Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supporting Information

Contents

1. Supporting Experimental Data

1.1 General Experimental Procedures

All experiments were conducted under an inert nitrogen atmosphere using standard Schlenk and glovebox techniques (MBraun, Labmaster SP). *n*-Hexane and *n*-pentane were degassed with nitrogen, dried over activated aluminium oxide (Solvent Purification System: Pure Solv 400−4−MD, Innovative Technology) and stored over 3Å molecular sieves. Chlorobenzene, fluorobenzene, 1,2-difluorobenzene and methylcyclohexane were dried over calcium hydride, distilled under N_2 atmosphere and stored over molecular sieves 3Å. C_6D_6 and C_6D_5Br (99.6% D, Sigma Aldrich) were dried over 3Å molecular sieves. 2,5-Norbornadiene (*nbd*) (Alfa Aesar, 97%) and dicyclopentadiene (*dcpd*) (Acros Organics) were dried over calcium hydride, distilled under N_2 atomsphere and stored over molecular sieves 3Å. Dicyclopentadiene was freshly cracked to cyclopentadiene prior to use. $[Ph_3C^+][B(C_6F_5)_4^-]$ (Boulder Scientific) was used as received, $[Ph_3C^+][Al(OC(CF_3)_3)_4^-]$,[S1] $[(BDI)Mg\textit{n}Bu]_2$,[S2] $MgCp_2$,[S3] $[(BDI)Mg^+\cdot C_6H_6][B(C_6F_5)_4^-]$[S4] and $[(BDI)Mg(\textit{n}Pr)]_2$[S4] were synthesized according to literature procedures. $[(BDI)Mg^+][B(C_6F_5)_4^-]$ was synthesized according to an adapted literature procedure using $[(BDI)Mg\textit{n}Bu]_2$ instead of $[(BDI)Mg(\textit{n}Pr)]_2$.[S4] $[(BDI)Mg^+\cdot C_6H_6][Al(OC(CF_3)_3)_4^-]$ was synthesized according to an adapted literature procedure (BDI = $HC[C(Me)N\text{-}DIPP]_2$, DIPP = 2,6-di*iso*propylphenyl).[S23] NMR spectra were recorded with a Bruker Avance III HD 400 MHz or a Bruker Avance III HD 600 MHz spectrometer. The spectra were referenced to the respective residual signals of the deuterated solvents.[S5] Elemental analysis was performed with a Euro EA 3000 (Euro Vector) analyzer. All crystal structures have been measured on a SuperNova (Agilent) diffractometer with dual Cu and Mo microfocus sources and Atlas S2 detector. The crystal structure data of the compounds have been deposited with the Cambridge Crystallographic Data Centre. CCDC 2073987 $[(BDI)Mg^+(\textit{nbd})][B(C_6F_5)_4^-]$, 2073988 $[(BDI)Mg^+(\textit{dcpd})][B(C_6F_5)_4^-]$, 2073989 $[(BDI)Mg(Cp)Mg(BDI)^+][B(C_6F_5)_4^-]$, 2073990 $[(BDI)Mg(C_6H_5F)\text{-}Cp\text{-}(C_6H_5F)Mg(BDI)^+][B(C_6F_5)_4^-]$, 2073991 $[(BDI\text{-}H)MgCp^+)][B(C_6F_5)_4^-]$, 2073992 (BDI)MgCp, 2073993 $[(BDI)Mg^+(\textit{nbd})][Al\{OC(CF_3)_3\}_4^-]$, 2073994 $[(BDI)Mg\text{-}Cp\text{-}Mg(BDI)^+][Al\{OC(CF_3)_3\}_4^-]$, 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.

1.2 Synthetic Procedures

Synthesis of [(BDI)Mg$^+$·*nbd*][B(C_6F_5)$_4^-$]

[(BDI)Mg(*n*Bu)]$_2$ (0.141 g, 0.141 mmol) and [Ph_3C^+][B(C_6F_5)$_4^-$] (0.276 g, 0.229 mmol) were dissolved in chlorobenzene (1.0 mL) and stirred until the solution became almost colorless (1 min). After addition of *nbd* (0.3 mL) a color change to intensive yellow was observed. The solution was stirred at room temperature for 5 minutes. For isolation of the *nbd* complex it is essential that product crystallization is fast (slow crystallization leads to isolation of the *r*DA decomposition product, see below). The crystallization procedure was as follows: the solution was layered with *n*-hexane (1.0 mL) and the solvents were left at room temperature to diffuse overnight. Subsequent scratching the glass wall of the vial with a spatula initiated immediate precipitation of a microcrystalline solid. After centrifugation, the resulting white powder was isolated and washed with *n*-hexane (6 x 1mL) after which it was dried *in vacuo* yielding the desired product (0.236 g, 0.195 mmol, 85 %). Crystals suitable for X-ray diffraction analysis were grown by recrystallization of the raw product at -20°C from a saturated *nbd*/chlorobenzene solution (1:1) under diffusion with *n*-pentane.^{1}H NMR (600 MHz, C_6D_5Br, 298K): δ 7.20 - 7.14 (m, 3H, Ar*H*), 7.07 - 7.05 (m, 3H, Ar*H*), 6.73 (br. s, 4H, C*H* (nbd)), 4.92 (s, 1H, CC*H*C), 3.36 (br. s, 2H, CH_2 (nbd)), 2.70 (hept, $^3J_{HH}$ = 6.9 Hz, 4H, C*H*Me$_2$), 1.91 (s, 2H, CH_2 (nbd)), 1.57 (s, 6H, CCH_3), 1.04 (d, $^3J_{HH}$ = 6.9 Hz, 12H, CH(CH_3)$_2$), 0.96 (d, $^3J_{HH}$ = 6.9 Hz, 12H, CH(CH_3)$_2$) ppm. ^{13}C{^{1}H} NMR (101 MHz, C_6D_5Br, 298K): δ 172.2 (s, N*C*(CH$_3$)), 148.9 (br. d, $^1J_{CF}$ = 237 Hz, B(*C*$_6$F$_5$)$_4$), 142.0 (s, Ar*C*), 141.7 (s, Ar*C*), 138.1 (br. pseudo-t, "J_{CF}" = 237 Hz, B(*C*$_6$F$_5$)$_4$), 127.5 (s, Ar*C*H), 124.9 (s, Ar*C*H), 97.0 (s, C*C*HC), 28.9 (s, *C*HMe$_2$), 24.3 (s, NC(*C*H$_3$)), 24.1 (s, CH*C*H$_3$) ppm. Signals for *nbd* and B-*C* of B(*C*$_6$F$_5$)$_4$) were not detected. ^{19}F{^{1}H} NMR (376 MHz, C_6D_5Br, 298K): δ -131.2 (br. s, 8F, *o*-C*F*), -160.3 (t, $^3J_{FF}$ = 21 Hz, 4F, *p*-C*F*), -165.2 (br. s, 8F, *m*-C*F*) ppm. ^{11}B{^{1}H} NMR (128 MHz, C_6D_5Br, 298K): δ -15.6 (s, *B*(C$_6$F$_5$)$_4$) ppm. Elemental analysis Calc. for $C_{60}H_{49}N_2BF_{20}Mg$ (M = 1213.15 g/mol): C, 59.40; H, 4.07; N, 2.31; Found: C, 59.78; H, 4.48; N, 1.91.

Synthesis of [(BDI)Mg(Cp)Mg(BDI)$^+$][B(C_6F_5)$_4^-$] via *r*DA decomposition

[(BDI)Mg(*n*Bu)]$_2$ (0.141 g, 0.141 mmol) and [Ph_3C^+][B(C_6F_5)$_4^-$] (0.276 g, 0.229 mmol) were dissolved in chlorobenzene (1.0 mL) and stirred until the solution became almost colorless (1 min). After addition of *nbd* (0.3 mL) a color change to intensive yellow was observed. The solution was stirred at room temperature for 5 minutes, subsequently layered with *n*-hexane (1.0 mL) and left at room temperature for 3 days. During this extended time, the *nbd* complex decomposed by *r*DA. Small crystals of the decomposition product grew which were washed with

n-hexane (4.0 mL) and dried under vacuum (0.142 g, 0.087 mmol, 38 %). Alternatively, heating a NMR sample of [(BDI)Mg^{+}·*nbd*][$B(C_6F_5)_4^-$] (0.020 mg, 0.017 mmol) in 0.5 mL C_6D_5Br overnight at 60 °C gave the target compound in 29 % isolated yield (0.008 g, 0.049 mmol). ^{1}H NMR (400 MHz, C_6H_4/C_6D_6 (400/200 µL), 298K): δ 6.19 (s, 5H, C*H* (Cp)), 5.21 (s, 2H, CC*H*C), 2.92 (hept, $^3J_{HH}$ = 6.9 Hz, 8H, C*H*Me_2), 1.88 (s, 12H, CCH_3), 1.45 (d, $^3J_{HH}$ = 6.9 Hz, 24H, CH(CH_3)$_2$), 1.32 (d, $^3J_{HH}$ = 6.9 Hz, 24H, CH(CH_3)$_2$) ppm. All signals at the aromatic region were obscured by PhF_2. ^{13}C{^{1}H} NMR (151 MHz, C_6H_4/C_6D_6 (400/200 µL, 298K): δ 171.4 (s, N*C*(CH_3)), 143.3 (s, Ar*C*), 141.8 (s, Ar*C*), 137.2 (br. d, $^1J_{CF}$ = 239 Hz, B(C_6F_5)$_4$), 126.9 (s, Ar*C*H), 107.7 (s, *C*H (Cp)), 94.7 (s, C*C*HC), 28.7 (s, *C*HMe_2), 24.1 (s, CH*C*H_3), 24.0 (s, NC(*C*H_3)), 23.8 (s, CH*C*H_3) ppm. One signal at the aromatic region and two signals of B(C_6F_5)$_4$ were obscured by PhF_2, B-*C* of B(C_6F_5)$_4$ was not detected. ^{19}F{^{1}H} NMR (565 MHz, C_6H_4/C_6D_6 (400/200 µL), 298K): δ -132.2 (m, 8F, *o*-C*F*), -163.6 (t, $^3J_{FF}$ = 21 Hz, 4F, *p*-C*F*), -167.3 (t, $^3J_{FF}$ = 21 Hz, 8F, *m*-C*F*) ppm. ^{11}B{^{1}H} NMR (193 MHz, C_6H_4/C_6D_6 (400/200 µL), 298K): δ -16.1 (s, *B*(C_6F_5)$_4$) ppm. Elemental analysis Calc. for $C_{87}H_{87}N_4BF_{20}Mg_2$ (M = 1628.07 g/mol): C, 64.18; H, 5.39; N, 3.44; Found: C, 63.99; H, 5.48; N, 3.00.

Synthesis of (BDI)MgCp

BDI-H (0.510 g, 1.22 mmol) and $MgCp_2$ (0.192 g, 1.24 mmol) were dissolved in chlorobenzene (5 mL) and heated to reflux for 4 days. After cooling down to room temperature, all volatiles were removed under vacuum leaving a yellow solid. The product was extracted with *n*-hexane (13 mL) and after filration crystallized at -30 °C (0.327 g, 0.0645 mmol, 52 %). ^{1}H NMR (400 MHz, C_6D_6, 298K): δ 7.19 - 7.14 (m, 6H, Ar*H*), 6.03 (s, 5H, C*H* (Cp)), 4.69 (s, 1H, CC*H*C), 2.97 (hept, $^3J_{HH}$ = 6.8 Hz, 4H, C*H*Me_2), 1.55 (s, 6H, CCH_3), 1.36 (d, $^3J_{HH}$ = 6.9 Hz, 12H, CH(CH_3)$_2$), 1.07 (d, $^3J_{HH}$ = 6.9 Hz, 12H, CH(CH_3)$_2$) ppm. ^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298K): δ 169.8 (s, N*C*(CH_3)), 145.2 (s, Ar*C*), 142.1 (s, Ar*C*), 126.0 (s, Ar*C*H), 124.1 (s, Ar*C*H), 106.2 (*C*H (Cp)), 94.3 (s, C*C*HC), 28.9 (s, *C*HMe_2), 24.6 (s, CH*C*H_3), 24.4 (s, NC(*C*H_3)), 23.9 (s, CH*C*H_3) ppm. Elemental analysis Calc. for $C_{34}H_{46}N_2Mg$ (M = 507.07 g/mol): C, 80.54; H, 9.14; N, 5.52; Found: C, 80.12; H, 9.19; N, 5.59.

Alternative synthesis of [(BDI)Mg(Cp)Mg(BDI)$^+$][$B(C_6F_5)_4^-$]

[(BDI)Mg(Cp)] (0.0642 g, 0.126 mmol) and [(BDI)Mg^{+}·C_6H_6][$B(C_6F_5)_4^-$] (0.150 g, 0.126 mmol) were dissolved in chlorobenzene (1 mL) and stirred until a suspension formed (1 min). The solution was filtrated and the remaining solid was washed with chlorobenzene (4 x 0.5 mL). The off-white solid was dried under vacuum. Crystals could be grown from a saturated chlorobenzene

solution layered with *n*-hexane at room temperature (0.158 g, 0.0970 mmol, 77 %). The NMR data match those of material obtained by the synthesis route *via* rDA decomposition of [(BDI)Mg^+·*nbd*][$B(C_6F_5)_4^-$].

Synthesis of [(BDI)Mg^+·*dcpd*][$B(C_6F_5)_4^-$]

[(BDI)Mg(*n*Pr)]$_2$ (0.0398 g, 0.0410 mmol) and [Ph_3C^+][$B(C_6F_5)_4^-$] (0.0720 g, 0.0781 mmol) were dissolved in chlorobenzene (0.3 mL) and stirred until the solution became almost colorless (1 min). After filtration, a mixture of *dcpd* (53 µL, 5 eq.) and methylcyclohexane (0.3 mL) was added and the reaction mixture left at room temperature for 1 day. Scratching the glass wall of the vial with a spatula initiated crystallization. The crystalline product was washed with *n*-hexane (3 x 0.5 mL) and dried under vacuum (0.0436 g, 0.0348 mmol, 45 %). ^{1}H NMR (400 MHz, C_6D_5Br, 298K): δ 7.20 - 7.16 (m, 2H, Ar*H*), 7.06 - 7.04 (m, 4H, Ar*H*), 5.94 (br. s, 2H, C*H* (dcpd)), 5.47 (br. s, 2H, C*H* (dcpd)), 4.95 (s, 1H, CC*H*C), 3.12 - 3.10 (m, 1H, C*H* (dcpd)), 2.76 (hept, $^3J_{HH}$ = 6.6 Hz, 4H, C*H*Me_2), 2.68 (br. s, 1H, C*H* (dcpd)), 2.60 - 2.58 (m, 1H, C*H* (dcpd)), 2.13 - 2.06 (m, 2H, C*H* (dcpd)), 1.58 (s, 6H, CC*H*$_3$), 1.46 - 1.44 (m, 1H, C*H* (dcpd)), 1.20 - 1.18 (m, 2H, C*H* (dcpd)), 1.06 (d, $^3J_{HH}$ = 6.6 Hz, 12H, CH(C*H*$_3$)$_2$), 0.90 (d, $^3J_{HH}$ = 6.6 Hz, 12H, CH(C*H*$_3$)$_2$) ppm. ^{13}C{^{1}H} NMR (151 MHz, C_6D_5Br, 298K): δ 173.3 (s, N*C*(CH_3)), 148.8 (br. d, $^1J_{CF}$ = 244 Hz, B(*C*$_6$F$_5$)$_4$), 142.1 (s, Ar*C*), 141.5 (s, Ar*C*), 138.7 (br. d, $^1J_{CF}$ = 244 Hz, B(*C*$_6$F$_5$)$_4$), 137.0 (br. d, $^1J_{CF}$ = 244 Hz, B(*C*$_6$F$_5$)$_4$), 133.0 (s, *C*H (dcpd)), 132.8 (s, *C*H (dcpd)), 132.7(s, *C*H (dcpd)), 127.4 (s, Ar*C*H), 124.9 (s, Ar*C*H), 96.9 (s, C*C*HC), 55.1 (s, *C*H (dcpd)), 50.7 (s, *C*H (dcpd)), 46.7 (s, *C*H (dcpd)), 45.7 (s, *C*H (dcpd)), 41.5 (s, *C*H_2 (dcpd)), 35.0 (s, *C*H_2 (dcpd)), 28.8 (s, *C*HMe_2), 24.4 (s, CH*C*H_3), 24.2 (s, NC(*C*H_3)), 24.1 (s, CH*C*H_3) ppm. One olefinic signal of *dcpd* and B-*C* of B(*C*$_6$F$_5$)$_4$ were not detected. ^{19}F{^{1}H} NMR (565 MHz, C_6D_5Br, 298K): δ -131.3 (br. s, 8F, *o*-C*F*), -160.0 (br. s, 4F, *p*-C*F*), -164.9 (br. s, 8F, *m*-C*F*) ppm. ^{11}B{^{1}H} NMR (193 MHz, C_6D_5Br, 298K): δ -15.7 (s, *B*(*C*$_6$F$_5$)$_4$) ppm. Elemental analysis Calc. for $C_{63}H_{53}N_2BF_{20}Mg$ (M = 1253.21 g/mol): C, 60.38; H, 4.26; N, 2.24; Found: C, 60.55; H, 4.67; N, 1.89.

Synthesis of [(BDI)Mg^+·*nbd*][$Al(OC(CF_3)_3)_4^-$]

[(BDI)Mg(*n*Bu)]$_2$ (0.0221 g, 0.0221 mmol) and [Ph_3C^+][$Al(OC(CF_3)_3)_4^-$] (0.0511 g, 0.0422 mmol) were dissolved in chlorobenzene (0.4 mL), stirred until the solution became almost colorless (1 min) and filtrated. After addition of *nbd* (0.05 mL) a color change to intensive yellow was observed. The solution was layered with *n*-hexane (0.5 mL) and stored at -20 °C overnight. The crystalline product was washed with *n*-pentane (3 x 0.2 mL) and dried under vacuum (0.0161 g, 0.0107 mmol, 25 %). ^{1}H NMR (600 MHz, C_6D_5Br, 298K): δ 7.23 (t, $^3J_{HH}$ = 7.7 Hz, 2H, Ar*H*), 7.11

(t, $^3J_{HH}$ = 7.7 Hz, 4H, Ar*H*), 6.81 (br. s, 4H, C*H* (nbd)), 4.95 (s, 1H, CC*H*C), 3.28 (br. s, 2H, CH_2 (nbd)), 2.66 (br. s, 4H, C*H*Me$_2$), 1.91 (s, 2H, CH_2 (nbd)), 1.57 (s, 6H, CCH_3), 1.07 (d, $^3J_{HH}$ = 6.6 Hz, 12H, CH(CH_3)$_2$), 0.99 (d, $^3J_{HH}$ = 6.6 Hz, 12H, CH(CH_3)$_2$) ppm. ^{13}C{^{1}H} NMR (151 MHz, C_6D_5Br, 298K): δ 172.7 (s, N*C*(CH$_3$), assigned in HMBC), 141.9 (s, Ar*C*, assigned in HMBC), 141.4 (s, Ar*C*, assigned in HMBC), 127.8 (s, Ar*C*H), 125.1 (s, Ar*C*H), 121.0 (s, *C*F$_3$), 96.8 (s, C*C*HC, assigned in HSQC and HMBC), 29.0 (s, *C*HMe$_2$), 24.4 (s, NC(*C*H$_3$)), 24.3 (s, CH*C*H$_3$) ppm. Signals for *nbd* and O-*C* of Al(O*C*(CF$_3$)$_3$)$_4^-$ were not detected. Signals were also not observed in temperature dependent NMR measurements (-20 °C and 50 °C). ^{19}F{^{1}H} NMR (376 MHz, C_6D_5Br, 298K): δ -74.3 (s, C*F*$_3$) ppm. ^{27}Al{^{1}H} NMR (156 MHz, C_6D_5Br, 298K): δ 35.7 (s, *Al*(OC(CF$_3$)$_3$)$_4$) ppm. Elemental analysis Calc. for $C_{52}H_{49}N_2AlF_{36}MgO_4$ (M = 1501.20 g/mol): C, 41.60; H, 3.29; N, 1.87; Found: C, 41.51; H, 3.36; N, 1.92.

Synthesis of [(BDI)Mg$^+$·C$_6$H$_6$][Al(OC(CF$_3$)$_3$)$_4^-$]

[(BDI)Mg$^+$·C$_6$H$_6$][Al(OC(CF$_3$)$_3$)$_4^-$] was synthesized to an adpated literature procedure.[S23] [(BDI)Mg(*n*Bu)]$_2$ (0.100 g, 0.100 mmol) and [Ph$_3$C$^+$][Al(OC(CF$_3$)$_3$)$_4^-$] (0.232 g, 0.251 mmol) were dissolved in chlorobenzene (2 mL). The brownish solution was stirred until colorless (1 min). Subsequently all volatiles were removed under reduced pressure and the material was layered with a 1:1 mixture of benzene and hexane (2 mL) overnight. The resulting white powder was washed with hexane (3 x 1 mL) and dried *in vacuo* yielding 0.249 g (0.167 mmol, 67 %) of the desired product. ^{1}H NMR (400 MHz, C_6D_5Br, 298K): δ 7.22 (t, $^3J_{HH}$ = 7.7 Hz, 2H, Ar*H*), 7.20 (s, 6H, C$_6H_6$), 7.10 (d, $^3J_{HH}$ = 7.7 Hz 4H, Ar*H*), 5.04 (s, 1H, CC*H*C), 2.72 (hept, $^3J_{HH}$ = 6.9 Hz, 4H, C*H*Me$_2$), 1.60 (s, 6H, CCH_3), 1.04 (d, $^3J_{HH}$ = 6.9 Hz, 12H, CH(CH_3)$_2$), 0.97 (d, $^3J_{HH}$ = 6.9 Hz, 12H, CH(CH_3)$_2$) ppm. ^{13}C{^{1}H} NMR (101 MHz, C_6D_5Br, 298K): δ 173.3 (s, N*C*(CH$_3$)), 142.1 (s, Ar*C*), 141.3 (s, Ar*C*), 128.7 (s, *C*$_6$H$_6$), 125.1 (s, Ar*C*H), 122.9 (s, Ar*C*H), 121.1 (s, *C*F$_3$), 96.3 (s, C*C*HC), 28.9 (s, *C*HMe$_2$), 24.7 (s, NC(*C*H$_3$)), 24.5 (s, CH*C*H$_3$), 24.3 (s, CH*C*H$_3$) ppm. O-*C* of Al(OC(CF$_3$)$_3$)$_4^-$ was not detected. ^{19}F{^{1}H} NMR (376 MHz, C_6D_5Br, 298K): δ -74.6 (s, C*F*$_3$) ppm. ^{27}Al{^{1}H} NMR (104 MHz, C_6D_5Br, 298K): δ 35.5 (s, *Al*(OC(CF$_3$)$_3$)$_4$) ppm. Elemental analysis Calc. for $C_{51}H_{47}N_2AlF_{36}MgO_4$ (M = 1487.18 g/mol): C, 41.19; H, 3.19; N, 1.88; Found: C, 40.85; H, 3.32; N, 1.79.

Alternative synthesis of [(BDI)Mg(Cp)Mg(BDI)$^+$][Al(OC(CF$_3$)$_3$)$_4^-$]

[(BDI)Mg(Cp)] (0.0141 g, 0.0278 mmol) and [(BDI)Mg$^+$·C$_6$H$_6$][Al(OC(CF$_3$)$_3$)$_4^-$] (0.0414 g, 0.0278 mmol) were dissolved in chlorobenzene (1.5 mL) and stirred until a suspension formed (2 h). The solution was filtrated and the remaining solid was washed with *n*-pentane (3 x 0.5 mL).

The off-white solid was dried under vacuum. Crystals could be grown from a saturated chlorobenzene solution at room temperature (0.0168 g, 0.00877 mmol, 32 %). ^{1}H NMR (400 MHz, C_6H_4/C_6D_6 (400/200 µL), 298K): δ 6.20 (s, 5H, C*H* (Cp)), 5.22 (s, 2H, CC*H*C), 2.92 (hept, $^{3}J_{HH}$ = 6.8 Hz, 8H, C*H*Me$_2$), 1.89 (s, 12H, CC*H*$_3$), 1.46 (d, $^{3}J_{HH}$ = 6.8 Hz, 24H, CH(C*H*$_3$)$_2$), 1.32 (d, $^{3}J_{HH}$ = 6.8 Hz, 24H, CH(C*H*$_3$)$_2$) ppm. All signals at the aromatic region were obscured by PhF_2. ^{13}C{^{1}H} NMR (151 MHz, C_6H_4/C_6D_6 (400/200 µL, 298K): δ 171.4 (s, N*C*(CH$_3$)), 143.3 (s, Ar*C*), 141.8 (s, Ar*C*), 126.9 (s, Ar*C*H), 121.4 (q, *C*F$_3$, $^{1}J_{CF}$ = 293.0 Hz), 107.7 (s, *C*H (Cp)), 94.7 (s, C*C*HC), 28.7 (s, *C*HMe$_2$), 24.1 (s, CH*C*H$_3$), 24.0 (s, NC(*C*H$_3$)), 23.8 (s, CH*C*H$_3$) ppm. One signal at the aromatic region was obscured by PhF_2, O-*C* of Al(OC(CF$_3$)$_3$)$_4^-$ was not detected. ^{19}F{^{1}H} NMR (565 MHz, C_6H_4/C_6D_6 (400/200 µL), 298K): δ -75.2 (s, C*F*$_3$) ppm. ^{27}Al{^{1}H} NMR (156 MHz, C_6H_4/C_6D_6 (400/200 µL), 298K): δ 35.1 (s, *Al*(OC(CF$_3$)$_3$)$_4$) ppm. Elemental analysis Calc. for $C_{79}H_{87}N_4AlF_{36}Mg_2O_4$ (M = 1916.12 g/mol): C, 49.52; H, 4.58; N, 2.92; Found: C, 49.05; H, 4.81; N, 2.68.

1.3 NMR Spectra of Synthesized Compounds

1.3.1 Spectra of free alkenes

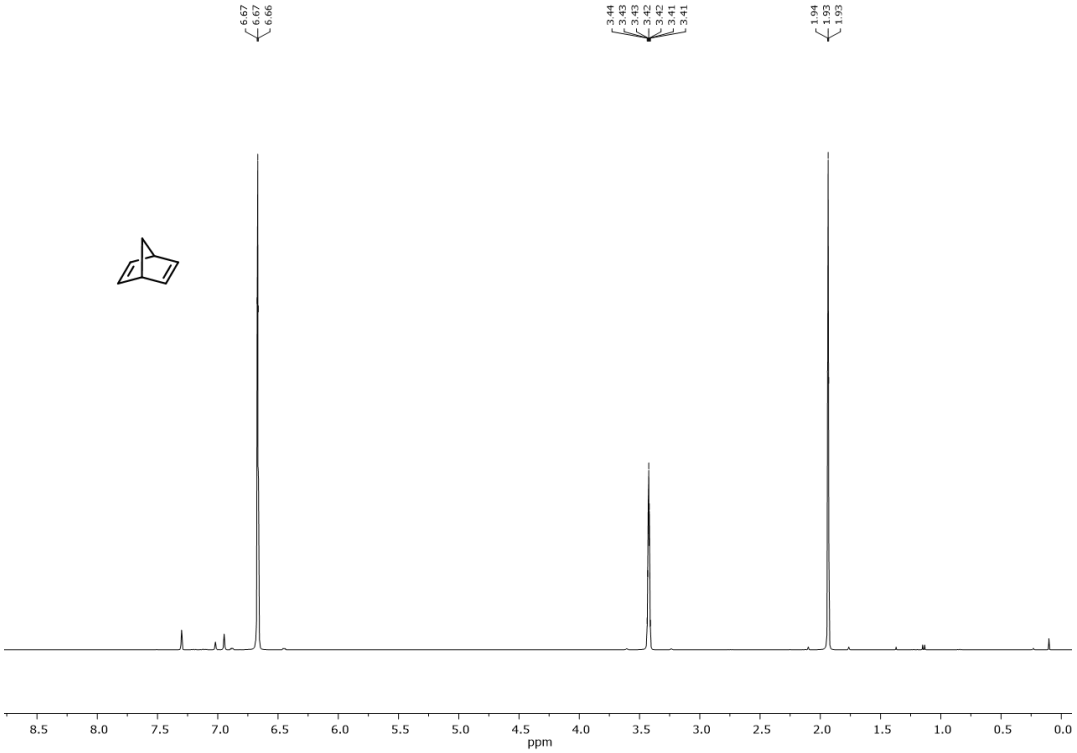

Figure S1: ^{1}H NMR spectrum (600 MHz, 298 K) of free *nbd* in C_6D_5Br.

