Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supporting Information

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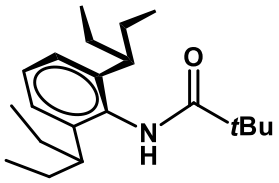
1. Materials and methods

All experiments, unless otherwise stated, were conducted in dry glassware under an inert nitrogen atmosphere by applying standard Schlenk techniques or gloveboxes (MBraun) using freshly dried and degassed solvents. Dichloromethane (DCM), diethyl ether (Et_2O) and methanol (MeOH) were purified by vacuum distillation. Toluene, benzene, pentanes and hexanes were degassed with nitrogen, dried over activated aluminum oxide (Innovative Technology, Pure Solv 400-4-MD, Solvent Purification System) and then stored under inert atmosphere over molecular sieves (3 Å). Deuterated benzene (C_6D_6) and toluene-d_8 were purchased from Deutero GmbH and Euriso-top, degassed and dried over molecular sieves (3 Å). *N,N,N',N'*-Tetramethylethylendiamine (TMEDA, 99.8% Sigma Aldrich) was dried over CaH_2, distilled and stored over molecular sieves (3 Å). Elemental iodine was sublimed and stored under nitrogen atmosphere. Following reagents were obtained commercially and used without further purification: *n*-butyllithium (^{n}BuLi (2.5 M in hexane, Sigma Aldrich), methyllithium (MeLi, 1.6 M in Et_2O, Sigma Aldrich), phosphorus pentachloride (PCl_5, reagent grade 95%, Sigma Aldrich), pivaloyl chloride (99%, Sigma Aldrich), triethylamine (NEt_3, >99.5%, Sigma Aldrich), di-*n*-butyl magnesium (Mg^nBu_2, 0.5 m in heptane, Sigma Aldrich) and potassium (chunks, washed with hexane, 98% trace metal basis, Sigma Aldrich). The following compounds were synthesized according to literature procedures: 2,6-Di(3-*iso*pentyl)aniline.[S1]

NMR spectra were measured on Bruker Avance III HD 400 MHz and Bruker Avance III HD 600 MHz spectrometers. Chemical shifts (δ) are denoted in ppm (parts per million), coupling constants in Hz (Hertz). For describing signal multiplicities common abbreviations are used: s (singlet), d (doublet), t (triplet), q (quartet), p (quintet), sept (septet), m (multiplet) and br (broad). Spectra were referenced to the solvent residual signal. Elemental analysis was performed with an Hekatech Eurovector EA3000 analyzer. All crystal structures have been measured on a SuperNova (Agilent) diffractometer with dual Cu and Mo microfocus sources and an Atlas S2 detector. Crystallographic data have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication numbers: CCDC 2020201 (^{DIPeP}Pivaloylamide), 2020202 ((^{DIPeP}BDI*)-H), 2020203 ((^{DIPeP}BDI*)Mg^{n}Bu), 2020204 ((^{DIPeP}BDI*)MgI), 2020205 ([(^{DIPeP}BDI*)Mg]$_2$) and (^{DIPeP}BDI)MgI 2020206.

2. Synthetic procedures

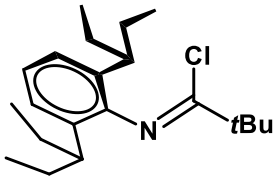
2.1 Synthesis of ^{DIPeP}Pivaloylamide



2,6-Di(3-*iso*pentyl)aniline (12.0 g, 51.0 mmol) and NEt_3 (7.10 mL, 51.0 mmol) were dissolved in DCM (250 mL) under air. Pivaloyl chloride (6.30 mL, 51.0 mmol), dissolved in DCM (30 mL), was added over the course of 2 h (HCl liberation!) and the reaction mixture subsequently heated to reflux for 3 h. The obtained colorless solution was chilled to room temperature, diluted with DCM (500 mL) and washed with water (3 x 200 mL). The aqueous phase was extracted with DCM (200 mL) and the combined organic phases were dried over $MgSO_4$. The solvent was removed under reduced pressure and the obtained off-white powder was recrystallized from boiling hexane, yielding colorless crystals of the ^{DIPeP}Pivaloylamide (9.74 g, 31.0 mmol, 61%) suitable for X-ray diffraction analysis.

^{1}H NMR (400.13 MHz, $CDCl_3$, 298K): δ = 0.76 (t, ^{3}J = 7.2 Hz, 12H, C**H$_3$**), 1.35 (s, 9H, C**H$_3$**-*t*Bu), 1.44-1.70 (m, 8H, C**H$_2$**), 2.53 (p, ^{3}J = 7.1 Hz, 2H, C**H**), 6.65 (s, 1H, N**H**), 7.04 (d, J = 7.7 Hz, 2H, C**H**-arom), 7.23-7.28 (m, 1H, C**H**-arom) ppm. **^{13}C NMR** (101.92 MHz, C_6D_6, 298K): δ = 12.5 (**C**H_3), 28.0 (**C**H_3-*t*Bu), 29.2 (**C**H_2), 39.2 (**C**$(CH_3)_3$-*t*Bu), 43.3 (**C**H), 123.9 (**C**-arom), 127.9 (**C**-arom), 134.6 (**C**-arom), 143.8 (**C**-arom), 176.5 (**C**O) ppm. **Elemental analysis** Calculated for $C_{21}H_{35}NO$ (M = 317.52 g/mol): C 79.44, H 11.11, N 4.41; Found: C 79.17, H 11.38, N 4.38.

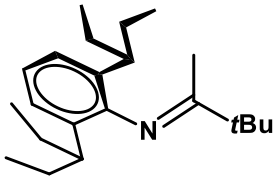
2.2 Synthesis of ^{DIPeP}Imidoyl chloride



^{DIPeP}Pivaloylamide (9.70 g, 30.6 mmol) was dissolved in toluene (80 mL). PCl_5 (6.3 g, 30.3 mmol) was added in one portion and the resulting suspension stirred at room temperature overnight (HCl liberation!). All volatiles from the obtained yellow solution were removed *in vacuo* and the remaining yellow liquid dried under high vacuum at 80 °C for 2 h. Vacuum distillation (140 °C, $1 \circ 10^{-3}$ mbar) gave ^{DIPeP}Imidoyl chloride as a colorless liquid (9.29 g, 28.0 mmol, 98%).

^{1}H NMR (400.13 MHz, C_6D_6, 298K): δ = 0.84 (t, ^{3}J = 7.4 Hz, 6H, C**H$_3$**), 0.96 (t, ^{3}J = 7.4 Hz, 6H, C**H$_3$**), 1.31 (s, 9H, C**H$_3$**-*t*Bu), 1.38-1.50 (m, 2H, C**H$_2$**), 1.56-1.68 (m, 4H, C**H$_2$**), 1.69-1.82 (m, 2H, C**H$_2$**), 2.40-2.48 (m, 2H, C**H**), 7.02-7.05 (m, 2H, C**H**-arom), 7.07-7.14 (m, 1H, C**H**-arom) ppm. **^{13}C NMR** (101.92 MHz, C_6D_6, 298K): δ = 12.2 (**C**H$_3$), 13.0 (**C**H$_3$), 28.0 (**C**H$_2$), 28.4 (**C**H$_3$-*t*Bu), 29.8 (**C**H$_2$), 43.4 (**C**H), 44.0 (**C**(CH$_3$)$_3$-*t*Bu), 124.2 (**C**-arom), 124.9 (**C**-arom), 134.2 (**C**-arom), 146.3 (**C**-arom), 153.4 (**C**Cl) ppm. **Elemental analysis** Calculated for $C_{21}H_{34}ClN$ (M = 335.96 g/mol): C 75.08, H 10.20, N 4.17; Found: C 74.45, H 9.88, N 4.03.

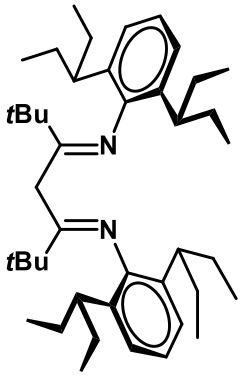
2.3 Synthesis of ^{DIPeP}Imine



Methyl lithium (12.5 mL, 20.0 mmol, 1.5 equivalents1.6 M in Et_2O) was added dropwise to a solution of ^{DIPeP}Imidoyl chloride (4.50 g, 13.0 mmol) in Et_2O (60 mL) at 0 °C. After completed addition the orange colored solution was allowed to reach room temperature and stirred at this temperature for 3 h. The solution was cooled to 0 °C and water (40 mL) was added carefully. The aqueous phase was extracted with Et_2O (100 mL) and the combined organic extracts dried over $MgSO_4$. The solvent was removed under reduced pressure to obtain ^{DIPeP}Imine as a sticky yellow liquid (3.82 g, 12 mmol, 92%).

^{1}H NMR (400.13 MHz, $CDCl_3$, 298K): δ = 0.74 (t, ^{3}J = 7.4 Hz, 6H, C**H$_3$**), 0.81 (t, ^{3}J = 7.4 Hz, 6H, C**H$_3$**), 1.27 (s, 9H, C**H$_3$**-*t*Bu), 1.35-1.42 (m, 2H, C**H$_2$**), 1.50-1.60 (m, 6H, C**H$_2$**), 1.62 (s, 3H, NCC**H$_3$**), 2.20-2.29 (m, 2H, C**H**), 6.96 (s, 3H, C**H**-arom) ppm. **^{13}C NMR** (101.92 MHz, $CDCl_3$, 298K): δ = 11.9 (**C**H$_3$), 12.9 (**C**H$_3$), 16.5 (NC**C**H$_3$), 27.1 (**C**H$_2$), 28.2 (**C**H$_3$-*t*Bu), 29.4 (**C**H$_2$), 40.6 (**C**(CH$_3$)$_3$-*t*Bu), 42.3 (**C**H), 122.1 (**C**-arom), 123.5 (**C**-arom), 133.1 (**C**-arom), 149.6 (**C**-arom), 175.1 (**C**N) ppm. **Elemental analysis** Calculated for $C_{22}H_{37}N$ (M = 315.55 g/mol): C 83.74, H 11.82, N 4.44; Found: C 84.26, H 11.74, N 5.26.

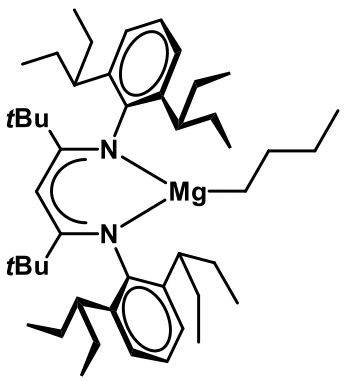
2.4 Synthesis of (^{DIPeP}BDI*)-H



^{DIPeP}Imine (3.80 g, 12.0 mmol) and TMEDA (1.80 mL, 12.0 mmol) were dissolved in hexane (50 mL) and the solution cooled to -80 °C. ^{n}BuLi (4.80 mL, 12.0 mmol, 2.5 M in hexane) was added dropwise at this temperature, yielding an orange solution, that was stirred at room temperature overnight. ^{DIPeP}Imidoyl chloride (4.03 g, 12.0 mmol), dissolved in hexane (10 mL), was slowly added to the reaction mixture affording a red solution, that was heated to reflux for 4 h. The resulting orange colored suspension was quenched with water (20 mL), extracted with Et_2O (150 mL) and the combined extracts washed with water (2 x 50 mL) and dried over $MgSO_4$. The solvent was removed *in vacuo* and the obtained yellow solid washed with cold MeOH (-30 °C, 150 mL), yielding the pro-ligand (^{DIPeP}BDI*)-H as a colorless powder in 66% yield (4.76 g, 8.00 mmol). Crystals suitable for X-ray diffraction analysis were obtained from a concentrated MeOH solution at room temperature.

^{1}H NMR (400.13 MHz, C_6D_6, 298K, *bis*-imine form): δ = 0.52-1.10 (br m, 24H, C**H$_3$**), 1.27 (s, 9H, C**H$_3$**-*t*Bu), 1.27-2.15 (br m, 16H, C**H$_2$**), 2.73 (br s, 2H, C**H**), 3.30 (s, 2H, C**H$_2$**-backbone), 6.91-7.12 (m, 6H, C**H**-arom) ppm. **^{13}C NMR** (101.92 MHz, C_6D_6, 298K, *bis*-imine form): δ = 9.6 (**C**H_3), 10.9 (**C**H_3), 13.0 (**C**H_3), 13.3 (**C**H_3), 25.2 (**C**H_2), 26.0 (**C**H_2), 26.2 (**C**H_2), 28.3 (**C**H_2), 29.5 (**C**H_3-*t*Bu), 32.7 (**C**H_2-backbone), 40.8 (**C**H), 42.1 (**C**H), 42.2 (**C**$(CH_3)_3$-*t*Bu), 123.5 (**C**-arom), 124.3 (**C**-arom), 128.4 (**C**-arom), 133.4 (**C**-arom), 136.0 (**C**-arom), 146.6 (**C**-arom), 173.2 (**C**N) ppm. **Elemental analysis** Calculated for $C_{43}H_{70}N_2$ (M = 615.55 g/mol): C 83.97, H 11.47, N 4.55; Found: C 83.92, H 11.34, N 4.58.

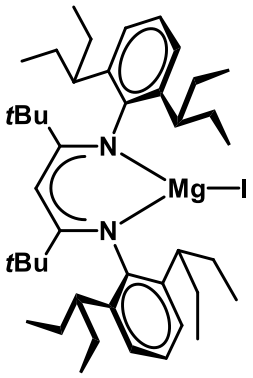
2.5 Synthesis of (^{DIPeP}BDI*)Mg^{n}Bu (1)



^{DIPeP}BDI*-H (3.20 g, 5.20 mmol) was dissolved in benzene (20 mL) and Mg^{n}Bu$_2$ (10.4 mL, 5.20 mmol, 0.5M in heptane) was added at room temperature. The solution was heated to 75 °C and stirred at this temperature overnight (17 h). The resulting pale brown solution was evaporated to dryness affording (^{DIPeP}BDI*)Mg^{n}Bu as colorless powder in quantitative yield (3.61 g, 5.19 mmol). Colorless crystals suitable for X-ray diffraction analysis were obtained from a saturated hexane solution at -20 °C.

^{1}H NMR (600.13 MHz, C_6D_6, 298K): δ = -0.63-(-0.57) (m, 2H, Mg-C**H$_2$**), 0.86 (t, ^{3}J = 7.1 Hz, 3H, Mg-(CH$_2$)$_3$C**H**$_3$), 0.85-0.91 (m, 2H, Mg-CH$_2$C**H$_2$**C$_2$H$_5$), 0.98 (t, ^{3}J = 7.4 Hz, 12H, C**H$_3$**), 0.99 (t, ^{3}J = 7.4 Hz, 12H, C**H**$_3$), 1.04-1.10 (m, 2H, Mg-(CH$_2$)$_2$C**H$_2$**CH$_3$), 1.19 (s, 18H, C**H$_3$**-*t*Bu), 1.62-1.73 (m, 8H, C**H$_2$**), 1.75-1.89 (m, 8H, C**H$_2$**), 3.00-3.06 (m, 4H, C**H**), 5.35 (s, 1H, C**H**-backbone), 6.98-7.06 (m, 6H, C**H**-arom) ppm. **^{13}C NMR** (150.92 MHz, C_6D_6, 298K): δ = 6.6 (Mg-**C**H$_2$), 9.9 (**C**H$_3$), 12.1 (**C**H$_3$), 14.3 (Mg-(CH$_2$)$_3$**C**H$_3$), 24.7 (**C**H$_2$), 26.2 (**C**H$_2$), 31.0 (Mg-CH$_2$**C**H$_2$C$_2$H$_5$), 31.2 (Mg-(CH$_2$)$_2$**C**H$_2$CH$_3$), 33.1 (**C**H$_3$-*t*Bu), 41.0 (**C**H), 44.0 (**C**(CH$_3$)$_3$-*t*Bu), 95.8 (**C**H-backbone), 123.7 (**C**-arom), 125.7 (**C**-arom), 138.7 (**C**-arom), 146.8 (**C**-arom), 176.2 (**C**N-backbone) ppm. **Elemental analysis** Calculated for $C_{47}H_{78}MgN_2$ (M = 695.46 g/mol): C 81.17, H 11.31, N 4.03; Found: C 81.13, H 11.02, N 4.11.

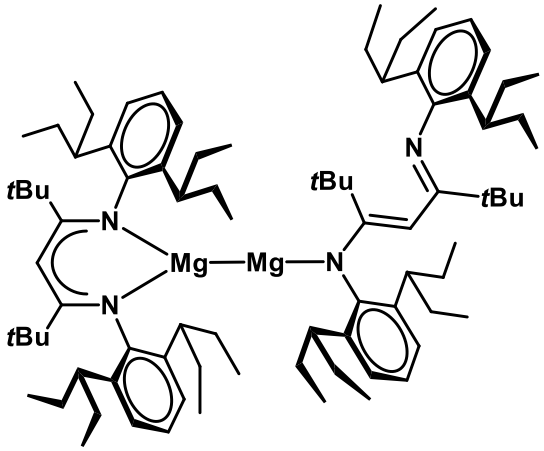
2.6 Synthesis of (^{DIPeP}BDI*)MgI (2)



(^{DIPeP}BDI*)Mg^{n}Bu (3.21 g, 4.62 mmol) and sublimed I_2 (1.23 g, 4.85 mmol, 1.05 eq.) were suspended in benzene (30 mL), vigorously stirred at 75 °C for 4 h and subsequently cooled to room temperature. Insoluble surplus material was filtered off and extracted with benzene (15 mL). All volatiles were removed *in vacuo*, yielding (^{DIPeP}BDI*)MgI as off white powder, that was washed with pentane (2 x 8 mL) and dried under high vacuum. The washings were concentrated to approximately 1/3 of its prior volume, filtered and slowly cooled to -20 °C. Overnight, block like crystals of (^{DIPeP}BDI*)MgI suitable for X-ray diffraction analysis deposited, that were isolated by decantation, washed with cold pentane (-20 °C, 1 x 0.5 mL) and dried under high vacuum. Combined yield: 3.13 g (4.09 mmol, 88%).

^{1}H NMR (600.13 MHz, C_6D_6, 298K): δ = 0.95 (t, ^{3}J = 7.4 Hz, 12H, C**H$_3$**), 1.00 (t, ^{3}J = 7.4 Hz, 12H, C**H**$_3$), 1.15 (s, 18H, C**H$_3$**-*t*Bu), 1.65-1.71 (m, 4H, C**H$_2$**), 1.74-1.81 (m, 8H, C**H$_2$**), 1.90-1.96 (m, 4H, C**H$_2$**), 2.97-3.01 (m, 4H, C**H**), 5.41 (s, 1H, C**H**-backbone), 6.98 (d, 7.7 Hz, 4H, C**H**-arom), 7.05-7.07 (m, 2H, C**H**-arom) ppm. **^{13}C NMR** (150.92 MHz, C_6D_6, 298K): δ = 10.2 (**C**H$_3$), 11.9 (**C**H$_3$), 24.5 (**C**H$_2$), 26.6 (**C**H$_2$), 33.0 (**C**H$_3$-*t*Bu), 41.4 (**C**H), 44.2 (**C**(CH$_3$)$_3$-*t*Bu), 96.5 (**C**H-backbone), 124.4 (**C**-arom), 126.1 (**C**-arom), 138.5 (**C**-arom), 145.3 (**C**-arom), 178.0 (**C**N-backbone) ppm. **Elemental analysis** Calculated for $C_{43}H_{69}IMgN_2$ (M = 765.25 g/mol): C 67.49, H 9.09, N 3.60; Found: C 67.51, H 9.11, N 3.60.

2.7 Synthesis of [(^{DIPeP}BDI*)Mg]$_2$ (3)



(^{DIPeP}BDI*)MgI (410 mg, 0.536 mmol) was dissolved in benzene (8 mL) and stirred over a potassium mirror (210 mg, 5.36 mmol, 10 eq.) at room temperature for 7 h. The mixture was filtered and the yellow solution evaporated to dryness. The crude product was dissolved in hexane (400 µL) and filtered. Leaving it standing overnight at -20 °C gave yellow crystalline blocks of [(^{DIPeP}BDI*)Mg]$_2$ suitable for X-ray diffraction analysis. The supernatant was decanted, the crystals washed with cold pentane (-20 °C, 1 x 0.5 mL) and dried *in vacuo.* Yield: 154 mg (0.121 mmol, 45%).

^{1}H NMR (400.13 MHz, tol-*d8*, 353K): δ = 0.76 (t, ^{3}J = 7.3 Hz, 6H, C**H$_3$**), 0.85 (t, ^{3}J = 7.4 Hz, 12H, C**H**$_3$), 0.88-0.92 (m, 6H, C**H$_3$**), 0.95 (t, ^{3}J = 7.4 Hz, 12H, C**H$_3$**), 0.99 (t, 12H, C**H$_3$**, superimposed by CH$_3$-*t*Bu), 0.99 (s, 9H, C**H$_3$**-*t*Bu), 1.13 (s, 18H, C**H$_3$**-*t*Bu), 1.35-1.42 (m, 4H, C**H$_2$**), 1.55 (s, 9H, C**H$_3$**-*t*Bu), 1.57-1.82 (m, 28H, C**H$_2$**), 2.71-2.80 (m, 4H, C**H**), 2.81-2.88 (m, 4H, C**H**), 4.10 (s, 1H, C**H**-backbone), 5.35 (s, 1H, C**H**-backbone), 6.81-6.98 (m, 12H, C**H**-arom) ppm. **^{13}C NMR** (101.92 MHz, tol-*d8*, 353K): δ = 11.3 (**C**H$_3$), 11.4 (**C**H$_3$), 12.0 (**C**H$_3$), 12.4 (**C**H$_3$), 24.5 (**C**H$_2$),12.6 (**C**H$_3$), 12.7 (**C**H$_3$), 25.4 (**C**H$_2$), 26.9 (**C**H$_2$), 27.3 (**C**H$_2$), 28.0 (**C**H$_2$), 28.8 (**C**H$_2$), 29.4 (**C**H$_2$), 31.8 (**C**H$_3$-*t*Bu), 33.2 (**C**H$_3$-*t*Bu), 33.3 (**C**H$_3$-*t*Bu), 38.7 (**C**(CH$_3$)$_3$-*t*Bu), 41.1 (**C**H), 41.3 (**C**H), 41.3 (**C**H), 44.2 (**C**(CH$_3$)$_3$-*t*Bu), 44.5 (**C**(CH$_3$)$_3$-*t*Bu), 94.7 (**C**H-backbone), 97.0 (**C**H-backbone), 119.9 (**C**-arom), 124.0 (**C**-arom), 124.1 (**C**-arom), 124.1 (**C**-arom), 125.7 (**C**-arom), 126.1 (**C**-arom), 133.1 (**C**-arom), 139.6 (**C**-arom), 144.3 (**C**-arom), 145.5 (**C**-arom), 147.3 (**C**-arom), 151.1 (**C**-arom), 169.5 (**C**N-backbone), 176.6 (**C**N-backbone) ppm. **Elemental analysis** Calculated for $C_{86}H_{138}Mg_2N_4$ (M = 1276.69 g/mol): C 80.91, H 10.90, N 4.39; Found: C 80.89, H 10.85, N 4.41.

