

Steric Control of Mg–Mg Bond Formation vs N₂ Activation in the Reduction of Bulky Magnesium Diamide Complexes

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Electronic Supplementary Information (45 pages)

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1. Experimental

General considerations.

All manipulations were carried out using standard Schlenk and glove box techniques under an atmosphere of high purity dinitrogen. Pentane was distilled over Na/K alloy (50:50), while hexane, methylcyclohexane, cyclohexane, THF and toluene were distilled over molten potassium. ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra were recorded on either Bruker AvanceIII 600 or Bruker AvanceIII 400 spectrometers and were referenced to the resonances of the solvent used. FTIR spectra were collected for solid samples or Nujol mulls on an Agilent Cary 630 attenuated total reflectance (ATR) spectrometer. High resolution mass spectra were recorded on an Agilent 6450 QTOF MS system (Santa Clara, CA, USA) with a dual ESI source. Microanalyses were carried out by the elemental analysis service at London Metropolitan University. The ICP analysis was carried out on a Perkin Elmer Avio 220 ICP-OES instrument. Melting points were determined in sealed glass capillaries under dinitrogen, and are uncorrected. The starting materials 4,5-dibromo-2,7-diethyl-9,9-dimethylxanthene,¹ TripNH₂,² 5% w/w K/KI³ and $[\text{Mg}(\text{CH}_2\text{SiMe}_3)_2]$ ⁴ were prepared by literature reported procedures. The gases CO, H₂ and N₂O were dried over P₂O₅ prior to use. All other reagents were used as received.

4,5-bis(2,4,6-triisopropylanilido)-2,7-diethyl-9,9-dimethyl-xanthene (^{Trip}NONH₂). An oven-dried 250 mL Schlenk flask was charged with a magnetic stir bar, 4,5-dibromo-2,7-diethyl-9,9-dimethylxanthene (7.25 g, 17 mmol), 2,4,6-triisopropyl aniline (7.5 g, 34.04 mmol), NaOBu^t (4.5 g, 47.6 mmol), Pd(OAc)₂ (153 mg, 0.68 mmol), DPEPhos (550 mg, 1.02 mmol), and toluene (~50 mL) under a N₂-atmosphere. The reaction mixture was then placed in a preheated oil bath at 100 °C and stirred for 5 days. The progress of the reaction was monitored by TLC. Upon completion, the reaction mixture was cooled to room temperature and diluted with hexane (100 mL), then filtered through celite. The organic layer was then washed with water and brine and dried over MgSO₄. Volatiles were removed under reduced pressure to obtain a brown solid, which was purified by flash column chromatography over neutral alumina using hexane as the eluent. The desired compound was obtained as a white solid (8.5 g, 71%), which could be recrystallized from a hexane solution stored at room temperature. M.p.: 173-177 °C; ^1H NMR (400 MHz, 298 K, C₆D₆) δ 1.05 (t, J = 7.6 Hz, 6H, CH₂CH₃), 1.19 (d, J = 6.9 Hz, 12H, *p*-CH(CH₃)₂), 1.27 (dd, J = 6.9, 4.8 Hz, 24H, *o*-CH(CH₃)₂), 1.62 (s, 6H, C(CH₃)₂), 2.30 (q, J = 7.6 Hz, 4H, CH₂CH₃), 2.87 (sept., J = 6.9 Hz, 2H, *p*-CH(CH₃)₂), 3.51 (sept., J = 6.9 Hz, 4H, *o*-CH(CH₃)₂), 5.92 (s, 2H, NH), 6.36 (d, J = 1.9 Hz, 2H, Ar-*H*), 6.68 (d, J = 2.0 Hz, 2H, Ar-*H*), 7.26 (s, 4H, Ar-*H*).; ^{13}C NMR (101 MHz, 298 K, C₆D₆) δ 16.8 (CH₂CH₃), 23.5 (*o*-CH(CH₃)₂), 24.5 (C(CH₃)₂), 24.9 (*p*-CH(CH₃)₂), 28.9 (*o*-CH(CH₃)₂), 29.5 (CH₂CH₃), 32.8 (C(CH₃)₂), 34.7 (*p*-CH(CH₃)₂), 109.8, 114.5, 122.2, 129.8, 133.7, 136.1, 136.8, 139.5, 147.6, 148.1

(Ar-C); IR ν/cm^{-1} (diamond ATR, neat): 672(w), 690(w), 742(w), 843(s), 878(s), 942(m), 1032(m), 1217(s), 1315(m), 1360(m), 1446(s), 1460(s), 1510(s), 1623(s), 2867(m), 2727(m), 2960(s), 3405(w), 3422(w); HRMS (ESI) m/z : $[\text{M} + \text{H}]^+$ calc. for $\text{C}_{49}\text{H}_{69}\text{N}_2\text{O}$: 701.5404; found: 701.5405.

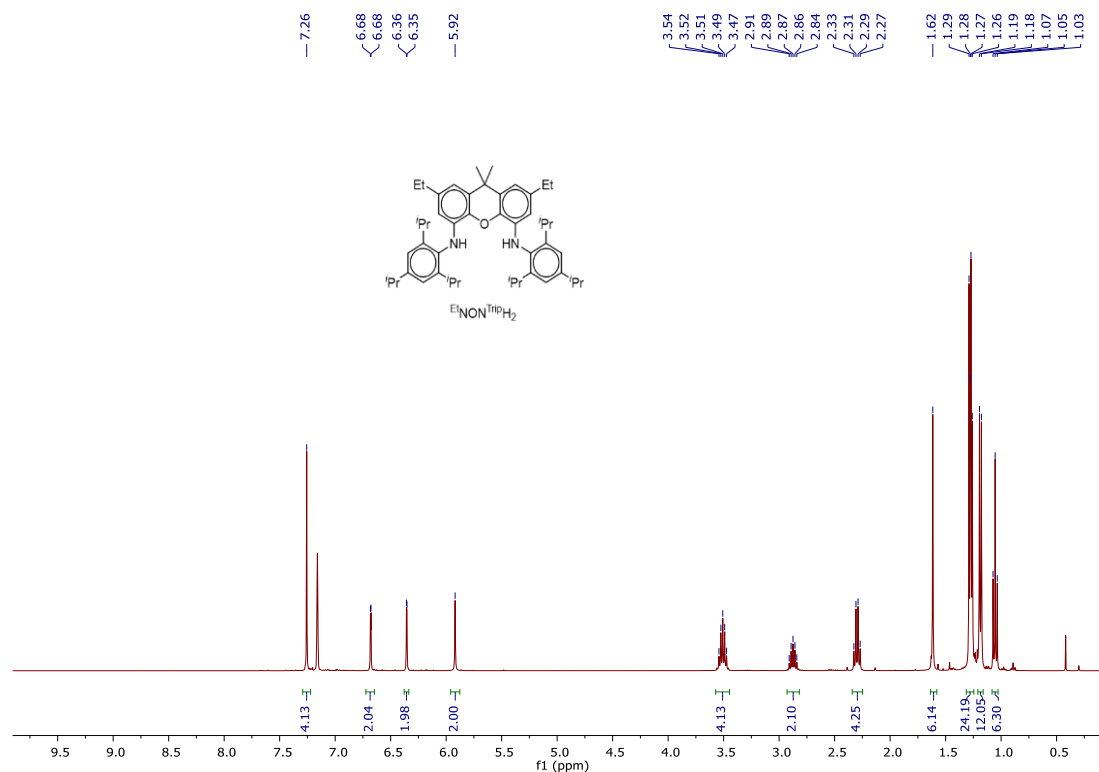


Figure S1. ^1H NMR spectrum (400 MHz, 298 K, C_6D_6) of TripNONH_2 .

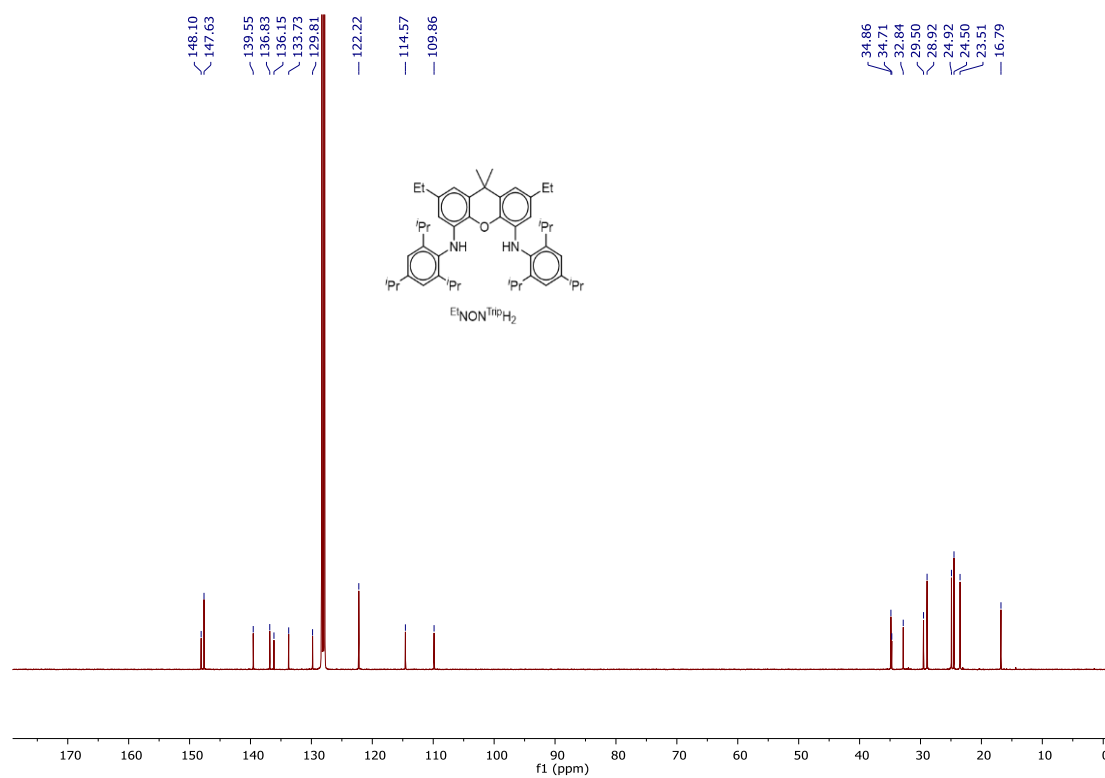


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of TripNONH_2 .

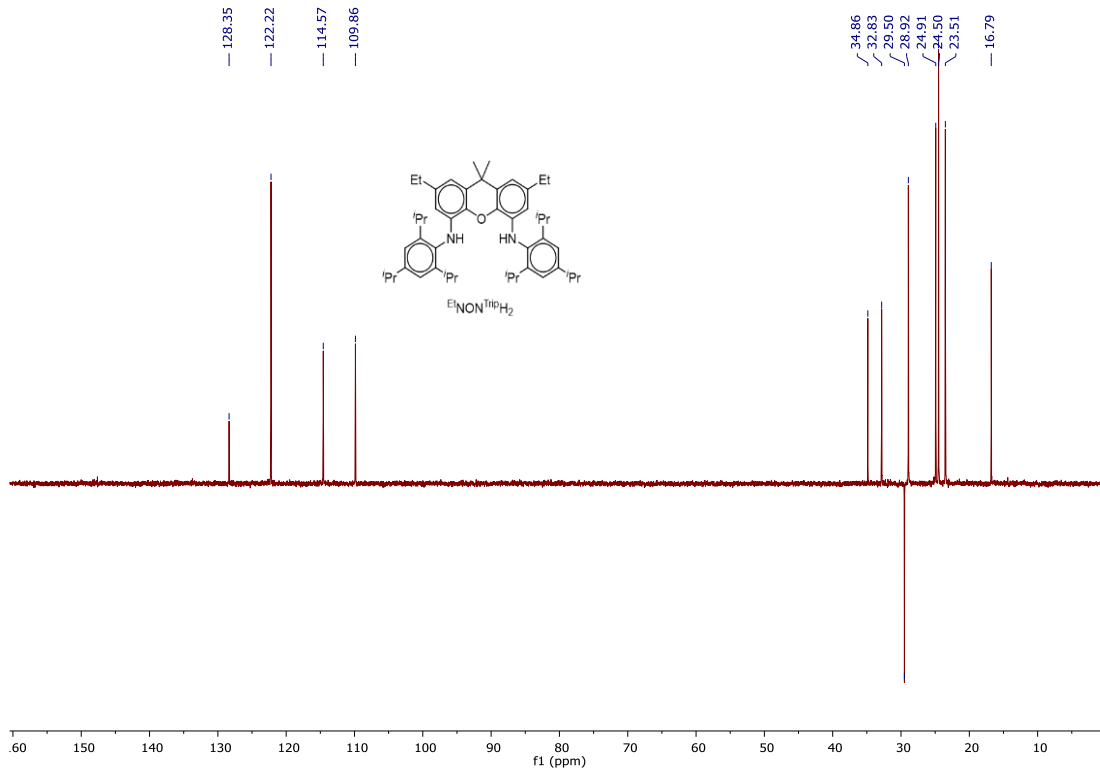


Figure S3. $^{13}\text{C}\{^1\text{H}\}$ (DEPT-135) NMR spectrum (101 MHz, 298 K, C_6D_6) of TripNONH_2 .

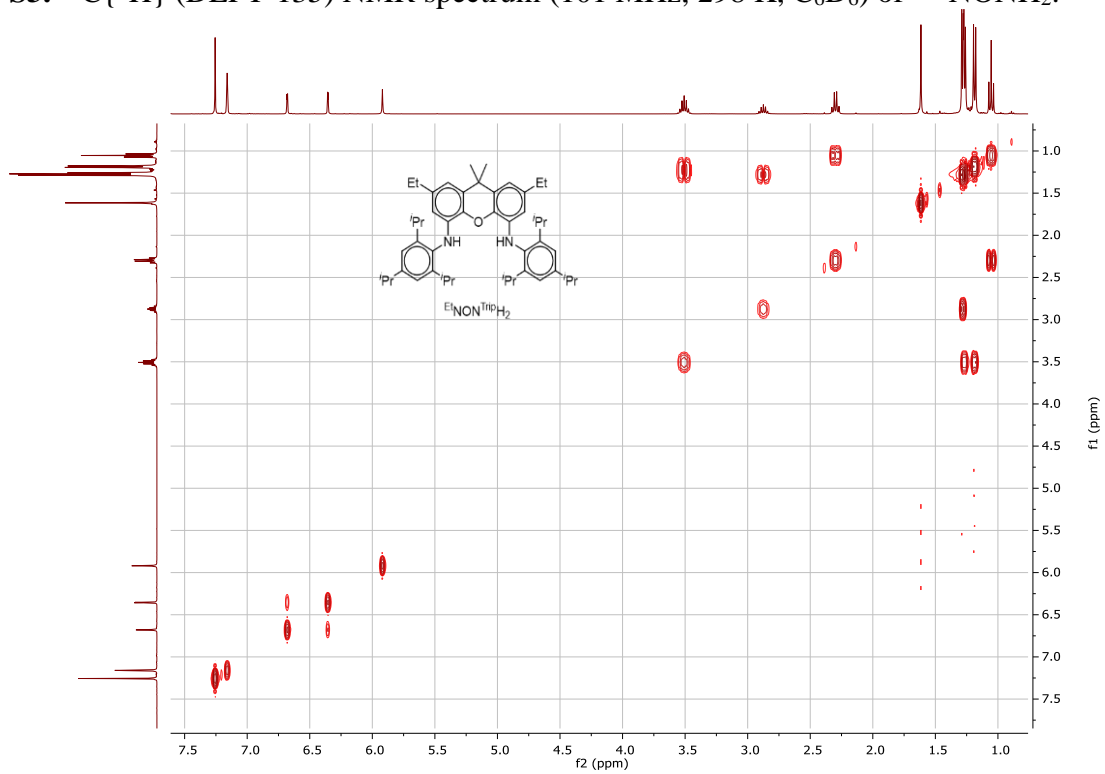


Figure S4. $^1\text{H}-^1\text{H}$ COSY NMR spectrum (101 MHz, 298 K, C_6D_6) of TripNONH_2 .

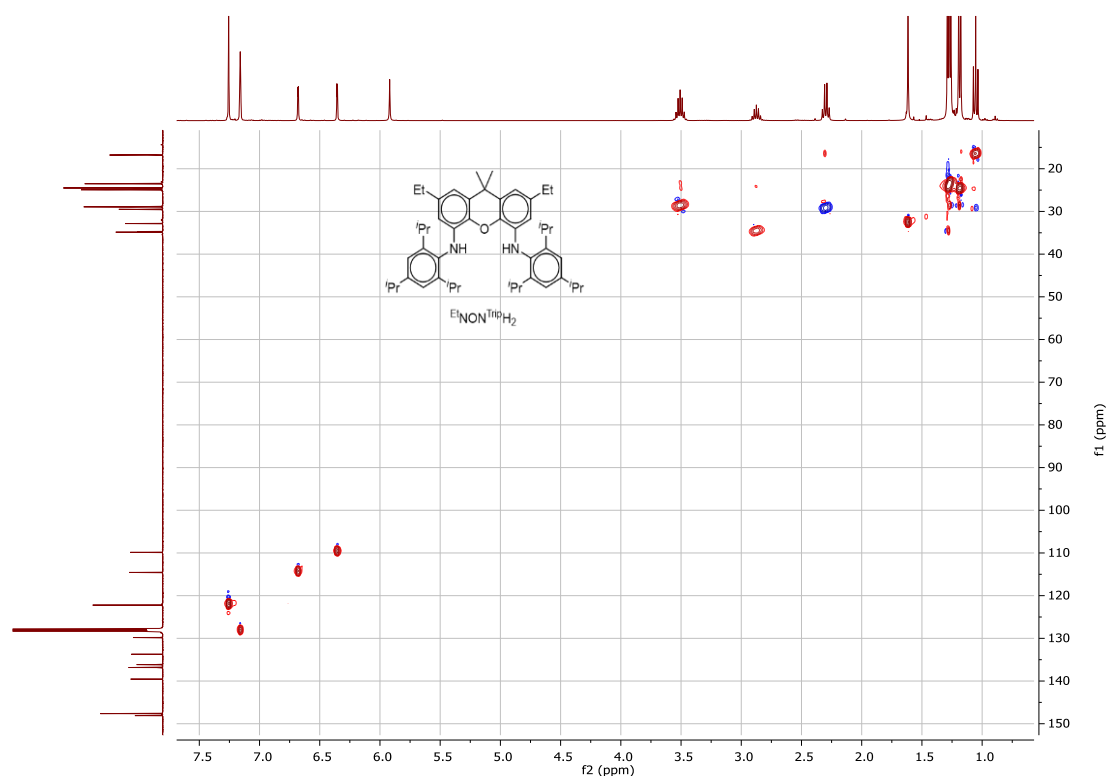


Figure S5. HSQC NMR spectrum (^1H : 400 MHz; ^{13}C : 101 MHz, 298 K, C_6D_6) of TripNONH_2 .

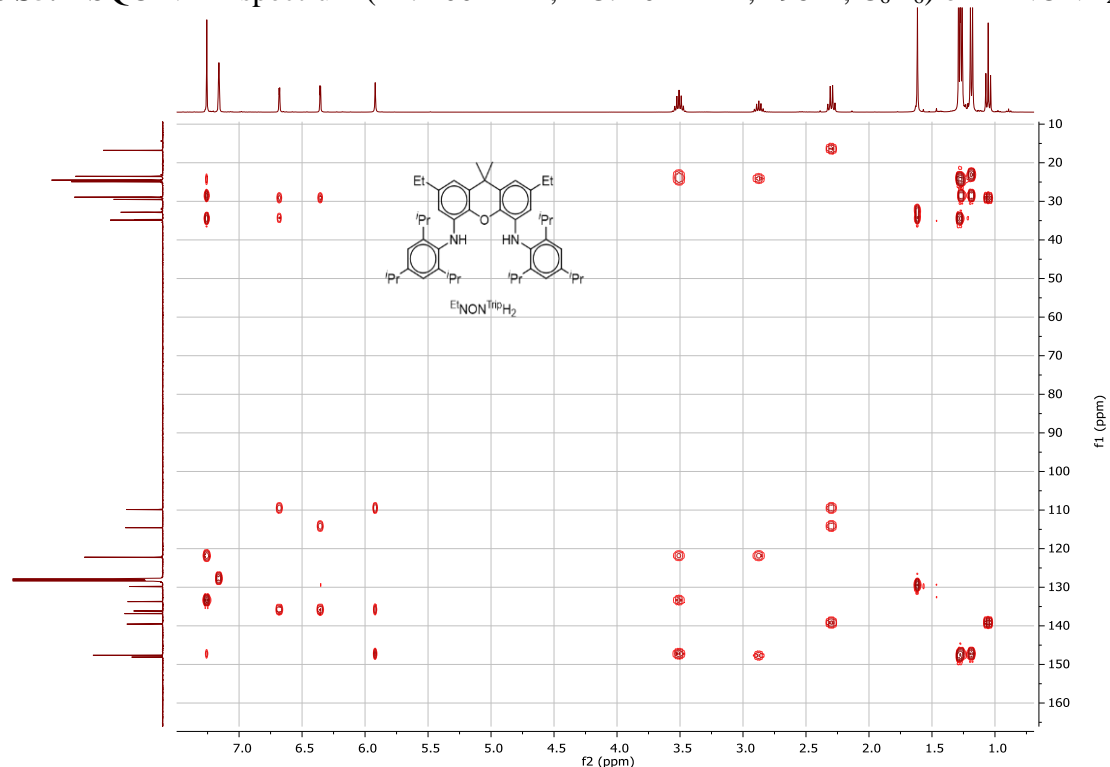


Figure S6. HMBC NMR spectrum (^1H : 400 MHz; ^{13}C : 101 MHz, 298 K, C_6D_6) of TripNONH_2 .

[Mg(TripNON)] (1). An oven-dried Teflon screw cap Schlenk flask was charged with a magnetic stir bar, TripNONH_2 (1.42 g, 2.0 mmol), and $[\text{Mg}(\text{CH}_2\text{SiMe}_3)_2]$ (0.4 g, 2.0 mmol) in a nitrogen-filled glove box. The flask was connected to a Schlenk line and methylcyclohexane (60 mL) was added under a N_2 -atmosphere. The reaction mixture was placed in a preheated oil bath at 90 °C and stirred for 20

mins. Upon completion of the reaction, as determined by $^1\text{H-NMR}$ spectroscopic monitoring, the reaction mixture was cooled to room temperature and volatiles were removed under vacuum to afford the desired compound as a pale yellow solid (1.30 g, 90%); M.p.: 240-243 °C; $^1\text{H NMR}$ (400 MHz, 298 K, C_6D_6) δ 1.10 (t, $J = 7.6$ Hz, 6H, CH_2CH_3), 1.25 (dd, $J = 11.6, 6.8$ Hz, 24H, $o\text{-CH}(\text{CH}_3)_2$), 1.33 (d, $J = 6.9$ Hz, 12H, $p\text{-CH}(\text{CH}_3)_2$), 1.62 (s, 6H, $\text{C}(\text{CH}_3)_2$), 2.36 (q, $J = 7.5$ Hz, 4H, CH_2CH_3), 2.94 (sept., $J = 6.9$ Hz, 2H, $p\text{-CH}(\text{CH}_3)_2$), 3.33 (sept., $J = 6.8$ Hz, 4H, $o\text{-CH}(\text{CH}_3)_2$), 6.05–6.12 (m, 2H, Ar-H), 6.42 (d, $J = 1.8$ Hz, 2H, Ar-H), 7.24 (s, 4H, Ar-H); $^{13}\text{C NMR}$ (101 MHz, 298 K, C_6D_6) δ 17.1 (CH_2CH_3), 24.4 ($o\text{-CH}(\text{CH}_3)_2$), 24.7 ($p\text{-CH}(\text{CH}_3)_2$), 26.0 ($o\text{-CH}(\text{CH}_3)_2$), 28.9 ($o\text{-CH}(\text{CH}_3)_2$), 29.6 ($\text{C}(\text{CH}_3)_2$), 30.1 (CH_2CH_3), 34.6 ($o\text{-CH}(\text{CH}_3)_2$), 35.6 ($\text{C}(\text{CH}_3)_2$), 108.0 112.1, 122.0, 131.5, 138.2, 140.9, 144.3, 144.5, 145.6, 147.2 (Ar-C); IR ν/cm^{-1} (diamond ATR, Nujol): 741(m), 850(m), 878(m), 922(w), 1571(w), 1617(m); anal. calc. for $\text{C}_{56}\text{H}_{80}\text{N}_2\text{OMg}$ **1** (C_7H_{14}): C, 81.87%; H, 9.82%; N, 3.41%; found: C 81.38%; H 9.60%; N 3.27%.

