.728443	-1.655017
C	5.451901	24.697853	0.862480
Mg	4.952019	17.720821	-0.506621
N	3.234096	16.536936	-0.630200

C	2.082846	16.939509	-1.147921
C	0.925375	15.972117	-1.247770
Al	7.104729	16.522424	1.009825
Mg	7.974164	16.527352	3.804503
N	7.910734	14.931367	5.129078
C	7.654924	15.044374	6.427167
C	7.604928	13.801403	7.287602
Al	9.810220	16.909952	1.569964
Mg	9.154584	15.458974	-0.640635
N	8.633949	13.433170	-0.877564
C	7.265632	13.293401	-1.423541
C	6.867409	11.836721	-1.624032
C	6.990106	11.067674	-0.309439
C	8.396764	11.225781	0.265050
C	8.750127	12.700413	0.403421
C	9.664561	13.050597	-1.850554
Mg	8.222234	18.900387	0.579348
N	8.613111	20.950393	0.817912
C	9.836430	21.166388	1.619345
C	10.129971	22.644825	1.845086
C	10.234286	23.374602	0.505469
C	8.975426	23.132844	-0.327595
C	8.728858	21.639186	-0.486452
C	7.391643	21.309761	1.551279
Al	10.303556	17.839054	-1.039934
Mg	12.480784	16.804822	0.513066
N	14.135899	17.983274	0.944178
C	15.260464	17.512343	1.465196
C	16.351955	18.476114	1.871589
Al	7.565749	17.471014	-1.667915
N	13.642361	15.096600	0.502118
C	13.180810	13.900946	-0.112818
C	12.480857	12.943219	0.637560
C	12.147791	11.726939	0.032605
C	12.456476	11.458530	-1.301381
C	13.090656	12.458292	-2.045609
C	13.456262	13.677505	-1.474251
C	12.108581	13.235632	2.060560
C	14.142644	14.748643	-2.272504
C	12.074674	10.152998	-1.943365
C	14.845147	15.040023	1.086911
C	15.575101	13.715019	1.139799
C	14.076134	19.361988	0.607579
C	14.545983	19.764664	-0.656742
C	14.491848	21.113699	-1.001435
C	13.982394	22.075328	-0.123960
C	13.504375	21.644865	1.113134
C	13.529623	20.299909	1.494838
C	15.098300	18.737409	-1.602601
C	12.997430	19.865167	2.830158
C	13.959591	23.530847	-0.504169
C	8.186642	13.625131	4.636705
C	9.501167	13.127900	4.704486
C	9.740947	11.809543	4.317179
C	8.721310	10.983519	3.838267
C	7.439593	11.523150	3.723217
C	7.149961	12.832560	4.117959
C	10.612722	14.000296	5.214782
C	9.000293	9.544983	3.492204
C	5.750179	13.368381	4.031220
C	15.536529	16.139592	1.619430
C	7.419233	16.267181	7.083884

C	7.378065	17.569928	6.569022
C	7.110811	18.665157	7.579446
N	7.552187	17.901236	5.281951
C	7.392440	19.282573	4.978190
C	8.504720	20.139197	4.991783
C	8.296160	21.513400	4.842461
C	7.020272	22.048243	4.656319
C	5.939771	21.165450	4.573128
C	6.104858	19.788006	4.722809
C	9.881408	19.570363	5.185771
C	6.809870	23.530896	4.515298
C	4.941061	18.842655	4.635418
C	3.303639	15.217705	-0.106265
C	3.049337	15.013960	1.260201
C	3.102213	13.718035	1.771842
C	3.415260	12.622273	0.964884
C	3.695383	12.857785	-0.382367
C	3.663888	14.141495	-0.932001
C	2.765561	16.189486	2.149249
C	4.015165	14.386981	-2.371634
C	3.485018	11.233239	1.539098
C	1.835168	18.261779	-1.567978
Mg	9.488364	17.541660	-3.814663
N	10.050447	19.083364	-5.107792
C	10.223884	18.967146	-6.416977
C	10.682962	20.163255	-7.220308
C	10.235567	20.373523	-4.536096
C	9.160859	21.277903	-4.533057
C	9.361459	22.561490	-4.018652
C	10.596905	22.963989	-3.507050
C	11.633267	22.027529	-3.477428
C	11.477638	20.738467	-3.988555
C	7.842810	20.871974	-5.128615
C	10.830990	24.380719	-3.053274
C	12.624344	19.770756	-3.984013
C	10.014256	17.772870	-7.132880
C	9.685438	16.496753	-6.660340
C	9.526361	15.429914	-7.723948
N	9.512925	16.162693	-5.371744
C	9.335170	14.771584	-5.127070
C	8.046845	14.228823	-4.995667
C	7.911389	12.840703	-4.880461
C	9.014218	11.986147	-4.889696
C	10.287785	12.555747	-4.978046
C	10.467528	13.934186	-5.079125
C	6.841779	15.125180	-5.016868
C	8.848403	10.497668	-4.751858
C	11.841946	14.535503	-5.133520
H	10.665703	20.696231	1.077388
H	9.714919	20.631662	2.564866
H	14.872530	21.424484	-1.972485
H	9.155342	22.180251	4.872785
H	7.817752	21.440193	-1.054037
H	9.557707	21.172920	-1.033580
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H	14.366757	14.407551	-3.285616

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H	5.554607	16.218368	0.558674
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H	5.973847	17.062543	-2.016563

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