3. NMR characterization

3.1 NMR spectroscopic data for ^{DIPeP}Pivaloylamide

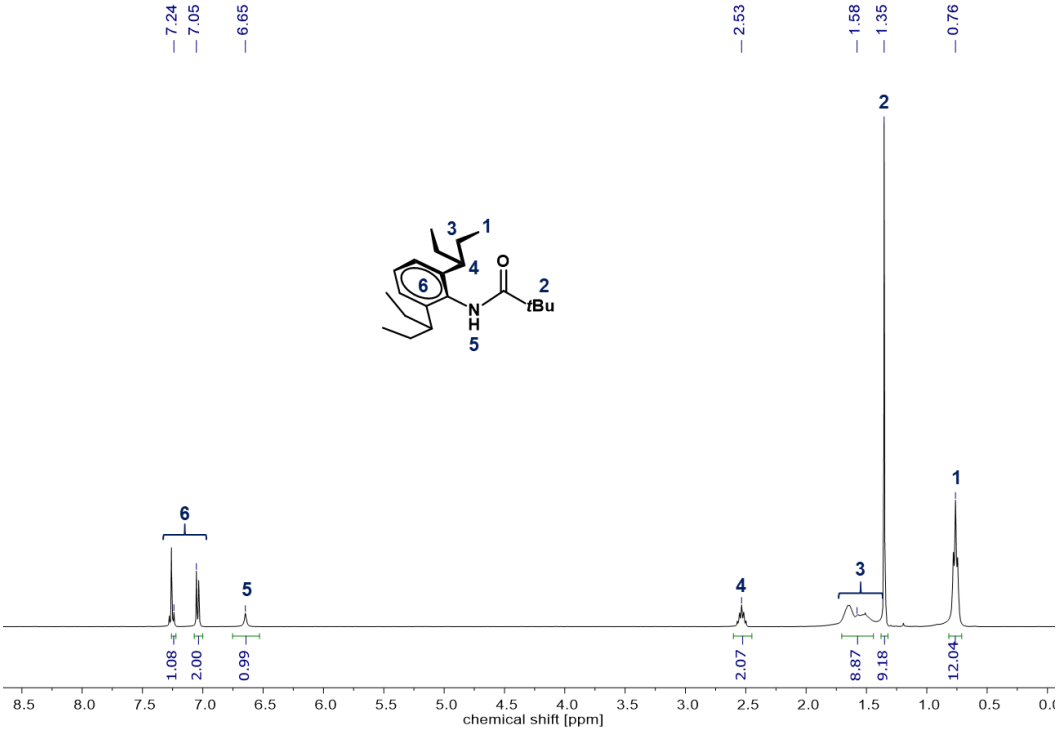


Figure S1. ^{1}H NMR (400.13 MHz, 298 K, $CDCl_3$) of ^{DIPeP}Pivaloylamide.

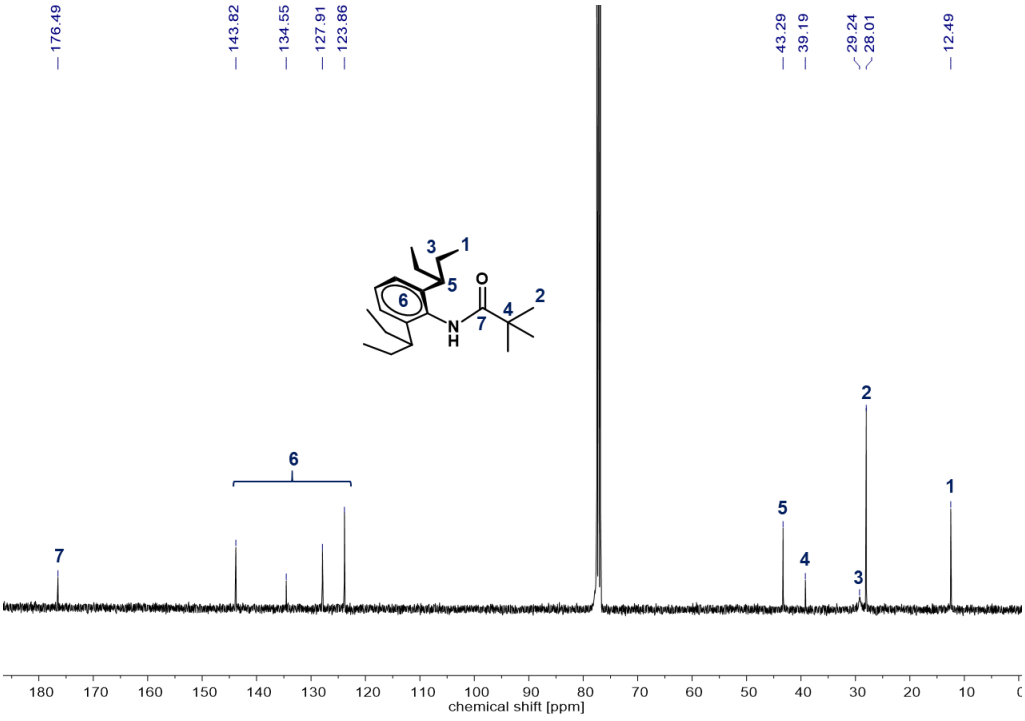


Figure S2. ^{13}C NMR (101.92 MHz, 298 K, $CDCl_3$) of ^{DIPeP}Pivaloylamide.

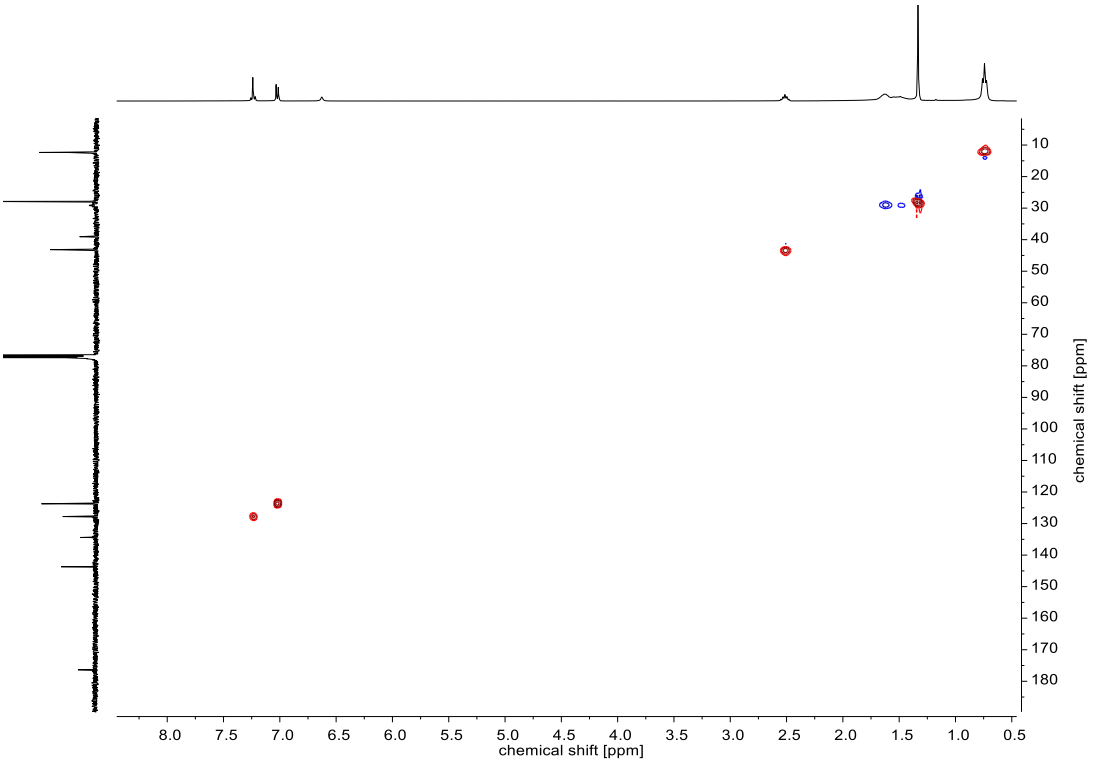


Figure S3. ^{1}H ^{13}C HSQC NMR (400.13/101.92 MHz, 298 K, $CDCl_3$) of ^{DIPeP}Pivaloylamide.

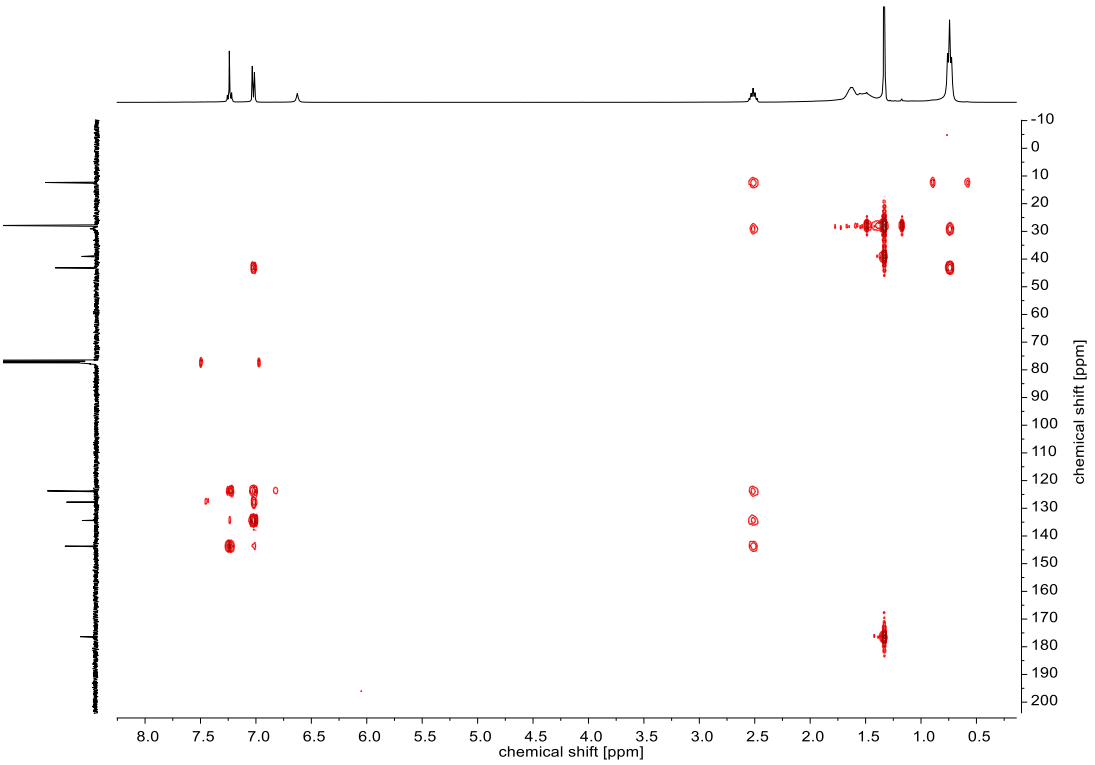


Figure S4. ^{1}H ^{13}C HMBC NMR (600.13/101.92 MHz, 298 K, $CDCl_3$) of ^{DIPeP}Pivaloylamide.

3.2 NMR spectroscopic data for ^{DIPeP}Imidoyl chloride

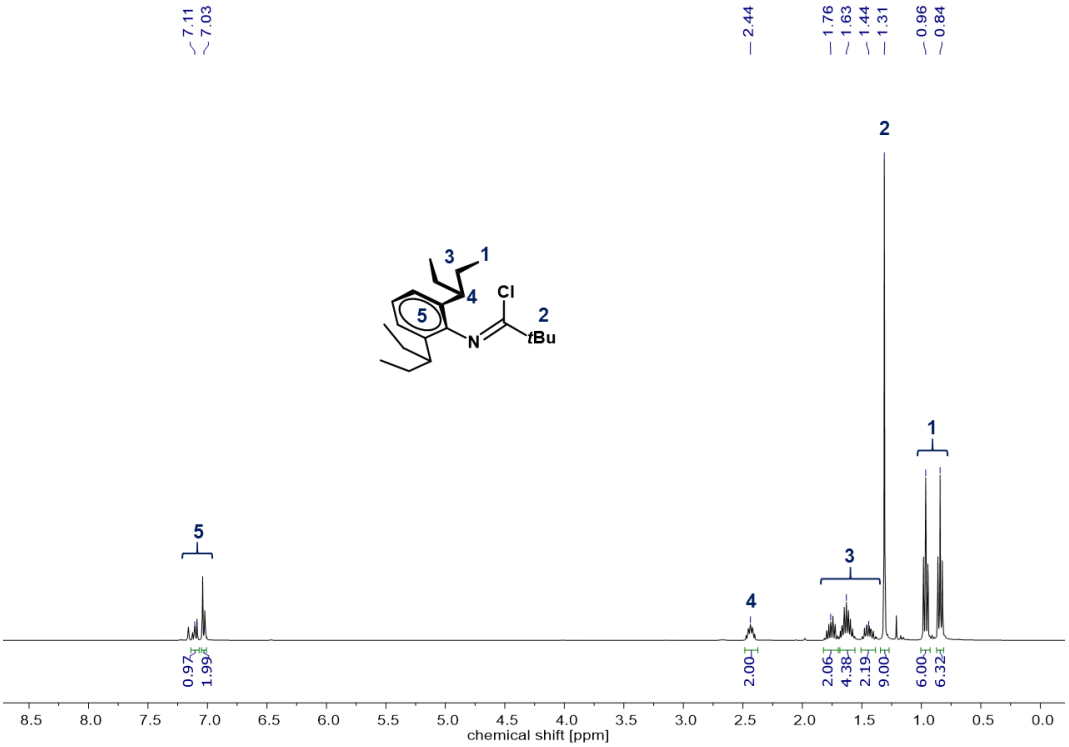


Figure S5. ^{1}H NMR (400.13 MHz, 298 K, C_6D_6) of ^{DIPeP}Imidoyl chloride.

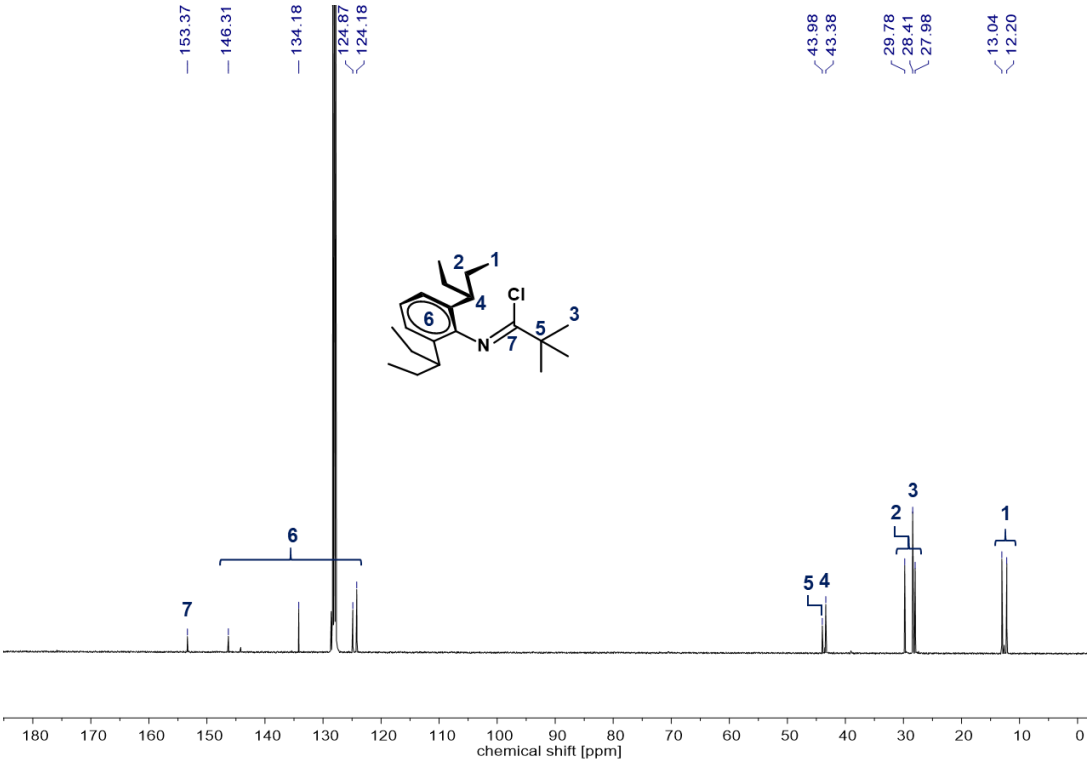


Figure S6. ^{13}C NMR (101.92 MHz, 298 K, C_6D_6) of ^{DIPeP}Imidoyl chloride.

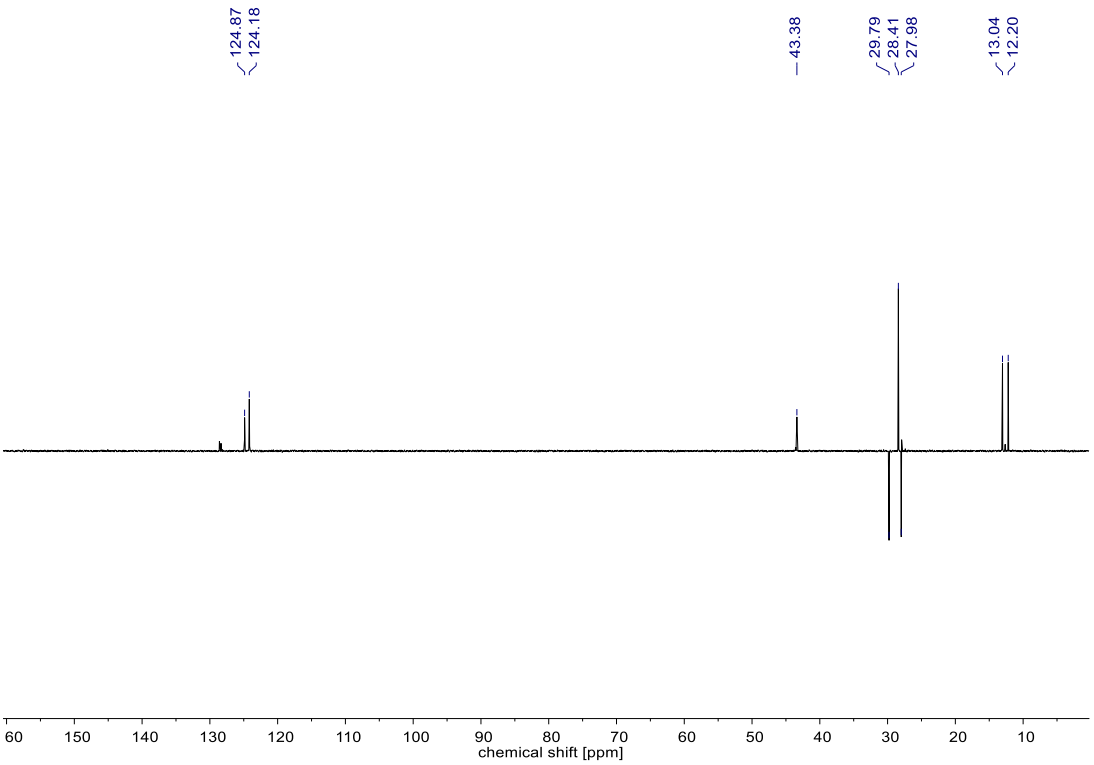


Figure S7. ^{13}C(DEPT 135) NMR (101.92 MHz, 298 K, C_6D_6) of ^{DIPeP}Imidoyl chloride.

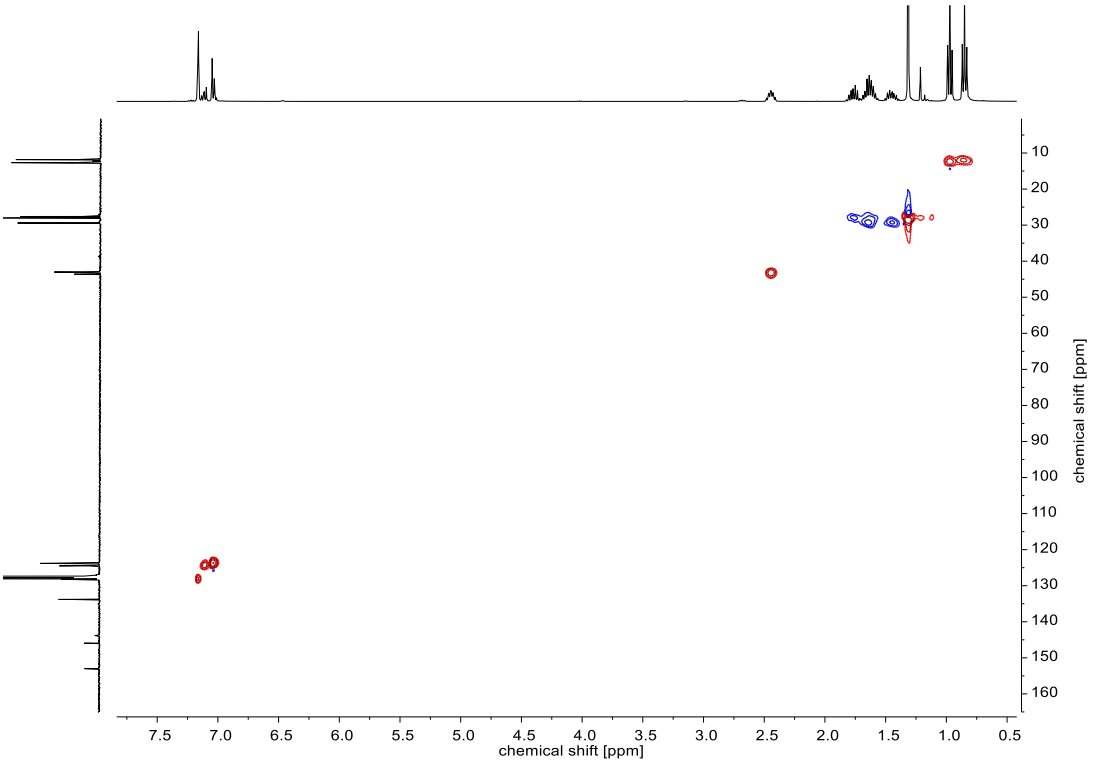


Figure S8. ^{1}H ^{13}C HSQC NMR (400.13/101.92 MHz, 298 K, C_6D_6) of ^{DIPeP}Imidoyl chloride.

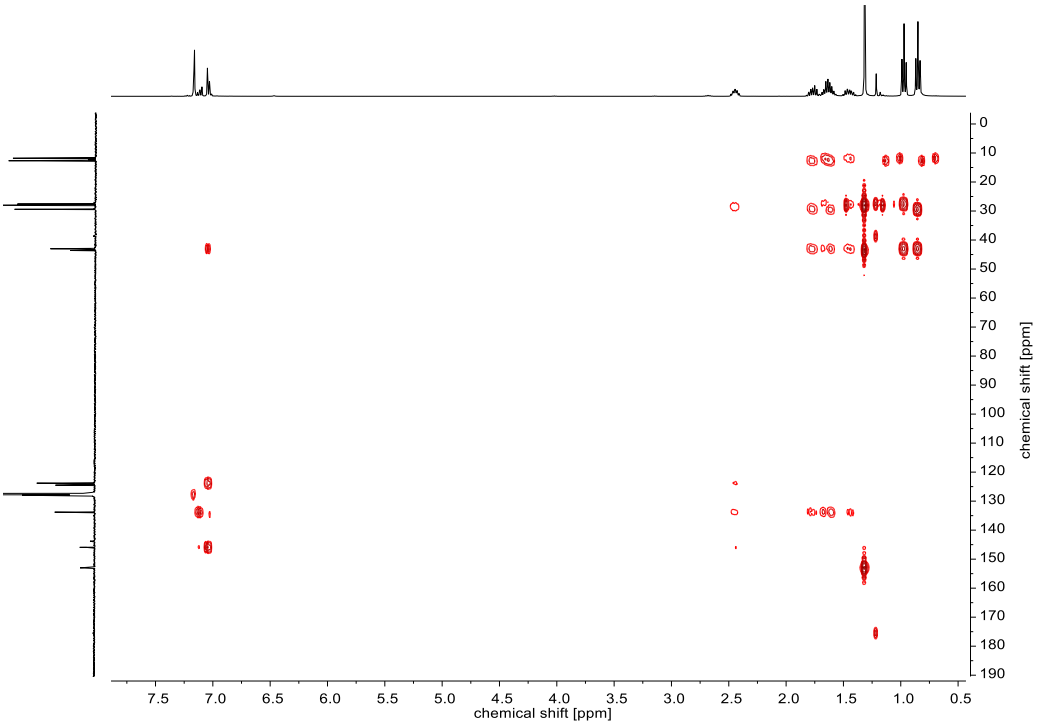


Figure S9. ^{1}H ^{13}C HMBC NMR (400.13/101.92 MHz, 298 K, C_6D_6) of ^{DIPeP}Imidoyl chloride.