N.B. NMR spectra for the compound acquired in C_6D_6 suggest a symmetrical, monomeric structure in solution, most likely with the magnesium centre coordinated by a molecule of benzene. Spectra acquired in cyclohexane- d_{12} are more complicated and are suggestive of an equilibrium mixture of monomeric and dimeric (likely involving Trip arene \rightarrow Mg intermolecular coordination, as has been seen in the solid state for closely related compounds⁵). These spectra are difficult to assign, though a tentative assignment of a section of variable temperature $^1\text{H NMR}$ spectra of **1** in cyclohexane- d_{12} is given below.

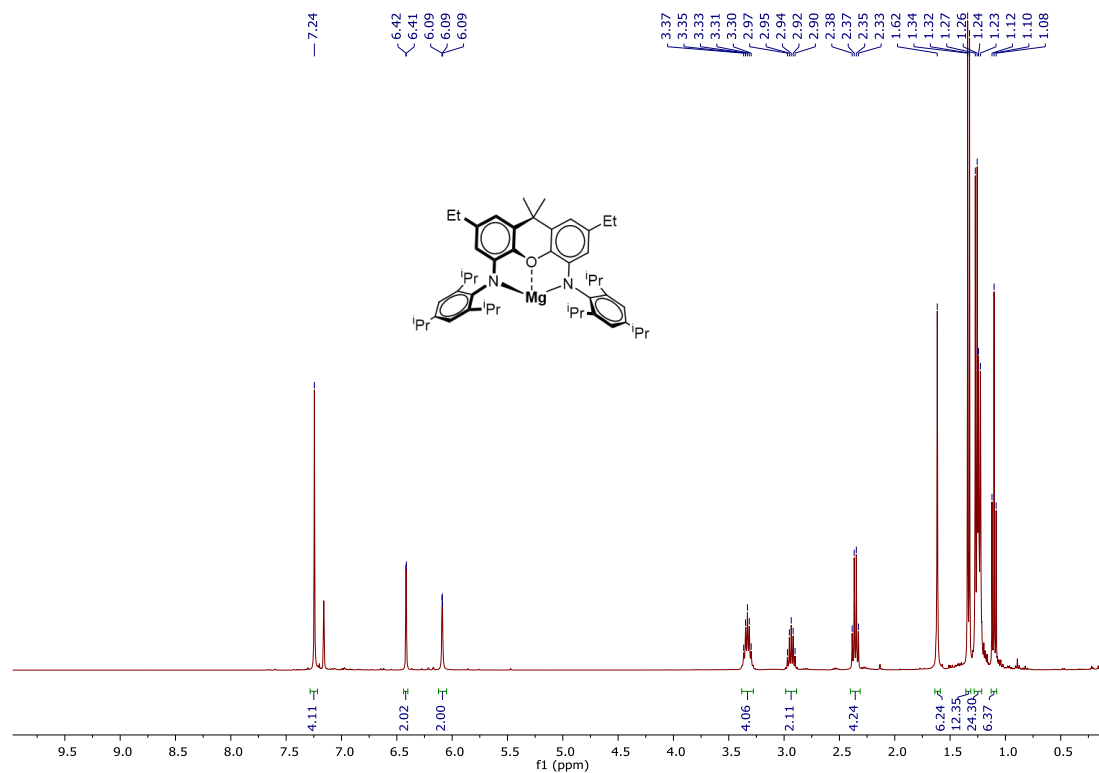


Figure S6. $^1\text{H NMR}$ spectrum (400 MHz, 298 K, C_6D_6) of **1**.

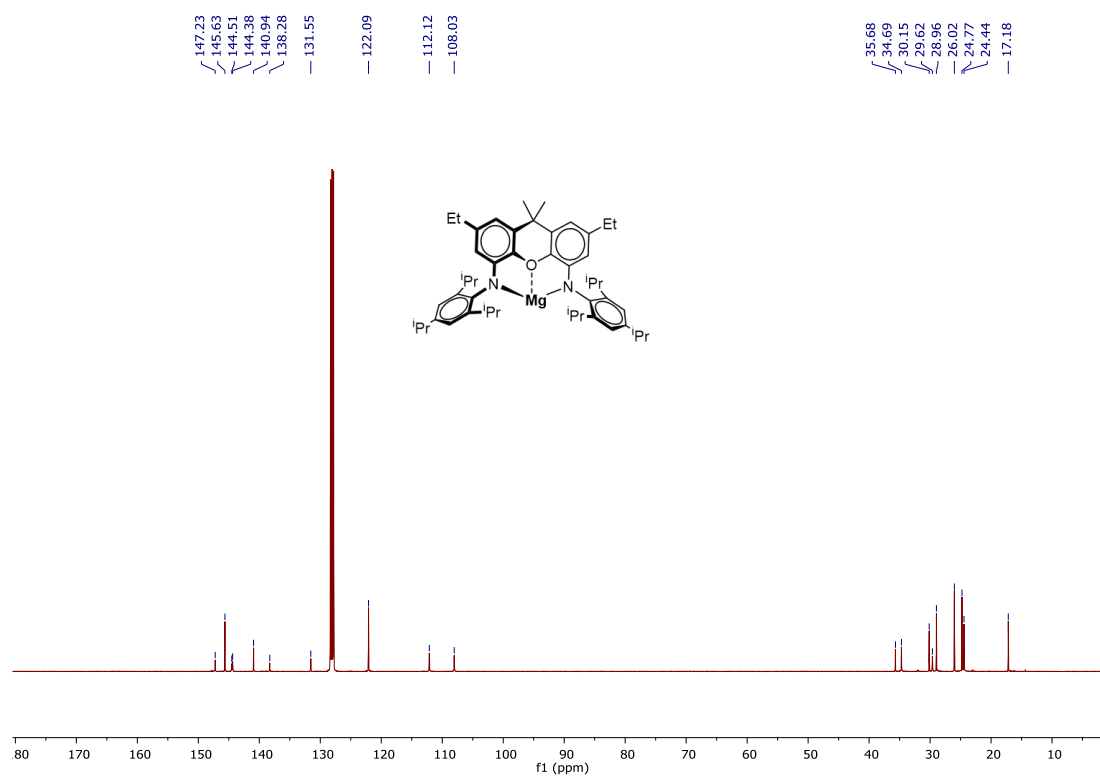


Figure S8. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of **1**.

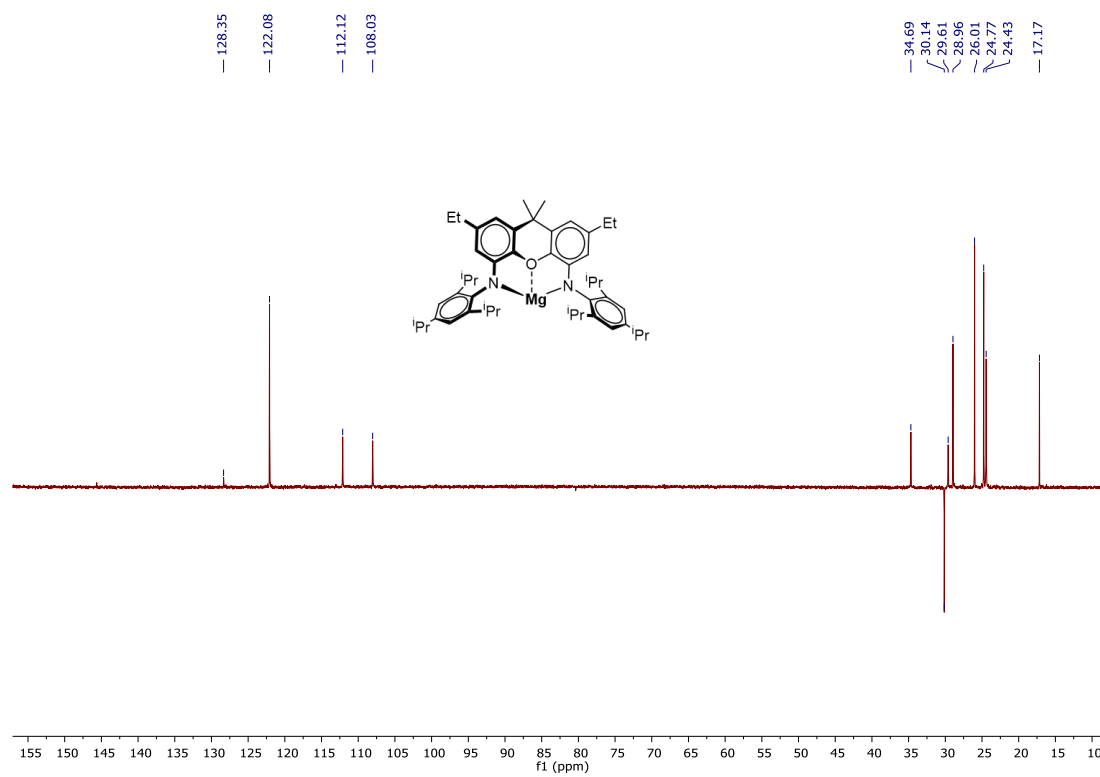


Figure S9. $^{13}\text{C}\{^1\text{H}\}$ (DEPT-135) NMR spectrum (101 MHz, 298 K, C_6D_6) of **1**.

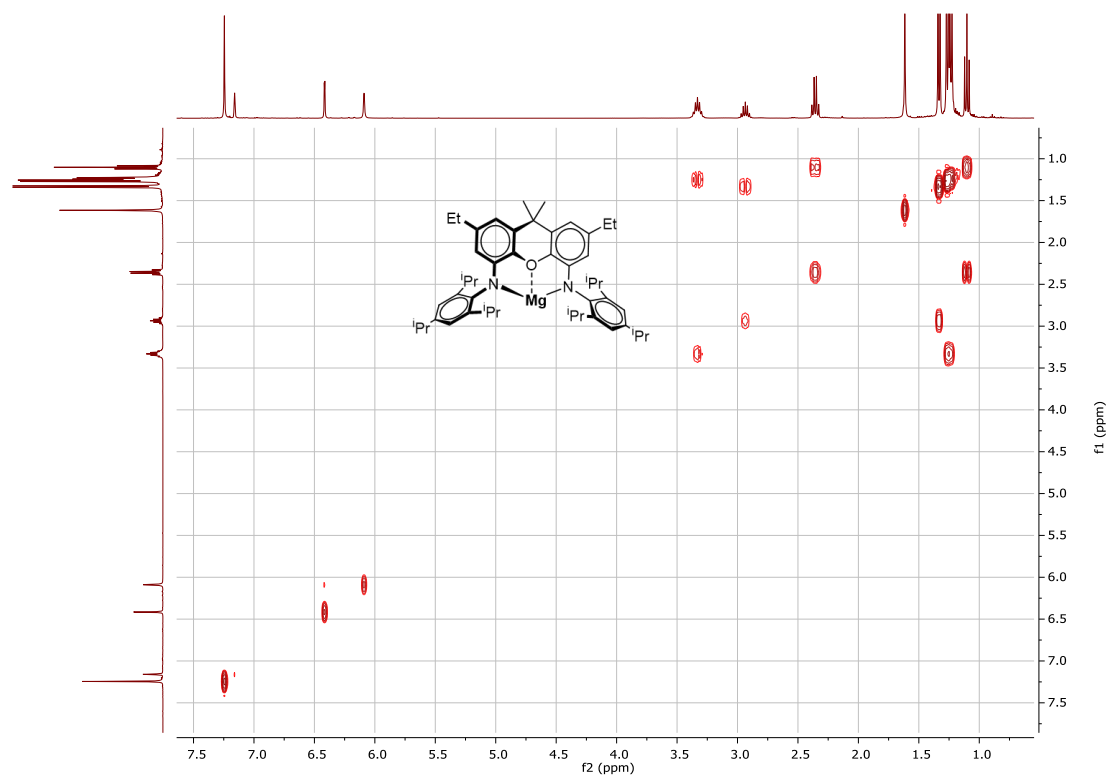


Figure S10. ^1H - ^1H COSY NMR spectrum (400 MHz, 298 K, C_6D_6) of **1**.

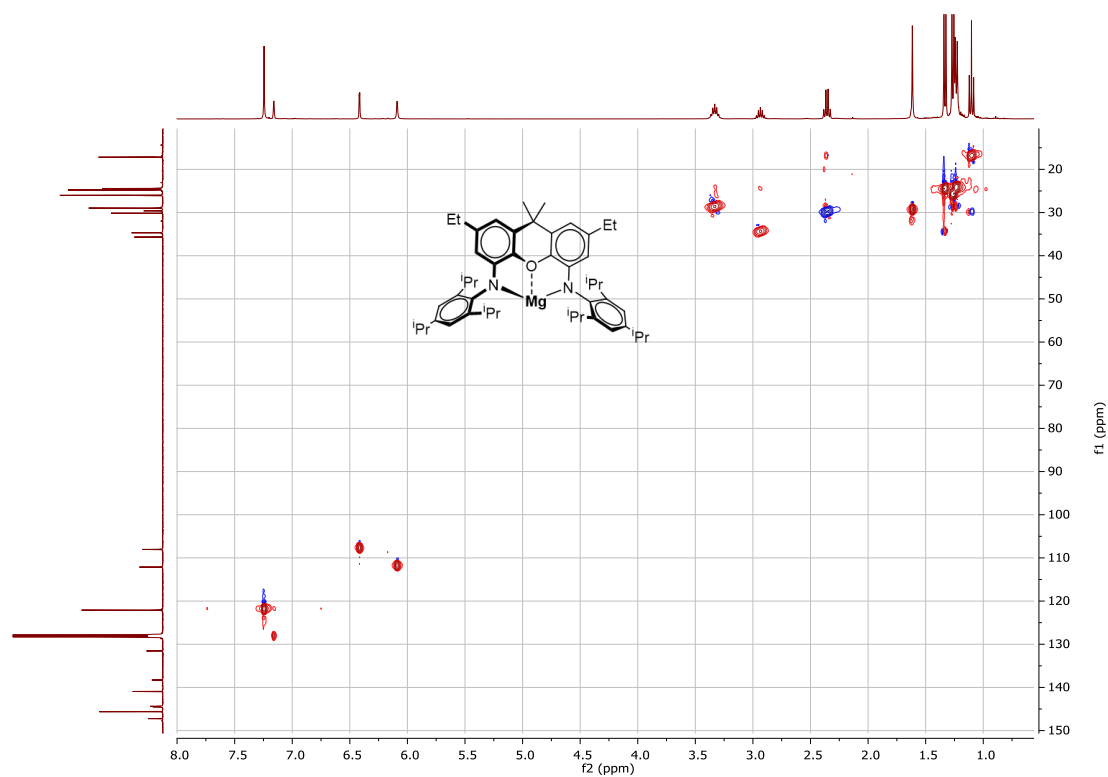


Figure S11. HSQC NMR spectrum (^1H : 400 MHz; ^{13}C : 101 MHz, 298 K, C_6D_6) of **1**.

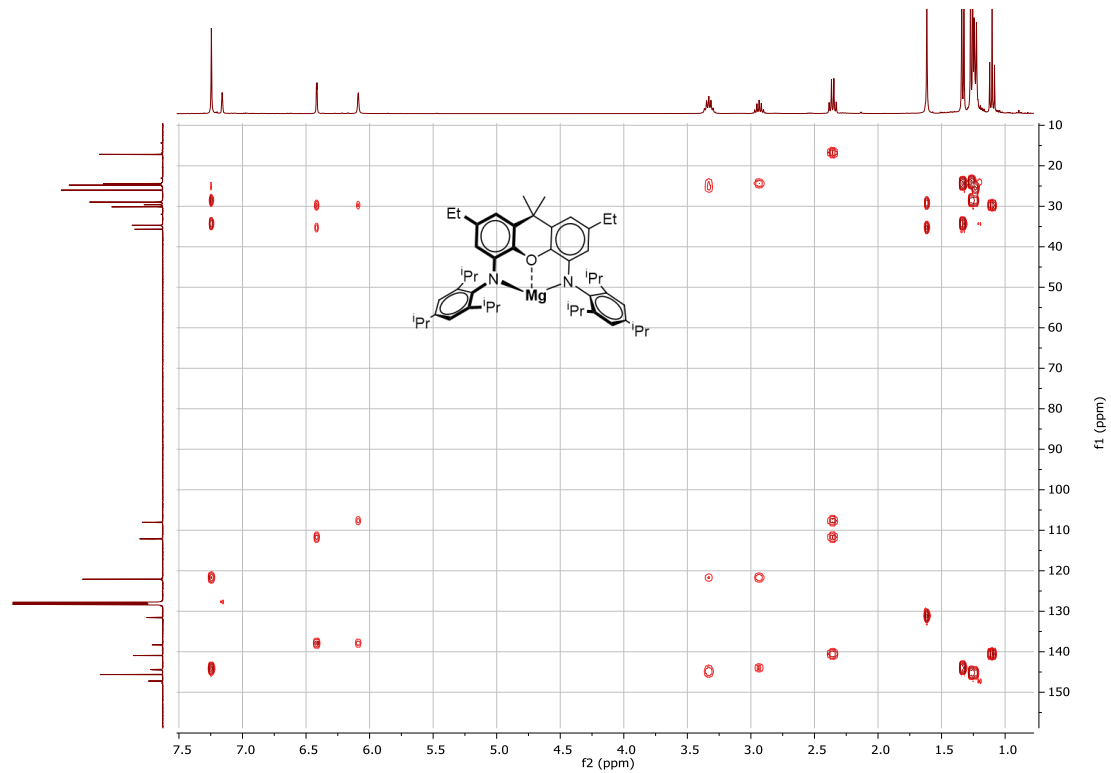


Figure 12. HMBC NMR spectrum (^1H : 400 MHz; ^{13}C : 101 MHz, 298 K, C_6D_6) of **1**.

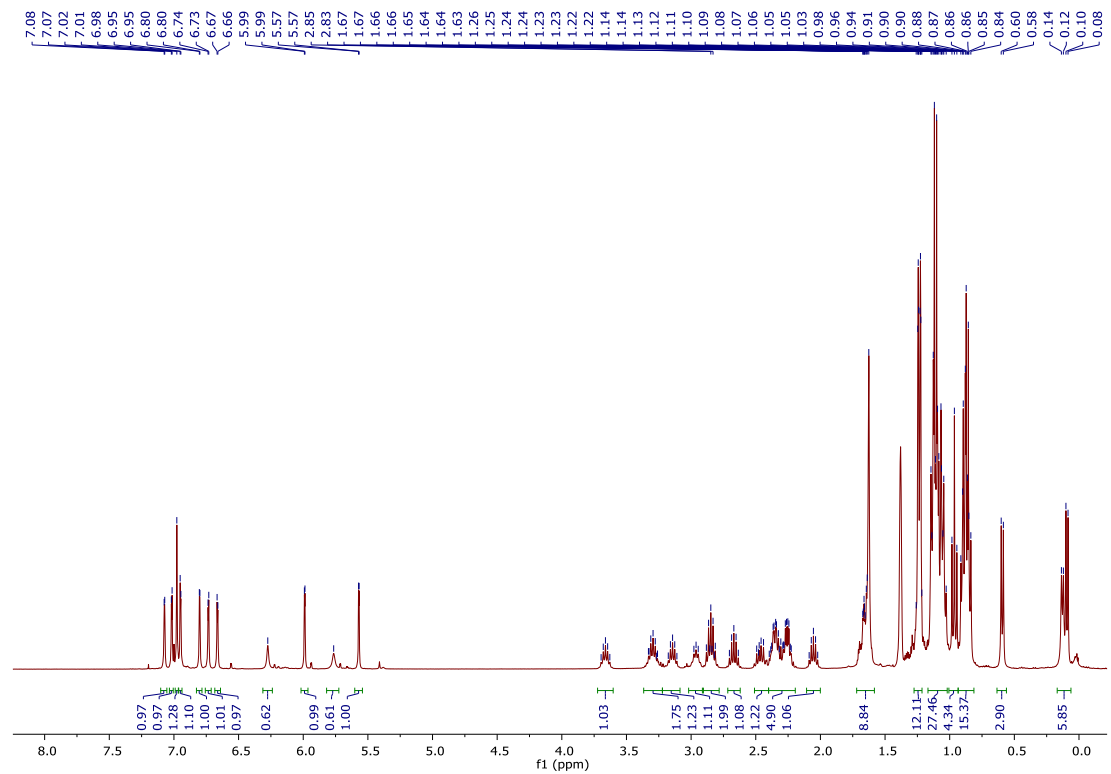


Figure S13. ^1H NMR spectrum (400 MHz, 298 K, C_6D_{12}) of **1**.

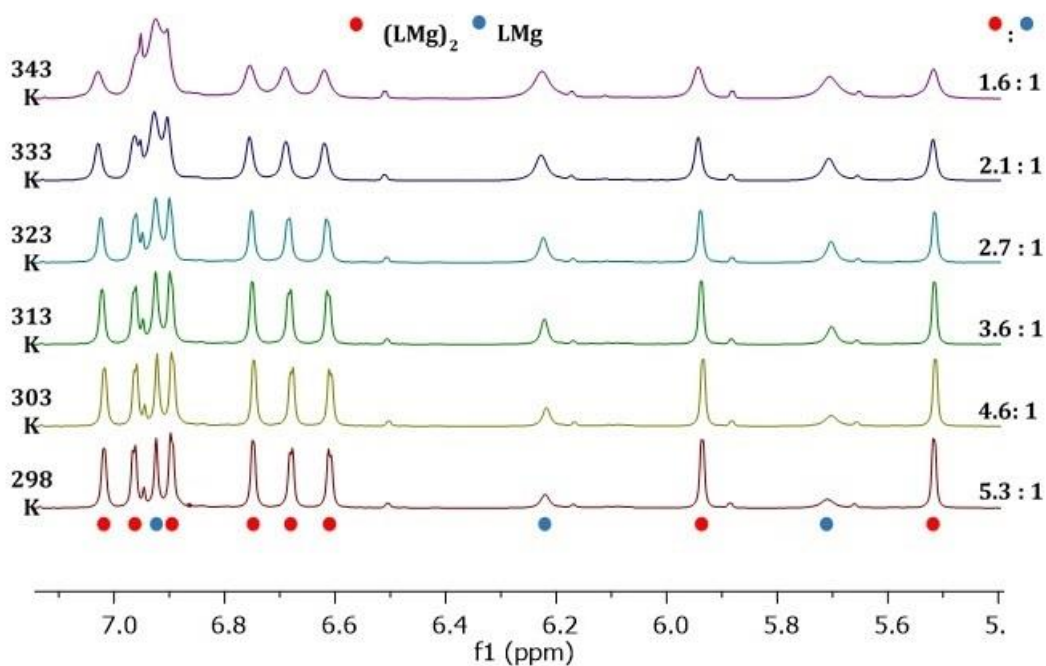


Figure S14. ^1H NMR spectra (400 MHz, 298-343 K, C_6D_{12}) of $[(\text{TripNON})\text{Mg}]_n$ ($n = 1$ or 2); $\text{L} = \text{TripNON}$.

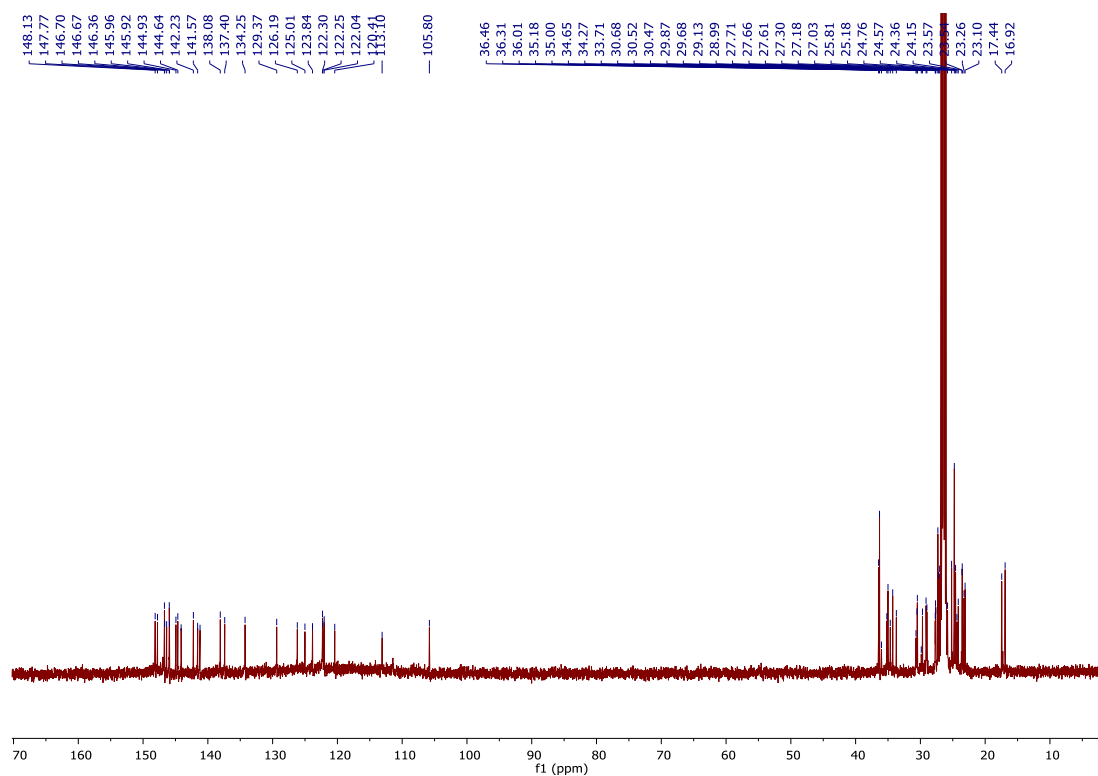


Figure S15. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, 298 K, C_6D_{12}) of **1**.