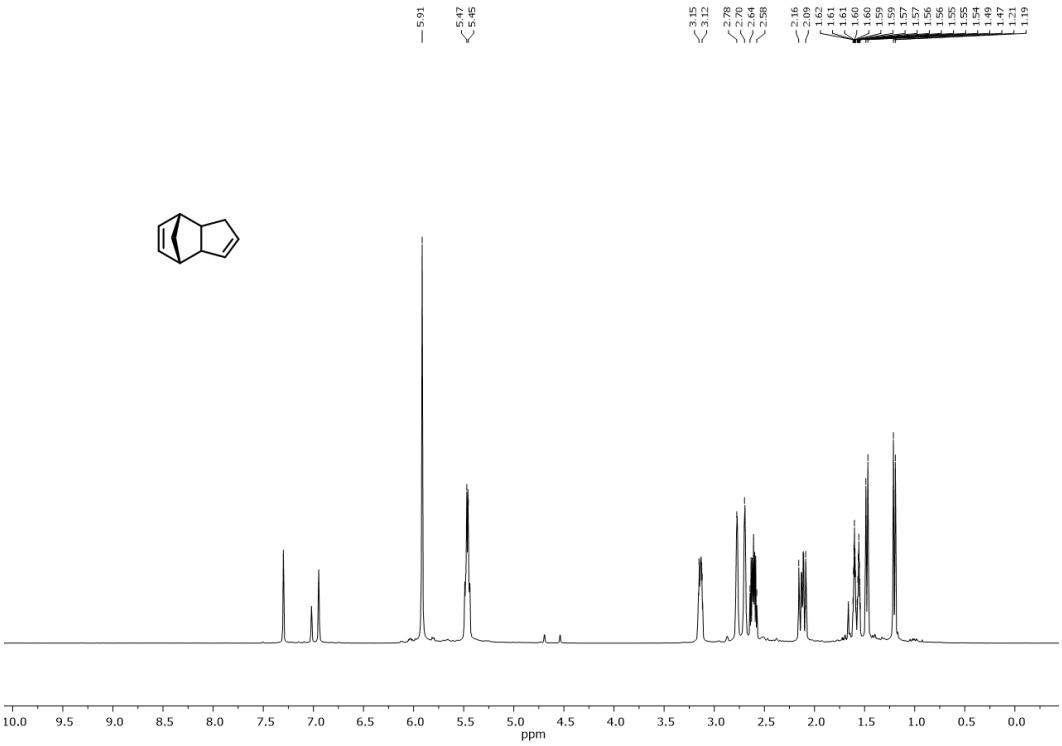

Figure S2: ^{1}H NMR spectrum (600 MHz, 298 K) of free *dcpd* in C_6D_5Br.

1.3.2 Spectra of [(BDI)Mg^{+}·*nbd*][B(C$_6$F$_5$)$_4^{-}$]

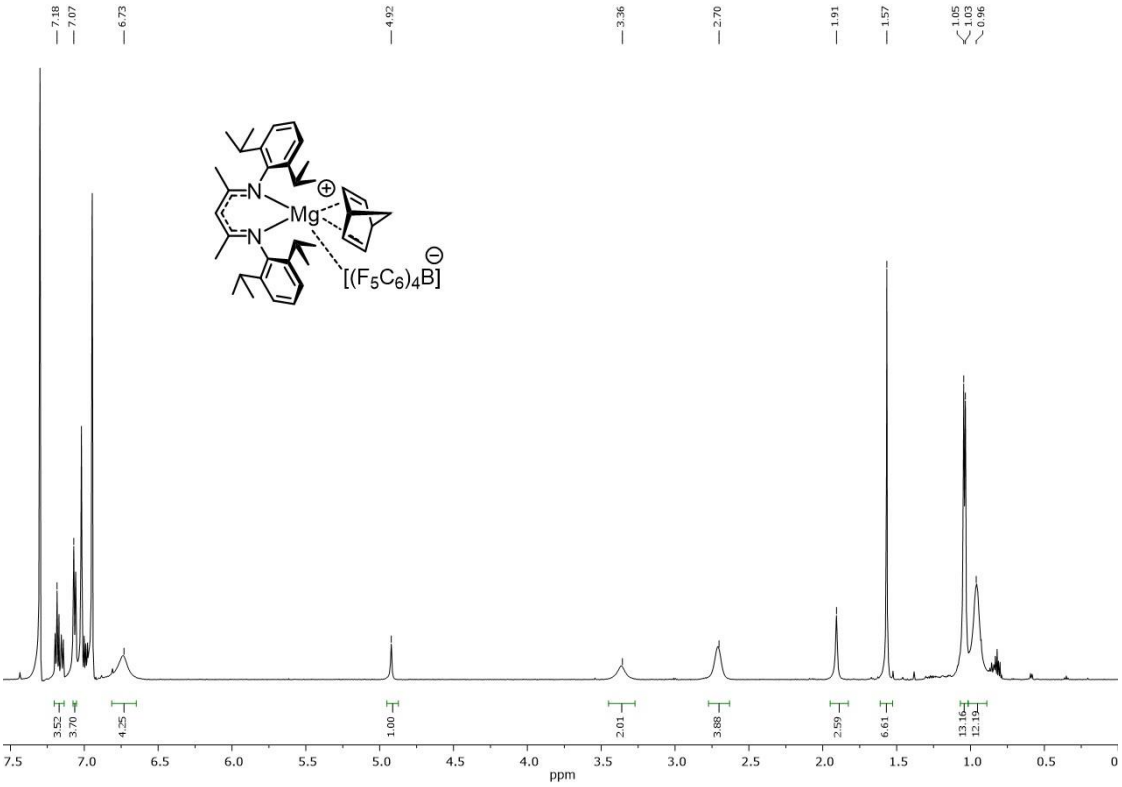

Figure S3: ^{1}H NMR spectrum (600 MHz, 298 K) of [(BDI)Mg^{+}·*nbd*][B(C$_6$F$_5$)$_4^{-}$] in C$_6$D$_5$Br.

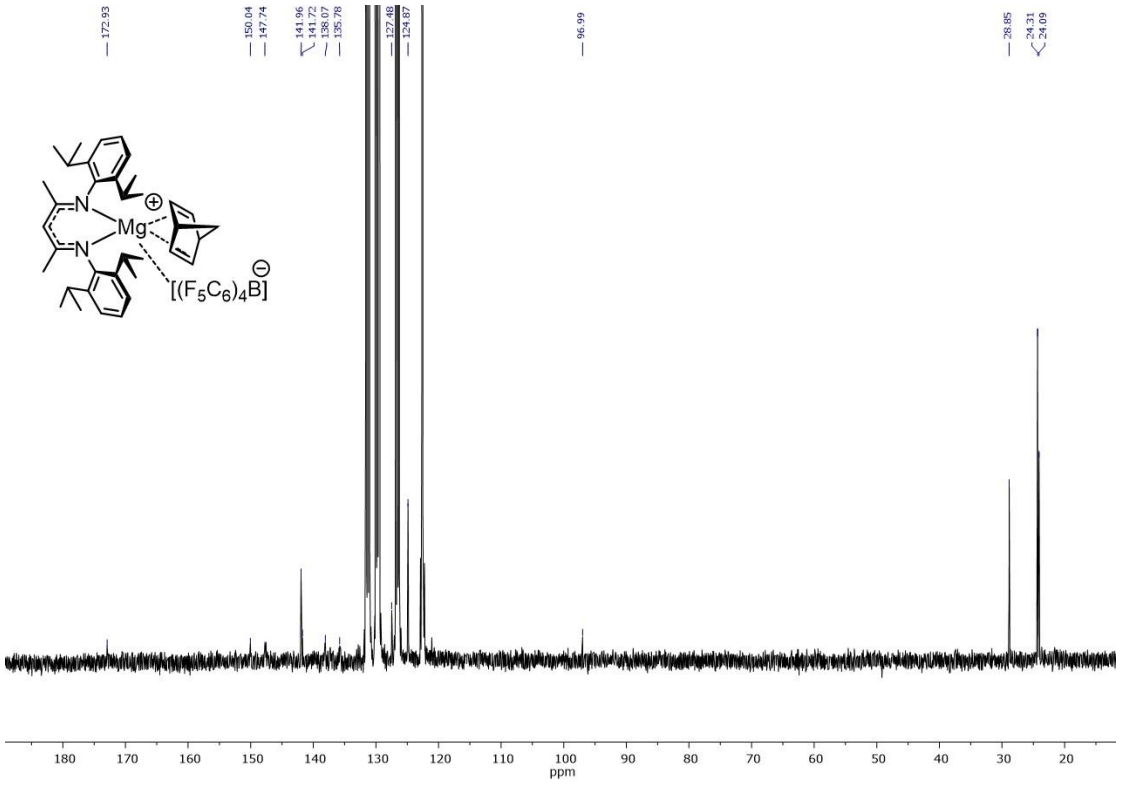

Figure S4: ^{13}C{^{1}H} NMR spectrum (101 MHz, 298 K) of [(BDI)Mg^{+}·*nbd*][B(C$_6$F$_5$)$_4^{-}$] in C$_6$D$_5$Br.

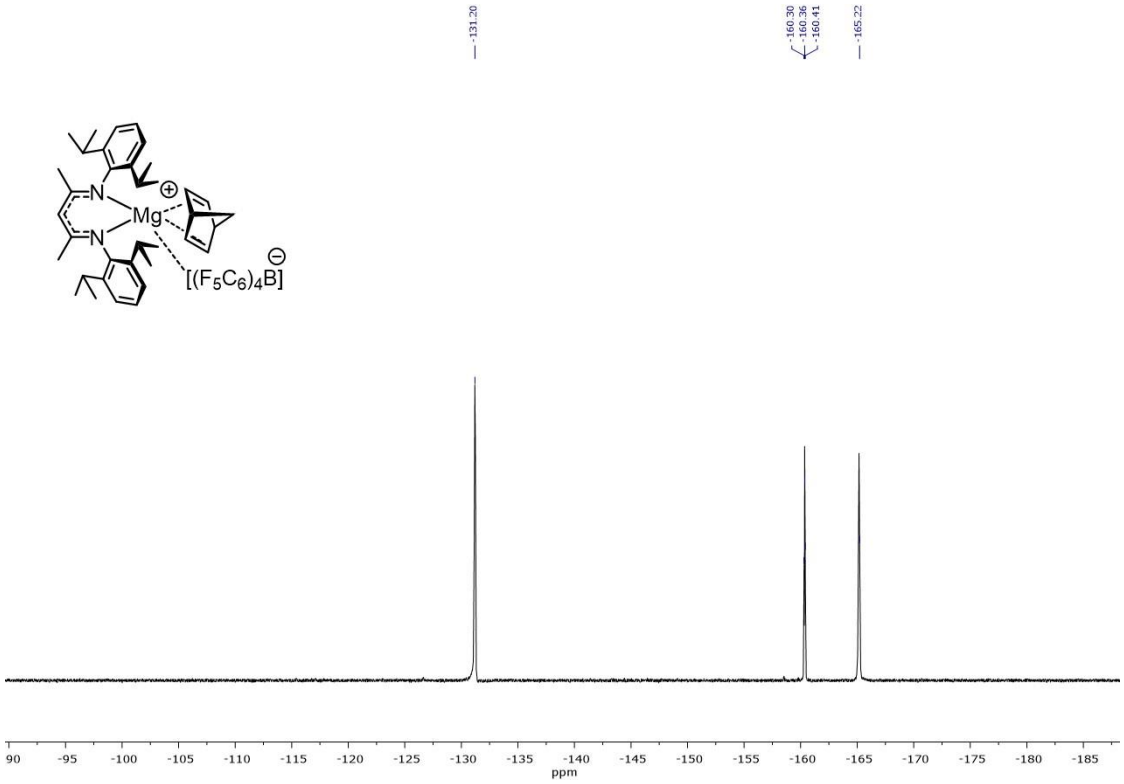

Figure S5: $^{19}F\{^{1}H\}$ NMR spectrum (376 MHz, 298 K) of [(BDI)Mg^{+}·*nbd*][$B(C_6F_5)_4^{-}$] in C_6D_5Br.

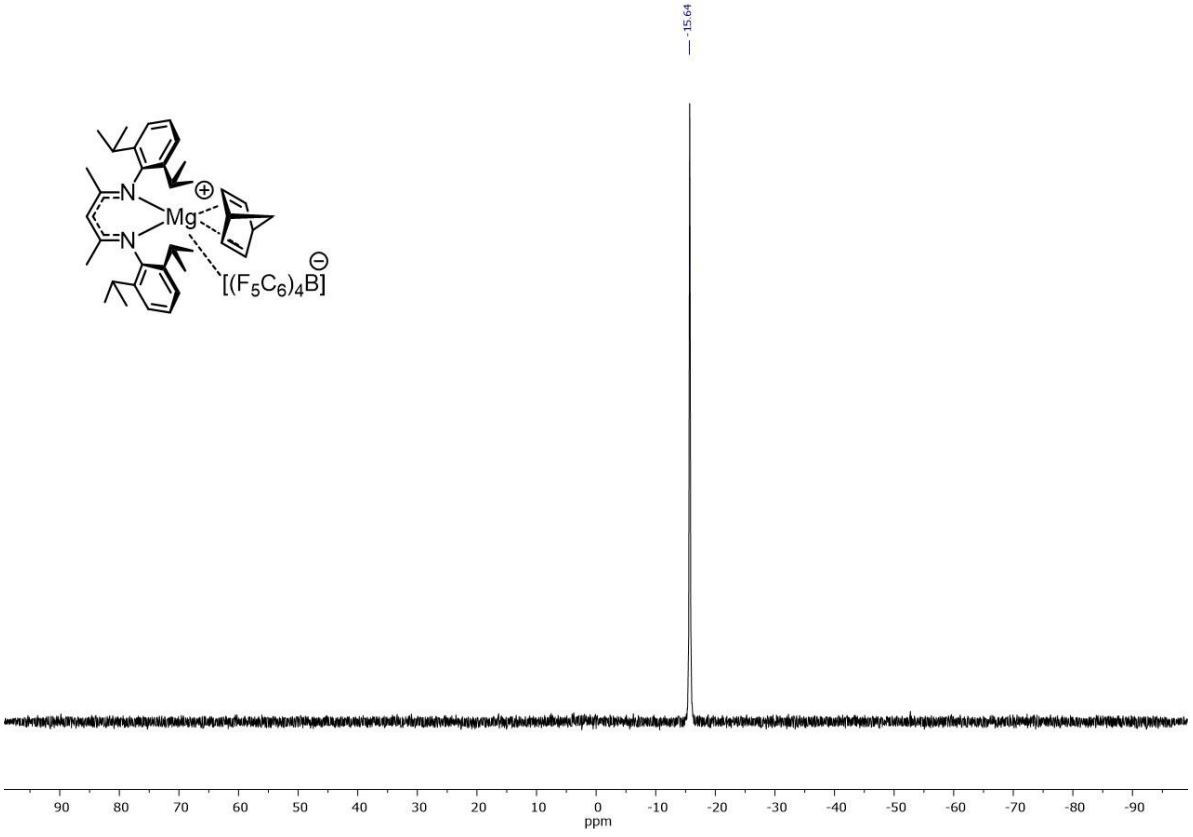

Figure S6: $^{11}B\{^{1}H\}$ NMR spectrum (128 MHz, 298 K) of [(BDI)Mg^{+}·*nbd*][$B(C_6F_5)_4^{-}$] in C_6D_5Br.

1.3.3 Spectra of [(BDI)Mg(Cp)]

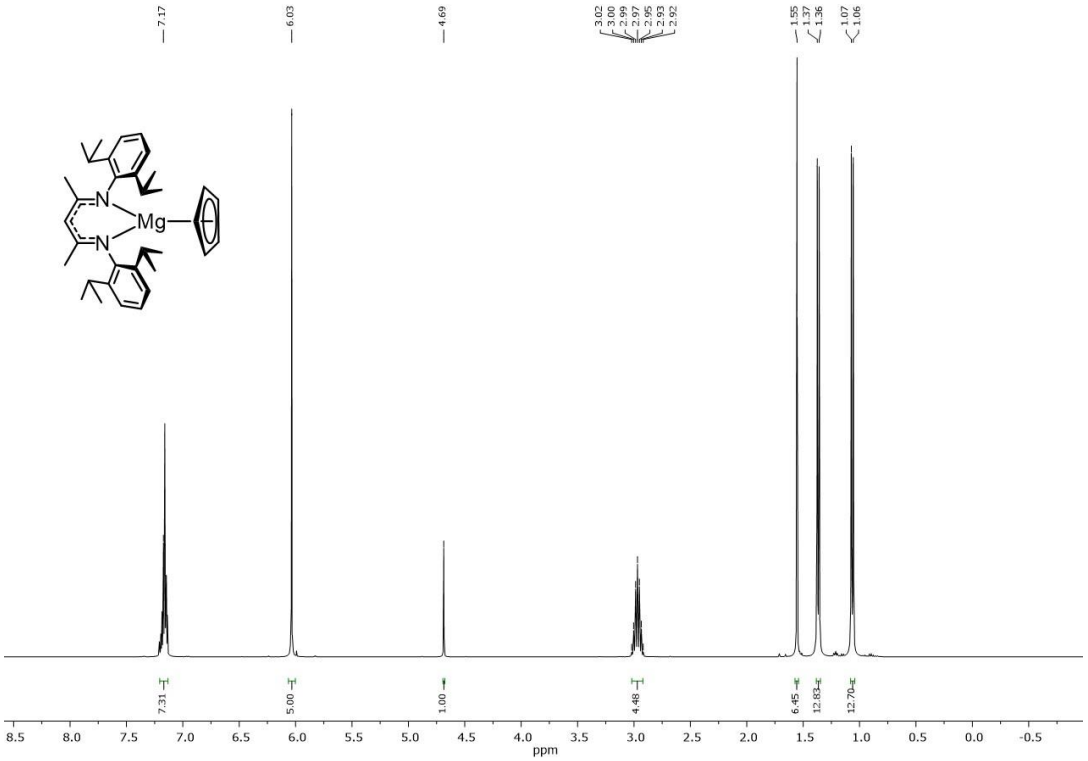

Figure S7: ^{1}H NMR spectrum (400 MHz, 298 K) of [(BDI)Mg(Cp)] in C_6D_6.

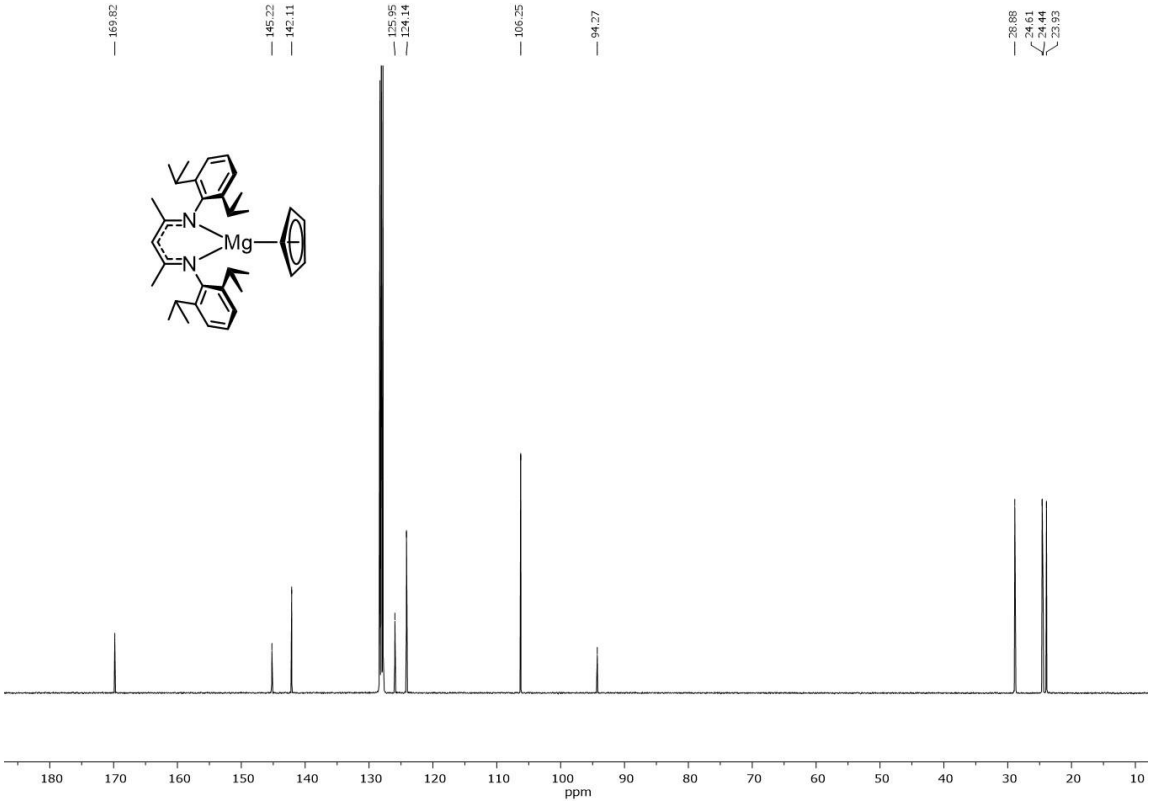

Figure S8: $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K) of [(BDI)Mg(Cp)] in C_6D_6.

1.3.4 Spectra of $[(BDI)Mg(Cp)Mg(BDI)^{+}][B(C_6F_5)_4^{-}]$

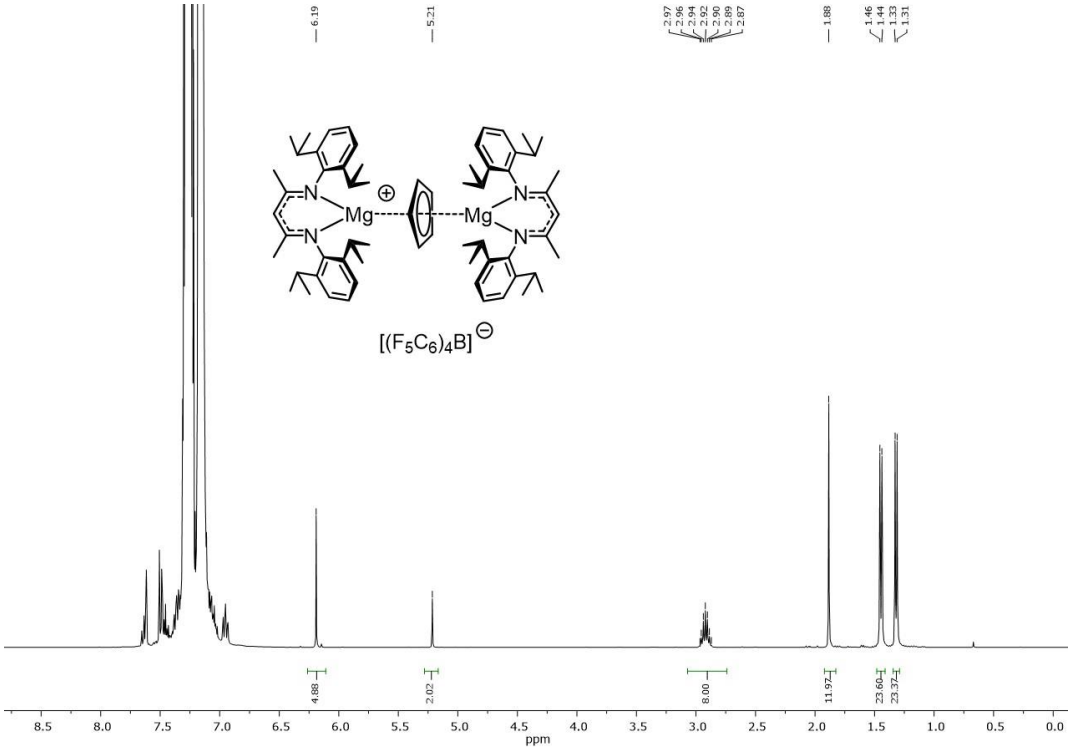

Figure S9: ^{1}H NMR spectrum (400 MHz, 298 K) of $[(BDI)Mg(Cp)Mg(BDI)^{+}][B(C_6F_5)_4^{-}]$ in $C_6H_4F_2/C_6D_6$.

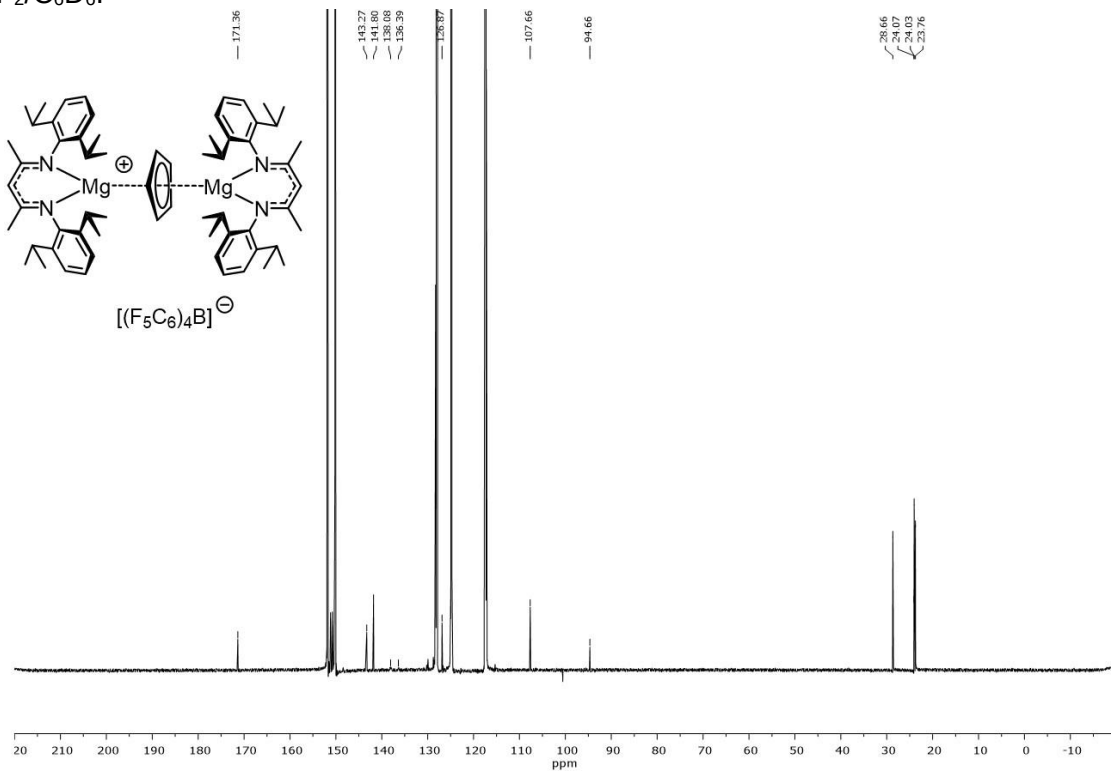

Figure S10: $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, 298 K) of $[(BDI)Mg(Cp)Mg(BDI)^{+}][B(C_6F_5)_4^{-}]$ in $C_6H_4F_2/C_6D_6$.

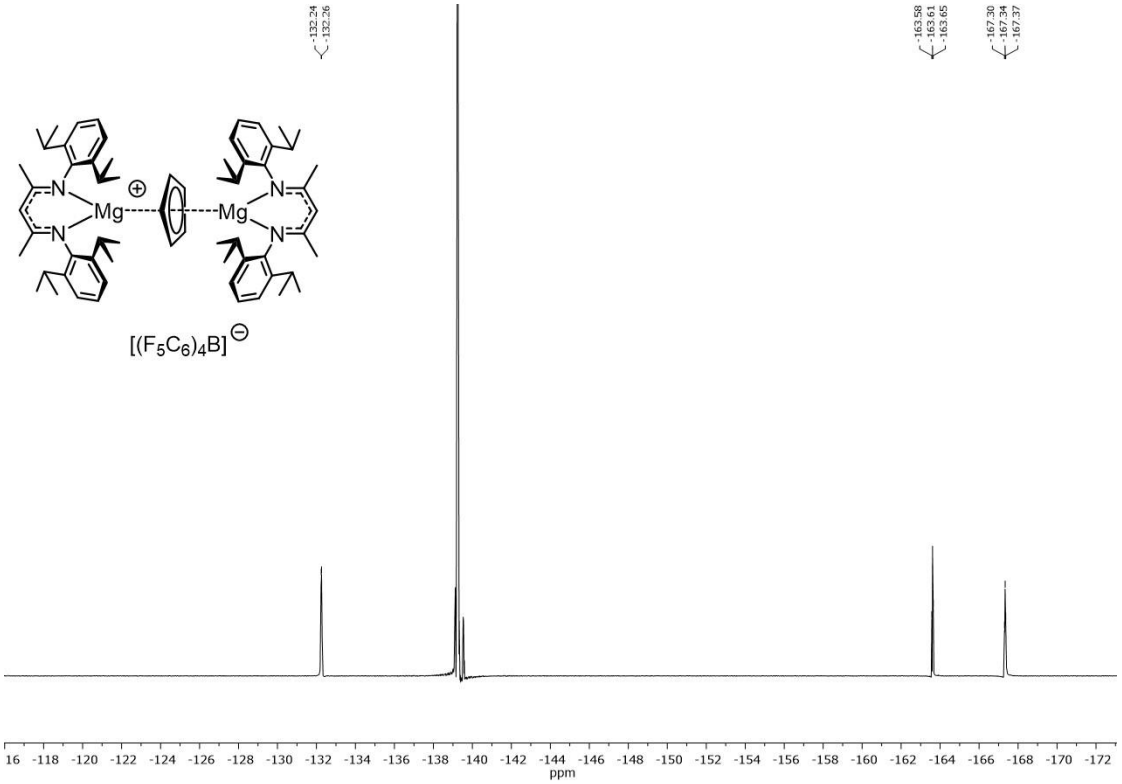

Figure S11: $^{19}F\{^{1}H\}$ NMR spectrum (565 MHz, 298 K) of [(BDI)Mg(Cp)Mg(BDI)$^{+}$][B(C_6F_5)$_4^{-}$] in $C_6H_4F_2/C_6D_6$.

