Supporting information for:

Addition of Carbon–Fluorine Bonds to a Mg(I)–Mg(I) bond: An Equivalent of Grignard Formation in Solution

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Table of Contents

1. General Experimental

All manipulations were carried out using standard Schlenk-line and glovebox techniques under an inert atmosphere of argon or dinitogen. A MBraun Labmaster glovebox was employed, operating at < 0.1 ppm O_2 and < 0.1 ppm H_2O. Solvents were dried over activated alumina from an SPS (solvent purification system) based upon the Grubbs design and degassed before use. Glassware was dried for 12 h at 120 °C prior to use. Benzene-d_6 and toluene-d_8 were stored over molecular sieves and distilled prior to use. NMR-scale reactions were conducted in J. Young's tap tubes and prepared in a glovebox. All heating mentioned was done using silicone oil baths. ^{1}H, ^{19}F and ^{13}C, NMR spectra were obtained on BRUKER 400 MHz or 500 MHz machines unless otherwise stated; all peak intensities are derived internal standard peak with values quoted in ppm. Data was processed using the MestReNova or Topsin software. Carbon-13 NMR data for magnesium fluoroaryl complexes has been assigned to the highest reasonable standard, given the resolution of the data obtained for $^{13}C\{^{1}H\}$ nuclei coupling to multiple ^{19}F nuclei (I=1/2) and quadrapolar ^{25}Mg nuclei (I = 5/2). For reactions containing multiple regioisomers $^{13}C\{^{1}H\}$ NMR data has not been reported. In these cases, further verification of the structures is given by protonation of the Mg–C bond to form hydrodefluorination products which have been compared to genuine synthetic or commercial samples. C^{IV} refers to quartnery carbons.

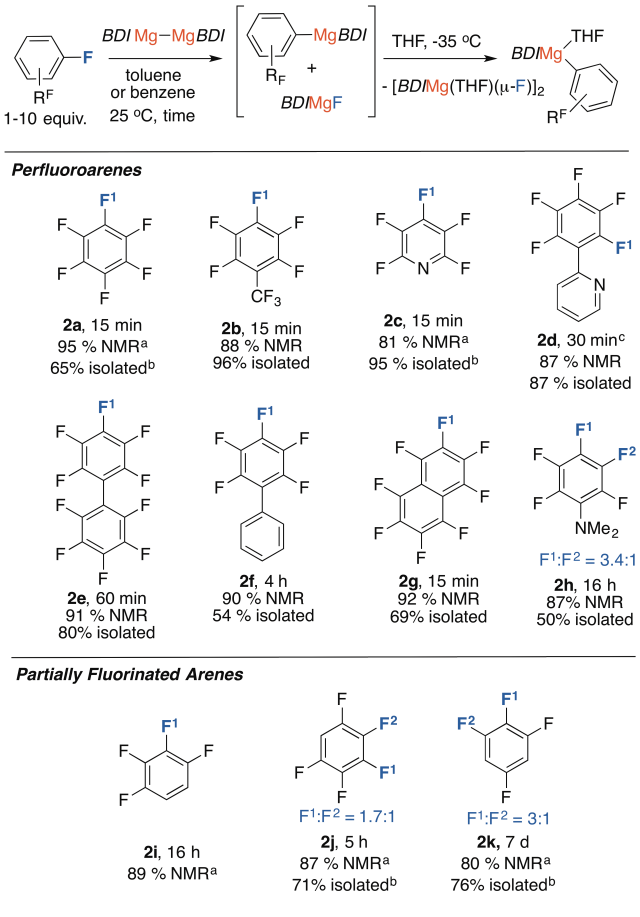
Fluorocarbons, where liquids at 25 ^{o}C were dried over activated molecular sieves and freeze-pump-thaw degassed before use. All other other chemicals were purchased from Fluorochem, Sigma Aldrich or Alfa Aeser and used without purification unless stated. *BDI*H, ^{Mes}*BDI*H,[i] *BDI*Mg–Mg*BDI*,[ii] and ^{Mes}*BDI*Mg–Mg*BDI*^{Mes},[iii] where prepared by literature procedures. *N,N*-Dimethylamino pentafluorobenzene was prepared by alkylation of the corresponding aniline according to the literature procedure.[iv]

2. Synthetic Procedures

2.1 General procedures for the oxidative addition of carbon–fluorine bonds to Mg–Mg:

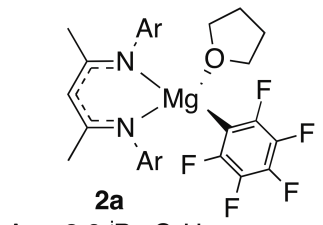
NMR scale: *BDI*Mg–Mg*BDI* (10 mg, 0.011 mmol) was dissolved in benzene-d_6 (0.6 mL) and the solution transferred into a Young's tap NMR tube equipped with a capillary tube containing a ferrocene standard solution; a t=0 ^{1}H NMR spectrum was recorded. The fluoroarene (0.11 mmol, 10 equiv.) was added using a micropipette and the reaction mixture was monitored by ^{1}H and ^{19}F NMR spectroscopy. NMR yields were recorded by comparison against the ferrocene internal standard, δ = 4.00 ppm.

Preparative scale (2a-j): *BDI*Mg–Mg*BDI* (100 mg, 0.11 mmol, approx. 0.03 M) was dissolved in toluene (4 mL) and the fluoroarene (0.11 mmol, 1 equiv. for non-volatile substrates **2d-g**; 0.16 mmol, 1.5 equiv. for volatile substrates **2a-c, 2h-j**) was added at 25 °C. After stirring the reaction mixture at this temperature for 24-48 h, tetrahydrofuran (0.1 mL) was added and the solution was transferred to the freezer. Crystals of [*BDI*Mg(μ-F)(THF)]$_2$ formed after overnight standing at -35 °C and were isolated by filtration.[v] The solvent was removed from the resultant supernatant under reduced pressure and the crude product extracted into n-hexane (2 mL). Complexes **2a-j** were isolated as solids by either removing the solvent, or following crystallization or precipitation by storage of the solutions at -35 °C.



a,bThe fluorine highlighted in blue is that of the carbon–fluorine bond that transforms to a carbon–magnesium bond, for regioisomeric products F^1 is the major and F^2 the minor product.cIsolated without THF coordinated.

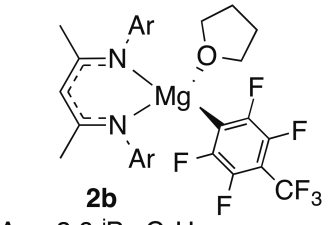
Table S1. Scope of the carbon–fluorine bond functionalization procedure.



2a

Ar = 2,6-^{i}Pr$_2$C$_6$H$_3$

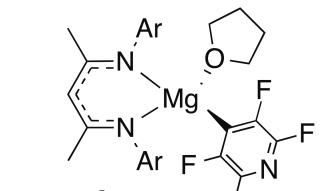
Compound 2a (50 mg, 0.07 mmol, 65 %[vi]): ^{1}H NMR (400 MHz, benzene-d_6, 298 K) δ (ppm): 0.82 (d, 6H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.01 (bm, 4H, O(CH$_2$)$_2$(CH_2)$_2$), 1.12 (d, 6H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.15 (d, 6H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.19 (d, 6H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.68 (s, 6H, CH_3), 3.17 (bm, 4H, O(CH_2)$_2$(CH$_2$)$_2$), 3.25 (sept, 2H, CH(CH$_3$)$_2$, $^3J_{HH}$ = 6.8 Hz), 3.33 (sept, 2H, CH(CH$_3$)$_2$, $^3J_{HH}$ = 6.8 Hz), 4.99 (s, 1H, CH), 7.00-7.13 (m, 6H, CH); ^{19}F NMR (376.5 MHz, benzene-d_6, 298 K) δ (ppm): -161.9 – -161.5 (m, 2F, *m*-C$_6$F$_5$), -157.7 (t, 1F, *p*-C$_6$F$_5$, $^3J_{FF}$ = 19.2 Hz), -112.7 (bs, 2F, *o*-C$_6$F$_5$); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 298 K) δ (ppm): 24.3 (*C*H$_3$), 24.6 (2 x *C*H$_3$), 24.6 (*C*H$_3$), 24.8 (*C*H$_3$), 24.9 (O(CH$_2$)$_2$(*C*H$_2$)$_2$), 27.9 (*C*H(CH$_3$)$_2$), 28.3 (*C*H(CH$_3$)$_2$), 69.6 (O(*C*H$_2$)$_2$(CH$_2$)$_2$), 95.5 (C(CH$_3$)*C*HC(CH$_3$)), 123.6 (*C*H), 124.5 (*C*H), 125.6 (*C*H), 136.6 (dm, *C*F, C$_6$F$_5$, *J* = 200.0 Hz), 139.9 (bd, *C*F, C$_6$F$_5$, *J* = 244.0 Hz), 142.1 (C^{IV}), 143.6 (C^{IV}), 145.4 (C^{IV}), 151.1 (dm, *C*F, C$_6$F$_5$, *J* = 219.0 Hz), 169.2 (*C*=N), *ipso* C^{IV} not observed; Anal. Calc. (MgC$_{39}$H$_{49}$F$_5$N$_2$O): C, 68.77; H, 7.25; N, 4.11. Found: C, 68.63; H, 7.29; N, 4.13.



2b

Ar = 2,6-^{i}Pr$_2$C$_6$H$_3$

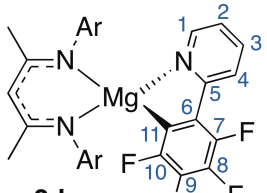
Compound 2b (79 mg, 0.11 mmol, 96 %): ^{1}H NMR (400 MHz, benzene-d_6, 298 K) δ (ppm): 0.79 (d, 6H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 0.99 (bm, 4H, O(CH$_2$)$_2$(CH_2)$_2$), 1.09 (d, 6H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.13 (d, 6H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.18 (d, 6H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.67 (s, 6H, CH_3), 3.14 (bm, 4H, O(CH_2)$_2$(CH$_2$)$_2$), 3.23 (sept, 2H, CH(CH$_3$)$_2$, $^3J_{HH}$ = 6.8 Hz), 3.28 (sept, 2H, CH(CH$_3$)$_2$, $^3J_{HH}$ = 6.8 Hz), 4.98 (s, 1H, CH), 7.02 (m, 2H, CH), 7.09 (m, 4H, CH); ^{19}F NMR (376.5 MHz, benzene-d_6, 298 K) δ (ppm): -142.2 – -141.8 (m, 2F, *m*-C$_6$F$_4$CF$_3$), -112.5 (bs, 2F, *o*-C$_6$F$_4$CF$_3$), -55.8 (t, 3F, C$_6$F$_4$C*F*$_3$, $^4J_{FF}$ = 21.4 Hz); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 298 K) δ (ppm): 24.2 (*C*H$_3$), 24.5 (*C*H$_3$), 24.5 (*C*H$_3$), 24.6 (*C*H$_3$), 24.7 (*C*H$_3$), 24.9 (O(CH$_2$)$_2$(*C*H$_2$)$_2$), 27.9 (*C*H(CH$_3$)$_2$), 28.3 (*C*H(CH$_3$)$_2$), 69.7 (O(*C*H$_2$)$_2$(CH$_2$)$_2$), 95.6 (C(CH$_3$)*C*HC(CH$_3$)), 123.6 (*C*H), 124.5 (*C*H), 125.6 (*C*H), 143.0 (dd, *C*F, C$_6$F$_4$CF$_3$, *J* = 263.2 Hz), 142.1 (C^{IV}), 143.5 (C^{IV}), 145.2 (C^{IV}), 151.1 (dm, *C*F, C$_6$F$_4$CF$_3$, *J* = 218.5 Hz), 169.4 (*C*=N), *ipso* C^{IV}, *para* C^{IV} and *C*F$_3$ not observed; Anal. Calc. (MgC$_{49}$H$_{49}$F$_7$N$_2$O): C, 65.71; H, 6.76; N, 3.83. Found: C, 65.60; H, 6.82; N, 3.94.



2c

Ar = 2,6-^{i}Pr$_2$C$_6$H$_3$

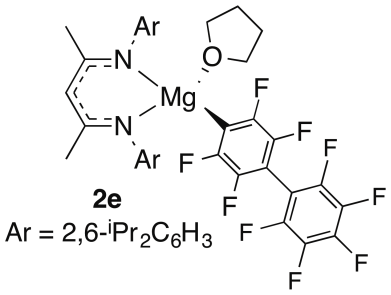
Compound 2c (71 mg, 0.11 mmol, 95 %): ^{1}H NMR (400 MHz, benzene-d_6, 298 K) δ (ppm): 0.75 (d, 6H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 0.96 (bm, 4H, O(CH$_2$)$_2$(CH_2)$_2$), 1.07 (d, 6H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.13 (d, 6H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.18 (d, 6H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.67 (s, 6H, CH_3), 3.28 (bm, 4H, O(CH_2)$_2$(CH$_2$)$_2$), 3.24 (sept, 4H, $^3J_{HH}$ = 6.4 Hz), 4.98 (s, 1H, C*H*), 6.98-7.03 (m, 2H, C*H*), 7.00-7.09 (m, 4H, C*H*); ^{19}F NMR (376.5 MHz, benzene-d_6, 298 K) δ (ppm): -119.4 (bs, 2F, *o*- C$_5$F$_4$N), -97.9 – -97.5 (m, 2F, *m*-C$_5$F$_4$N); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 298 K) δ (ppm): 24.2 (*C*H$_3$), 24.4 (*C*H$_3$), 24.5 (*C*H$_3$), 24.6 (*C*H$_3$), 24.9 (O(CH$_2$)$_2$(*C*H$_2$)$_2$), 24.9 (*C*H$_3$), 27.8 (*C*H(CH$_3$)$_2$), 28.3 (*C*H(CH$_3$)$_2$), 69.7 (O(*C*H$_2$)$_2$(CH$_2$)$_2$), 95.6 (C(CH$_3$)*C*HC(CH$_3$)), 123.6 (*C*H), 124.5 (*C*H), 125.6 (*C*H), 142.0 (C^{IV}), 143.4 (ddd, *C*F, C$_5$F$_4$N, *J* = 198.0 Hz, *J* = 24.0 Hz, *J* = 6.0 Hz), 143.5 (C^{IV}), 145.1 (C^{IV}), 147.3 (dm, *C*F, C$_5$F$_4$N, *J* = 185.0 Hz), 154.7 (t, C^{IV}, C$_5$F$_4$N, *J* = 63.0 Hz), 169.4 (*C*=N); Anal. Calc. (MgC$_{38}$H$_{49}$F$_4$N$_3$O): C, 68.72; H, 7.44; N, 6.33. Found: C, 68.60; H, 7.58; N, 6.22.



2d

Ar = 2,6-^{i}Pr$_2$C$_6$H$_3$

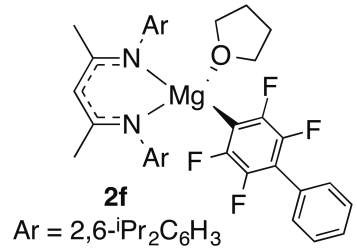
Compound 2d (66 mg, 0.10 mmol, 87 %): ^{1}H NMR (400 MHz, benzene-d_6, 298 K) δ (ppm): 0.26 (d, 6H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.13 (d, 6H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.29 (d, 6H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.57 (d, 6H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.73 (s, 6H, CH_3), 2.90 (sept, 2H, C*H*(CH$_3$)$_2$, $^3J_{HH}$ = 6.8 Hz), 3.65 (sept, 2H, C*H*(CH$_3$)$_2$, $^3J_{HH}$ = 6.8 Hz), 4.95 (s, 1H, C*H*), 6.38 (ddd, 1H, Py-C^2*H*), 6.88 (dd, 2H, Ar*H*, $^3J_{HH}$ = 7.6 Hz, $^4J_{HH}$ = 1.6 Hz), 6.92 (m, 1H, Py-C^3*H*), 6.99 (t, 2H, Ar*H*, $^3J_{HH}$ = 7.6 Hz), 7.14 (dd, 2H, Ar*H*, $^3J_{HH}$ = 7.6 Hz, $^4J_{HH}$ = 1.6 Hz), 7.88 (dm, 1H, Py-C^4*H* $^3J_{HH}$ = 8.4 Hz), 8.31 (dm, 1H, Py-C^1*H*, $^3J_{HH}$ = 4.8 Hz); ^{19}F NMR (376.5 MHz, benzene-d_6, 298 K) δ (ppm): -157.7 (t, 1F, *m*^{b}-C$_6$F$_4$), -150.3 – -150.0 (m, 1F, *p* or *m*^{a}-C$_6$F$_4$), -136.5 – - 136.3 (m, 1F, *p* or *m*^{a}-C$_6$F$_4$), -106.8 – 106.5 (m, 1F, *o*-C$_6$F$_4$); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 298 K) δ (ppm): 23.5 (CH(*C*H$_3$)$_2$), 23.7 (2 x *C*H$_3$), 24.0 (d, CH(*C*H$_3$)$_2$, *J* = 3.5 Hz[vii]), 24.1 (CH(*C*H$_3$)$_2$), 24.3 (CH(*C*H$_3$)$_2$), 27.7 (*C*^{A}H(CH$_3$)$_2$), 29.1 (*C*^{B}H(CH$_3$)$_2$), 94.2 (C(CH$_3$)*C*HC(CH$_3$)), 122.2 (*C*^{2}H, C$_5$H$_4$N), 123.4 (*C*H), 123.7 (*C*H), 124.0 (d, *C*^{4}H, C$_5$H$_4$N, *J* = 22.4 Hz), 125.4 (*C*H), 140.1 (*C*^{3}H, C$_5$H$_4$N), 141.7 (C^{IV}), 142.2 (C^{IV}), 144.2 (C^{IV}), 147.4 (*C*^{1}H, C$_5$H$_4$N), 169.4 (*C*=N), *C*F and C^{IV} signals 5-11 could not be identified; Anal. Calc. (MgC$_{40}$H$_{45}$F$_4$N$_3$): C, 71.91; H, 6.79; N, 3.64. Found: C, 71.78; H, 6.68; N, 6.44.



2e

Ar = 2,6-^{i}Pr$_2$C$_6$H$_3$

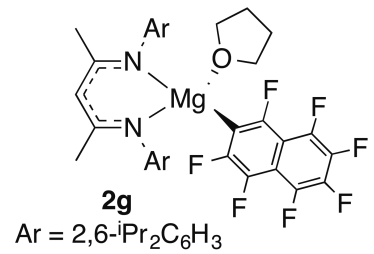
Compound 2e (75 mg, 0.09 mmol, 80 %): ^{1}H NMR (400 MHz, benzene-d_6, 298 K) δ (ppm): 0.96 (d, 6H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 1.03 (bm, 4H, O(CH$_2$)$_2$(CH_2)$_2$), 1.18 (d, 12H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 1.22 (d, 6H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 1.72 (s, 6H, CH_3), 3.22 (bm, 4H, O(CH_2)$_2$(CH$_2$)$_2$), 3.29 (sept, 2H, CH(CH$_3$)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 3.43 (sept, 2H, CH(CH$_3$)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 5.04 (s, 1H, CH), 7.00-7.14 (m, 6H, CH); ^{19}F NMR (376.5 MHz, benzene-d_6, 298 K) δ (ppm): -162.1 – -161.8 (m, 2F, -C$_6$F$_4$-*m*-C$_6$F$_5$), -155.0 (t, 1F, $^{3}J_{FF}$ = 21.4 Hz, -C$_6$F$_4$-*p*-C$_6$F$_5$), -140.2 – -139.8 (m, 2F, *m*-C$_6$F$_4$-C$_6$F$_5$), -139.6 – -139.4 (m, 2F, -C$_6$F$_4$-*o*-C$_6$F$_5$), -113.1 (bs, 2F, *o*-C$_6$F$_4$-C$_6$F$_5$); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 298 K) δ (ppm): 24.3 (*C*H$_3$), 24.6 (*C*H$_3$), 24.7 (*C*H$_3$), 24.8 (*C*H$_3$), 25.0 (O(CH$_2$)$_2$(*C*H$_2$)$_2$), 28.0 (*C*H(CH$_3$)$_2$), 28.4 (*C*H(CH$_3$)$_2$), 69.7 (O(*C*H$_2$)$_2$(CH$_2$)$_2$), 95.6 (C(CH$_3$)*C*HC(CH$_3$)), 103.7 (t, C$_{12}$F$_9$, C^{IV}, *J* = 20.0 Hz), 105.0 (t, C$_{12}$F$_9$, C^{IV}, *J* = 22.1 Hz), 123.6 (*C*H), 124.6 (*C*H), 125.6 (*C*H), 137.8 (dm, C$_{12}$F$_9$, *C*F, *J* = 255.0 Hz),142.1 (C^{IV}), 143.1 (dm, C$_{12}$F$_9$, *C*F, *J* = 256.0 Hz), 143.6 (C^{IV}), 145.4 (C^{IV}), 150.2 (dm, C$_{12}$F$_9$, CF, *J* = 220.0 Hz), 169.3 (*C*=N), assignment of the remaining three C^{IV} and CF signals was not possible due to complicated ^{13}C-^{19}F coupling; Anal. Calc. (MgC$_{45}$H$_{49}$F$_9$N$_2$O): C, 65.18; H, 5.96; N, 3.38. Found: C, 65.07; H, 6.16; N, 3.47.