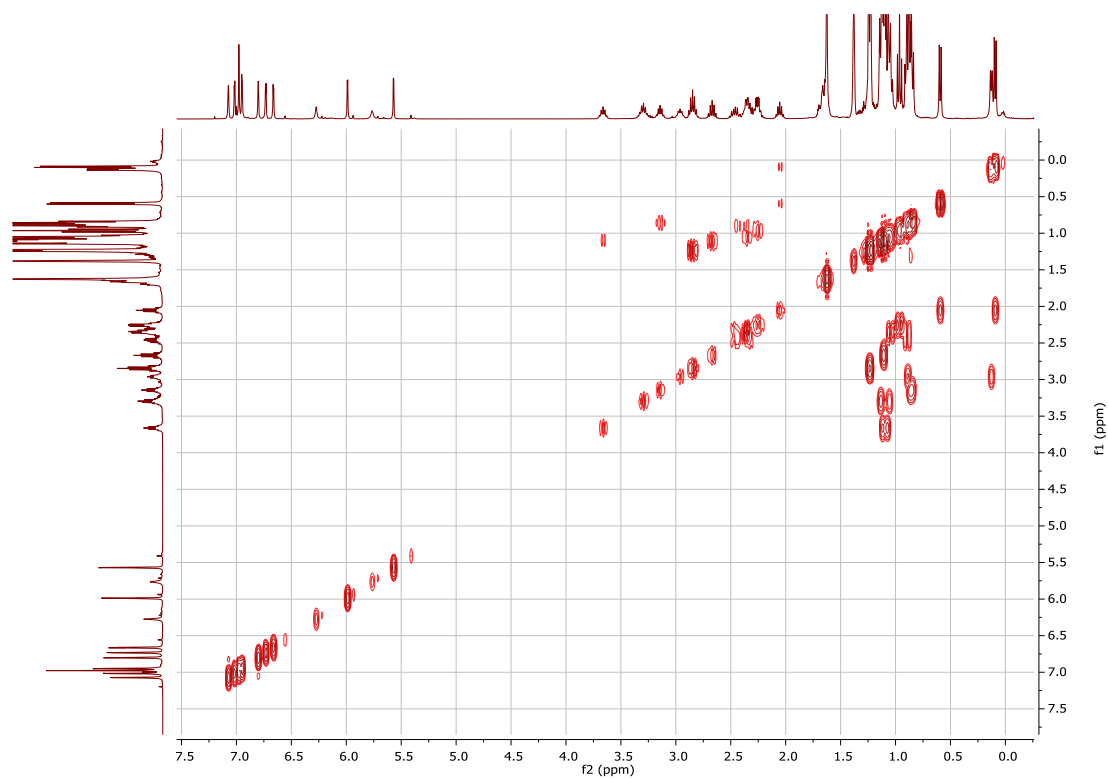


Figure S16. ^1H - ^1H COSY NMR spectrum (400 MHz, 298 K, C_6D_{12}) of **1**.

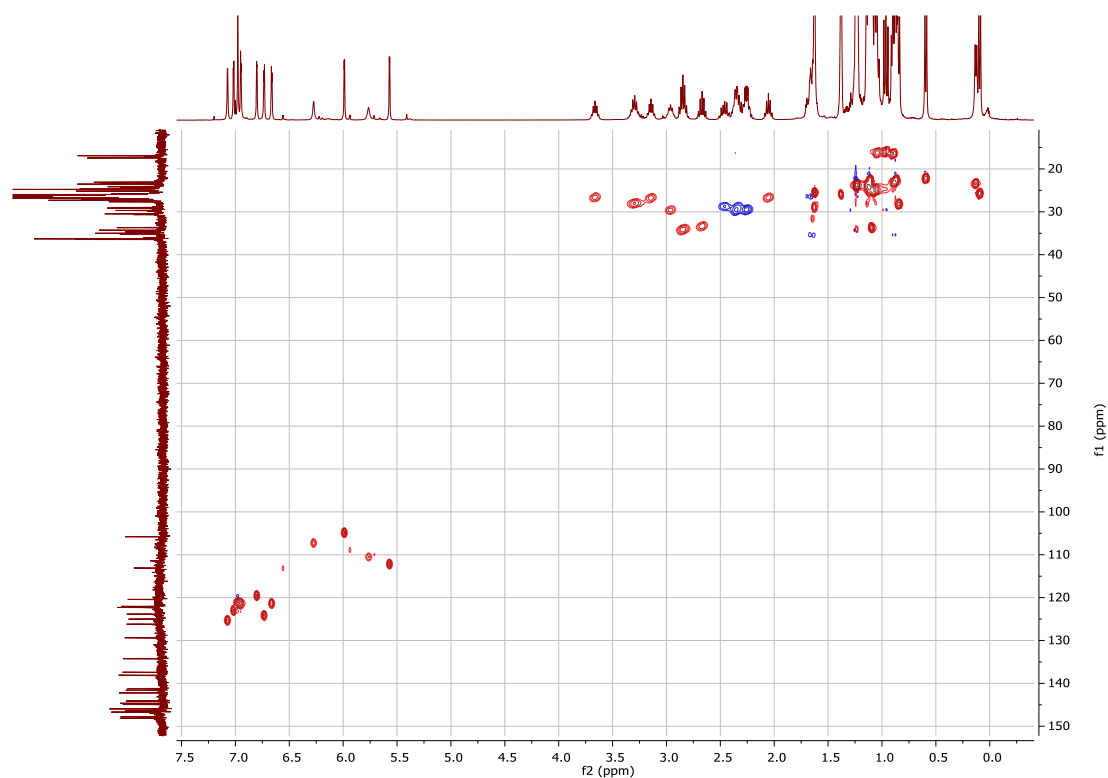


Figure S17. HSQC NMR spectrum (^1H : 400 MHz; ^{13}C : 101 MHz, 298 K, C_6D_{12}) of **1**.

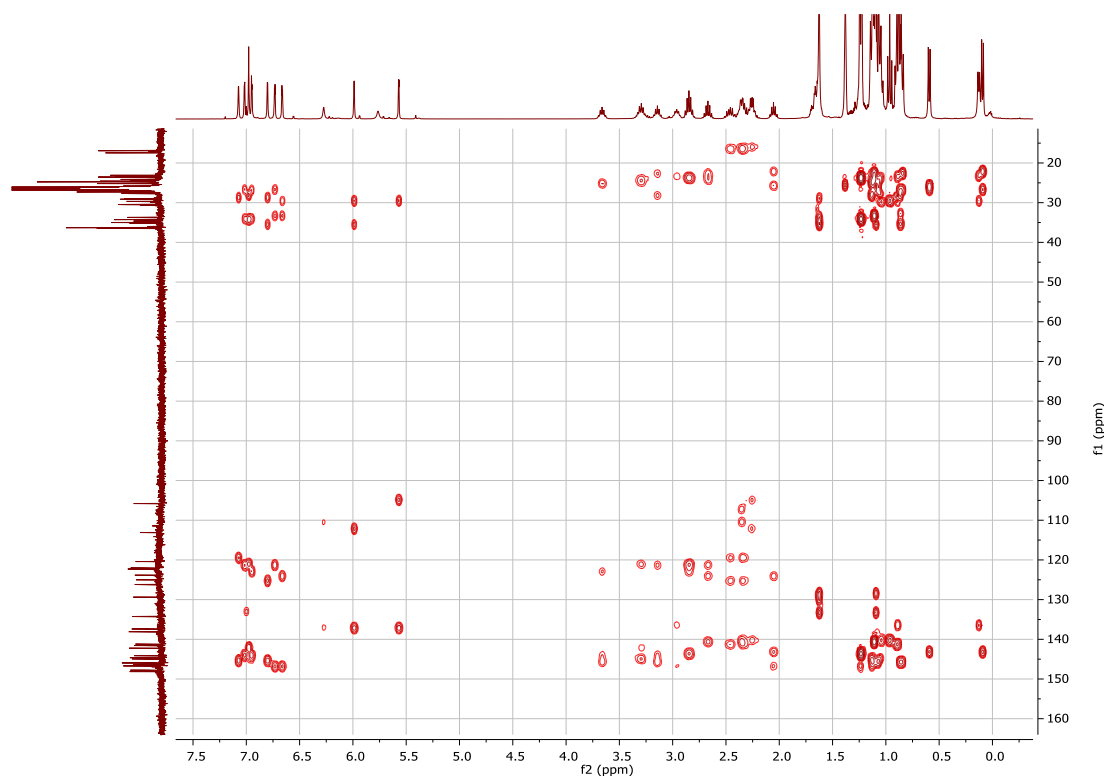


Figure S18. HMBC NMR spectrum (^1H : 400 MHz; ^{13}C : 101 MHz, 298 K, C_6D_{12}) of **1**.

[[K(TripNON)Mg]₂] (2). A 100 mL oven dried Schlenk flask was charged with a magnetic stir bar, [(TripNON)Mg] (1.45 g, 2.0 mmol) and K/KI (5% w/w, 4.8 g, 6.0 mmol). The flask was connected to a Schlenk line and methylcyclohexane (60 mL) added under a positive pressure of N_2 . The reaction mixture was allowed to stir overnight (~ 16 hrs.) to give a dark red/orange solution and then filtered *via* cannula. Volatiles were removed from the filtrate under vacuum to afford a red-orange solid, which was extracted with *n*-pentane (60 mL). The bright orange solution was then concentrated to *ca.* 20 mL and stored at $-30\text{ }^\circ\text{C}$ for 24 hours to obtain bright orange crystals of **2** (0.85 g, 56%). M.p.: $210\text{--}215\text{ }^\circ\text{C}$; ^1H NMR (400 MHz, 298 K, C_6D_6) δ 0.54 (d, $J = 6.9\text{ Hz}$, 6H, $\text{CH}(\text{CH}_3)_2$), 0.80 – 0.87 (m, 12H, $\text{CH}(\text{CH}_3)_2$), 0.95 (m, 18H, $\text{CH}_2\text{CH}_3 + \text{CH}(\text{CH}_3)_2$), 1.11 (t, $J = 7.6\text{ Hz}$, 6H, CH_2CH_3), 1.29 (m, 12H, $\text{CH}(\text{CH}_3)_2$), 1.35–1.38 (m, 6H, $\text{CH}(\text{CH}_3)_2$), 1.42 (m, 12H, $\text{CH}(\text{CH}_3)_2$), 1.51 (m, 12H, $\text{CH}(\text{CH}_3)_2$), 1.68 (s, 12H, $\text{C}(\text{CH}_3)_2$), 2.11 (q, $J = 7.5\text{ Hz}$, 4H, CH_2CH_3), 2.40 (m, 6H, $\text{CH}_2\text{CH}_3 + \text{CH}(\text{CH}_3)_2$), 2.97–3.09 (m, 2H, $\text{CH}(\text{CH}_3)_2$), 3.21–3.35 (m, 2H, $\text{CH}(\text{CH}_3)_2$), 3.80 (sept., $J = 6.5\text{ Hz}$, 4H, $\text{CH}(\text{CH}_3)_2$), 3.93–4.07 (m, 2H, $\text{CH}(\text{CH}_3)_2$), 5.78 (d, $J = 1.8\text{ Hz}$, 2H, Ar-*H*), 6.03 (d, $J = 1.8\text{ Hz}$, 2H, Ar-*H*), 6.22 (d, $J = 1.8\text{ Hz}$, 2H, Ar-*H*), 6.30 (d, $J = 1.8\text{ Hz}$, 2H, Ar-*H*), 6.96 (d, $J = 2.2\text{ Hz}$, 2H, Ar-*H*), 7.04 (d, $J = 2.3\text{ Hz}$, 2H, Ar-*H*), 7.13 (d, $J = 2.3\text{ Hz}$, 2H, Ar-*H*), 7.26–7.30 (m, 2H, Ar-*H*); ^{13}C NMR (101 MHz, 298 K, C_6D_6) δ 16.7, 17.3 (CH_2CH_3), 20.8, 22.4, 23.8, 24.1, 24.3 ($\text{CH}(\text{CH}_3)_2$), 24.6 ($\text{C}(\text{CH}_3)_2$), 24.8, 24.9, 25.3, 25.4, 25.7, 25.9 ($\text{CH}(\text{CH}_3)_2$), 27.8 ($\text{CH}(\text{CH}_3)_2$), 29.0 ($\text{CH}(\text{CH}_3)_2$), 29.9, 30.0 (CH_2CH_3), 30.2, 31.2, 33.7 ($\text{CH}(\text{CH}_3)_2$), 34.6 ($\text{C}(\text{CH}_3)_2$), 35.0 ($\text{CH}(\text{CH}_3)_2$), 36.01 ($\text{C}(\text{CH}_3)_2$),

105.0, 106.3, 111.9, 112.1, 120.7, 121.4, 122.7, 123.2, 131.8, 135.4, 138.1, 140.2, 141.2, 141.8, 142.1, 143.1, 143.3, 146.1, 146.7, 147.2, 147.8, 148.8, 149.0, 151.9 (Ar-C); IR ν/cm^{-1} (diamond ATR, Nujol): 677(m), 698(m), 755(m), 845(m), 870(m), 922(m), 938(m), 1025(s), 1572(w), 1609(w); anal. calc. for $\text{C}_{108}\text{H}_{156}\text{N}_4\text{O}_2\text{K}_2\text{Mg}_2$ (**2**·pentane): C, 77.71%; H, 9.42%; N, 3.36%; found: C, 77.49%; H, 9.36%; N, 3.31%.



Figure S19. Photographs of isolated crystals of **2**.

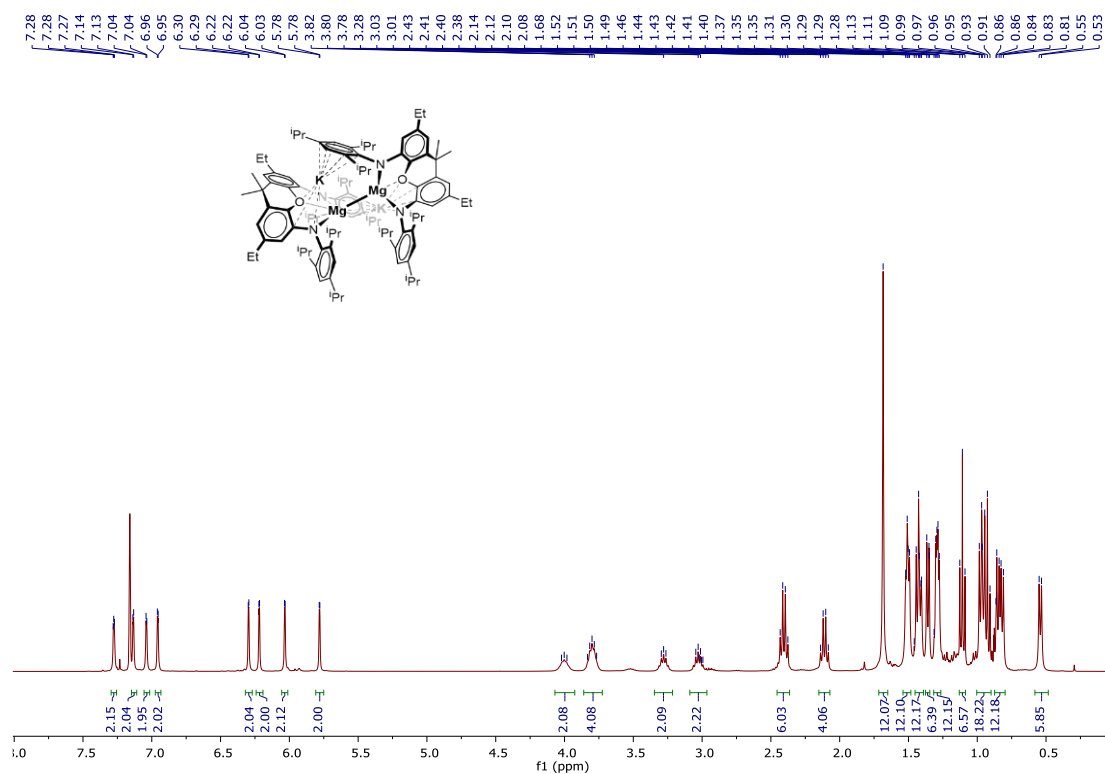


Figure S20. ^1H NMR spectrum (400 MHz, 298 K, C_6D_6) of **2**.

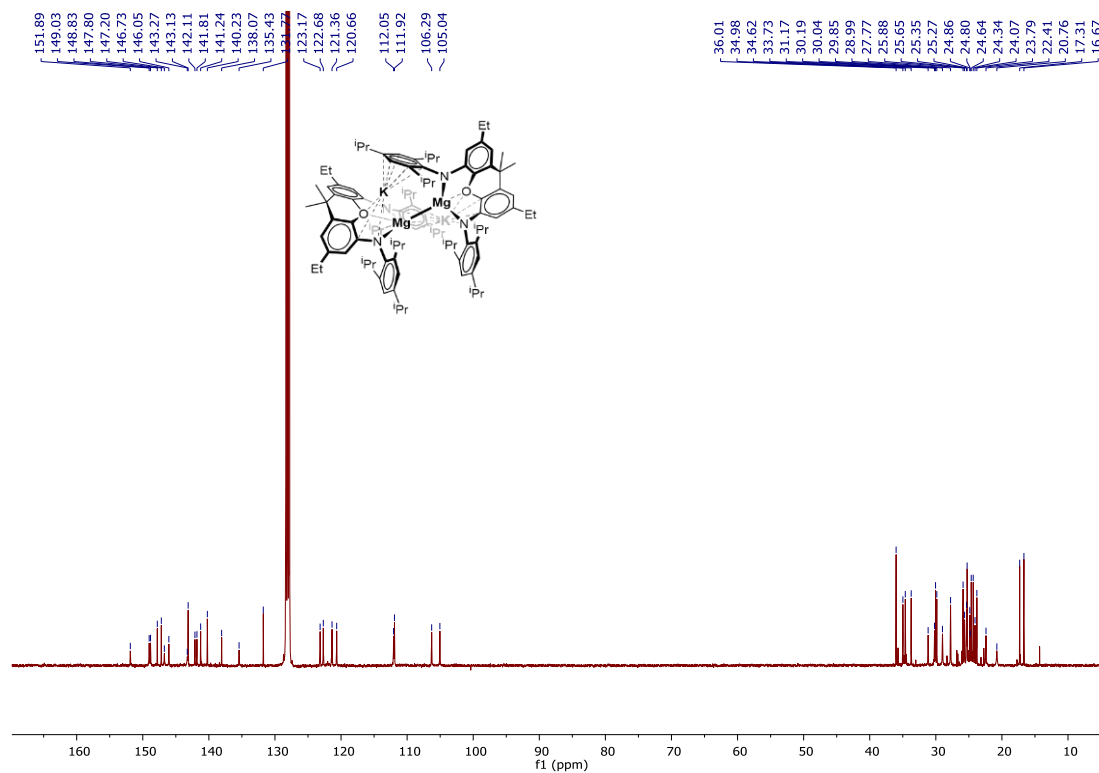


Figure S21. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of **2**.

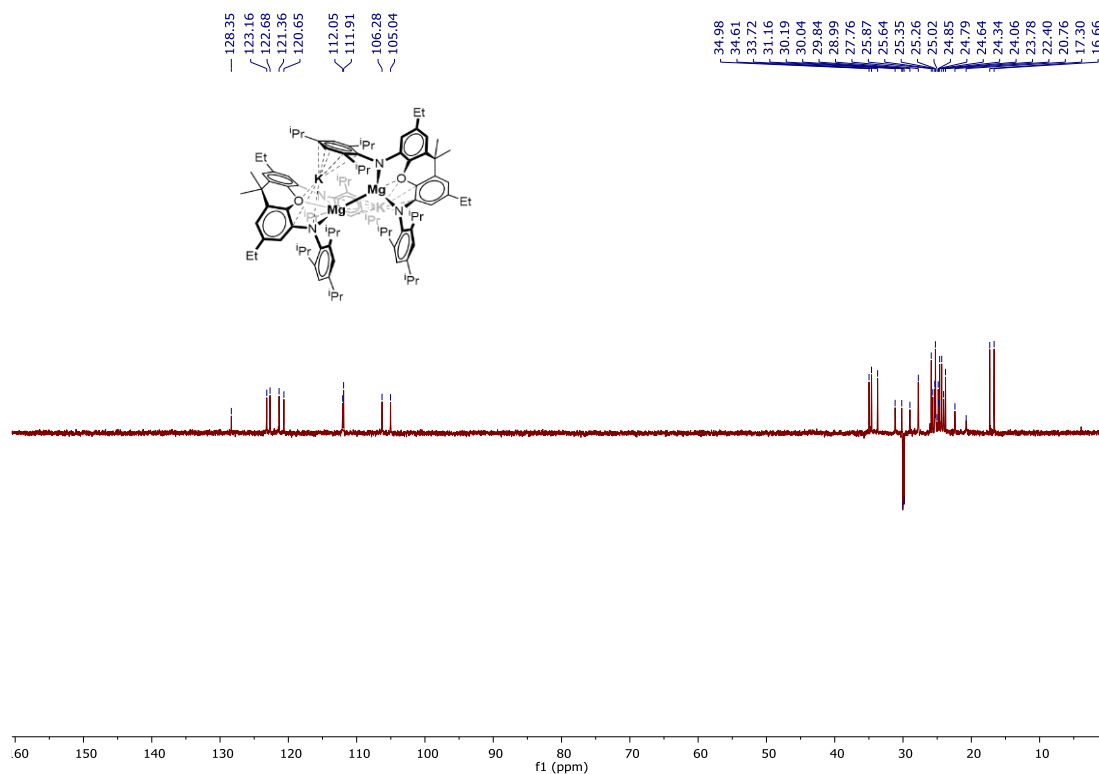


Figure S22. $^{13}\text{C}\{^1\text{H}\}$ (DEPT-135) NMR spectrum (101 MHz, 298 K, C_6D_6) of **2**.

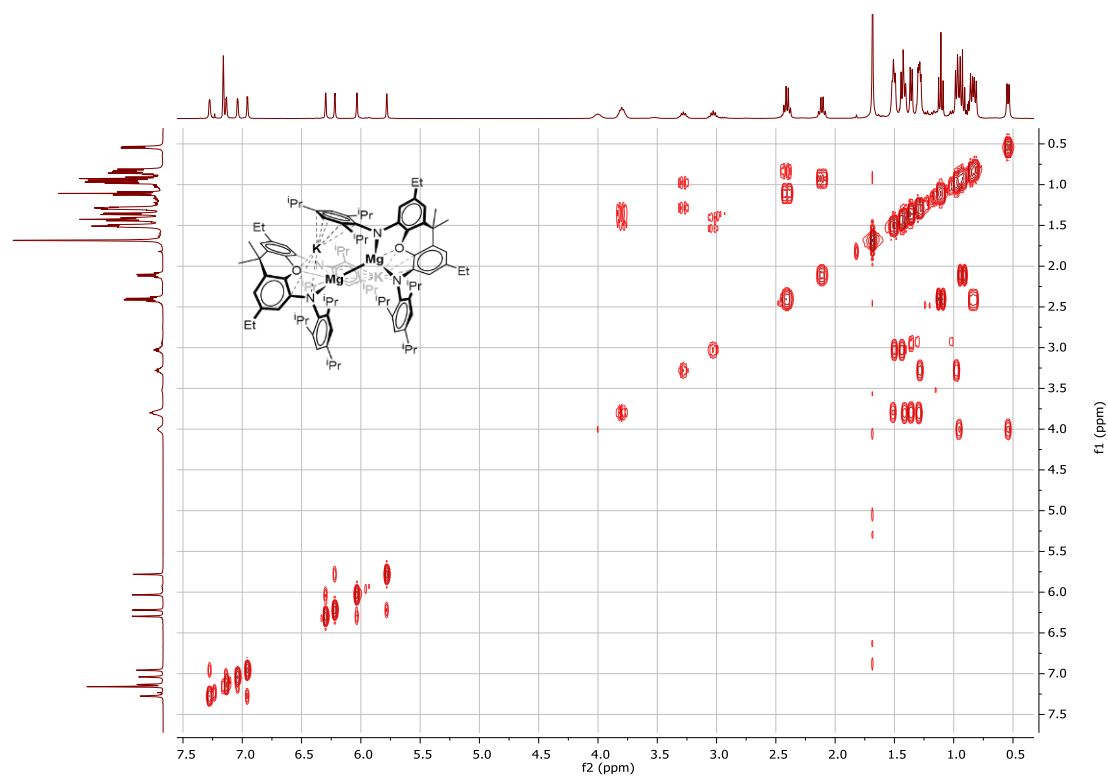


Figure S23. ^1H - ^1H COSY NMR spectrum (400 MHz, 298 K, C_6D_6) of **2**.