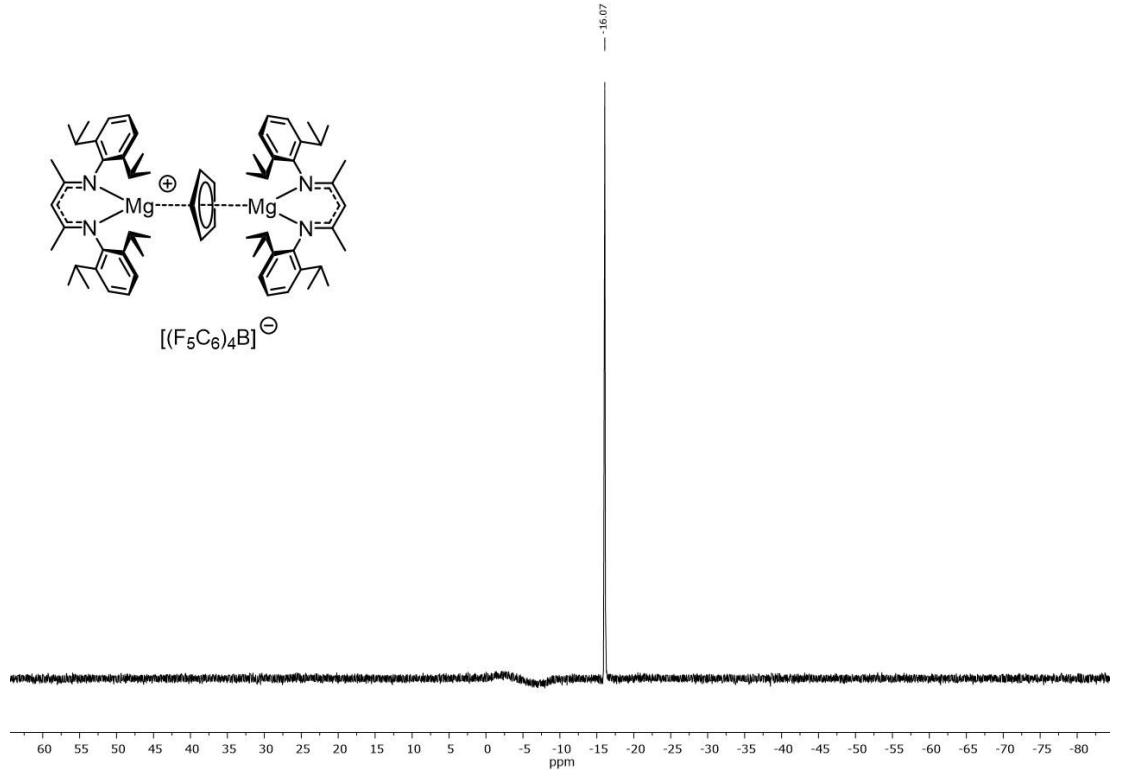

Figure S12: $^{11}B\{^{1}H\}$ NMR spectrum (193 MHz, 298 K) of [(BDI)Mg(Cp)Mg(BDI)$^{+}$][B(C_6F_5)$_4^{-}$] in $C_6H_4F_2/C_6D_6$.

1.3.5 Spectra of [(BDI)Mg^{+}·*dcpd*][B(C$_6$F$_5$)$_4^{-}$]

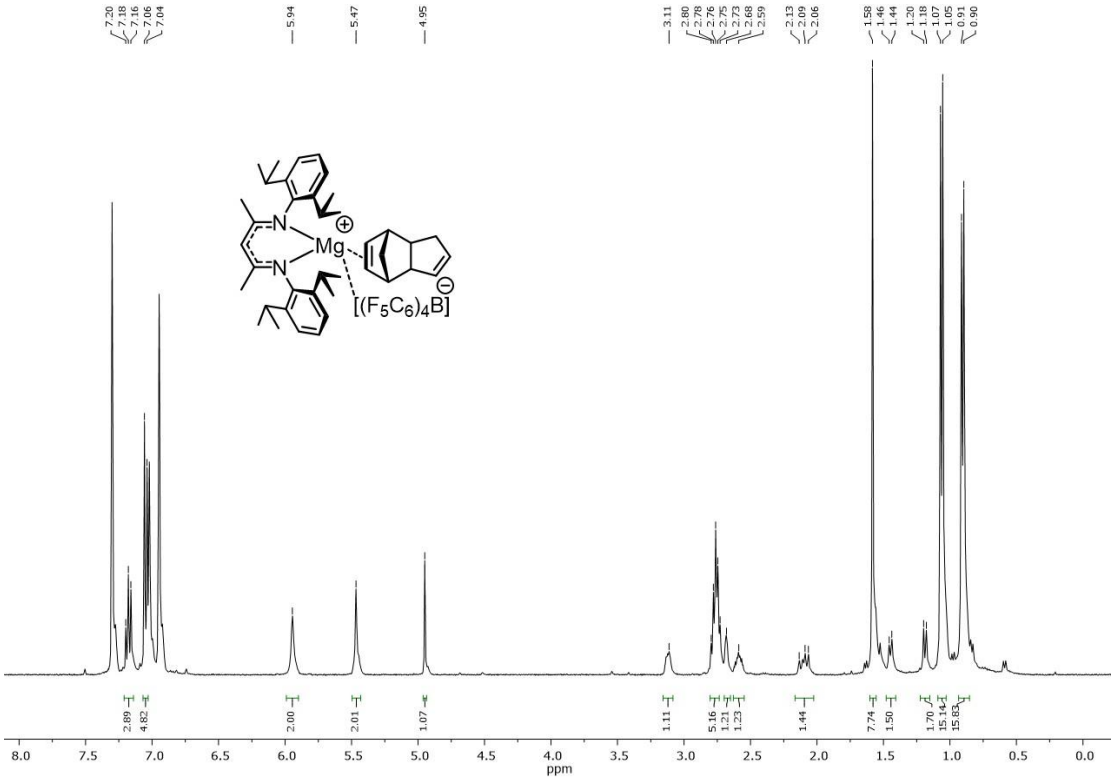

Figure S13: ^{1}H NMR spectrum (400 MHz, 298 K) of [(BDI)Mg^{+}·*dcpd*][B(C$_6$F$_5$)$_4^{-}$] in C$_6$D$_5$Br.

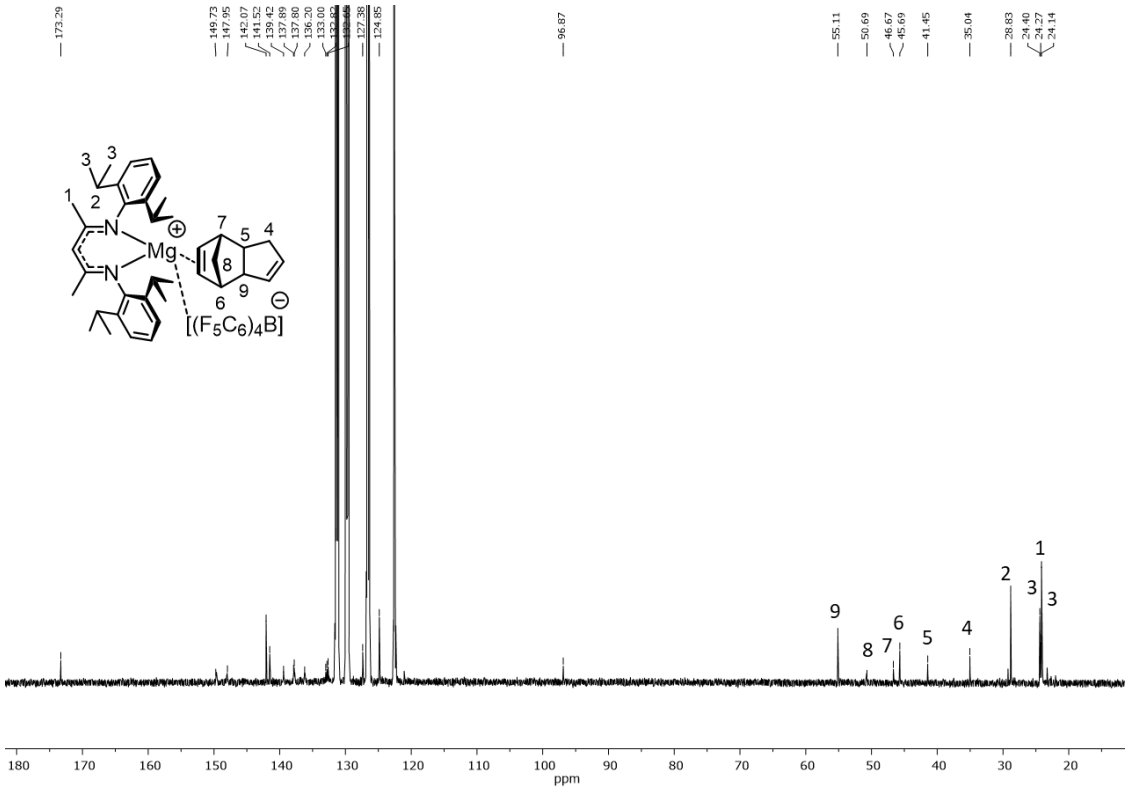

Figure S14: ^{13}C{^{1}H} NMR spectrum (151 MHz, 298 K) of [(BDI)Mg^{+}·*dcpd*][B(C$_6$F$_5$)$_4^{-}$] in C$_6$D$_5$Br.

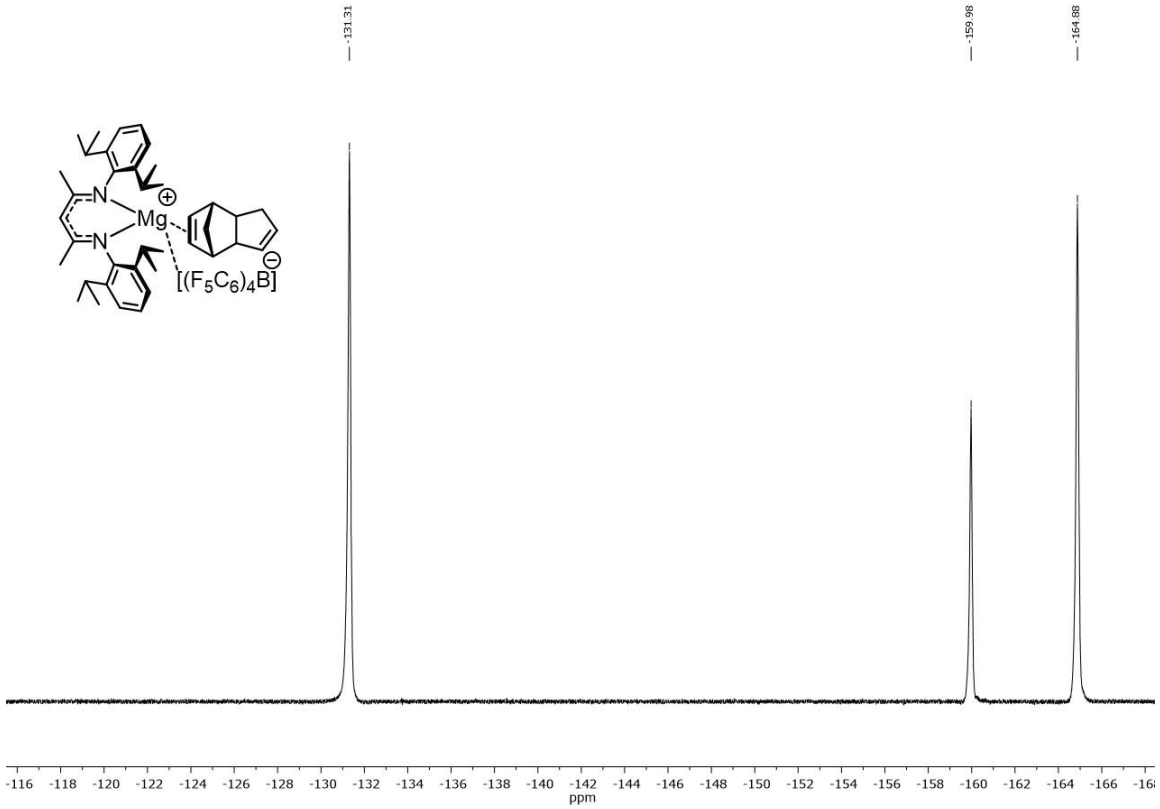

Figure S15: $^{19}F\{^{1}H\}$ NMR spectrum (565 MHz, 298 K) of [(BDI)Mg^{+}·*dcpd*][$B(C_6F_5)_4^{-}$] in C_6D_5Br.

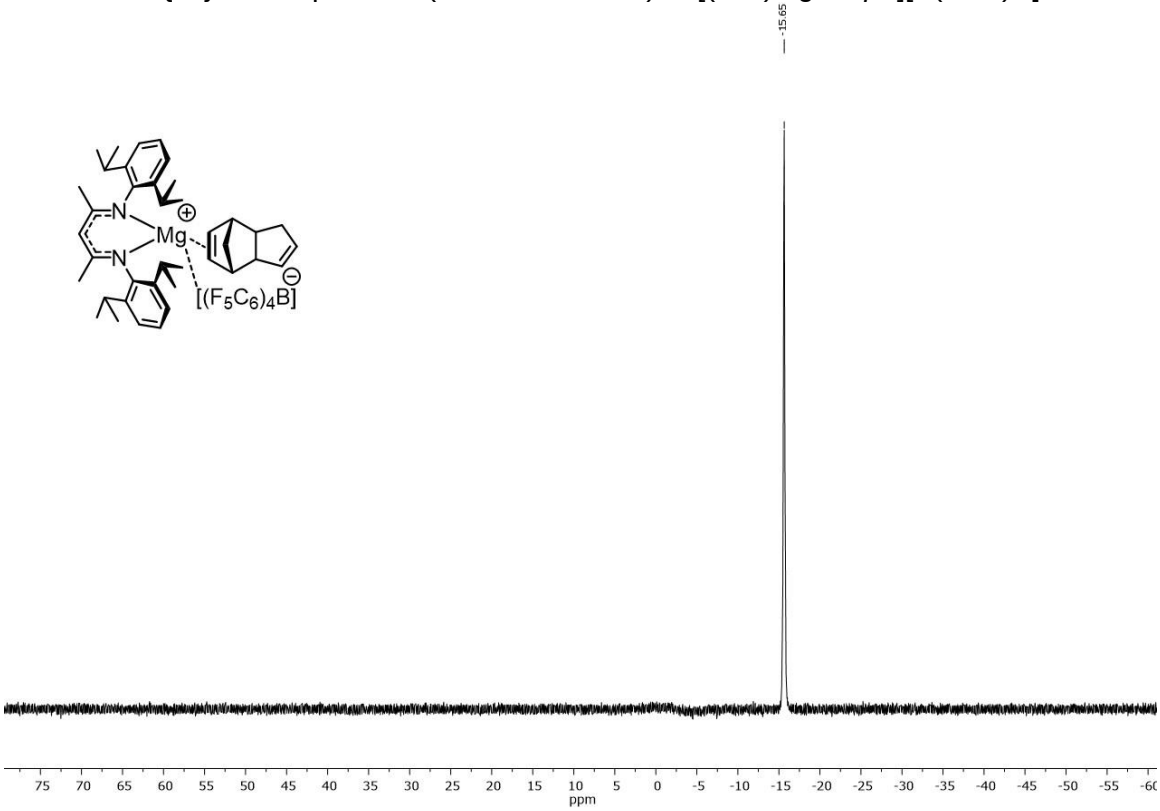

Figure S16: $^{11}B\{^{1}H\}$ NMR spectrum (565 MHz, 298 K) of [(BDI)Mg^{+}·*dcpd*][$B(C_6F_5)_4^{-}$] in C_6D_5Br.

1.3.6 Spectra of [(BDI)Mg^{+}·*nbd*][Al(OC(CF$_3$)$_3$)$_4^{-}$]

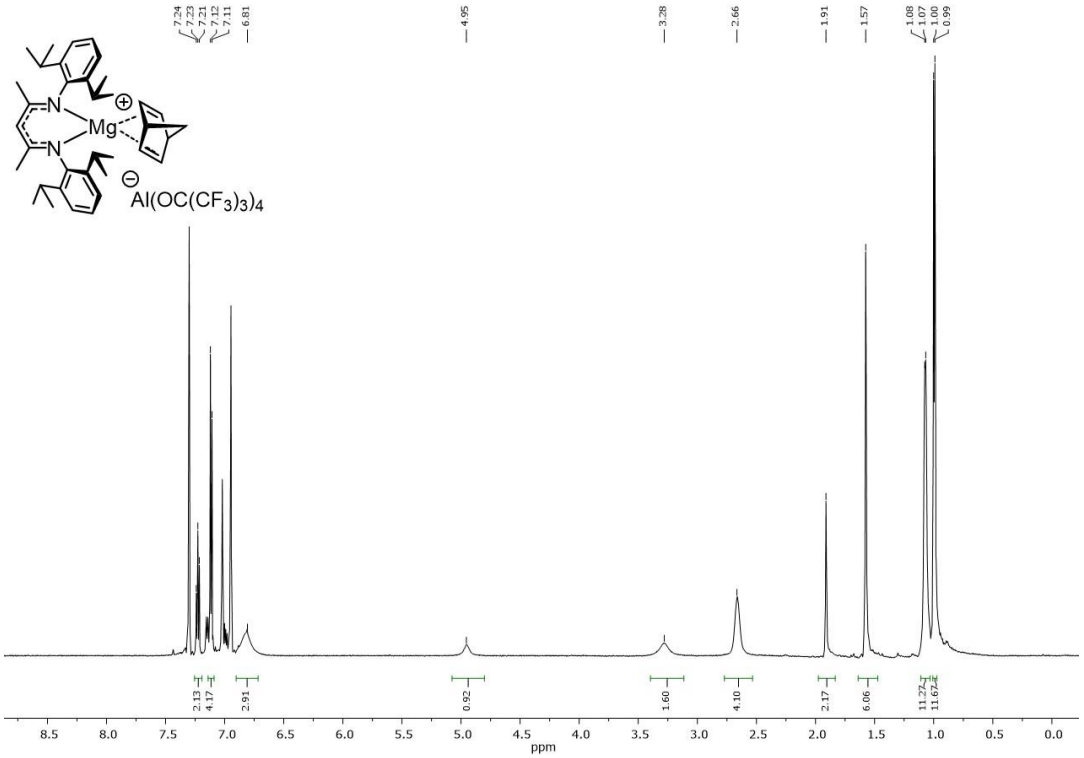

Figure S17: ^{1}H NMR spectrum (600 MHz, 298 K) of [(BDI)Mg^{+}·*nbd*][Al(OC(CF$_3$)$_3$)$_4^{-}$] in C_6D_5Br.

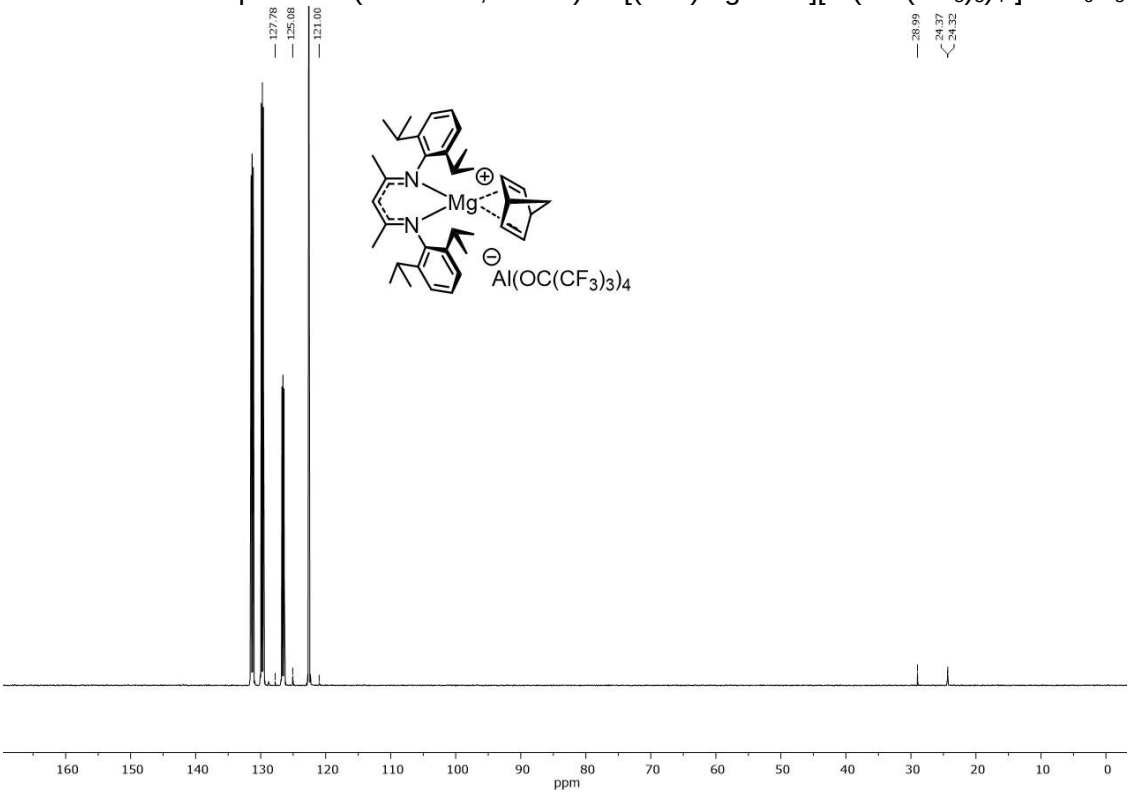

Figure S18: $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, 298 K) of [(BDI)Mg^{+}·*nbd*][Al(OC(CF$_3$)$_3$)$_4^{-}$] in C_6D_5Br.

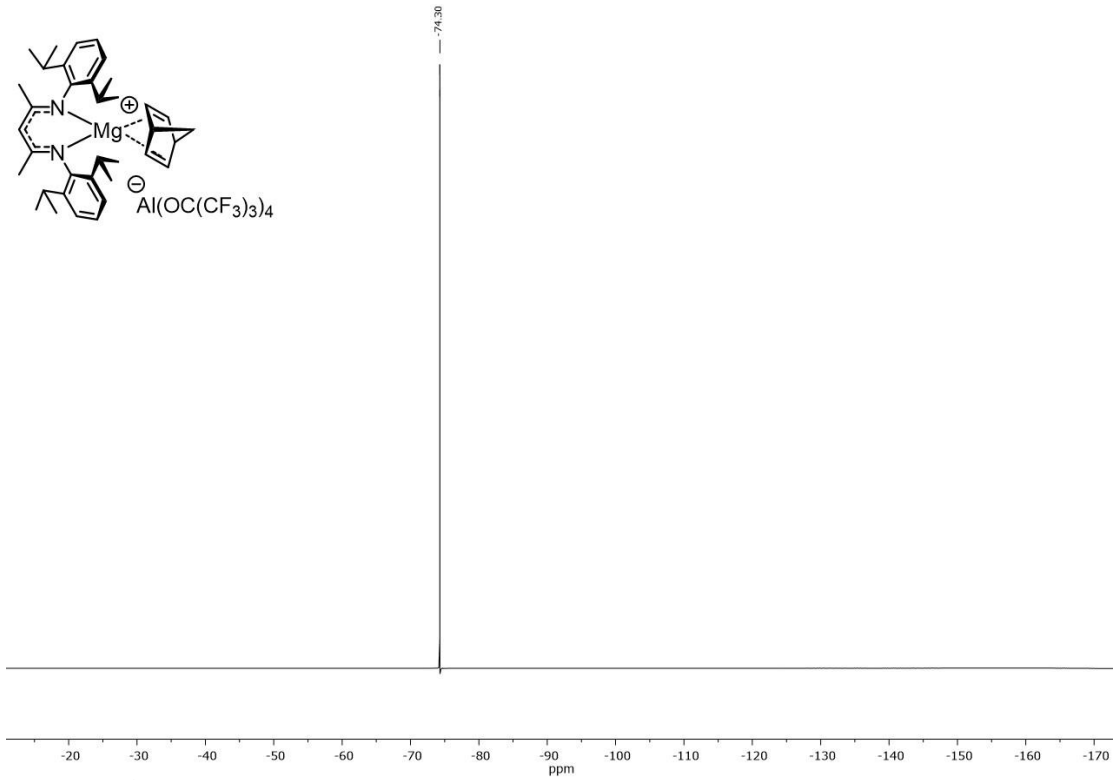

Figure S19: $^{19}F\{^{1}H\}$ NMR spectrum (376 MHz, 298 K) of [(BDI)Mg^{+}·*nbd*][$Al(OC(CF_3)_3)_4^{-}$] in C_6D_5Br.

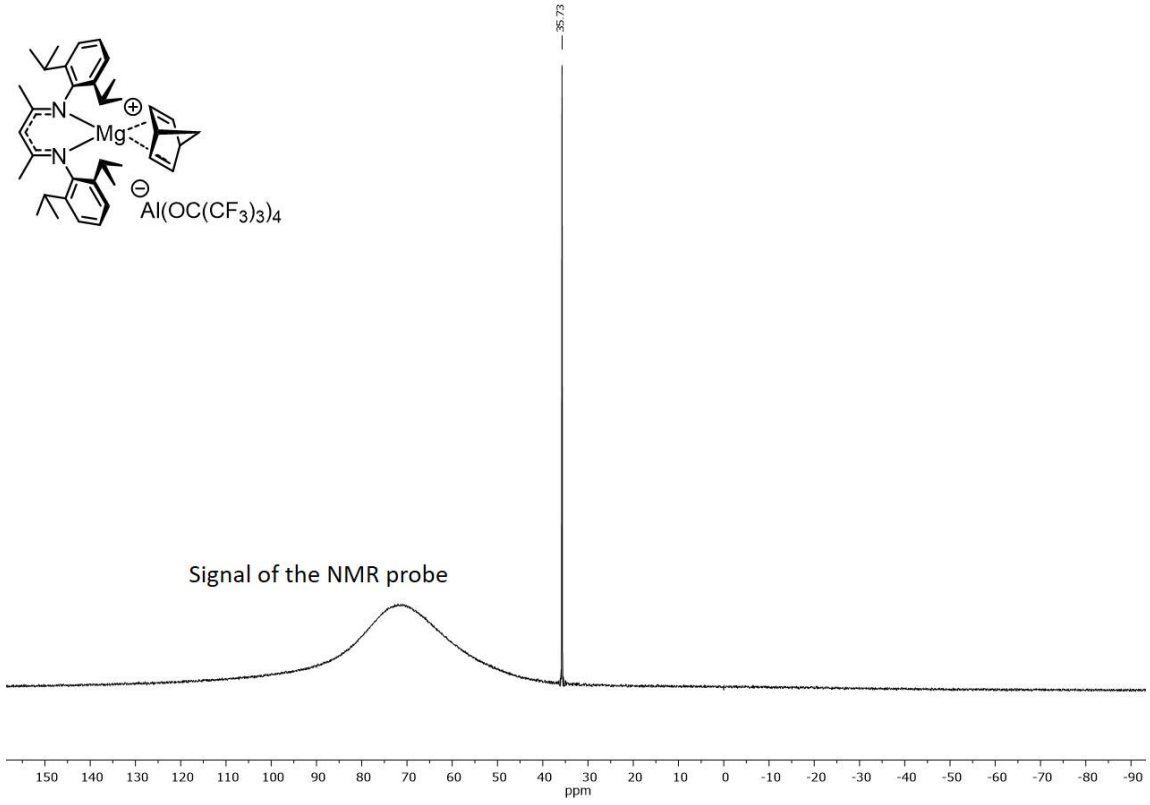

Figure S20: $^{27}Al\{^{1}H\}$ NMR spectrum (156 MHz, 298 K) of [(BDI)Mg^{+}·*nbd*][$Al(OC(CF_3)_3)_4^{-}$] in C_6D_5Br.

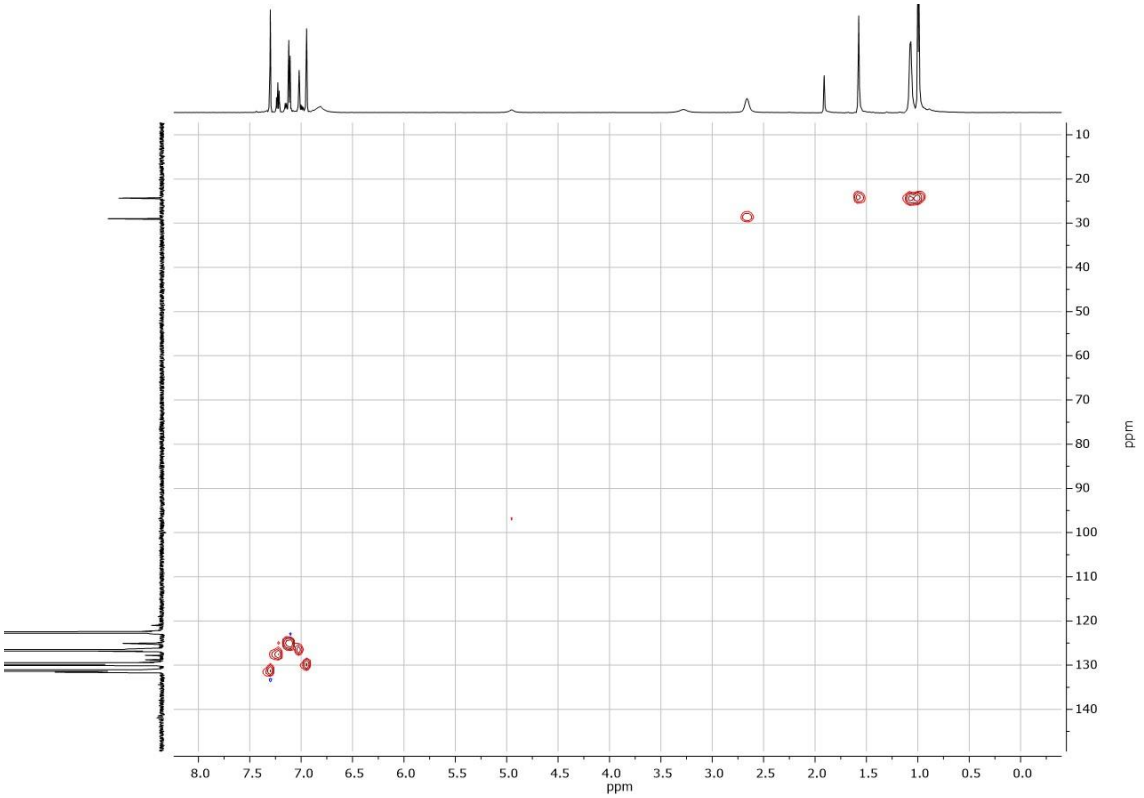

Figure S21: 2-dimensional HSQC spectrum of [(BDI)Mg^{+}·*nbd*][$Al(OC(CF_3)_3)_4^{-}$] in C_6D_5Br.