3.3 NMR spectroscopic data for ^{DIPeP}Imine

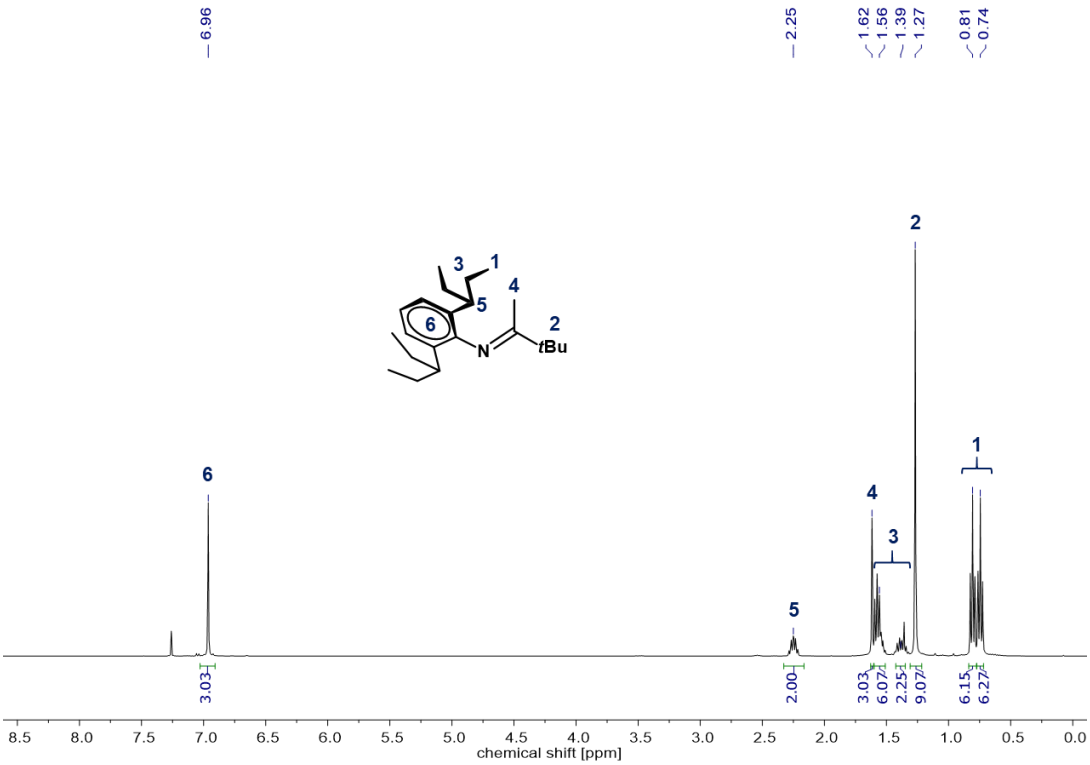


Figure S10. ^{1}H NMR (400.13 MHz, 298 K, $CDCl_3$) of ^{DIPeP}Imine.

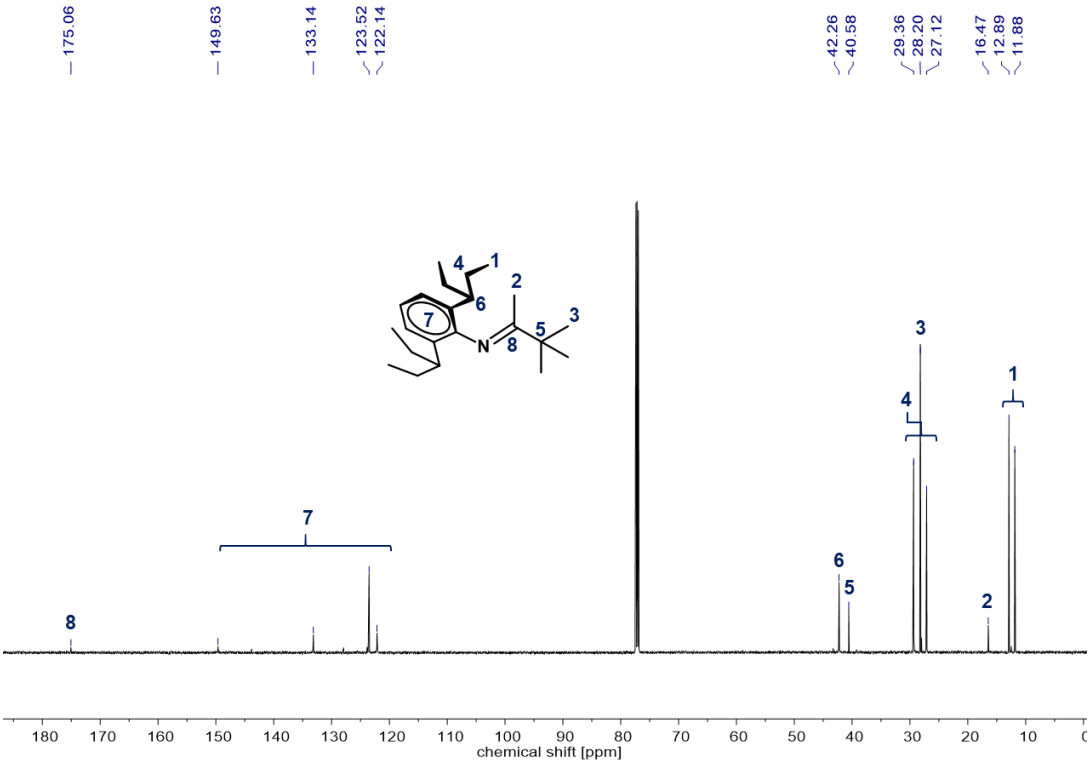


Figure S11. ^{13}C NMR (101.92 MHz, 298 K, $CDCl_3$) of ^{DIPeP}Imine.

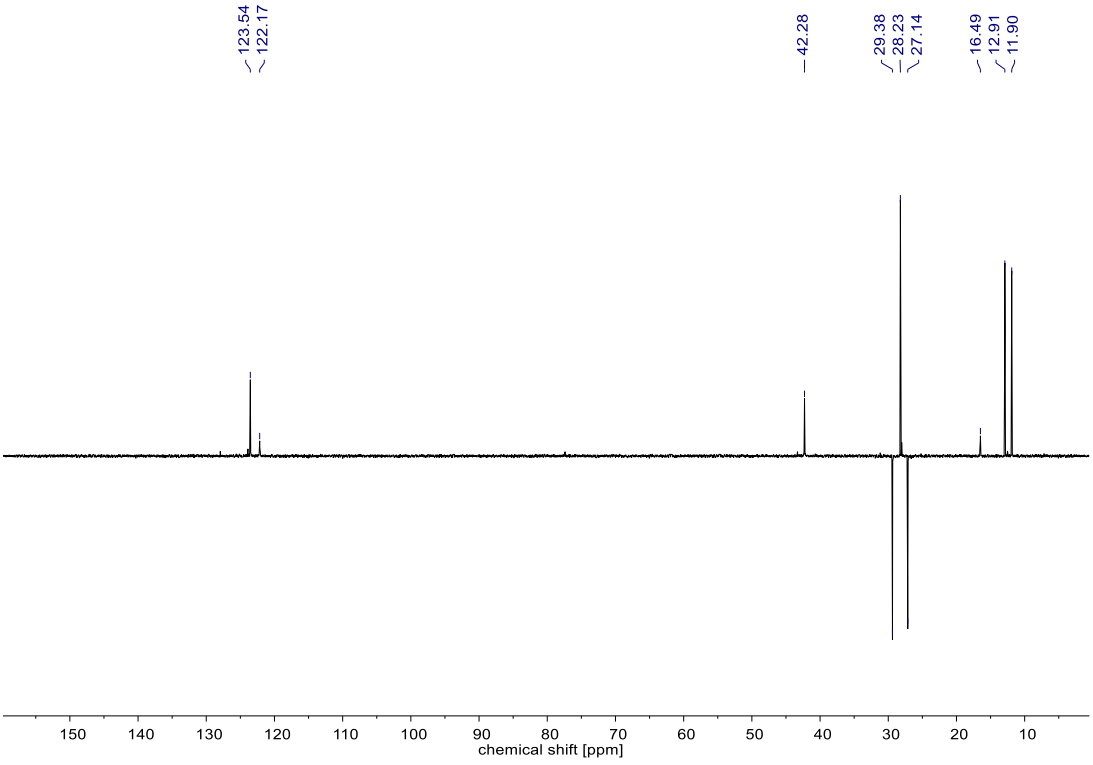


Figure S12. ^{13}C(DEPT 135) NMR (101.92 MHz, 298 K, $CDCl_3$) of ^{DIPeP}Imine.

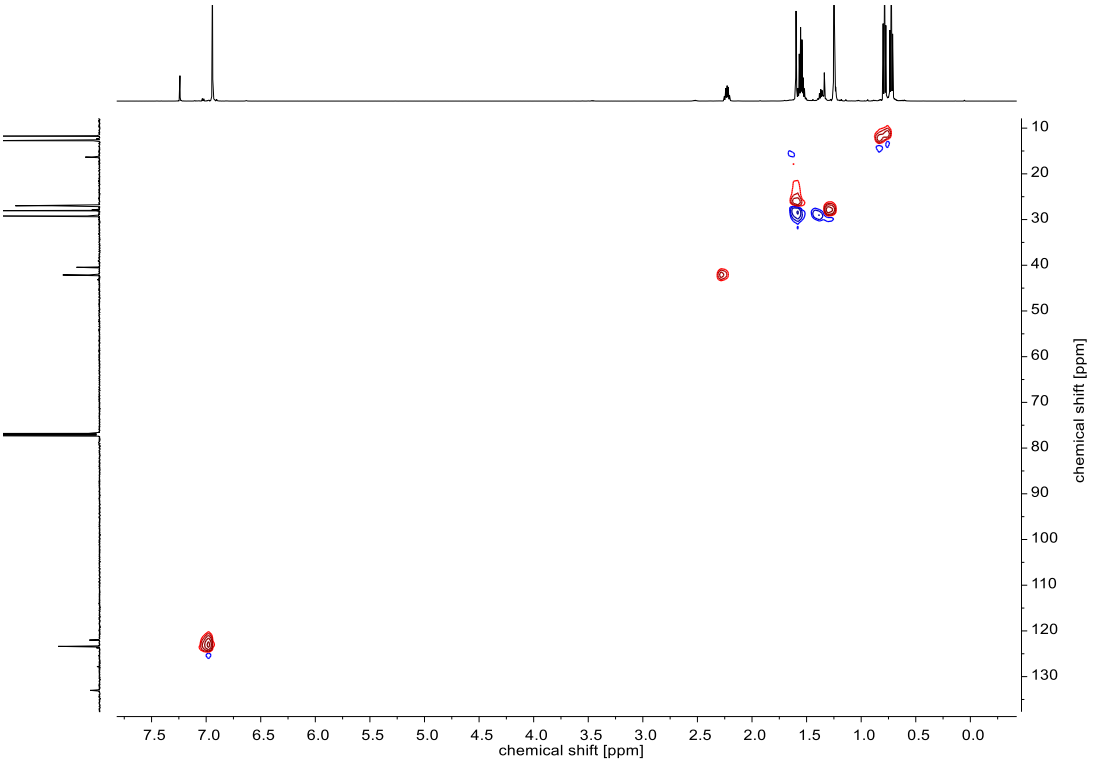


Figure S13. ^{1}H ^{13}C HSQC NMR (400.13/101.92 MHz, 298 K, C_6D_6) of ^{DIPeP}Imine.

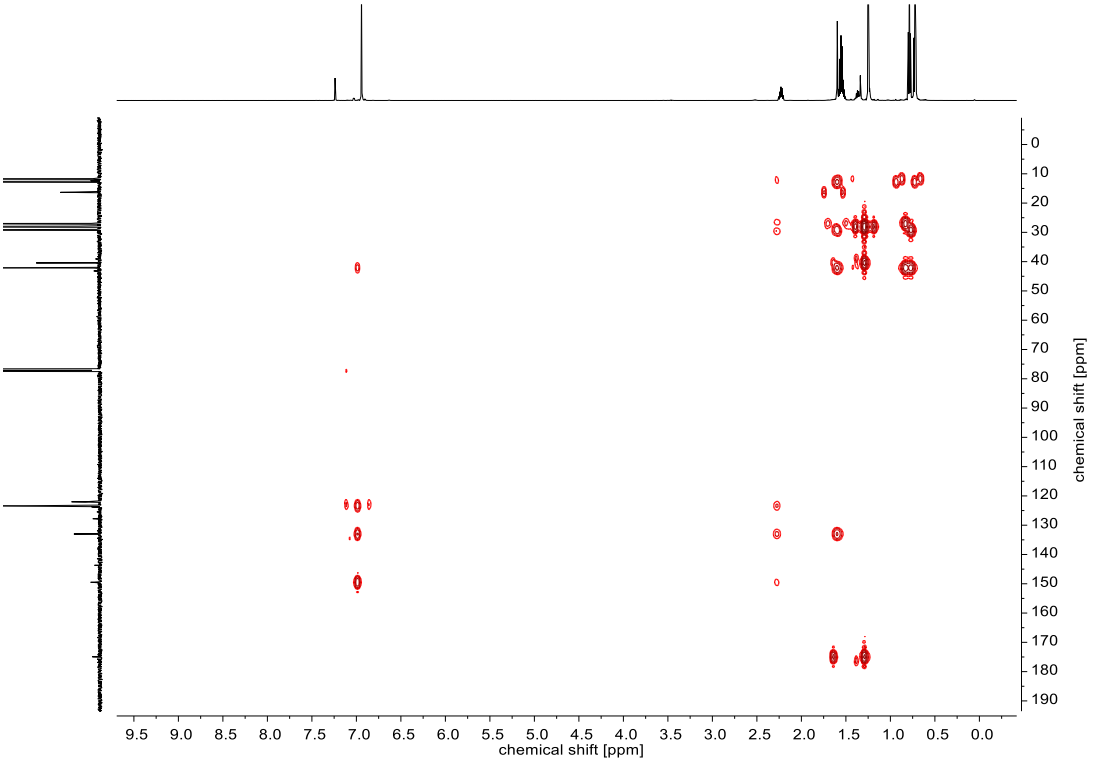


Figure S14. ^{1}H ^{13}C HMBC NMR (400.13/101.92 MHz, 298 K, C_6D_6) of ^{DIPeP}Imine.

3.4 NMR spectroscopic data for (^{DIPeP}BDI*)-H

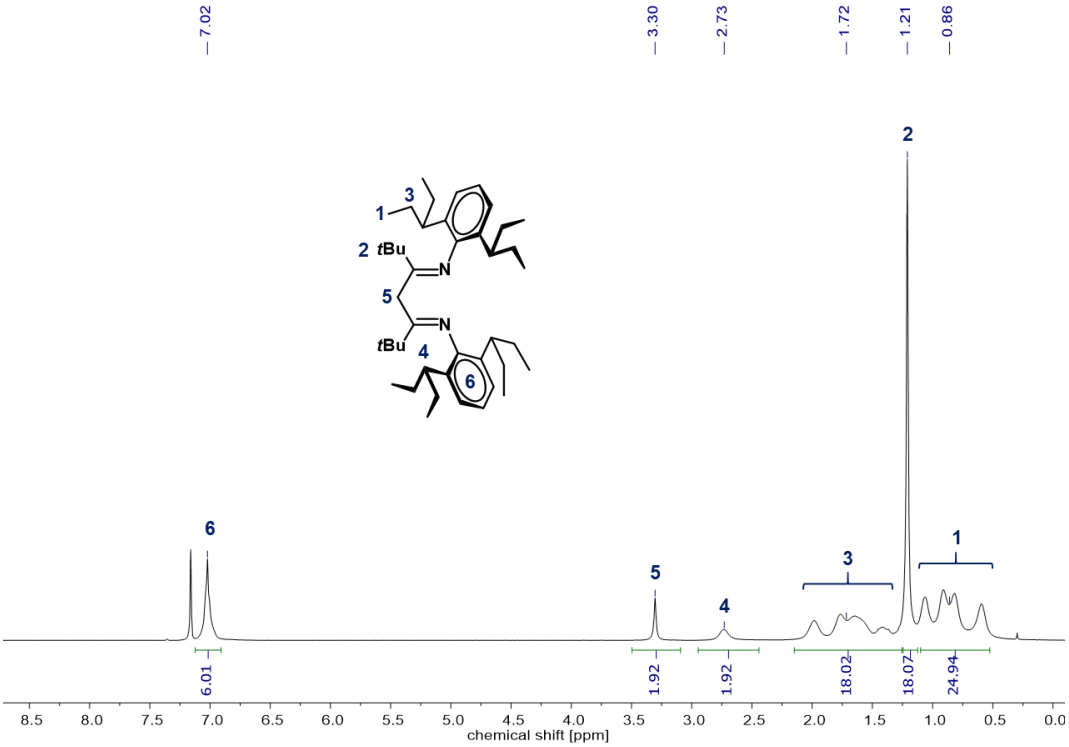


Figure S15. ^{1}H NMR (400.13 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)-H.

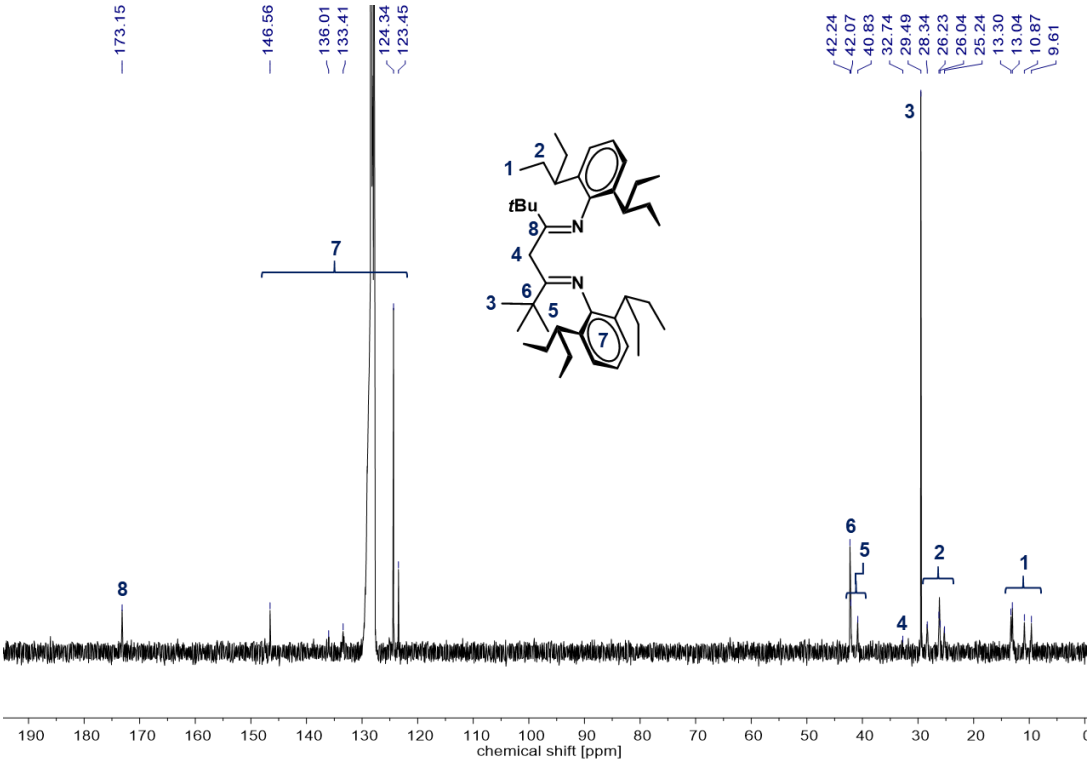


Figure S16. ^{13}C NMR (101.92 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)-H.

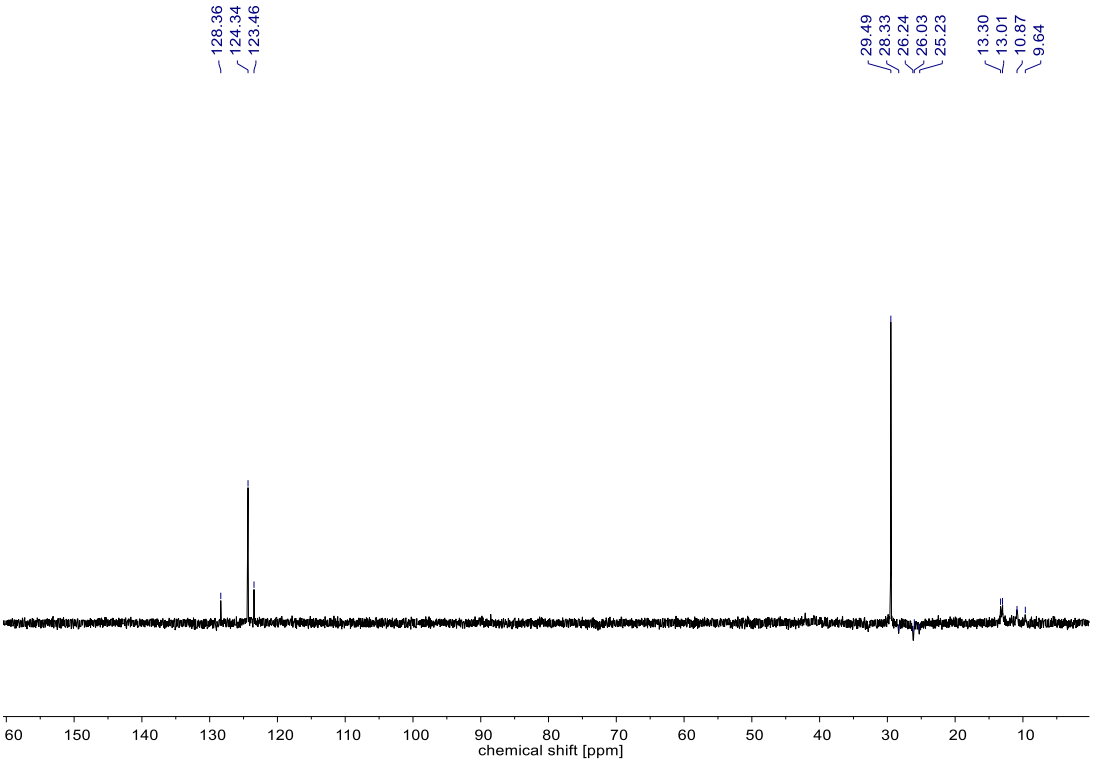


Figure S17. ^{13}C(DEPT 135) NMR (101.92 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)-H.