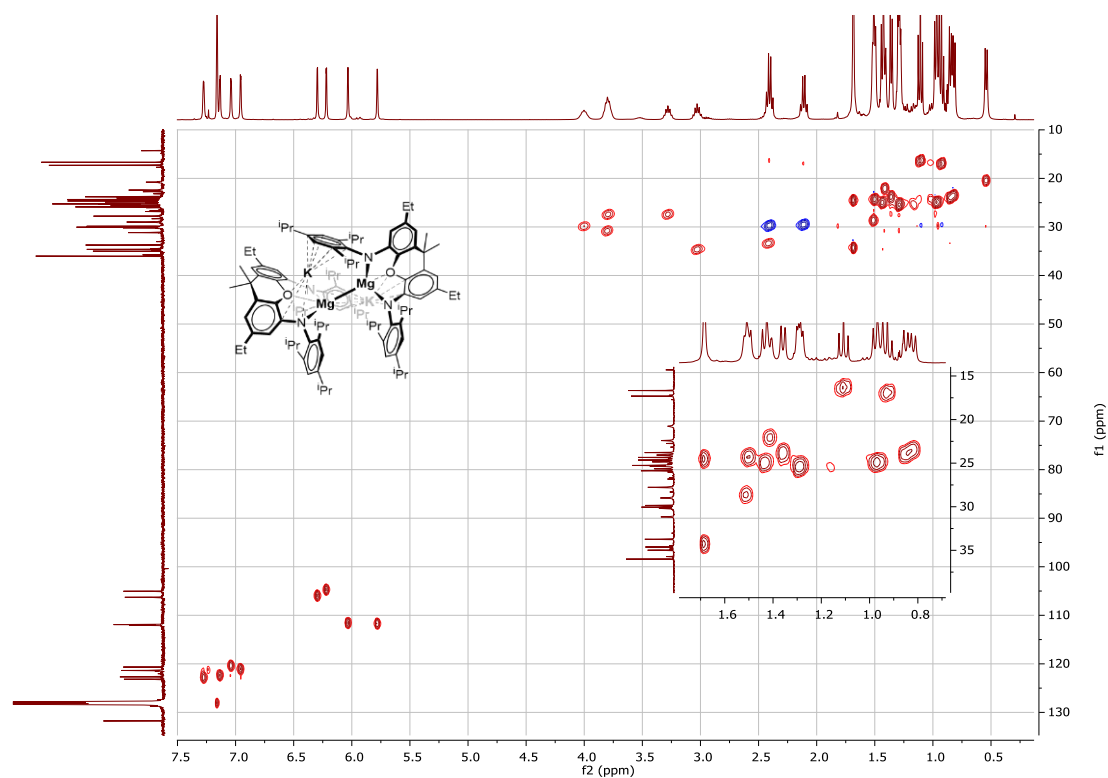


Figure S24. HSQC NMR spectrum (^1H : 400 MHz; ^{13}C : 101 MHz, 298 K, C_6D_6) of **2**.

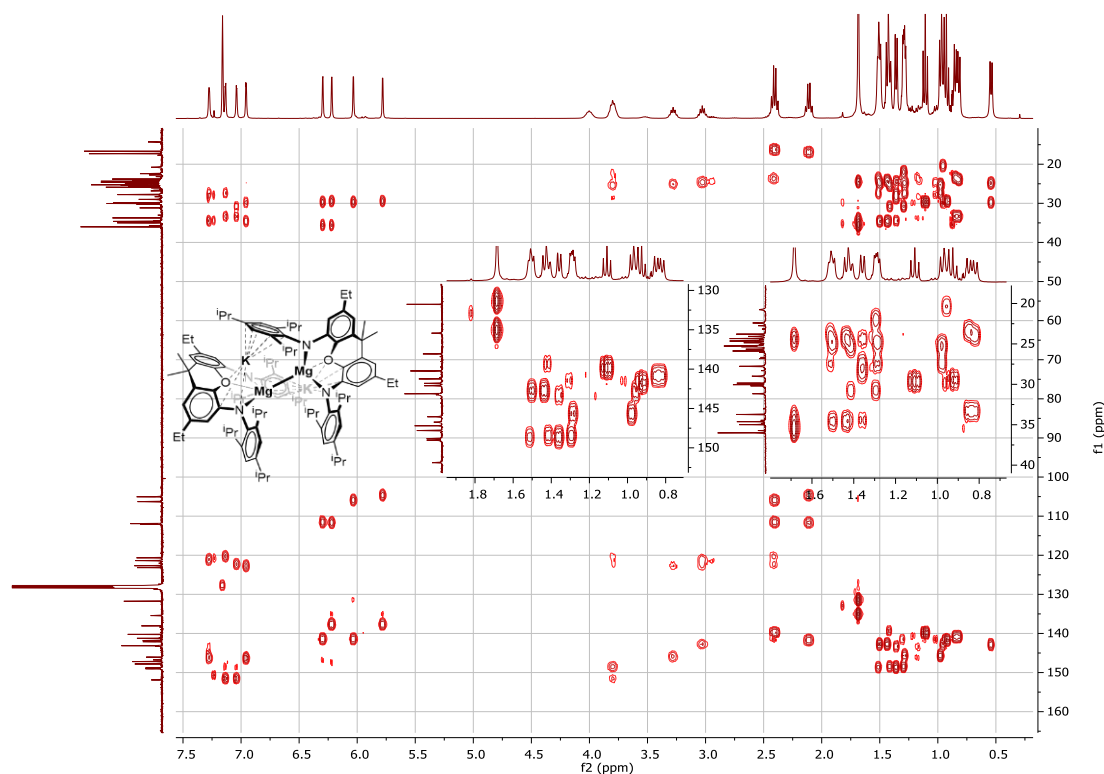


Figure S25. HMBC NMR spectrum (^1H : 400 MHz; ^{13}C : 101 MHz, 298 K, C_6D_6) of **2**.

[[K(TripNON)Mg] $_2$ (μ -C $_2$ O $_2$)] (3). An oven dried 50 mL Teflon screw cap Schlenk flask was charged with **2** (77.0 mg, 0.05 mmol) and cyclohexane (10 mL) under an N_2 atmosphere. The resultant suspension was then freeze-thaw degassed and the flask back-filled with carbon monoxide (~ 1 bar). The reaction mixture was then sealed and ultra-sonicated to give a clear pale-yellow solution. The reaction mixture was stored at room temperature and stored overnight, yielding colorless crystals. The supernatant was decanted, and the crystals dried under vacuum to afford the desired compound as a colourless crystalline solid (48 mg, 61%). Single crystals of **3** suitable for X-ray diffraction analysis were obtained from a benzene solution at room temperature. M.p.: 178-180 $^\circ\text{C}$ (decomp.); ^1H NMR (400 MHz, 298 K, C_6D_6) δ 1.09 (d, $J = 6.9$ Hz, 24H, $\text{CH}(\text{CH}_3)_2$), 1.14 (t, $J = 7.6$ Hz, 12H, CH_2CH_3), 1.19 (d, $J = 6.9$ Hz, 24H, $\text{CH}(\text{CH}_3)_2$), 1.29 (d, $J = 6.9$ Hz, 24H, $\text{CH}(\text{CH}_3)_2$), 1.68 (s, 12H, $\text{C}(\text{CH}_3)_2$), 2.39 (q, $J = 7.5$ Hz, 8H, CH_2CH_3), 2.92 (sept., $J = 6.9$ Hz, 4H, $\text{CH}(\text{CH}_3)_2$), 3.64 (sept., $J = 6.9$ Hz, 8H, $\text{CH}(\text{CH}_3)_2$), 5.80 (d, $J = 1.8$ Hz, 4H, Ar- H), 6.43 (d, $J = 1.8$ Hz, 4H, Ar- H), 7.15 (s, 8H, Ar- H); ^{13}C NMR (101 MHz, 298 K, C_6D_6) δ 17.2 (CH_2CH_3), 23.9, 24.5, 24.7 ($\text{CH}(\text{CH}_3)_2$), 28.4 ($\text{CH}(\text{CH}_3)_2$), 30.2 (CH_2CH_3), 30.6 ($\text{C}(\text{CH}_3)_2$), 33.6 ($\text{CH}(\text{CH}_3)_2$), 35.3 ($\text{C}(\text{CH}_3)_2$), 55.3 ($\text{OC}\equiv\text{CO}$), 107.5, 108.6, 121.1, 130.4, 138.1, 140.8, 142.2, 147.5, 147.6, 148.8 (Ar- C); IR ν/cm^{-1} (diamond ATR, Nujol): 699(w), 848(m), 924(w), 942(w), 1182(m); anal. calc. for $\text{C}_{100}\text{H}_{132}\text{N}_4\text{O}_4\text{K}_2\text{Mg}_2$ C, 75.97%; H, 8.42%; N, 3.54%; Found: C, 75.80%; H, 8.55%; N, 3.40%.



Figure 26. Photographs of isolated crystals of **3**.

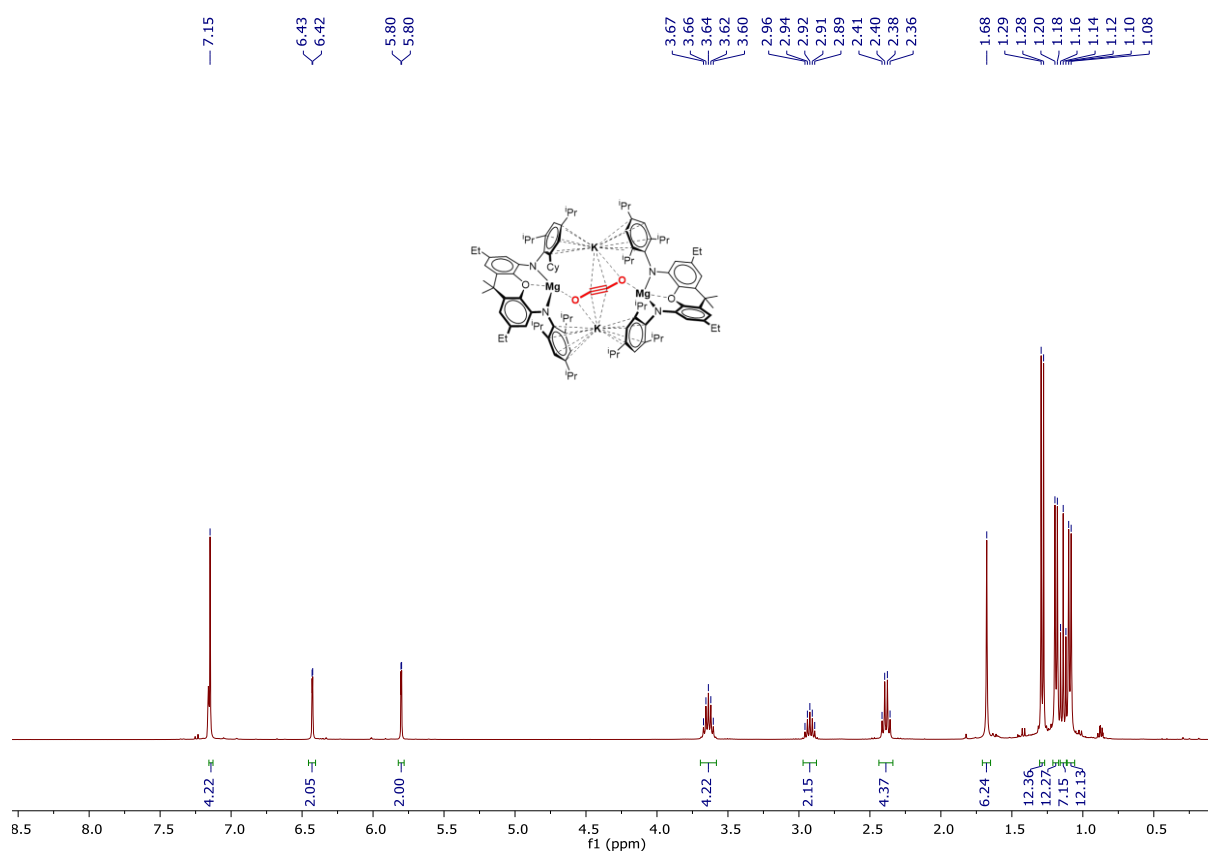


Figure S27. ¹H NMR spectrum (400 MHz, 298 K, C₆D₆) of **3**.

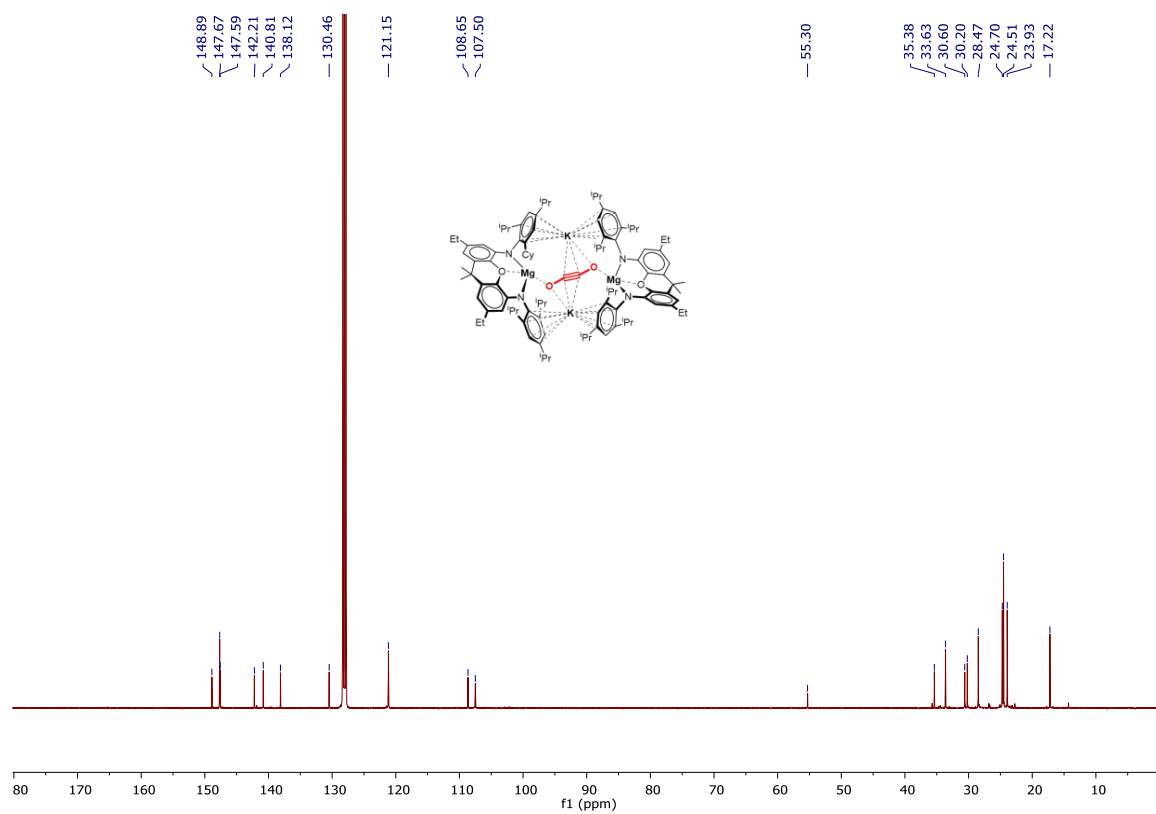


Figure S28. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (400 MHz, 298 K, C_6D_6) of **3**.

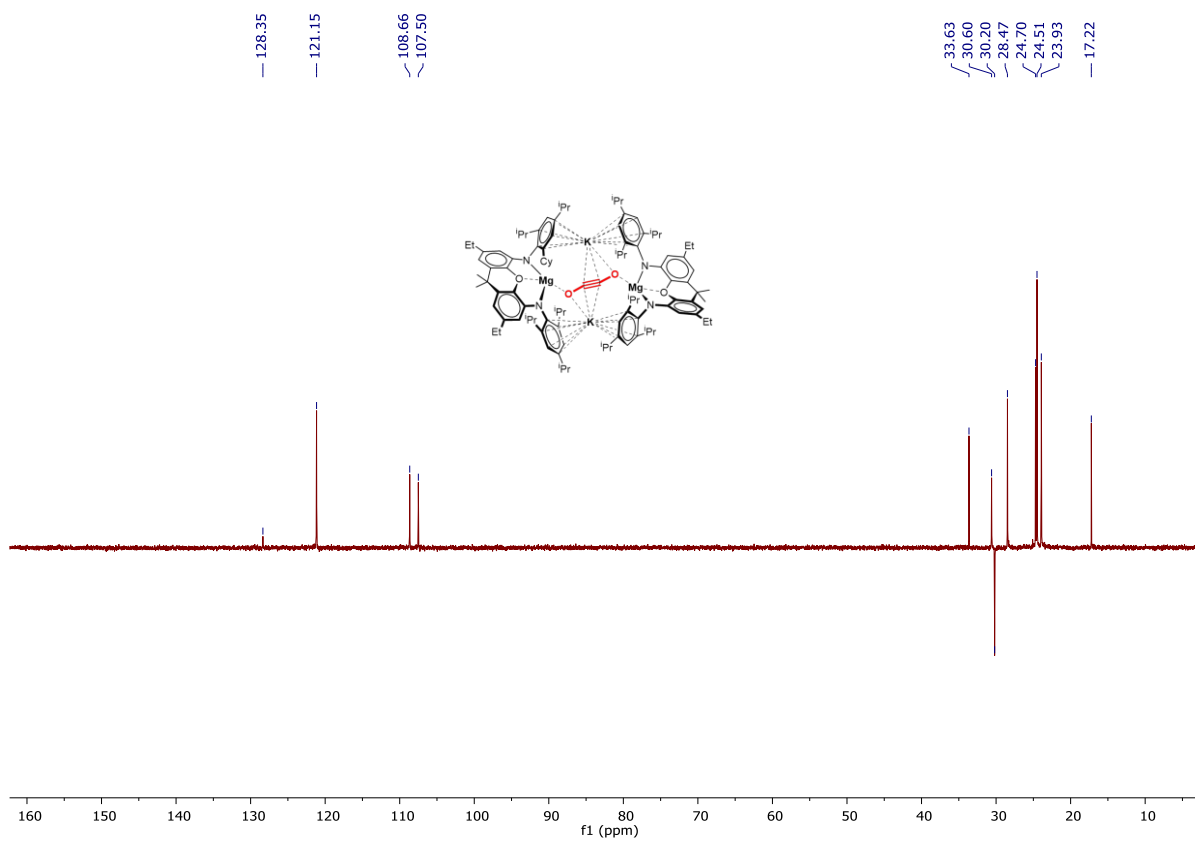


Figure S29. $^{13}\text{C}\{^1\text{H}\}$ (DEPT-135) NMR spectrum (400 MHz, 298 K, C_6D_6) of **3**.

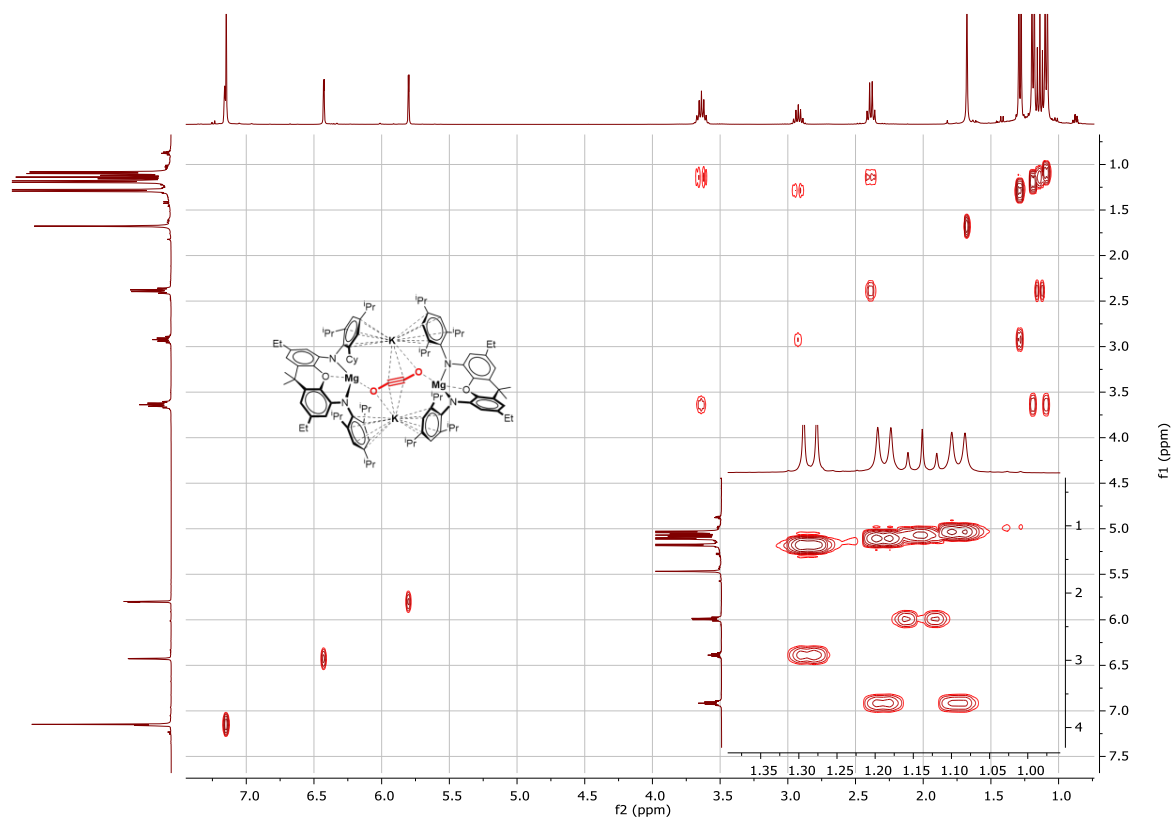


Figure S30. ^1H - ^1H COSY NMR spectrum (400 MHz, 298 K, C_6D_6) of **3**.

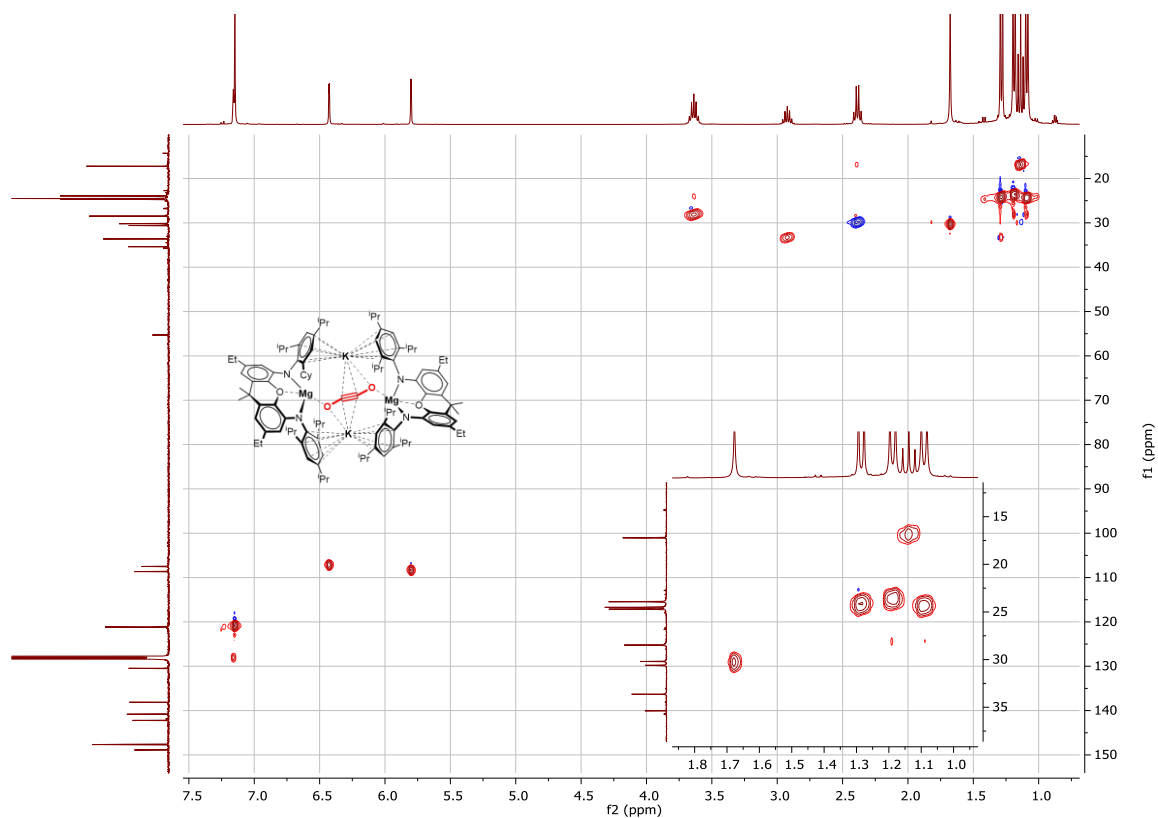


Figure S31. HSQC NMR spectrum (^1H : 400 MHz; ^{13}C : 101 MHz, 298 K, C_6D_6) of **3**.