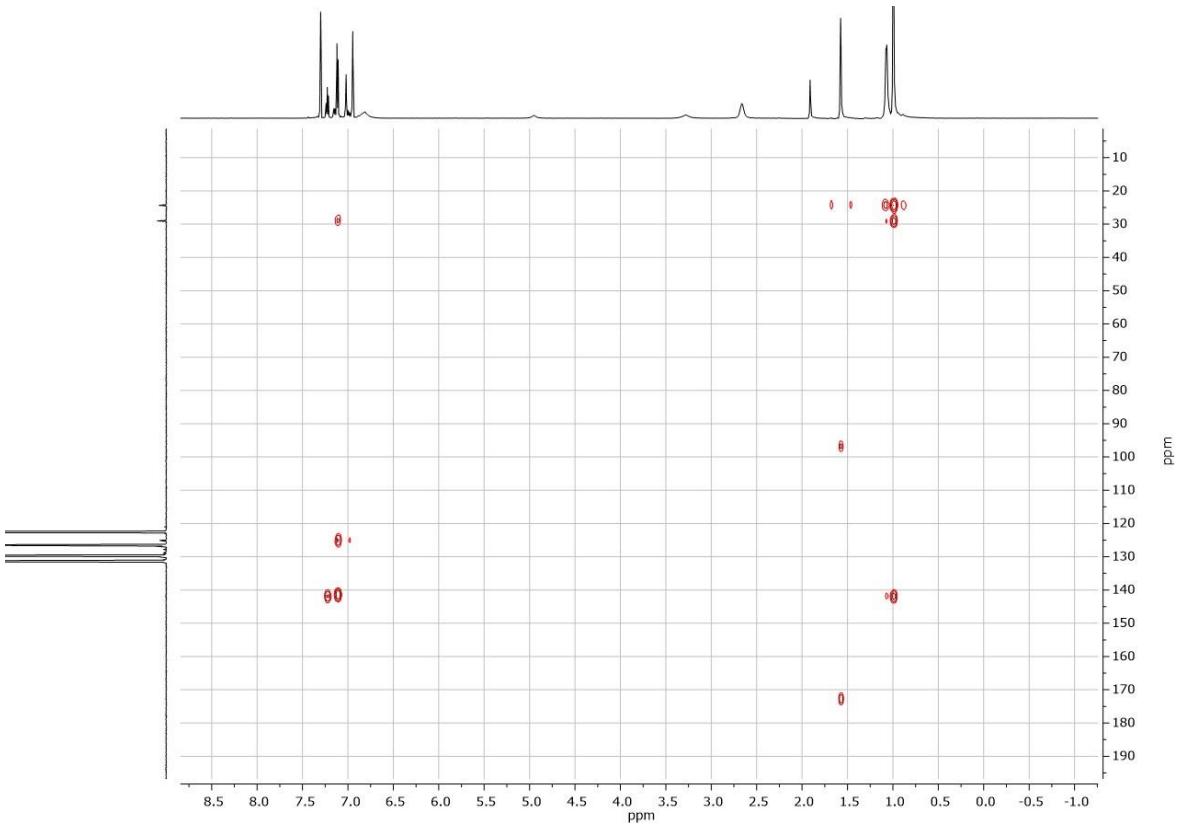

Figure S22: 2-dimensional HMBC spectrum of [(BDI)Mg^{+}·*nbd*][$Al(OC(CF_3)_3)_4^{-}$] in C_6D_5Br.

1.3.7 Spectra of $[(BDI)Mg^{+}\cdot C_6H_6][Al(OC(CF_3)_3)_4^{-}]$

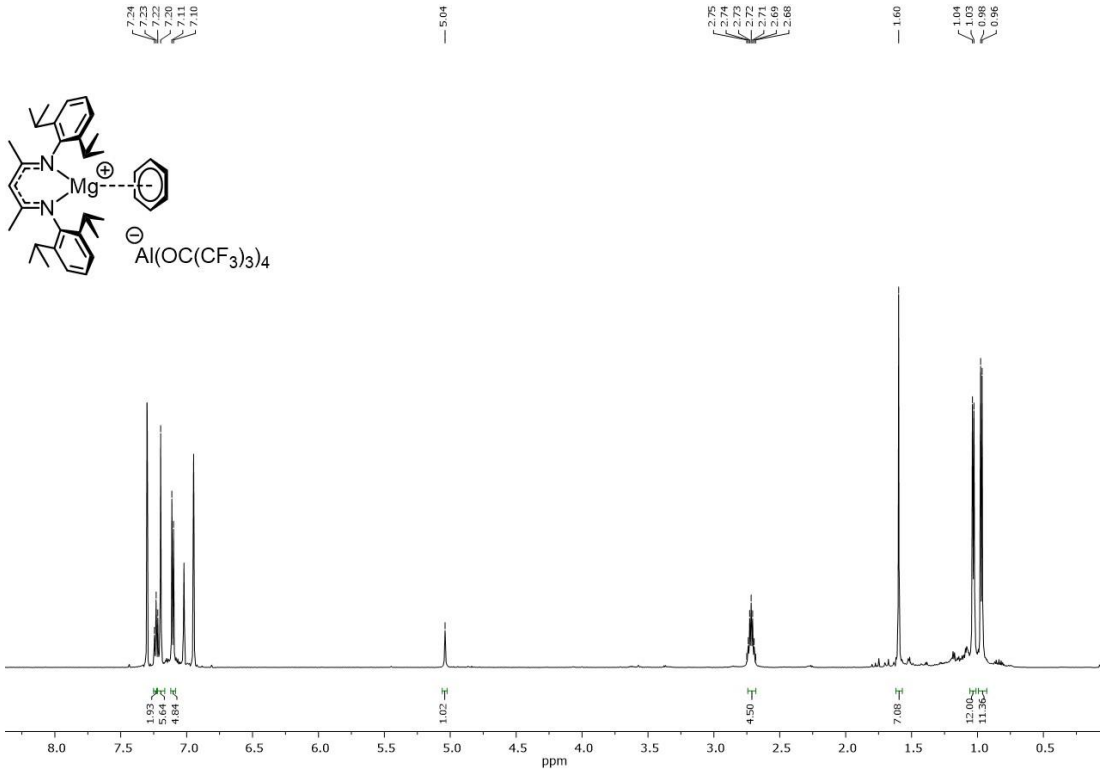

Figure S23: ^{1}H NMR spectrum (400 MHz, 298 K) of $[(BDI)Mg^{+}\cdot C_6H_6][Al(OC(CF_3)_3)_4^{-}]$ in C_6D_5Br.

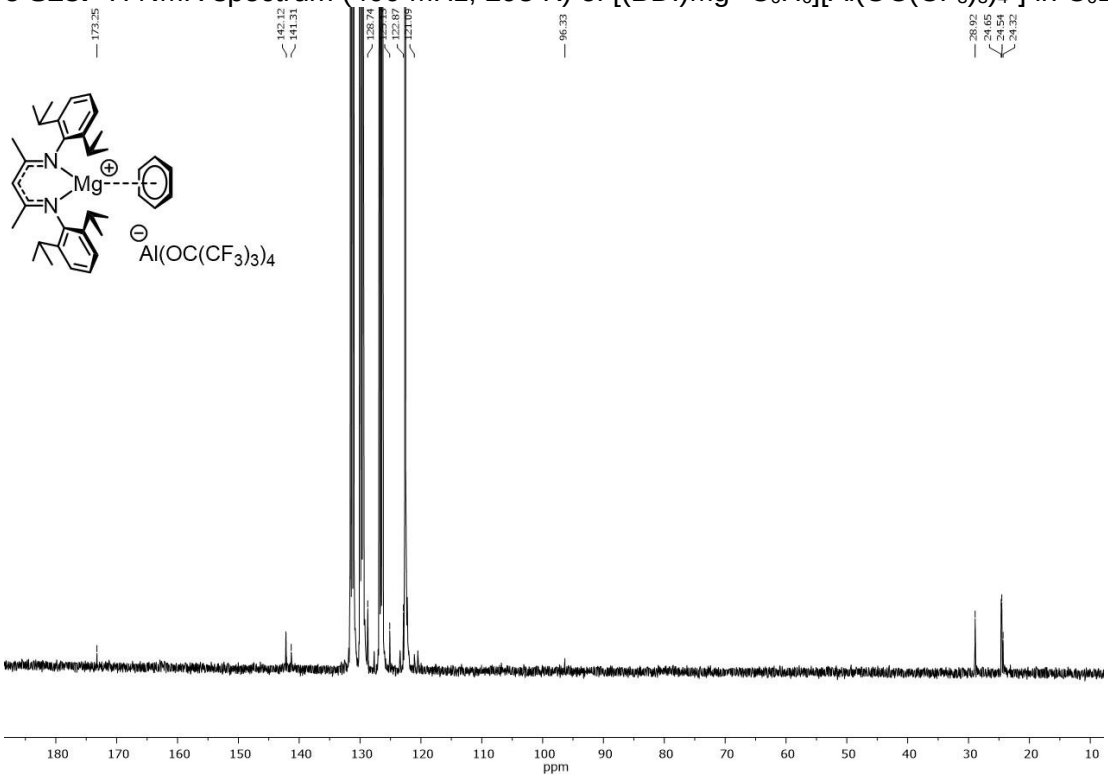

Figure S24: $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K) of $[(BDI)Mg^{+}\cdot C_6H_6][Al(OC(CF_3)_3)_4^{-}]$ in C_6D_5Br.

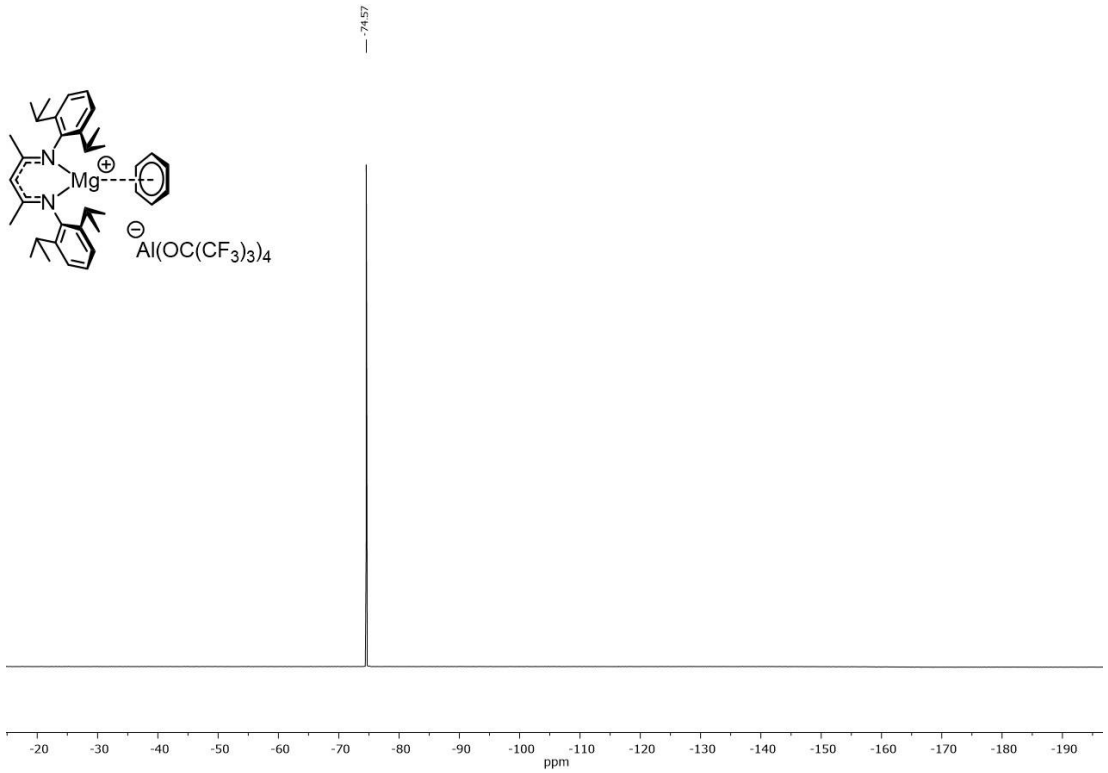

Figure S25: $^{19}F\{^{1}H\}$ NMR spectrum (376 MHz, 298 K) of $[(BDI)Mg^{+}\cdot C_6H_6][Al(OC(CF_3)_3)_4^{-}]$ in C_6D_5Br.

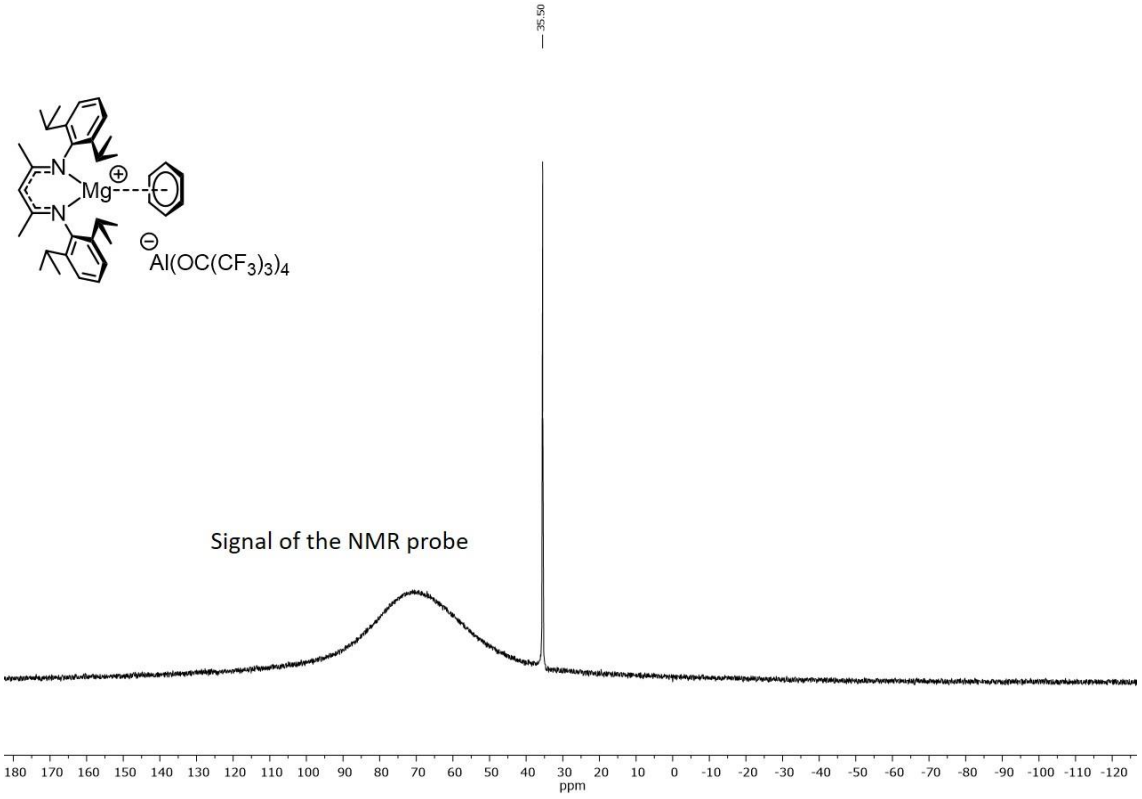

Figure S26: $^{27}Al\{^{1}H\}$ NMR spectrum (104 MHz, 298 K) of $[(BDI)Mg^{+}\cdot C_6H_6][Al(OC(CF_3)_3)_4^{-}]$ in C_6D_5Br.

1.3.8 Spectra of $[(BDI)Mg(Cp)Mg(BDI)^+][Al(OC(CF_3)_3)_4^-]$

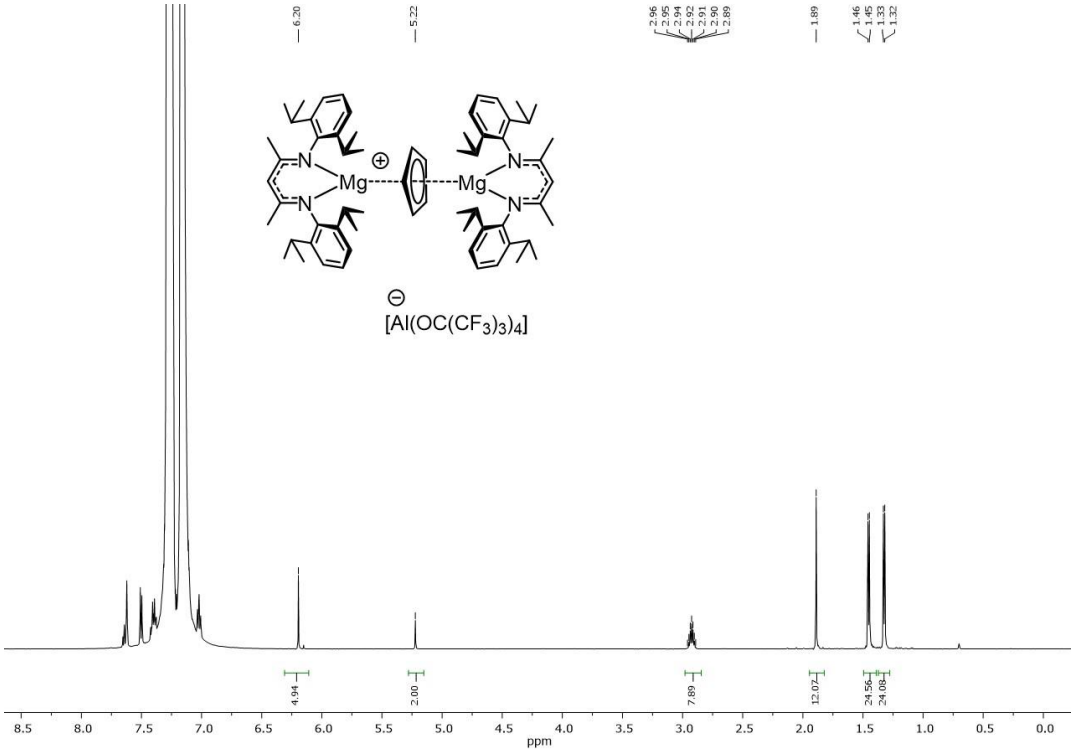

Figure S27: ^{1}H NMR spectrum (400 MHz, 298 K) $[(BDI)Mg(Cp)Mg(BDI)^+][Al(OC(CF_3)_3)_4^-]$ in $C_6H_4F_2/C_6D_6$.

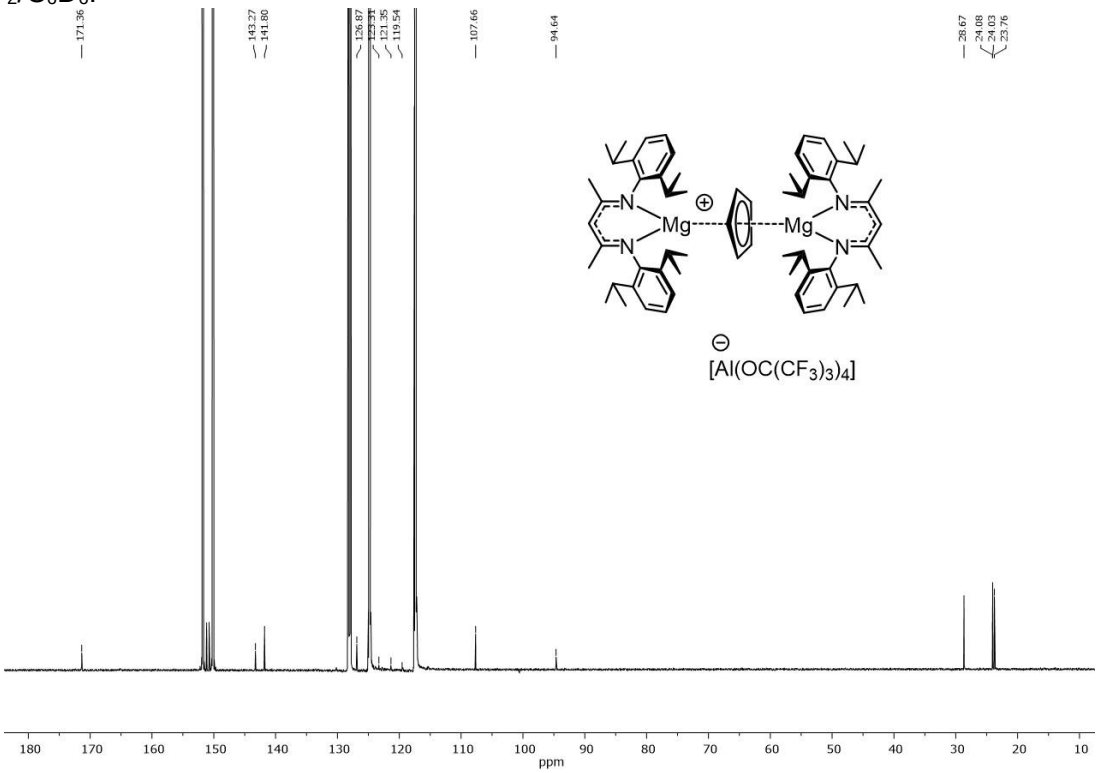

Figure S28: $^{13}C\{^1H\}$ NMR spectrum (151 MHz, 298 K) of $[(BDI)Mg(Cp)Mg(BDI)^+][Al(OC(CF_3)_3)_4^-]$ in $C_6H_4F_2/C_6D_6$.

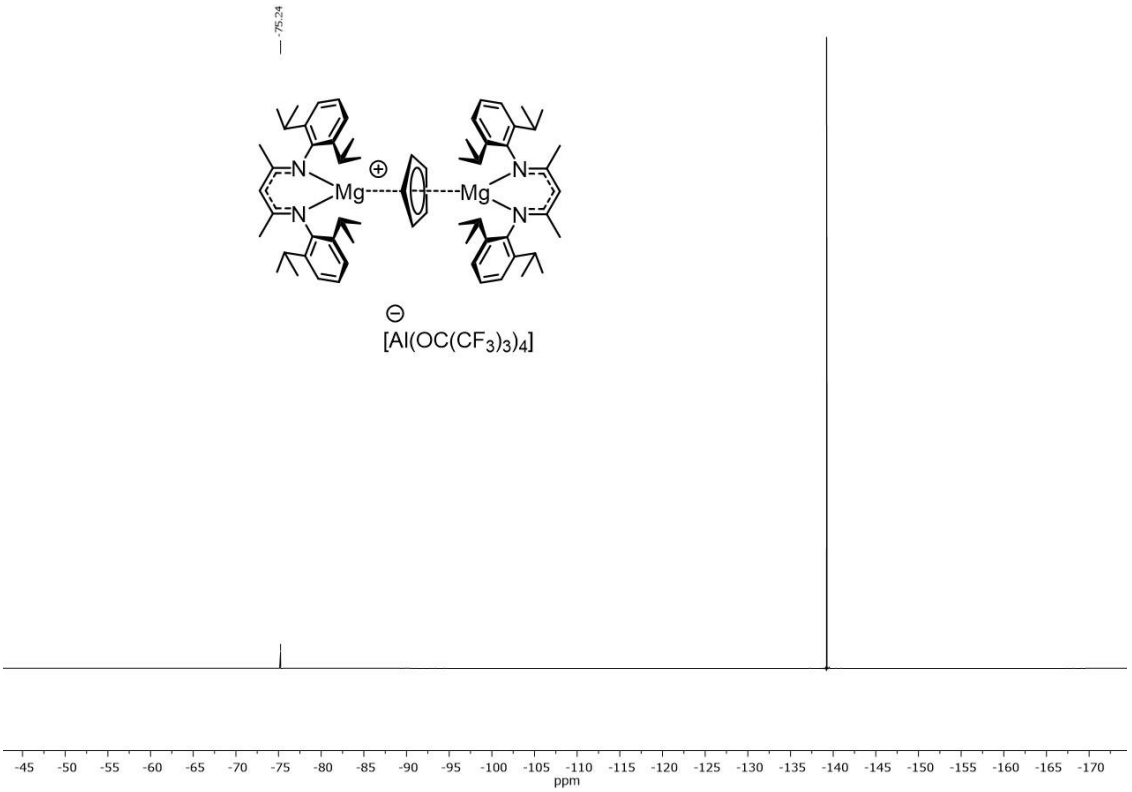

Figure S29: $^{19}F\{^{1}H\}$ NMR spectrum (565 MHz, 298 K) of $[(BDI)Mg(Cp)Mg(BDI)^{+}][Al(OC(CF_3)_3)_4^{-}]$ in $C_6H_4F_2/C_6D_6$.

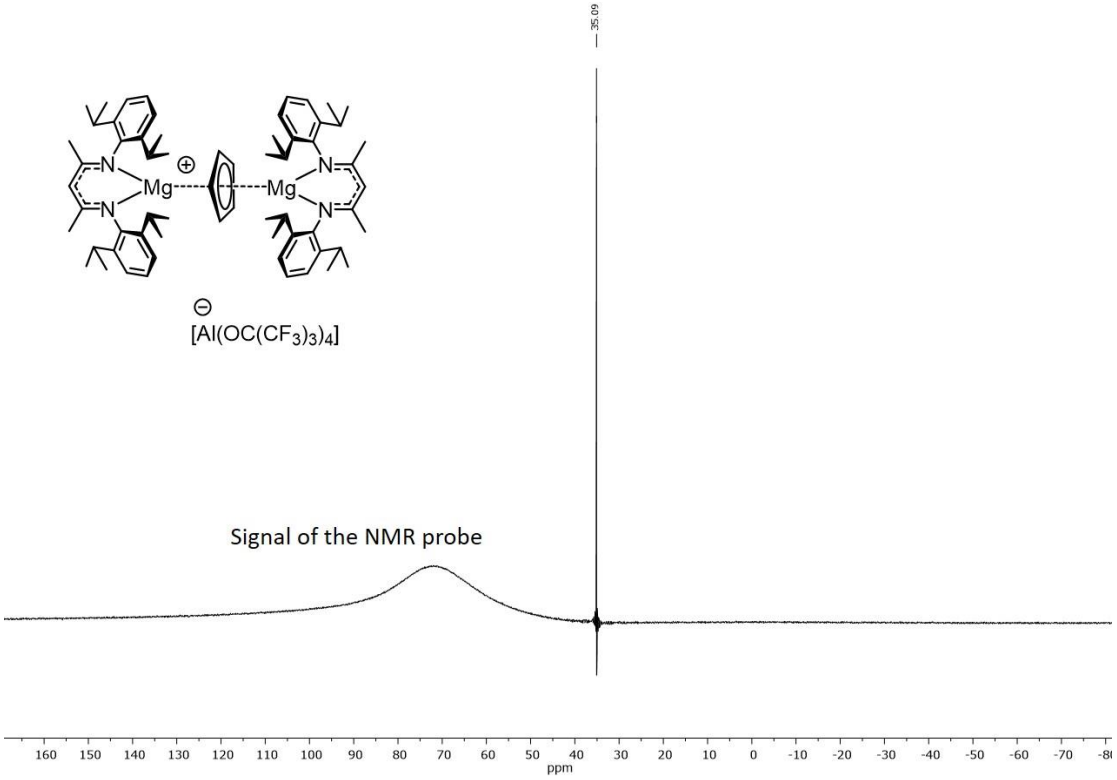

Figure S30: $^{27}Al\{^{1}H\}$ NMR spectrum (156 MHz, 298 K) of $[(BDI)Mg(Cp)Mg(BDI)^{+}][Al(OC(CF_3)_3)_4^{-}]$ in $C_6H_4F_2/C_6D_6$.