2f

Ar = 2,6-^{i}Pr$_2$C$_6$H$_3$

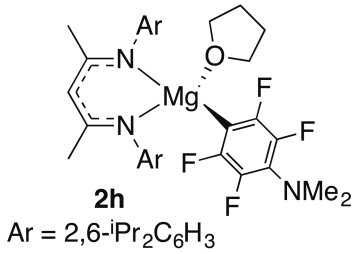
Compound 2f (45 mg, 0.06 mmol, 54 %[viii]): ^{1}H NMR (400 MHz, benzene-d_6, 298 K) δ (ppm): 0.98 (d, 6H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.4 Hz), 1.0 (bm, 4H, O(CH$_2$)$_2$(CH_2)$_2$), 1.15-1.27 (m, 18H, CH(CH_3)$_2$), 1.73 (s, 6H, CH_3), 3.28 (bm and sept, 6H, O(CH_2)$_2$(CH$_2$)$_2$ and CH(CH$_3$)$_2$), 3.50 (sept, 2H, CH(CH$_3$)$_2$, $^{3}J_{HH}$ = 6.4 Hz), 5.04 (s, 1H, CH), 7.06-7.15 (m, 9H, CH), 7.57 (dm, 2H, $^{3}J_{HH}$ = 6.8 Hz); ^{19}F NMR (376.5 MHz, benzene-d_6, 298 K) δ (ppm): -145.1 – -144.8 (m, 2F, *m*-C$_6$F$_4$-C$_6$H$_5$), -113.9 (bs, 2F, *o*-C$_6$F$_4$-C$_6$H$_5$); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 298 K) δ (ppm): 24.3 (*C*H$_3$), 24.7 (3 x *C*H$_3$), 24.9 (*C*H$_3$), 24.9 (O(CH$_2$)$_2$(*C*H$_2$)$_2$), 28.0 (*C*H(CH$_3$)$_2$), 28.4 (*C*H(CH$_3$)$_2$), 69.7 (O(*C*H$_2$)$_2$(CH$_2$)$_2$), 95.5 (C(CH$_3$)*C*HC(CH$_3$)), 119.3 (t, C^{IV}, C$_{12}$F$_4$H$_5$, *J* = 17.0 Hz), 123.6 (*C*H), 124.5 (*C*H), 125.5 (*C*H), 128.2 (*C*H), 128.6 (*C*H), 130.8 (*C*H), 134.7 (t, C^{IV}, C$_{12}$F$_4$H$_5$, *J* = 86.0 Hz), 142.1 (C^{IV}), 143.3 (dm, *C*F, C$_{12}$F$_4$H$_5$, *J* = 251.0 Hz), 143.7 (C^{IV}), 145.6 (C^{IV}), 151.6 (dm, *C*F, C$_{12}$F$_4$H$_5$, *J* = 218.0 Hz), 169.1 (*C*(CH$_3$)CH*C*(CH$_3$)), *ipso* C^{IV} signal could not be assigned; Anal. Calc. (MgC$_{45}$H$_{54}$F$_4$N$_2$O): C, 73.12; H, 7.36; N, 3.79. Found: C, 72.99; H, 7.45; N, 3.83.



2g

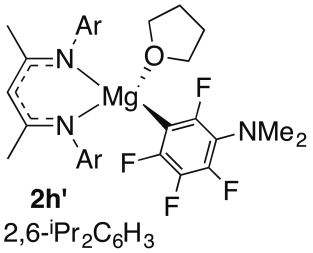
Ar = 2,6-^{i}Pr$_2$C$_6$H$_3$

Compound 2g (60 mg, 0.08 mmol, 69 %): ^{1}H NMR (400 MHz, benzene-d_6, 298 K) δ (ppm): 0.79 (d, 6H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 0.99 (bm, 4H, O(CH$_2$)$_2$(CH_2)$_2$), 1.09 (d, 6H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 1.13 (d, 6H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 1.18 (d, 6H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 1.67 (s, 6H, CH_3), 3.28 (m, 6H, CH(CH$_3$)$_2$ and O(CH_2)$_2$(CH$_2$)$_2$), 3.41 (bs, 2H, CH(CH$_3$)$_2$), 5.00 (s, 1H, CH), 7.00-7.12 (m, 6H, CH); ^{19}F NMR (376.5 MHz, benzene-d_6, 298 K) δ (ppm): -160.5 – -160.3 (m, 1F, C$_{10}$F$_7$), -159.0 – -158.6 (m, 1F, C$_{10}$F$_7$), -154.2 – -153.7 (m, 1F, C$_{10}$F$_7$), -148.8 – -148.4 (m, 1F, C$_{10}$F$_7$), -146.7 – -146.1 (m, 1F, C$_{10}$F$_7$), -107.7 (bs, 1F, *o*-C$_{10}$F$_7$), -90.7 (bs, 1F, *o*-C$_{10}$F$_7$); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 298 K) δ (ppm): 24.3 (*C*H$_3$), 24.6 (2 x *C*H$_3$), 24.7 (*C*H$_3$), 24.8 (*C*H$_3$), 25.0 (O(CH$_2$)$_2$(*C*H$_2$)$_2$), 28.0 (*C*H(CH$_3$)$_2$), 28.3 (*C*H(CH$_3$)$_2$), 69.7 (O(*C*H$_2$)$_2$(CH$_2$)$_2$), 95.7 (C(CH$_3$)*C*HC(CH$_3$)), 123.7 (*C*H), 124.4 (*C*H), 125.6 (*C*H), 142.1 (C^{IV}), 143.4 (C^{IV}), 145.5 (C^{IV}), 169.6 (*C*=N), ^{13}C resonances for the fluoroaryl unit could not be assigned; Due to the low purity of this complex attempts to acquire satisfactory CHN analysis failed.



2h

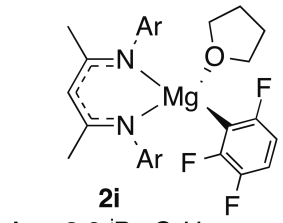
Ar = 2,6-^{i}Pr$_2$C$_6$H$_3$



2h'

Ar = 2,6-^{i}Pr$_2$C$_6$H$_3$

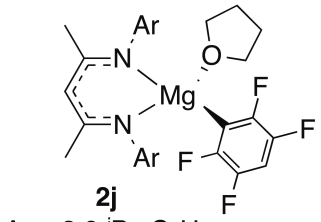
Compound 2h and 2h' (3.4:1, 40 mg, 0.06 mmol, 50 %[8]): ^{1}H NMR (400 MHz, benzene-d_6, 298 K) δ (ppm): 0.83-1.20 (bm, CH(CH_3)$_2$ and O(CH$_2$)$_2$(CH_2)$_2$ for **2h** and **2h'**), 1.70 (s, **2h'** CH_3), 1.72 (s, **2h** CH_3), 3.20-3.55 (bm, CH(CH_3)$_2$ and O(CH_2)$_2$(CH$_2$)$_2$ for **2h** and **2h'**), 4.98 (s, **2h'** CH), 5.01 (s, **2h** CH_3), 7.05-7.15 (bs, CH for **2h** and **2h'**); ^{19}F NMR (376.5 MHz, benzene-d_6, 298 K) δ (ppm): -165.2 (m, 1F, **2h'** *m* or *p*- C$_6$F$_4$NMe$_2$), -149.9 (m, 2F, **2h** *m*-C$_6$F$_4$NMe$_2$), -145.2 (m, 1F, **2h'** *m* or *p*- C$_6$F$_4$NMe$_2$), -114.7 (bs, 2F, **2h** *o*-C$_6$F$_4$NMe$_2$), -95.2 (bs, 1F, **2h'** *o*-C$_6$F$_4$NMe$_2$), one ^{19}F signal not observed; Due to the sensitivity of these complexes repeated attempts to acquire satisfactory CHN analysis failed. Addition of a drop of methanol gave a mixture of *N,N*-dimethylamino-2,3,5,6-tetrafluorobenzene (^{19}F NMR (376.5 MHz, benzene-d_6, 298 K) δ (ppm): -151.8 (m, 2H, *o*-C$_6$F$_4$HNMe$_2$), -141.1 (m, 2H, *m*-C$_6$F$_4$HNMe$_2$)) and *N,N*-dimethylamino-2,3,4,6-tetrafluorobenzene (^{19}F NMR (376.5 MHz, benzene-d_6, 298 K) δ (ppm): -164.8 (m, 1H), -142.3 (m, 1H), -141.4 (m, 1H), -124.5 (m, 1H)). The minor component was assigned by comparison of the ^{19}F NMR data against a synthetic sample of *N,N*-dimethylamino-2,3,4,5-tetrafluorobenzene.



2i

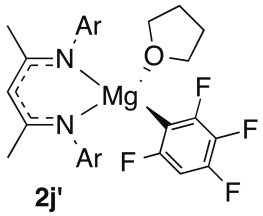
Ar = 2,6-^{i}Pr$_2$C$_6$H$_3$

Compound 2i (71 mg, 0.11 mmol, 100 %[ix]): ^{1}H NMR (400 MHz, benzene-d_6, 298 K) δ (ppm): 0.91 (bs, 6H, CH(CH_3)$_2$), 1.06 (bs, 4H, O(CH$_2$)$_2$(CH_2)$_2$), 1.12-1.29 (bm, 18H, CH(CH_3)$_2$), 1.73 (s, 6H, CH_3), 3.29 (bm, 6H, CH(CH_3)$_2$ and O(CH_2)$_2$(CH$_2$)$_2$), 3.46 bs, 2H, CH(CH_3)$_2$), 5.02 (s, 1H, CH_3), 6.49 (m, 1H, CH, C$_6$F$_3$H$_3$), 6.69 (m, 1H, CH, C$_6$F$_3$H$_3$), 7.05-7.15 (bs, 6H, CH); ^{19}F NMR (376.5 MHz, benzene-d_6, 298 K) δ (ppm): -145.8 – -146.1 (m, 1F, *m*-C$_6$F$_3$H$_2$), -110.1 – -108.9 (bs, 1F, *o*-C$_6$F$_3$H$_2$), -91.0 – -90.0 (bs, 1F, *o*-C$_6$F$_3$H$_2$); ^{13}C{^{1}H} NMR (125 MHz, benzene-d_6, 298 K) δ (ppm): 23.9 (*C*H$_3$), 24.3 (*C*H$_3$), 24.4 (*C*H$_3$), 24.6 (O(CH$_2$)$_2$(*C*H$_2$)$_2$), 27.6 (*C*H(CH$_3$)$_2$), 27.9 (*C*H(CH$_3$)$_2$), 69.2 (O(*C*H$_2$)$_2$(CH$_2$)$_2$), 95.1 (C(CH$_3$)*C*HC(CH$_3$)), 108.8 (dm, *C*H, C$_6$F$_3$H$_2$, J = 38.3), 115.0 (dd, *C*H, C$_6$F$_3$H$_2$, J = 20.6 Hz, J = 9.5 Hz), 125.01 (*C*H), 128.0 (*C*H), 142.7 (C^{IV}), 143.4 (C^{IV}), 145.5 (C^{IV}), 146.8 (ddd, CF, C$_6$F$_3$H$_2$, J = 245.0, J = 24.1, J = 4.8), 156.1 (ddd, C^{IV}, C$_6$F$_3$H$_2$, J = 222.5, J = 32.8, J = 9.1), 165.5 (dd, C^{IV}, C$_6$F$_3$H$_2$, J = 219.9, J = 29.1), 168.9 (*C*=N), *ipso* C^{IV} signal could not be assigned; Due to the sensitivity of these complexes repeated attempts to acquire satisfactory CHN analysis failed.



2j

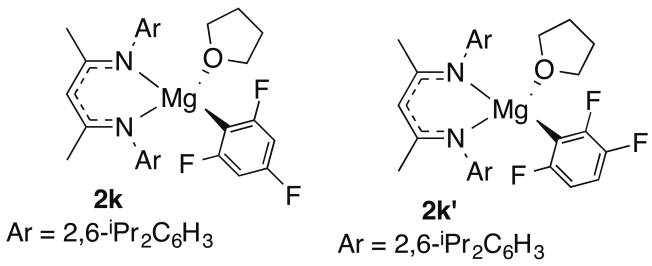
Ar = 2,6-^{i}Pr$_2$C$_6$H$_3$



2j'

Ar = 2,6-^{i}Pr$_2$C$_6$H$_3$

Compound 2j and **2j'** (1.7:1, 66 mg, 0.1 mmol, 71 %[x]): ^{1}H NMR (400 MHz, benzene-d_6, 298 K) δ (ppm): 0.78-1.27 (m, **2j 2j'**, CH(CH_3)$_2$ and O(CH$_2$)$_2$(CH_2)$_2$), 1.71 (s, **2j** and **2j'** CH_3), 3.14-3.48 (m, **2j**, **2j'** CH(CH$_3$)$_2$ and O(CH_2)$_2$(CH$_2$)$_2$), 4.99 (s, **2j'** C*H*), 5.01 (s, **2j** C*H*), 6.44 (m, **2j'** C$_6$F$_4$H), 6.62 (m, **2j** C$_6$F$_4$H), 7.02-7.14 (m, **2j**, **2j'** C*H*). ^{19}F NMR (376.5 MHz, benzene-d_6, 298 K) δ (ppm): -169.1 (m, 1F, **2j'**, *m or p*-C$_6$F$_4$H), -141.3 (m, 2F, **2j**, *m*-C$_6$F$_4$H), -138.2 (m, 1F, **2j'**, *m or p*-C$_6$F$_4$H), -115.1 (, 2F, **2j**, *o*-C$_6$F$_4$H);), -108.1 (bs, 1H, **2j'**, *o*-C$_6$F$_4$H), -87.6 (bs, 1H, **2j'**, *o*-C$_6$F$_4$H). Due to the sensitivity of these complexes repeated attempts to acquire satisfactory CHN analysis failed. Addition of a drop of methanol gave a mixture of 1,2,4,5-tetrafluorobenzene, 1,2,3,5-tetrafluorobenzene and 1,2,3,4,5-pentafluorobenzene (from minor C–H activation pathway).



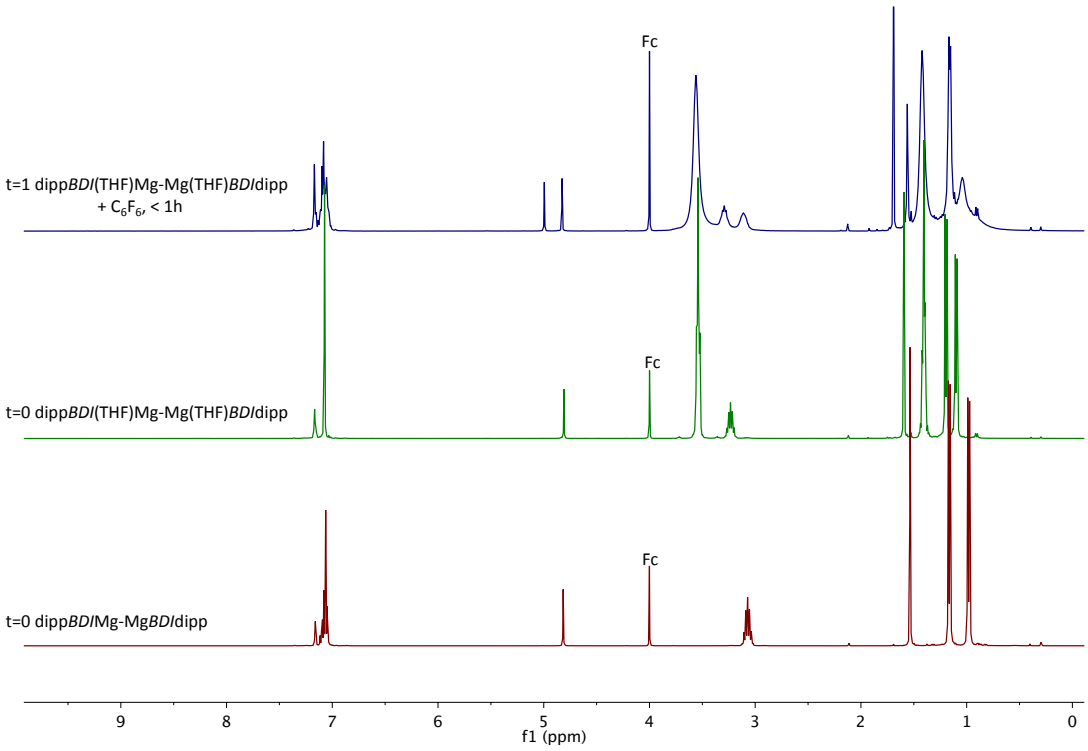
Preparative scale (2k and **2k'):** *BDI*Mg–Mg*BDI* (100 mg, 0.11 mmol, approx. 0.03 M) was dissolved in toluene (4 mL) and the 1,2,3,5-tetrafluorobenzene (1.1 mmol, 10 equiv.) was added at 25 °C. After stirring the reaction mixture at this temperature for 7 days, tetrahydrofuran (0.25 mL) was added and the solution was transferred to the freezer. Crystals of [*BDI*Mg(μ-F)(THF)]$_2$ formed after overnight standing at -35 °C and were isolated by filtration. The solvent was removed from the resultant supernatant under reduced pressure and the crude product extracted into n-hexane (2 mL). Complexes **2k**/**2k'** could be further purified by crystallization (**2k** and **2k'** 3:1, 64 mg, 0.1 mmol, 76 %[xi]): ^{1}H NMR (400 MHz, benzene-d_6, 298 K) δ (ppm): 0.85-1.28 (bm, **2k**, **2k'** CH(CH_3)$_2$ and O(CH$_2$)$_2$(CH_2)$_2$)), 1.68 (s, **2k'** CH_3), 1.73 (s, **2k** CH_3), 3.15-3.53 (bm, **2k, 2k'** CH(CH$_3$)$_2$ and O(CH$_2$)$_2$(CH_2)$_2$)**)**, 4.85 (s, **2k'** CH), 4.99 (s, 1H, **2k** CH), 6.42-6.57 (m, **2k**, **2k'** CH^F), 7.05-7.16 (bm, CH of **2k**, **2k'**); ^{19}F NMR (376.5 MHz, benzene-d_6, 298 K) δ (ppm): -135.5 (m, 1F, **2k'**, $C_6F_3H_2$), -119.2 (m, 1F, **2k'**, $C_6F_3H_2$), -117.0 (m, 1F, **2k'**, $C_6F_3H_2$)**,** -114.7 (m, 1F, **2k**, *p*-$C_6F_3H_2$), -81.6 (bs, 2F, **2k**, *o*-$C_6F_3H_2$); Addition of a drop of methanol gave a mixture of 1,2,3-trifluorobenzene, 1,2,4-trifluorobenzene and 1,2,3,5-tetrafluorobenzene (from minor C–H activation pathway).

[*BDI*Mg(μ-F)(THF)]$_2$: ^{1}H NMR (400 MHz, benzene-d_6, 298 K) δ (ppm): 0.97 (d, 12H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.10 (d, 12H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.50 (bm, 4H, O(CH$_2$)$_2$(CH_2)$_2$), 1.49 (s, 6H, CH_3), 3.02 (sept, 4H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 3.54 (bs, 4H, O(CH_2)$_2$(CH$_2$)$_2$), 4.84 (s, 1H, CH), 6.97-7.12 (m, 6H, CH); ^{19}F NMR (376.5 MHz, benzene-d_6, 298 K) δ (ppm): -187.9.

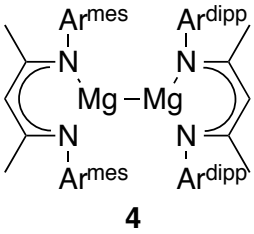
[*BDI*Mg(μ-F)]$_2$: ^{1}H NMR (400 MHz, benzene-d_6, 298 K) δ (ppm): 0.96 (d, 12H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.10 (d, 12H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.48 (s, 6H, CH_3), 3.02 (sept, 4H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 4.84 (s, 1H, CH), 6.97-7.12 (m, 6H, CH); ^{19}F NMR (376.5 MHz, benzene-d_6, 298 K) δ (ppm): -187.9.