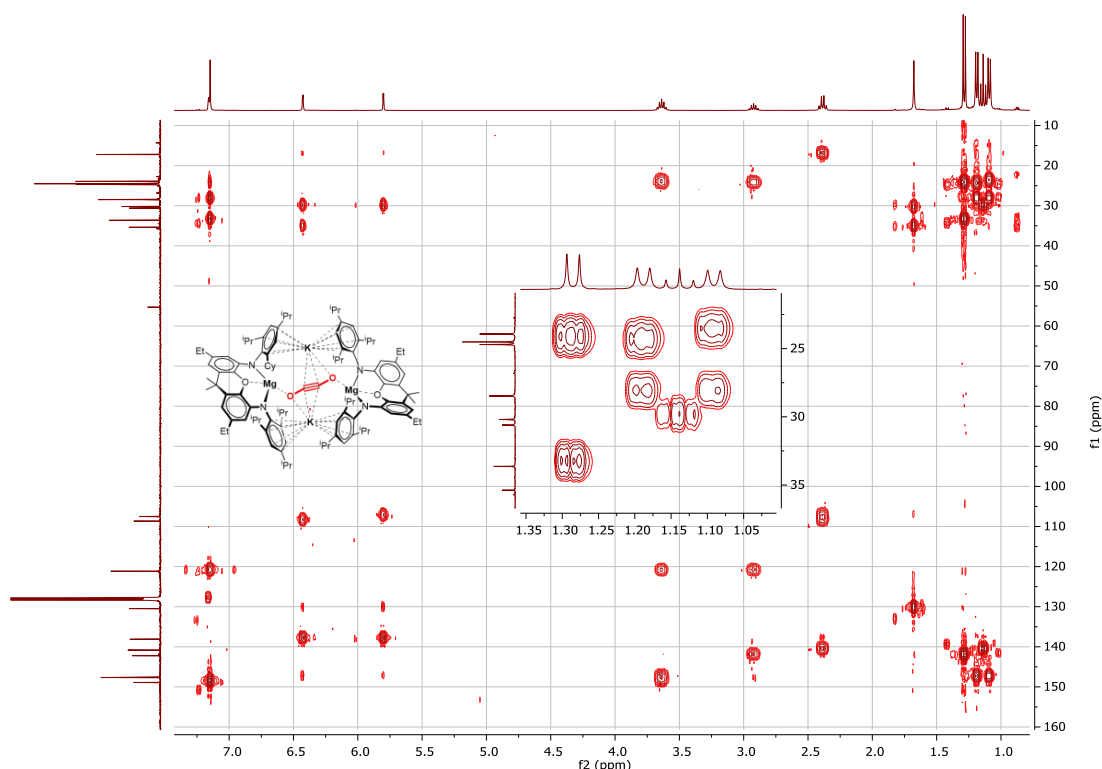


Figure S32. HMBC NMR spectrum (^1H : 400 MHz; ^{13}C : 101 MHz, 298 K, C_6D_6) of **3**.

[[K(^{Trip}NON)Mg(μ -H)]₂ (4**).** An oven dried 50 mL Teflon screw cap Schlenk flask was charged with **2** (230 mg, 0.15 mmol) and hexane (5 mL) under a N_2 -atmosphere. The suspension was freeze-thaw degassed, then the flask backfilled with H_2 (~1 bar). The reaction mixture was then placed in a preheated oil bath at 80 °C for 36 hours (without stirring) during which time the colour of the reaction mixture changed from bright orange to pale yellow. The mixture was then cooled to room temperature and stored at 4 °C for 2 days, resulting in the deposition of pale-yellow crystals of **4**. The supernatant was decanted, and the crystals dried under vacuum to afford the desired compound as a pale yellow crystalline solid (119 mg, 52%). M.p.: 262-264 °C; ^1H NMR (400 MHz, 298 K, C_6D_6) δ 0.86–0.92 (m, n-hexane), 1.05 (d, $J = 6.9$ Hz, 24H, $\text{CH}(\text{CH}_3)_2$), 1.15 (t, $J = 7.5$ Hz, 12H, CH_2CH_3), 1.25 (dd, $J = 7.3, 3.9$ Hz, 54H, $\text{CH}(\text{CH}_3)_2 + \text{n-hexane}$), 1.68 (s, 12H, $\text{C}(\text{CH}_3)_2$), 2.39 (q, $J = 7.5$ Hz, 8H, CH_2CH_3), 2.91 (m, 4H, $\text{CH}(\text{CH}_3)_2$), 3.04 (s, 2H, Mg-H), 3.64 (sept., $J = 6.8$ Hz, 8H, $\text{CH}(\text{CH}_3)_2$), 5.90–5.95 (m, 4H, Ar-H), 6.43 (d, $J = 1.8$ Hz, 4H, Ar-H), 7.14 (s, 8H, Ar-H); ^{13}C NMR (101 MHz, 298 K, C_6D_6) δ 14.3 (n-hexane), 17.4 (CH_2CH_3), 23.0 (n-hexane), 24.2, 24.3, 24.5, 25.3 ($\text{CH}(\text{CH}_3)_2$), 28.3 ($\text{CH}(\text{CH}_3)_2$), 30.2 (CH_2CH_3), 31.0 ($\text{C}(\text{CH}_3)_2$), 31.9 (n-hexane), 33.6 ($\text{CH}(\text{CH}_3)_2$), 35.2 ($\text{C}(\text{CH}_3)_2$), 107.4, 108.5, 121.3, 129.9, 137.9, 140.8, 142.5, 146.8, 146.9, 147.29 (Ar-C); IR ν/cm^{-1} (diamond ATR, Nujol): 672(m), 887(s), 923(w), 1115(m), 1580(m), 1618(m); anal. calc. for $\text{C}_{98}\text{H}_{134}\text{K}_2\text{Mg}_2\text{N}_4\text{O}_2$ C, 77.09%; H, 8.85%; N, 3.67%; Found: C, 75.72%; H, 8.56%; N, 3.35%.

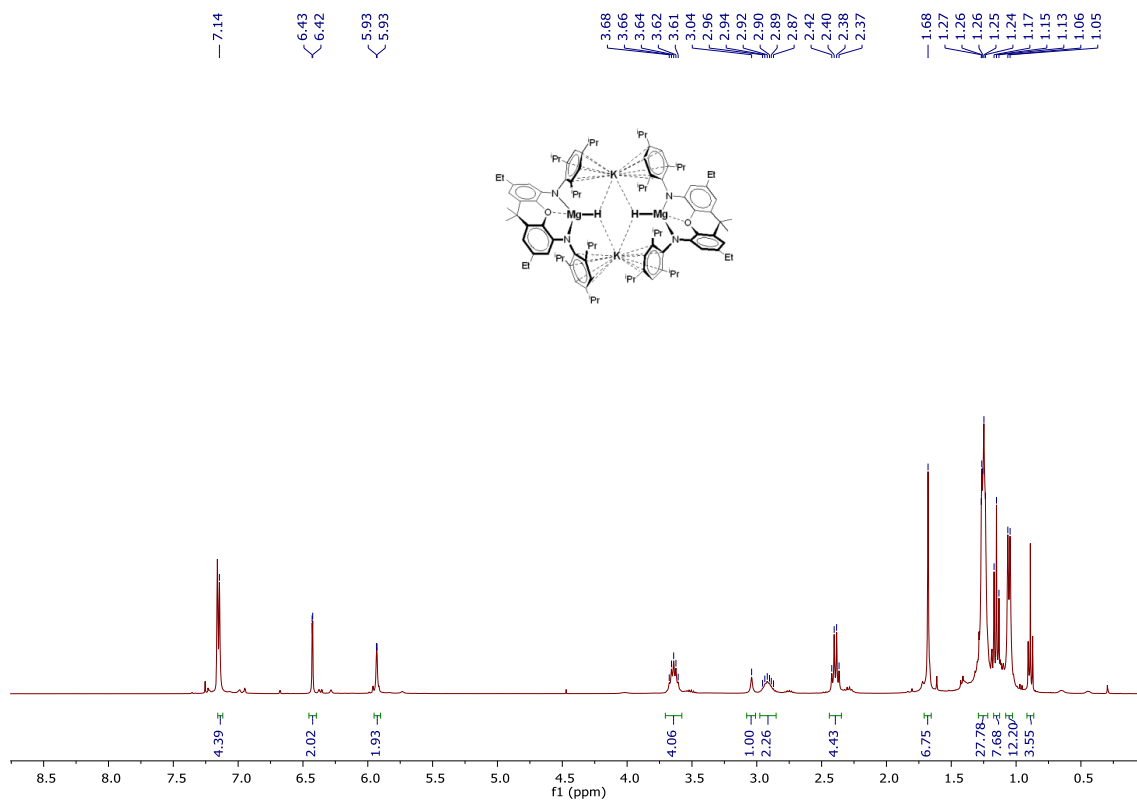


Figure S33. ^1H NMR spectrum (400 MHz, 298 K, C_6D_6) of 4.

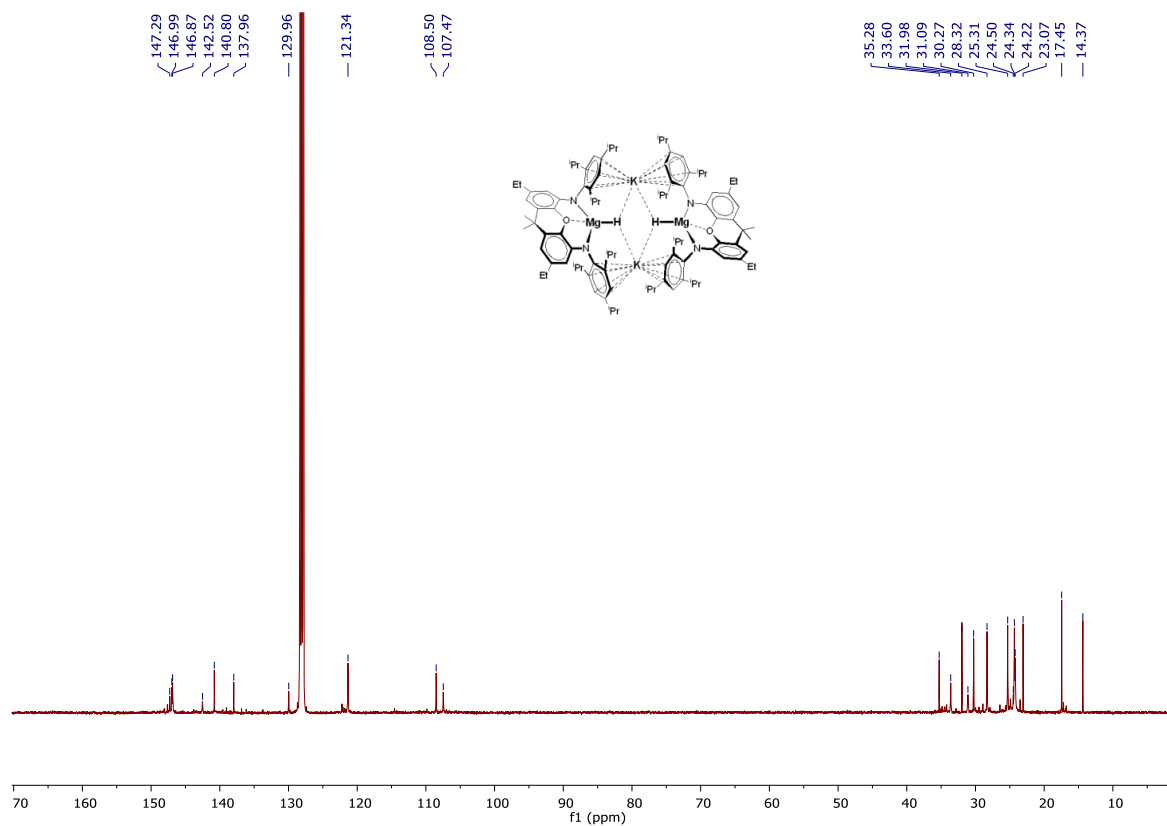


Figure S34. ^{13}C NMR spectrum (101 MHz, 298 K, C_6D_6) of 4.

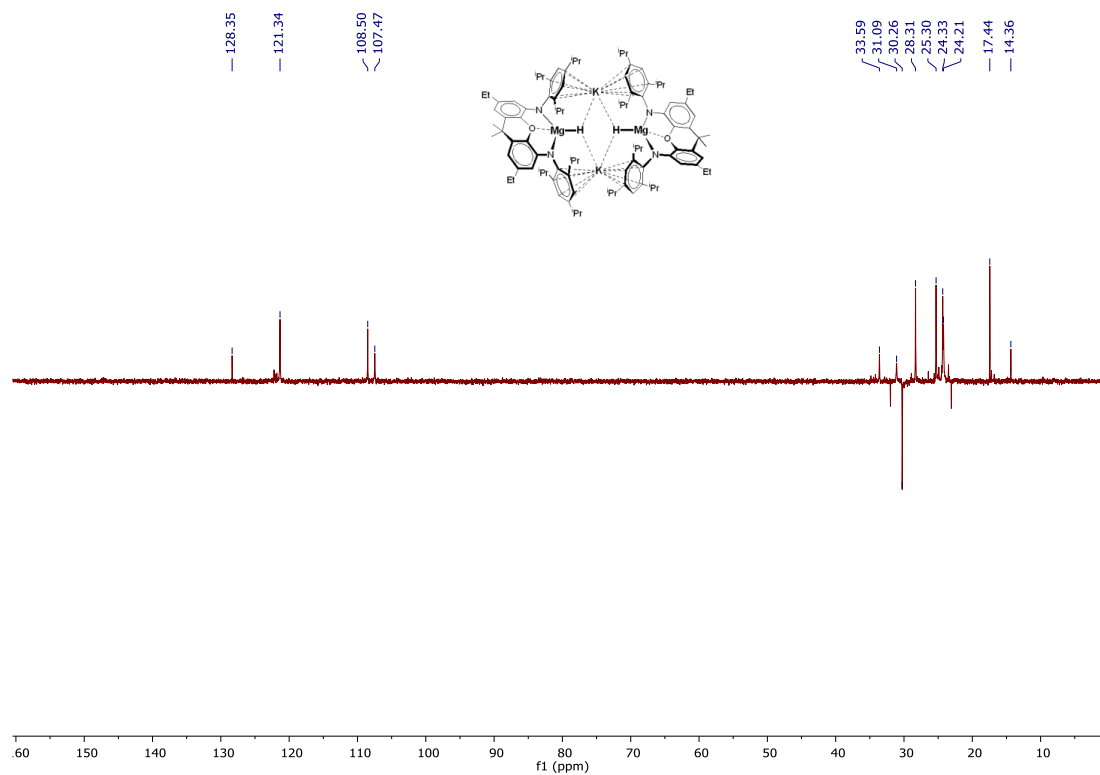


Figure S35. DEPT-135 $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (400 MHz, 298 K, C_6D_6) of **4**.

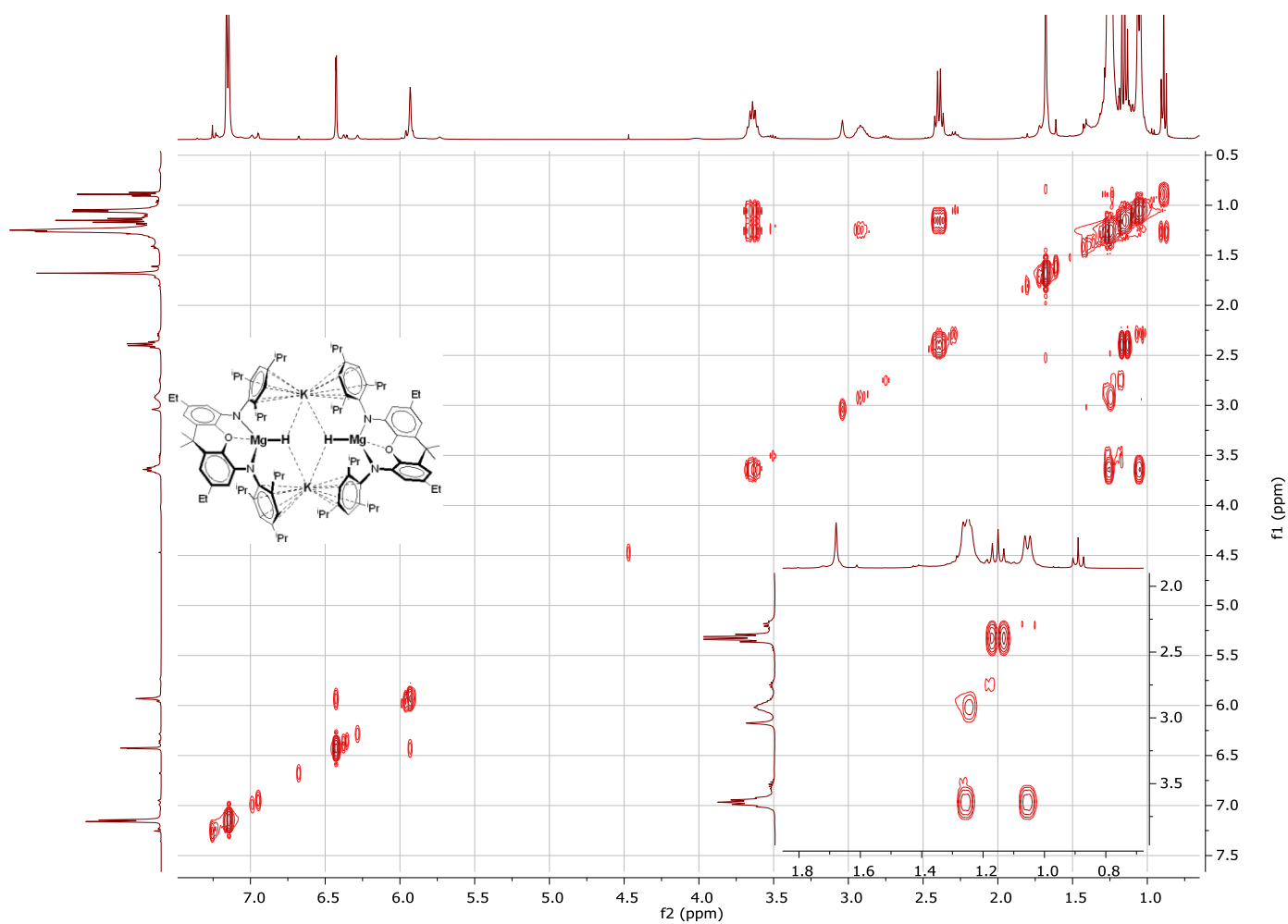


Figure S36. $^1\text{H}\text{-}^1\text{H}$ COSY NMR spectrum (401 MHz, 298 K, C_6D_6) of **4**.

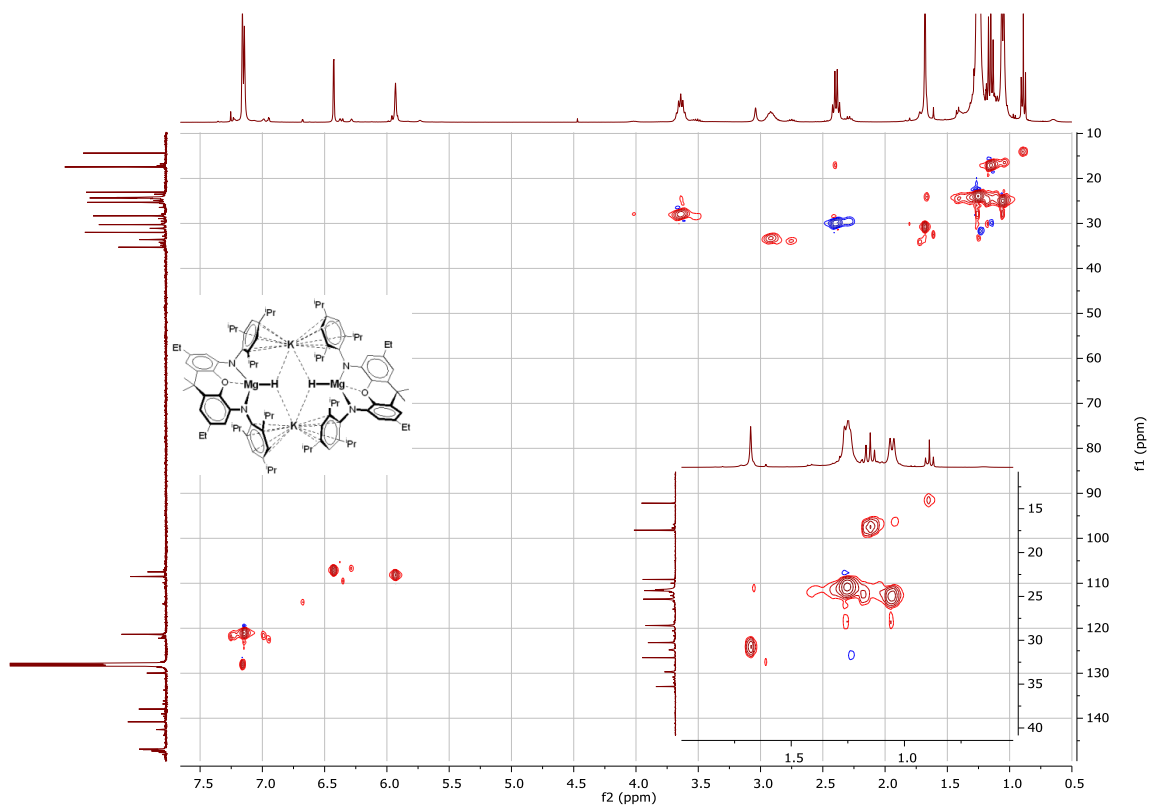


Figure S37. ^1H - ^{13}C HSQC NMR spectrum (401 MHz, ^{13}C : 101 MHz, 298 K, C_6D_6) of **4**.

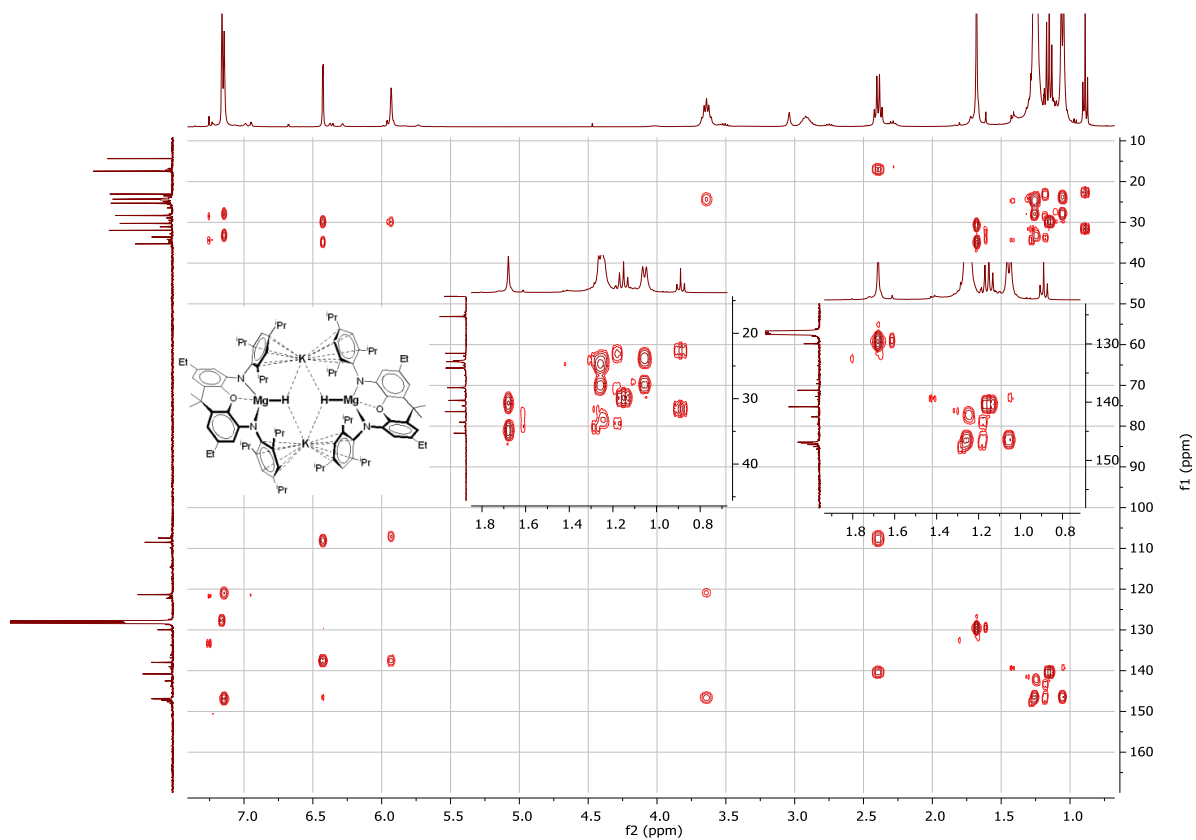


Figure S38. ^1H - ^{13}C HMBC NMR spectrum (401 MHz, ^{13}C : 101 MHz, 298 K, C_6D_6) of **4**.