1.4 Spectra for *retro*-Diels-Alder reaction of [(BDI)Mg$^+$(*nbd*)][B(C$_6$F$_5$)$_4^-$]

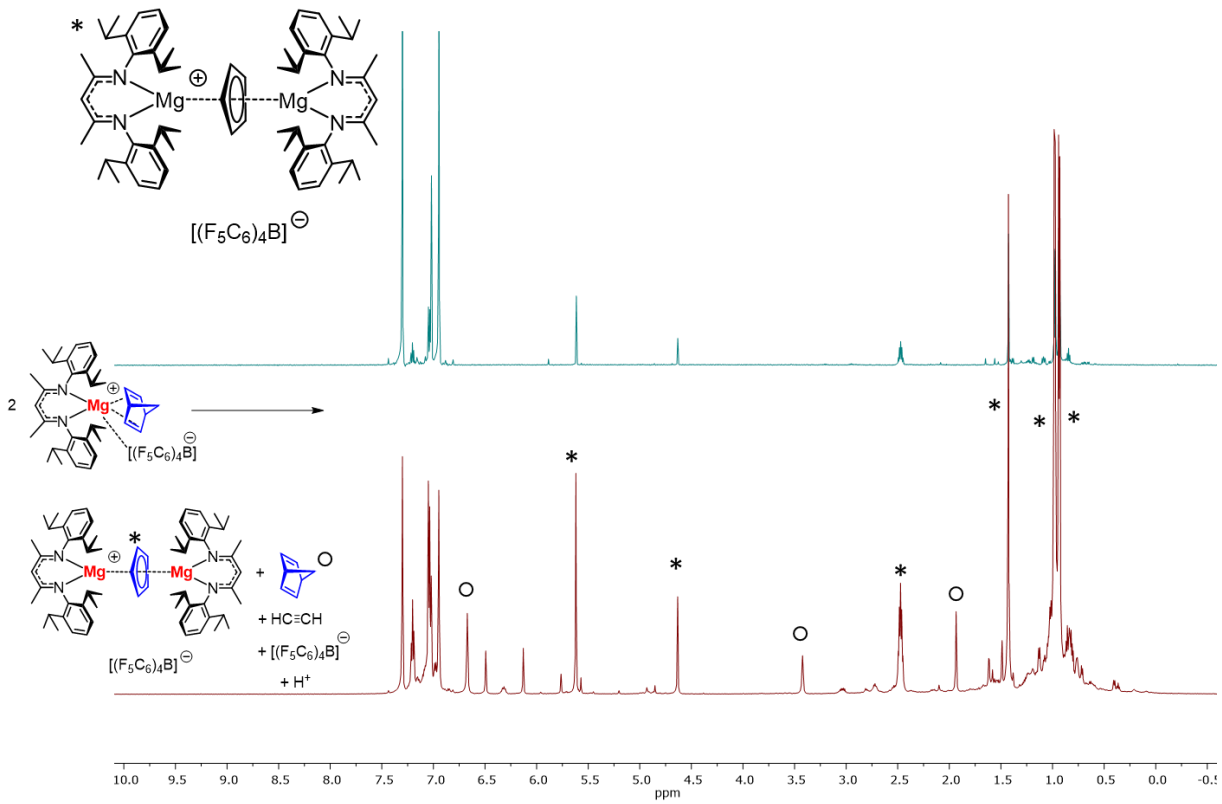

Figure S31: ^{1}H NMR spectrum of [(BDI)Mg(Cp)Mg(BDI)$^+$][B(C$_6$F$_5$)$_4^-$] (top) and *in situ* ^{1}H NMR spectrum of [(BDI)Mg(Cp)Mg(BDI)$^+$][B(C$_6$F$_5$)$_4^-$] after storing sample of [(BDI)Mg$^+$(*nbd*)][B(C$_6$F$_5$)$_4^-$] at room temperature under inert atmosphere for 14 days (bottom), solvent: C$_6$D$_5$Br.

1.5 Spectra for *retro*-Diels-Alder reaction of [(BDI)Mg$^+$(*nbd*)][Al(OC(CF$_3$)$_3$)$_4^-$]

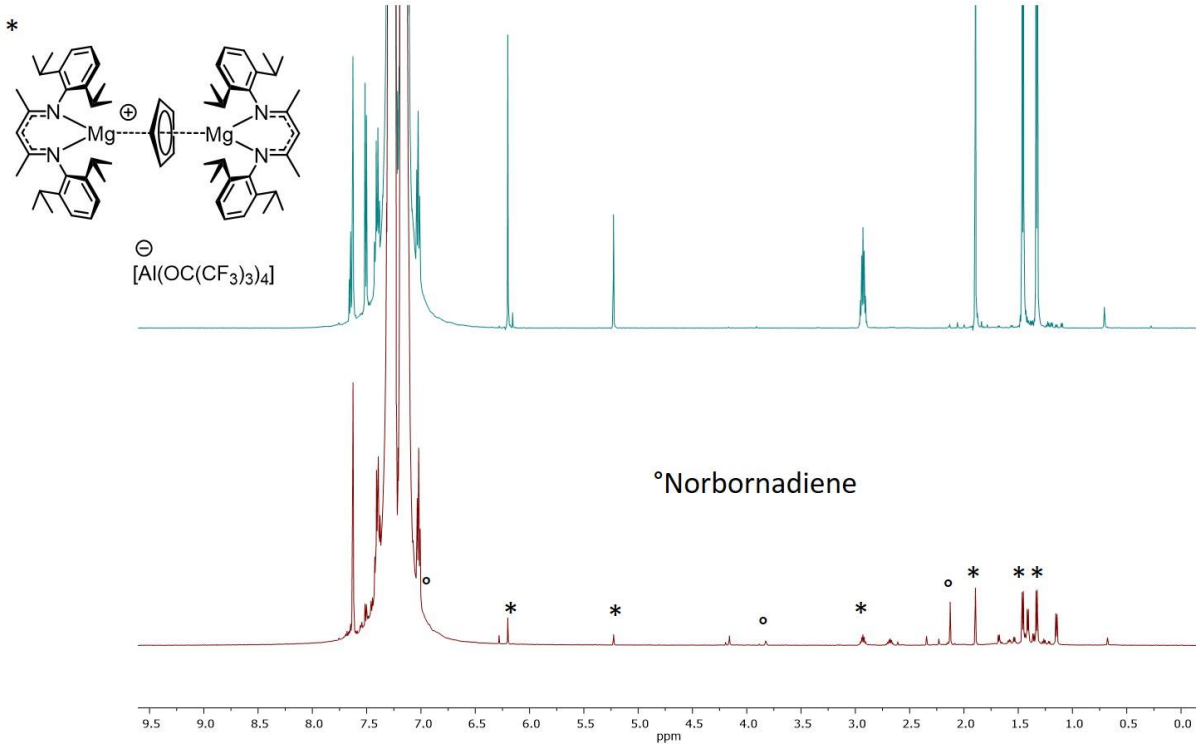

Figure S32: ^{1}H NMR spectrum of [(BDI)Mg(Cp)Mg(BDI)$^+$][Al(OC(CF$_3$)$_3$)$_4^-$] (top) and *in situ* ^{1}H NMR spectrum of [(BDI)Mg(Cp)Mg(BDI)$^+$][Al(OC(CF$_3$)$_3$)$_4^-$] after crystallization attempt of [(BDI)Mg$^+$(*nbd*)][Al(OC(CF$_3$)$_3$)$_4^-$] from [(BDI)Mg(*n*Bu)]$_2$, [Ph$_3$C$^+$][Al(OC(CF$_3$)$_3$)$_4^-$] and *nbd* at room temperature under inert atmosphere for 21 days (bottom), solvent: C$_6$H$_4$F$_2$/C$_6$D$_6$ (400/200 µL).

1.6 Single Crystal X-Ray Diffraction

1.6.1 Structure determination of [(BDI)Mg^{+}·*nbd*][$B(C_6F_5)_4^{-}$]

A colorless crystal of compound [(BDI)Mg^{+}·*nbd*][$B(C_6F_5)_4^{-}$] 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 (v40.18b) software package.[S7] Using Olex2,[S9] the structure was solved with the ShelXT[S10] structure solution program using Intrinsic Phasing and refined with the ShelXL[S11] refinement package using Least Squares minimization. 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 positions of the hydrogen atoms at C1, C2, C4 and C5 (*nbd* ligand) were observed from difference Fourier maps and refined.

Additionally, voids with heavily disordered solvent (mixture of chlorobenzene/*n*-pentane) were found within the crystal. A suitable disorder model for these solvent molecules could not be built. Therefore, their contribution to the structure factors was secured by back-Fourier transformation using the solvent mask routine[S13, S14] of the program Olex2.[S9] The solvent accessible voids treated this way had a size of 1884.3 $Å^3$ (15.6% of the unit cell) and contained 407.6 electrons/unit cell. Crystallographic and refinement data are summarized in Table S1 (see below).

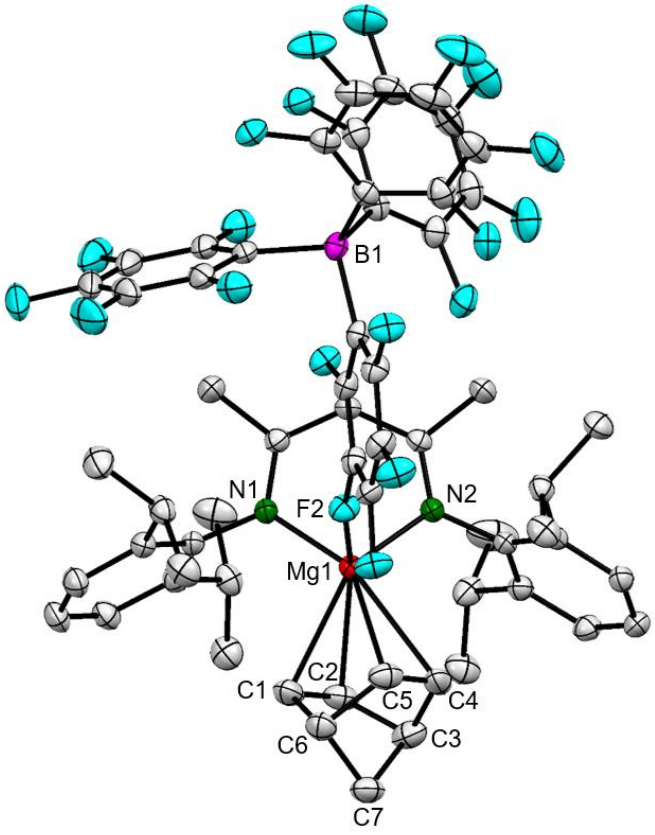

Figure S33: ORTEP representation of [(BDI)Mg^{+}·*nbd*][$B(C_6F_5)_4^{-}$] (probability level 50%). Hydrogen atoms were omitted for clarity.

1.6.2 Structure determination of [(BDI)Mg(Cp)]

A colorless crystal of compound [(BDI)Mg(Cp)] 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 (v38.46) software package.[S7] Using Olex2,[S9] the structure was solved with the ShelXT[S10] structure solution program using Intrinsic Phasing and refined with the ShelXL[S11] 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.

Rotational disorder of one methyl group was observed and modeled. The relative occupancies of the two alternative orientations were refined to 0.67(3) and 0.33(3), respectively. Crystallographic and refinement data are summarized in Table S1 (see below).

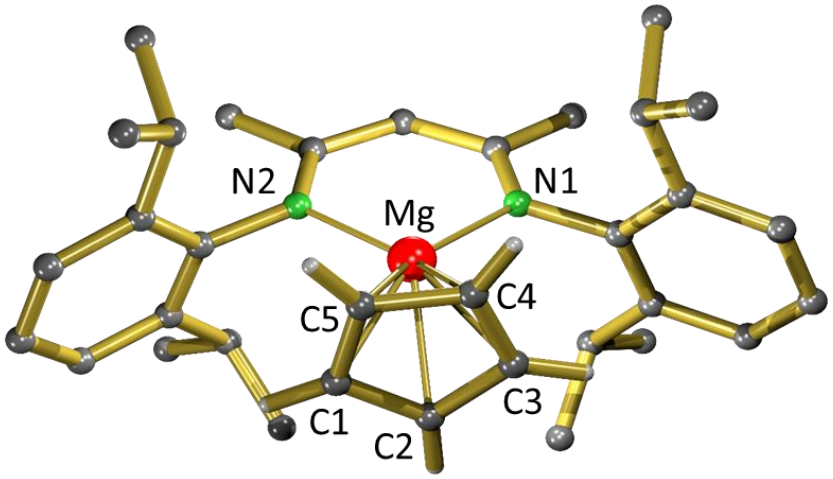

Figure S34: Crystal structure of [(BDI)Mg(Cp)]. Hydrogen atoms omitted for clarity, except hydrogen atoms at double bonds. Selected bond length (Å) and angles (°): Mg–C1 2.3788(17), Mg–C2 2.3589(17), Mg–C3 2.3622(17), Mg–C4 2.3729(18), Mg–C5 2.3821(17), Mg–$C^{centroid}$ 2.0463(9), Mg–N1 2.0410(14), Mg–N2 2.0403(14), C1=C2 1.414(2), C2=C3 1.409(3), C3=C4 1.409(3), C4=C5 1.409(3), C5=C1 1.401(3), N–Mg–N 94.68(6).

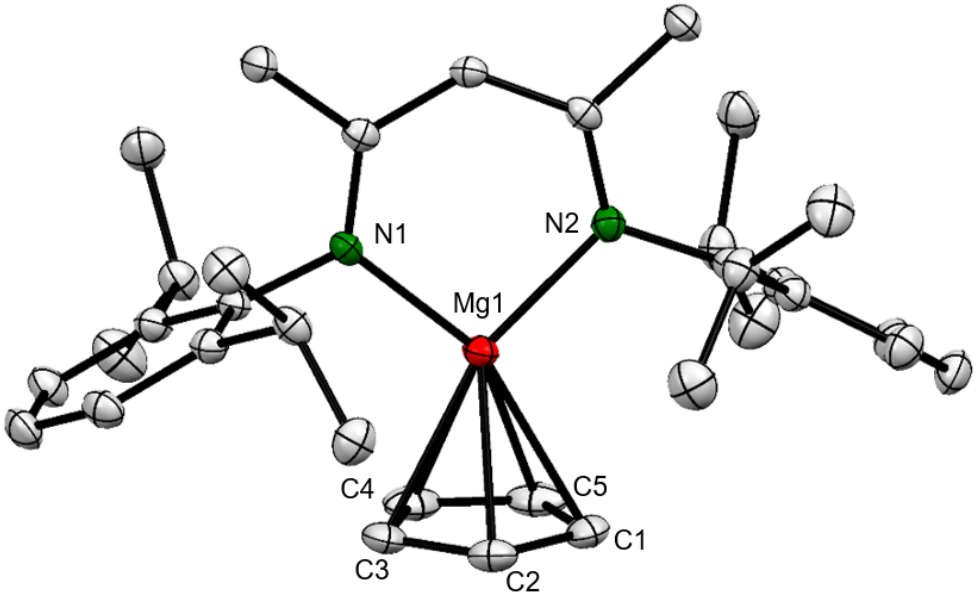

Figure S35: ORTEP representation of [(BDI)Mg(Cp)] (probability level 50%). Hydrogen atoms were omitted for clarity.

1.6.3 Structure determination of [(BDI)Mg(Cp)Mg(BDI)$^+$][B(C_6F_5)$_4^-$]

A colorless crystal of compound [(BDI)Mg(Cp)Mg(BDI)$^+$][B(C_6F_5)$_4^-$] 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 (v39.46) software package.[S6] The X-ray diffraction pattern obtained shows the presence of weak superstructure reflections. Omission of the superstructure reflections leads to a triclinic unit cell (a = 13.2113(3), b = 14.1171(3), 22.9280(6), α = 90.2656(19), β = 93.9099(19), γ = 111.280(2)). The average structure obtained in space group *P*-1 is chemically reasonable. However, inclusion of the superstructure reflections is preferable and the solution in the resulting supercell is reported.

Using Olex2,[S9] the structure was solved with the ShelXT[S10] structure solution program using Intrinsic Phasing and refined with the ShelXL[S11] 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 DIPP moiety, 6 additional *i*Pr groups and both Cp ligands was observed. It was modeled with the help of similarity restraints (SIMU, SADI) and rigid bond restraints (RIGU).[S12] The relative occupancies of the two alternative orientations were refined to 0.661(6)/0.339(6) (DIPP), 0.821(9)/ 0.179(9) (*i*Pr), 0.881(10)/0.119(10) (*i*Pr), 0.825(7)/0.175(7) (*i*Pr), 0.854(15)/0.146(15) (*i*Pr), 0.687(11)/0.313(11) (*i*Pr), 0.811(11)/0.189(11) (*i*Pr), 0.815(8)/0.185(8) (Cp) and 0.774(10)/0.226(10) (Cp), respectively. Crystallographic and refinement data are summarized in Table S1 (see below).

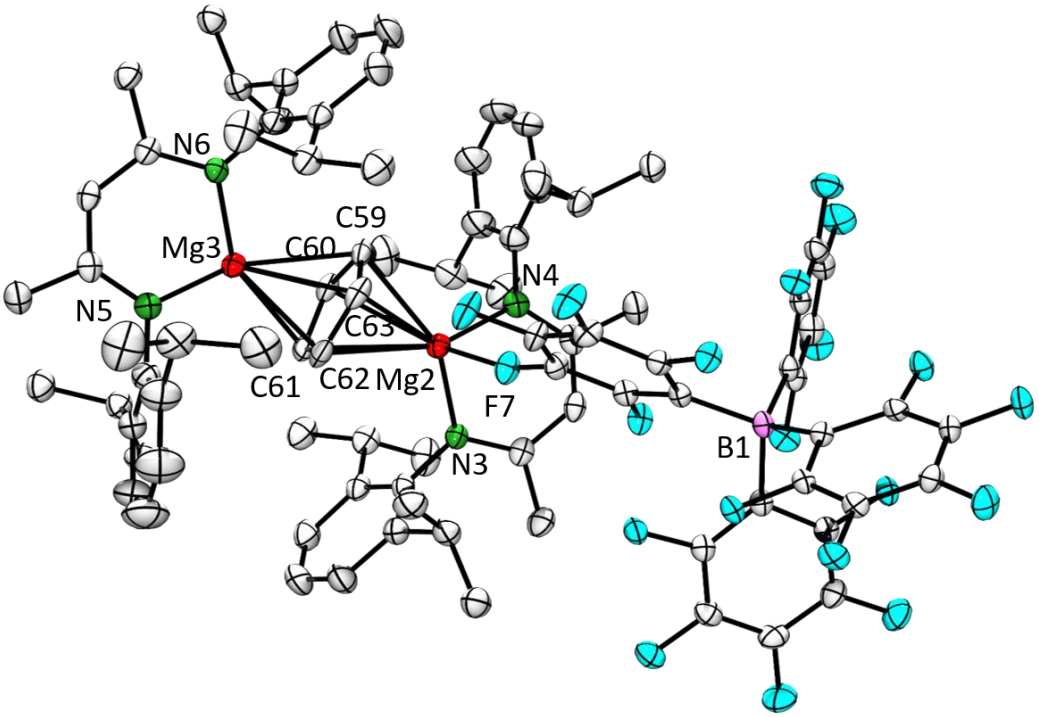

Figure S36: ORTEP representation of section from polymeric chain of [(BDI)Mg(Cp)Mg(BDI)$^{+}$][B(C_6F_5)$_4^{-}$] (probability level 50%). Hydrogen atoms were omitted for clarity. Selected bond length (Å): Mg2–C59 2.504(5), Mg2–C60 2.570(7), Mg2–C61 2.542(5), Mg2–C62 2.464(5), Mg2–C63 2.439(7), Mg2–N3 2.0115(18), Mg2–N4 2.0180(18), Mg3–C59 2.401(5), Mg3–C60 2.397(7), Mg3–C61 2.491(4), Mg3–C62 2.555(5), Mg3–C63 2.505(7), Mg3–N5 2.0210(18), Mg3–N6 2.0118(17), C59=C60 1.424(9), C60=C61 1.406(9), C61=C62 1.405(8), C62=C63 1.426(6), C63=C59 1.415(11), Mg2–F7 2.2735(13), Mg3–F22 2.2101(13).

1.6.4 Structure determination of [(BDI)Mg(C_6H_5F)(Cp)Mg(BDI)(C_6H_5F)$^{+}$][B(C_6F_5)$_4^{-}$]

A colorless crystal of compound [(BDI)Mg(C_6H_5F)(Cp)Mg(BDI)(C_6H_5F)$^{+}$][B(C_6F_5)$_4^{-}$] 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 (v38.46) software package.[S8] Using Olex2, [S9] the structure was solved with the ShelXT[S10] structure solution program using Intrinsic Phasing and refined with the ShelXL[S11] 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 fluorobenzene moiety was observed and was modeled with the help of similarity restraints (SIMU, SADI) and rigid bond restraints (RIGU).[S12] The relative occupancies of the two alternative orientations were refined to 0.528(8) and 0.472(8), respectively.

Additionally, voids with heavily disordered solvent (mixture of fluorobenzene/benzene) were found within the crystal. A suitable disorder model for these solvent molecules could not be built. Therefore, their contribution to the structure factors was secured by back-Fourier transformation using the solvent mask routine[S13-S14] of the program Olex2.[S9] The solvent accessible voids treated this way had a size of 372.0 Å^3 (7.9% of the unit cell) and contained 93.2 electrons/unit cell. Crystallographic and refinement data are summarized in Table S1 (see below).

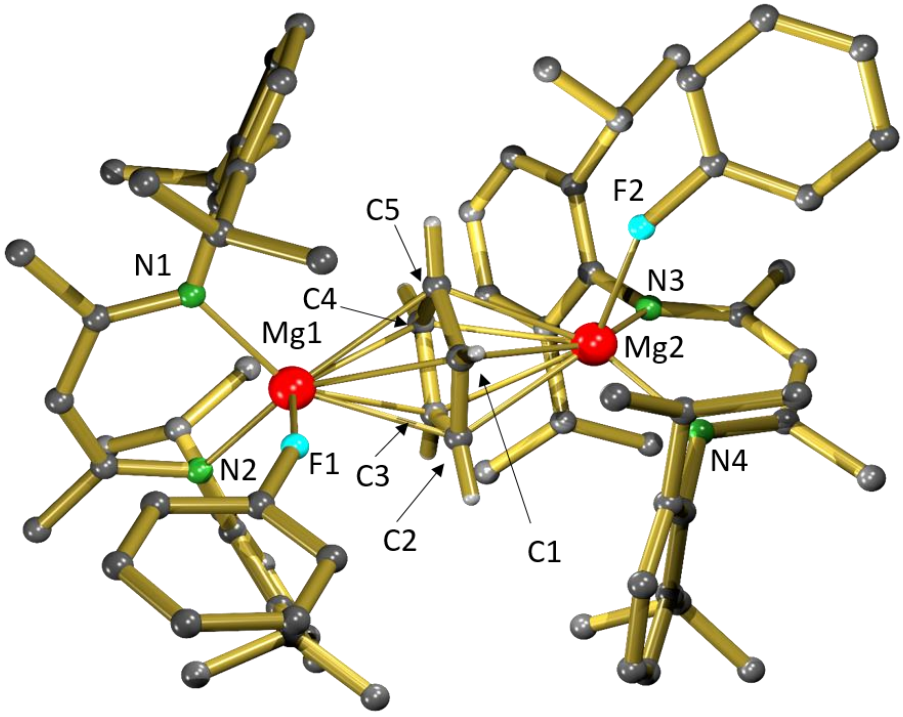

Figure S37: Crystal structure of cationic unit [(BDI)Mg(C_6H_5F)(Cp)Mg(BDI)(C_6H_5F)$^+$]. Counter anion and hydrogen atoms except hydrogen atoms at double bonds omitted for clarity. Selected bond length (Å): Mg1–C1 2.4357(16), Mg1–C2 2.4086(16), Mg1–C3 2.4820(16), Mg1–C4 2.5473(16), Mg1–C5 2.5202(16), Mg1–N1 2.0258(14), Mg1–N2 2.0199(13), Mg2–C1 2.4110(16), Mg2–C2 2.4747(16), Mg2–C3 2.5431(16), Mg2–C4 2.5255(16), Mg2–C5 2.4514(16), Mg2–N3 2.0176(13), Mg2–N4 2.0255(14), C1=C2 1.415(3), C2=C3 1.403(3), C3=C4 1.404(2), C4=C5 1.406(2), C5=C1 1.412(3), Mg1–F1 2.1861(11), Mg2–F2 2.1590(11).

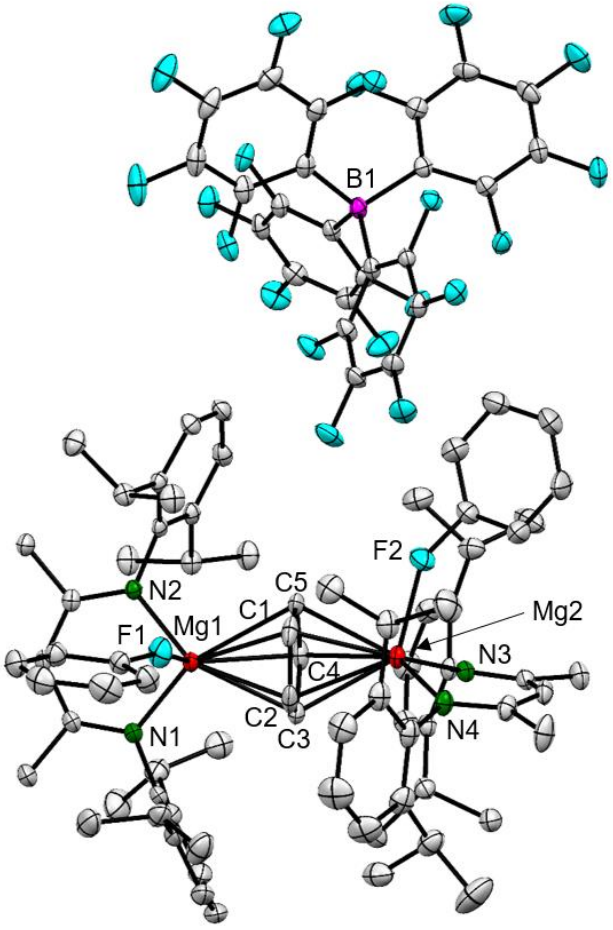

Figure S38: ORTEP representation of $[(BDI)Mg(C_6H_5F)(Cp)Mg(BDI)(C_6H_5F)^+][B(C_6F_5)_4^-]$ (probability level 50%). Hydrogen atoms were omitted for clarity.

1.6.5 Structure determination of $[(BDI\text{-}H)Mg^+(Cp)][B(C_6F_5)_4^-]$

A colorless crystal of compound $[(BDI\text{-}H)Mg^+(Cp)][B(C_6F_5)_4^-]$ 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 (v40.18b) software package.[S7] Using Olex2,[S9] the structure was solved with the ShelXT[S10] structure solution program using Intrinsic Phasing and refined with the ShelXL[S11] 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 the Cp ligand was observed, and was modeled with the help of similarity restraints (SIMU, SADI) and rigid bond restraints (RIGU).[S12] The relative occupancies of the two alternative

orientations were refined to 0.68(3) and 0.32(3), respectively. Crystallographic and refinement data are summarized in Table S1 (see below).

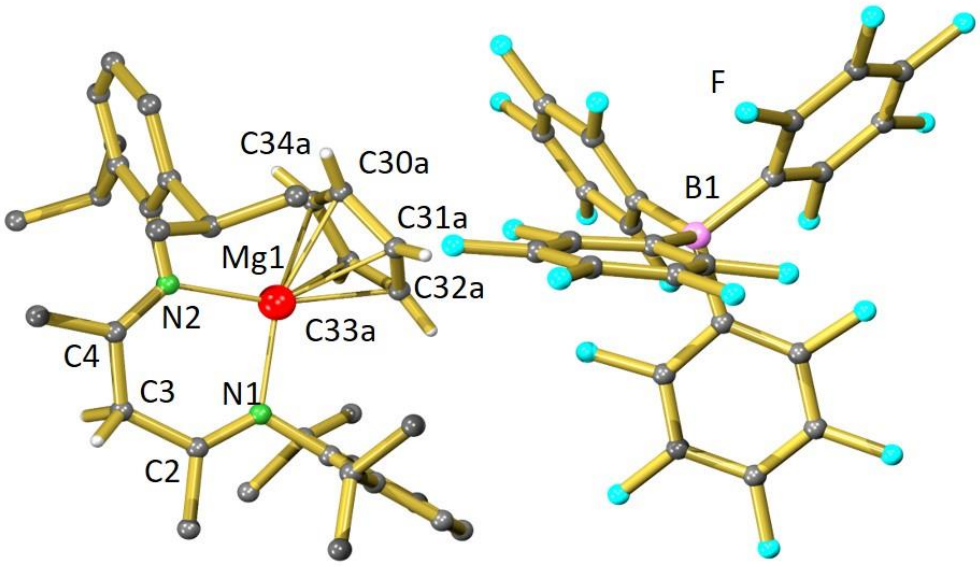

Figure S39: Crystal structure of [(BDI-H)Mg^{+}(Cp)][$B(C_6F_5)_4^{-}$]. Hydrogen atoms omitted for clarity, except hydrogen atoms at double bonds. Selected bond length (Å) and angles (°): Mg1–C30a 2.44(3), Mg1–C31a 2.35(4), Mg1–C32a 2.26(3), Mg1–C33a 2.264(13), Mg1–C34a 2.38(2), Mg1–N1 2.0813(16), Mg1–N2 2.0923(15), C30a=C31a 1.38(13), C31a=C32a 1.399(13), C32a=C33a 1.396(12), C33a=C34a 1.391(10), C34a=C30a 1.387(13), C2–C3 1.506(2), C3–C4 1.507(2), N–Mg–N 91.51(6).