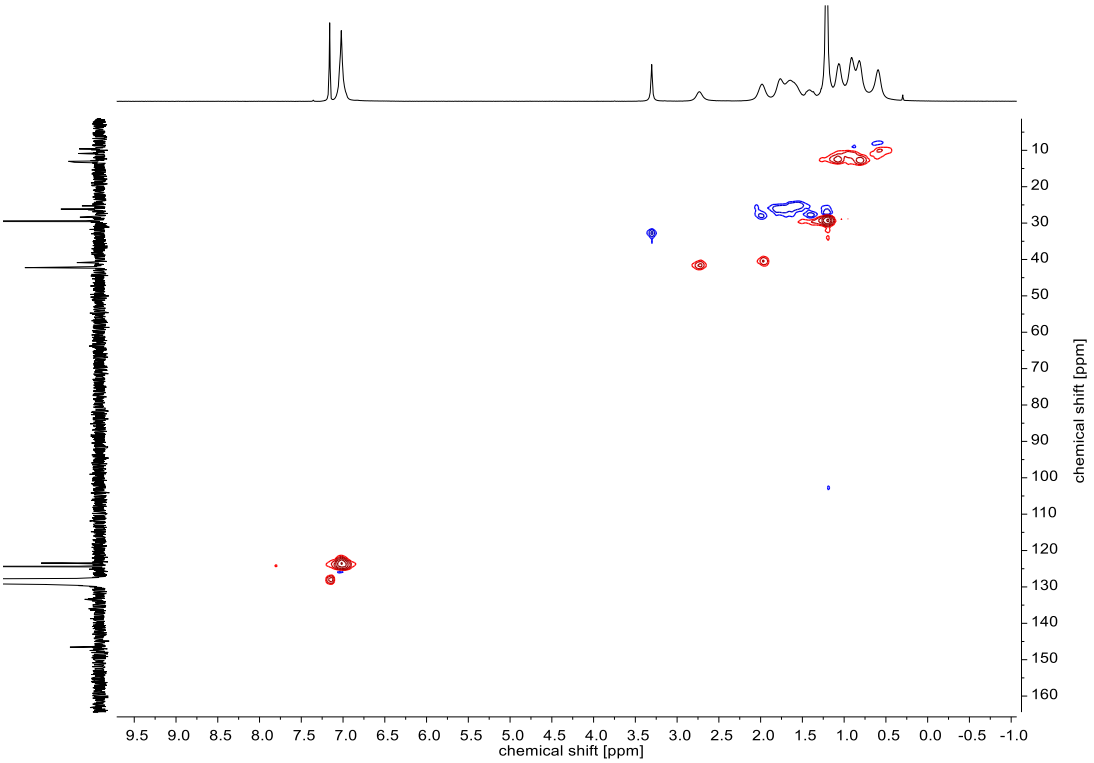


Figure S18. ^{1}H ^{13}C HSQC NMR (400.13/101.92 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)-H.

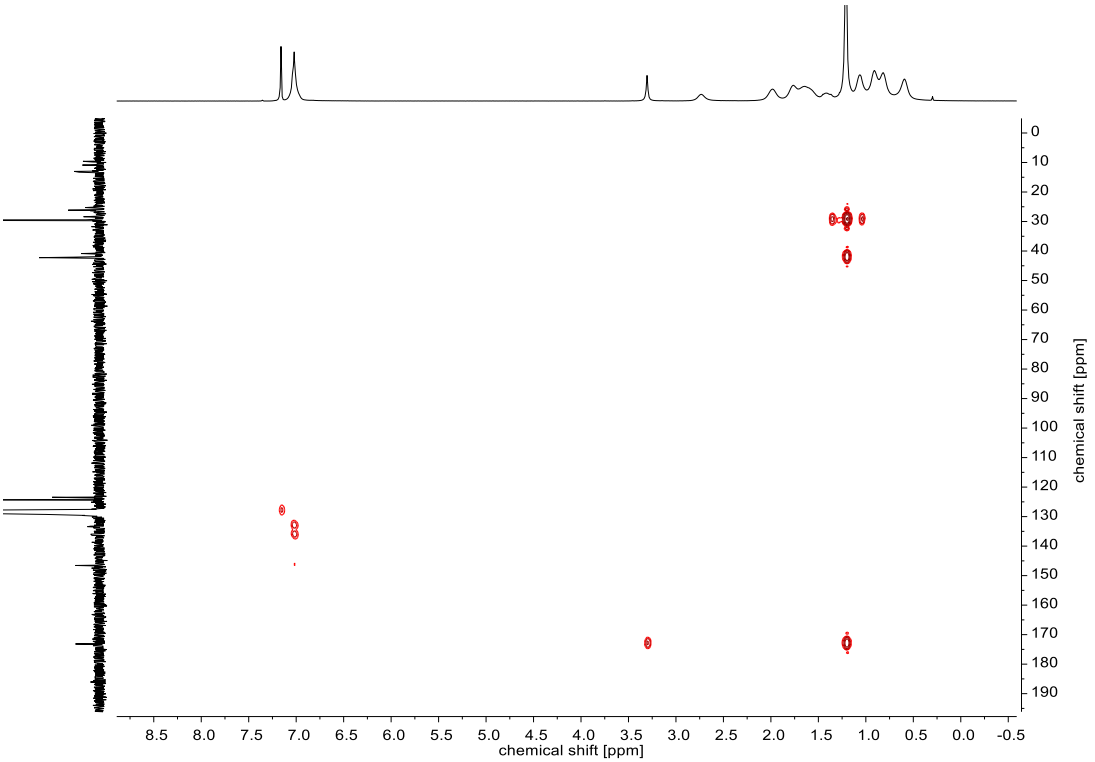


Figure S19. ^{1}H ^{13}C HMBC NMR (400.13/101.92 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)-H.

3.5 NMR spectroscopic data for (^{DIPeP}BDI*)Mg^{n}Bu

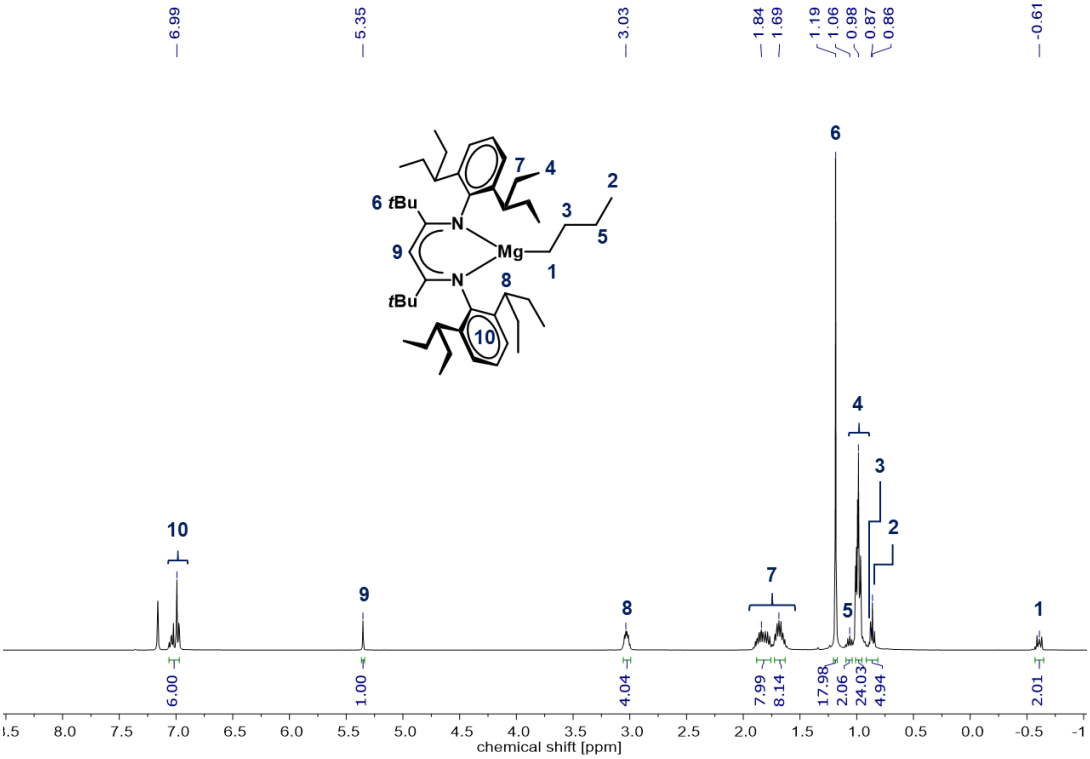


Figure S20. ^{1}H NMR (600.13 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)Mg^{n}Bu.

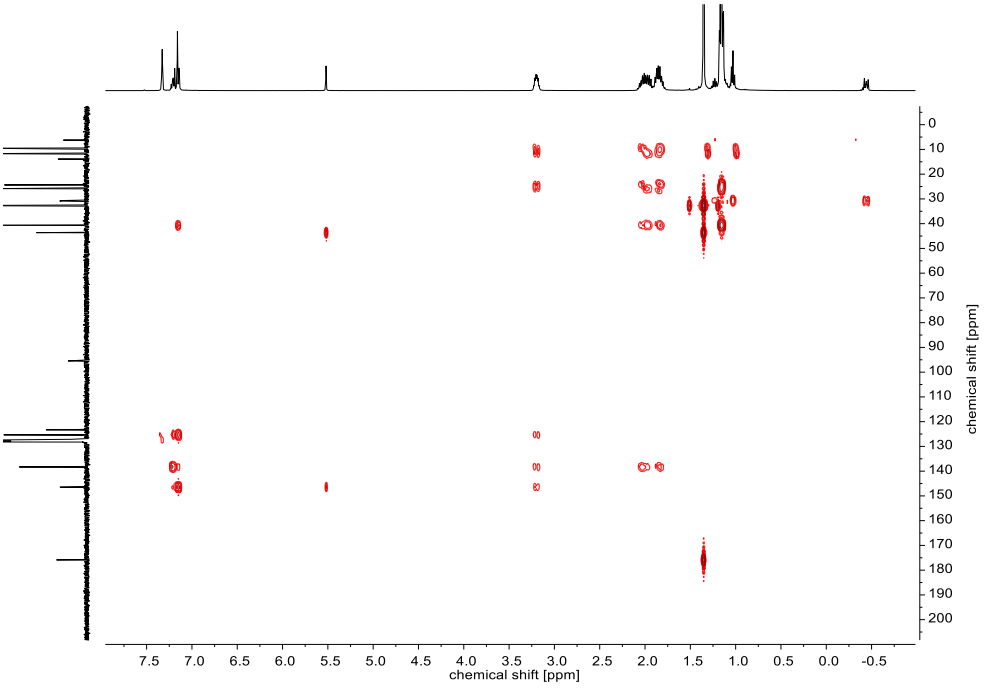


Figure S21. ^{1}H-^{1}H COSY NMR (600.13 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)Mg^{n}Bu.

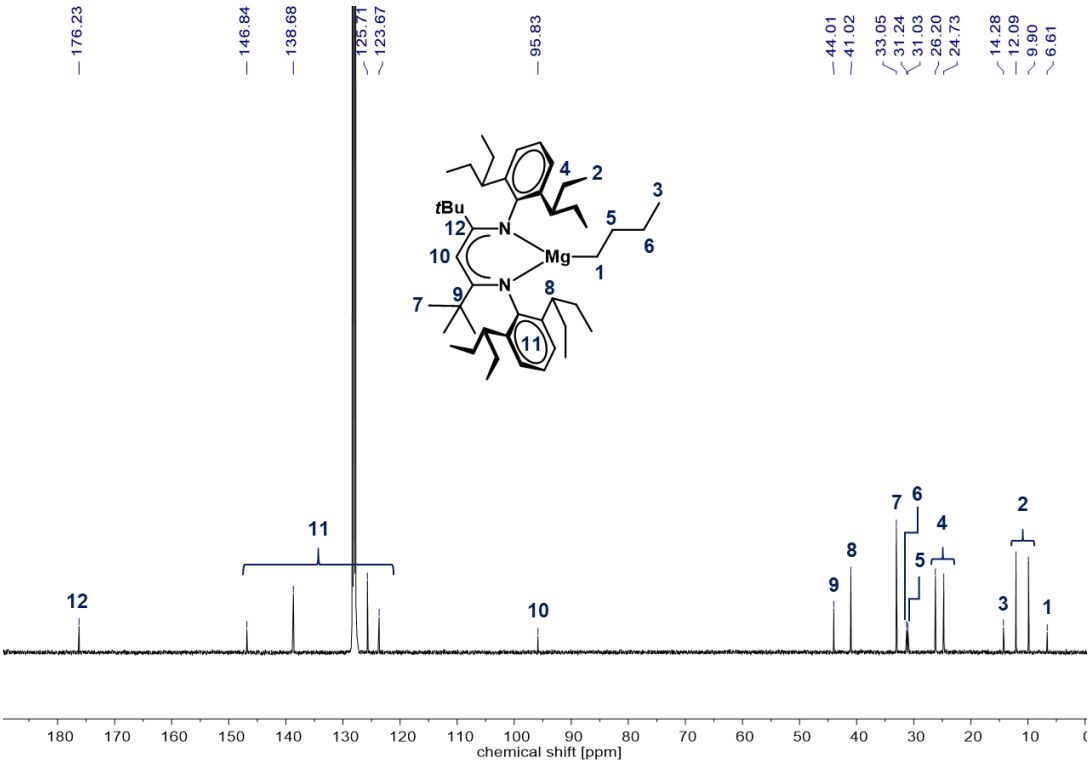


Figure S22. ^{13}C NMR (150.92 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)Mg^{n}Bu.

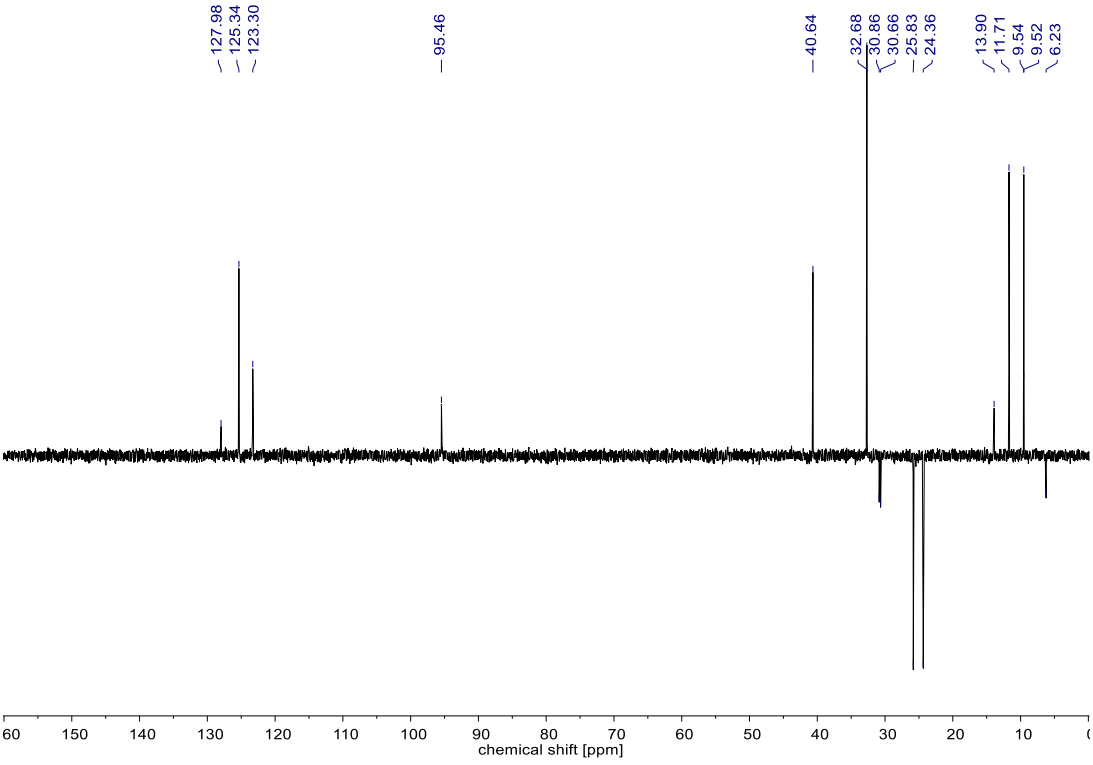


Figure S23. ^{13}C(DEPT 135) NMR (150.92 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)Mg^{n}Bu.

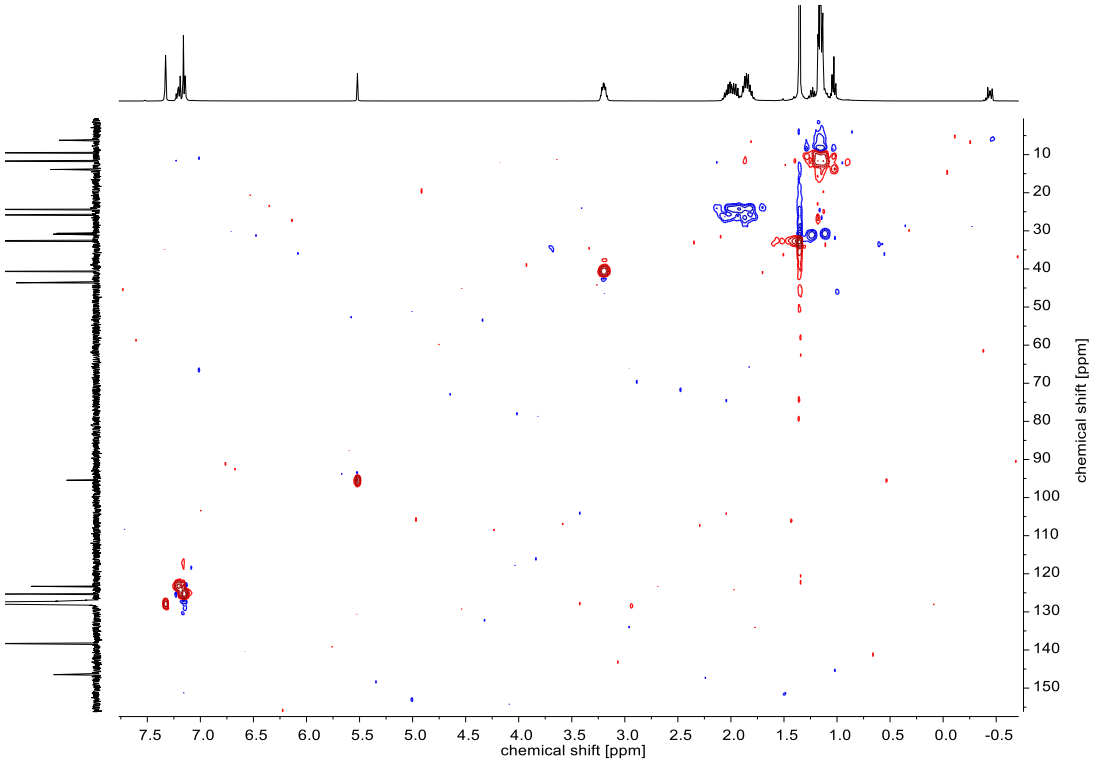


Figure S24. ^{1}H ^{13}C HSQC NMR (600.13/150.92 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)Mg^{n}Bu.

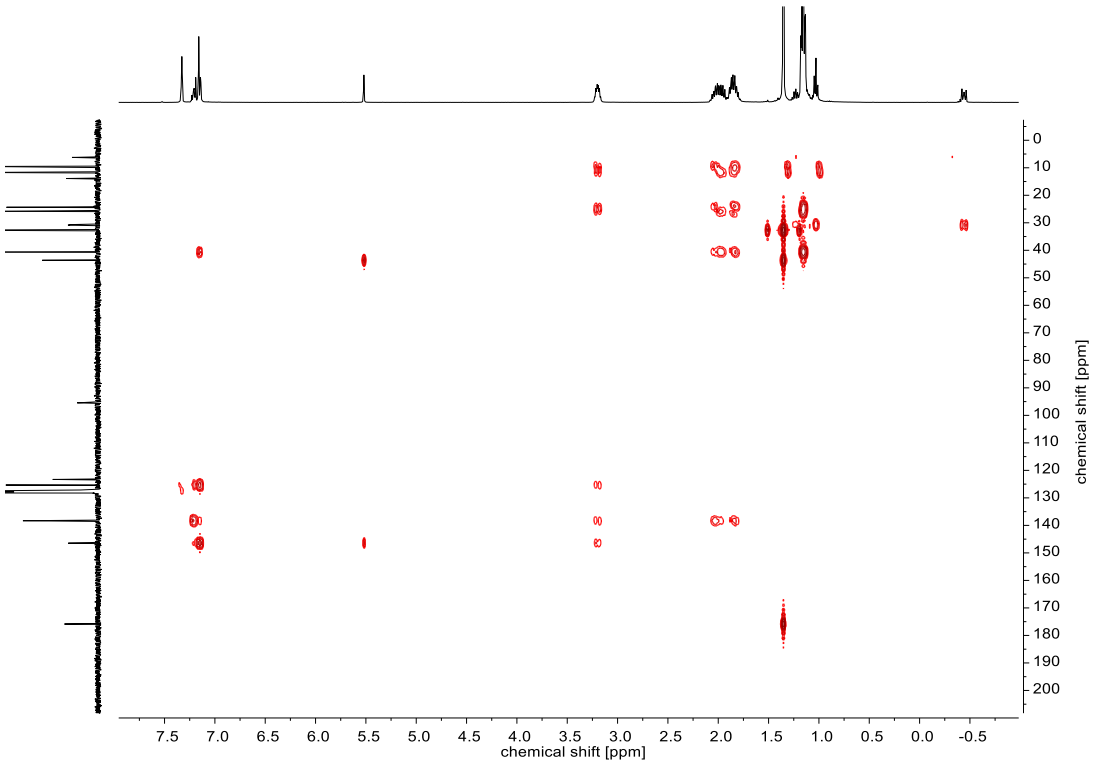


Figure S25. ^{1}H ^{13}C HMBC NMR (600.13/150.92 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)Mg^{n}Bu.

3.6 NMR spectroscopic data for (^{DIPeP}BDI*)MgI

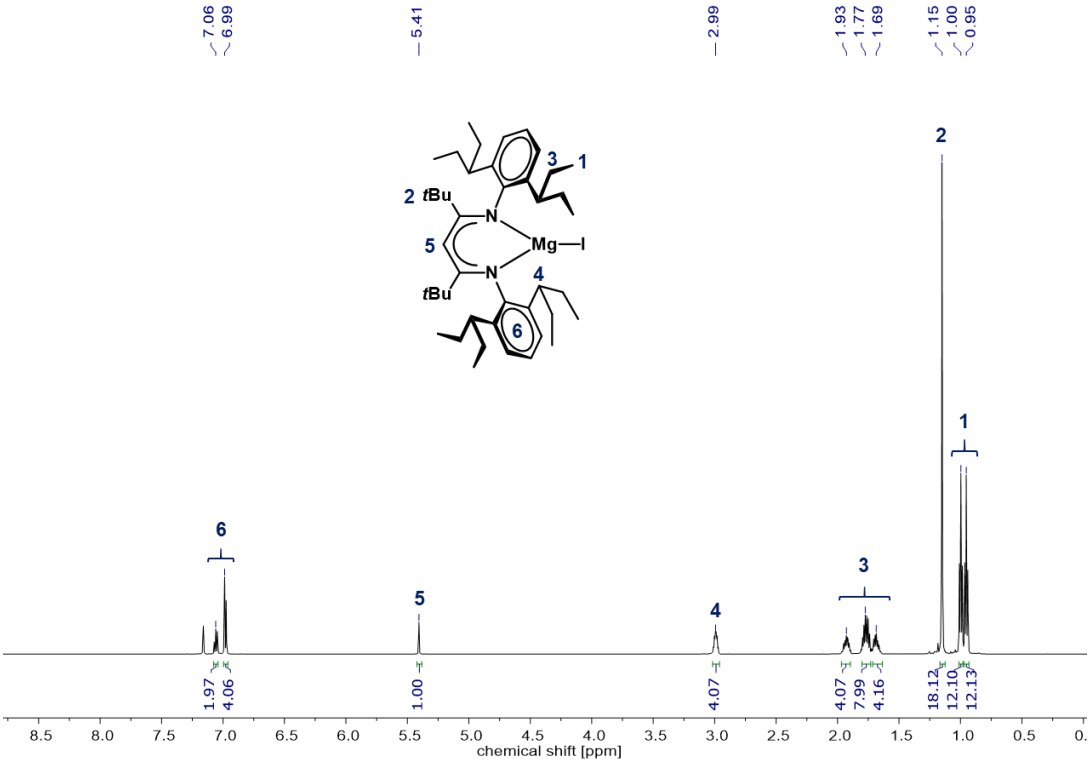


Figure S26. ^{1}H NMR (600.13 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)MgI.