[[K^(TripNON)(THF)Mg(μ -H)]₂ (5**).** An oven dried 50 mL Teflon screw cap Schlenk flask was charged with **2** (230 mg, 0.15 mmol) and hexane (5 mL) under a N₂-atmosphere. The suspension was freeze-thaw degassed, then the flask back-filled with H₂ (~1 bar). The reaction mixture was then placed in a preheated oil bath at 80 °C for 36 hours (without stirring) during which time the colour of the reaction mixture changed bright orange to yellow. It was then cooled to room temperature and THF (*ca.* 0.1 mL) was added under an N₂ atmosphere, then the mixture stored at 4 °C for 2 days. During this time pale yellow crystals of **5** deposited at the bottom of the flask. The supernatant was decanted, and the crystals dried under vacuum to afford the title compound as a pale yellow crystalline solid (163 mg, 65%). M.p.: 150-155 °C (decomp.); ¹H NMR (400 MHz, 298 K, C₆D₆ + THF-*d*₈) δ 1.08 (m, 12H, CH₂CH₃), 1.22 (m, 72H, CH(CH₃)₂), 1.51 (m, 8H, O(CH₂CH₂)₂), 1.63 (m, 12H, C(CH₃)₂), 2.22–2.37 (m, 8H, CH₂CH₃), 2.84 (m, 4H, CH(CH₃)₂), 3.53 (m, 10H, O(CH₂CH₂)₂ + Mg-H), 3.64–3.86 (m, 8H, CH(CH₃)₂), 5.74 (m, 4H, Ar-H), 6.13 (m, 4H, Ar-H), 7.09 (m, 8H, Ar-H); Due to the poor solubility of **5** in C₆D₆ a few drops of THF-*d*₈ (~0.1 mL) were added to NMR sample before recording the NMR spectra. Even with this solvent mixture, the solubility of the compound was not sufficient to acquire a meaningful ¹³C NMR spectrum; IR ν /cm⁻¹ (diamond ATR, Nujol): 741(w), 851(s), 876(s), 940(w), 1035(s), 1179(s), 1572(s), 1615(s); anal. calc. for C₁₀₆H₁₅₀N₄O₄K₂Mg₂: C, 76.18%; H, 9.09%; N, 3.35%; found: C, 75.97%; H, 9.00%; N, 3.12%.

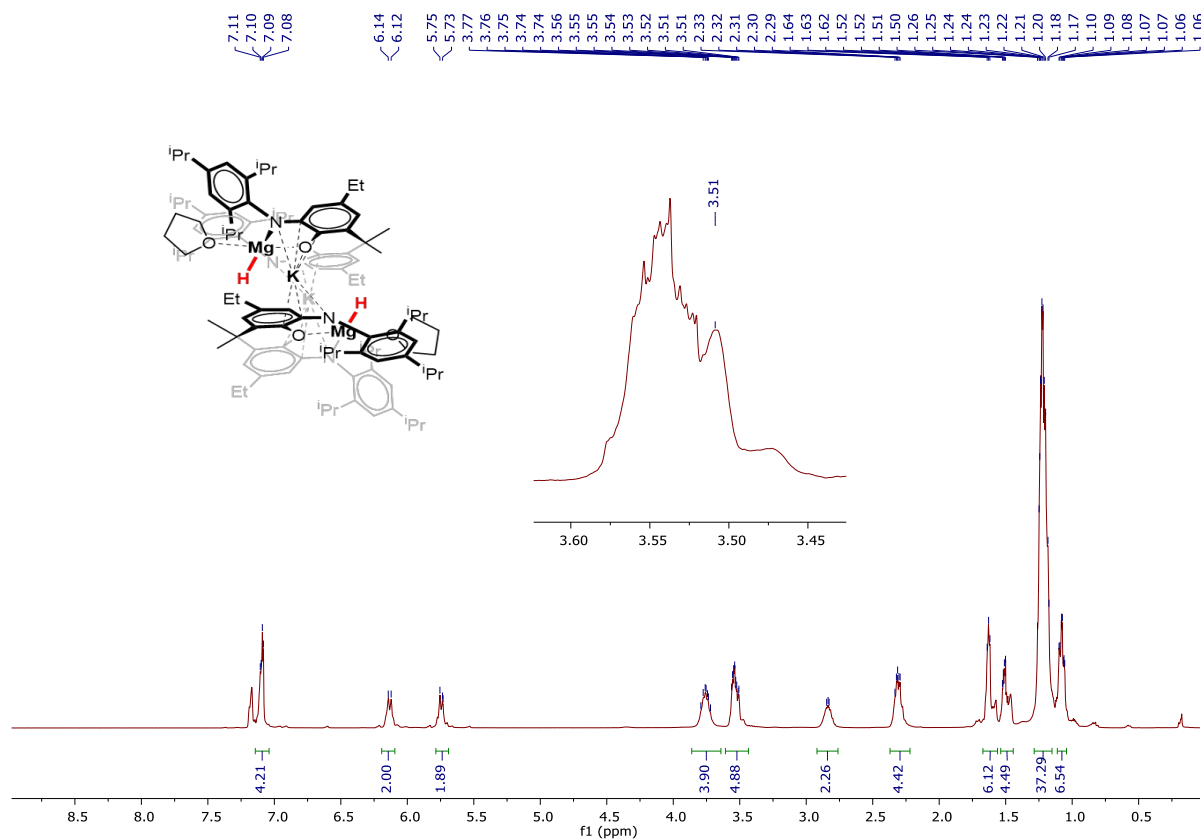


Figure S39. ¹H NMR spectrum (400 MHz, 298 K, C₆D₆ + ~0.1 mL THF-*d*₈) of **5**.

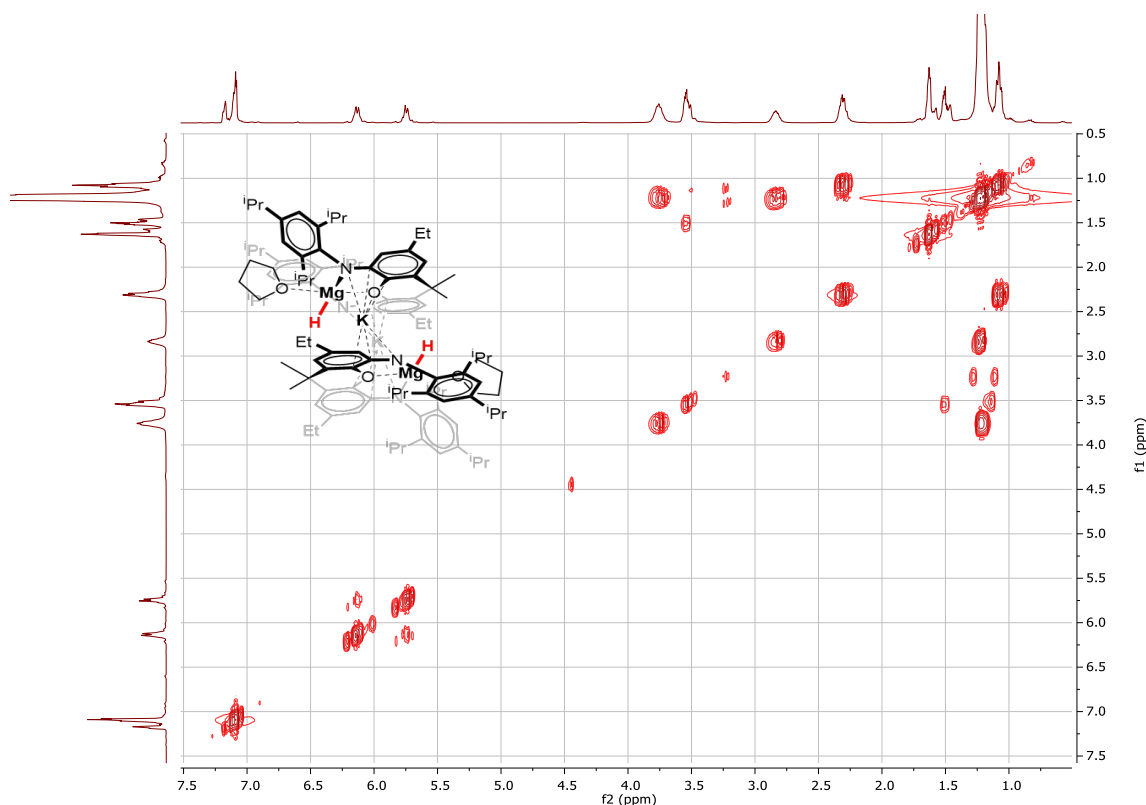


Figure S40. ^1H - ^1H COSY NMR spectrum (401 MHz, 298 K, C_6D_6 + ~0.1 mL $\text{THF-}d_8$) of **5**.

[[K(TripNON)Mg] $_2$ (μ -O)] (6**).** An oven dried 50 mL Teflon screw cap Schlenk flask was charged with **2** (76.0 mg, 0.05 mmol) and pentane (5 mL) under an N_2 -atmosphere. The suspension was freeze-thaw degassed and the flask backfilled with N_2O (~1 bar). The reaction mixture was then ultrasonicated, during which time the bright orange suspension immediately changed to a colourless solution. It was then stored at room temperature overnight, depositing colourless crystals of the title compound. The supernatant was decanted, and the crystals dried under vacuum to afford the desired compound as a colorless crystalline solid (37 mg, 48 %). Single crystals of **6** suitable for X-ray diffraction analysis were obtained from the filtrate stored at -30 °C. M.P.: >300 °C; ^1H NMR (400 MHz, C_6D_6) δ 0.55 – 0.73 (m, 6H, $\text{CH}(\text{CH}_3)_2$), 0.87 (t, $J = 7.1$ Hz, 12H, pentane), 1.01–1.29 (m, 84H, pentane+ CH_2CH_3 + $\text{CH}(\text{CH}_3)_2$), 1.39 – 1.43 (m, 6H, $\text{CH}(\text{CH}_3)_2$), 1.67 (s, 6H, $\text{C}(\text{CH}_3)_2$), 1.72 (s, 6H, $\text{C}(\text{CH}_3)_2$), 2.20 – 2.50 (m, 10H, CH_2CH_3 + $\text{CH}(\text{CH}_3)_2$), 2.75 (sept, $J = 6.9$ Hz, 4H, $\text{CH}(\text{CH}_3)_2$), 3.54 (m, 4H, $\text{CH}(\text{CH}_3)_2$), 3.95 – 4.09 (m, 2H, $\text{CH}(\text{CH}_3)_2$), 5.73 (s, 2H, Ar- H), 5.96 (d, $J = 1.8$ Hz, 2H, Ar- H), 6.28 (s, 2H, Ar- H), 6.34 – 6.41 (m, 2H, Ar- H), 6.92 – 7.02 (m, 4H, Ar- H), 7.16 (m, 2H, Ar- H), 7.22 (s, 2H, Ar- H); Once crystallised, the title compound had very poor solubility in non-coordinating deuterated solvents, which prevented the acquisition of meaningful ^{13}C NMR spectra. IR ν/cm^{-1} (diamond ATR, Nujol): 674(w), 877(w), 923(w), 1174(w), 1579(w), 1614(w); N.B. a reproducible microanalysis could not be obtained as the compound consistently co-crystallised with small amounts of the pro-ligand, TripNONH_2 , which could not be separated by recrystallisations.

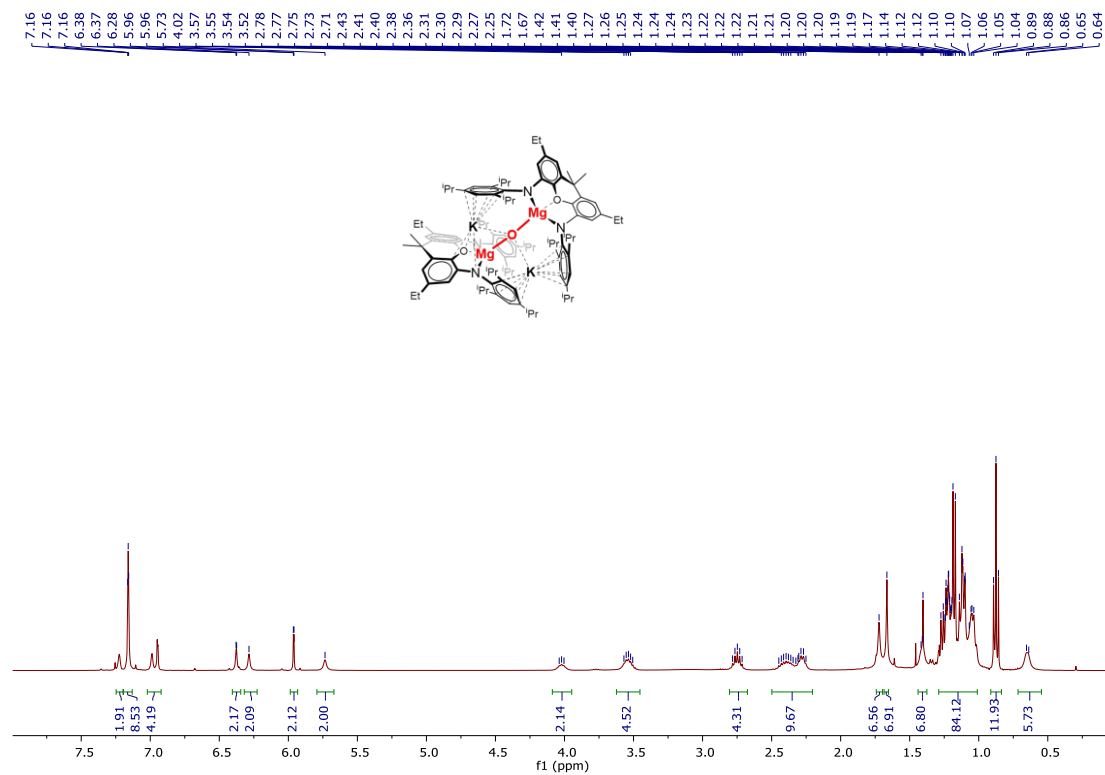


Figure S41. ^1H NMR spectrum (400 MHz, 298 K, C_6D_6) of **6**.

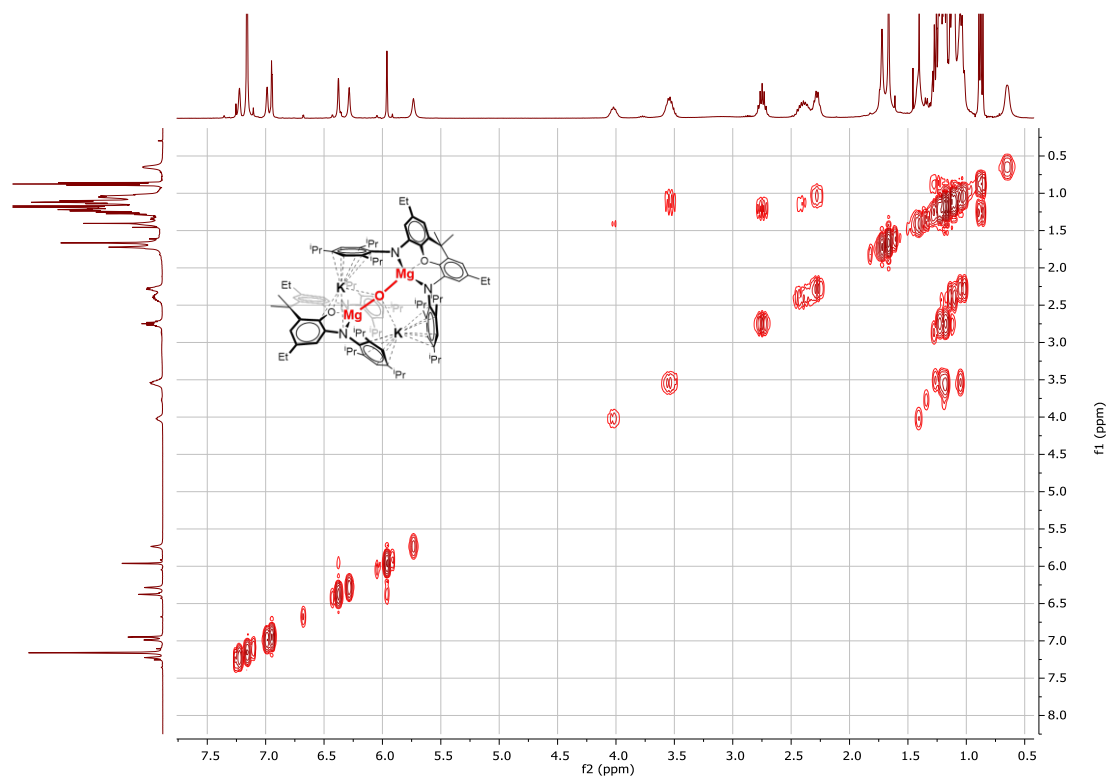


Figure S42. ^1H - ^1H COSY NMR spectrum (401 MHz, 298 K, C_6D_6) of **6**.

Treatment of $[\{K(\text{Tri}^{\text{p}}\text{NON})\text{Mg}\}_2]$ (2) with THF. When orange solutions of **2** (*ca.* 20 mg) in cyclohexane (*ca.* 1 mL) are treated with THF (*ca.* 0.1 mL) at room temperature there is an immediate precipitation of metal, and change in colour of the solution to yellow. NMR spectroscopic analysis of the soluble material shows the major product (*ca.* 70%) to be $[(\text{Tri}^{\text{p}}\text{NON})\text{Mg}(\text{THF})_2]$, by comparison with the NMR spectra of that compound prepared as below. The remaining components of the soluble fraction could not be identified. The metallic precipitate was digested in concentrated nitric acid and analysed by ICP-OES. This showed it to contain a K:Mg ratio of 6.4:1.

$[(\text{Tri}^{\text{p}}\text{NON})\text{Mg}(\text{THF})_2]$. An oven-dried Teflon screw cap Schlenk flask was charged with $\text{Tri}^{\text{p}}\text{NONH}_2$ (0.7 g, 1.0 mmol), under an N_2 atmosphere. Methylcyclohexane (10 mL) and $\text{MgBu}_2 \cdot 2\text{THF}$ (1.0 mL, 1.0 mmol) were then added. The reaction mixture was then placed in a preheated oil bath at 90 °C and stirred for 2 hours. The mixture was then cooled to room temperature and volatiles removed under vacuum to afford a semi-solid mass. The solid mass was then extracted with pentane (~10 mL) and stored at room temperature for 2 hours, during which time colourless crystals deposited at bottom the flask (0.473 g, 55%); M.p.: 205-210 °C; ^1H NMR (400 MHz, C_6D_6) δ 0.79–0.96 (m, 4H, OCH_2CH_2), 1.15–1.22 (m, 18H, $\text{CH}_2\text{CH}_3 + \text{CH}(\text{CH}_3)_2$), 1.28-1.45 (m, 28H, $\text{CH}(\text{CH}_3)_2 + \text{OCH}_2\text{CH}_2$), 1.68 (s, 6H, $\text{C}(\text{CH}_3)_2$), 2.43 (q, $J = 7.6$ Hz, 4H, CH_2CH_3), 2.92 (m, 6H, $\text{OCH}_2\text{CH}_2 + \text{CH}(\text{CH}_3)_2$), 3.64 (m, 4H, $\text{CH}(\text{CH}_3)_2$), 3.81 (s, 4H, OCH_2CH_2), 6.07 (d, $J = 1.7$ Hz, 2H, Ar-*H*), 6.37 (d, $J = 1.8$ Hz, 2H, Ar-*H*), 7.22 (s, 4H, Ar-*H*); ^{13}C NMR (101 MHz, 298 K, C_6D_6) δ 17.3 (CH_2CH_3), 24.5 (OCH_2CH_2), 24.7, 24.8, 25.4 ($\text{CH}(\text{CH}_3)_2$), 26.2 ($\text{C}(\text{CH}_3)_2$), 28.0 ($\text{CH}(\text{CH}_3)_2$), 30.3 (CH_2CH_3), 34.6 ($\text{CH}(\text{CH}_3)_2$), 35.4 ($\text{C}(\text{CH}_3)_2$), 70.3 (OCH_2CH_2), 105.8, 110.7, 121.5, 130.2, 137.7, 140.2, 143.2, 145.9, 147.7, 148.8 (Ar-*C*); IR ν/cm^{-1} (diamond ATR, Nujol): 744(w), 847(m), 876(s), 923(s), 1574(s) 1628(s); N.B. a reproducible microanalysis could not be obtained as the compound consistently co-crystallised with small amounts of the pro-ligand, $\text{Tri}^{\text{p}}\text{NONH}_2$, which could not be separated by recrystallisations.

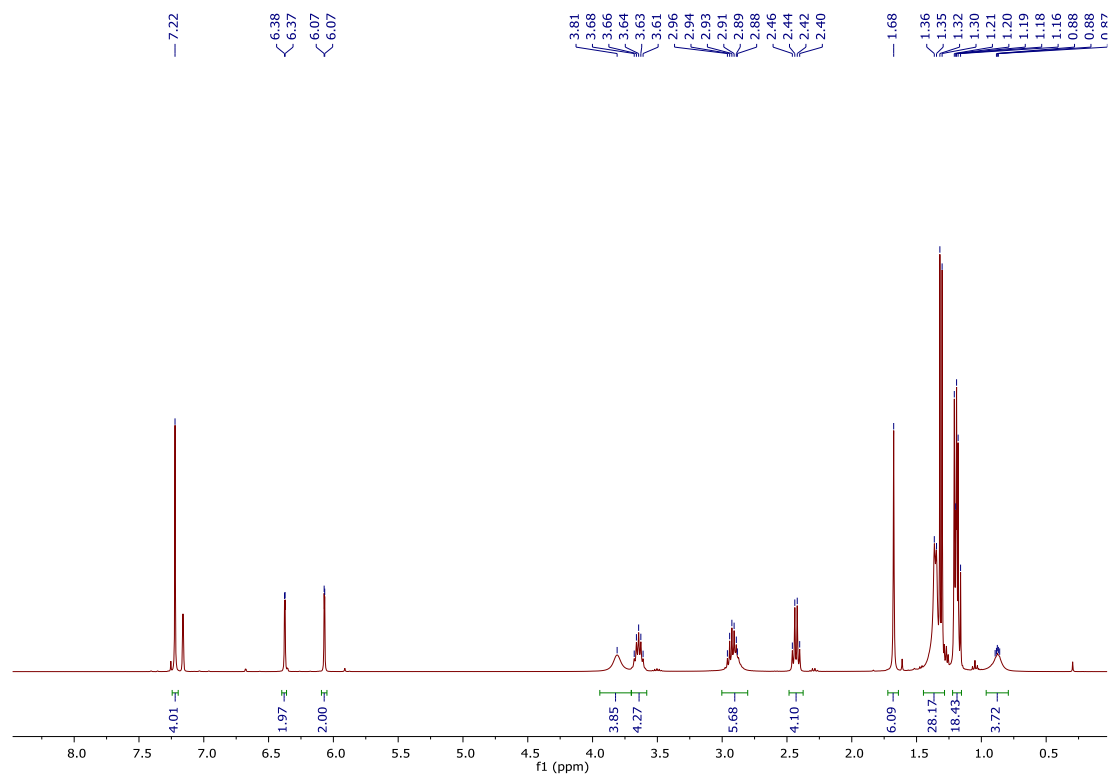


Figure S43. ^1H NMR spectrum (400 MHz, 298 K, C_6D_6) of $[(\text{TriipNON})\text{Mg}(\text{THF})_2]$.