NMR scale reaction of *BDI*Mg–Mg*BDI*.(THF)$_2$ with C_6F_6: *BDI*Mg–Mg*BDI* (10 mg, 0.011 mmol) was dissolved in benzene-d$_6$ (0.6 mL) and the solution transferred into a Young's tap NMR tube equipped with a capillary tube containing a ferrocene standard solution; a t=0 ^{1}H NMR spectrum was recorded. To the solution was added a drop of tetrahydrofuran where an immediate colour change from yellow to orange was observed. A further ^{1}H NMR was recorded, clearly showing the formation of the THF adduct, as evidenced by the upfield shifts in the NMR signals. Hexafluorobenzene (13 μL, 0.11 mmol, 10 equiv.) was added using a micropipette. After approximately 45 minutes a ^{1}H NMR spectrum was recorded, showing full conversion of *BDI*Mg–Mg*BDI* to *BDI*MgC$_6$F$_5$.THF and 0.5 [*BDI*Mg(μ-F)(THF)]$_2$.

Figure S1: Stack plot of the formation of *BDI*Mg–Mg*BDI*.$(THF)_2$ and subsequent reaction with C_6F_6 to form *BDI*MgC_6F_5.THF (**2a**) and 0.5 [*BDI*Mg(μ-F)$(THF)]_2$ at 25 °C in benzene-d_6.



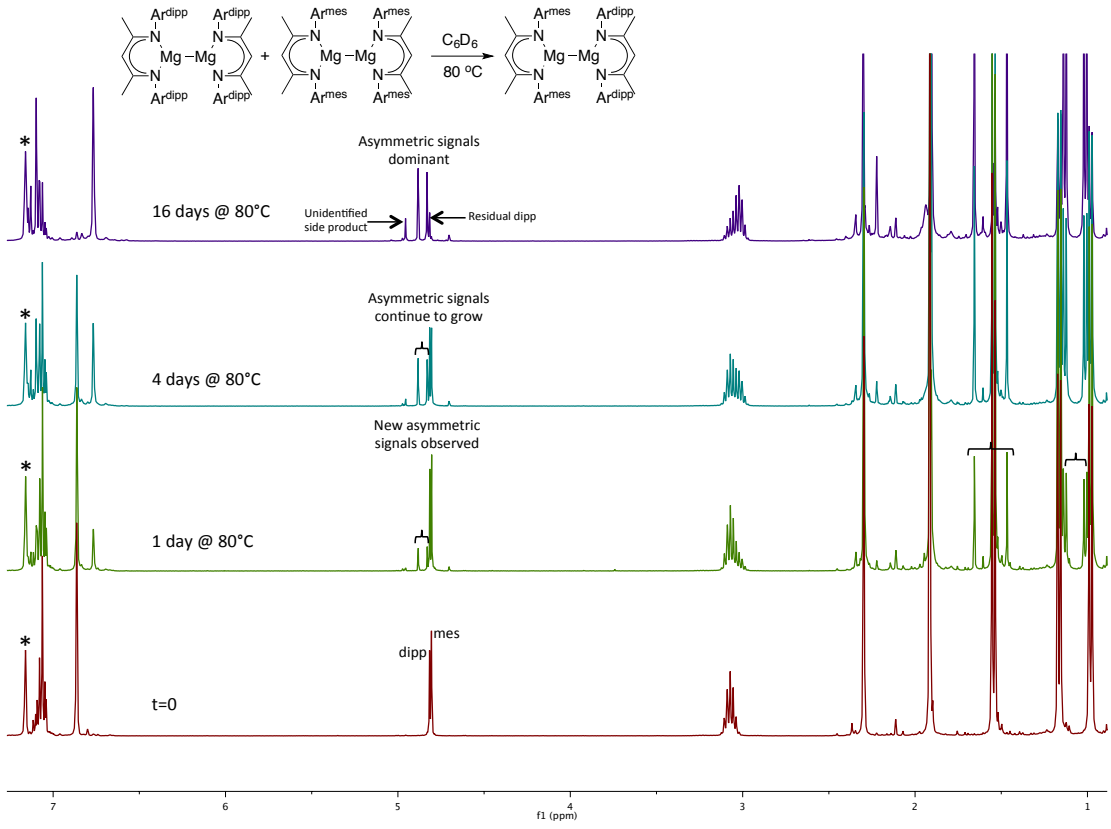
2.2 Cross-over experiment to form 4



4

Synthesis of **4** **^{mes}BDIMg–MgBDI^{dipp}:** To a Young's tap ampoule was added **^{mes}BDIMg–MgBDI^{mes}** (73 mg, 0.1 mmol) and **^{dipp}BDIMg–MgBDI^{dipp}** (90 mg, 0.1 mmol) in toluene (5 mL). The ampoule has heated at 353 K and the reaction was monitored by taking NMR aliquots. After 10 days it was necessary to add more **^{mes}BDIMg–MgBDI^{mes}** to the reaction (**^{mes}BDIMg–MgBDI^{mes}** has lower solution stability and degrades over time). After a total of 2 weeks at 353 K, the solution was filtered to remove a significant amount of black precipitate and the filtrate was reduced *in vacuo*. The yellow crystalline solid was washed with hexane (3 mL) to yield compound **4** in high purity (70 mg, 0.09 mmol, 43 %). ^{1}H NMR (400 MHz, benzene-d_6, 298 K) δ (ppm): 1.01 (d, 12H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 1.13 (d, 12H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 1.47 (s, 6H, C(CH_3)CHC(CH_3)^{mes}), 1.66 (s, 6H, C(CH_3)CHC(CH_3)^{dipp}), 1.91 (s, 12H, *o*-CH_3^{mes}), 2.30 (s, 6H, *p*-CH_3^{mes}), 3.02 (sept, 4H, CH(CH$_3$)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 4.83 (s, 1H, C(CH$_3$)CHC(CH$_3$)^{mes}), 4.88 (s, 1H, C(CH$_3$)CHC(CH$_3$)^{dipp}), 6.77 (s, 4H, CH^{mes}), 7.07-7.15 (m, 6H, CH^{dipp});^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 298 K) δ (ppm): 18.8 (*o*-CH_3^{mes}), 20.8 (*p*-CH_3^{mes}), 23.0 (C(CH_3)CHC(CH_3)^{mes}), 23.4 (CH(CH_3)$_2$), 23.6 (C(CH_3)CHC(CH_3)^{dipp}), 24.4 (CH(CH_3)$_2$), 28.0 (CH(CH$_3$)$_2$), 95.0 (C(CH$_3$)CHC(CH$_3$)^{dipp}), 95.7 (C(CH$_3$)CHC(CH$_3$)^{mes}), 123.3 (CH^{dipp}), 124.8 (CH^{dipp}), 128.0 (CH^{dipp}), 129.3 (CH^{mes}), 131.0 (C^{IV}), 132.1 (C^{IV}), 141.5 (C^{IV}), 144.8 (C^{IV}), 145.7 (C^{IV}), 166.6 (C(CH$_3$)CHC(CH$_3$) dipp or mes), 166.9 (C(CH$_3$)CHC(CH$_3$) dipp or mes); Anal. Calc. ($Mg_2C_{52}H_{70}N_4$): C, 78.09; H, 8.82; N, 7.01. Found: C, 77.94; H, 8.86; N, 7.00.

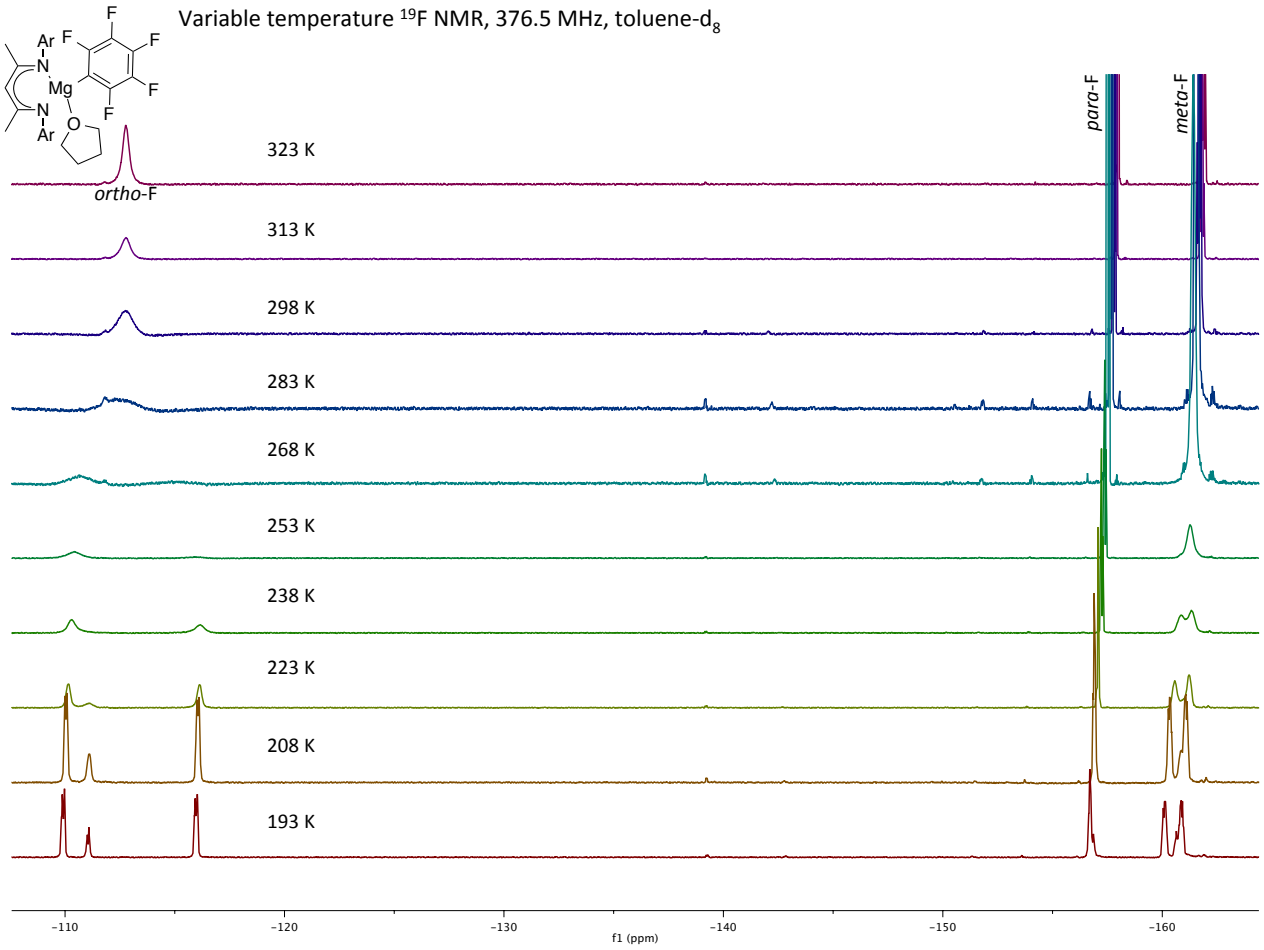
Figure S2: Stack plot of the formation of compound **4** from compounds **1** and **3** at 80 °C over time; solvent peak marked with asterisk.



3. Variable Temperature ^{19}F NMR data

Variable temperature ^{19}F NMR data was collected on both isolated and purified samples of **2a** along with the reaction mixture obtained from the addition of hexafluorobenzene to **1**. The data are presented below. **2a** shows a decoalescence of the *ortho*- and *meta*-fluorine resonances upon cooling suggesting hindered rotation about the Mg–C bond. This process has been quantified. A minor species is also observed at low temperature and may be due to an as yet unidentified ligand redistribution / Schlenk equilibrium process.

Figure S3: Variable temperature ^{19}F NMR spectra of compound **2a** over the temperature range 193 – 323 K.



VT NMR data was fitted using line shape analysis with the DNMR programme integrated into Topsin v3.1. The ^{19}F resonances of **2a** were fitted over the 223 to 333 K range with an initial line broadening factor of 2 Hz. Fits for *k* were optimized to the experimental data with reasonable accuracy and the modelled data are presented below, a minor unassigned species observable at the lowest temperatures was not included in the model. The activation parameters for the exchange process are as follows: $\mathbf{\Delta H^{\ddagger} = 7.6\ kcal\ mol^{-1}}$, $\mathbf{\Delta S^{\ddagger} = -15.0\ cal\ K^{-1}\ mol^{-1}}$, $\mathbf{\Delta G^{\ddagger}_{298K} = 12.1\ kcal\ mol^{-1}}$.

Figure S4. Modelled ^{19}F resonances of **2a** from 223 to 323K.

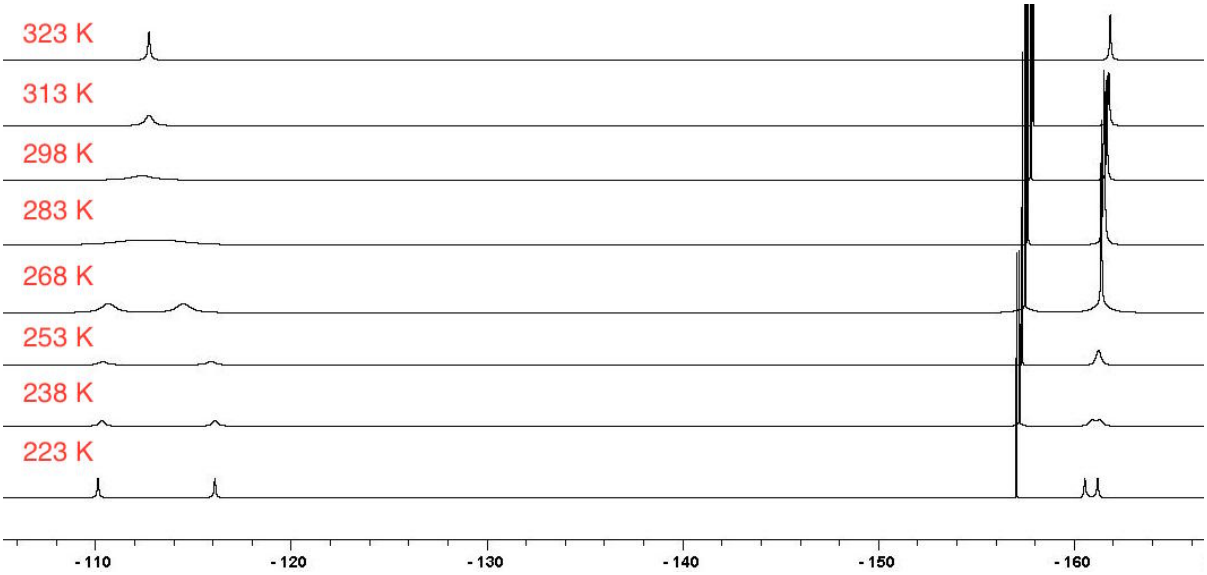
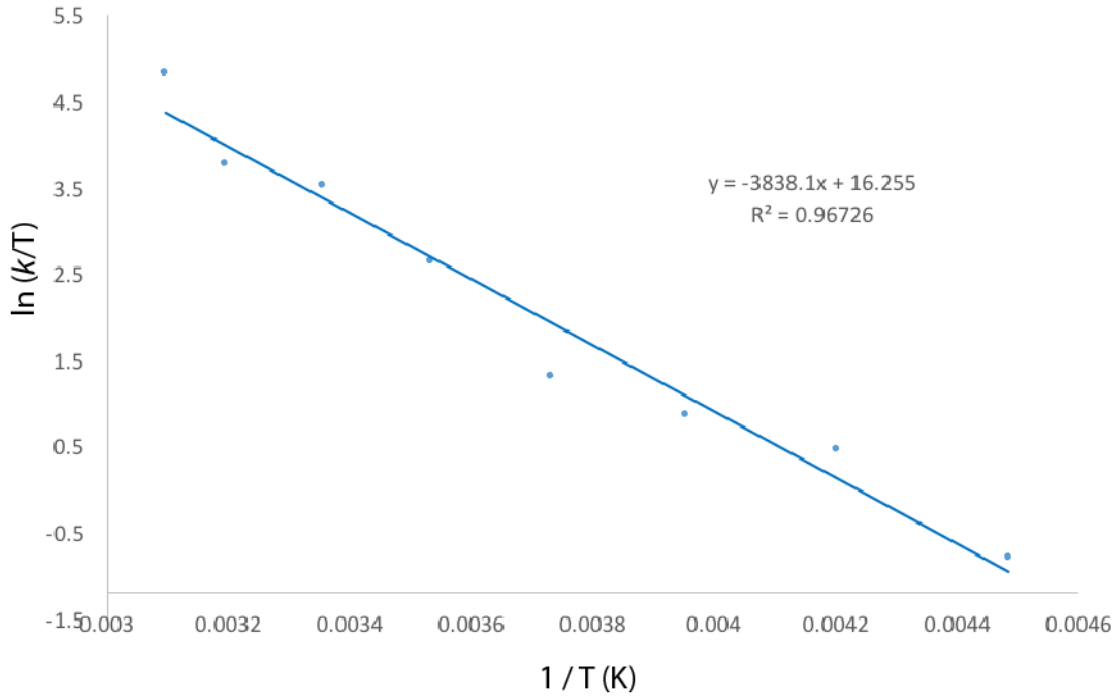
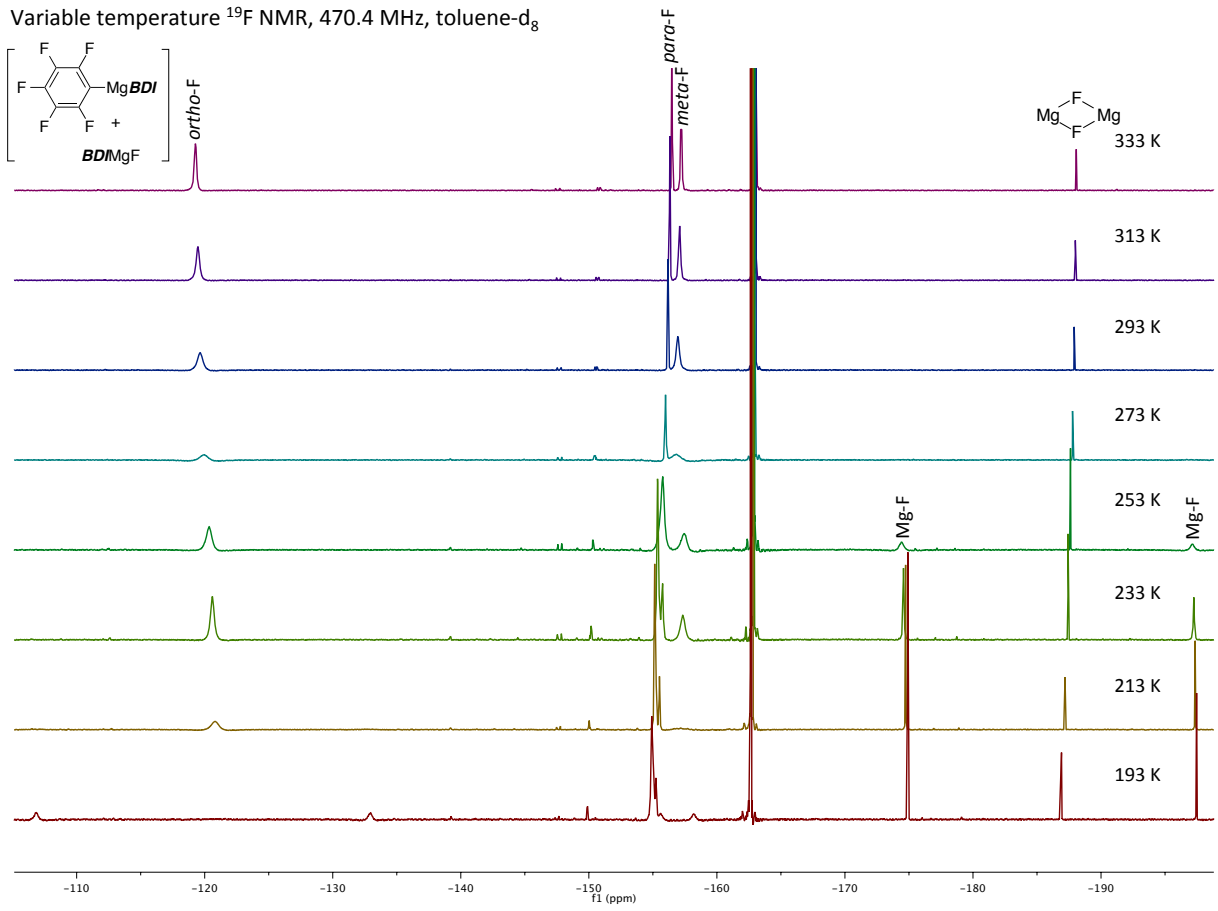


Figure S5. Eyring analysis: ln(k/T) versus 1/T.