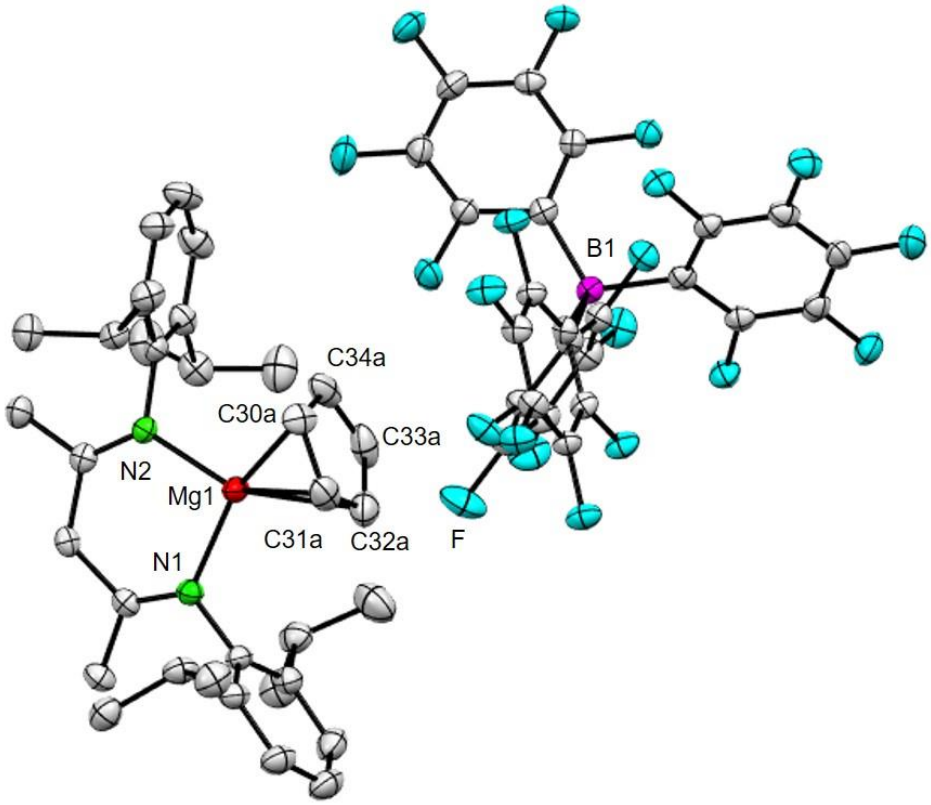

Figure S40: ORTEP representation of [(BDI-H)Mg^{+}(Cp)][$B(C_6F_5)_4^{-}$] (probability level 50%). Hydrogen atoms were omitted for clarity.

1.6.6 Structure determination of [(BDI)Mg^{+}·*dcpd*][$B(C_6F_5)_4^{-}$]

A colorless crystal of compound [(BDI)Mg^{+}·*dcpd*][$B(C_6F_5)_4^{-}$] 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.[S15] Using Olex2,[S9] the structure was solved with the ShelXT[S10] structure solution program using Intrinsic Phasing and refined with the ShelXL[S11] refinement package using Least Squares minimization. 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 positions of the hydrogen atom at C30 and C31 were observed from difference Fourier maps and refined.

Disorder within the *dcpd* ligand was observed, and was modeled with the help of similarity restraints (SIMU, SADI) and rigid bond restraints (RIGU).[S12] The relative occupancies of the two alternative orientations were refined to 0.59(2) and 0.41(2), respectively. Crystallographic and refinement data are summarized in Table S1 (see below).

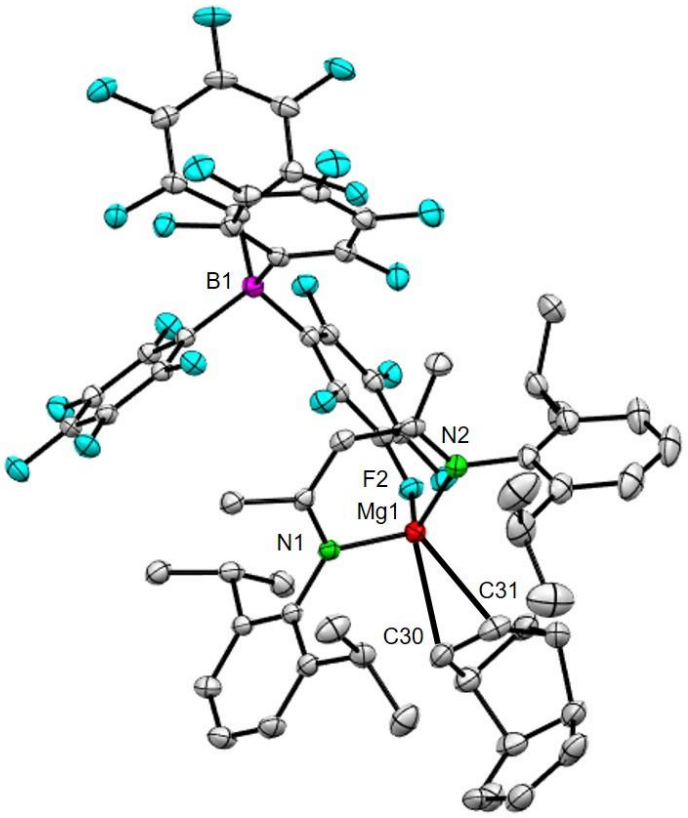

Figure S41: ORTEP representation of [(BDI)Mg^{+}·*dcpd*][$B(C_6F_5)_4^-$] (probability level 50%). Hydrogen atoms were omitted for clarity.

1.6.7 Structure determination of [(BDI)Mg(Cp)Mg(BDI)$^+$][$Al(OC(CF_3)_3)_4^-$]

A colorless crystal of compound [(BDI)Mg(Cp)Mg(BDI)$^+$][$Al(OC(CF_3)_3)_4^-$] 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.[S7] Using Olex2,[S9] the structure was solved with the ShelXT[S10] structure solution program using Intrinsic Phasing and refined with the ShelXL[S11] 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 *i*Pr group, one $C(CF_3)_3$ group und three additional CF_3 groups was observed. It was modeled with the help of similarity restraints (SIMU, SADI). The relative occupancies of the two alternative orientations were refined to 0.827(15)/0.173(15) (*i*Pr), 0.895(5)/0.105(5) ($C(CF_3)_3$), 0.735(17)/0.265(17) (CF_3), 0.72(3)/0.28(3) (CF_3) and 0.749(17)/0.251(17) (CF_3), respectively.

Additionally, the crystal under investigation suffered from twinning by pseudo-merohedry (twin law -1 0 0 / 0 -1 0 / 0 0 1). The fractional contributions of the two twin domains were refined to 0.8784(9) and 0.1216(9). Crystallographic and refinement data are summarized in Table S1 (see below).

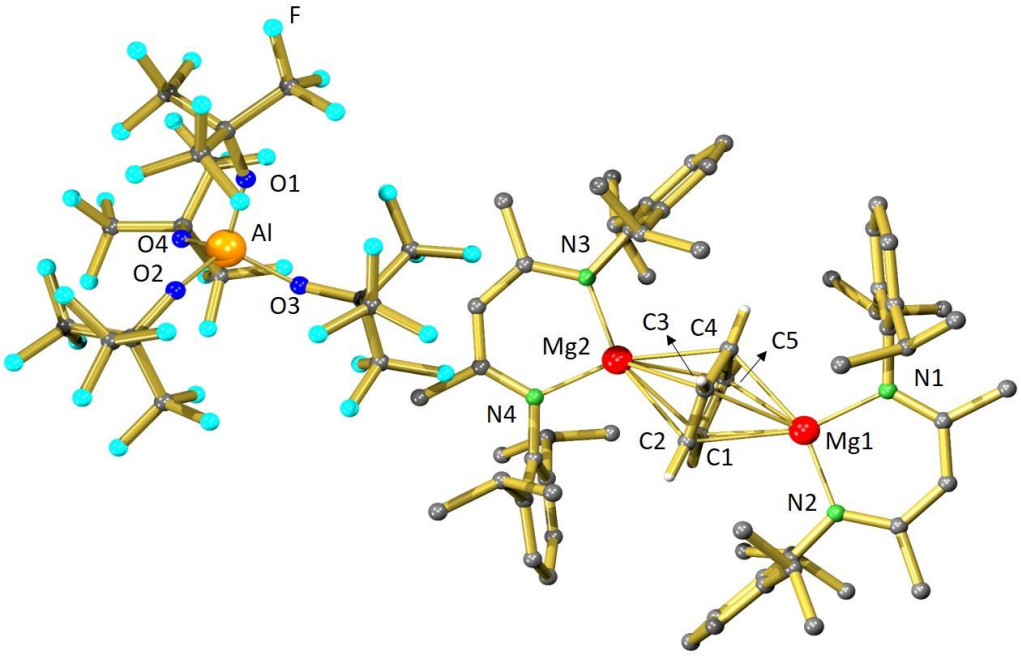

Figure S42: Crystal structure of $[(BDI)Mg(Cp)Mg(BDI)^+][Al(OC(CF_3)_3)_4^-]$. Hydrogen atoms omitted for clarity, except hydrogen atoms at double bonds. Selected bond length (Å): Mg1–C1 2.476(4), Mg1–C2 2.478(4), Mg1–C3 2.443(3), Mg1–C4 2.424(4), Mg1–C5 2.441(4), Mg1–N1 1.990(3), Mg1–N2 1.990(3), Mg2–C1 2.515(4), Mg2–C2 2.496(4), Mg2–C3 2.424(4), Mg2–C4 2.490(4), Mg2–C5 2.459(4), Mg2–N3 1.998(3), Mg2–N4 1.984(3), C1=C2 1.399(6), C2=C3 1.416(6), C3=C4 1.425(5), C4=C5 1.424(5), C5=C1 1.415(6).

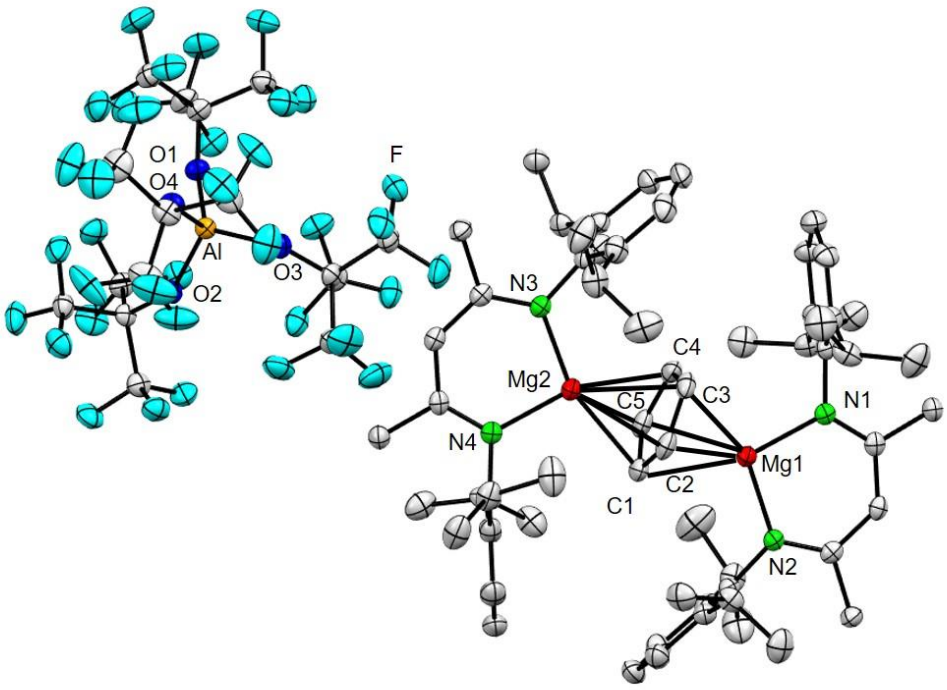

Figure S43: ORTEP representation of [(BDI)Mg(Cp)Mg(BDI)$^+$][Al(OC(CF$_3$)$_3$)$_4^-$] (probability level 50%). Hydrogen atoms were omitted for clarity.

1.6.8 Structure determination of [(BDI)Mg$^+$·*nbd*][Al(OC(CF$_3$)$_3$)$_4^-$]

A yellow crystal of the composition [(BDI)Mg$^+$·*nbd*][Al(OC(CF$_3$)$_3$)$_4^-$]·2(C$_6$H$_5$Cl) 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.[S22] Using Olex2,[S9] the structure was solved with the ShelXT[S10] structure solution program using Intrinsic Phasing and refined with the ShelXL[S11] 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 a 2,6-di*iso*propylphenyl moiety (DIPP), two *i*Pr groups, two C(CF$_3$)$_3$ groups and of both co-crystallized chlorobenzene molecules was observed. It was modeled with the help of similarity restraints (SIMU, SADI) and a rigid bond restraint (RIGU)[S12]. The relative occupancies

of the two alternative orientations were refined to 0.516(7)/0.484(7) (DIPP), 0.556(9)/0.444(9) (*i*Pr), 0.66(3)/0.34(3) (*i*Pr), 0.718(3)/0.282(3) ($C(CF_3)_3$), 0.710(3)/0.290(3) ($C(CF_3)_3$) and 0.572(4)/0.428(4) (chlorobenzene), respectively. In case of the first chlorobenzene molecule, the phenyl rings were refined as regular hexagons (AFIX 66). The disorder of the second chlorobenzene was too severe and no satisfying disorder model could be built. Therefore, the contribution of this solvent molecule to the structure factors was secured by back-Fourier transformation using the solvent mask routine[S13-S14] of the program Olex2.[S9] The solvent accessible voids treated this way had a size of 735.2 $Å^3$ (10.2% of the unit cell) and contained 215.6 electrons/unit cell. Crystallographic and refinement data are summarized in Table S1 (see below).

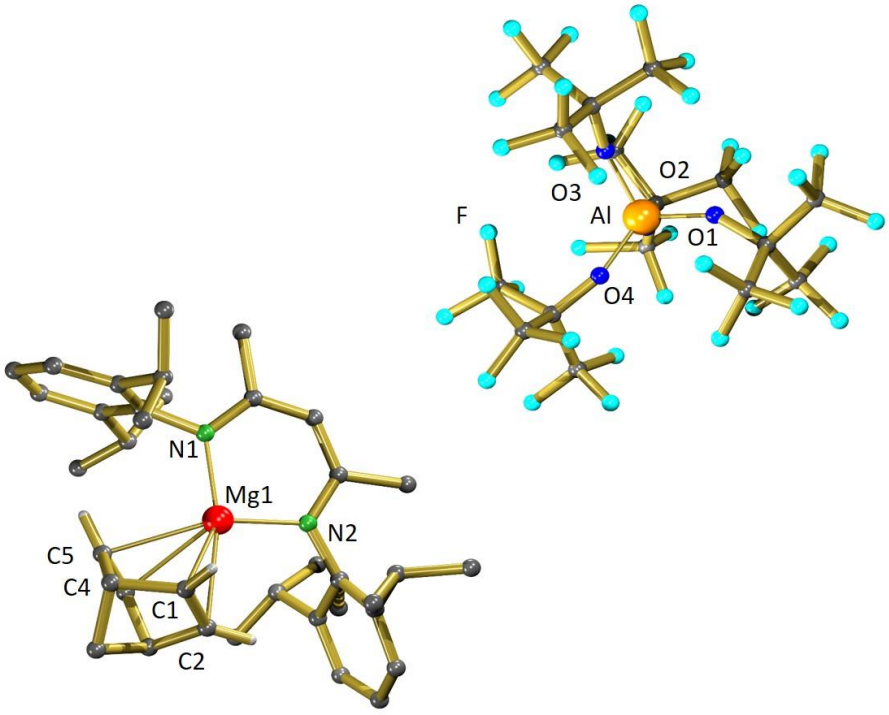

Figure S44: Crystal structure of [(BDI)Mg^{+}·*nbd*][$Al(OC(CF_3)_3)_4^{-}$]. Hydrogen atoms omitted for clarity, except hydrogen atoms at double bonds. Selected bond length (Å): Mg1–N1 1.9916(18), Mg1–N2 1.9886(18), Mg1–C1 2.519(3), Mg1–C2 2.587(3), Mg1–C4 2.580(3), Mg1–C5 2.524(2), C1–C2 1.338(4), C4–C5 1.333(5).

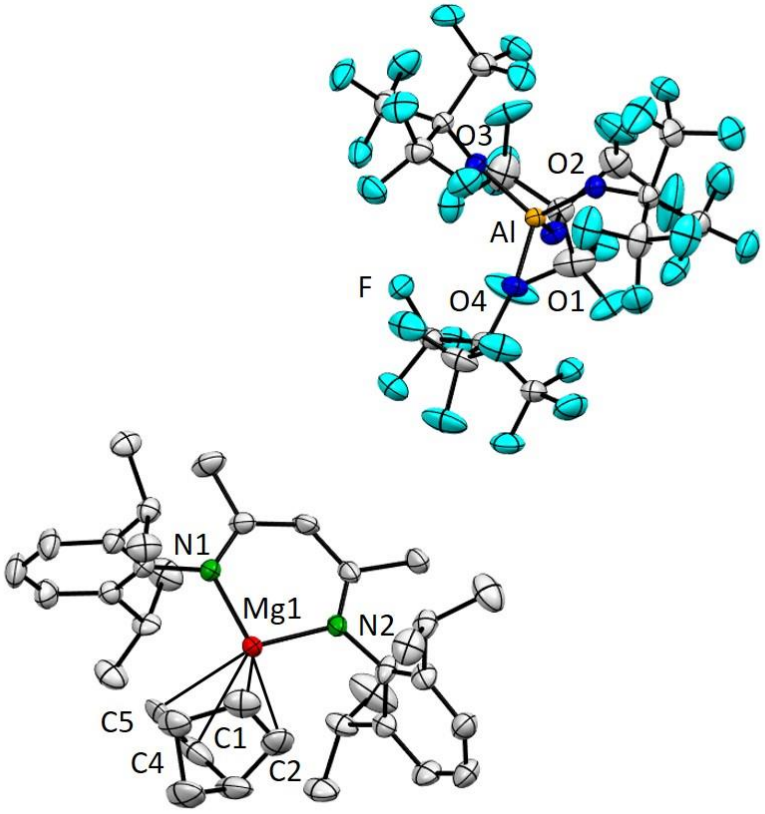

Figure S45: ORTEP representation of [(BDI)Mg^{+}·*nbd*][$Al(OC(CF_3)_3)_4^{-}$] (probability level 50%). Hydrogen atoms were omitted for clarity.

Table S1. Crystal data and structure refinement.

Identification code	[(BDI)Mg^{+}·*nbd*] [$B(C_6F_5)_4^-$]	[(BDI)Mg(Cp)]	[(BDI)Mg(Cp)Mg(BDI)$^{+}$] [$B(C_6F_5)_4^-$]
Empirical formula	$C_{60}H_{49}BF_{20}MgN_2$	$C_{34}H_{46}MgN_2$	$C_{174}H_{174}B_2F_{40}Mg_4N_8$
Formula weight	1213.13	507.04	3256.06
Temperature/K	100.0(1)	100.0(2)	100.0(1)
Crystal system	monoclinic	triclinic	triclinic
Space group	C2/c	P-1	P-1
a/Å	40.5682(4)	9.2377(4)	14.1185(3)
b/Å	14.32480(10)	12.4708(7)	25.0351(5)
c/Å	21.1084(2)	13.7451(6)	25.6684(5)
α/°	90	74.655(4)	111.8037(19)
β/°	98.9620(10)	87.535(4)	101.0099(17)
γ/°	90	78.126(4)	100.4072(16)
Volume/$Å^3$	12117.00(19)	1494.22(13)	7947.3(3)
Z	8	2	2
ρ_{calc}g/cm^3	1.330	1.127	1.361
μ/mm^{-1}	1.148	0.675	1.097
F(000)	4960.0	552.0	3384.0
Crystal size/mm^3	0.232 × 0.13 × 0.105	0.279 × 0.161 × 0.125	0.42 × 0.33 × 0.193
Crystal color	colorless	colorless	colorless
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	7.616 to 147.5	6.668 to 145.852	6.592 to 147.47
Index ranges	-49 ≤ h ≤ 46, -17 ≤ k ≤ 17, -25 ≤ l ≤ 26	-11 ≤ h ≤ 11, -14 ≤ k ≤ 15, -11 ≤ l ≤ 16	-17 ≤ h ≤ 16, -31 ≤ k ≤ 24, -28 ≤ l ≤ 31
Reflections collected	47636	9006	51180
Independent reflections	12062 [R_{int} = 0.0249, R_{sigma} = 0.0201]	5648 [R_{int} = 0.0346, R_{sigma} = 0.0497]	30713 [R_{int} = 0.0297, R_{sigma} = 0.0413]
Data/restraints/parameters	12062/0/783	5648/0/345	30713/739/2430
Goodness-of-fit on F^2	1.025	1.046	1.020
Final R indexes [I>=2σ (I)]	R_1 = 0.0393, wR_2 = 0.0947	R_1 = 0.0509, wR_2 = 0.1335	R_1 = 0.0485, wR_2 = 0.1300
Final R indexes [all data]	R_1 = 0.0443, wR_2 = 0.0977	R_1 = 0.0549, wR_2 = 0.1384	R_1 = 0.0676, wR_2 = 0.1433
Largest diff. peak/hole / e $Å^{-3}$	0.33/-0.27	0.27/-0.33	0.39/-0.34

Table S1. Crystal data and structure refinement (continued).

Identification code	[(BDI)Mg(C_6H_5F)(Cp)Mg(BDI)(C_6H_5F)$^+$][B(C_6F_5)$_4^-$]	[(BDI-H)Mg$^+$(Cp)][B(C_6F_5)$_4^-$]	[(BDI)Mg$^+$·*dcpd*][B(C_6F_5)$_4^-$]
Empirical formula	$C_{99}H_{97}BF_{22}Mg_2N_4$	$C_{58}H_{47}BF_{20}MgN_2$	$C_{63}H_{53}BF_{20}MgN_2$
Formula weight	1820.23	1187.09	1253.19
Temperature/K	100.0(2)	100.0(1)	100.0(1)
Crystal system	triclinic	monoclinic	triclinic
Space group	P-1	$P2_1/n$	P-1
a/Å	12.6804(4)	15.9261(2)	12.5647(6)
b/Å	16.3144(5)	20.4561(2)	13.9361(6)
c/Å	22.7319(7)	17.1852(2)	18.4496(4)
α/°	90.874(2)	90	97.935(3)
β/°	90.208(3)	106.9367(14)	98.421(3)
γ/°	92.266(3)	90	115.012(4)
Volume/Å^3	4698.4(2)	5355.89(13)	2823.1(2)
Z	2	4	2
ρ_{calc}g/cm^3	1.287	1.472	1.474
μ/mm^{-1}	1.016	1.285	1.251
F(000)	1892.0	2424.0	1284.0
Crystal size/mm^3	0.236 × 0.098 × 0.076	0.236 × 0.066 × 0.041	0.14 × 0.058 × 0.037
Crystal color	colorless	colorless	colorless
Radiation	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)	CuKα (λ = 1.54184)
2Θ range for data collection/°	6.624 to 145.844	6.662 to 147.504	7.18 to 147.732
Index ranges	-15 ≤ h ≤ 15, -20 ≤ k ≤ 19, -27 ≤ l ≤ 27	-19 ≤ h ≤ 14, -24 ≤ k ≤ 23, -20 ≤ l ≤ 21	-15 ≤ h ≤ 14, -17 ≤ k ≤ 17, -22 ≤ l ≤ 14
Reflections collected	28675	20676	18589
Independent reflections	17831 [R_{int} = 0.0346, R_{sigma} = 0.0498]	10462 [R_{int} = 0.0319, R_{sigma} = 0.0430]	10978 [R_{int} = 0.0285, R_{sigma} = 0.0479]
Data/restraints/parameters	17831/288/1219	10462/273/795	10978/120/821
Goodness-of-fit on F^2	1.014	1.035	1.015
Final R indexes [I>=2σ (I)]	R_1 = 0.0436, wR_2 = 0.1132	R_1 = 0.0406, wR_2 = 0.0991	R_1 = 0.0402, wR_2 = 0.0965
Final R indexes [all data]	R_1 = 0.0492, wR_2 = 0.1191	R_1 = 0.0555, wR_2 = 0.1082	R_1 = 0.0570, wR_2 = 0.1057
Largest diff. peak/hole / e Å^{-3}	0.31/-0.29	0.31/-0.31	0.26/-0.29

Table S1. Crystal data and structure refinement (continued).

Identification code	[(BDI)Mg(Cp)Mg(BDI)$^+$] [Al(OC(CF$_3$)$_3$)$_4^-$]	[(BDI)Mg$^+$·*nbd*] [Al(OC(CF$_3$)$_3$)$_4^-$]
Empirical formula	$C_{79}H_{87}AlF_{36}Mg_2N_4O_4$	$AlC_{64}Cl_2F_{36}H_{59}MgN_2O_4$
Formula weight	1916.12	1726.32
Temperature/K	100.0(1)	100.0(2)
Crystal system	monoclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$
a/Å	19.6397(3)	17.66188(8)
b/Å	21.7453(3)	20.93276(9)
c/Å	20.3018(4)	19.46075(10)
α/°	90	90
β/°	90.637(2)	93.1584(4)
γ/°	90	90
Volume/Å^3	8669.8(2)	7183.94(6)
Z	4	4
ρ_{calc}g/cm^3	1.468	1.596
μ/mm^{-1}	1.496	2.316
F(000)	3928.0	3488.0
Crystal size/mm^3	0.51 × 0.321 × 0.155	0.539 × 0.308 × 0.244
Crystal color	colorless	yellow
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.956 to 145.932	6.206 to 145.404
Index ranges	-24 ≤ h ≤ 24, -26 ≤ k ≤ 26, -25 ≤ l ≤ 18	-21 ≤ h ≤ 21, -25 ≤ k ≤ 25, -22 ≤ l ≤ 23
Reflections collected	67462	55377
Independent reflections	16934 [R_{int} = 0.0331, R_{sigma} = 0.0243]	14090 [R_{int} = 0.0204, R_{sigma} = 0.0150]
Data/restraints/parameters	16934/2929/1379	14090/3968/1325
Goodness-of-fit on F^2	1.149	1.033
Final R indexes [I>=2σ (I)]	R_1 = 0.0707, wR_2 = 0.2100	R_1 = 0.0549, wR_2 = 0.1464
Final R indexes [all data]	R_1 = 0.0759, wR_2 = 0.2217	R_1 = 0.0578, wR_2 = 0.1490
Largest diff. peak/hole / e Å^{-3}	0.63/-0.54	0.70/-0.74

2. Computational Details

General

All calculations were carried out using Gaussian 16A.[S16] All methods were used as implemented. All structures were fully optimized on a ωB97XD/6-31+G** level of theory.[S17-S19] For the coordination energies the frequencies were calculated at ωB97XD/6-31G* level of theory as every larger basis set lead to convergency problems. For the mechanism the frequencies were calculated at ωB97XD/6-31+G** level of theory. Energies were obtained on a ωB97XD/6-311+G**//6-31+G** level of theory. Topological analyses were carried out using AIMAll V17 with the wave functions obtained from the ωB97XD/6-311+G**//6-31+G** calculations.[S20-S21]

Table S2. NPA Charges of Mg alkene complexes as their $B(C_6F_5)_4^-$ salts.