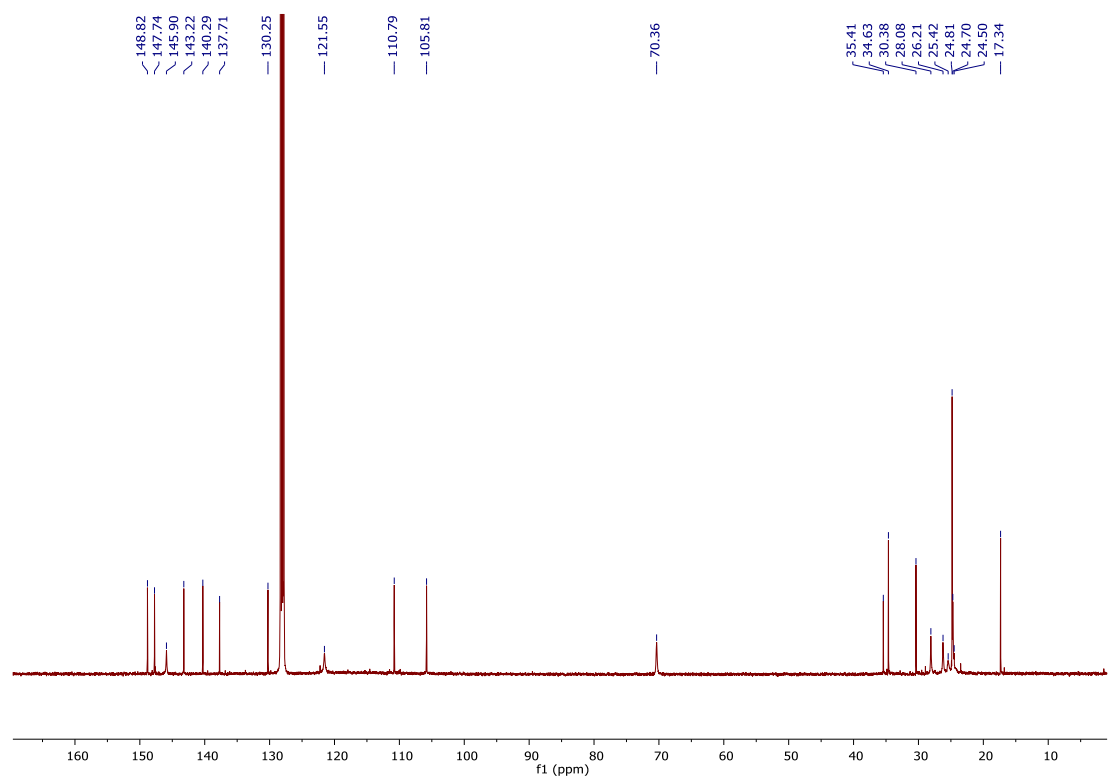


Figure S44. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum (101 MHz, 298 K, C_6D_6) of $[(\text{TriipNON})\text{Mg}(\text{THF})_2]$.

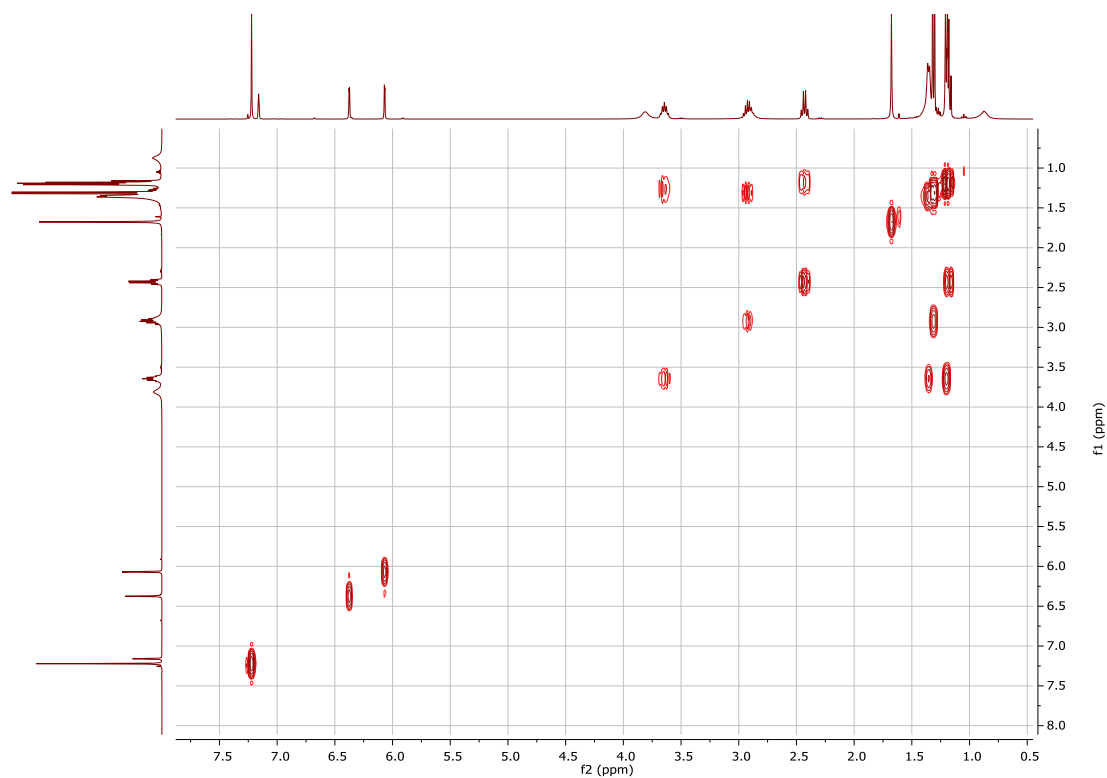


Figure S45. ¹H-¹H COSY NMR spectrum (400 MHz, 298 K, C₆D₆) of [(^{Triip}NON)Mg(THF)₂].

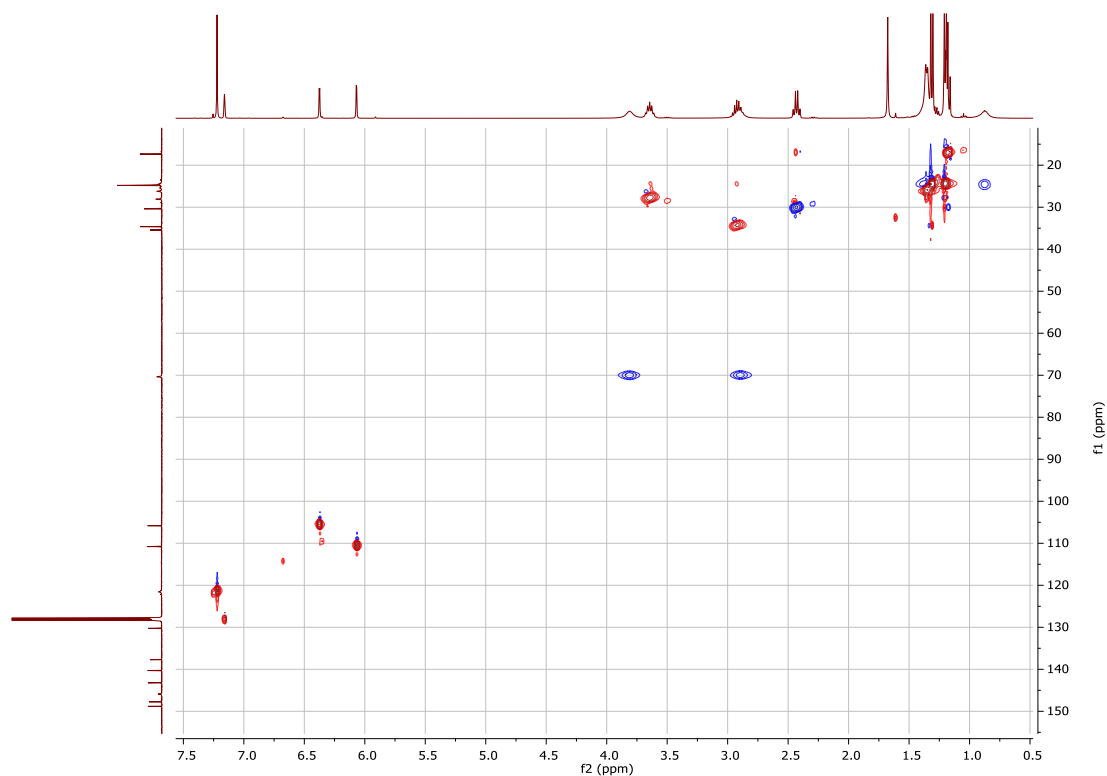


Figure S46. HSQC NMR spectrum (¹H: 400 MHz; ¹³C: 101 MHz, 298 K, C₆D₆) of [(^{Triip}NON)Mg(THF)₂].

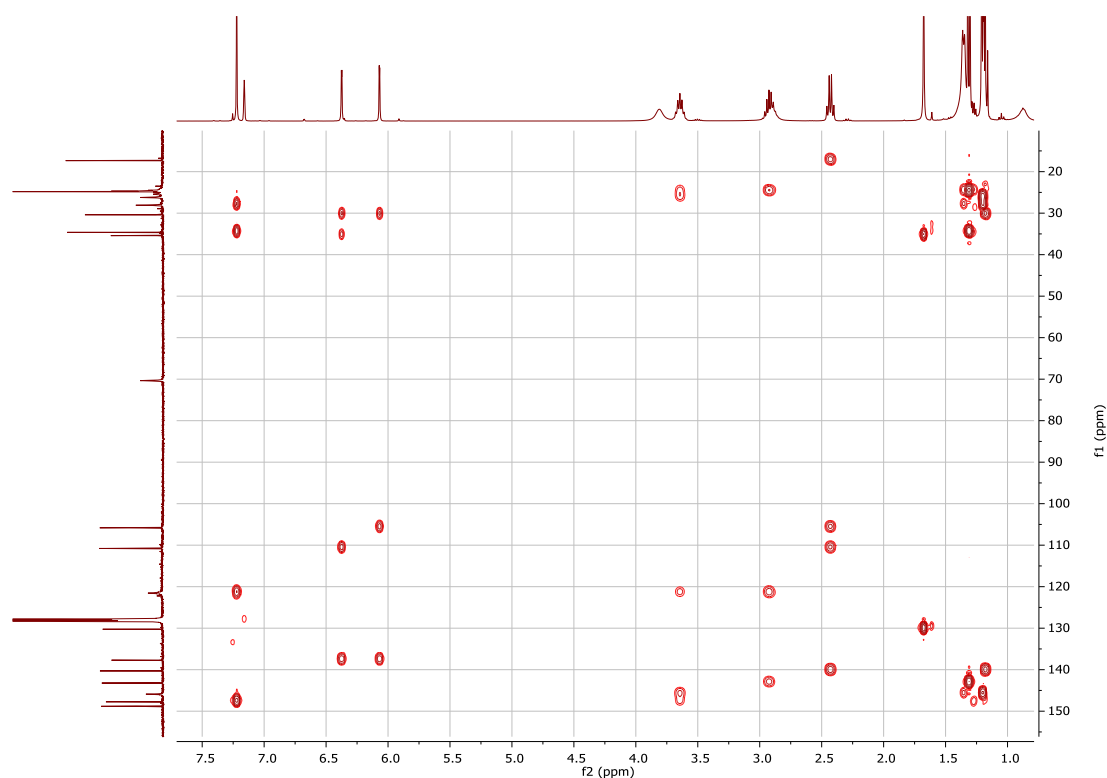


Figure S47. HMBC NMR spectrum (^1H : 400 MHz; ^{13}C : 101 MHz, 298 K, C_6D_6) of $[(\text{Tri}^p\text{NON})\text{Mg}(\text{THF})_2]$.

2. X-Ray Crystallography

Crystals of compounds 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 Cu $K\alpha$ radiation (1.54180 Å) or the MX1 beamline of the Australian Synchrotron ($\lambda = 0.71090$ Å). The software package Blu-Ice⁶ was used for synchrotron data acquisition, while the program XDS⁷ was employed for synchrotron data reduction.. All structures were solved by direct methods and refined on F^2 by full matrix least squares (SHELX18⁸) using all unique data. Hydrogen atoms, except hydrides, are typically included in calculated positions (riding model). Crystal data, details of data collections and refinements for all structures can be found in their CIF files and are summarized in Table S1.

Table S1. Crystal data for compounds **2-6**, and ^{Trip}NONH₂.

	2 ·(pentane) ₃	3 ·(benzene) ₅	4 ·(hexane)
empirical formula	C ₁₁₃ H ₁₆₈ K ₂ Mg ₂ N ₄ O ₂	C ₁₃₀ H ₁₆₂ K ₂ Mg ₂ N ₄ O ₄	C ₁₀₄ H ₁₄₈ K ₂ Mg ₂ N ₄ O ₂
formula weight	1741.32	1971.45	1613.08
crystal system	Triclinic	Monoclinic	Triclinic
space group	<i>P</i> -1	<i>C</i> 2/ <i>c</i>	<i>P</i> -1
<i>a</i> (Å)	17.4631(4)	58.863(2)	16.5142(3)
<i>b</i> (Å)	18.2690(3)	9.92670(10)	16.8828(3)
<i>c</i> (Å)	19.2800(3)	34.1523(12)	19.9517(3)
α (deg.)	102.560(2)	90	90.887(2)
β (deg.)	105.430(2)	144.652(8)	90.703(2)
γ (deg.)	92.826(2)	90	106.972(2)
vol (Å ³)	5749.7(2)	11545.2(14)	4785.76(15)
<i>Z</i>	2	4	2
<i>T</i> (K)	123.01(10)	123.01(10)	123.01(10)
ρ (calcd) (g.cm ⁻³)	1.106	1.134	1.119
μ (mm ⁻¹)	1.168	1.238	1.3774
<i>F</i> (000)	1904	4256	1756
reflections collected	82755	110724	35909
unique reflections	24135	12367	16821
<i>R</i> _{int}	0.0731	0.0855	0.0953
R1 indices [<i>I</i> >2 σ (<i>I</i>)] ^a	0.0959	0.0468	0.0825
wR2 indices (all data) ^b	0.2582	0.1165	0.2274
Largest peak and hole (e.Å ⁻³)	1.227, -0.662	0.319, -0.379	1.092, -0.693
CCDC No.	2309546	2309549	2309545

Table S1 (contd.). Crystal data for compounds **2-6**, and ^{Trip}NONH₂.

	5 ·(hexane) ₂	6 ·(pentane)	^{Trip} NONH ₂
empirical formula	C ₁₁₈ H ₁₇₈ K ₂ Mg ₂ N ₄ O ₄	C ₁₀₃ H ₁₄₄ K ₂ Mg ₂ N ₄ O ₃	C ₄₉ H ₆₈ N ₂ O
formula weight	1843.45	1613.03	701.05
crystal system	Orthorhombic	Orthorhombic	Triclinic
space group	<i>Pbca</i>	<i>P2₁2₁2₁</i>	<i>P</i> -1
<i>a</i> (Å)	19.617(4)	18.18420(10)	13.0578(3)
<i>b</i> (Å)	21.324(4)	22.16750(10)	13.4792(4)
<i>c</i> (Å)	25.718(5)	24.56070(10)	13.9769(3)
α (deg.)	90	90	67.548(2)
β (deg)	90	90	70.378(2)
γ (deg.)	90	90	81.771(2)
vol (Å ³)	10758(4)	9900.38(8)	2141.24(10)
<i>Z</i>	4	4	2
<i>T</i> (K)	100(2)	123.01(10)	123.01(10)
ρ (calcd) (g.cm ⁻³)	1.138	1.082	1.087
μ (mm ⁻¹)	0.153	1.332	0.476
<i>F</i> (000)	4032	3504	768
reflections collected	185007	48050	29245
unique reflections	10924	19486	9054
<i>R</i> _{int}	0.0543	0.0310	0.0297
R1 indices [<i>I</i> >2 σ (<i>I</i>)] ^a	0.0646	0.0438	0.0482
wR2 indices (all data) ^b	0.1901	0.1266	0.1284
Largest peak and hole (e.Å ⁻³)	0.939, -0.462	1.125, -0.259	0.336, -0.269
CCDC No.	2309548	2309547	2309550

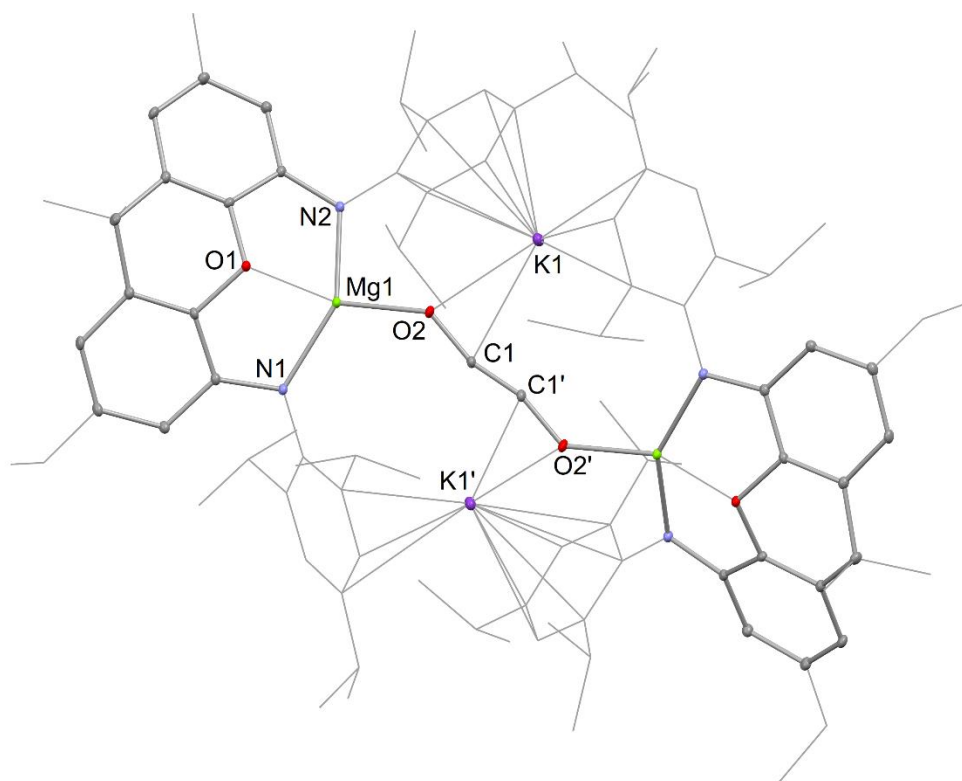


Figure S48. The molecular structure of **3** (20% ellipsoids; Trip, methyl and ethyl substituents shown as wire-frame for clarity; hydrogen atoms omitted). Selected bond lengths (Å) and angles (°): Mg(1)-O(2) 1.9029(11), Mg(1)-N(2) 2.0394(13), Mg(1)-N(1) 2.0455(12), Mg(1)-O(1) 2.0533(11), O(2)-C(1) 1.3049(18), C(1)-C(1') 1.2060(10), C(1)'-C(1)-O(2) 163.4(2), C(1)-O(2)-Mg(1) 134.51(10).

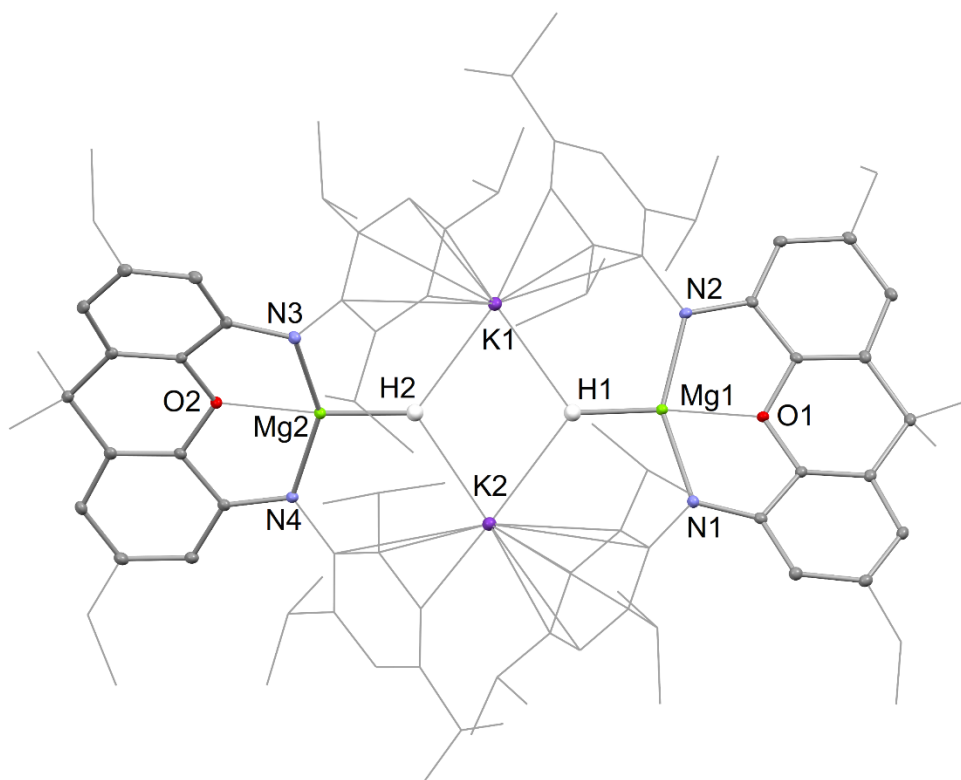


Figure S49. The molecular structure of **4** (20% ellipsoids; Trip, methyl and ethyl substituents shown as wire-frame for clarity; hydrogen atoms, except hydrides, omitted). Selected bond lengths (Å) and angles (°): Mg(1)-O(1) 2.073(2), Mg(1)-N(1) 2.049(3), Mg(1)-N(2) 2.045(3), Mg(1)-H(2) 1.76(5), Mg(2)-O(2) 2.066(2), Mg(2)-N(4) 2.053(3), Mg(2)-N(3) 2.058(3), Mg(2)-H(4) 1.86(5), K(2)-H(2) 2.74(5), K(2)-H(4) 2.63(5), K(1)-H(2) 2.74(5), K(1)-H(4) 2.72(5), N(4)-Mg(2)-N(3) 148.97(11), N(2)-Mg(1)-N(1) 148.84(12).

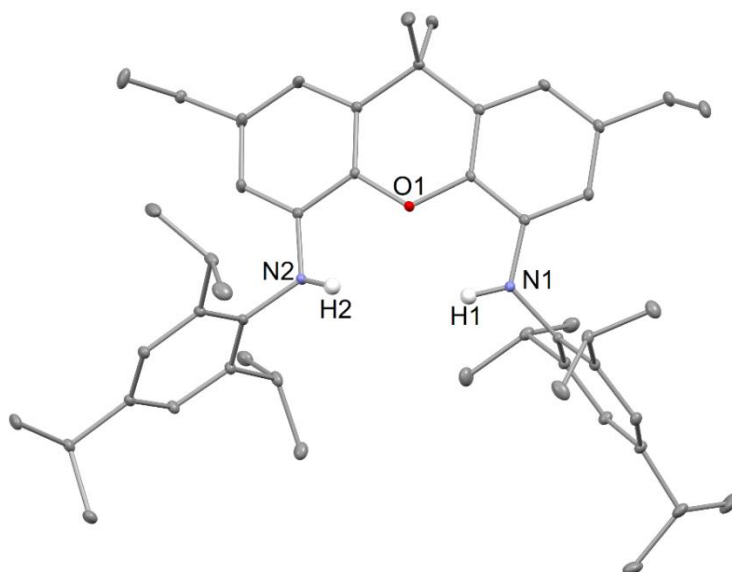


Figure S50. The molecular structure of TriipNONH_2 (20% ellipsoids; hydrogen atoms, except amine protons, omitted).

3. Computational Studies

All the DFT calculations were performed using Gaussian16 suite of programs.⁹ Hybrid DFT functional (wB97XD)¹⁰ along with SDD basis sets¹¹ for Mg, K atoms (additional polarization¹² for Mg and K atoms) and 6-31G** basis sets¹³ for the rest of the atoms were employed for the computation. Frequency calculations were performed to locate minima for the optimized structure.

Table S2. DFT computed natural charges for selected atoms in **2**.

	Natural charges
K1	0.89863
K2	0.90150
Mg3	0.97047
Mg4	0.97503
O5	-0.63415
O6	-0.63451
N7	-0.90820
N8	-0.91590
N9	-0.90814
N10	-0.91611

Table S3. DFT computed Wiberg indices for **2**.

Atom Label	Wiberg bond index	Atom Label	Wiberg bond index	Atom Label	Wiberg bond index
Mg3	0.0000	Mg3	0.0000	Mg3	0.0000
O6	0.0164	N7	0.0510	N10	0.0488
Atom Label	Wiberg bond index	Atom Label	Wiberg bond index	Atom Label	Wiberg bond index
Mg4	0.0000	Mg4	0.0000	Mg4	0.0000
O5	0.0164	N8	0.0493	N9	0.0517
Atom Label	Wiberg bond index				
Mg3	0.0000				
Mg4	0.6937				

Table S4. DFT computed NBO second order perturbation analysis for **2**.