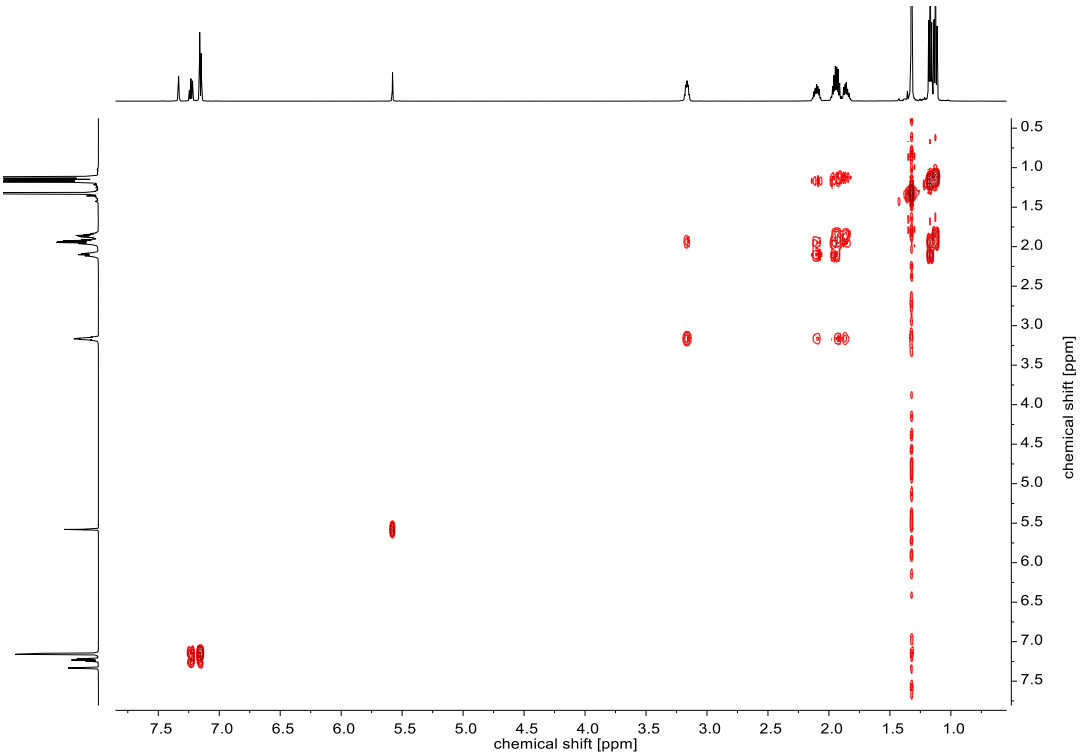


Figure S27. ^{1}H-^{1}H COSY NMR (600.13 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)MgI.

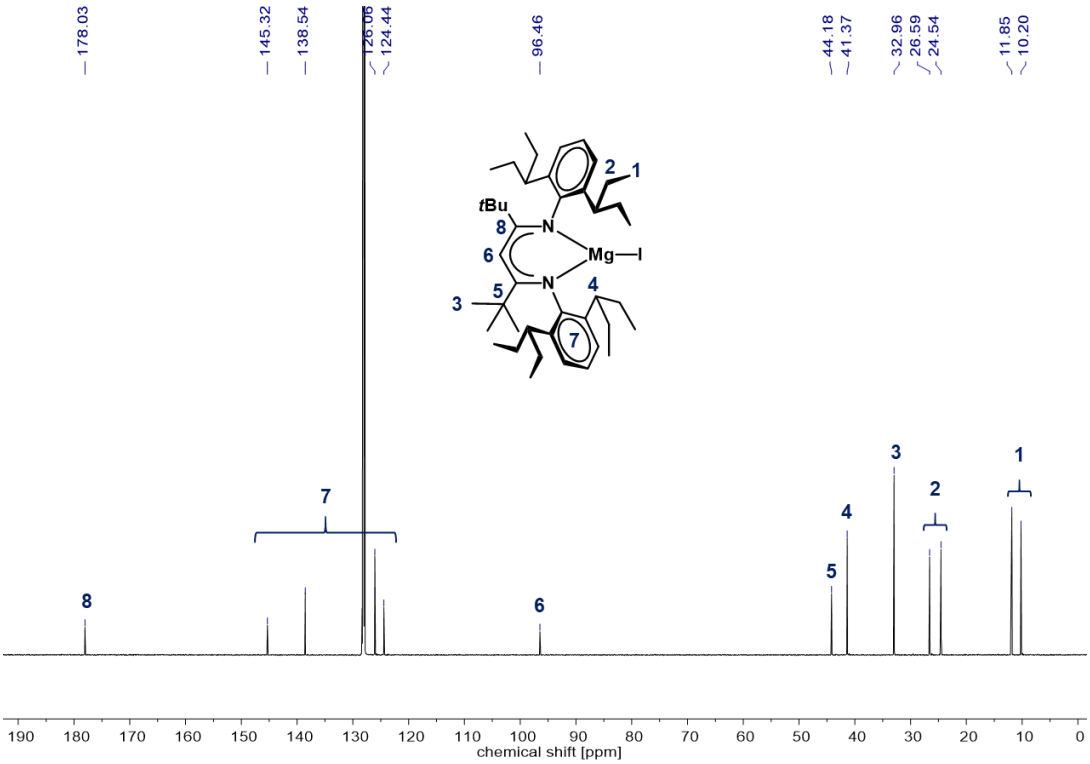


Figure S28. ^{13}C NMR (150.92 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)MgI.

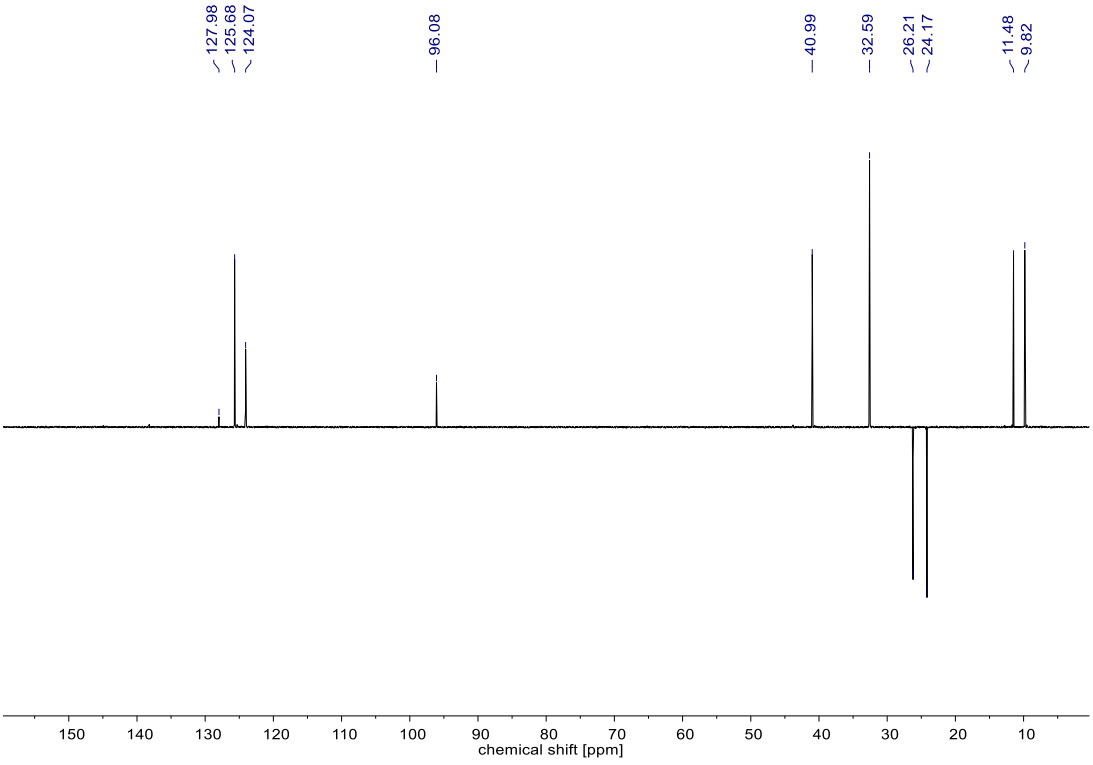


Figure S29. ^{13}C(DEPT 135) NMR (150.92 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)MgI.

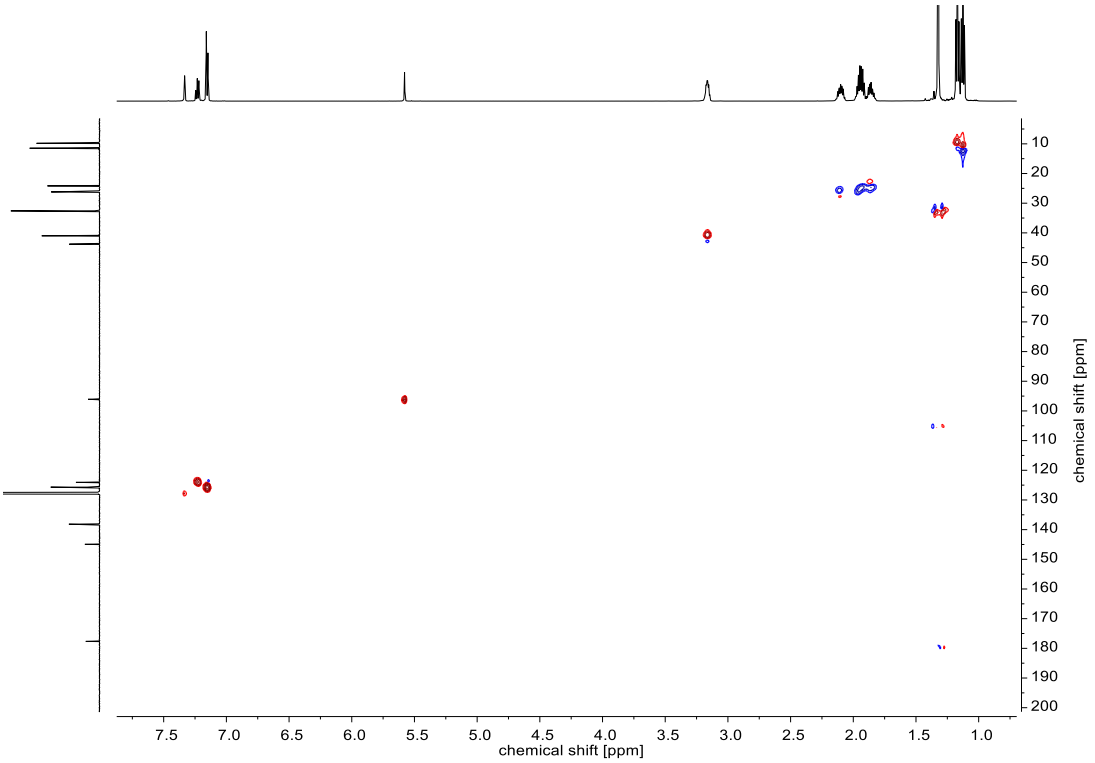


Figure S30. ^{1}H ^{13}C HSQC NMR (600.13/150.92 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)MgI.

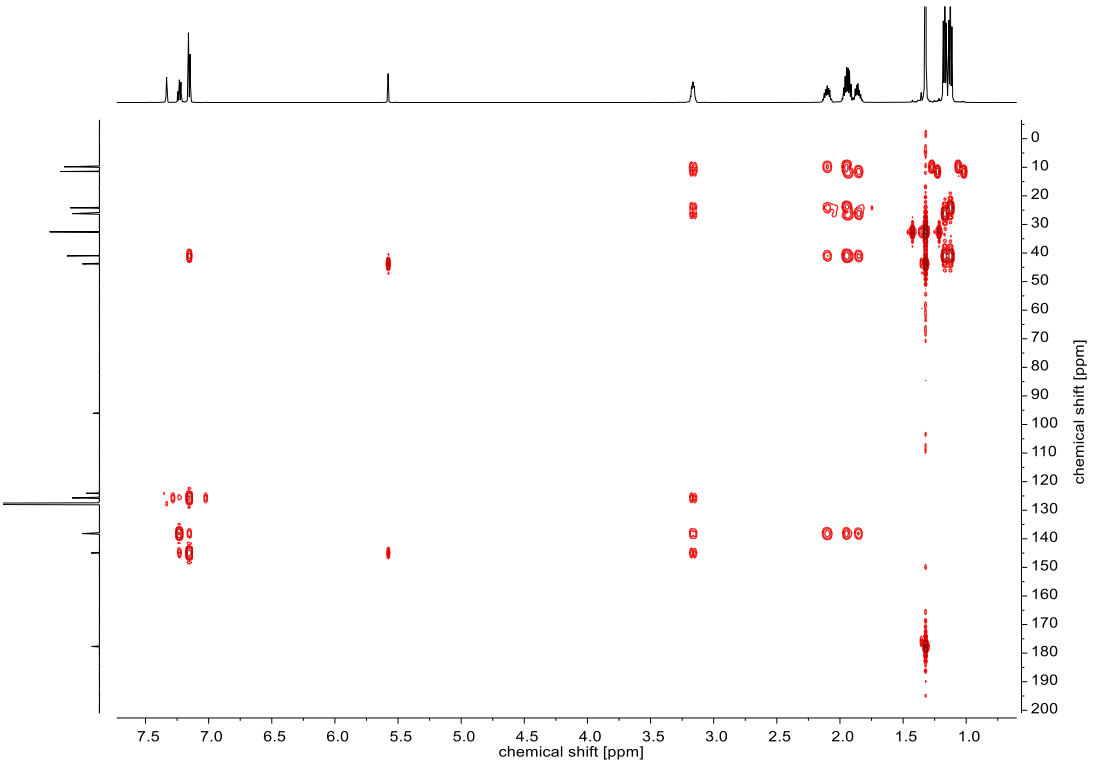


Figure S31. ^{1}H ^{13}C HMBC NMR (600.13/150.92 MHz, 298 K, C_6D_6) of (^{DIPeP}BDI*)MgI.

3.7 NMR spectroscopic data for [(^{DIPeP}BDI*)Mg]$_2$

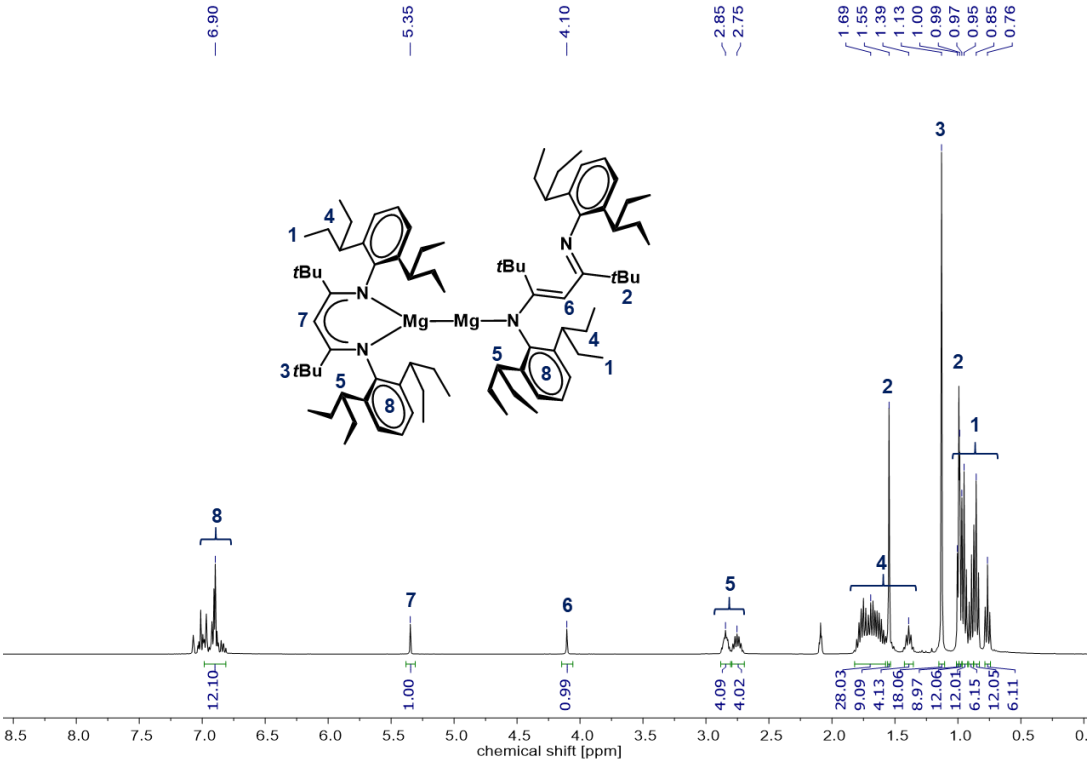


Figure S32. ^{1}H NMR (400.13 MHz, 353 K, tol-*d8*) of [(^{DIPeP}BDI*)Mg]$_2$.

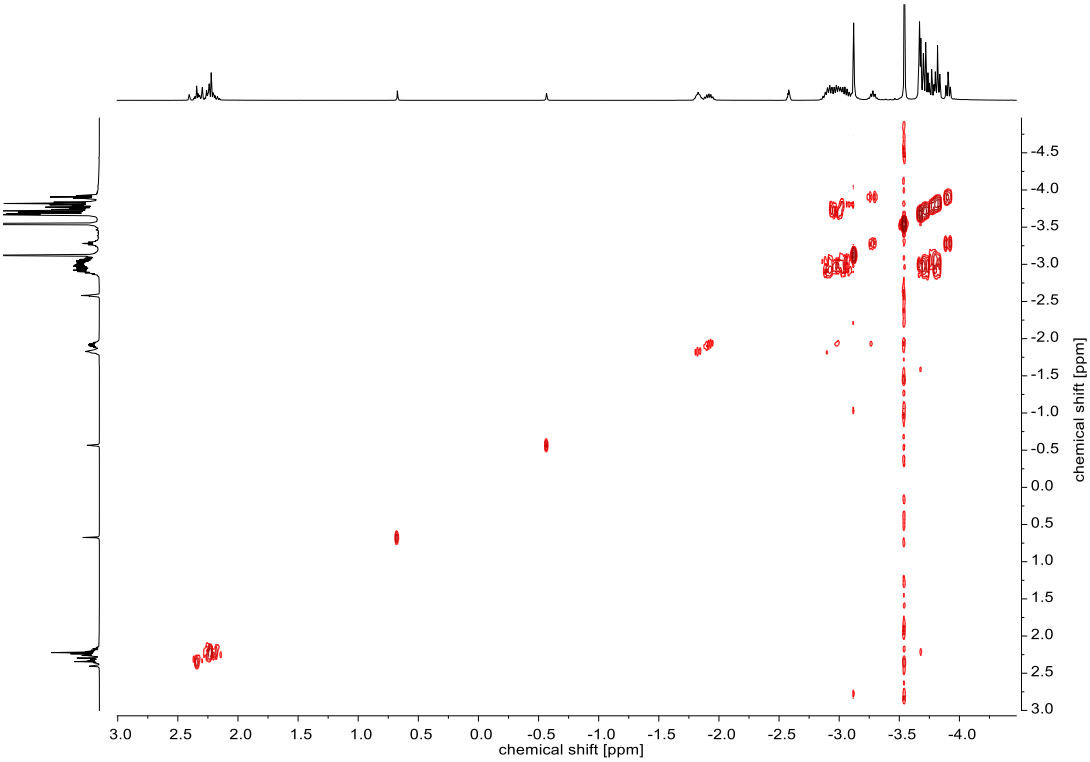


Figure S33. ^{1}H-^{1}H COSY NMR (400.13 MHz, 353 K, tol-*d8*) of [(^{DIPeP}BDI*)Mg]$_2$.

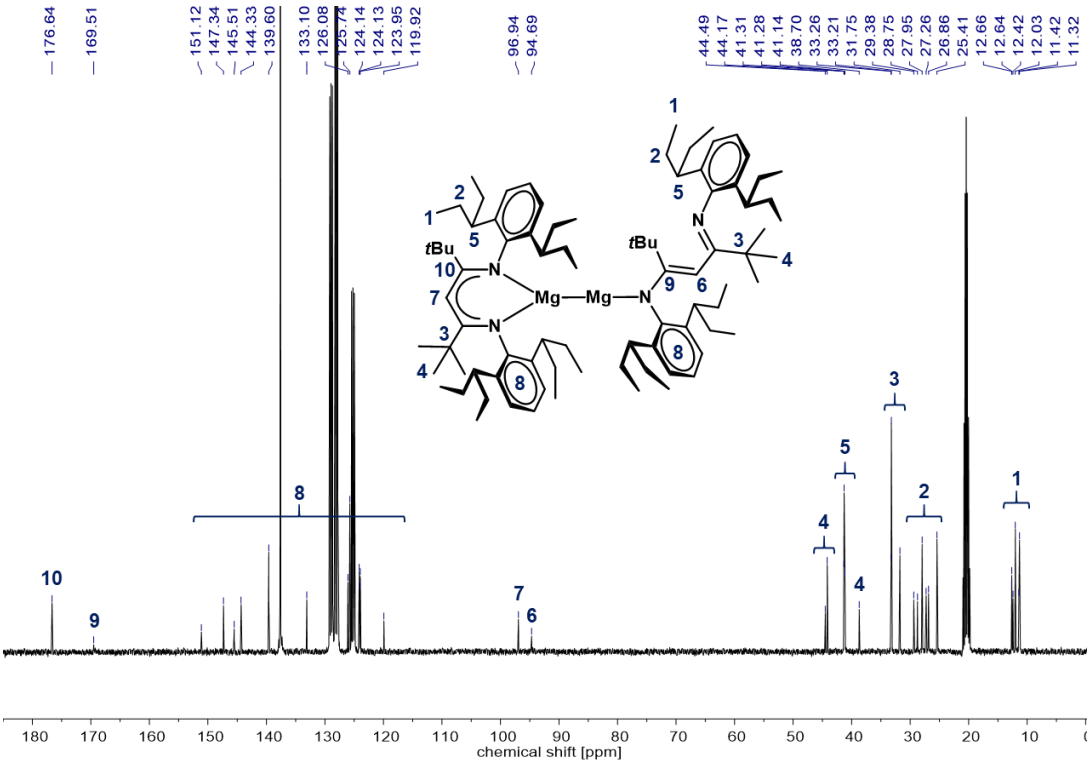


Figure S34. ^{13}C NMR (101.92 MHz, 353 K, tol-*d8*) of [(^{DIPeP}BDI*)Mg]$_2$.