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 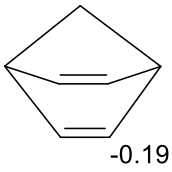
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 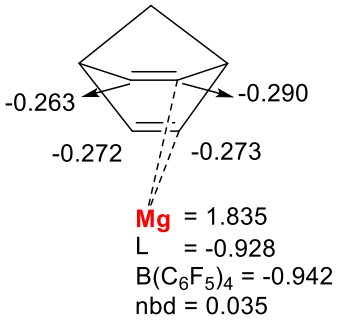
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 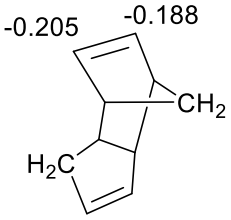
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 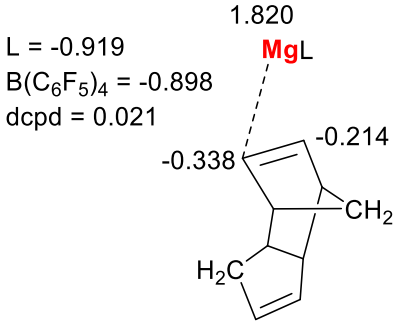
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 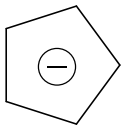
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 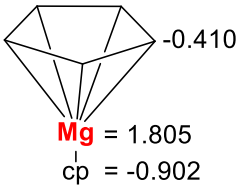
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 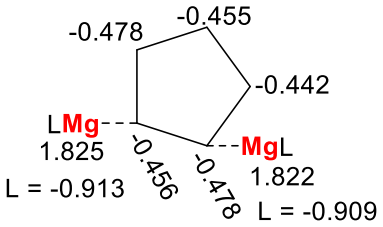
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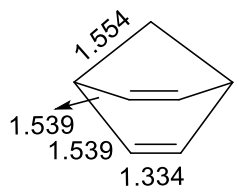
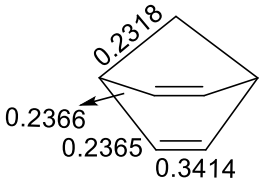
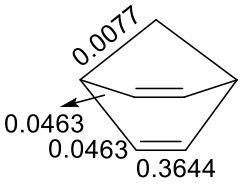
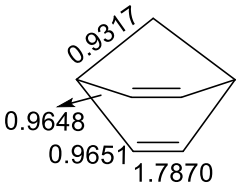
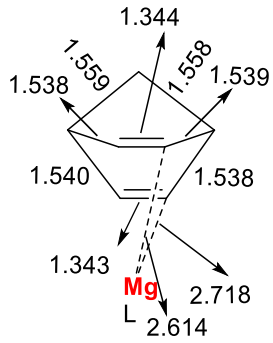
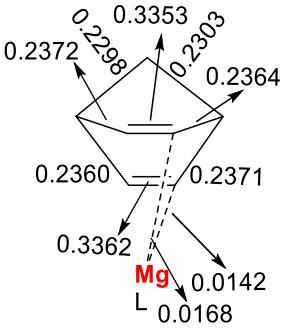
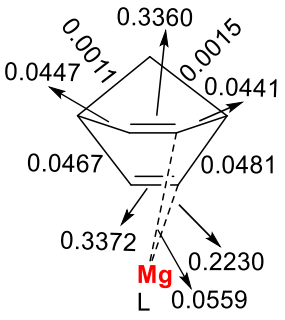
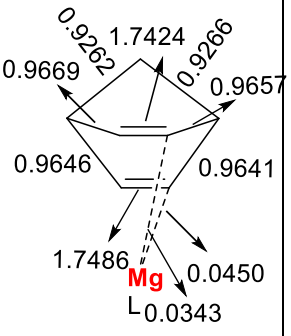
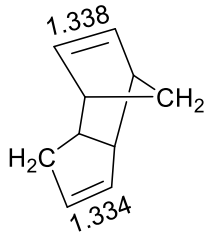
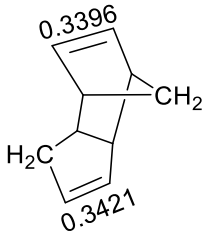
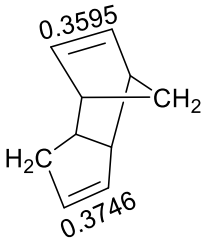
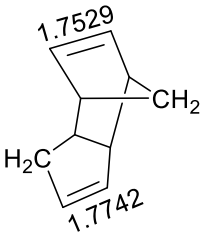
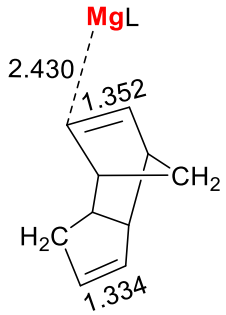
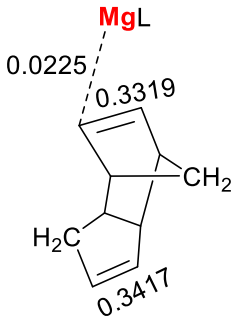
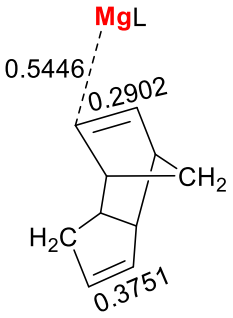
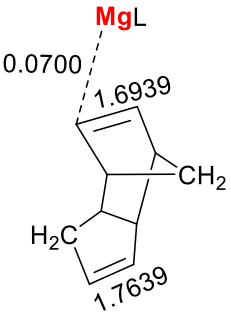
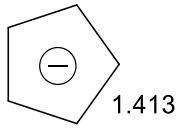
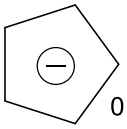
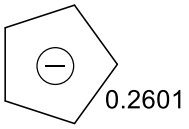
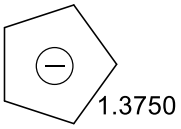
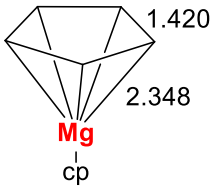
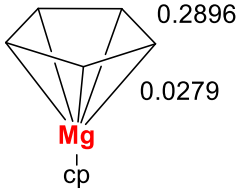
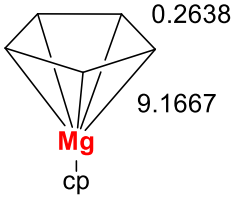
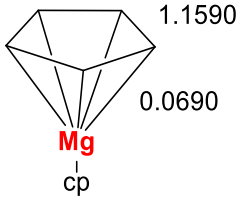
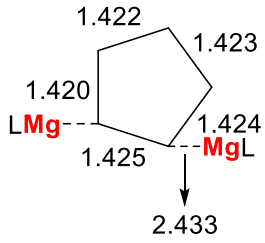
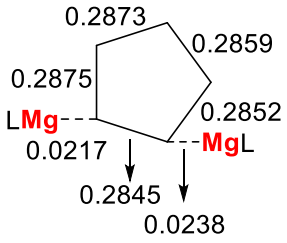
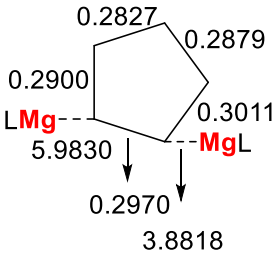
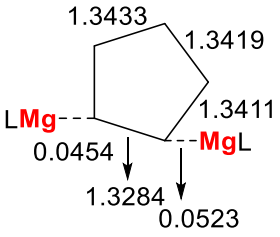
Table S3. Coordination Energies.

[(BDI)Mg$^+$][B(C$_6$F$_5$)$_4^-$] + alkene → [(BDI)Mg$^+$(*alkene*)][B(C$_6$F$_5$)$_4^-$]		
Alkene	ΔE [kcal/mol]	ΔH [kcal/mol]
nbd	-11.39	-7.04
dcpd	-9.58	-14.30
[(BDI)Mg$^+$·C$_6$H$_6$][B(C$_6$F$_5$)$_4^-$] + alkene → [(BDI)Mg$^+$·*alkene*][B(C$_6$F$_5$)$_4^-$] + C$_6$H$_6$		
Alkene	ΔE [kcal/mol]	ΔH [kcal/mol]
nbd	-4.59	-1.11
dcpd	-2.78	-8.37

Table S4. QTAIM pictures of free alkenes and of Mg alkene complexes as their $B(C_6F_5)_4^-$ salts.

Bond distance [Å]	Electron density [a.u.]	Bond ellipticity [a.u.]	Delocalization index [a.u.]
nbd 			
[(BDI)Mg$^+$·*nbd*] 			
dcpd 			
[(BDI)Mg$^+$·*dcpd*] 			

cp				
Cp_2Mg				
[(BDI)Mg(Cp)Mg(BDI)$^+$]				

[(BDI)Mg$^+$·*nbd*][B(C_6F_5)$_4^-$]

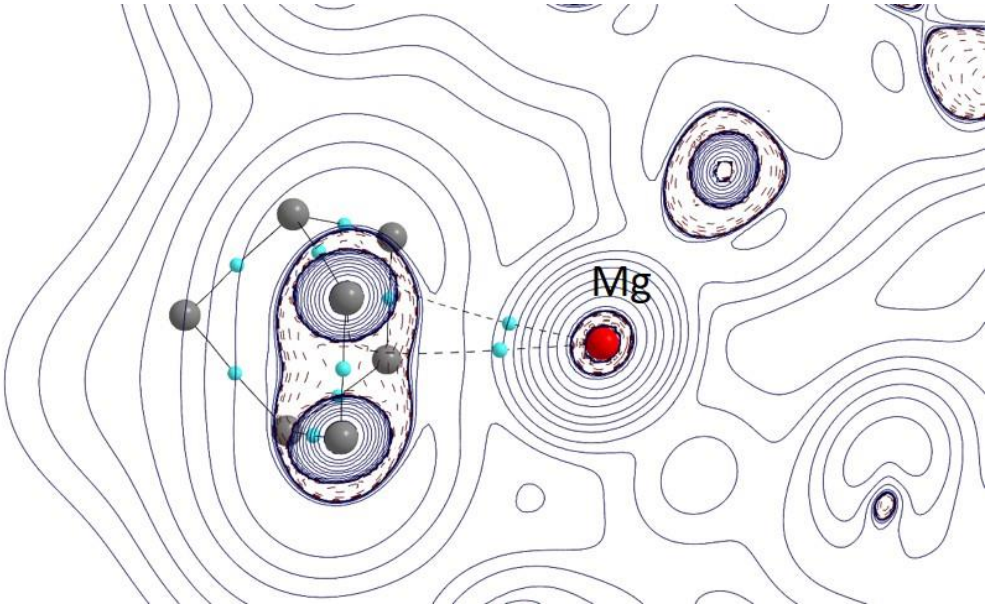


Figure S46: Laplacian of the electron density in the plane of the double bond closest to Mg.

[(BDI)Mg^{+}·*dcpd*][B(C$_6$F$_5$)$_4^{-}$]

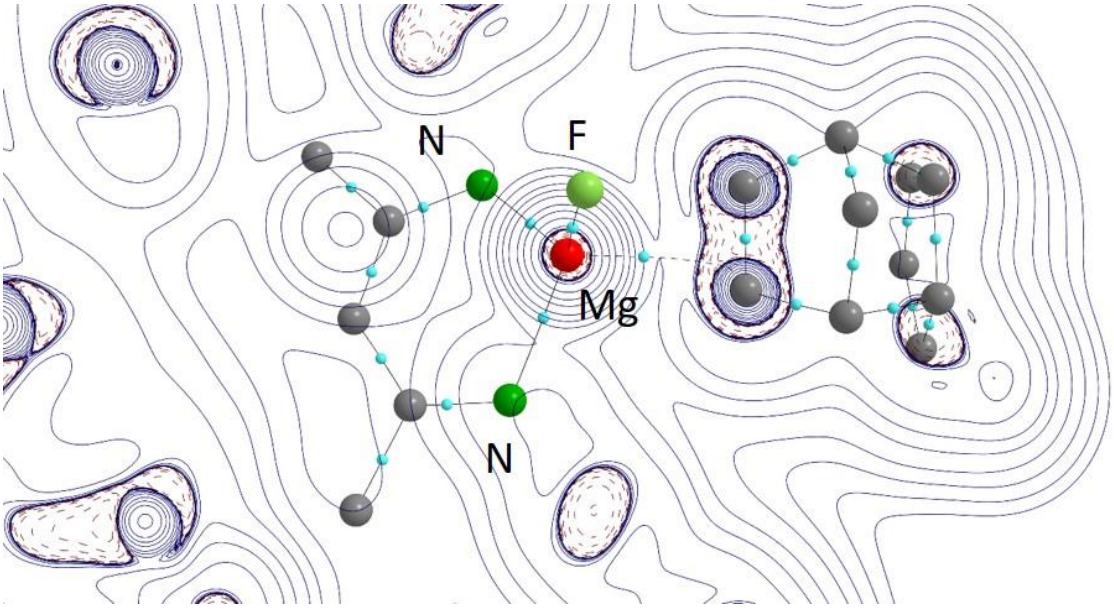


Figure S47: Laplacian of the electron density in the plane of Mg and the coordinating double bond.

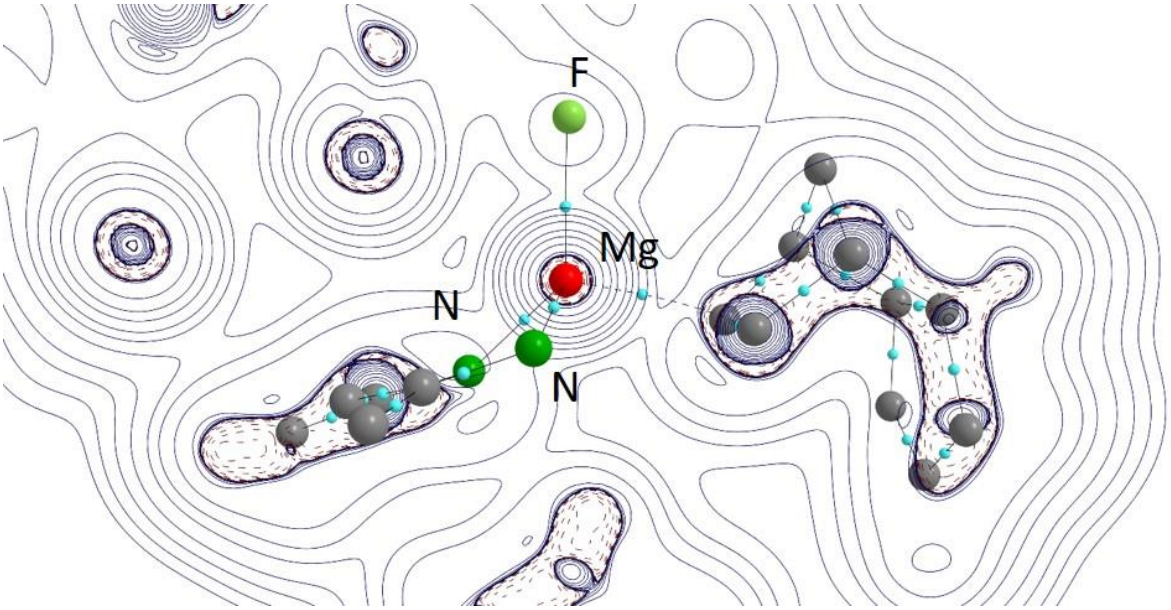


Figure S48: Laplacian of the electron density in the plane of Mg and the coordinated carbon and the adjacent sp^3 carbon.

[(BDI)Mg(Cp)Mg(BDI)$^+$][B(C$_6$F$_5$)$_4^-$]

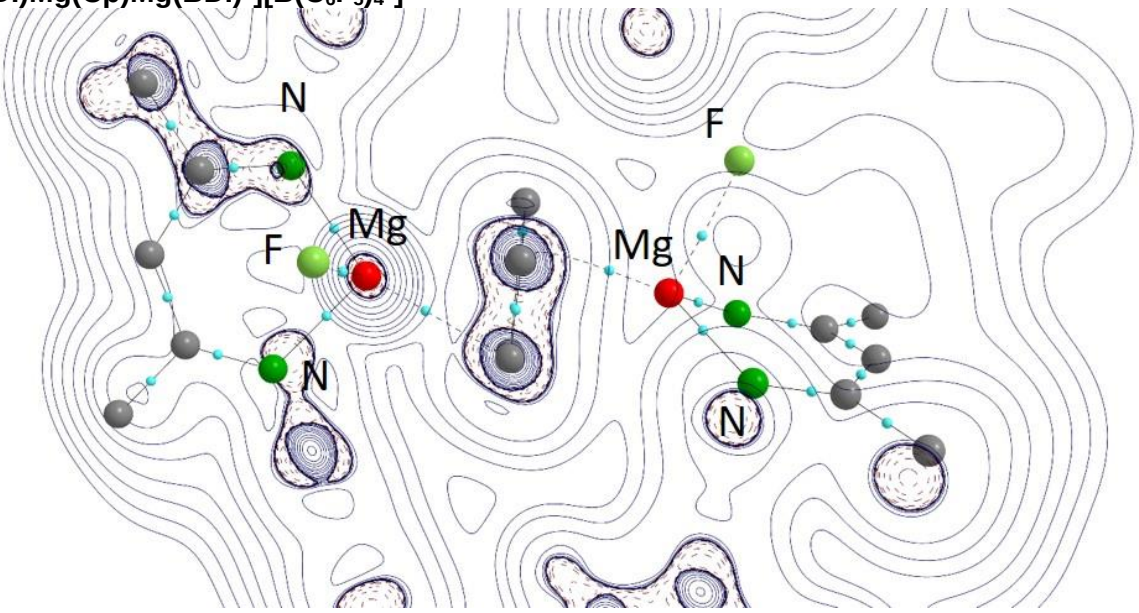
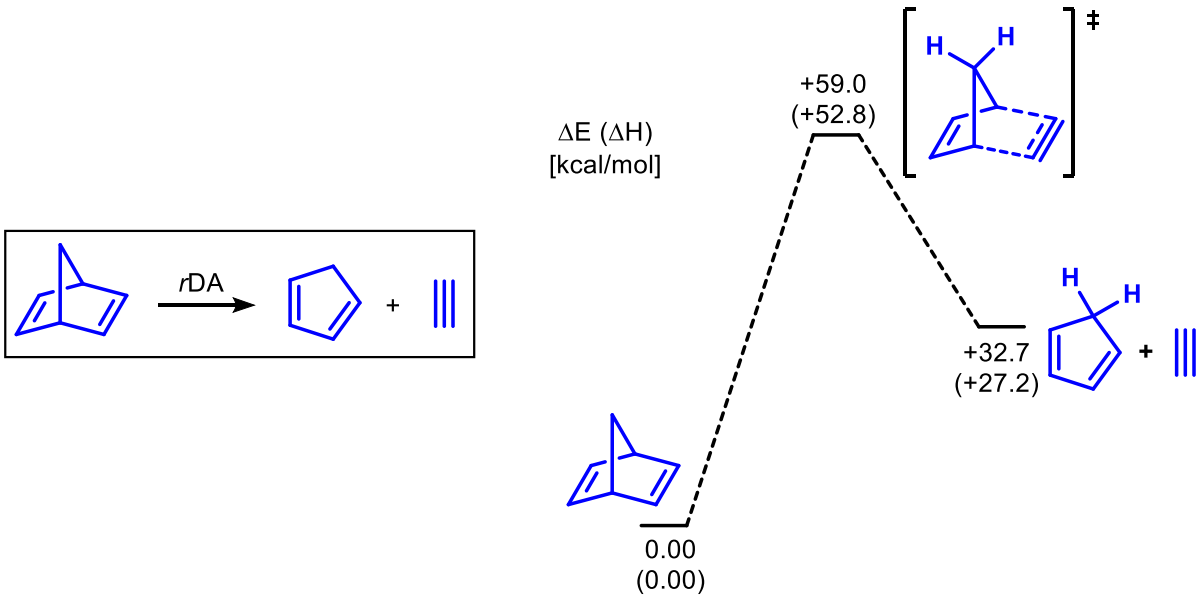
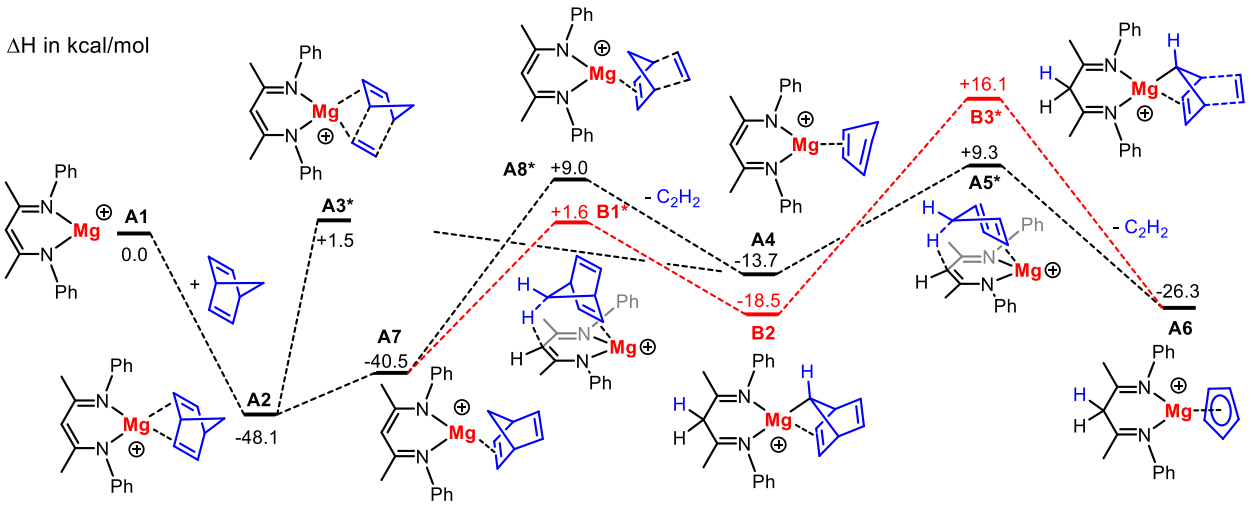


Figure S49: Laplacian of the electron density in the plane of Mg and the coordinating double bond



Scheme S1: Energies for *retro*-Diels-Alder reaction of norbornadiene to cyclopentadiene and acetylene without catalyst.

Preliminary DFT calculations on a model system, $HC[C(Me)N(Ph)]_2Mg^+$, which for simplicity does not include the weakly coordinating anion $B(C_6F_5)_4^-$, are inconclusive. Without competition by solvent or $B(C_6F_5)_4^-$, Mg···*nbd* complexation (**A2**) is highly exothermic (ΔH = -48.1 kcal/mol). The subsequent concerted elimination of acetylene is very endothermic (**A2**-**A3***, +49.6 kcal/mol). The alternative route **A7**-**A8*** also has a high barrier of +49.5 kcal/mol. Although Mg-complexation leads to a decrease of the activation energy by nearly 10 kcal/mol (*cf.* Scheme S1), both *r*DA reactions are unlikely. The subsequent CpH deprotonation step is feasible (**A4**-**A5***, +23.0 kcal/mol). The alternative route *via nbd* deprotonation features a difficult first step (**A7**-**B1***, +42.1 kcal/mol) and although *r*DA of deprotonated *nbd* is much easier (**B2**-**B3***, +34.6 kcal/mol), the barrier is still too high for a facile reaction. Comprehensive calculation studies on the full system, including the influence of anion and solvent and considering non-concerted radical routes as well quadricyclene intermediates, is in progress.



Scheme S2: Energy profile for the *r*DA decomposition of *nbd* by the model system $HC[C(Me)N(Ph)]_2Mg^+$; ωB97XD/6-311+G**//ωB97XD/6-31+G**, ΔH in kcal/mol.

XYZ Coordinates

21

$Mg(cp)_2$

Mg	0.000011	-0.000037	-0.000048
C	2.013714	-0.009151	-1.207692
C	2.013681	-1.151446	-0.364526
C	2.013813	1.145782	-0.381917
C	2.013760	-0.702516	0.982362
C	2.013844	0.717273	0.971644
C	-2.013888	-0.009027	-1.207622
C	-2.013770	1.145850	-0.381772
C	-2.013837	-1.151376	-0.364538
C	-2.013649	0.717249	0.971764
C	-2.013687	-0.702545	0.982382
H	2.025189	-0.017394	-2.290040
H	2.025156	-2.183375	-0.691171
H	2.025360	2.172598	-0.724197
H	2.025275	-1.332090	1.862811
H	2.025410	1.360093	1.842458
H	-2.025509	-0.017191	-2.289968
H	-2.025282	2.172692	-0.723977
H	-2.025436	-2.183282	-0.691251
H	-2.025050	1.360010	1.842624
H	-2.025133	-1.332176	1.862790

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$[(BDI)Mg(Cp)Mg(BDI)^+][B(C_6F_5)_4]$

Mg	3.362566	1.979683	0.135979
Mg	2.148670	-2.159036	-0.109820
F	-6.146567	-1.190344	-2.565318
F	-8.160365	0.803812	-1.743710
F	-5.799284	-2.717125	-0.357026
F	-4.467541	-2.173144	-4.381575
F	-5.821853	3.002884	1.291302
F	-7.980847	1.254591	1.025480
F	-3.861769	2.587757	-0.863605
F	-2.449442	0.378722	-0.039166
F	-5.305627	3.372422	3.852056
F	-4.079449	-1.398040	1.602591
F	0.084588	-2.432865	-0.417094
F	-4.143602	1.406769	5.346139
F	-1.783423	-1.771560	-4.130108
F	-0.823335	-0.430927	-1.966035
F	3.052064	2.713034	-1.880948
F	-7.775133	-4.139964	0.640667
F	-3.530788	-0.978830	4.172235
F	-8.649416	2.823810	-3.364682
F	-9.973406	-0.203278	2.011980
F	-4.376081	4.615921	-2.500541
F	-9.909578	-2.926947	1.842978
F	-6.789767	4.770909	-3.785369
N	2.327018	3.507292	0.954924
N	2.193151	-3.450859	1.443127
N	2.868046	-3.459757	-1.505267
N	5.181584	2.802775	0.542268
C	-4.837268	-1.031399	-2.337409
C	2.843222	4.726749	0.995109
C	0.986144	3.262420	1.390867
C	0.799915	2.724935	2.683468
C	-5.996216	1.609463	-1.157393
C	-6.808540	-2.024331	0.204241
C	-4.964224	0.781885	1.286608
C	-6.788437	-0.636835	0.247150
C	-7.193279	1.722216	-1.858901
C	-0.098669	3.440216	0.514982
C	-4.408252	-0.378459	-1.181380
C	4.206446	5.009958	0.755563
H	4.479152	6.057817	0.821154
C	2.283370	-3.015673	2.801946
C	-7.834412	-2.806560	0.723760
C	-0.493934	2.386035	3.076767
H	-0.671833	1.965283	4.060345
C	-3.989151	-1.529570	-3.315419
C	3.708926	3.311150	-2.938438
C	-4.406742	1.208686	4.053548
C	0.056683	3.948629	-0.910107
H	1.096295	4.259732	-1.055793
C	-2.624967	-1.324689	-3.189205
C	-5.247351	1.981161	1.936229
C	-3.028912	-0.216585	-1.097825
C	-5.082330	2.620097	-1.439644
C	1.958270	-4.728268	1.162223
C	1.954044	5.907643	1.317439
H	1.357680	6.170903	0.436779
H	2.540487	6.780885	1.608622
H	1.250044	5.666535	2.117578
C	4.816996	-3.242697	2.566022
H	4.618758	-2.953860	1.526506
C	3.570103	-2.893071	3.370612
C	-7.894038	-0.077553	0.889104
C	3.837685	-0.361068	0.649485
H	4.758721	-0.590306	1.169581
C	-7.476196	2.771708	-2.730333
C	5.295497	4.118930	0.700026
C	-1.571495	2.559670	2.220920
H	-2.566683	2.267950	2.528085
C	1.136195	-2.628622	3.520340
C	-4.374450	-0.178779	2.105227
C	6.291746	1.939431	0.785992
C	3.726365	-3.044555	-2.568140
C	1.976834	2.505618	3.626728
H	2.825457	2.164802	3.019314
C	2.584847	-0.072643	1.256042
H	2.382002	-0.078381	2.318552
C	1.638461	0.181033	0.222973
H	0.597814	0.455112	0.347092
C	-8.944198	-0.811930	1.418629
C	2.063042	-5.288813	-0.128701
H	1.804338	-6.339838	-0.191719
C	4.054493	4.639468	-2.813427
H	3.841916	5.173296	-1.892138
C	-4.993684	2.204093	3.288850
C	3.675183	-0.281797	-0.759747
H	4.435790	-0.475138	-1.504180
C	-4.090712	-0.000116	3.449774
C	-2.148902	-0.640793	-2.087262
C	-1.372787	3.088882	0.958896
H	-2.223588	3.212977	0.302611
C	2.609030	-4.752885	-1.309486
C	2.423721	3.804911	4.312933
H	2.789941	4.541868	3.593290
H	3.236879	3.601183	5.020214
H	1.592875	4.251085	4.871148
C	6.942415	1.321861	-0.302605
C	2.313354	0.041823	-1.023882
H	1.863571	0.178241	-1.996388
C	-8.915369	-2.197234	1.336488
C	-5.314185	3.682918	-2.295495
C	6.648034	1.620175	2.110788
C	3.206957	-2.350266	-3.681178
C	3.674640	-2.434567	4.684020
H	4.652007	-2.333523	5.143842
C	-6.534078	3.762885	-2.950980
C	-0.924064	-3.306258	-0.817899
C	6.656217	4.761466	0.882882
H	6.758494	5.122235	1.911251
H	6.744803	5.631964	0.225616
H	7.478516	4.075928	0.674695
C	5.105354	-4.751190	2.558815
H	5.225026	-5.127760	3.581233
H	6.033324	-4.955808	2.011292
H	4.306512	-5.317845	2.073656
C	1.551127	-5.671651	2.272373
H	1.624831	-6.714210	1.959346
H	0.512335	-5.469559	2.555604
H	2.162201	-5.522856	3.166205
C	1.713719	-2.147893	-3.875281
H	1.230828	-2.167010	-2.892317
C	-0.847100	5.157464	-1.194779
H	-1.903027	4.869106	-1.211705
H	-0.610552	5.584226	-2.175884
H	-0.726595	5.941616	-0.439926
C	2.546502	-2.094882	5.420306
H	2.648035	-1.742820	6.442456
C	6.058922	-2.476869	3.031405
H	5.870171	-1.402154	3.104195
H	6.880971	-2.619370	2.325033
H	6.409321	-2.826307	4.009437
C	5.115988	-3.254320	-2.446297
C	-0.249228	-2.597300	2.893939
H	-0.173917	-3.044294	1.900174
C	6.547199	1.659291	-1.730439
H	5.462653	1.810107	-1.734580
C	-0.244063	2.827889	-1.916374
H	0.386063	1.952356	-1.741952
H	-0.075563	3.174368	-2.942628
H	-1.286731	2.504404	-1.832912
C	1.696911	1.429925	4.680703
H	0.977273	1.779046	5.429741
H	2.614396	1.166836	5.213649
H	1.297851	0.512384	4.237415
C	1.293542	-2.184734	4.835030
H	0.416059	-1.886129	5.402187
C	3.967580	2.532433	-4.048212
H	3.683761	1.485405	-4.069002
C	7.963819	0.409729	-0.041317
H	8.474950	-0.074392	-0.866967
C	8.335969	0.098762	1.260519
H	9.131723	-0.616737	1.444549
C	4.089498	-1.915501	-4.671684
H	3.697571	-1.395650	-5.540846
C	7.679574	0.702515	2.321694
H	7.966159	0.448709	3.338943
C	-0.713597	-1.142174	2.730274
H	-0.903295	-0.683329	3.706205
H	-1.641380	-1.075721	2.156774
H	0.036315	-0.532529	2.223360
C	5.939015	2.222709	3.314952
H	5.152364	2.893286	2.955854
C	5.263039	1.140543	4.165691
H	4.532490	0.562695	3.588783
H	4.738786	1.599249	5.010141
H	5.995887	0.437073	4.576749
C	5.738530	-3.905109	-1.219662
H	4.943945	-4.125880	-0.501338
C	4.701008	5.229819	-3.897088
H	4.989843	6.274105	-3.839405
C	5.953782	-2.827333	-3.477702
H	7.023512	-3.004252	-3.401955
C	4.977773	4.489343	-5.044389
H	5.479892	4.959776	-5.883222
C	4.616323	3.145308	-5.117524
H	4.836865	2.566840	-6.008681
C	1.346879	-0.812228	-4.533741
H	1.850869	0.035472	-4.056767
H	0.270193	-0.651350	-4.459974
H	1.610419	-0.796199	-5.596908
C	2.867325	-5.769366	-2.404968
H	3.349716	-5.333591	-3.280381
H	1.910374	-6.206039	-2.714394
H	3.487577	-6.588524	-2.030745
C	6.719553	-2.946506	-0.533836
H	7.542859	-2.664895	-1.200167
H	7.159259	-3.422322	0.348737
H	6.226395	-2.023525	-0.211025
C	5.452293	-2.162789	-4.586402
H	6.120634	-1.832072	-5.375753
C	7.181371	2.973876	-2.203665
H	6.856793	3.821288	-1.595878
H	6.897184	3.180264	-3.241195
H	8.274400	2.910617	-2.150563
C	6.848419	0.543341	-2.731642
H	7.921881	0.463297	-2.939703
H	6.349282	0.752793	-3.683562
H	6.502916	-0.433209	-2.379929
C	6.899577	3.048941	4.182024
H	7.654273	2.410006	4.655047
H	6.349183	3.560573	4.979156
H	7.429208	3.802555	3.592048
B	-5.533653	0.340503	-0.204463
C	-1.294873	-3.396354	3.680822
H	-0.996569	-4.441572	3.811389
H	-2.255509	-3.371344	3.156309
H	-1.461945	-2.967843	4.674417
C	1.138934	-3.306698	-4.706504
H	1.562012	-3.289557	-5.717396
H	0.051298	-3.225235	-4.782919
H	1.385717	-4.279006	-4.268045
C	6.432132	-5.229510	-1.564908
H	5.749966	-5.918899	-2.070861
H	6.797339	-5.716923	-0.654170
H	7.291901	-5.067822	-2.225464
C	-0.680287	-4.124900	-1.897522
C	-1.721169	-4.944319	-2.325233
C	-2.946788	-4.924443	-1.664663
C	-2.116483	-3.250306	-0.132334
C	-3.140904	-4.085813	-0.569882
H	0.282446	-4.112444	-2.386596
H	-1.568880	-5.590585	-3.183770
H	-3.758834	-5.556331	-2.008313
H	-2.262721	-2.556109	0.684696
H	-4.098492	-4.048948	-0.067913