Donor NBO	Acceptor NBO	E(2) kcal/mol
(1.81177) BD (1)Mg 3-Mg 4 (50.15%) 0.7081*Mg 3 s(90.40%)p 0.11(9.59%)d 0.00(0.01%) (49.85%) 0.7061*Mg 4 s(90.33%)p 0.11(9.66%)d 0.00(0.01%)	(0.09757) LV (1) K 1 s(99.35%)p 0.01(0.56%)d 0.00(0.08%)	27.70
(1.81177) BD (1)Mg 3-Mg 4 (50.15%) 0.7081*Mg 3 s(90.40%)p 0.11(9.59%)d 0.00(0.01%) (49.85%) 0.7061*Mg 4 s(90.33%)p 0.11(9.66%)d 0.00(0.01%)	(0.09499) LV (1) K 2 s(99.31%)p 0.01(0.61%)d 0.00(0.08%)	26.22
(1.95517) LP (1) O 5 s(29.05%)p 2.44(70.92%)d 0.00(0.03%)	(0.14747) BD*(1)Mg 3-Mg 4 (49.85%) 0.7061*Mg 3 s(90.40%)p 0.11(9.59%)d 0.00(0.01%) (50.15%) -0.7081*Mg 4 s(90.33%)p 0.11(9.66%)d 0.00(0.01%)	6.39
(1.88554) LP (1) N 8 s(30.11%)p 2.32(69.87%)d 0.00(0.02%)	(0.14747) BD*(1)Mg 3-Mg 4 (49.85%) 0.7061*Mg 3 s(90.40%)p 0.11(9.59%)d 0.00(0.01%) (50.15%) -0.7081*Mg 4 s(90.33%)p 0.11(9.66%)d 0.00(0.01%)	12.11
(1.87021) LP (1) N 9 s(29.33%)p 2.41(70.66%)d 0.00(0.02%)	(0.14747) BD*(1)Mg 3-Mg 4 (49.85%) 0.7061*Mg 3 s(90.40%)p 0.11(9.59%)d 0.00(0.01%) (50.15%) -0.7081*Mg 4 s(90.33%)p 0.11(9.66%)d 0.00(0.01%)	12.35
(1.95511) LP (1) O 6 s(29.05%)p 2.44(70.92%)d 0.00(0.03%)	(0.14747) BD*(1)Mg 3-Mg 4 (49.85%) 0.7061*Mg 3 s(90.40%)p 0.11(9.59%)d 0.00(0.01%) (50.15%) -0.7081*Mg 4 s(90.33%)p 0.11(9.66%)d 0.00(0.01%)	6.43
(1.86999) LP (1) N 7 s(29.33%)p 2.41(70.66%)d 0.00(0.02%)	(0.14747) BD*(1)Mg 3-Mg 4 (49.85%) 0.7061*Mg 3 s(90.40%)p 0.11(9.59%)d 0.00(0.01%) (50.15%) -0.7081*Mg 4 s(90.33%)p 0.11(9.66%)d 0.00(0.01%)	12.33
(1.88565) LP (1) N 10 s(30.06%)p 2.33(69.92%)d 0.00(0.02%)	(0.14747) BD*(1)Mg 3-Mg 4 (49.85%) 0.7061*Mg 3 s(90.40%)p 0.11(9.59%)d 0.00(0.01%) (50.15%) -0.7081*Mg 4 s(90.33%)p 0.11(9.66%)d 0.00(0.01%)	12.03

Table S5. Computed BCP descriptors for **2** (atomic units).

	$\rho(r)$	$\nabla^2\rho(r)$	$G(r)$	$V(r)$	$H(r)$	ε
Mg3-Mg4	0.025	-0.020	0.0002	-0.006	-0.0056	0.05
K2-Mg3	0.006	0.013	0.003	-0.002	0.0003	0.51
Mg3-O6	0.024	0.155	0.011	-0.013	-0.0017	0.05
Mg3-N7	0.041	0.242	0.015	-0.019	-0.0037	0.11
Mg3-N10	0.039	0.226	0.014	-0.018	-0.0036	0.12
Mg4-O5	0.024	0.155	0.011	-0.013	-0.0017	0.06
Mg4-N8	0.039	0.226	0.014	-0.018	-0.0036	0.12
Mg4-N9	0.041	0.242	0.015	-0.019	-0.0038	0.11

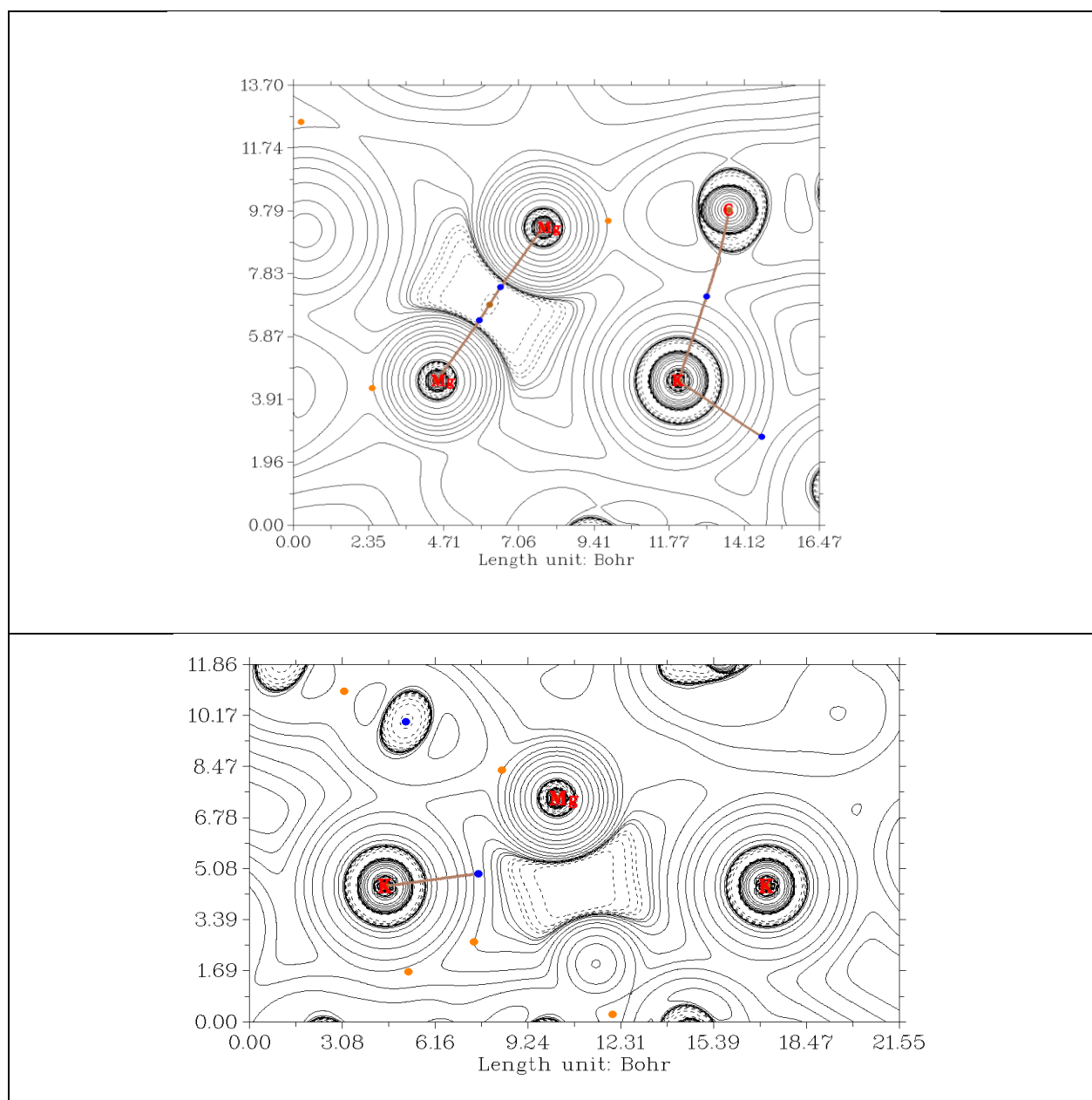
**Figure S51.** Laplacian distributions for **2**, showing a non-nuclear attractor (NNA, brown dot) at the centre of the Mg-Mg vector (top), and an MgK₂ plane (bottom). Blue dots represent bond critical points, whereas orange dots represent ring critical points.

Table S6. CMO analysis for **2**.

MO 393 (occ): orbital energy = -0.19334 a.u. (HOMO) 0.807*[125]: BD (1)Mg 3-Mg 4	(1.81177) BD (1)Mg 3-Mg 4 (50.15%) 0.7081*Mg 3 s(90.40%)p 0.11(9.59%)d 0.00(0.01%) (49.85%) 0.7061*Mg 4 s(90.33%)p 0.11(9.66%)d 0.00(0.01%)
MO 394 (vir): orbital energy = 0.05508 a.u. (LUMO) 0.665*[395]: LV (1) K 2(lv) -0.264*[394]: LV (1) K 1(lv) -0.226*[499]: BD*(2) C64- C82*	(0.09499) LV (1) K 2 s(99.31%)p 0.01(0.61%)d 0.00(0.08%) (0.09757) LV (1) K 1 s(99.35%)p 0.01(0.56%)d 0.00(0.08%) (0.36262) BD*(2) C 64- C 82 (51.63%) 0.7186* C 64 s(0.02%)p99.99(99.93%)d 2.63(0.05%) (48.37%) -0.6955* C 82 s(0.03%)p99.99(99.93%)d 1.20(0.04%)

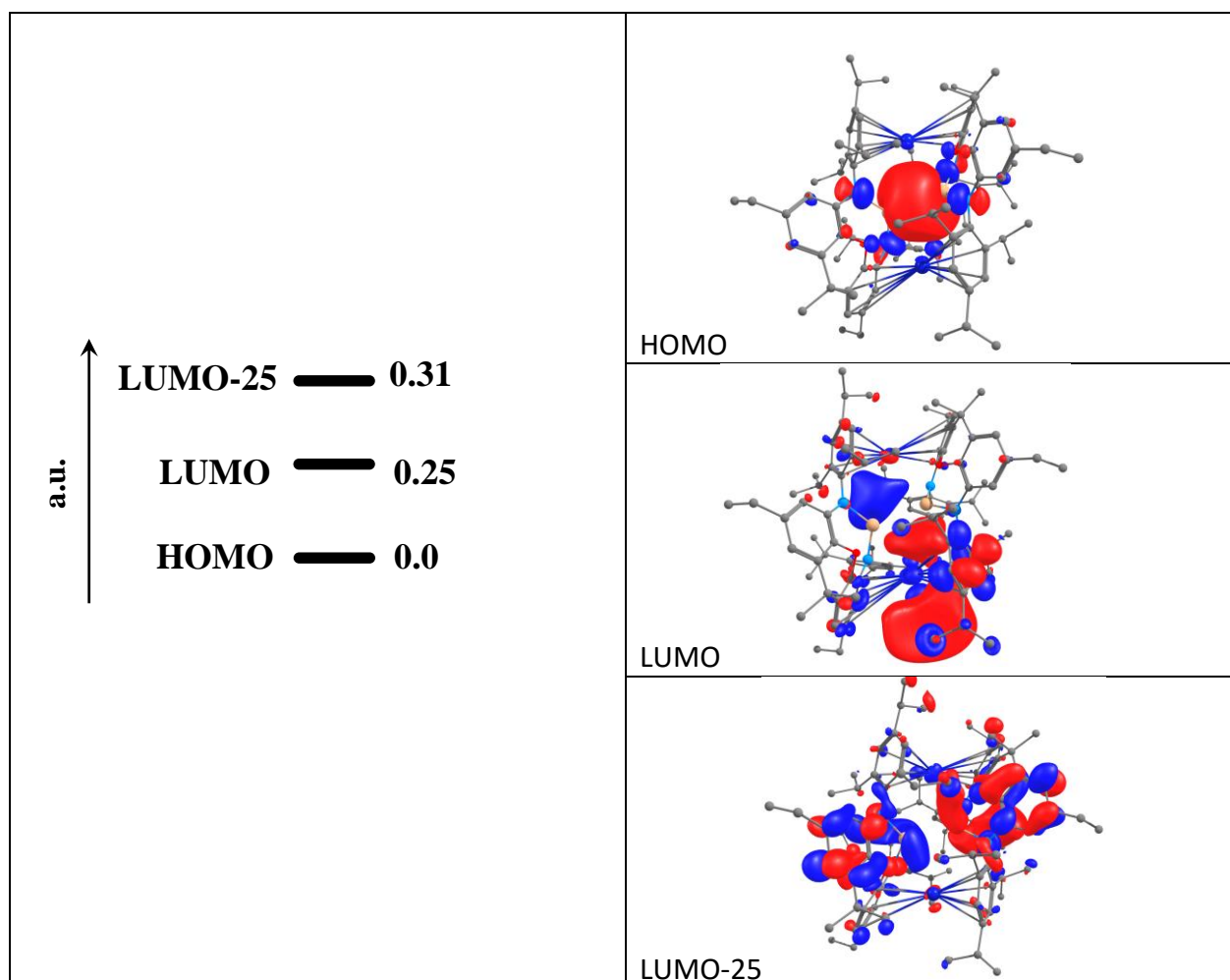
**Figure S52.** Selection of DFT computed MO's for **2**.

Table S7. Cartesian coordinates for the optimised geometry of **2**.

K	-2.206019000	-0.416994000	-2.507099000
K	2.135377000	-0.612715000	2.589437000
Mg	1.343789000	-0.227510000	-0.678402000
Mg	-1.379359000	-0.037778000	0.742242000
O	-3.232672000	-1.107339000	0.141653000
O	3.060532000	-1.493879000	-0.058863000
N	1.577430000	-1.607654000	-2.254499000
N	-2.702871000	1.447149000	-0.035862000
N	-1.777513000	-1.351627000	2.341713000
N	2.838015000	1.111353000	0.044184000
C	0.586716000	-1.834221000	-3.223455000
C	-4.250878000	-0.317625000	-0.391247000
C	-3.684380000	-2.037314000	1.078670000
C	2.584281000	-2.532150000	-2.129802000
C	0.439313000	-0.922327000	-4.305263000
C	3.396485000	-2.486666000	-0.980862000
C	-1.735227000	3.535611000	-0.896324000
C	-1.584850000	-2.085482000	-5.054448000
C	-2.886193000	-2.153555000	2.232385000
C	-0.342678000	-2.902696000	-3.110698000
C	-4.873170000	-2.701766000	0.849271000
C	-0.247479000	-3.890493000	2.135345000
H	-0.999150000	-3.488566000	1.456426000
C	-0.032468000	-2.855962000	3.229104000
C	-5.462684000	-0.888366000	-0.728408000
C	-1.105349000	2.783506000	-2.053249000
H	-0.860405000	1.787331000	-1.659955000
C	-0.821491000	-1.676660000	3.317108000
C	-0.246576000	-3.940882000	-2.003175000
H	0.552384000	-3.624521000	-1.333100000
C	-1.534669000	-4.030153000	-1.179190000
H	-1.809514000	-3.064422000	-0.742350000
H	-1.414040000	-4.739116000	-0.354716000
H	-2.374338000	-4.389779000	-1.781944000
C	-2.517476000	2.852496000	0.057220000
C	-0.646306000	-1.056826000	-5.174816000
H	-0.767349000	-0.349117000	-5.990310000
C	-6.138799000	1.297374000	-1.524417000
C	1.503730000	0.139476000	-4.552506000
H	1.726997000	0.623821000	-3.592813000
C	-3.929652000	1.051401000	-0.490167000
C	-4.920121000	1.840860000	-1.114517000
H	-4.740612000	2.905556000	-1.235657000
C	-3.359479000	-3.077053000	3.181880000
H	-2.804596000	-3.204274000	4.107913000
C	4.503830000	-3.277698000	-0.744423000
C	-1.395347000	-3.006087000	-4.026816000
H	-2.095123000	-3.830147000	-3.914405000
C	2.941704000	-3.523470000	-3.061594000
H	2.370512000	-3.603421000	-3.982978000
C	-6.421649000	-0.054632000	-1.315517000
H	-7.391115000	-0.445802000	-1.604036000
C	4.167354000	-0.813601000	0.449292000
C	-2.096580000	2.644072000	-3.221402000
H	-3.060539000	2.233600000	-2.900075000
H	-1.679939000	2.021573000	-4.026494000
H	-2.305826000	3.627617000	-3.655234000
C	5.309224000	-3.022774000	0.538620000
C	-5.294380000	-3.611192000	1.826682000

H	-6.221308000	-4.161360000	1.706647000
C	-5.638425000	-2.383355000	-0.444312000
C	-1.485281000	0.422595000	4.599523000
H	-1.656420000	0.904171000	3.627873000
C	-0.561131000	-0.768431000	4.378742000
C	4.009105000	0.585624000	0.512613000
C	-4.536229000	-3.800088000	2.982471000
C	2.825230000	2.525156000	-0.088587000
C	1.085883000	1.223082000	-5.549354000
H	0.972344000	0.815084000	-6.559873000
H	1.857514000	1.995110000	-5.598916000
H	0.146448000	1.711491000	-5.271369000
C	-3.100887000	3.584630000	1.117518000
C	-7.117473000	-2.764288000	-0.327208000
H	-7.649415000	-2.538502000	-1.255218000
H	-7.603237000	-2.229065000	0.492805000
H	-7.224058000	-3.838483000	-0.154582000
C	1.026154000	-4.140905000	1.321912000
H	1.407103000	-3.221225000	0.865465000
H	0.831779000	-4.850859000	0.512434000
H	1.818194000	-4.576724000	1.938852000
C	5.310441000	-1.511262000	0.787980000
C	0.494943000	-1.018494000	5.261449000
H	0.691049000	-0.308446000	6.057231000
C	-5.021058000	-3.170436000	-1.622411000
H	-5.055419000	-4.247099000	-1.427582000
H	-3.974308000	-2.895805000	-1.772628000
H	-5.573219000	-2.961213000	-2.545494000
C	-3.909513000	2.903081000	2.213061000
H	-3.711687000	1.827696000	2.142829000
C	-2.914778000	4.965681000	1.173385000
H	-3.368479000	5.519237000	1.991335000
C	0.986639000	-3.073684000	4.160322000
H	1.582922000	-3.981636000	4.081753000
C	-2.153050000	5.654297000	0.233218000
C	-1.566329000	4.914792000	-0.788019000
H	-0.960318000	5.433914000	-1.525264000
C	0.107983000	-5.328700000	-2.554950000
H	-0.685061000	-5.703456000	-3.212619000
H	0.223713000	-6.043349000	-1.732927000
H	1.043447000	-5.309239000	-3.116583000
C	4.812140000	-4.248126000	-1.704983000
H	5.670970000	-4.898295000	-1.578835000
C	4.029231000	-4.372347000	-2.852934000
C	-2.797382000	-2.119237000	-5.970596000
H	-2.495285000	-1.661890000	-6.921427000
C	2.158868000	3.326866000	0.859748000
C	1.443765000	2.691992000	2.037457000
H	1.083172000	1.719895000	1.674577000
C	1.287298000	-2.165173000	5.173221000
C	3.468170000	3.146935000	-1.185305000
C	4.401790000	-5.367883000	-3.928182000
H	3.494239000	-5.837881000	-4.325666000
H	5.005921000	-6.171727000	-3.493149000
C	0.207766000	3.393305000	-2.541823000
H	0.051010000	4.318998000	-3.107165000
H	0.715115000	2.691145000	-3.209918000
H	0.877217000	3.612571000	-1.708090000
C	-5.024658000	-4.725006000	4.074271000
H	-4.178112000	-5.286216000	4.487731000
H	-5.713392000	-5.464295000	3.650604000
C	-2.851553000	-0.068493000	5.106769000

H	-3.334223000	-0.729100000	4.385629000
H	-3.516843000	0.780025000	5.292868000
H	-2.728863000	-0.614838000	6.049015000
C	6.733216000	-3.575782000	0.425936000
H	7.273444000	-3.119467000	-0.407640000
H	6.713638000	-4.658744000	0.278176000
H	7.292639000	-3.392104000	1.347070000
C	2.803231000	-0.526372000	-5.034946000
H	3.199836000	-1.219511000	-4.292478000
H	3.567085000	0.230373000	-5.238231000
H	2.620785000	-1.079831000	-5.963231000
C	-0.768080000	-5.218814000	2.701190000
H	-0.028049000	-5.678909000	3.366375000
H	-0.966596000	-5.924034000	1.886870000
H	-1.696120000	-5.079896000	3.258378000
C	-7.134563000	2.184548000	-2.235658000
H	-7.183705000	3.157491000	-1.733362000
H	-8.135168000	1.743805000	-2.168986000
C	-3.485949000	3.370595000	3.611268000
H	-2.403282000	3.308946000	3.742135000
H	-3.964971000	2.752777000	4.377226000
H	-3.785299000	4.407009000	3.800389000
C	4.610670000	-3.707969000	1.734607000
H	5.186956000	-3.543516000	2.651873000
H	4.521291000	-4.785440000	1.563256000
H	3.602398000	-3.312703000	1.879639000
C	0.210474000	3.469168000	2.497174000
H	0.473817000	4.392687000	3.024957000
H	-0.372738000	2.857989000	3.192475000
H	-0.430577000	3.730668000	1.653048000
C	-5.419954000	3.120771000	2.037445000
H	-5.658973000	4.189845000	2.083555000
H	-5.972849000	2.616689000	2.837385000
H	-5.774462000	2.730904000	1.081742000
C	-0.931545000	1.474031000	5.564164000
H	-0.861904000	1.083455000	6.585494000
H	-1.602732000	2.335963000	5.595476000
H	0.058856000	1.835720000	5.269505000
C	2.178211000	4.713969000	0.723486000
H	1.664815000	5.325352000	1.460383000
C	3.470937000	4.538901000	-1.268608000
H	3.966559000	5.010208000	-2.112867000
C	2.407828000	2.472009000	3.215371000
H	2.733307000	3.436113000	3.620137000
H	3.315538000	1.937862000	2.912554000
C	6.368538000	-0.778645000	1.338794000
H	7.293681000	-1.269996000	1.619554000
C	4.122122000	2.333198000	-2.295162000
H	3.700436000	1.322385000	-2.244822000
C	2.837222000	5.344515000	-0.325601000
C	-3.932885000	-1.259043000	-5.388172000
H	-4.273827000	-1.668034000	-4.427511000
H	-4.799587000	-1.238938000	-6.056297000
H	-3.612917000	-0.220778000	-5.238823000
C	5.089591000	1.270600000	1.112590000
H	5.038459000	2.352379000	1.199853000
C	2.484754000	-2.403426000	6.078428000
H	2.633630000	-3.489370000	6.132334000
C	-3.301356000	-3.532785000	-6.272207000
H	-2.491701000	-4.174883000	-6.629513000
H	-4.080885000	-3.502075000	-7.039188000
H	-3.739588000	-4.000999000	-5.383939000

C	3.819198000	2.906669000	-3.685673000
H	2.753740000	3.111197000	-3.815842000
H	4.135398000	2.200556000	-4.459544000
H	4.362834000	3.840370000	-3.865541000
C	6.246683000	0.602090000	1.515654000
C	-6.764799000	2.393691000	-3.709217000
H	-7.493145000	3.033996000	-4.216078000
H	-6.727368000	1.434425000	-4.236265000
H	-5.779684000	2.863447000	-3.796749000
C	2.288168000	-1.890705000	7.507368000
H	2.251459000	-0.796410000	7.541833000
H	3.121535000	-2.206282000	8.142074000
H	1.360607000	-2.274269000	7.940958000
C	5.643845000	2.212871000	-2.120976000
H	6.105169000	3.207792000	-2.112063000
H	6.077588000	1.647410000	-2.952831000
H	5.906908000	1.705470000	-1.192135000
C	5.175970000	-4.708843000	-5.075903000
H	4.580738000	-3.914458000	-5.536969000
H	5.435523000	-5.436952000	-5.850745000
H	6.100606000	-4.256206000	-4.704914000
C	-5.725516000	-3.959799000	5.203072000
H	-6.591146000	-3.413282000	4.816460000
H	-5.046812000	-3.228545000	5.653129000
H	-6.069747000	-4.638259000	5.989895000
C	7.406019000	1.404101000	2.064004000
H	7.031660000	2.161915000	2.762007000
H	8.068532000	0.746964000	2.638161000
C	8.205229000	2.092376000	0.951108000
H	8.595281000	1.353743000	0.244048000
H	9.049018000	2.656178000	1.360547000
H	7.570904000	2.785267000	0.389935000
C	3.755021000	-1.798290000	5.456463000
H	3.954897000	-2.221178000	4.464640000
H	4.635054000	-1.994275000	6.077018000
H	3.658033000	-0.708178000	5.364896000
C	-1.896033000	7.145853000	0.344875000
H	-1.493076000	7.477091000	-0.621281000
C	-3.167476000	7.956609000	0.616101000
H	-3.585870000	7.727855000	1.602030000
H	-3.937117000	7.746283000	-0.132054000
H	-2.949757000	9.029313000	0.594819000
C	-0.825620000	7.421930000	1.409892000
H	-0.590610000	8.490225000	1.468106000
H	0.094396000	6.877723000	1.178126000
H	-1.170394000	7.092125000	2.396365000
C	2.787219000	6.854603000	-0.468225000
H	2.433483000	7.258234000	0.489600000
C	1.766291000	7.254627000	-1.542508000
H	1.682246000	8.343783000	-1.622980000
H	0.778894000	6.848930000	-1.303644000
H	2.062419000	6.860698000	-2.521200000
C	4.159618000	7.474361000	-0.751769000
H	4.545016000	7.162818000	-1.728435000
H	4.890188000	7.178927000	0.006713000
H	4.093190000	8.567125000	-0.759637000
H	1.916892000	1.929891000	4.036540000

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