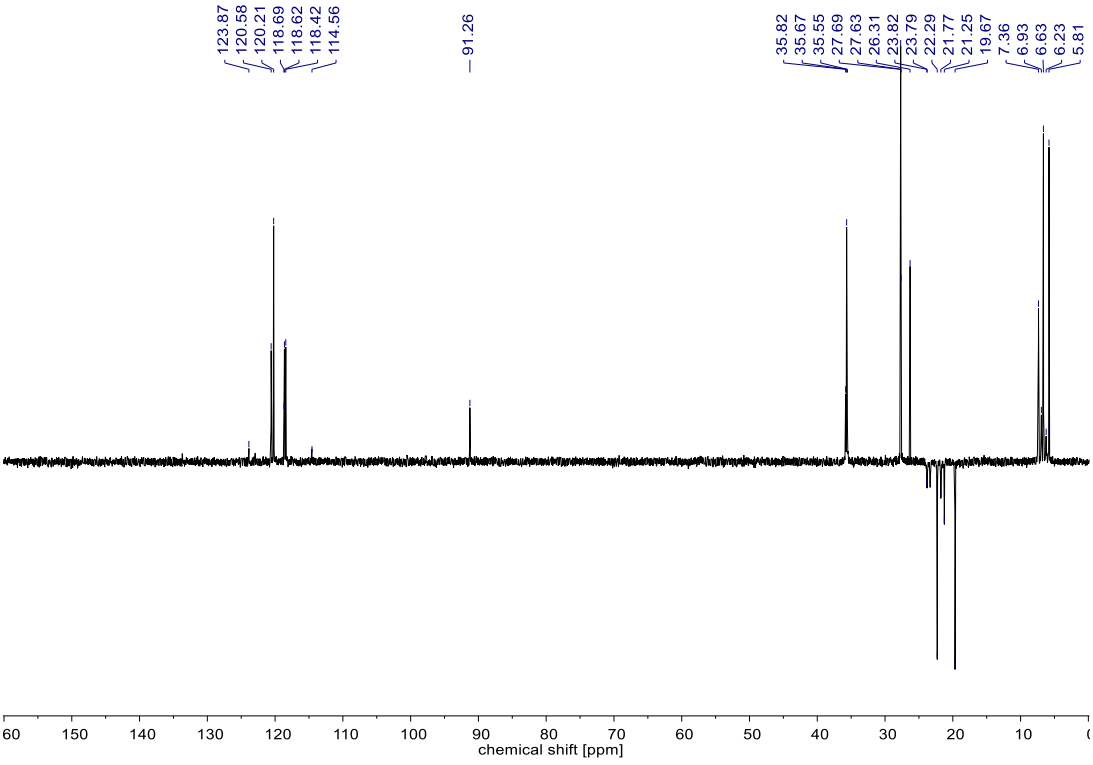


Figure S35. ^{13}C(DEPT 135) NMR (101.92 MHz, 353 K, tol-*d8*) of [(^{DIPeP}BDI*)Mg]$_2$.

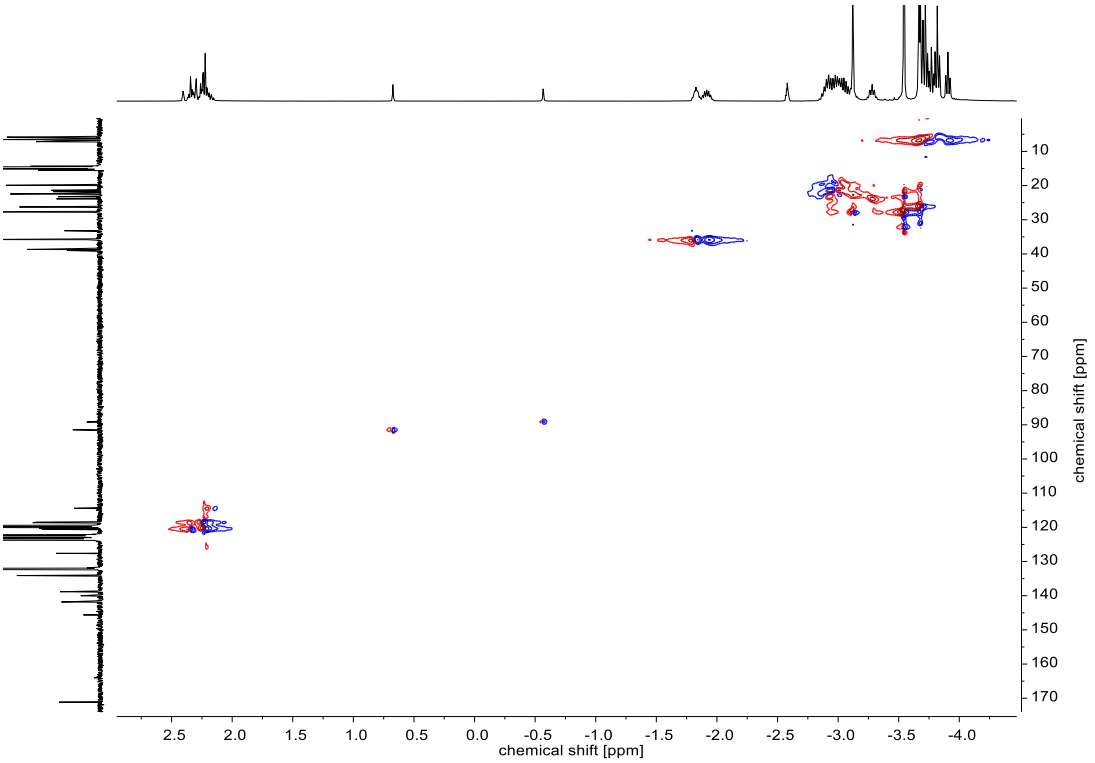


Figure S36. ^{1}H ^{13}C HSQC NMR (400.13/101.92 MHz, 353 K, tol-*d8*) of [(^{DIPeP}BDI*)Mg]$_2$.

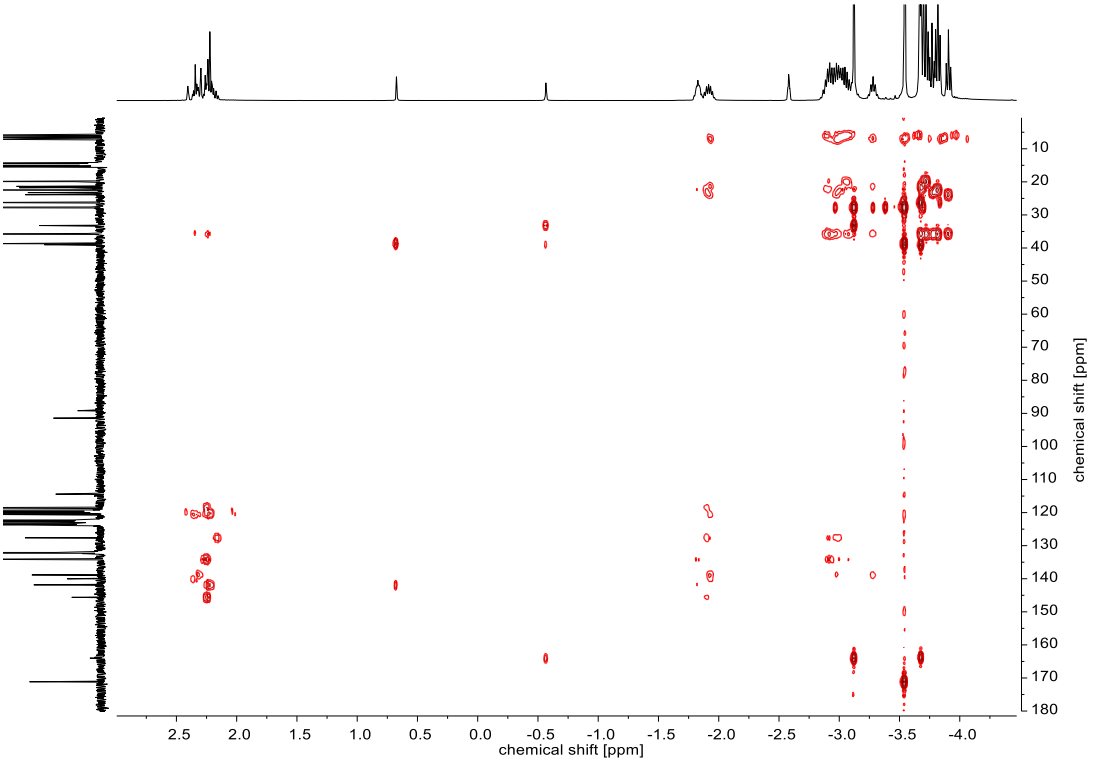


Figure S37. ^{1}H ^{13}C HMBC NMR (400.13/101.92 MHz, 353 K, tol-*d8*) of [(^{DIPeP}BDI*)Mg]$_2$.

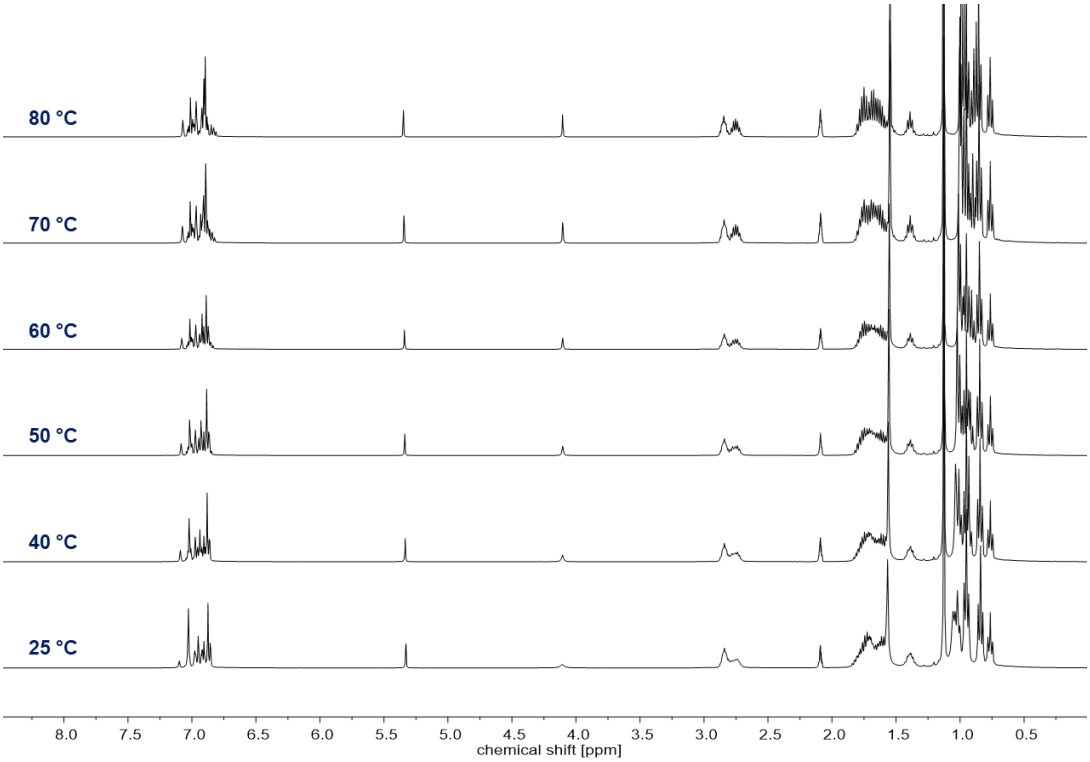


Figure S38. Temperature dependent ^{1}H NMR (600.13 MHz,tol-*d8*) of [(^{DIPeP}BDI*)Mg]$_2$.

4. Crystal structure determination

The crystal structure data of the compounds mentioned below has been deposited with the Cambridge Crystallographic Data Centre. CCDC 2020201 (^{DIPeP}Pivaloylamide), 2020202 ((^{DIPeP}BDI*)-H), 2020203 ((^{DIPeP}BDI*)Mg^{n}Bu), 2020204 ((^{DIPeP}BDI*)MgI), 2020205 ([(^{DIPeP}BDI*)Mg]$_2$) and 2020206 ((^{DIPeP}BDI)MgI) contain the supplementary crystallographic data for the compounds. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

4.1 Crystal structure of ^{DIPeP}Pivaloylamide

A colorless crystal of compound ^{DIPeP}Pivaloylamide was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then flash cooled to 100.0(1) K in a nitrogen gas stream and kept at this temperature during the experiment. The crystal structure was measured on a SuperNova diffractometer with Atlas S2 detector using a CuKα microfocus source. The measured data was processed with the CrysAlisPro (v40.67a) software package.[S2] Using Olex2,[S3] the structure was solved with the ShelXT[S4] structure solution program using Intrinsic Phasing and refined with the ShelXL[S5] refinement package using Least Squares Minimization. The asymmetric unit contains two independent molecules. All non-hydrogen atoms were refined anisotropically. Most hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The nitrogen bound hydrogen atoms were observed from difference Fourier maps and refined. Disorder of the *t*Bu groups of both independent molecules as well as the dipep moiety in one molecule was observed. The disorder was modeled with the help of similarity restraints (SIMU, SADI) and rigid bond restraints (RIGU).[S6] Additionally, a FLAT restraint was used for the aromatic ring of the less occupied orientation of the dipep group. The relative occupancies of the two alternative orientations of each group were refined to 0.64(5)/0.36(5) (*t*Bu), 0.862(6)/0.138(6) (*t*Bu) and 0.847(2)/0.153(2) (dipep), respectively. Crystallographic and refinement data are summarized in Table S1.

Table S1 Crystal data and structure refinement for ^{DIPeP}Pivaloylamide.

Identification code	hasj200604b
Empirical formula	$C_{21}H_{35}NO$
Formula weight	317.50
Temperature/K	100.0(1)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.9088(3)
b/Å	20.8368(11)
c/Å	19.7657(10)
α/°	90
β/°	98.387(4)
γ/°	90
Volume/Å^3	4037.3(3)
Z	8
ρ_{calc}g/cm^3	1.045
μ/mm^{-1}	0.473
F(000)	1408.0
Crystal size/mm^3	0.425 × 0.079 × 0.07
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.198 to 145.632
Index ranges	-12 ≤ h ≤ 8, -24 ≤ k ≤ 16, -23 ≤ l ≤ 24
Reflections collected	14248
Independent reflections	7787 [R_{int} = 0.0368, R_{sigma} = 0.0476]
Data/restraints/parameters	7787/1943/667
Goodness-of-fit on F^2	1.168
Final R indexes [I>=2σ (I)]	R_1 = 0.0758, wR_2 = 0.1508
Final R indexes [all data]	R_1 = 0.0854, wR_2 = 0.1553
Largest diff. peak/hole / e Å^{-3}	0.27/-0.28

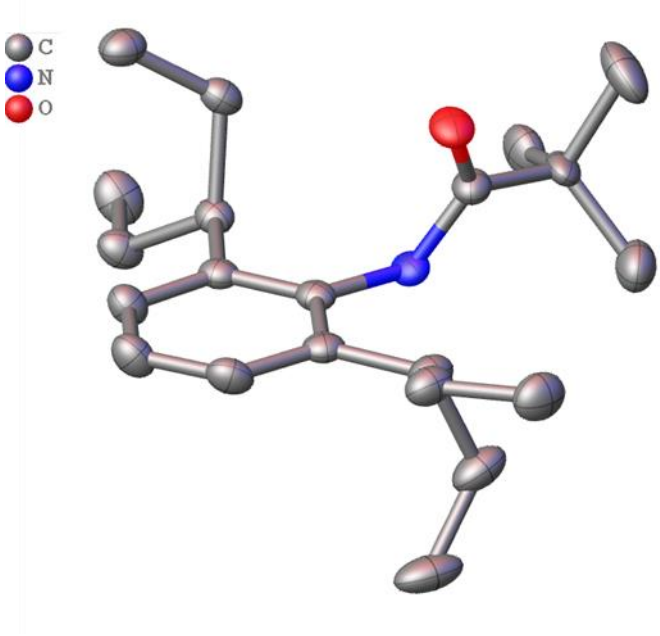


Figure S39. Solid state structure of ^{DIPeP}Pivaloylamide (molecule 1 of 2 independent molecules). Ellipsoids represent 50% probability. Hydrogen atoms and disorder have been omitted for clarity.

4.2 Crystal structure of (^{DIPeP}BDI*)-H

A colorless crystal of compound (^{DIPeP}BDI*)-H was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then flash cooled to 100.0(2) K in a nitrogen gas stream and kept at this temperature during the experiment. The crystal structure was measured on a SuperNova diffractometer with Atlas S2 detector using a CuKα microfocus source. The measured data was processed with the CrysAlisPro (v40.67a) software package.[S2] Using Olex2,[S3] the structure was solved with the ShelXT[S4] structure solution program using Intrinsic Phasing and refined with the ShelXL[S5] refinement package using Least Squares Minimization. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. Disorder of one *t*Bu groups was observed, and was modeled with the help of similarity restraints (SADI) and rigid bond restraints (RIGU).[S6] The relative occupancies of the two alternative orientations were refined to 0.871(9) and 0.129(9). Crystallographic and refinement data are summarized in Table S2.

Table S2 Crystal data and structure refinement for (^{DIPeP}BDI*****)-H

Identification code	hasj200604a
Empirical formula	$C_{43}H_{70}N_2$
Formula weight	615.01
Temperature/K	100.0(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	11.9665(2)
b/Å	23.6431(4)
c/Å	15.0792(3)
α/°	90
β/°	112.986(3)
γ/°	90
Volume/Å^3	3927.57(16)
Z	4
ρ_{calc}g/cm^3	1.040
μ/mm^{-1}	0.434
F(000)	1368.0
Crystal size/mm^3	0.303 × 0.24 × 0.149
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.384 to 145.398
Index ranges	-13 ≤ h ≤ 14, -20 ≤ k ≤ 29, -18 ≤ l ≤ 13
Reflections collected	14599
Independent reflections	7553 [R_{int} = 0.0198, R_{sigma} = 0.0261]
Data/restraints/parameters	7553/33/452
Goodness-of-fit on F^2	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0378, wR_2 = 0.0932
Final R indexes [all data]	R_1 = 0.0435, wR_2 = 0.0979
Largest diff. peak/hole / e Å^{-3}	0.23/-0.18

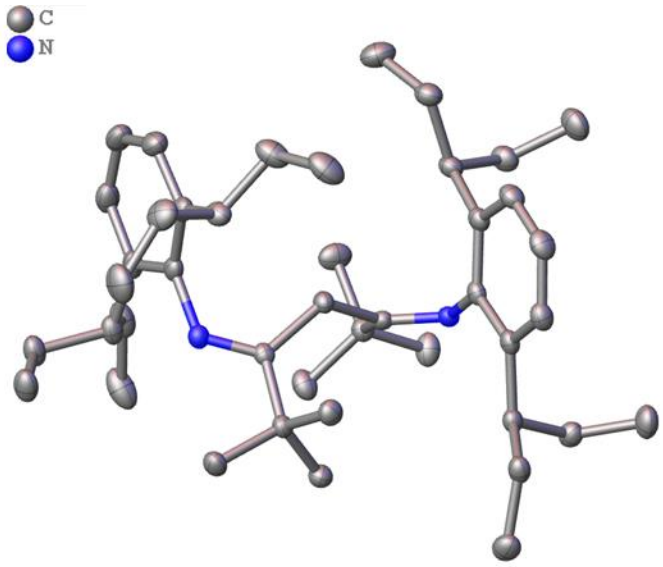


Figure S40. Solid state structure of (^{DIPeP}BDI*****)-H. Ellipsoids represent 50% probability. Hydrogen atoms and disorder have been omitted for clarity.

4.3 Crystal structure of (^{DIPeP}BDI*)Mg^{n}Bu (10% (^{DIPeP}BDI*)MgEt impurity)

A colorless crystal of compound (^{DIPeP}BDI*****)Mg^{n}Bu was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then flash cooled to 100.0(1) K in a nitrogen gas stream and kept at this temperature during the experiment. The crystal structure was measured on a SuperNova diffractometer with Atlas S2 detector using a CuKα microfocus source. The measured data was processed with the CrysAlisPro (v40.53) software package.[S7] Using Olex2,[S3] the structure was solved with the ShelXT[S4] structure solution program using Intrinsic Phasing and refined with the ShelXL[S5] refinement package using Least Squares Minimization. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. Conformational disorder of one dipep moiety, which is connected to a substitutional disorder between metal bound *n*-butyl groups and ethyl groups was observed. The disorder was modeled with the help of similarity restraints (SIMU, SADI) and rigid bond restraints (RIGU).[S6] The relative

occupancies of the two alternative molecules were refined to 0.894(2) and 0.106(2). Crystallographic and refinement data are summarized in Table S3.

Table S3 Crystal data and structure refinement for (^{DIPeP}BDI*****)Mg^{n}Bu.

Identification code	hasj190708a
Empirical formula	$C_{46.79}H_{77.58}MgN_2$
Formula weight	692.47
Temperature/K	100.0(1)
Crystal system	triclinic
Space group	P-1
a/Å	10.1571(4)
b/Å	10.6195(3)
c/Å	21.6789(5)
α/°	97.526(2)
β/°	99.465(2)
γ/°	105.672(3)
Volume/Å^3	2182.57(12)
Z	2
ρ_{calc}g/cm^3	1.054
μ/mm^{-1}	0.569
F(000)	769.0
Crystal size/mm^3	0.452 × 0.404 × 0.328
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.414 to 147.328
Index ranges	-12 ≤ h ≤ 11, -10 ≤ k ≤ 12, -23 ≤ l ≤ 26
Reflections collected	14348
Independent reflections	8484 [R_{int} = 0.0227, R_{sigma} = 0.0315]
Data/restraints/parameters	8484/688/551
Goodness-of-fit on F^2	1.047
Final R indexes [I>=2σ (I)]	R_1 = 0.0391, wR_2 = 0.0979
Final R indexes [all data]	R_1 = 0.0435, wR_2 = 0.1008
Largest diff. peak/hole / e Å^{-3}	0.28/-0.24

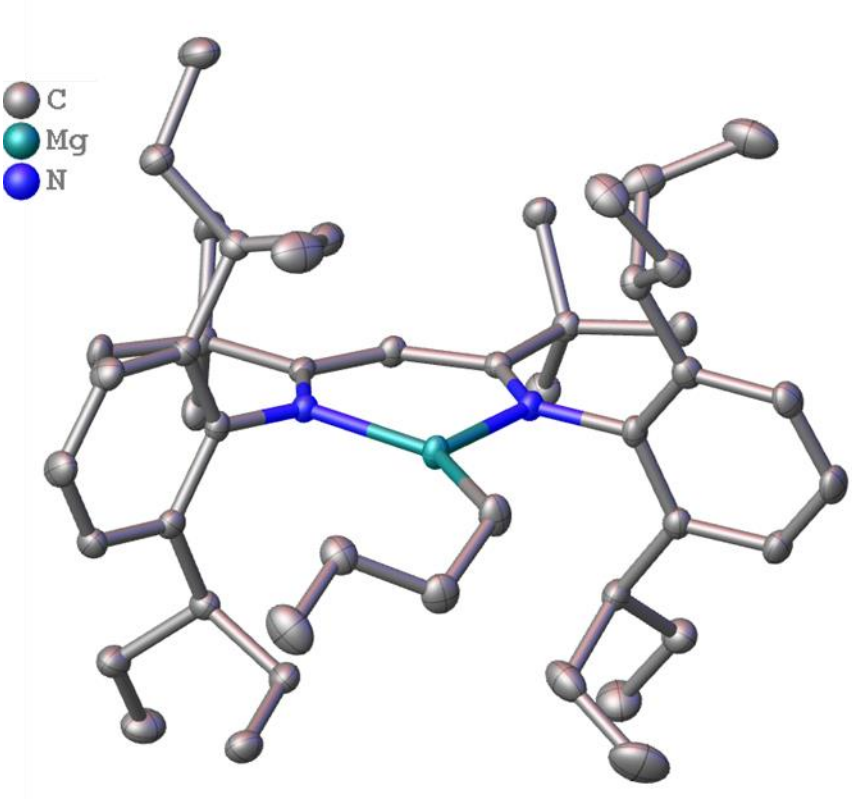


Figure S41. Solid state structure of (^{DIPeP}BDI*)Mg^{n}Bu. Ellipsoids represent 50% probability. Hydrogen atoms and disorder have been omitted for clarity.