The reaction mixture from the addition of **1** to hexafluorobenzene also shows a decoalescence of the *ortho*- and *meta*-fluorine resonances upon cooling suggesting hindered rotation about the Mg–C bond. In addition to [*BDI*Mg(μ-F)]$_2$, observable at room temperature, two new magnesium fluoride resonances become clear at low temperatures. While we have been unable to resolve this complex processes addition of a drop of THF yields a mixture of **2a** and [*BDI*Mg(μ-F)(THF)].

Figure S6: Variable temperature ^{19}F NMR spectra of the products from the reaction of compound **1** with hexafluorobenzene over the temperature range 193 – 333 K.



4. X-ray Crystallographic Data

The X-ray crystal structure of ^{mes}BDIMg–MgBDI^{mes}

This structure is the same as that reported by Bonyhady *et al*.[iii] in 2010 (CCDC refcode GUPQUE). The complex was found to have crystallographic C_2 symmetry about an axis that bisects the Mg1···Mg1A vector.

The X-ray crystal structure of 2a

The crystal of **2a** that was studied was found to be a three component twin in a *ca*. 44:12:44 ratio – despite the comparatively low contribution of component two, ignoring this component and modelling the data as a two component twin using components 1 and 3 gave poor results. The lattice for component 2 is related to that of component 1 by the approximate twin law [–0.21 0.80 –0.12 –1.20 –0.18 –0.12 –0.37 0.04 0.96], whilst that for component 3 is related to that of component 1 by the approximate twin law [1.00 –0.04 –0.01 0.00 –1.00 0.00 0.00 0.00 1.00]. Despite a *ca*. 47 hour data collection, the data collected for the crystal of **2a** was weak (overall I/σ *ca*. 3.1), and the presence of three differently orientated lattices in the crystal was clearly a contributing factor in this weak scattering.

The structure was found to contain two crystallographically independent complexes, **2a-A** and **2a-B**. The THF ligand in complex **2a-A** was found to be disordered, with two orientations of *ca*. 77 and 23% occupancy identified for the middle two carbon atoms of the C_4 chain [C42A and C43A]. The geometries of both orientations were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and only the non-hydrogen atoms of the major occupancy orientation were refined anisotropically (those of the minor occupancy orientation were refined isotropically).

The X-ray crystal structure of 2b

The C36-based CF_3 unit in the structure of **2b** was found to be disordered. Two orientations were identified of *ca*. 80 and 20% occupancy, their geometries were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and only the atoms of the major occupancy orientation were refined anisotropically (those of the minor occupancy orientation were refined isotropically).

The X-ray crystal structure of 2d

Close inspection of the diffraction data for the crystal of **2d** that was studied showed a small (*ca*. 13%) but not insignificant twin component. Attempts to model this twinning, however, did not improve upon the results obtained without considering the twinning, and so no twin models were used in the final refinements. This unresolved twining may, however, be the root cause of some anomalous intensities.

The X-ray crystal structure of 4

The crystal of **4** that was studied was found to be a two component twin in a *ca*. 81:19 ratio, with the two lattices related by the approximate twin law [–1.00 0.00 –0.62 0.00 –1.00 0.00 0.00 0.00 1.00]. The complex was found to have crystallographic C_2 symmetry about an axis that passes through C2, Mg1, Mg2 and C22.

The X-ray crystal structure of [*BDI*Mg(μ-F)(THF)]$_2$

The complex in the structure of **[*BDI*Mg(μ-F)(THF)]$_2$** was found to have crystallographic C_{2h} symmetry; the C_2 axis passes through the two bridging fluorine atoms F1 and F1A, whilst the mirror plane is perpendicular to this and passes through the metal centres Mg1 and Mg1A. The unique O20-based THF ligand was found to be disordered across the mirror plane, and this disorder was modelled by using one complete 50% occupancy orientation for the THF ligand (the operation of the mirror plane generates a second 50% occupancy orientation). The geometry of this unique orientation was optimised, and the non-hydrogen atoms were refined anisotropically. The C31-based included hexane solvent molecule has crystallographic C_{2h} symmetry.

This structure is isomorphous to the (μ-H)$_2$ analogue reported by Green *et al*.[xii] in 2008 (CCDC refcode XOLXEC), though that reports the unit cell using the *C*-face setting whereas the body-centred, *I*, setting is reported here. The (μ-F)$_2$ complex itself was reported in 2002 as a different solvate (and in a different unit cell) by Hao *et al*.[xiii] (CCDC refcode QADPOB).

Figure S7: The crystal structure of the C_2-symmetric complex **^{mes}BDIMg–MgBDI^{mes}** (50% probability ellipsoids).

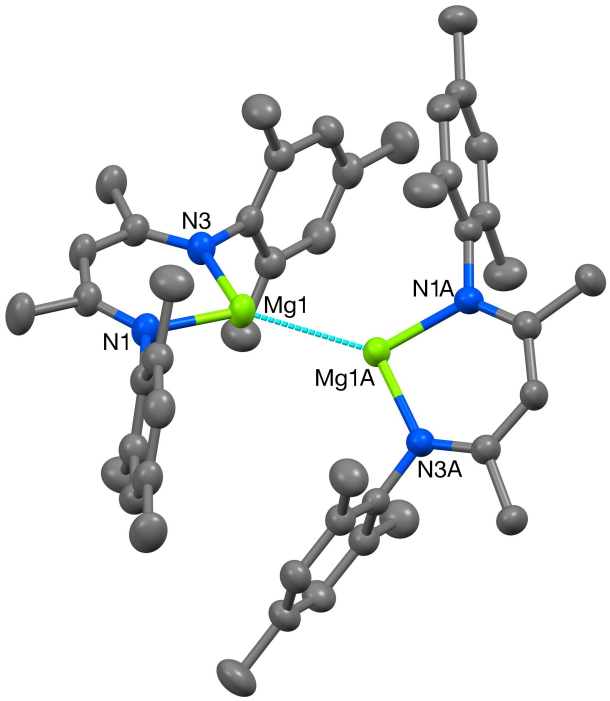


Figure S8: The structure one (**2a-A**) of the two independent complexes present in the crystal of **2a** (50% probability ellipsoids).

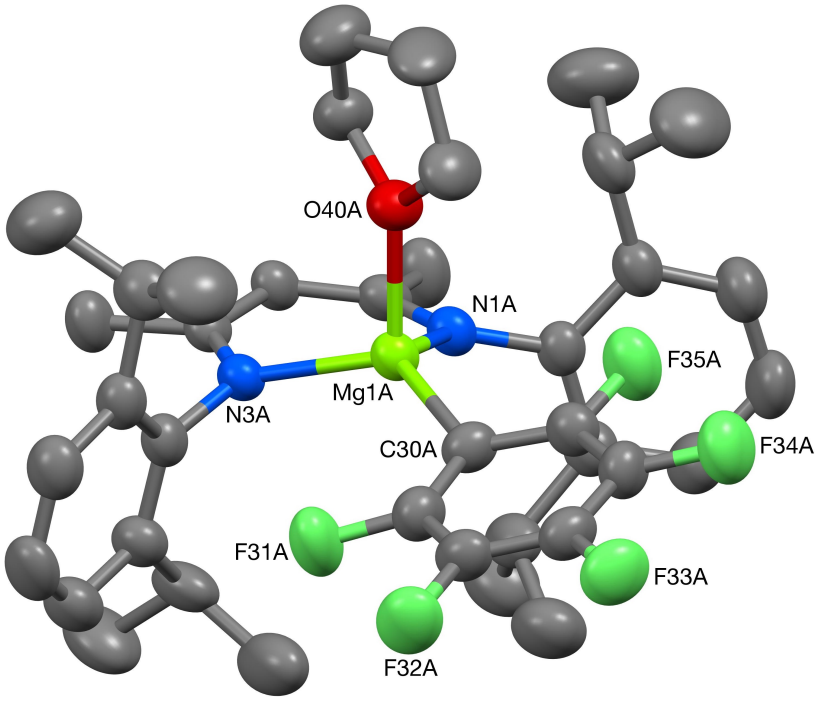


Figure S9: The structure one (**2a-B**) of the two independent complexes present in the crystal of **2a** (50% probability ellipsoids).

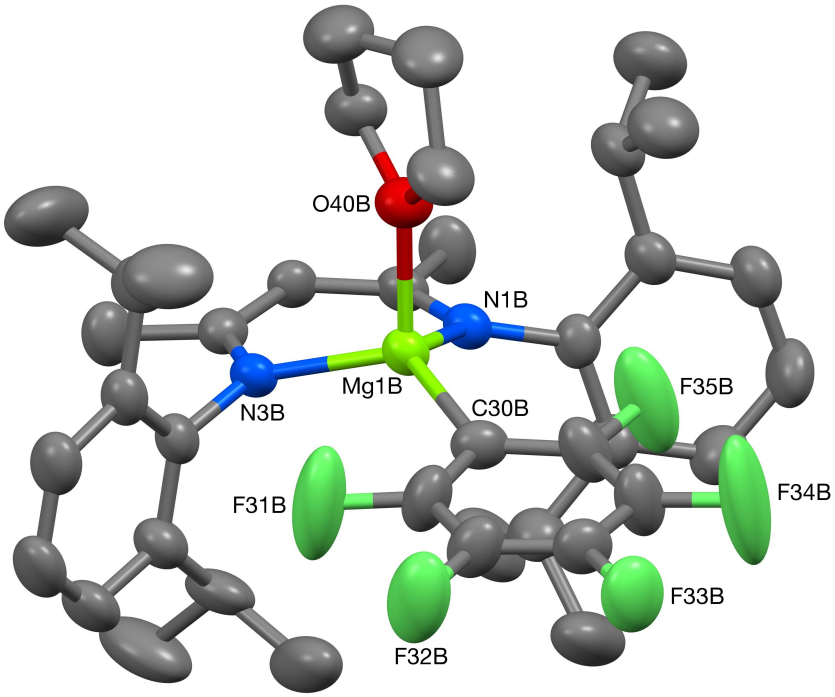


Figure S10: The crystal structure of **2b** (50% probability ellipsoids).

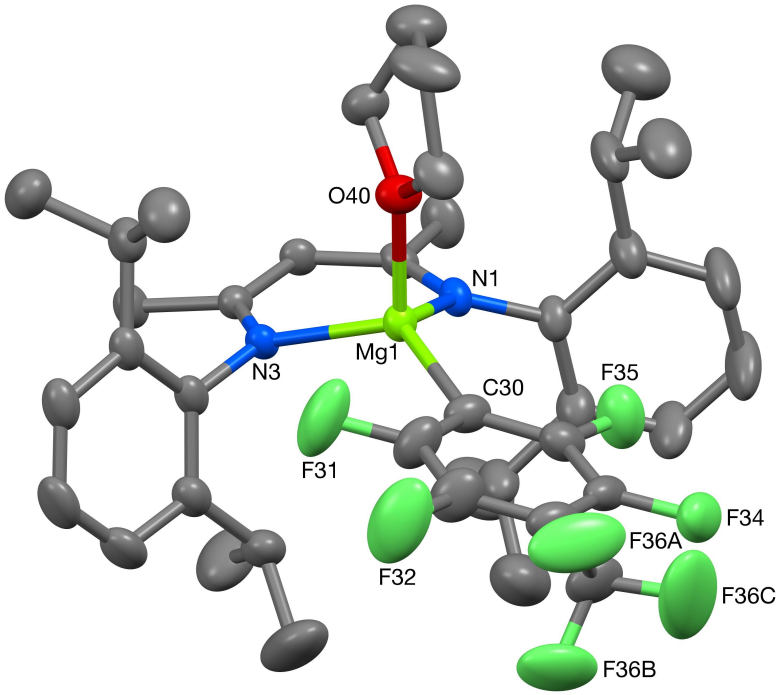


Figure S11: The crystal structure of **2c** (50% probability ellipsoids).

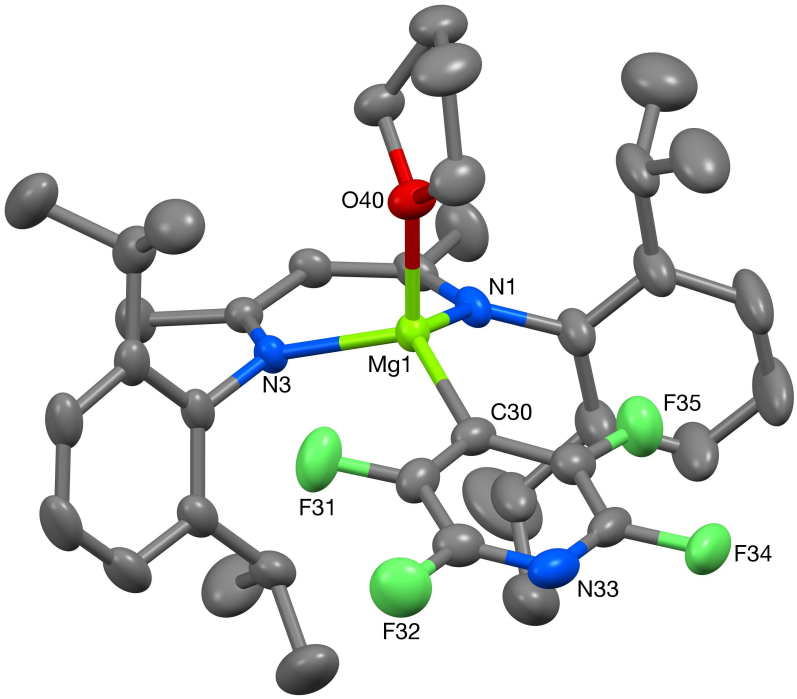


Figure S12: The crystal structure of **2d** (50% probability ellipsoids).

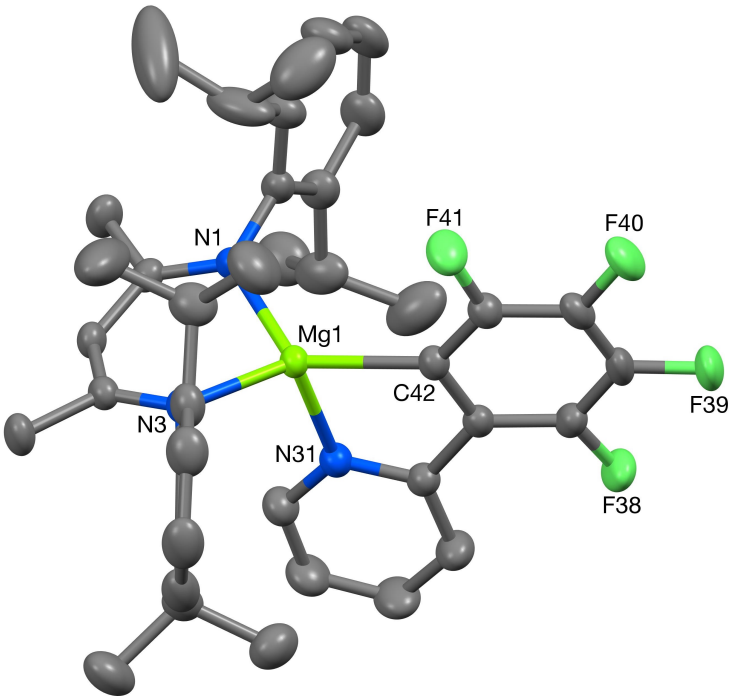


Figure S13: The crystal structure of the C_2-symmetric complex **4** (50% probability ellipsoids).

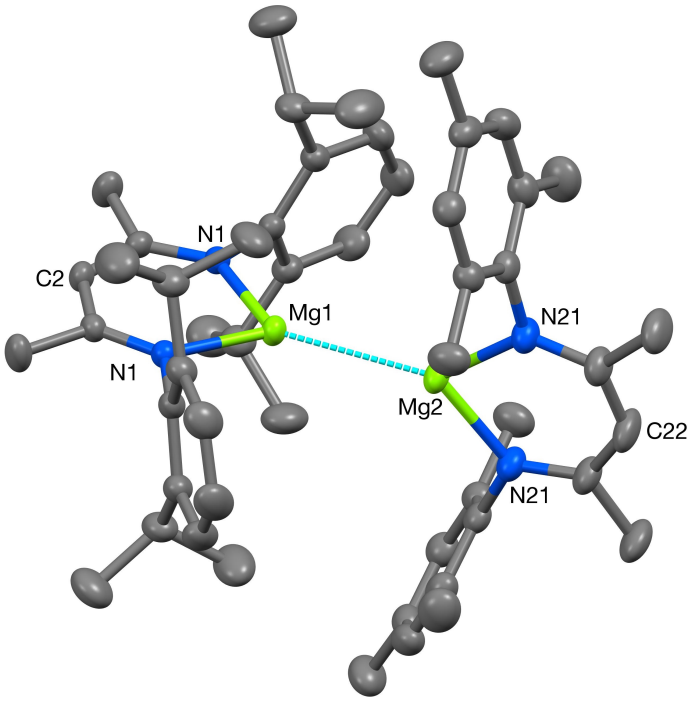


Figure S14: The crystal structure
of the C_{2h}-symmetric complex **[*BDI*Mg(μ-F)(THF)]$_2$** (50% probability ellipsoids).

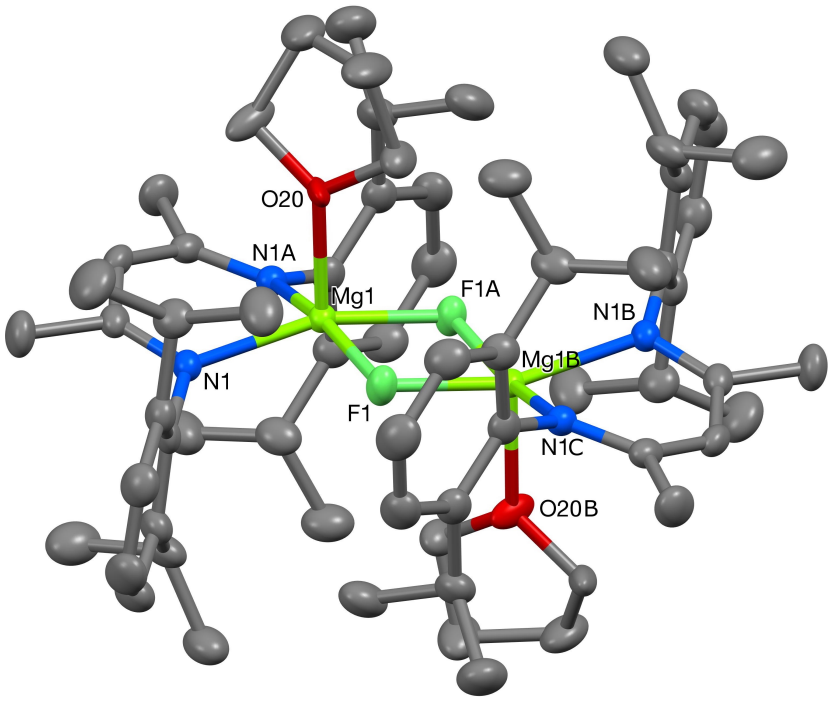


Table S2. Crystal Data, Data Collection and Refinement Parameters for the structures of **^{mes}BDIMg–MgBDI^{mes}**, **2a**, **2b**, **2c**, **2d**, **4** and **[*BDI*Mg(μ-F)(THF)]**.

data	^{mes}BDIMg–MgBDI^{mes}	2a	2b	2c
formula	$C_{46}H_{58}Mg_2N_4$	$C_{39}H_{49}F_5MgN_2O$	$C_{40}H_{49}F_7MgN_2O$	$C_{38}H_{49}F_4MgN_3O$
solvent	—	—	—	—
formula weight	715.58	681.11	731.12	664.11
colour, habit	pale yellow blocks	colourless plates	colourless blocks	pale brown blocks
temperature / K	173(2)	173(2)	173(2)	173(2)
crystal system	monoclinic	triclinic	monoclinic	monoclinic
space group	*P*2/*n* (no. 13)	*P*-1 (no. 2)	*I*2/*a* (no. 15)	*C*2/*c* (no. 15)
***a* / Å**	13.4857(6)	12.8601(11)	14.9886(4)	34.4121(8)
***b* / Å**	8.2720(4)	15.9403(14)	14.8728(4)	14.8141(3)
***c* / Å**	19.9081(8)	18.1538(13)	36.1312(9)	14.8714(4)
α / deg	90	84.244(7)	90	90
β / deg	101.058(4)	89.380(6)	98.802(3)	100.005(2)
γ / deg	90	88.675(7)	90	90
***V* / Å^3**	2179.59(16)	3701.6(5)	7959.6(3)	7465.9(3)
Z	2 [b]	4 [c]	8	8
***D*$_c$ / g cm^{-3}**	1.090	1.222	1.220	1.182
radiation used	Cu-Kα	Cu-Kα	Mo-Kα	Mo-Kα
μ / mm^{-1}	0.742	0.896	0.109	0.100
2θ max / deg	148	150	56	57
no. of unique reflns				
measured (R_{int})	4199 (0.0411)	33969 (0.0922)	8344 (0.0233)	7786 (0.0228)
obs, $\|F_o\| > 4\sigma(\|F_o\|)$	2876	11317	6112	5779

no. of variables	243	896	487	434
R_1**(obs),** wR_2**(all)** [a]	0.0502, 0.1472	0.0715, 0.2208	0.0555, 0.1456	0.0485, 0.1317

Table S2. continued…

data	**2d**	**4**	**[*BDI*Mg(μ-F)(THF)]$_2$**
formula	$C_{40}H_{45}F_4MgN_3$	$C_{52}H_{70}Mg_2N_4$	$C_{66}H_{98}F_2Mg_2N_4O_2$
solvent	—	—	C_6H_{14}
formula weight	668.10	799.74	1152.27
colour, habit	colourless blocks	yellow blocky needles	colourless blocks
temperature / K	173(2)	173(2)	173(2)
crystal system	monoclinic	monoclinic	monoclinic
space group	*C*2/*c* (no. 15)	*C*2/*c* (no. 15)	*I*2/*m* (no. 12)
***a* / Å**	31.6147(4)	18.2530(6)	11.9516(5)
***b* / Å**	16.0108(2)	13.8247(3)	18.2934(7)
***c* / Å**	15.04066(19)	21.1714(6)	15.7645(6)
α / deg	90	90	90
β / deg	101.3341(12)	110.993(3)	99.934(4)
γ / deg	90	90	90
***V* / Å^3**	7464.77(17)	4987.8(3)	3395.0(2)
Z	8	4 [b]	2 [d]
***D*$_c$ / g cm^{-3}**	1.189	1.065	1.127
radiation used	Cu-Kα	Cu-Kα	Mo-Kα
μ / mm^{-1}	0.830	0.692	0.087
2θ max / deg	148	147	56
no. of unique reflns			
measured (*R*$_{int}$)	7157 (0.0193)	8912 (0.0505)	3484 (0.0189)
obs, |*F*$_o$| > 4σ(|*F*$_o$|)	6030	7263	2678
no. of variables	443	274	221
***R*$_1$(obs),** ***wR*$_2$(all)** [a]	0.0387, 0.1083	0.0458, 0.1363	0.0467, 0.1171

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]\}^{1/2}$; $w^{-1} = \sigma^2(F_o^2) + (aP)^2 + bP$. [b] The molecule has crystallographic C_2 symmetry. [c] The are two crystallographically independent complexes. [d] The molecule has crystallographic C_{2h} symmetry.