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cp(-)

C	0.420496	-1.126321	-0.000015
C	-0.941262	-0.747968	-0.000019
C	1.201181	0.051870	-0.000014
C	-1.002253	0.664050	-0.000007
C	0.321848	1.158366	-0.000017
H	0.800904	-2.145218	0.000092
H	-1.792757	-1.424604	0.000083
H	2.287757	0.098817	0.000096
H	-1.908927	1.264739	0.000091
H	0.612971	2.206281	0.000073

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$[(BDI)Mg^{\cdot}\text{-}nbd][B(C_6F_5)_4]$

Mg	3.204863	-0.014152	-0.616594
F	-0.368805	0.167039	0.140651
F	1.447893	-0.109426	-1.794620
F	0.670360	-0.459931	-4.365845
F	-2.007307	-0.576737	-4.964656
F	-3.819155	-0.360462	-3.066057
F	-1.906869	1.344630	2.419219
F	-1.737410	3.937408	2.878779
F	-2.712126	5.747073	1.088374
F	-3.853380	4.858677	-1.228803
F	-4.044129	2.246240	-1.718666
F	-1.368139	-2.427363	0.106887
F	-1.170756	-4.065294	2.162843
F	-2.560478	-3.612503	4.463269
F	-4.228905	-1.451006	4.614697
F	-4.484451	0.196560	2.543020
F	-4.032013	-2.484322	-1.159381
F	-6.488230	-3.392147	-1.647764
F	-8.666164	-1.816907	-1.153072
F	-8.300964	0.689711	-0.144014
F	-5.882219	1.612262	0.361916
N	2.788398	1.405940	0.730121
N	3.032094	-1.530032	0.679372
C	5.055013	1.398442	-1.945346
H	4.733191	2.387987	-1.636912
C	5.702822	0.476707	-1.212091
H	6.028614	0.557939	-0.181625
C	5.981623	-0.723170	-2.134281
H	6.726219	-1.433150	-1.781698
C	4.624865	-1.336405	-2.520245
H	4.317760	-2.345019	-2.267015
C	3.973925	-0.417368	-3.251095
H	3.008361	-0.505482	-3.733647
C	4.894389	0.812699	-3.358498
H	4.637157	1.527717	-4.137797
C	6.258937	0.064802	-3.449384
H	7.122940	0.730876	-3.381676
H	6.341311	-0.577794	-4.329329
C	1.276144	2.245562	2.469975
H	1.933480	3.097932	2.652955
H	0.831179	1.919108	3.409021
H	0.465955	2.600536	1.823596
C	1.984258	1.118815	1.760165
C	1.715386	-0.187883	2.200830
H	1.009485	-0.263395	3.018679
C	2.248901	-1.410695	1.753806
C	1.861157	-2.644925	2.530508
H	1.003662	-3.120028	2.043019

H	1.569454	-2.395394	3.551243
H	2.666704	-3.381910	2.554403
C	3.237472	2.743173	0.517731
C	2.561067	3.588118	-0.379544
C	3.096005	4.852109	-0.640809
H	2.582505	5.518074	-1.328574
C	4.270448	5.273097	-0.031561
H	4.668749	6.261112	-0.239088
C	4.937433	4.421810	0.843892
H	5.860586	4.757104	1.305941
C	4.446107	3.146836	1.126580
C	5.198318	2.211588	2.063995
H	4.913691	1.189985	1.787910
C	4.776137	2.404952	3.528297
H	4.952120	3.438369	3.846587
H	5.355336	1.743130	4.180676
H	3.719256	2.176490	3.679370
C	6.722091	2.332102	1.939788
H	7.056211	2.293357	0.897524
H	7.205014	1.517163	2.488561
H	7.092062	3.268506	2.370089
C	1.293090	3.139576	-1.085724
H	0.985362	2.191713	-0.636983
C	0.134349	4.121471	-0.890970
H	-0.018204	4.342874	0.168570
H	-0.790825	3.691850	-1.286825
H	0.310141	5.069798	-1.409245
C	1.552924	2.902650	-2.580832
H	1.860951	3.829853	-3.075450
H	0.647628	2.540987	-3.079188
H	2.347877	2.165490	-2.747289
C	3.699116	-2.751657	0.365070
C	3.063245	-3.739274	-0.409704
C	3.819377	-4.837186	-0.831066
H	3.348187	-5.607735	-1.434461
C	5.160465	-4.962011	-0.494439
H	5.729230	-5.822584	-0.832150
C	5.771495	-3.985229	0.286043
H	6.817872	-4.098401	0.550654
C	5.060813	-2.868471	0.726179
C	5.721404	-1.807195	1.596655
H	5.247289	-0.851161	1.349431
C	5.444729	-2.047718	3.088746
H	4.377296	-2.011751	3.314269
H	5.937716	-1.279227	3.693667
H	5.828143	-3.026028	3.398110
C	7.228744	-1.661809	1.366975
H	7.784277	-2.519099	1.760994
H	7.599085	-0.773891	1.888505
H	7.480519	-1.560784	0.306976
C	1.599422	-3.636815	-0.812116
H	1.163073	-2.773760	-0.302909
C	0.808128	-4.877696	-0.378224
H	1.127221	-5.767199	-0.932027
H	-0.257996	-4.728399	-0.564514
H	0.938649	-5.080336	0.687887
C	1.440241	-3.405555	-2.321761
H	1.965199	-2.504399	-2.654597
H	0.381655	-3.291653	-2.576016
H	1.836024	-4.249875	-2.896654
C	-2.210407	-0.140916	-1.326508
C	-0.840858	-0.040422	-1.096719
C	0.104814	-0.164307	-2.091816
C	-0.261736	-0.352886	-3.411400
C	-1.611639	-0.414242	-3.702053
C	-2.546486	-0.302532	-2.669166
C	-3.056597	1.640020	0.345922
C	-2.443882	2.153087	1.485876
C	-2.335948	3.513954	1.757122
C	-2.829370	4.438617	0.852489
C	-3.405360	3.982654	-0.323985
C	-3.488742	2.617114	-0.551535
C	-2.918267	-0.984308	1.216670
C	-2.099521	-2.107333	1.197180
C	-1.970771	-2.991894	2.263006
C	-2.680564	-2.775396	3.430669
C	-3.526443	-1.677693	3.501568
C	-3.631495	-0.831557	2.407962
C	-4.806727	-0.372471	-0.411123
C	-5.063058	-1.652966	-0.901859
C	-6.327402	-2.156096	-1.162733
C	-7.435962	-1.359549	-0.912669
C	-7.243927	-0.085761	-0.404261
C	-5.953456	0.375451	-0.158058
B	-3.249474	0.042670	-0.042803

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nbd

C	-1.239280	0.667028	-0.519958
H	-1.929293	1.334526	-1.021075
C	-1.239172	-0.667407	-0.519698
H	-1.929051	-1.335244	-1.020552
C	-0.000067	-1.119045	0.273066
H	0.000075	-2.154443	0.614721
C	1.239390	-0.667358	-0.519554
H	1.929233	-1.335617	-1.019889
C	1.239503	0.666988	-0.519794
H	1.929410	1.334990	-1.020372
C	-0.000086	1.119241	0.272379
H	0.000048	2.154861	0.613362
C	-0.000240	0.000473	1.351504
H	-0.900260	0.000695	1.972921
H	0.899556	0.000710	1.973213

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[(BDI)Mg^{+}·dcpd][B(C_6F_5)$_4^-$]

Mg	2.440627	0.012643	0.346991
F	-0.427507	0.096167	0.058668
F	1.286954	0.037330	2.051902
F	0.420181	-0.086414	4.633898
F	-2.282301	-0.168323	5.136762
F	-4.016219	-0.137168	3.166058
F	-4.078881	-2.439141	1.442130
F	-6.505168	-3.421877	1.925508
F	-8.734624	-1.992901	1.248275
F	-8.448141	0.446898	0.064845
F	-6.061188	1.444004	-0.434475
F	-4.327780	2.280444	1.688173
F	-4.367727	4.853931	1.000175
F	-3.269447	5.664490	-1.366360
F	-2.081877	3.827657	-2.988502
F	-2.005456	1.271763	-2.320404
F	-4.519434	0.076212	-2.488874
F	-4.215894	-1.680242	-4.460398
F	-2.598399	-3.860813	-4.131905
F	-1.300490	-4.211914	-1.764783
F	-1.509357	-2.434608	0.179871
N	2.290918	1.430764	-1.038252
N	2.377243	-1.537379	-0.908663
C	0.978313	2.283720	-2.924621
H	0.319502	2.907714	-2.312763
H	0.406499	1.922547	-3.777898
H	1.786712	2.930194	-3.276595
C	1.511163	1.146059	-2.089494
C	1.138330	-0.159581	-2.463877
H	0.438490	-0.217748	-3.287788
C	1.620759	-1.399980	-1.999487
C	1.273011	-2.615585	-2.819580
H	2.059847	-2.806414	-3.554808
H	0.343560	-2.454740	-3.367674
H	1.172398	-3.504895	-2.194824
C	2.826354	2.747018	-0.890176
C	4.095005	3.023278	-1.445438
C	4.613602	4.311465	-1.300624
H	5.578007	4.555098	-1.733016
C	3.925109	5.291293	-0.594568
H	4.343413	6.288159	-0.498253
C	2.715269	4.980447	0.009415
H	2.199681	5.738520	0.591192
C	2.150691	3.709686	-0.119676
C	4.905605	1.932948	-2.137851
H	4.619518	0.981090	-1.671916
C	4.576497	1.808619	-3.632122
H	3.535965	1.520306	-3.796929
H	5.208659	1.043894	-4.096434
H	4.757477	2.757831	-4.148248
C	6.414886	2.113180	-1.936505
H	6.798514	2.978744	-2.486154
H	6.950510	1.236757	-2.309955
H	6.667880	2.237479	-0.878663
C	0.873350	3.372196	0.629099
H	0.479905	2.435298	0.222807
C	-0.220622	4.429158	0.463478
H	0.039275	5.367680	0.963545
H	-1.154342	4.069692	0.904977
H	-0.401210	4.650614	-0.591621
C	1.189110	3.163458	2.119452
H	1.983654	2.423180	2.270847
H	0.298901	2.833711	2.665625
H	1.534305	4.099451	2.571195
C	3.113220	-2.731814	-0.636820
C	4.312686	-2.988741	-1.339902
C	5.105785	-4.064956	-0.936569
H	6.028048	-4.275829	-1.470758
C	4.744919	-4.871023	0.134969
H	5.378233	-5.700021	0.434438
C	3.559732	-4.614751	0.809301
H	3.268262	-5.257015	1.635484
C	2.726200	-3.556767	0.439386
C	4.787102	-2.135796	-2.511026
H	4.062852	-1.331891	-2.674228
C	6.145700	-1.478888	-2.227455
H	6.116967	-0.820923	-1.353629
H	6.455361	-0.874492	-3.085934
H	6.923264	-2.230090	-2.053942
C	4.883171	-2.960853	-3.804472
H	5.697761	-3.690645	-3.743993
H	5.083864	-2.307323	-4.659339
H	3.963695	-3.516118	-4.005298
C	1.420437	-3.354141	1.192307
H	0.888389	-2.514580	0.733895
C	1.659101	-3.030216	2.673374
H	2.125190	-3.874592	3.192052
H	0.709267	-2.818605	3.174925
H	2.317055	-2.166411	2.805975
C	0.510470	-4.582892	1.059653
H	0.317882	-4.819466	0.011546
H	-0.452176	-4.396905	1.542840
H	0.964341	-5.460760	1.531848
C	-2.352589	-0.060632	1.466866
C	-0.976241	0.012047	1.289260
C	-0.069918	-0.011877	2.326344
C	-0.473470	-0.075837	3.645203
C	-1.836256	-0.117751	3.882936
C	-2.731928	-0.103639	2.809994
C	-4.920328	-0.426597	0.513826
C	-5.136464	-1.677744	1.092474
C	-6.384723	-2.219199	1.353500
C	-7.519216	-1.497136	1.010842
C	-7.367240	-0.257104	0.413550
C	-6.091241	0.245248	0.171584
C	-3.240951	1.615097	-0.306746
C	-3.775474	2.613086	0.508661
C	-3.817512	3.958663	0.174935
C	-3.267507	4.373915	-1.028435
C	-2.664656	3.434608	-1.847492
C	-2.642640	2.096631	-1.467849
C	-2.999568	-1.041304	-1.055874
C	-3.676484	-0.946246	-2.274321
C	-3.551502	-1.854155	-3.315045
C	-2.732772	-2.962893	-3.153297
C	-2.065138	-3.126770	-1.952488
C	-2.202012	-2.174113	-0.948017
B	-3.370107	0.030880	0.153147
C	4.602430	0.944789	1.471443
H	4.576047	1.747386	0.738371
C	4.675577	-0.380356	1.216331
H	4.756959	-0.843793	0.236269
C	4.991942	-1.086087	2.518635
H	4.763587	-2.152074	2.544307
C	4.278385	-0.162879	3.527571
H	4.586351	-0.344176	4.560912
H	3.187741	-0.199687	3.474628
C	4.875177	1.132133	2.943749
H	4.560376	2.080928	3.377590
C	6.413068	0.810634	3.105593
H	6.702670	1.073017	4.128894
C	7.919127	0.469498	1.321316
C	6.482596	-0.729472	2.834797
H	6.775479	-1.276456	3.734049
C	7.348444	1.401883	2.085997
C	7.511234	-0.933283	1.698389
H	8.377130	-1.512229	2.038666
H	7.094355	-1.484121	0.845078
H	7.516306	2.470434	1.991817
H	8.615683	0.674809	0.514155

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dcpd

C	1.033207	0.676473	1.277710
H	0.923630	1.342682	2.125465
C	0.995899	-0.660737	1.295618
H	0.858542	-1.296177	2.162978
C	1.022497	-1.138055	-0.145966
H	1.322281	-2.176392	-0.301517
C	1.915467	-0.046231	-0.773319
H	1.910896	-0.058999	-1.869389
H	2.945103	-0.073170	-0.406335
C	1.091552	1.113042	-0.173512
H	1.448233	2.127934	-0.358431
C	-0.306138	0.796364	-0.819920
H	-0.312090	1.196864	-1.841028
C	-2.238636	0.165899	0.377728
C	-0.352901	-0.769146	-0.795062
H	-0.378724	-1.174887	-1.810601
C	-1.534055	1.210541	-0.059214
C	-1.632419	-1.158196	-0.018178
H	-2.324899	-1.740474	-0.637704
H	-1.412041	-1.773638	0.863655
H	-1.795899	2.249906	0.116077
H	-3.151869	0.236624	0.961516

4
Acetylene

C	0.055194	-0.409503	0.438548
C	-0.055194	0.409503	-0.438548
H	0.152910	-1.134804	1.214679
H	-0.152910	1.134804	-1.214679

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A1

Mg	0.000055	-0.990323	0.003677
N	1.530675	0.202554	0.004287
N	-1.530636	0.202501	0.002842
C	2.463904	2.467077	0.008795
H	3.099950	2.282364	0.879243
H	2.140029	3.506592	0.023792
H	3.084410	2.303806	-0.877124
C	1.286878	1.525401	0.007164
C	-0.000017	2.099991	0.008599
H	-0.000040	3.181662	0.011768
C	-1.286928	1.525340	0.005861
C	-2.463934	2.467035	0.006359
H	-3.088222	2.298238	-0.875828
H	-2.139985	3.506609	0.013778
C	2.878288	-0.295927	0.000145
C	3.517235	-0.587544	1.206900
C	4.801734	-1.127208	1.199382
H	5.298041	-1.345177	2.139227
C	5.447700	-1.382729	-0.008436
H	6.447767	-1.802330	-0.011788
C	4.806490	-1.096575	-1.212018
H	5.306451	-1.291057	-2.155076
C	3.522036	-0.557044	-1.211087
C	-2.878296	-0.295975	-0.000820
C	-3.519961	-0.579777	1.206363
C	-4.804472	-1.119348	1.199401
H	-5.302886	-1.331322	2.139500
C	-5.447731	-1.382656	-0.008221
H	-6.447828	-1.802189	-0.011112
C	-4.803778	-1.104395	-1.212153
H	-5.301642	-1.304859	-2.155067
C	-3.519275	-0.564885	-1.211784
H	-3.018692	-0.359551	2.145166
H	-3.017179	-0.333714	-2.147486
H	3.014031	-0.372939	2.145986
H	3.021897	-0.320142	-2.146394
H	-3.096260	2.287807	0.880685

52
A2
Mg 0.000662 -0.057545 0.002412
C -0.166658 -2.143018 -1.403398
H -0.511883 -1.732663 -2.346885
C 1.087554 -2.152036 -0.913168
H 1.988597 -1.732486 -1.350506
C 1.046256 -2.938017 0.411501
H 2.013354 -3.257988 0.792386
C 0.167725 -2.147956 1.404119
H 0.514230 -1.741633 2.348865
C -1.086561 -2.151937 0.914024
H -1.986481 -1.731538 1.352884
C -1.047527 -2.933709 -0.413278
H -2.015561 -3.249637 -0.795161
C -0.002174 -4.016209 -0.002650
H 0.324921 -4.639458 -0.837935
H -0.331031 -4.641245 0.830605
N 1.484236 1.248431 0.077982
N -1.483521 1.247661 -0.074739
C 2.465753 3.499199 0.114233
H 3.191603 3.161745 0.858802
H 2.157993 4.516764 0.353422
H 2.979877 3.517859 -0.851639
C 1.277096 2.569976 0.062267
C 0.000024 3.160381 0.000663
H -0.000237 4.242897 0.000209
C -1.276760 2.569308 -0.060721
C -2.465864 3.497860 -0.114277
H -3.189559 3.161030 -0.861241
H -2.158313 4.516030 -0.351099
C 2.795500 0.689666 0.066681
C 3.259359 0.013145 1.198661
C 4.478831 -0.662004 1.165855
H 4.835566 -1.172176 2.055043
C 5.242871 -0.670691 0.001454
H 6.192647 -1.193850 -0.024343
C 4.784599 0.006080 -1.129026
H 5.377199 0.007615 -2.038218
C 3.565750 0.678491 -1.101118
C -2.795005 0.689146 -0.065384
C -3.565347 0.675102 1.102266
C -4.784774 0.003578 1.128049
H -5.377481 0.002890 2.037171
C -5.243433 -0.669345 -0.004526
H -6.193650 -1.191790 0.019517
C -4.479216 -0.657806 -1.168825
H -4.836271 -1.165079 -2.059541
C -3.259192 0.016395 -1.199468
H -3.198932 1.186456 1.987966
H -2.670026 0.049412 -2.112630
H 2.670533 0.044153 2.112126
H 3.199628 1.192579 -1.985341
H -2.982531 3.514409 0.850279

52
A3*
C -0.448927 -2.057897 -1.527190
H -1.380975 -1.981686 -2.059333
C 0.791355 -1.959215 -1.420292
H 1.787741 -1.732415 -1.761118
C 1.196866 -2.862264 0.615587
H 2.267120 -3.033690 0.610017
C 0.558536 -1.942880 1.463517
H 1.069732 -1.230296 2.104120
C -0.837886 -2.065817 1.294963
H -1.603537 -1.458923 1.768812
C -1.084653 -3.065926 0.340304
H -2.075751 -3.434899 0.102945
C 0.166607 -3.895666 0.257400
H 0.326810 -4.463529 -0.655657
H 0.128349 -4.602270 1.103928
Mg -0.013918 -0.133796 -0.109316
N 1.469777 1.178817 0.015188
N -1.510063 1.163874 -0.023350
C 2.437094 3.421634 0.215204
H 3.062841 3.167671 1.075963
H 2.123933 4.460979 0.305569
H 3.065107 3.320628 -0.675046
C 1.250217 2.493182 0.131332
C -0.031585 3.074740 0.175030
H -0.038064 4.152832 0.268721
C -1.305902 2.480797 0.099387
C -2.501241 3.401217 0.153689
H -3.188187 3.190346 -0.670792
H -2.198200 4.446345 0.102677
H -3.060483 3.249291 1.081842
C 2.795989 0.656405 -0.053018
C 3.460573 0.254047 1.108801
C 4.709355 -0.358792 1.027510
H 5.221408 -0.657671 1.936620
C 5.303612 -0.580294 -0.213617
H 6.276870 -1.055178 -0.275204
C 4.647446 -0.174423 -1.374593
H 5.111566 -0.327717 -2.343749
C 3.398498 0.439069 -1.296532
C -2.828823 0.623069 -0.088160
C -3.576319 0.409740 1.074059
C -4.817166 -0.218820 1.004141
H -5.393002 -0.372532 1.911164
C -5.320746 -0.647411 -0.223354
H -6.288470 -1.134552 -0.275282
C -4.580024 -0.435164 -1.384100
H -4.973670 -0.749205 -2.345720
C -3.338180 0.194973 -1.317821
H -2.766824 0.388739 -2.222604
H 2.886934 0.770131 -2.196933
H 3.000686 0.442296 2.075437
H -3.181100 0.746200 2.029077

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A4
Mg 0.049060 -0.342320 0.057511
N 1.571279 0.909288 0.054842
N -1.416554 0.978600 0.037977
C 2.607168 3.130366 0.050403
H 3.157075 3.021430 -0.889370
H 3.293876 2.852822 0.855131
H 2.328443 4.176815 0.168181
C 1.393718 2.234195 0.055068
C 0.127616 2.853928 0.059732
H 0.153190 3.935661 0.071629
C -1.163514 2.295836 0.045173
C -2.331027 3.252015 0.039199
H -1.997288 4.285899 0.116921
H -3.009135 3.036625 0.870053
H -2.910950 3.141771 -0.882082
C 2.877998 0.332574 0.018427
C 3.458925 -0.145418 1.196046
C 4.684891 -0.807425 1.153814
H 5.134831 -1.165265 2.074342
C 5.334821 -1.002040 -0.063178
H 6.289504 -1.515870 -0.094956
C 4.756034 -0.526922 -1.239251
H 5.260217 -0.669867 -2.189585
C 3.530224 0.133658 -1.201749
C -2.758368 0.489007 0.009120
C -3.379958 0.091683 1.196031
C -4.639238 -0.504441 1.161725
H -5.118611 -0.802411 2.088683
C -5.284347 -0.711908 -0.056374
H -6.264845 -1.174987 -0.081787
C -4.668073 -0.311865 -1.241288
H -5.168709 -0.462101 -2.192353
C -3.408234 0.283065 -1.211201
H 3.073525 0.504437 -2.115372
H 2.954001 0.023727 2.143780
H -2.873848 0.262201 2.142569
H -2.921037 0.593866 -2.131389
C -1.462118 -2.792625 -0.259789
H -1.877738 -3.808282 -0.355406
C -0.781139 -2.675790 1.071527
H -1.296357 -2.734111 2.022044
C 0.560282 -2.568349 0.884230
H 1.324070 -2.535209 1.653070
C 0.839807 -2.546779 -0.572086
H 1.833222 -2.483039 -1.003260
C -0.337900 -2.636813 -1.242987
H -0.462280 -2.667376 -2.318268
H -2.318360 -2.119825 -0.408003

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A5*
Mg -0.028219 0.590468 -0.769593
C -0.933828 2.497269 -1.835522
H -1.570404 2.330891 -2.696254
C 0.516734 2.619868 -1.863215
H 1.136118 2.561098 -2.750438
C 0.953925 2.889320 -0.578455
H 1.978505 3.059171 -0.274584
C -1.359276 2.694347 -0.534081
H -2.387242 2.689428 -0.197927
C -0.194296 2.891816 0.329791
H -0.090331 1.903962 1.248861
H -0.240255 3.638817 1.123324
N 1.507596 -0.075830 0.390577
N -1.433357 -0.247795 0.445555
C 2.423863 0.129325 2.676471
H 3.410752 0.175768 2.214788
H 2.356122 -0.802210 3.247856
H 2.314449 0.951866 3.387467
C 1.316638 0.188694 1.659614
C 0.015584 0.640568 2.126586
H 0.018034 0.908767 3.180142
C -1.234044 0.018120 1.709673
C -2.269735 -0.209157 2.776985
H -2.737642 0.745698 3.043205
H -1.799305 -0.604455 3.679179
H -3.054723 -0.890623 2.449288
C 2.732994 -0.636879 -0.082648
C 3.112714 -1.927465 0.289647
C 4.282202 -2.480788 -0.224322
H 4.575370 -3.482776 0.070932
C 5.069839 -1.756657 -1.117190
H 5.979844 -2.191036 -1.516368
C 4.682434 -0.473735 -1.497150
H 5.292555 0.096793 -2.189547
C 3.513508 0.085821 -0.986497
C -2.637194 -0.824973 -0.059967
C -2.557141 -2.051375 -0.722173
C -3.698073 -2.607726 -1.295448
H -3.633330 -3.567604 -1.796863
C -4.916898 -1.937082 -1.222844
H -5.804146 -2.370191 -1.671543
C -4.992362 -0.706965 -0.572584
H -5.938159 -0.178429 -0.515554
C -3.856372 -0.147088 0.005815
H 3.218063 1.091360 -1.271178
H 2.488996 -2.494096 0.974626
H -1.606476 -2.576413 -0.762585
H -3.915134 0.812421 0.510455

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A6
Mg 0.000000 -0.599464 -0.229602
H 0.000002 3.211595 -1.518043
N 1.472712 0.919485 -0.164636
N -1.472707 0.919492 -0.164637
C 2.480665 3.162611 -0.144325
H 3.429034 2.707301 -0.428814
H 2.568968 3.501610 0.894539
H 2.294951 4.045045 -0.761170
C 1.337211 2.193170 -0.246677
C 0.000005 2.857636 -0.475188
H 0.000011 3.785911 0.109185
C -1.337201 2.193176 -0.246668
C -2.480652 3.162619 -0.144297
H -2.294925 4.045077 -0.761104
H -2.568971 3.501576 0.894581
H -3.429018 2.707325 -0.428818
C 2.780390 0.358322 0.062037
C 3.262051 0.243168 1.362996
C 4.485949 -0.384219 1.584152
H 4.865379 -0.477346 2.596096
C 5.216140 -0.894192 0.512922
H 6.166510 -1.385958 0.688971
C 4.722075 -0.775812 -0.785030
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15
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15
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