4.4 Crystal structure of (^{DIPeP}BDI*)MgI

A colorless crystal of compound (^{DIPeP}BDI*)MgI was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then flash cooled to 100.0(1) K in a nitrogen gas stream and kept at this temperature during the experiment. The crystal structure was measured on a SuperNova diffractometer with Atlas S2 detector using a MoKα microfocus source. The measured data was processed with the CrysAlisPro (v40.18b) software package.[S8] Using Olex2,[S3] the structure was solved with the ShelXT[S4] structure solution program using Intrinsic Phasing and refined with the ShelXL[S5] refinement package using Least Squares Minimization. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in ideal positions and refined as riding

atoms with relative isotropic displacement parameters. Crystallographic and refinement data are summarized in Table S4.

Table S4 Crystal data and structure refinement for (^{DIPeP}BDI*****)MgI.

Identification code	hasj190517a
Empirical formula	$C_{43}H_{69}IMgN_2$
Formula weight	765.21
Temperature/K	100.0(1)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.8072(3)
b/Å	18.5224(3)
c/Å	21.5987(4)
α/°	90
β/°	104.313(2)
γ/°	90
Volume/Å^3	4189.32(15)
Z	4
ρ_{calc}g/cm^3	1.213
μ/mm^{-1}	0.809
F(000)	1624.0
Crystal size/mm^3	0.356 × 0.164 × 0.087
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.47 to 58.902
Index ranges	-14 ≤ h ≤ 14, -25 ≤ k ≤ 20, -28 ≤ l ≤ 29
Reflections collected	27312
Independent reflections	10031 [R_{int} = 0.0388, R_{sigma} = 0.0510]
Data/restraints/parameters	10031/0/438
Goodness-of-fit on F^2	1.064
Final R indexes [I>=2σ (I)]	R_1 = 0.0452, wR_2 = 0.1032
Final R indexes [all data]	R_1 = 0.0640, wR_2 = 0.1132
Largest diff. peak/hole / e Å^{-3}	1.88/-1.00

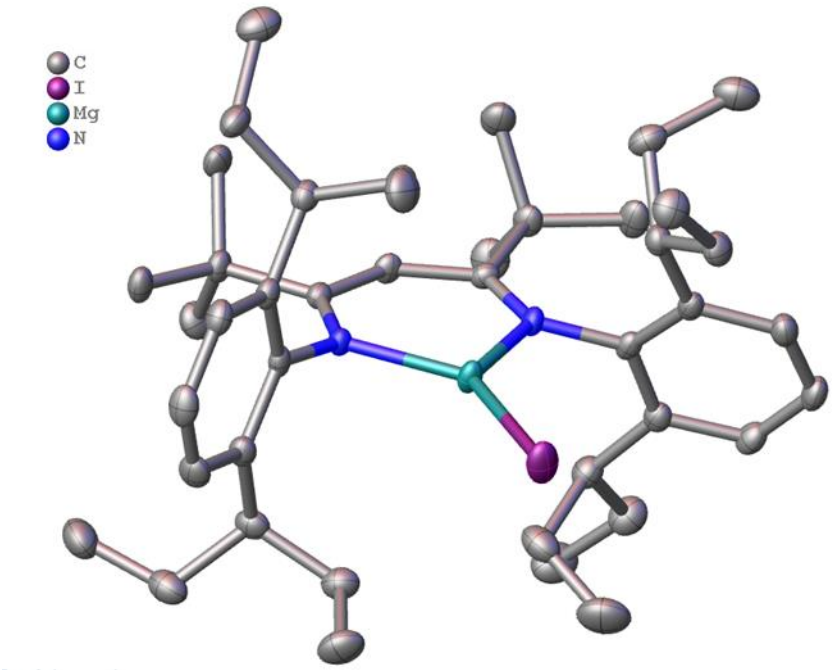


Figure S42. Solid state structure of (^{DIPeP}BDI***)MgI. Ellipsoids represent 50% probability. Hydrogen atoms have been omitted for clarity.

4.5 Crystal structure of [(^{DIPeP}BDI^{tBu})Mg]$_2$

A yellow crystal of compound [(^{DIPeP}BDI***)Mg]$_2$ was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then flash cooled to 100.0(2) K in a nitrogen gas stream and kept at this temperature during the experiment. The crystal structure was measured on a SuperNova diffractometer with Atlas S2 detector using a CuKα microfocus source. The measured data was processed with the CrysAlisPro (v40.53) software package.[S7] Using Olex2,[S3] the structure was solved with the ShelXT[S4] structure solution program using Intrinsic Phasing and refined with the ShelXL[S5] refinement package using Least Squares Minimization. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. Disorder of two isopentyl groups and one methyl group was observed. The disorder was modeled with the help of similarity restraints (SIMU, SADI) and rigid bond restraints (RIGU).[S6] The relative occupancies of

the two alternative orientations of each group were refined to 0.778(7)/0.222(7) (isopentyl), 0.518(9)/0.482(9) (isopentyl) and 0.52(4)/0.48(4) (Me), respectively. Crystallographic and refinement data are summarized in Table S5.

Table S5 Crystal data and structure refinement for $[(^{DIPeP}BDI^{*})Mg]_2$.

Identification code	hasj190725a
Empirical formula	$C_{86}H_{138}Mg_2N_4$
Formula weight	1276.62
Temperature/K	100.0(2)
Crystal system	triclinic
Space group	P-1
a/Å	11.0072(4)
b/Å	16.9342(8)
c/Å	21.7042(7)
α/°	91.446(3)
β/°	95.022(3)
γ/°	97.171(3)
Volume/Å^3	3995.9(3)
Z	2
ρ_{calc}g/cm^3	1.061
μ/mm^{-1}	0.587
F(000)	1412.0
Crystal size/mm^3	0.164 × 0.072 × 0.043
Radiation	CuKα (λ = 1.54184)
2Θ range for data collection/°	8.13 to 145.494
Index ranges	-11 ≤ h ≤ 13, -20 ≤ k ≤ 20, -26 ≤ l ≤ 21
Reflections collected	26690
Independent reflections	15298 [R_{int} = 0.0633, R_{sigma} = 0.0921]
Data/restraints/parameters	15298/213/926
Goodness-of-fit on F^2	1.006
Final R indexes [I>=2σ (I)]	R_1 = 0.0845, wR_2 = 0.2180
Final R indexes [all data]	R_1 = 0.1091, wR_2 = 0.2475
Largest diff. peak/hole / e Å^{-3}	0.75/-0.46

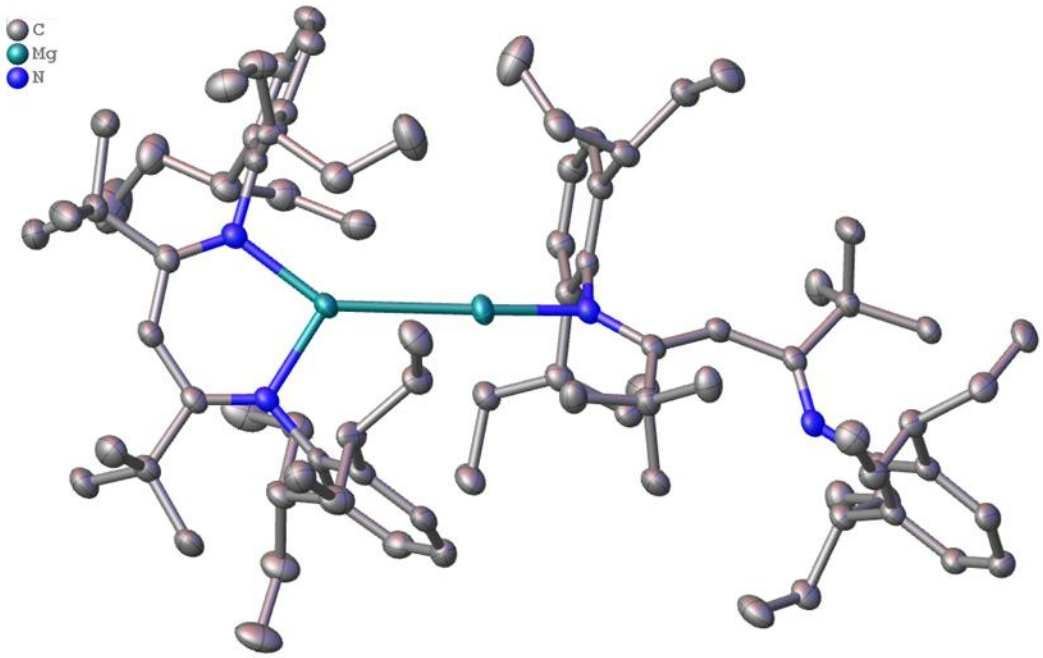


Figure S43. Solid state structure of [(^{DIPeP}BDI^{tBu})Mg]$_2$. Ellipsoids represent 50% probability. Hydrogen atoms and disorder have been omitted for clarity.

4.6 Crystal structure of (^{DIPeP}BDI)MgI

A colorless crystal of compound (^{DIPeP}BDI*)MgI was embedded in inert perfluoropolyalkylether (viscosity 1800 cSt; ABCR GmbH) and mounted using a Hampton Research CryoLoop. The crystal was then flash cooled to 100.0(1) K in a nitrogen gas stream and kept at this temperature during the experiment. The crystal structure was measured on a SuperNova diffractometer with Atlas S2 detector using a MoKα microfocus source. The measured data was processed with the CrysAlisPro (v40.18b) software package.[S8] Using Olex2,[S3] the structure was solved with the ShelXT[S4] structure solution program using Intrinsic Phasing and refined with the ShelXL[S5] refinement package using Least Squares Minimization. All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. Crystallographic and refinement data are summarized in Table S6.

Table S6 Crystal data and structure refinement for (^{DIPeP}BDI)MgI .

Identification code	hasj181101a
Empirical formula	$C_{37}H_{57}IMgN_2$
Formula weight	681.05
Temperature/K	100.0(1)
Crystal system	orthorhombic
Space group	Pbca
a/Å	16.7941(4)
b/Å	19.6395(4)
c/Å	21.8990(6)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	7222.9(3)
Z	8
ρ_{calc}g/cm^3	1.253
μ/mm^{-1}	0.930
F(000)	2864.0
Crystal size/mm^3	0.371 × 0.248 × 0.094
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.85 to 59.628
Index ranges	-23 ≤ h ≤ 23, -26 ≤ k ≤ 18, -27 ≤ l ≤ 30
Reflections collected	34505
Independent reflections	8886 [R_{int} = 0.0309, R_{sigma} = 0.0305]
Data/restraints/parameters	8886/0/380
Goodness-of-fit on F^2	1.029
Final R indexes [I>=2σ (I)]	R_1 = 0.0316, wR_2 = 0.0658
Final R indexes [all data]	R_1 = 0.0437, wR_2 = 0.0717
Largest diff. peak/hole / e Å^{-3}	1.19/-1.06

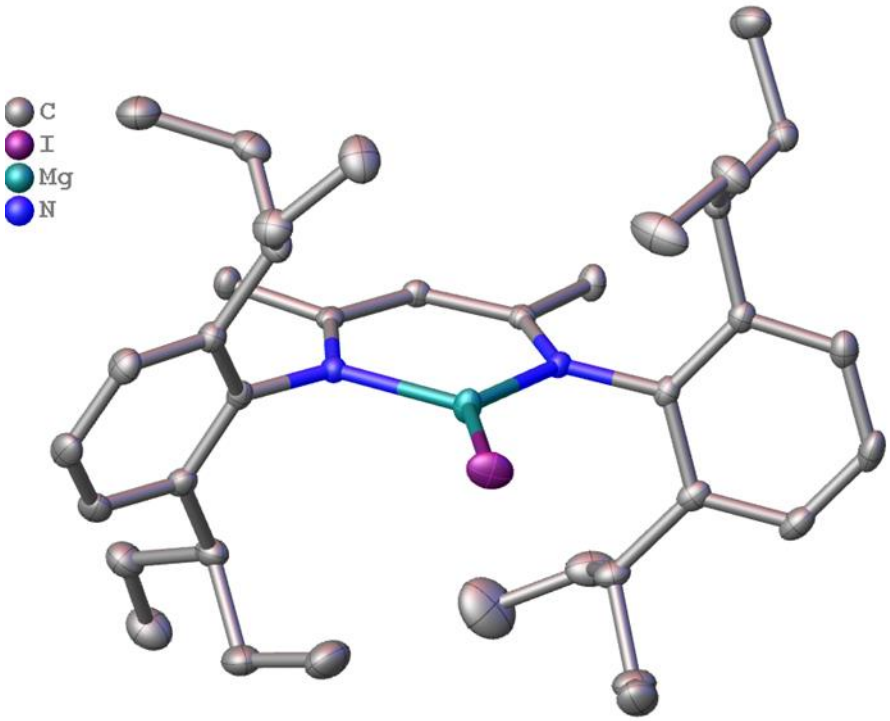


Figure S44. Solid state structure of (^{DIPeP}BDI)MgI. Ellipsoids represent 50% probability. Hydrogen atoms have been omitted for clarity.

5. DFT Calculations

5.1 General Methods

All calculations were carried out using Gaussian 16A.[S9] All methods were used as implemented. All structures were fully optimized on a B3PW91/def2SVP level of theory.[S7] All structures were characterized as true minima (Nimag=0) by frequency calculations on the same level of theory. Energies were determined at a B3PW91/def2TZVP level of theory. In all cases Grimme`s third dispersion correction with Becke-Johnson damping (GD3BJ) was added.[S10] Solvation effects were approximated using a PCM field of benzene.[S11] Charges were calculated via NBO Analyses.[S12] All structures were evaluated using Molecule 2.3.[S13] Topological analyses were carried out using AIMAll (v17).[S14],[S15]

5.2 Natural Population Analysis (NPA)

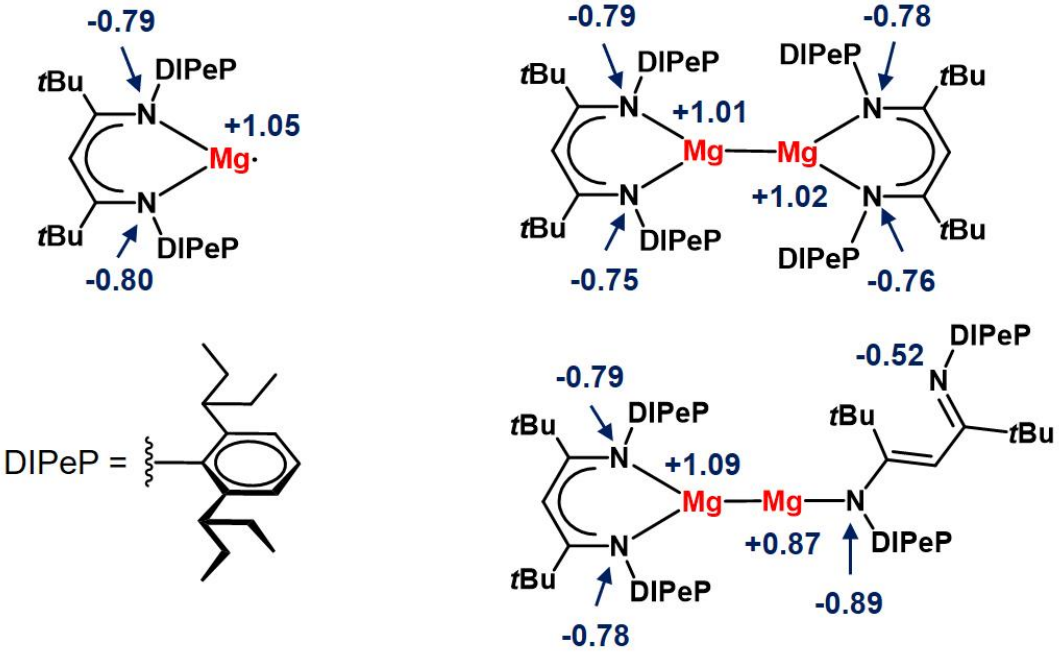


Figure S45. Selected NPA charges calculated for (^{DIPeP}BDI*)Mg•, symmetric [(^{DIPeP}BDI*)Mg]$_2$ and [(^{DIPeP}BDI*)Mg]$_2$ with one cleaved Mg-N bond (**3**). A slight polarization of the Mg-Mg bond in the asymmetric dimer is indicated by the different charges of the three-coordinate Mg (+1.09) and the two-coordinate Mg (+0.87).

5.3 Atoms-In-Molecules Analysis

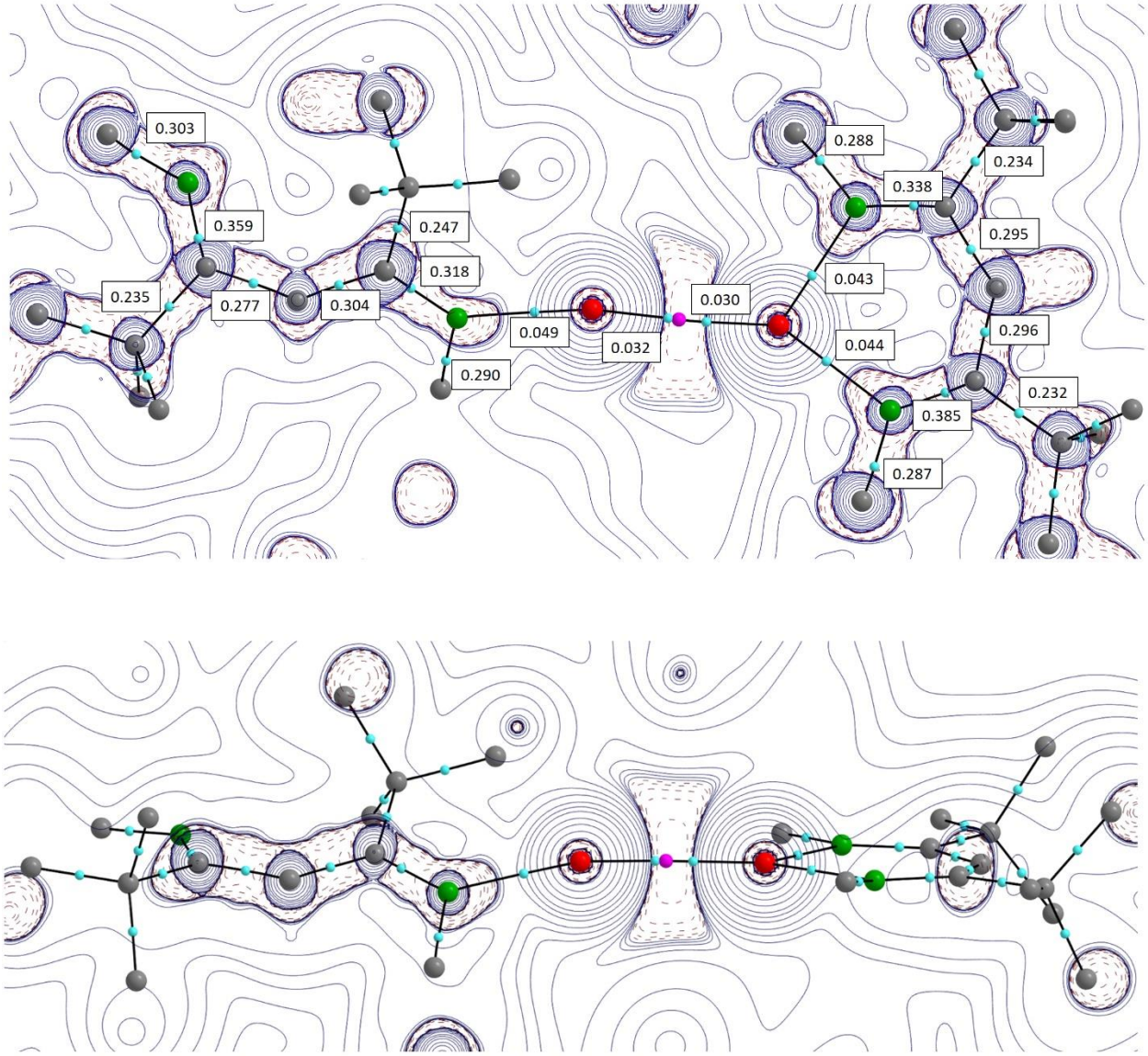


Figure S46. Contour plots of the negative Laplacian, $-\nabla^2\rho(\mathbf{r})$, in [(^{DIPeP}BDI*)Mg]$_2$ (**3**). The Non-Nuclear-Attractor is shown in purple. Boxed numbers are related to the electron density in bond-critical-points (in light-blue).