Table S2 provides a summary of the crystallographic data for the structures of **1**, **2a**, **2b**, **2c**, **2d**, **4** and **[*BDI*Mg(μ-F)(THF)]$_2$**. Data were collected using Agilent Diffraction Xcalibur PX Ultra A (**1**, **2a**, **2d** and **4**) and Xcalibur 3 E (**2b**, **2c** and **[*BDI*Mg(μ-F)(THF)]$_2$**) diffractometers, and the structures were refined using the SHELXTL, SHELX-97, and SHELX-2013 program systems.[xiv] CCDC 1497405 to 1497411.

5. DFT Calculations

Calculations were conducted in Gaussian09. Unless indicated otherwise, all minima were confirmed by frequency calculations and solid-state data were used as an input for the atom coordinates. A series of functionals and basis-sets were tested, benchmarking the data against solid-state data on **2b, 2d** along with the known structures of [*BDI*Mg(μ-F)(THF)]$_2$ and [*BDI*Mg–Mg*BDI*]. The results of these experiments are presented in section 4.1, the ωB97X functional and a hybrid 6,31G+(d,p) (C,H,N,O,F) / Lanl2DZ (Mg) basis-set gave the best results in terms of computational cost and accurate modelling of key bond angles and distances about the Mg centre.

5.1 Benchmarking Studies

Table S3. Calculated bond angles (°) and bond lengths (Å) in **2b**.

Functional	**B3LYP**	**B3LYP**	**ωB97X**	**ωB97XD**	**Xray**
Basis-set	6,31G(d,p) (C,H,N,O,F) 6,311G(d,p) (Mg)	6,31G+(d,p) (C,H,N,O,F) LanL2DZ (Mg)	6,31G+(d,p) (C,H,N,O,F) LanL2DZ (Mg)	6,31G+(d,p) (C,H,N,O,F) LanL2DZ (Mg)	
Mg–C	2.17	2.18	**2.16**	2.15	2.176(2)
Mg---F35	3.25	3.31	**3.24**	3.25	3.2
Mg---F31	3.34	3.33	**3.35**	3.30	3.4
Mg–N1	2.09	2.07	**2.04**	2.03	2.0512(16)
Mg–N3	2.08	2.07	**2.05**	2.04	2.0524(16)
Mg–O	2.12	2.06	**2.01**	2.01	2.0318(15)
N–Mg–N	95.0	95.2	**93.5**	93.1	93.99(6)

Table S4. Calculated bond angles (°) and bond lengths (Å) in **2d**.

Functional	**B3LYP**	**B3LYP**	**ωB97X**	**ωB97XD**	**Xray**
Basis-set	6,31G(d,p) (C,H,N,O,F) 6,311G(d,p) (Mg)	6,31G+(d,p) (C,H,N,O,F) LanL2DZ (Mg)	6,31G+(d,p) (C,H,N,O,F) LanL2DZ (Mg)	6,31G+(d,p) (C,H,N,O,F) LanL2DZ (Mg)	
Mg–N1	2.08	2.06	**2.04**	2.02	2.0402(13)
Mg–N3	2.08	2.06	**2.04**	2.02	2.0467(13)
Mg–N31	2.20	2.17	**2.16**	2.13	2.1293(13)
N–Mg–N	95.3	95.7	**94.3**	93.6	94.89(5)

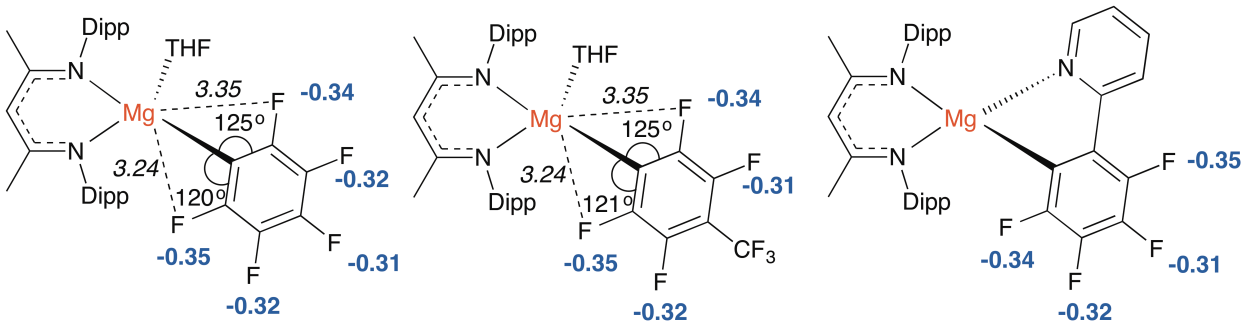
Table S5. Calculated bond angles (°) and bond lengths (Å) in [**LMg(μ-F)(THF)]$_2$**.

Functional	**B3LYP**	**B3LYP**	**ωB97X**	**ωB97XD**	**Xray**
Basis-set	6,31G(d,p) (C,H,N,O,F) 6,311G(d,p) (Mg)	6,31G+(d,p) (C,H,N,O,F) LanL2DZ (Mg)	6,31G+(d,p) (C,H,N,O,F) LanL2DZ (Mg)	6,31G+(d,p) (C,H,N,O,F) LanL2DZ (Mg)	
Mg–F1	1.99	2.00	**1.99**	1.99	1.9529(10) 1.9529(10)
Mg–F1A	1.98	2.00	**1.97**	1.97	
Mg–N1	2.19	2.17	**2.13**	2.13	2.1372(14)
Mg–N10	2.19	2.18	**2.13**	2.13	2.1372(14)
N–Mg–N	88	88	**88**	88	87.19(7)

5.2 NBO Calculations

NBO calculations were run using NBO v5.9 within g09. ωB97X functional and a hybrid 6,31G+(d,p) (C,H,N,O,F) / Lanl2DZ (Mg) basis-set.

Figure S15: Calculated bond angles (°) and bond lengths (Å) in **2a**, **2b** and **2d** (left to right) along with NBO data (NPA charges in bold and blue).



5.3 Thermodynamics and Solvation: C–F Bond Cleavage Reaction

Based on the benchmarking, basis sets using an effective core potential on Mg were used in place of more costly approaches. Structures were optimised from X-ray coordinates where available separetly using the ωB97X functional with and without a dispersion correction. All mimina for both dispersion corrected and uncorrected data sets were confirmed by frequency calculations.

Figure S16: Graphical representations of **1** (a) 2.98 Å structure, (b) 2.85 Å structure Data quoted are for coordinates generated with ωB97XD functional and a hybrid 6,31G+(d,p) (C,H,N,O,F) / Lanl2DZ (Mg) basis-set.

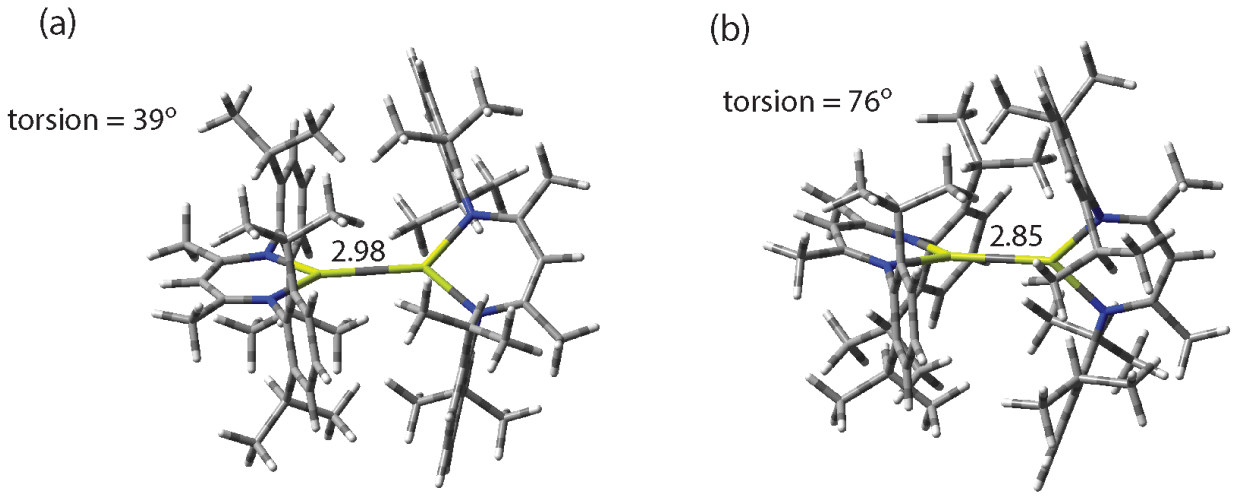


Figure S17: Graphical representations of Mg–C_6F_5/Mg–F species. Data quoted are for coordinates generated with ωB97XD functional and a hybrid 6,31G+(d,p) (C,H,N,O,F) / Lanl2DZ (Mg) basis-set. (a) [Mg]–C_6F_5(THF), (b) [Mg]–C_6F_5, (c) [Mg]–F/C_6F_5–[Mg] and (d) [Mg]–F–[Mg]–C_6F_5.

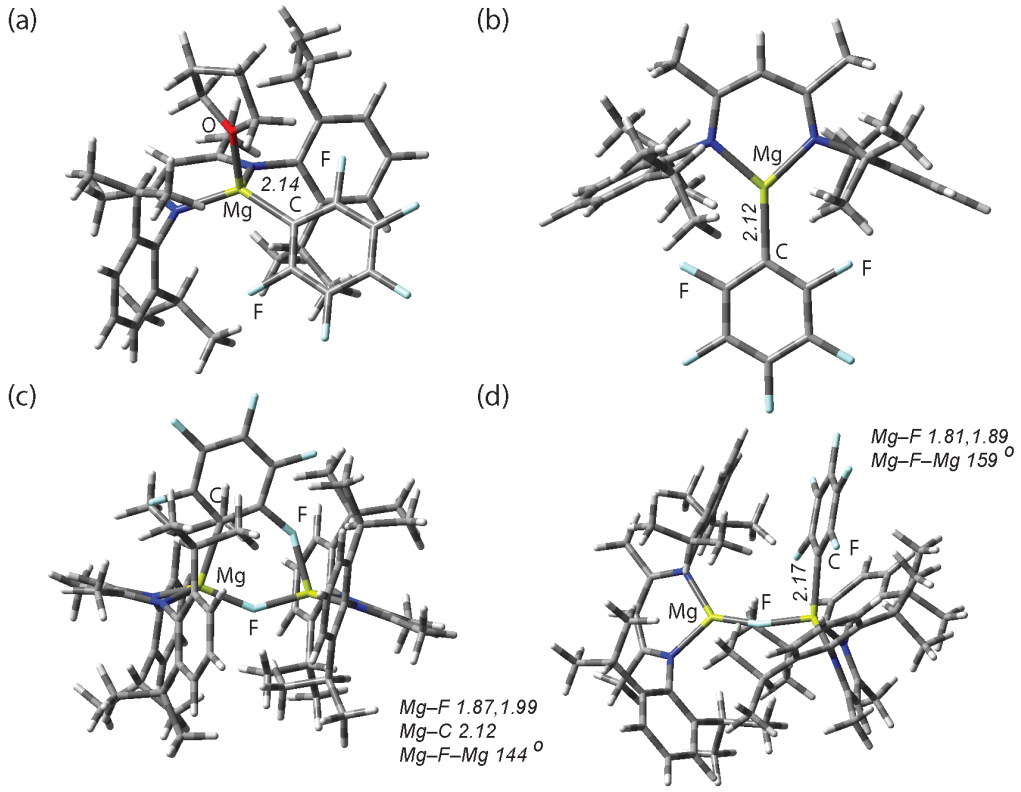


Figure S18: Graphical representations of Mg–F species. Data quoted are for coordinates generated with ωB97XD functional and a hybrid 6,31G+(d,p) (C,H,N,O,F) / Lanl2DZ (Mg) basis-set. (a) [Mg]–F, [Mg]–F/F–[Mg], (c) [Mg]–F–[Mg]–F and (d) [Mg]–F/F–[Mg](THF)$_2$.

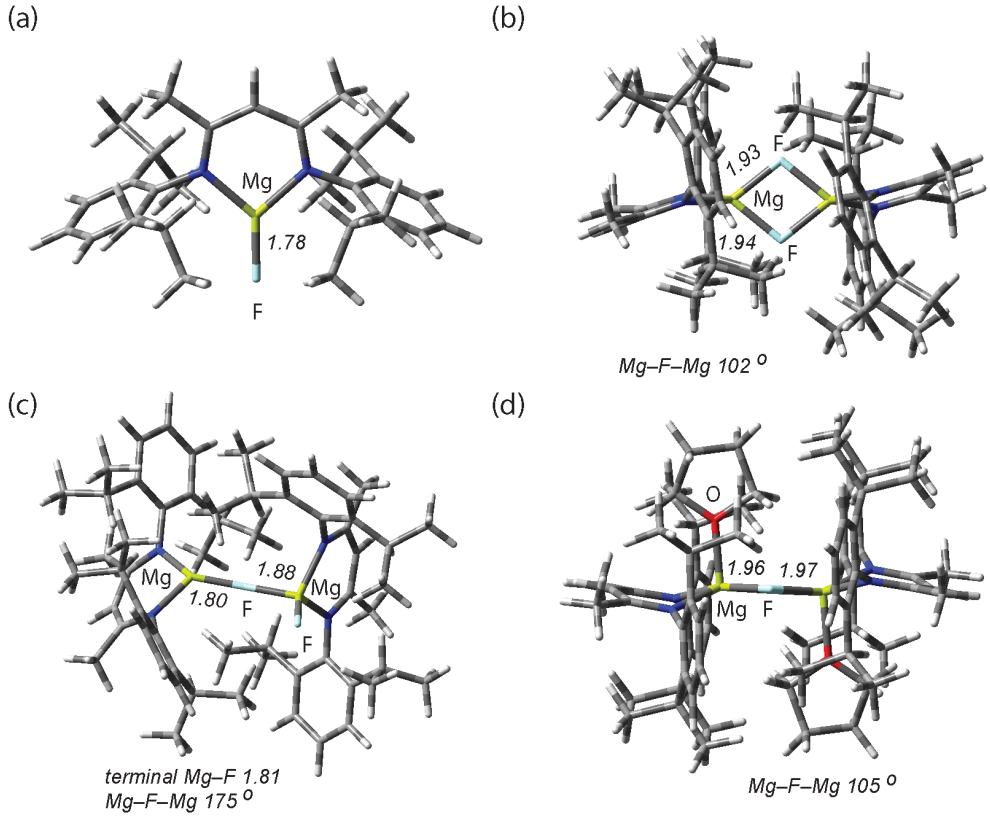
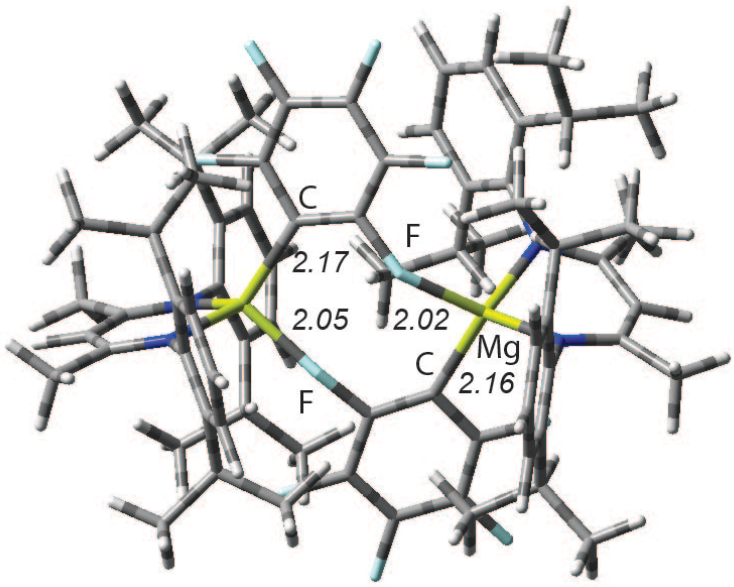


Figure S19: Graphical representations of [Mg]–C_6F_5/C_6F_5–[Mg]. Data quoted are for coordinates generated with ωB97XD functional and a hybrid 6,31G+(d,p) (C,H,N,O,F) / Lanl2DZ (Mg) basis-set.



6. Z Matrices

[Mg]–[Mg] (2.9 A, torsion = 76°)
wB97X
6,31G+(d,p) / Lanl2DZ
Sum of electronic and zero-point Energies= -2477.933597
Sum of electronic and thermal Energies= -2477.863112
Sum of electronic and thermal Enthalpies= -2477.862168
Sum of electronic and thermal Free Energies= -2478.039890

Low energy vibrations = 16.22, 27.29, 31.93 cm^{-1}

0 1

Mg	-1.14354700	-0.94644100	0.28881600
N	-3.00649200	-1.14748300	1.16558700
N	-1.34989200	-2.75029300	-0.69339900
C	-4.90166500	-2.43007000	2.10023600
C	-3.63436800	-2.33182500	1.27163600
C	-3.24703300	-3.50773600	0.60724400
C	-2.25910200	-3.67778200	-0.38291400
C	-2.27059500	-4.99390900	-1.13313500
C	-3.70214100	0.02553600	1.63821100
C	-3.36789900	0.62292900	2.87106400
C	-4.09619600	1.74020200	3.29917700
C	-5.11411100	2.28090400	2.52338800
C	-5.40578400	1.71350000	1.28620100
C	-4.71589800	0.58928100	0.82576700
C	-2.24254100	0.09906800	3.75466700
C	-1.22422600	1.21079400	4.06027800
C	-2.78222600	-0.51497600	5.05762100
C	-5.03542100	0.03533400	-0.55988300
C	-4.43761000	0.94907600	-1.64528300
C	-6.54257600	-0.15746500	-0.79238900
C	-0.42186500	-2.96787600	-1.77385300
C	0.77693200	-3.68109300	-1.55181700
C	1.70935000	-3.76888700	-2.59087400
C	1.46589200	-3.18626000	-3.83086500
C	0.27202400	-2.50522800	-4.04552300
C	-0.68226200	-2.37702800	-3.03027800
C	1.09376500	-4.33807000	-0.21295000
C	2.23767800	-3.60662100	0.50562300
C	1.43931100	-5.82925100	-0.37114900
C	-1.97733900	-1.62298200	-3.31562400
C	-1.70872200	-0.19754400	-3.82249500
C	-2.86078400	-2.39607800	-4.31045000
H	-4.79638100	-1.90048400	3.05116800
H	-5.15119100	-3.47370300	2.29939200
H	-5.74596200	-1.97181500	1.57257500
H	-3.86477600	-4.37638100	0.80156500
H	-2.32102200	-4.82079200	-2.21321700
H	-3.12222400	-5.60760200	-0.83620400
H	-1.35227600	-5.55958400	-0.94609700
H	-3.85890900	2.19236400	4.25838500
H	-5.66898600	3.14579600	2.87343500
H	-6.18411500	2.15225900	0.66815600
H	-1.72401600	-0.69377900	3.20222400
H	-0.81606400	1.62971900	3.13289000
H	-0.39188600	0.82192700	4.65794700
H	-1.68464000	2.02889300	4.62594700
H	-3.31553500	0.23612700	5.65270300
H	-1.96009700	-0.90779200	5.66791000
H	-3.47565500	-1.33788400	4.85314600
H	-4.55920100	-0.94629800	-0.65612700
H	-4.88535300	1.94963200	-1.59733700
H	-4.62929000	0.53674700	-2.64355600
H	-3.35374300	1.06544600	-1.52364500
H	-6.99420100	-0.77815200	-0.01060700
H	-6.71470100	-0.64617200	-1.75785300
H	-7.07437300	0.80076400	-0.80885600
H	2.64166300	-4.30183000	-2.42392700
H	2.20074400	-3.26567400	-4.62592000
H	0.07751400	-2.06002800	-5.01791300
H	0.20294500	-4.26265400	0.42074200
H	3.16550700	-3.65929400	-0.07705200
H	2.43256800	-4.05597400	1.48622300
H	2.00339100	-2.54701400	0.65901800
H	0.65872800	-6.37559100	-0.91213900
H	1.56556200	-6.29462700	0.61281700
H	2.37801300	-5.95968500	-0.92188300
H	-2.53333100	-1.54434800	-2.37296700
H	-1.11111300	0.37619100	-3.10504100
H	-2.64998700	0.34037300	-3.98222900
H	-1.16771000	-0.20757700	-4.77688100
H	-2.35756700	-2.50103100	-5.27920100
H	-3.80633400	-1.86620600	-4.47538000
H	-3.09306100	-3.40122600	-3.94150700
Mg	1.07320400	0.91086200	0.39633300
N	1.32463000	2.79263300	-0.42438600
N	2.91365800	1.01691200	1.33220100
C	2.16503900	5.11803700	-0.47622300
C	2.17814700	3.69935600	0.06009500
C	3.12946200	3.42746400	1.06418300
C	3.52755200	2.18553000	1.58603000
C	4.78161000	2.19645600	2.43982400
C	0.48206800	3.11276900	-1.54733700
C	0.85876100	2.64020900	-2.82824200
C	0.02135300	2.91368200	-3.91400400
C	-1.17553300	3.60570000	-3.74573600
C	-1.54802100	4.03816400	-2.47879700
C	-0.73079100	3.80967700	-1.36524100
C	2.15163700	1.84941000	-3.02260200
C	3.38091800	2.77227400	-3.11333700
C	2.11165200	0.90918200	-4.23498200
C	-1.19192100	4.29886300	0.00302800
C	-2.40473400	3.49431700	0.49678000
C	-1.52511800	5.80132100	-0.00353600
C	3.61563500	-0.19561700	1.67781600
C	4.58564500	-0.69641700	0.77764900
C	5.30285000	-1.84451300	1.12493300
C	5.07066200	-2.50097500	2.33003900
C	4.08346900	-2.02765900	3.18648000
C	3.33579600	-0.88535900	2.87550600
C	4.82992900	-0.05131500	-0.58330600
C	4.28767700	-0.95943600	-1.70258300
C	6.31204900	0.27633900	-0.82515700
C	2.23242200	-0.44659500	3.83039800
C	2.78645600	-0.02719400	5.20239300
C	1.18679200	-1.56463700	3.99101900
H	2.03834400	5.13483100	-1.56205000
H	3.08957400	5.63821400	-0.21975000
H	1.32847700	5.67857800	-0.04410000
H	3.71374900	4.27911900	1.39158200
H	4.64097300	1.61809000	3.35740000
H	5.06153100	3.21765500	2.70336100
H	5.61943400	1.73755700	1.90294800
H	0.29503100	2.56464800	-4.90394400
H	-1.81702500	3.79866100	-4.59998100
H	-2.48969100	4.56431600	-2.34746700
H	2.28590800	1.22239600	-2.12978800
H	3.27516300	3.46882100	-3.95409500
H	4.28989200	2.17883100	-3.27467800
H	3.52088000	3.35386300	-2.19723400

H	1.23139200	0.25862000	-4.20959900
H	2.99945200	0.26765100	-4.23650600
H	2.10987100	1.46643600	-5.17944700
H	-0.37547800	4.13425200	0.71540400
H	-3.25801000	3.61617000	-0.18196500
H	-2.71686600	3.83016700	1.49211900
H	-2.17743700	2.42406800	0.55890300
H	-0.69992600	6.40130000	-0.40224400
H	-1.74274100	6.14546200	1.01379900
H	-2.40986100	6.00537500	-0.61772000
H	6.05250100	-2.23219600	0.44000900
H	5.64398400	-3.38503500	2.59127500
H	3.88611900	-2.55444800	4.11655400
H	4.27309500	0.89195300	-0.61945500
H	4.80361700	-1.92790500	-1.70209700
H	4.44223900	-0.49424800	-2.68379400
H	3.21529500	-1.15692000	-1.58078900
H	6.71385000	0.92162600	-0.03621600
H	6.43251900	0.79565600	-1.78300400
H	6.92348000	-0.63292200	-0.86069300
H	1.73534100	0.42501200	3.38790800
H	3.28394400	-0.86866700	5.69928000
H	1.97485600	0.31606800	5.85500900
H	3.51373100	0.78655500	5.11041800
H	0.74731400	-1.82804100	3.02173000
H	0.37863500	-1.25049000	4.66191500
H	1.63838000	-2.46943000	4.41416900

[Mg]–[Mg] (3.0 A, torsion = 46 °)
wB97X
6,31G+(d,p) / Lanl2DZ
Sum of electronic and zero-point Energies= -2477.928809
Sum of electronic and thermal Energies= -2477.857931
Sum of electronic and thermal Enthalpies= -2477.856987
Sum of electronic and thermal Free Energies= -2478.037039

Low energy vibrations = 19.95 23.18 30.90 cm^{-1}

0 1

C	1.16977200	-4.28802200	0.49287900
C	-1.16911500	-4.28810700	-0.49368200
C	0.00040400	-4.88602000	-0.00052500
H	0.00052200	-5.96892100	-0.00070400
C	-1.16973200	4.28790200	0.49322600
C	1.16916400	4.28801000	-0.49329500
C	-0.00034100	4.88591600	-0.00010200
H	-0.00042000	5.96881800	-0.00018200
C	-2.26555400	-5.24851600	-0.91664600
H	-3.12215800	-5.17672700	-0.23724000
H	-2.63933700	-5.01561000	-1.91742200
H	-1.90406700	-6.27767400	-0.90550500
C	2.26639500	-5.24833900	0.91558500
H	3.12283500	-5.17644700	0.23597600
H	2.64037200	-5.01544000	1.91628600
H	1.90500600	-6.27753300	0.90447100
C	-2.26635000	5.24818400	0.91600700
H	-3.12292900	5.17609900	0.23659600
H	-2.64009300	5.01540800	1.91682800
H	-1.90506400	6.27741000	0.90466100
C	2.26566900	5.24841600	-0.91610000
H	3.12207100	5.17674600	-0.23641600
H	2.63974300	5.01541700	-1.91674400
H	1.90414100	6.27756300	-0.90516500
C	2.66633900	2.54012600	-1.07594900
C	3.74347000	2.41301000	-0.17139100
C	2.85094300	2.28304000	-2.45116300
C	4.99327100	2.02310700	-0.66262600
C	4.12477400	1.92094600	-2.90289300
C	5.19219700	1.79244000	-2.02048000
H	5.82557700	1.91290400	0.02698300
H	4.28120700	1.73516300	-3.96241500
H	6.17395800	1.51000200	-2.38876300
C	-2.66659700	2.53986300	1.07619400
C	-2.85101800	2.28274800	2.45142500
C	-3.74379400	2.41258500	0.17174600
C	-4.12474100	1.92042100	2.90327800
C	-4.99346700	2.02240000	0.66308700
C	-5.19221600	1.79167900	2.02096000
H	-4.28105200	1.73464700	3.96281900
H	-5.82580600	1.91201100	-0.02645300
H	-6.17388500	1.50903600	2.38933200
C	-2.66635500	-2.54021600	-1.07615700
C	-2.85098800	-2.28302300	-2.45134500
C	-3.74343100	-2.41305000	-0.17154100
C	-4.12481500	-1.92082400	-2.90300400
C	-4.99321800	-2.02299800	-0.66269900
C	-5.19219000	-1.79227200	-2.02053700
H	-4.28127900	-1.73496500	-3.96250800
H	-5.82546800	-1.91269900	0.02696400
H	-6.17394500	-1.50973900	-2.38876300
C	2.66659900	-2.53997400	1.07597800
C	3.74379700	-2.41257500	0.17153600
C	2.85097700	-2.28286500	2.45121100
C	4.99344000	-2.02235400	0.66291300
C	4.12467100	-1.92046300	2.90309200
C	5.19215600	-1.79166100	2.02079900
H	5.82579600	-1.91192800	-0.02660000
H	4.28094800	-1.73467000	3.96263500
H	6.17380500	-1.50898200	2.38919500
Mg	-0.00012500	1.50267400	0.00000700
Mg	0.00010300	-1.50280000	-0.00008600
C	-1.71227300	2.40599800	3.45754900
H	-0.80639000	2.67862100	2.90360200
C	-3.57308100	2.68942900	-1.31800100
H	-2.59679600	3.16549200	-1.46189200
C	3.57256100	2.68969400	1.31836400
H	2.59620300	3.16562600	1.46220400
C	1.71227000	2.40603300	-3.45739000
H	0.80629500	2.67856400	-2.90355300
C	-3.57250300	-2.68981900	1.31819700
H	-2.59626400	-3.16601300	1.46197300
C	-1.71233300	-2.40594800	-3.45760300
H	-0.80636400	-2.67856100	-2.90379000
C	3.57309200	-2.68925600	-1.31823900
H	2.59692500	-3.16554600	-1.46216900
C	1.71222000	-2.40619200	3.45730700
H	0.80635700	-2.67882300	2.90333200
N	1.37479200	-2.96419900	0.58581600
N	-1.37440500	-2.96429800	-0.58623400
N	-1.37477100	2.96407500	0.58606100
N	1.37440700	2.96420900	-0.58599100
C	-3.57964400	1.37414700	-2.11140100
H	-4.55061700	0.87491000	-2.02321000
H	-3.38443400	1.55636400	-3.17558300
H	-2.82404100	0.67426600	-1.73538000
C	-4.64347700	3.64839000	-1.86483400
H	-5.64216600	3.19914200	-1.81883100
H	-4.67265400	4.58838900	-1.30249700
H	-4.43583300	3.88482000	-2.91445500
C	-1.97947000	3.51196500	4.49326800
H	-2.12322800	4.48632000	4.01430600

H	-2.87768100	3.29010800	5.08176800
H	-1.13540800	3.59654100	5.18713900
C	-1.44943000	1.06594000	4.16400300
H	-0.59974600	1.15438400	4.85118300
H	-2.32320900	0.74862200	4.74625400
H	-1.22299600	0.27627600	3.43912400
C	1.44971300	1.06586400	-4.16372700
H	0.60005100	1.15407600	-4.85096800
H	2.32359400	0.74863700	-4.74587800
H	1.22338000	0.27623800	-3.43877400
C	1.97939700	3.51196200	-4.49317300
H	2.12312700	4.48634100	-4.01424800
H	2.87760100	3.29012100	-5.08168700
H	1.13531700	3.59647400	-5.18703000
C	4.64279400	3.64871600	1.86539900
H	4.67187600	4.58879500	1.30319000
H	4.43505700	3.88497700	2.91503800
H	5.64154800	3.19961000	1.81939000
C	3.57919400	1.37432000	2.11162900
H	2.82364400	0.67443200	1.73551500
H	4.55020300	0.87514300	2.02343100
H	3.38393300	1.55642500	3.17582000
C	-1.44972600	-1.06571900	-4.16382000
H	-0.59999100	-1.15388400	-4.85097300
H	-2.32354500	-0.74848000	-4.74606100
H	-1.22350200	-0.27612800	-3.43880400
C	-1.97949600	-3.51172200	-4.49354300
H	-2.12311900	-4.48620300	-4.01479800
H	-2.87777300	-3.28982100	-5.08192600
H	-1.13547500	-3.59605400	-5.18749400
C	-3.57873500	-1.37447600	2.11150500
H	-4.54961100	-0.87502600	2.02341600
H	-3.38344400	-1.55668000	3.17567700
H	-2.82301600	-0.67479300	1.73535700
C	-4.64296700	-3.64857500	1.86524700
H	-5.64161500	-3.19923600	1.81920600
H	-4.67225300	-4.58866700	1.30307400
H	-4.43529100	-3.88485500	2.91489500
C	3.57929300	-1.37385100	-2.11145800
H	4.55013700	-0.87436200	-2.02320900
H	3.38413300	-1.55600000	-3.17566100
H	2.82349700	-0.67422700	-1.73535500
C	4.64371500	-3.64785600	-1.86526000
H	5.64229800	-3.19837500	-1.81920700
H	4.67313200	-4.58794400	-1.30308200
H	4.43610600	-3.88416300	-2.91491500
C	1.97944000	-3.51220400	4.49298000
H	2.12323000	-4.48653500	4.01398100
H	2.87764000	-3.29033800	5.08149300
H	1.13537300	-3.59683400	5.18683900
C	1.44931000	-1.06618700	4.16382700
H	0.59957400	-1.15468500	4.85093600
H	2.32304000	-0.74889000	4.74616700
H	1.22291900	-0.27647900	3.43898500

[Mg]–F
wB97X
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -1338.852059
Sum of electronic and thermal Energies= -1338.816133
Sum of electronic and thermal Enthalpies= -1338.815188
Sum of electronic and thermal Free Energies= -1338.919897

Low energy vibrations = 29.08 31.86 47.5 cm^{-1}

0 1

Mg	0.00006300	-0.18937500	-0.72066400
N	1.47740900	0.08642300	0.58051500
C	1.27227000	0.23504400	1.89656000
C	-0.00000300	0.30231500	2.49659200
H	-0.00002600	0.41869000	3.57339100
C	2.47234700	0.32500000	2.81371300
H	3.10065500	-0.56649800	2.70988400
H	2.16643300	0.42026100	3.85623500
H	3.09940100	1.18450300	2.55207300
C	2.81601400	0.02755700	0.04691700
C	3.40170900	-1.22903800	-0.20603400
C	4.66380300	-1.26598800	-0.80862500
H	5.12721100	-2.22548200	-1.01837800
C	5.33023100	-0.09433300	-1.15093900
H	6.30760500	-0.14201700	-1.62047000
C	4.73657700	1.14035000	-0.90121400
H	5.25955400	2.04912100	-1.18284000
C	3.47573500	1.22429700	-0.30448000
C	2.66755300	-2.52635900	0.11360600
H	1.83200400	-2.28065800	0.78119900
C	2.08181900	-3.14745900	-1.17023300
H	1.41415900	-2.45888700	-1.70327100
H	1.51940200	-4.05831700	-0.93072500
H	2.88879200	-3.42163700	-1.86062500
C	3.55747800	-3.53816800	0.85154500
H	4.37497600	-3.89330800	0.21388900
H	2.96781500	-4.41314100	1.14648200
H	3.99843900	-3.10033300	1.75407300
C	2.79663200	2.57503600	-0.10640600
H	2.03592900	2.45880600	0.67445900
C	2.07057900	2.99399200	-1.39825400
H	2.78965800	3.13591500	-2.21325500
H	1.52213300	3.93197000	-1.25334100
H	1.35712600	2.22803600	-1.72757300
N	-1.47737300	0.08630600	0.58047700
C	-1.27225600	0.23489700	1.89652200
C	-2.47236700	0.32470000	2.81365400
H	-3.10052500	-0.56690200	2.70981800
H	-2.16648900	0.42001300	3.85618200
H	-3.09955300	1.18409900	2.55199600
C	-2.81596300	0.02732700	0.04687700
C	-3.40139400	-1.22931600	-0.20650600
C	-4.66348400	-1.26631900	-0.80908100
H	-5.12668000	-2.22583800	-1.01920000
C	-5.33021100	-0.09468500	-1.15092100
H	-6.30760700	-0.14244300	-1.62040000
C	-4.73683300	1.14002900	-0.90076100
H	-5.26001500	2.04881600	-1.18195400
C	-3.47595900	1.22403300	-0.30406900
C	-2.66704800	-2.52664100	0.11272900
H	-1.83127500	-2.28097900	0.78006400
C	-2.08169400	-3.14753900	-1.17138000
H	-1.41410700	-2.45884600	-1.70435700
H	-1.51923900	-4.05845300	-0.93216500
H	-2.88881400	-3.42158500	-1.86163900
C	-3.55673000	-3.53849000	0.85089500
H	-4.37457900	-3.89339900	0.21355900
H	-2.96703800	-4.41358200	1.14541400
H	-3.99722500	-3.10074700	1.75369600
C	-2.79714000	2.57483700	-0.10555700
H	-2.03654300	2.45857100	0.67541100

C	-3.76254100	3.67765300	0.35113800
H	-3.20515000	4.58966700	0.59134400
H	-4.48536200	3.93372600	-0.43153400
H	-4.32250500	3.37327900	1.24218100
C	-2.07091900	2.99419100	-1.39718700
H	-2.78988000	3.13608000	-2.21230100
H	-1.52272700	3.93227200	-1.25199200
H	-1.35722800	2.22845600	-1.72650300
F	-0.00003000	-0.82378200	-2.38922800
C	3.76178300	3.67808000	0.35023000
H	4.48486600	3.93395600	-0.43226300
H	3.20426500	4.59015300	0.58994000
H	4.32147800	3.37407600	1.24156700

[Mg]–F–[Mg]–C_6F_5
wB97X
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -3305.314760
Sum of electronic and thermal Energies= -3305.234572
Sum of electronic and thermal Enthalpies= -3305.233628
Sum of electronic and thermal Free Energies= -3305.428193