5.4 XYZ coordinates

115
(^{DIPeP}BDI*)Mg Monomer

Mg	0.023529	-0.014227	-1.219313
N	1.538708	-0.163500	0.187744
N	-1.547929	0.007365	0.146974
C	1.256030	-0.345697	1.483680
C	-2.790836	-0.286797	-0.477834
C	-1.312656	0.081168	1.459491
C	-3.487211	0.671981	-1.258240
C	2.812584	0.227429	-0.306454
C	-3.219718	-1.647455	-0.482920
C	-0.037370	-0.162137	2.013308
H	-0.055178	-0.213413	3.090634
C	3.233308	1.563151	-0.060307
C	-2.392862	-2.723213	0.204963
H	-1.987941	-2.296937	1.134535
C	3.584376	-0.608601	-1.152803
C	4.808659	-0.130661	-1.634621
H	5.414205	-0.775712	-2.274630
C	-2.423867	0.453413	2.486328
C	-3.203777	1.656459	1.953479
C	-1.856943	0.861168	3.856391
C	-3.394934	-0.709446	2.721707
C	-2.174758	2.186119	-2.732695
H	-1.391122	1.401550	-2.702550
H	-2.819467	1.901374	-3.582287
C	-3.002594	2.101833	-1.436556
H	-2.329342	2.338309	-0.596121
C	2.337372	-0.770477	2.524966
C	3.260240	-1.825137	1.910234
C	1.713981	-1.414894	3.777176
C	3.174300	0.428341	2.997352
C	3.080894	-1.961441	-1.621802
H	2.322178	-2.298602	-0.896961
C	-4.626431	0.265359	-1.965482
H	-5.169818	1.001902	-2.560683
C	-4.361819	-1.994337	-1.207538
H	-4.696290	-3.032563	-1.215541
C	2.299794	2.551316	0.616527
H	1.658242	1.993441	1.312312
C	-3.169996	-3.995509	0.571571
H	-3.551341	-4.459115	-0.354606
H	-2.444785	-4.723456	0.970261
C	5.271789	1.140180	-1.315444
H	6.239397	1.484427	-1.687911
C	4.474443	1.983583	-0.547014
H	4.815656	2.998550	-0.337327
C	-1.177586	-3.112608	-0.661628
H	-1.502662	-3.843176	-1.422222
H	-0.844987	-2.239921	-1.256123
C	-4.304869	-3.841452	1.574193
H	-4.832713	-4.797625	1.713188

H	-5.046036	-3.097034	1.246775
H	-3.932503	-3.525421	2.559196
C	-5.074443	-1.047549	-1.937498
H	-5.965788	-1.339653	-2.497473
C	-1.512896	3.530032	-2.994988
H	-2.237719	4.308776	-3.275547
H	-0.782095	3.450940	-3.814367
H	-0.973683	3.884627	-2.102944
C	-4.126696	3.153145	-1.486139
H	-3.650658	4.143500	-1.559769
H	-4.671917	3.031545	-2.438918
C	4.995705	-3.351213	-0.513325
H	4.379636	-3.749140	0.305422
H	5.512418	-2.455131	-0.137972
H	5.764108	-4.105346	-0.744130
C	3.017966	3.618831	1.449967
H	3.763206	3.119070	2.089044
H	3.593332	4.298279	0.800443
C	1.344354	3.160097	-0.432421
H	0.833550	2.330473	-0.959502
H	0.540357	3.705437	0.088964
C	2.389031	-1.766840	-2.987027
H	1.704171	-0.898105	-2.916186
H	3.154988	-1.463297	-3.722029
C	1.999644	4.056520	-1.471013
H	1.260340	4.416929	-2.200513
H	2.779744	3.516616	-2.028333
H	2.465643	4.942210	-1.011988
C	4.160831	-3.047799	-1.747865
H	3.661829	-3.975156	-2.071505
H	4.830416	-2.781254	-2.584722
C	-5.126599	3.181541	-0.339336
H	-5.930817	3.903138	-0.551602
H	-4.655584	3.486357	0.605515
H	-5.596576	2.199238	-0.179010
C	-0.006418	-3.650907	0.145242
H	-0.295984	-4.522117	0.752504
H	0.374533	-2.877609	0.828924
H	0.822777	-3.967185	-0.504288
C	2.074423	4.438541	2.319936
H	1.471841	3.787445	2.974365
H	1.373519	5.037233	1.718015
H	2.630541	5.136674	2.964029
C	1.597067	-2.956955	-3.506055
H	0.818492	-3.259285	-2.788654
H	2.230844	-3.834686	-3.702505
H	1.088077	-2.700657	-4.447768
H	3.971104	-2.186834	2.668621
H	2.685656	-2.688916	1.546145
H	3.843148	-1.423597	1.077693
H	2.521373	-1.846139	4.388188
H	1.187007	-0.691949	4.416523
H	1.015557	-2.224384	3.518472
H	3.849256	0.106021	3.806158
H	3.791175	0.838285	2.188963
H	2.533336	1.229927	3.393643

H	-2.681911	1.242405	4.477316
H	-1.412317	0.017222	4.403828
H	-1.103015	1.657450	3.770488
H	-3.942484	1.984101	2.700838
H	-2.535442	2.504288	1.740609
H	-3.748823	1.404031	1.041013
H	-4.141891	-0.417860	3.477041
H	-3.933415	-0.986802	1.808370
H	-2.864194	-1.594536	3.100351

230
[(^{DIPeP}BDI*)Mg]2 Dimer

Mg	-1.505525	0.033906	0.210338
Mg	1.612953	0.091653	0.158832
N	-3.179999	1.420099	-0.080880
N	-2.884625	-1.617625	0.462563
N	3.021175	1.710303	0.412100
N	3.257393	-1.286963	-0.237388
C	-4.410714	1.122749	0.342485
C	-2.271279	-2.890527	0.591381
C	4.351175	1.590236	0.294856
C	-4.193300	-1.442927	0.620234
C	2.834753	-2.485770	-0.866839
C	4.538435	-0.971784	-0.078105
C	-1.782794	-3.571202	-0.546324
C	4.981604	0.345333	0.163445
H	6.054880	0.409780	0.213153
C	-2.923485	2.597527	-0.830774
C	2.432034	2.896380	0.923411
C	2.987551	-2.568670	-2.283031
C	2.234896	-3.548507	-0.150009
C	-2.143183	-3.467197	1.887148
C	1.802119	3.827560	0.065274
C	-4.785064	-0.168864	0.748612
H	-5.825489	-0.227754	1.028920
C	-3.191791	2.597870	-2.219178
C	2.456315	3.112214	2.328611
C	-2.813682	-2.832565	3.097746
H	-3.808946	-2.504472	2.757404
C	-2.417316	3.755001	-0.192370
C	2.526821	-3.703892	-2.949571
H	2.625143	-3.769755	-4.033154
C	3.740173	-1.484577	-3.039254
H	4.614364	-1.232582	-2.420383
C	-2.133406	4.880148	-0.966708
H	-1.743098	5.778715	-0.487002
C	1.265172	4.993184	0.623656
H	0.792205	5.726830	-0.030507
C	-5.290742	-2.564362	0.512117
C	-5.962091	-2.317722	-0.857455
C	-6.346744	-2.434585	1.628540
C	-4.843659	-4.030844	0.517589
C	-0.609054	-2.278256	-2.317774
H	-0.547269	-1.349716	-1.720875
H	0.236461	-2.879176	-1.958653

C	1.929263	4.305127	2.833576
H	1.976871	4.502756	3.905805
C	-1.913626	-3.015681	-1.954524
H	-2.739739	-2.283481	-1.951517
C	-5.630231	2.116718	0.446106
C	-5.475998	3.542912	-0.100011
C	-5.954902	2.252446	1.947993
C	-6.852662	1.531628	-0.292521
C	-2.289403	3.746233	1.315187
H	-3.222910	3.284889	1.678780
C	1.965202	-4.769013	-2.253241
H	1.626576	-5.661078	-2.785144
C	-1.187931	-4.823954	-0.371842
H	-0.845696	-5.370496	-1.249852
C	5.745577	-1.978228	-0.070159
C	5.476131	-3.416998	-0.524526
C	6.227310	-2.032320	1.395389
C	6.908390	-1.468643	-0.948609
C	-1.499208	-4.700563	2.004551
H	-1.388929	-5.158591	2.987693
C	-3.879079	1.408468	-2.865135
H	-4.270564	0.791112	-2.044865
C	1.838976	-4.682135	-0.875342
H	1.413316	-5.518033	-0.323879
C	3.062370	2.069840	3.252614
H	3.827074	1.537830	2.670482
C	1.352197	5.249649	1.988216
H	0.950621	6.178217	2.399752
C	-3.046261	-3.797385	4.269634
H	-2.076686	-4.204382	4.605114
H	-3.407473	-3.200756	5.121789
C	-2.353718	4.878697	-2.343401
H	-2.123647	5.767150	-2.936081
C	5.353631	2.808301	0.286347
C	4.879658	3.944460	-0.630406
C	6.742979	2.412624	-0.254988
C	5.584811	3.375814	1.693311
C	-2.891171	3.750880	-2.955956
H	-3.108097	3.776789	-4.025284
C	1.772930	3.606694	-1.437903
H	2.648335	2.987199	-1.676208
C	-2.111424	-1.565252	3.607509
H	-1.268510	-1.859988	4.250824
H	-1.660422	-1.028040	2.758839
C	-4.038082	-4.926814	4.026321
H	-4.145692	-5.555504	4.923756
H	-3.729594	-5.581618	3.197993
H	-5.035217	-4.531474	3.779177
C	-1.036845	-5.388218	0.886950
H	-0.568396	-6.368732	1.001769
C	-0.393687	-1.954441	-3.787205
H	-0.129623	-2.850793	-4.367546
H	0.435565	-1.242714	-3.898676
H	-1.281553	-1.505835	-4.252658
C	3.771292	2.658795	4.477948
H	4.414465	3.490763	4.154313

H	3.039609	3.106535	5.169500
C	-2.242946	-4.082675	-3.010950
H	-2.368668	-3.563518	-3.973420
H	-1.365888	-4.737949	-3.154005
C	2.066922	-3.662307	1.363057
H	1.169624	-4.291415	1.484905
C	-3.462679	5.968281	1.898758
H	-4.313491	5.459397	2.378607
H	-3.752113	6.179364	0.858197
H	-3.325990	6.935270	2.407442
C	-5.090579	1.825234	-3.710021
H	-5.717185	2.501859	-3.106242
H	-4.769733	2.423484	-4.578411
C	-2.898925	0.495825	-3.623261
H	-2.023814	0.329670	-2.972836
H	-3.363688	-0.497268	-3.739914
C	1.884656	4.924139	-2.229217
H	0.876463	5.355909	-2.357855
H	2.448597	5.655442	-1.628146
C	2.026277	0.994275	3.645012
H	1.421566	0.745190	2.752287
H	2.561266	0.067911	3.905939
C	1.750056	-2.369456	2.117213
H	0.920199	-1.864172	1.587267
H	2.615352	-1.688349	2.089822
C	-1.152296	2.820908	1.783407
H	-0.712348	2.284419	0.924879
H	-0.317858	3.416051	2.172811
C	-2.445748	0.999535	-4.986162
H	-1.682113	0.334973	-5.416771
H	-2.003827	2.003612	-4.925499
H	-3.281712	1.044092	-5.700766
C	0.532421	2.788557	-1.807718
H	0.530759	1.867113	-1.196358
H	-0.358475	3.332940	-1.476305
C	1.095832	1.375706	4.786118
H	0.318497	0.611464	4.933984
H	0.587250	2.331504	4.591223
H	1.638804	1.472403	5.738233
C	1.322919	-2.587306	3.561939
H	0.531976	-3.349989	3.627426
H	0.923395	-1.658494	3.990533
H	2.157246	-2.907170	4.203850
C	4.290189	-1.930692	-4.400494
H	3.455732	-2.250779	-5.048068
H	4.706113	-1.040058	-4.898137
C	4.611746	1.633335	5.226924
H	3.997319	0.819733	5.642731
H	5.155411	2.095644	6.064994
H	5.356730	1.169674	4.559783
C	-2.199935	5.121439	1.979414
H	-1.947256	4.955147	3.040453
H	-1.340903	5.673224	1.568143
C	2.959740	-0.168662	-3.203825
H	2.315529	-0.243609	-4.095797
H	2.268442	-0.026791	-2.357108

C	-3.480748	-4.927708	-2.754175
H	-3.664041	-5.616871	-3.593107
H	-4.377742	-4.300533	-2.639948
H	-3.383923	-5.534927	-1.842071
C	-3.056837	-0.640460	4.361029
H	-3.570000	-1.165733	5.181408
H	-3.829582	-0.242879	3.684650
H	-2.525075	0.211199	4.806375
C	-5.928183	0.645955	-4.186115
H	-6.242785	0.014251	-3.339509
H	-5.372130	0.000511	-4.883197
H	-6.837126	0.984803	-4.706338
C	5.368989	-3.004644	-4.355593
H	5.012662	-3.930687	-3.880545
H	6.245959	-2.661217	-3.786139
H	5.713298	-3.261948	-5.369139
C	0.363604	2.395191	-3.262811
H	1.275899	1.958647	-3.690871
H	0.064998	3.248414	-3.889223
H	-0.429363	1.642241	-3.346627
C	3.218051	-4.427676	2.046669
H	2.972463	-4.501462	3.116887
H	4.134121	-3.819804	1.998330
C	3.500429	-5.831542	1.532698
H	2.605826	-6.470553	1.607719
H	4.297317	-6.306875	2.125532
H	3.820728	-5.838399	0.480384
C	2.572682	4.809874	-3.584695
H	3.605255	4.444260	-3.472948
H	2.626477	5.792327	-4.079624
H	2.053724	4.125469	-4.268106
C	-1.621140	1.829288	2.824443
H	-2.508164	1.280748	2.470402
H	-1.914623	2.330699	3.759922
H	-0.840486	1.097386	3.066116
C	3.886923	1.033449	-3.308072
H	4.438171	1.166159	-2.366367
H	3.337513	1.960672	-3.513892
H	4.624663	0.907518	-4.115594
H	-7.024108	-3.300672	1.587181
H	-5.880707	-2.422943	2.625093
H	-6.974673	-1.538087	1.540833
H	-5.736014	-4.652878	0.345680
H	-4.127110	-4.260444	-0.272089
H	-4.405611	-4.342415	1.468921
H	-6.722272	-3.091129	-1.051140
H	-6.443577	-1.332913	-0.905300
H	-5.217163	-2.364786	-1.665824
H	-6.818913	2.921847	2.085503
H	-6.193070	1.286374	2.413415
H	-5.103652	2.684999	2.495633
H	-6.422170	4.073280	0.090450
H	-4.686852	4.111204	0.393233
H	-5.289289	3.574773	-1.178983
H	-7.662349	2.277133	-0.308120
H	-6.603046	1.287490	-1.334423

H	-7.257956	0.626089	0.176693
H	6.397102	-4.000269	-0.368979
H	4.680035	-3.903148	0.038977
H	5.217752	-3.482819	-1.586371
H	7.666789	-2.261042	-1.039510
H	6.568834	-1.214512	-1.962921
H	7.415824	-0.586624	-0.537649
H	7.057561	-2.749837	1.493072
H	6.575815	-1.051030	1.745557
H	5.419543	-2.354163	2.068122
H	7.342819	3.327858	-0.369206
H	7.301561	1.756668	0.428301
H	6.683432	1.924340	-1.238259
H	5.667752	4.710823	-0.683334
H	4.698338	3.584826	-1.652043
H	3.975509	4.434813	-0.261085
H	6.397194	4.118907	1.655550
H	4.693458	3.879749	2.081515
H	5.885365	2.587453	2.398567

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[(^{DIPeP}BDI*)Mg]2 Dimer; open Mg-N cleaved

Mg	3.133840	0.095581	0.105523
N	3.889261	1.971586	-0.378033
N	4.997645	-0.799777	0.197746
C	5.181632	2.224782	-0.532444
C	6.166747	1.224659	-0.368672
H	7.169862	1.594927	-0.532863
C	6.136607	-0.138080	-0.002259
C	5.786753	3.626454	-0.851117
C	4.786318	4.757665	-1.108315
H	4.145102	4.570517	-1.974313
H	5.356108	5.677560	-1.311822
H	4.136566	4.954879	-0.250463
C	6.640931	4.051047	0.359335
H	6.023184	4.110865	1.267762
H	7.074429	5.047596	0.180267
H	7.463680	3.352124	0.560300
C	6.671097	3.526224	-2.108810
H	7.527762	2.851672	-1.980362
H	7.067201	4.521760	-2.362131
H	6.088911	3.166563	-2.970959
C	7.567859	-0.766499	0.068040
C	8.107237	-0.800209	-1.375910
H	7.459072	-1.409804	-2.021081
H	9.115405	-1.243603	-1.391725
H	8.167606	0.203685	-1.817822
C	8.487651	0.109445	0.942482
H	8.667896	1.108054	0.524420
H	9.467258	-0.381492	1.048107
H	8.066320	0.238425	1.950973
C	7.689006	-2.186687	0.637181
H	7.411811	-2.240554	1.696315
H	8.744165	-2.491111	0.557217
H	7.090967	-2.928753	0.100660

C	2.786704	2.842695	-0.553877
C	2.197170	3.477019	0.566057
C	1.016592	4.204249	0.371174
H	0.574983	4.743869	1.210412
C	0.392914	4.254430	-0.871706
H	-0.544105	4.802013	-0.994362
C	0.978105	3.616354	-1.964046
H	0.497072	3.681711	-2.941788
C	2.188147	2.930059	-1.835902
C	3.222859	4.795552	2.471324
H	3.760358	5.347831	1.684232
C	4.080350	4.754029	3.728916
H	4.386379	5.765575	4.036365
H	4.997064	4.164286	3.564380
H	3.548365	4.299729	4.578660
C	2.893593	2.308782	-3.028165
H	3.972687	2.420071	-2.835298
C	2.602449	2.996087	-4.366846
H	3.089273	2.402912	-5.158897
H	1.523736	2.929937	-4.586154
C	3.070175	4.440300	-4.470291
H	2.601766	5.076275	-3.703840
H	2.822904	4.867999	-5.453901
H	4.161230	4.515709	-4.342001
C	2.630260	0.797186	-3.142637
H	2.356212	0.387479	-2.152294
H	1.726518	0.638344	-3.748913
C	4.864077	-2.114825	0.714948
C	4.936053	-2.311113	2.116679
C	4.730506	-3.594794	2.626880
H	4.791200	-3.762258	3.703148
C	4.455135	-4.670495	1.785499
H	4.302883	-5.668448	2.202508
C	4.356711	-4.461416	0.415498
H	4.127336	-5.303569	-0.241357
C	4.544716	-3.192092	-0.143101
C	5.985805	-1.568604	4.317445
H	6.762066	-2.303808	4.047197
C	6.635870	-0.408835	5.059958
H	5.896763	0.325503	5.415020
H	7.348554	0.127768	4.412978
H	7.190257	-0.763778	5.941843
C	4.472972	-3.025116	-1.648476
H	4.517342	-1.944037	-1.855127
C	3.161204	-3.571525	-2.228691
H	3.182110	-3.460254	-3.324955
H	3.113887	-4.659414	-2.048008
C	1.913235	-2.907309	-1.679400
H	1.876028	-1.842874	-1.959219
H	1.887296	-2.954515	-0.580657
H	0.992772	-3.373974	-2.054280
C	5.692133	-3.676167	-2.327753
H	6.596306	-3.423728	-1.754108
H	5.594788	-4.773510	-2.253766
C	5.901132	-3.267732	-3.779714
H	6.034160	-2.178017	-3.870572

H	5.050911	-3.548978	-4.419095
H	6.798331	-3.747977	-4.199517
C	2.060681	2.557474	2.944894
H	1.731465	1.639457	2.426109
H	2.757418	2.216088	3.726053
C	0.870387	3.218492	3.624611
H	1.176292	4.067832	4.254157
H	0.353118	2.499134	4.278097
C	3.805389	0.024178	-3.716263
H	4.106408	0.418149	-4.699661
H	3.564132	-1.039647	-3.850397
H	4.680326	0.095716	-3.050134
Mg	0.386146	-0.216037	0.244170
N	-1.538076	-0.810755	-0.011505
N	-5.843574	0.430202	0.378413
C	-2.727746	-0.259393	0.361457
C	-3.902449	-0.992043	0.253299
H	-3.703634	-2.021508	-0.038641
C	-5.323621	-0.751234	0.409168
C	-2.643199	1.152919	0.946715
C	-1.208534	1.624702	1.169309
H	-0.644130	1.768639	0.229018
H	-0.653225	0.987198	1.883958
H	-1.219888	2.622032	1.625467
C	-3.299032	2.146108	-0.022330
H	-2.771867	2.146154	-0.989096
H	-3.254588	3.167325	0.390449
H	-4.349205	1.869345	-0.180030
C	-3.335612	1.165599	2.312291
H	-4.391693	0.898888	2.209836
H	-3.274198	2.167026	2.763258
H	-2.855834	0.448394	2.996941
C	-6.116200	-2.075770	0.633806
C	-7.623808	-1.888185	0.805200
H	-7.863465	-1.193866	1.616884
H	-8.075524	-2.862380	1.050996
H	-8.110008	-1.510815	-0.100130
C	-5.889635	-3.050497	-0.534664
H	-6.168854	-2.586770	-1.491762
H	-6.520441	-3.943295	-0.398800
H	-4.848935	-3.393993	-0.617601
C	-5.585423	-2.689752	1.941005
H	-4.506564	-2.877092	1.891626
H	-6.097028	-3.642879	2.150984
H	-5.768735	-2.011608	2.789157
C	-1.553894	-2.043324	-0.718105
C	-1.507072	-3.269415	-0.011102
C	-1.490512	-4.464494	-0.737727
H	-1.465861	-5.418100	-0.207786
C	-1.517567	-4.458002	-2.130385
H	-1.509356	-5.400873	-2.682479
C	-1.547821	-3.247866	-2.817497
H	-1.554498	-3.254196	-3.908627
C	-1.562921	-2.026257	-2.133823
C	-1.489505	-3.258020	1.504761
H	-2.035108	-2.350882	1.809884

C	-2.225392	-4.453071	2.122062
H	-3.196667	-4.560411	1.613166
H	-1.679713	-5.388757	1.917628
C	-2.449221	-4.320503	3.621879
H	-2.984891	-3.387867	3.861597
H	-1.500889	-4.310904	4.181445
H	-3.049797	-5.157333	4.009782
C	-0.055374	-3.106723	2.046989
H	0.413756	-2.225973	1.568596
H	-0.097080	-2.850974	3.118613
C	0.860180	-4.299701	1.833049
H	1.893875	-4.056861	2.115699
H	0.875684	-4.607758	0.776785
H	0.547817	-5.169362	2.431576
C	-1.608158	-0.708111	-2.879307
H	-1.159117	0.045447	-2.208692
C	-3.059142	-0.241204	-3.109990
H	-3.569481	-0.213536	-2.136196
H	-3.039724	0.799891	-3.471126
C	-3.861123	-1.102228	-4.071402
H	-4.872480	-0.695314	-4.198715
H	-3.964903	-2.131692	-3.695655
H	-3.402137	-1.155207	-5.071584
C	-0.765631	-0.713664	-4.160095
H	0.251986	-1.049319	-3.898787
H	-1.145821	-1.459590	-4.876379
C	-0.705956	0.643663	-4.848074
H	-0.426045	1.437162	-4.136280
H	-1.676365	0.925029	-5.283582
H	0.033363	0.648720	-5.663708
C	-7.150076	0.880687	0.296329
C	-7.772996	1.480643	1.423993
C	-9.030757	2.068600	1.281675
H	-9.502633	2.527169	2.154191
C	-9.696194	2.086036	0.059665
H	-10.680378	2.550959	-0.032199
C	-9.081431	1.503373	-1.043358
H	-9.594016	1.518112	-2.008721
C	-7.824988	0.898295	-0.956133
C	-7.061519	1.552640	2.760613
H	-6.297791	0.756269	2.773447
C	-7.976121	1.313235	3.968760
H	-7.359024	1.358802	4.880436
H	-8.694453	2.146875	4.063880
C	-8.722706	-0.012216	3.947832
H	-9.381934	-0.090722	3.070374
H	-9.344154	-0.134697	4.848619
H	-8.021311	-0.860880	3.911708
C	-6.328914	2.904500	2.850197
H	-5.637233	2.963499	1.995068
H	-7.069195	3.707293	2.688360
C	-5.576796	3.160052	4.150622
H	-4.936384	4.052240	4.065974
H	-4.928615	2.310723	4.417927
H	-6.259773	3.330761	4.996617
C	-7.224105	0.299258	-2.215899

H	-6.290662	-0.215695	-1.937591
C	-6.859635	1.403269	-3.221837
H	-6.443532	0.941487	-4.132676
H	-7.789187	1.909064	-3.538822
C	-5.874374	2.426804	-2.681533
H	-5.656487	3.206817	-3.427725
H	-4.925032	1.948782	-2.404026
H	-6.269022	2.918618	-1.779526
C	-8.174683	-0.740303	-2.838461
H	-8.528351	-1.412459	-2.040465
H	-9.077817	-0.224841	-3.207084
C	-7.586087	-1.579543	-3.963945
H	-7.282862	-0.967358	-4.826849
H	-8.320384	-2.314558	-4.328869
H	-6.698962	-2.138095	-3.628573
H	2.306706	5.378979	2.661805
H	5.297903	-2.098326	4.997675
C	2.858393	3.405201	1.930098
H	3.807464	2.867595	1.778715
H	0.128594	3.591790	2.906702
C	5.251882	-1.146863	3.037164
H	5.937970	-0.479854	2.492118
C	3.998230	-0.303105	3.330514
H	4.268719	0.493210	4.041426
H	3.718885	0.243896	2.412733
C	2.789866	-1.072223	3.835734
H	1.954074	-0.389795	4.051524
H	3.013382	-1.625946	4.760864
H	2.441543	-1.798290	3.086988

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