Lowest energy frequencies = 23.23 32.60 37.87cm^{-1}

0 1

Mg	-1.35403300	-0.85492500	0.23668700
N	-1.76143400	-2.85168300	0.05183700
C	-1.77057900	-3.68398700	1.10187900
C	-1.76429100	-3.27322200	2.44844500
H	-1.76748800	-4.07430500	3.17797000
C	-1.86035300	-1.97381600	2.98080000
N	-1.80047500	-0.85288800	2.25256800
C	-1.80267500	-5.18217700	0.86430300
H	-2.58977600	-5.45732100	0.15677500
H	-1.96427400	-5.72166500	1.79884900
H	-0.85372300	-5.51787500	0.43092700
C	-2.02654000	-1.88352100	4.48624300
H	-2.29024000	-2.85449300	4.90849300
H	-2.79347200	-1.15587700	4.76427200
H	-1.09018800	-1.55203000	4.95061100
C	-1.96051600	-3.39450000	-1.26959600
C	-3.26229600	-3.36783800	-1.82539400
C	-3.44385500	-3.88912900	-3.10916600
H	-4.43087700	-3.87613400	-3.55811000
C	-2.37479300	-4.40503700	-3.83821400
H	-2.53911100	-4.80040500	-4.83583600
C	-1.09744100	-4.39693900	-3.29191900
H	-0.26378500	-4.78462600	-3.87133800
C	-0.86781900	-3.89724200	-2.00480600
C	-4.43713100	-2.76843800	-1.05148400
H	-4.05280600	-1.88024100	-0.53097000
C	-5.58849100	-2.30403300	-1.95519800
H	-5.22900200	-1.65218500	-2.75448300
H	-6.31777600	-1.74524500	-1.35694900
H	-6.11880700	-3.15469000	-2.40058800
C	-4.99019800	-3.72924100	0.01858900
H	-5.29016700	-4.68013900	-0.43921600
H	-5.87578500	-3.28942000	0.49377700
H	-4.26161600	-3.93411400	0.80715600
C	0.55282700	-3.87553300	-1.45089200
H	0.49934300	-3.62470800	-0.38513400
C	1.26332600	-5.23266000	-1.57860700
H	0.67508600	-6.04024400	-1.12870800
H	2.23796800	-5.19252200	-1.07808400
H	1.43847700	-5.49378200	-2.62879500
C	1.38464500	-2.77709500	-2.13568400
H	1.48478200	-2.97796800	-3.21008600
H	2.38944700	-2.73748300	-1.69605000
H	0.90445800	-1.79976000	-2.01639400
C	-2.09323400	0.41329700	2.87256900
C	-1.08186700	1.16116600	3.50975200
C	-1.40907700	2.40194900	4.06419300
H	-0.63719000	2.98793700	4.55764800
C	-2.70216700	2.90791600	3.97782400
H	-2.93971400	3.87478200	4.40997600
C	-3.68641900	2.17614800	3.31883800
H	-4.68897200	2.58546300	3.23670000
C	-3.40372500	0.92892100	2.75347400
C	0.36472900	0.68082200	3.54047400
H	0.38116800	-0.31739600	3.09218400
C	0.93447200	0.58280100	4.96409900
H	0.97635600	1.56939500	5.44018900
H	1.95522800	0.18009600	4.94211200
H	0.32397000	-0.06612000	5.60034800
C	1.25804000	1.59620700	2.68168000
H	0.79630200	1.77720100	1.70360400
H	2.27187200	1.17754200	2.57671200
H	1.37486700	2.58317100	3.14476300
C	-4.49523700	0.14023300	2.03506400
H	-3.99618300	-0.59148200	1.38904400
C	-5.38162100	1.01699500	1.13800900
H	-6.01511300	1.69242800	1.72489700
H	-6.04471200	0.38272400	0.53781100
H	-4.77921300	1.62320800	0.45330400
C	-5.35996600	-0.65278400	3.03160400
H	-4.75882100	-1.36938500	3.60113900
H	-6.13801400	-1.21404600	2.50047200
H	-5.85040700	0.02463700	3.74148200
C	-2.22263200	0.77626700	-0.91776400
C	-2.04995100	2.04266300	-0.38778700
F	-1.16740800	2.19510700	0.69265200
C	-2.67732500	3.19173000	-0.84230800
F	-2.50147700	4.41317800	-0.23257900
C	-3.49350500	3.09203200	-1.95936700
C	-3.67345400	1.85933000	-2.57117400
F	-4.46803900	1.76689900	-3.69068900
C	-3.03959100	0.74451500	-2.03542800
F	-3.24316700	-0.46063200	-2.70444900
F	-4.09870400	4.21534900	-2.47178300
F	0.51766400	-0.49188500	0.05135800
Mg	2.08111200	0.44861200	0.01309800
N	2.56355500	2.33094800	-0.52963500
N	3.90227400	-0.27453600	0.39335500
C	3.80824000	2.74250500	-0.28573200
C	1.59456200	3.16352800	-1.21354300
C	4.84087300	0.62972200	0.75047000
C	4.22881500	-1.68129700	0.36927500
C	4.77559000	1.99512200	0.44514300
C	4.31349400	4.07604000	-0.79524200
C	1.10515600	2.73064200	-2.46776500
C	1.08287300	4.34344100	-0.61913300
C	6.04614900	0.16211000	1.54100600
C	4.94617900	-2.22043100	-0.73198500
C	3.78541300	-2.53012500	1.40659100
H	5.65214900	2.56859800	0.72689300
H	3.59973200	4.56860600	-1.45526100
H	5.24876100	3.91767200	-1.34005100
H	4.53225700	4.74551000	0.04290100
C	0.14751900	3.50516000	-3.12963900
C	1.62887400	1.47985700	-3.16075600
C	0.13461400	5.08856500	-1.32812900
C	1.47890500	4.84342500	0.76916800
H	6.47685500	-0.75487600	1.13441600

H	6.82053400	0.93007800	1.57758300
H	5.73054400	-0.05667500	2.56879200
C	5.20053300	-3.59761700	-0.74807900
C	5.49181700	-1.43645900	-1.93222500
C	4.05705300	-3.90204000	1.33439700
C	3.03497000	-2.01696200	2.62882400
H	-0.22597400	3.17963400	-4.09572000
C	-0.33220100	4.68390900	-2.57277500
H	2.17951200	0.87917500	-2.42570800
C	0.51070800	0.59547400	-3.73238000
C	2.64540100	1.86323500	-4.25059500
H	-0.27009600	5.98954900	-0.87903700
H	2.21297600	4.14723200	1.19387500
C	0.26117000	4.88353700	1.71389300
H	5.74699500	-4.01580700	-1.58905000
C	4.76415200	-4.44011300	0.26898900
H	5.72812900	-2.21185500	-2.67423100
C	6.81820600	-0.70678500	-1.64506800
C	4.50492000	-0.48396400	-2.61801000
H	3.71262800	-4.55374800	2.13224400
H	2.90813000	-0.93294200	2.51874400
C	3.84215600	-2.25634000	3.91745500
C	1.64149400	-2.65802900	2.73506600
H	-1.08292400	5.27106200	-3.09224400
H	-0.24219100	0.36106700	-2.97152300
H	0.92831300	-0.34638300	-4.10608700
H	0.00005500	1.08163800	-4.57064900
H	2.16829600	2.49916000	-5.00521100
H	3.03426600	0.96969200	-4.75130600
H	3.48939900	2.41760000	-3.82430700
H	-0.45273700	5.64916100	1.39001700
H	0.58334100	5.13651900	2.73185100
H	-0.27528800	3.93374100	1.73667300
H	4.97193200	-5.50450000	0.22612200
H	7.52286500	-1.35365200	-1.11125300
H	7.28414900	-0.40486800	-2.59030500
H	6.65707700	0.20126700	-1.05582900
H	4.35772700	0.43009800	-2.03598700
H	4.90193700	-0.19224200	-3.59742700
H	3.53256400	-0.96389400	-2.78084800
H	3.32388300	-1.82195500	4.78019400
H	3.96726600	-3.32843600	4.10818300
H	4.84059300	-1.81015000	3.85358700
H	1.70979900	-3.75070400	2.78328000
H	1.12775900	-2.32142500	3.64311800
H	1.01335000	-2.40055400	1.87516500
C	2.11160900	6.24809500	0.71636100
H	1.36790500	6.99019300	0.40460500
H	2.47066100	6.53858100	1.71036000
H	2.94934700	6.30661400	0.01626800

[Mg]–C_6F_5/F–[Mg]
wB97X
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -3305.342040
Sum of electronic and thermal Energies= -3305.261815
Sum of electronic and thermal Enthalpies= -3305.260870
Sum of electronic and thermal Free Energies= -3305.455814

Lowest energy vibrations = 20.18 31.77 35.01 cm^{-1}

0 1

Mg	-1.60663700	0.79364000	-0.75802400
N	-1.80216300	2.63718900	-1.56441300
C	-2.85346300	2.97726300	-2.32858200
C	-3.96644500	2.15352600	-2.57275900
H	-4.71704700	2.57791200	-3.22791900
C	-2.86316800	4.32511600	-3.02502100
H	-2.56194200	5.13030600	-2.35067000
H	-3.85483900	4.54778800	-3.42156300
H	-2.15256700	4.32648400	-3.85995900
C	-0.73848400	3.59926600	-1.39348600
C	-0.70881400	4.40214600	-0.23100600
C	0.32203000	5.34008800	-0.10391900
H	0.35958400	5.97866100	0.77223900
C	1.31742300	5.45367000	-1.06964900
H	2.11626100	6.17827200	-0.94366600
C	1.29325800	4.63215800	-2.19161600
H	2.08526900	4.71287700	-2.92935200
C	0.26189700	3.70770500	-2.38293200
C	-1.77383400	4.26885500	0.85736600
H	-2.04853000	3.20846400	0.92292200
C	-1.27254600	4.69603500	2.24541300
H	-0.31708300	4.22011600	2.49356700
H	-2.00559300	4.40783100	3.00428700
H	-1.13848200	5.78214300	2.30948400
C	-3.05574100	5.04980900	0.51233700
H	-2.82272100	6.10614500	0.33027100
H	-3.76468200	4.99669100	1.34631700
H	-3.55396400	4.64523900	-0.37312400
C	0.24040800	2.82725600	-3.62833700
H	-0.78581400	2.47327700	-3.77660200
C	0.65270900	3.58490700	-4.89985100
H	0.48096900	2.95749300	-5.78128100
H	1.71753000	3.84339900	-4.88592800
H	0.08152100	4.51237500	-5.02076600
N	-3.45639400	0.15613700	-1.27808300
C	-4.25857400	0.86663800	-2.08676100
C	-5.56234600	0.25749500	-2.56610700
H	-6.10974900	-0.22629100	-1.75423800
H	-6.20085000	1.01597700	-3.02130300
H	-5.36101900	-0.51603600	-3.31730000
C	-3.91987400	-1.12327000	-0.79440300
C	-4.56146500	-1.19597700	0.46148400
C	-5.00622400	-2.44631200	0.90648000
H	-5.51622800	-2.52236300	1.86201100
C	-4.79520000	-3.59610600	0.15226200
H	-5.14021300	-4.55814400	0.51930500
C	-4.14389600	-3.51080100	-1.07504800
H	-3.97717700	-4.41355800	-1.65418000
C	-3.71338900	-2.27927400	-1.57749300
C	-4.80620500	0.04749200	1.31341500
H	-4.09936200	0.81877500	0.98862300
C	-4.55882200	-0.20242800	2.80886500
H	-3.57284000	-0.64707300	2.97947800
H	-4.60527500	0.74283500	3.35727400
H	-5.31214300	-0.87403300	3.23661600
C	-6.22709800	0.60338100	1.10482500
H	-6.97784700	-0.15976200	1.34378600
H	-6.39667900	1.46500500	1.76033900
H	-6.38797700	0.93144500	0.07315100
C	-3.03294100	-2.19451500	-2.93978000
H	-3.15476300	-1.17105200	-3.31270700
C	-3.66201500	-3.13603700	-3.97802100
H	-3.23621800	-2.93775400	-4.96768200
H	-3.46177000	-4.18735000	-3.74229900
H	-4.74815400	-3.00246800	-4.03716700
C	-1.52475200	-2.46472500	-2.82038600
H	-1.34497300	-3.47021200	-2.42465000
H	-1.04372600	-2.39103000	-3.80342500
H	-1.02965400	-1.75453900	-2.14821700
Mg	1.37987900	-0.81381400	0.47842700

N	3.37715000	-0.33658300	0.28588600
C	4.25787200	-1.07572200	0.97995800
C	4.00307400	-2.36697500	1.47627700
H	4.80574600	-2.80826300	2.05398200
C	5.63925300	-0.52041900	1.26998400
H	6.08230300	-0.04393000	0.39203700
H	6.30992000	-1.30682000	1.61979400
H	5.56998300	0.24169100	2.05472100
C	3.85415400	0.84190600	-0.39411200
C	4.27737500	0.72460200	-1.74139200
C	4.74537000	1.87010000	-2.39356700
H	5.08368700	1.80114600	-3.42209600
C	4.77246700	3.10743100	-1.75333800
H	5.13414800	3.98502300	-2.28086300
C	4.33677800	3.21174500	-0.43831800
H	4.35233300	4.17837300	0.05803300
C	3.88719200	2.08803500	0.26465300
C	4.22337200	-0.61834700	-2.47142700
H	3.31813800	-1.13352300	-2.12050300
C	4.13118300	-0.47358100	-3.99811200
H	3.32692300	0.20294000	-4.29978700
H	3.94078000	-1.45219300	-4.45143200
H	5.07184400	-0.10067800	-4.42108400
C	5.42550300	-1.52359600	-2.13619000
H	6.36680800	-1.01237400	-2.37331800
H	5.37906900	-2.44216000	-2.73513300
H	5.44373600	-1.81861900	-1.08456500
C	3.44959100	2.24200300	1.71593800
H	3.26265100	1.24168600	2.12035600
C	2.14434200	3.04794200	1.80941700
H	2.30239600	4.08263000	1.48485300
H	1.77543500	3.06577100	2.84374400
H	1.36336300	2.62357500	1.16829900
N	1.77968500	-2.82382900	0.60898200
C	2.91216900	-3.21237000	1.21526700
C	3.08100000	-4.66432100	1.61430300
H	3.22551600	-5.29264000	0.72795700
H	3.94760600	-4.78834700	2.26539000
H	2.19221600	-5.04027400	2.12894800
C	0.84941400	-3.83476000	0.17902500
C	1.06620700	-4.49825100	-1.04971500
C	0.13464000	-5.45155200	-1.47212200
H	0.29188000	-5.96912700	-2.41493100
C	-0.99523200	-5.74192400	-0.71135400
H	-1.71217300	-6.48030600	-1.05782700
C	-1.19509300	-5.08711500	0.49973400
H	-2.07478200	-5.31697700	1.09516300
C	-0.27596200	-4.14321500	0.97132700
C	2.27418400	-4.18761800	-1.92812000
H	2.95145900	-3.54067200	-1.35888600
C	1.84870000	-3.41423000	-3.18774100
H	1.36552900	-2.46537800	-2.92726700
H	2.72049700	-3.19596300	-3.81591700
H	1.13899800	-4.00113500	-3.78383700
C	3.05309000	-5.45470500	-2.31827900
H	2.45796800	-6.10703800	-2.96796300
H	3.96441200	-5.18449000	-2.86413800
H	3.34416600	-6.03626300	-1.43666100
C	-0.48781600	-3.50238000	2.33693600
H	0.36078200	-2.83585400	2.52791900
C	-0.51649500	-4.55553500	3.45855500
H	-0.61611000	-4.06811500	4.43497400
H	-1.36436300	-5.23980900	3.33619500
H	0.39968200	-5.15569800	3.47088800
C	-1.76881800	-2.65803600	2.37163100
H	-2.65983700	-3.27949900	2.22875700
H	-1.86059600	-2.14805300	3.33908700
H	-1.77389900	-1.89922500	1.58064600
F	0.01545200	-0.16696300	-0.71930100
C	1.13109800	1.58974500	-3.43221200
H	2.16543600	1.89722400	-3.24238800
H	0.80688300	0.97974500	-2.58162700
H	1.11271900	0.95932100	-4.33016500
C	4.53423200	2.90331600	2.58397000
H	4.69970600	3.94548500	2.28650000
H	4.22891400	2.90194000	3.63640800
H	5.49224900	2.37893400	2.50473400
C	0.44937500	0.08955600	2.28746100
C	1.15808200	0.06948200	3.48185100
C	-0.74542200	0.75355300	2.39536000
C	0.73169700	0.66539700	4.66098800
C	-1.25298700	1.37989000	3.52324700
C	-0.48884100	1.33164600	4.67843800
F	2.39495300	-0.56878700	3.52375100
F	1.48494900	0.61335500	5.80694500
F	-0.93546700	1.93281100	5.82734200
F	-2.45991100	2.04049300	3.51410100
F	-1.61834200	0.84814000	1.24496600

[Mg]–C_6F_5
wB97X
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -1966.403877
Sum of electronic and thermal Energies= -1966.358854
Sum of electronic and thermal Enthalpies= -1966.357910
Sum of electronic and thermal Free Energies= -1966.484591

Lowest energy vibrations = 19.44 22.59 30.20 cm^{-1}

0 1

Mg	-0.00010000	-0.30547600	-0.00024300
N	-1.47916100	-1.65636700	-0.06790900
C	-1.26931900	-2.98136500	-0.07101300
C	-0.00023700	-3.58458500	0.00012400
H	-0.00028100	-4.66760400	0.00024300
C	1.26891400	-2.98145900	0.07118800
N	1.47890600	-1.65649600	0.06776600
C	-2.46405700	-3.90675300	-0.15476200
H	-3.14081600	-3.74633900	0.69160700
H	-2.15317700	-4.95207600	-0.16151400
H	-3.04323400	-3.70554000	-1.06270400
C	2.46352500	-3.90697600	0.15534400
H	2.15254200	-4.95227000	0.16186800
H	3.04231200	-3.70592200	1.06357500
H	3.14068400	-3.74654800	-0.69069600
C	-2.82697600	-1.14022500	-0.12230500
C	-3.53128600	-0.92002000	1.07946100
C	-4.79226000	-0.32295700	1.01165700
H	-5.34649000	-0.13436200	1.92578700
C	-5.34639600	0.04819600	-0.21017500
H	-6.32286600	0.52066700	-0.24270500
C	-4.64380600	-0.18178600	-1.38765600
H	-5.08143800	0.11319200	-2.33705700
C	-3.37989400	-0.78059800	-1.36670100
C	-2.91141500	-1.26799500	2.42895200
H	-2.14480200	-2.03408400	2.26081800
C	-2.21299700	-0.03813000	3.03888400
H	-1.43235700	0.35927500	2.37936800
H	-1.75314800	-0.29159800	4.00112000
H	-2.93368200	0.77166000	3.19813100

C	-3.92805400	-1.84941400	3.42282700
H	-4.66110900	-1.09849300	3.73761300
H	-3.41372300	-2.20178400	4.32355700
H	-4.47375100	-2.69326500	2.98673000
C	-2.61429200	-0.99308800	-2.66795700
H	-1.77534000	-1.66717000	-2.45680100
C	-3.47380800	-1.65894300	-3.75374500
H	-3.91219900	-2.59615600	-3.39385800
H	-2.86403900	-1.88163300	-4.63637200
H	-4.29304700	-1.00595400	-4.07504700
C	-2.03147900	0.33677000	-3.18074200
H	-2.83550600	1.04399500	-3.41581500
H	-1.43880300	0.17731700	-4.08909800
H	-1.38874500	0.81598900	-2.43111400
C	2.82676900	-1.14049200	0.12234400
C	3.53129100	-0.92051100	-1.07933400
C	4.79232000	-0.32357300	-1.01140300
H	5.34672200	-0.13515800	-1.92546600
C	5.34629000	0.04769400	0.21046900
H	6.32280100	0.52007500	0.24309700
C	4.64348000	-0.18205700	1.38786400
H	5.08097900	0.11300200	2.33730500
C	3.37951300	-0.78074200	1.36678100
C	2.91162500	-1.26862000	-2.42888400
H	2.14491000	-2.03461600	-2.26077700
C	3.92839900	-1.85029200	-3.42248300
H	4.66155300	-1.09947700	-3.73728900
H	3.41419300	-2.20280300	-4.32323000
H	4.47396800	-2.69409300	-2.98612800
C	2.21345700	-0.03877200	-3.03912700
H	1.43262900	0.35870700	-2.37987300
H	1.75384300	-0.29228700	-4.00146600
H	2.93423000	0.77095800	-3.19823700
C	2.61373000	-0.99299600	2.66797600
H	1.77469600	-1.66696500	2.45680300
C	2.03109600	0.33700800	3.18058000
H	2.83522100	1.04415200	3.41557000
H	1.43838700	0.17776400	4.08895100
H	1.38843000	0.81620000	2.43087800
C	3.47308200	-1.65886300	3.75388400
H	3.91131100	-2.59621200	3.39414700
H	2.86324900	-1.88131000	4.63652800
H	4.29243900	-1.00597800	4.07509600
C	0.00011100	1.81775600	-0.00016000
C	1.14370500	2.56700900	-0.23813300
F	2.34608200	1.91359100	-0.48516100
C	1.17522600	3.95493000	-0.24493700
F	2.33768400	4.64555000	-0.48734700
C	0.00039400	4.65076700	-0.00010500
C	-1.17457600	3.95516700	0.24468300
F	-2.33690900	4.64598800	0.48709400
C	-1.14332300	2.56722800	0.23780900
F	-2.34585400	1.91403100	0.48473200
F	0.00054500	6.02246500	-0.00008000

[Mg]–C_6F_5(THF)
wB97X
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -2198.654504
Sum of electronic and thermal Energies= -2198.604406
Sum of electronic and thermal Enthalpies= -2198.603461
Sum of electronic and thermal Free Energies= -2198.738199

Lowest energy vibrations = 24.76 34.03 40.82 cm^{-1}

0 1

Mg	-0.11876000	-0.45483800	-0.28347300
N	-1.88187500	-0.99006100	0.60736100
C	-1.92227100	-2.06502400	1.41567000
C	-0.79607500	-2.67246100	1.99722600
H	-1.00609300	-3.52281800	2.63551100
C	0.54409500	-2.21505300	2.02802500
N	1.02251400	-1.26975400	1.22015800
C	-3.26901200	-2.66769100	1.76964900
H	-3.87909800	-1.96680400	2.34690300
H	-3.14791500	-3.58309300	2.35094700
H	-3.83524400	-2.89764600	0.86047600
C	1.44716200	-2.86385100	3.05900500
H	0.85882300	-3.37974700	3.81939200
H	2.08330600	-2.12005200	3.54737000
H	2.11299600	-3.59543500	2.58759100
C	-3.10314800	-0.25367600	0.38454900
C	-3.51677800	0.69553400	1.34807400
C	-4.70316100	1.40117300	1.12933200
H	-5.03109800	2.12963300	1.86589300
C	-5.46395700	1.20031500	-0.01830700
H	-6.38137500	1.75981900	-0.17094500
C	-5.03154900	0.28917900	-0.97434700
H	-5.61518500	0.14505500	-1.87998400
C	-3.85583300	-0.44639900	-0.79134400
C	-2.69711500	0.99424200	2.60096300
H	-1.77020600	0.41160700	2.54362500
C	-2.31375500	2.48317300	2.66691600
H	-1.80816100	2.79797300	1.74984100
H	-1.65196600	2.66826700	3.52198100
H	-3.20114400	3.11464400	2.79404800
C	-3.43372600	0.58113400	3.88727800
H	-4.38218200	1.12272000	3.98597100
H	-2.82057400	0.81254600	4.76612000
H	-3.65365400	-0.49147600	3.90485300
C	-3.40577600	-1.40759100	-1.88283000
H	-2.50939100	-1.91871000	-1.51661200
C	-4.46571000	-2.47465000	-2.19920500
H	-4.74248600	-3.04030000	-1.30281300
H	-4.08988600	-3.18256500	-2.94845900
H	-5.37817500	-2.01965800	-2.60121700
C	-3.01972900	-0.63071000	-3.15358100
H	-3.88971900	-0.11169700	-3.57215300
H	-2.63104000	-1.30848700	-3.92503500
H	-2.25937300	0.12768600	-2.93222000
C	2.36590500	-0.76944100	1.36594300
C	3.47037600	-1.49488200	0.87182700
C	4.74637900	-0.93222100	0.97889300
H	5.60374600	-1.47769300	0.59456800
C	4.93624100	0.31840200	1.55392000
H	5.93321300	0.74089700	1.62695700
C	3.83855300	1.03413500	2.02200900
H	3.99104900	2.01634300	2.45699600
C	2.54414100	0.51410400	1.93192100
C	3.31271200	-2.83769700	0.16743900
H	2.28517100	-3.18409400	0.32816600
C	4.26422300	-3.91185100	0.71897600
H	5.30991000	-3.66457900	0.50467600
H	4.05391300	-4.88203100	0.25427100
H	4.16499000	-4.02109800	1.80436300
C	3.51448600	-2.66789400	-1.34870000
H	2.82233700	-1.91868300	-1.74302600
H	3.35896700	-3.62113900	-1.87132100
H	4.53239100	-2.32475300	-1.56589000
C	1.35871800	1.31189400	2.46544900
H	0.47102700	1.01773900	1.89165300
C	1.52616500	2.82749600	2.28993900
H	2.29681800	3.23336400	2.95534000

H	0.58590800	3.33651800	2.52789200
H	1.79855700	3.07647500	1.25776600
C	1.08090300	0.95693800	3.93729800
H	0.85182100	-0.10843800	4.05229000
H	0.22669900	1.52908100	4.31878600
H	1.95404500	1.18955300	4.55887800
C	0.49694700	1.45110600	-1.07676100
C	1.77985000	1.63217000	-1.56579800
F	2.61893700	0.51967100	-1.71187500
C	2.31451400	2.85834800	-1.93705500
F	3.59731400	2.97404100	-2.41736500
C	1.51856700	3.98950100	-1.82230700
C	0.21875700	3.87200000	-1.35041000
F	-0.57012900	4.99277800	-1.24660000
C	-0.25166300	2.61352600	-0.99904600
F	-1.56491800	2.54869200	-0.53266800
O	0.11391900	-1.73797000	-1.84228000
C	-0.07416200	-3.19412300	-1.71372800
H	-0.90464200	-3.35520700	-1.02362800
H	0.84109600	-3.62226200	-1.29360300
C	-0.32273500	-3.65174300	-3.14489400
H	-1.37151200	-3.48758600	-3.41910700
H	-0.09153700	-4.71009700	-3.28744900
C	0.60286100	-2.72830900	-3.95758000
H	1.62980300	-3.10877400	-3.93416500
H	0.29638500	-2.64161200	-5.00280000
C	0.51266300	-1.38659000	-3.22730000
H	1.45532400	-0.84193800	-3.16891400
H	-0.26839500	-0.73860000	-3.62949900
F	2.01242800	5.21844000	-2.18478600

[Mg]–F–[Mg]–F
wB97X
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -2677.763953
Sum of electronic and thermal Energies= -2677.691864
Sum of electronic and thermal Enthalpies= -2677.690920
Sum of electronic and thermal Free Energies= -2677.869091

Lowest energy vibrations = 26.34 31.65 38.25 cm^{-1}

0 1

Mg	2.01757300	0.22483700	0.34923800
N	3.10956700	-0.27036200	-1.30107800
C	3.50177900	0.63216300	-2.20549800
C	3.25402800	2.01809000	-2.11450500
H	3.60362400	2.60486200	-2.95584000
C	2.72770500	2.76491800	-1.04063600
N	2.23944300	2.23336200	0.08442900
C	4.29193900	0.16635400	-3.41267400
H	5.20511400	-0.34894000	-3.09520500
H	4.56865000	1.00595700	-4.05189300
H	3.71523600	-0.55191300	-4.00602500
C	2.77984100	4.27383700	-1.17952000
H	3.04525800	4.56597700	-2.19680200
H	3.52401300	4.69568600	-0.49350100
H	1.81720000	4.72521500	-0.91812300
C	3.51349700	-1.64851600	-1.42766900
C	4.64326000	-2.10233100	-0.71243300
C	4.98602800	-3.45710900	-0.78410900
H	5.85122100	-3.81386800	-0.23212100
C	4.23901700	-4.35332500	-1.54024700
H	4.52045000	-5.40088700	-1.58357700
C	3.12276200	-3.89817800	-2.23505200
H	2.53224800	-4.60086600	-2.81692200
C	2.74284500	-2.55296400	-2.19127600
C	5.48668500	-1.17201200	0.15185700
H	5.08495600	-0.15680500	0.04668800
C	5.37881700	-1.56686200	1.63530400
H	4.34698900	-1.44820600	1.98420900
H	6.02484500	-0.92622300	2.24750100
H	5.69531000	-2.60613300	1.78777600
C	6.95209600	-1.14281800	-0.31443600
H	7.42700900	-2.12395600	-0.19444800
H	7.52314500	-0.42150900	0.28113600
H	7.03340100	-0.85653400	-1.36963100
C	1.47215500	-2.11638300	-2.91008400
H	1.44448300	-1.02135500	-2.90580900
C	1.42022400	-2.58859400	-4.37074700
H	2.30590000	-2.26264500	-4.92741000
H	0.53227700	-2.18265500	-4.86931500
H	1.36528600	-3.68101300	-4.44011300
C	0.24419700	-2.61348900	-2.12666300
H	0.23761000	-3.70878500	-2.06405500
H	-0.69242800	-2.29868600	-2.60575700
H	0.28052400	-2.22146800	-1.10537900
C	1.91643500	3.07944700	1.20346800
C	0.57660500	3.42470100	1.47187800
C	0.28643200	4.20338900	2.59800200
H	-0.74476600	4.47929700	2.80537800
C	1.29487800	4.62656400	3.45493500
H	1.05618800	5.22781200	4.32660200
C	2.61355500	4.26153500	3.19555000
H	3.39640000	4.57430800	3.88010000
C	2.94691200	3.48866300	2.08056600
C	-0.56067400	2.96030900	0.57329000
H	-0.11341800	2.36797500	-0.23118600
C	-1.31870700	4.13621500	-0.06194100
H	-1.78706000	4.76484500	0.70495600
H	-2.10655400	3.77686700	-0.73482100
H	-0.63898100	4.76962800	-0.64253800
C	-1.53058200	2.05039300	1.35024200
H	-0.99502800	1.21084500	1.81554100
H	-2.34404900	1.70967600	0.68365400
H	-2.02928900	2.59035200	2.16363300
C	4.38511500	3.02938500	1.87509100
H	4.49097300	2.69350900	0.83733600
C	4.67281200	1.81768600	2.78154700
H	4.60414700	2.10877700	3.83745600
H	5.68549600	1.43677500	2.59916700
H	3.95473800	1.00690400	2.60756200
C	5.41158700	4.14812900	2.10611900
H	5.18942100	5.03248800	1.49729900
H	6.41495600	3.79451500	1.84415700
H	5.43984900	4.45965600	3.15667400
F	0.17893100	-0.11573000	-0.00521000
Mg	-1.61213300	-0.41031000	-0.09747500
N	-2.42442900	-1.99543100	0.80296600
N	-3.01479000	-0.07910500	-1.49551000
C	-3.26588200	-2.74702600	0.08648900
C	-2.05940400	-2.36118100	2.15540900
C	-3.75878400	-1.14755800	-1.85717200
C	-3.37360300	1.23806500	-1.97870200
C	-3.77716000	-2.38132300	-1.18328900
C	-3.72929900	-4.08214800	0.62769300
C	-1.02980500	-3.29236700	2.40629100
C	-2.72063300	-1.70799000	3.22268400
C	-4.65189100	-1.07726300	-3.08333100
C	-2.67758300	1.88021900	-3.03077800
C	-4.44902900	1.89946900	-1.32975600
H	-4.39344300	-3.13945800	-1.65340100
H	-2.95939500	-4.84090800	0.44997200

H	-4.64710500	-4.40599700	0.13465300
H	-3.89783500	-4.03959300	1.70654800
C	-0.71434000	-3.59399500	3.73631400
C	-0.21380000	-3.94320200	1.29708900
C	-2.37362900	-2.04729200	4.53309300
C	-3.80351800	-0.66426700	2.96147000
H	-4.86045100	-0.05205800	-3.39088300
H	-4.15092100	-1.58200500	-3.91741200
H	-5.59752900	-1.59425400	-2.90472100
C	-3.09533700	3.16255700	-3.41548700
C	-1.47957900	1.31541100	-3.79632600
C	-4.82965800	3.17400300	-1.76235800
C	-5.22943300	1.25914800	-0.18242000
H	0.08202200	-4.30315400	3.94153400
C	-1.38368200	-2.99076400	4.79243100
H	-0.62143000	-3.60409500	0.33800800
C	1.26383500	-3.50964900	1.37578600
C	-0.30267600	-5.47964800	1.33109300
H	-2.87242500	-1.56105400	5.36449800
H	-3.54778900	-0.15047500	2.02427500
C	-3.88381700	0.40761800	4.05819400
H	-2.56701800	3.65732600	-4.22568700
C	-4.16132100	3.80817800	-2.80154500
H	-1.32417500	2.01894000	-4.62629400
C	-1.70679300	-0.05543000	-4.44706200
C	-0.18271700	1.34633000	-2.97288400
H	-5.66265700	3.67507600	-1.27869800
H	-4.66666400	0.38612700	0.16755200
C	-6.60909900	0.76172900	-0.65124400
C	-5.40004800	2.21697700	1.00903700
H	-1.12288500	-3.23723300	5.81653000
H	1.39099000	-2.43194600	1.52783200
H	1.80185300	-3.80836800	0.46658400
H	1.75699700	-3.99975700	2.22489300
H	0.15517700	-5.87476000	2.24530200
H	0.24040000	-5.90480800	0.47939200
H	-1.33644400	-5.84025500	1.29677000
H	-4.29347800	0.00196000	4.99018000
H	-4.54568400	1.22006700	3.73901100
H	-2.89747000	0.83145000	4.27545000
H	-4.46571400	4.79662300	-3.12992700
H	-2.61427000	-0.05568800	-5.06058800
H	-0.85866300	-0.29736300	-5.09839000
H	-1.79212600	-0.84701200	-3.69865100
H	-0.17243500	0.60642300	-2.16648900
H	0.68245100	1.13307000	-3.61148000
H	-0.02068500	2.33444400	-2.52753700
H	-7.14401000	0.28489100	0.17837600
H	-7.21751600	1.59939600	-1.01300200
H	-6.52238000	0.03325700	-1.46257000
H	-6.04147000	3.06767300	0.75345400
H	-5.87485400	1.69232200	1.84610500
H	-4.43823600	2.61325500	1.35221100
F	2.36229500	-0.49446900	1.98021000
C	-5.17960200	-1.32307800	2.75387000
H	-5.45663000	-1.90832800	3.63882500
H	-5.95348100	-0.56202400	2.59364100
H	-5.18054000	-1.99128800	1.88631000

[Mg]–F/F–[Mg]
wB97X
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -2677.801366
Sum of electronic and thermal Energies= -2677.729565
Sum of electronic and thermal Enthalpies= -2677.728621
Sum of electronic and thermal Free Energies= -2677.905951

Lowest energy vibrations = 19.83 29.43 35.25 cm^{-1}

0 1

Mg	0.03764900	1.46351800	-0.45494000
F	0.04381500	0.42089600	1.18471600
N	1.55286500	2.82212000	-0.76816400
C	1.37909500	3.91971700	-1.52316500
C	0.15824800	4.31531300	-2.09663600
H	0.20843500	5.18642700	-2.73742800
C	2.54413400	4.86418800	-1.75829100
H	2.89400500	5.28285000	-0.80830100
H	2.24644100	5.68668600	-2.40958800
H	3.39939800	4.35224200	-2.20874100
C	2.84843300	2.67615100	-0.14167300
C	3.03854200	3.15394400	1.17035000
C	4.31956200	3.08047800	1.73161800
H	4.48180900	3.45582400	2.73854300
C	5.38288200	2.53317800	1.02409500
H	6.37004900	2.48408300	1.47339400
C	5.17627500	2.04029300	-0.26331300
H	6.01111800	1.61098500	-0.80719600
C	3.91928200	2.11253100	-0.87117200
C	1.90067400	3.75071100	1.99207200
H	1.00254500	3.76738900	1.36234200
C	1.59853800	2.87465800	3.22067900
H	1.25225400	1.88190000	2.91345000
H	0.81858400	3.33384500	3.83833200
H	2.49296100	2.75287100	3.84376800
C	2.19717000	5.20075400	2.40967900
H	3.06057400	5.25233700	3.08336600
H	1.33573400	5.62659500	2.93741200
H	2.40985700	5.83215600	1.53970800
C	3.70873700	1.59858600	-2.29185700
H	2.93651000	2.21731800	-2.76404100
C	4.96954800	1.69387700	-3.16316300
H	4.71728900	1.46853500	-4.20487000
H	5.72953700	0.96897500	-2.84892700
H	5.41545900	2.69446100	-3.12690900
N	-1.41856400	2.78382400	-1.05225900
C	-1.13541000	3.85128300	-1.81725100
C	-2.27182400	4.68348800	-2.37772900
H	-2.81817600	5.18291100	-1.56943600
H	-1.89407100	5.44586900	-3.06030600
H	-2.99547600	4.06006700	-2.91098300
C	-2.79756600	2.59842600	-0.66298400
C	-3.27819000	3.25920600	0.48960100
C	-4.59579800	3.02358800	0.89380100
H	-4.98002700	3.51882900	1.78121600
C	-5.42404800	2.16231200	0.17847000
H	-6.44071200	1.98027600	0.51395200
C	-4.95289300	1.55808300	-0.98240200
H	-5.61021400	0.90912000	-1.55408400
C	-3.64983200	1.78671700	-1.43796200
C	-2.40109000	4.23143100	1.27374500
H	-1.54085800	4.48975300	0.64543500
C	-1.85093100	3.58797100	2.55667900
H	-1.24895000	2.69917600	2.33599800
H	-1.22076700	4.30269300	3.10048300
H	-2.66990200	3.28233500	3.21920800
C	-3.13631100	5.54078500	1.60365600
H	-3.94545900	5.37913400	2.32505000
H	-2.43945900	6.26061500	2.04735300
H	-3.57149300	5.99377300	0.70584600

C	-3.19916300	1.20874400	-2.77386000
H	-2.24374200	1.67858900	-3.03342100
C	-4.19810100	1.52671700	-3.89978800
H	-3.79607000	1.19221700	-4.86263800
H	-5.15268600	1.01150300	-3.74268600
H	-4.40524400	2.60069900	-3.96949500
C	-2.96121400	-0.30232500	-2.68050200
H	-3.87691600	-0.82422400	-2.38211800
H	-2.63739200	-0.69984700	-3.65004200
H	-2.18232600	-0.53041900	-1.94701600
Mg	0.03196300	-1.40991400	0.50247600
N	1.52285200	-2.80378300	0.77976600
C	1.34963400	-3.87422600	1.57311700
C	0.13114200	-4.23418100	2.17679100
H	0.17775400	-5.08338300	2.84658400
C	2.50526400	-4.82849400	1.82472300
H	2.89990400	-5.21706700	0.88048200
H	2.17887700	-5.67047800	2.43638800
H	3.33808200	-4.33326300	2.33247600
C	2.79816400	-2.70305100	0.10761900
C	2.90617300	-3.16174400	-1.22261200
C	4.16955700	-3.16518000	-1.82503400
H	4.27865100	-3.53028100	-2.84103800
C	5.28842800	-2.69221300	-1.14728300
H	6.26086800	-2.70179600	-1.63004300
C	5.15671700	-2.19095200	0.14553500
H	6.03285900	-1.80857300	0.65841400
C	3.91941500	-2.19514500	0.79787900
C	1.68175600	-3.65985400	-1.98679800
H	0.81358300	-3.10837000	-1.60409400
C	1.76572600	-3.37852000	-3.49374700
H	2.00589500	-2.32801800	-3.68718600
H	0.80314500	-3.59987700	-3.96697000
H	2.52214700	-4.00357200	-3.98283300
C	1.42281400	-5.15710800	-1.73815300
H	2.29762900	-5.75091100	-2.03101000
H	0.56585300	-5.50016700	-2.33121900
H	1.20231000	-5.36059100	-0.68526100
C	3.77873800	-1.65228400	2.21664000
H	3.02521900	-2.25288600	2.73885600
C	3.26803900	-0.20501200	2.18376700
H	3.95728100	0.42371700	1.61395300
H	3.19291900	0.20211700	3.19933500
H	2.27771200	-0.12643900	1.72472900
N	-1.43186100	-2.71600300	1.09782800
C	-1.15999500	-3.76861200	1.88643900
C	-2.30363600	-4.57852200	2.46450200
H	-2.87546500	-5.06433000	1.66655500
H	-1.93032100	-5.34921100	3.14016700
H	-3.00392100	-3.94026200	3.01183900
C	-2.79916200	-2.54535100	0.66611500
C	-3.22887500	-3.19535100	-0.51139400
C	-4.54185900	-2.98860300	-0.94731700
H	-4.88658300	-3.48219600	-1.85251100
C	-5.41078900	-2.15944700	-0.24419100
H	-6.42324700	-2.00042800	-0.60328900
C	-4.98356200	-1.55152600	0.93276800
H	-5.67033200	-0.92042100	1.48936800
C	-3.68843400	-1.75266800	1.42059600
C	-2.31723900	-4.13747500	-1.29414900
H	-1.37807600	-4.23924800	-0.73806700
C	-1.97365900	-3.57604700	-2.68377600
H	-1.41722700	-2.63577900	-2.60795100
H	-1.36210200	-4.29461600	-3.24326000
H	-2.88329300	-3.38320600	-3.26555900
C	-2.93441900	-5.54100000	-1.42393900
H	-3.85142500	-5.51898400	-2.02442200
H	-2.22864200	-6.22043800	-1.91583000
H	-3.18541500	-5.96257600	-0.44442600
C	-3.27297400	-1.15404400	2.75899400
H	-2.33871500	-1.63933300	3.06335900
C	-4.31549300	-1.41524900	3.85873900
H	-3.93268600	-1.07176500	4.82621500
H	-5.24805800	-0.87401700	3.66227300
H	-4.55834800	-2.48061500	3.94442200
C	-2.99085600	0.34780400	2.63363700
H	-3.88481000	0.88434500	2.29833200
H	-2.67926700	0.76202500	3.60021500
H	-2.18797800	0.53840200	1.91527800
F	0.00746600	-0.36512700	-1.12788500
C	3.19471600	0.15122800	-2.26789100
H	3.90136200	-0.48823900	-1.73112000
H	2.21718500	0.06387300	-1.78307400
H	3.09206000	-0.23545400	-3.28964900
C	5.07669200	-1.73381700	3.03190700
H	5.82517100	-1.02219600	2.66380900
H	4.87320800	-1.47925500	4.07745900
H	5.51506900	-2.73802500	3.00246900

[Mg]–F/F–[Mg] (THF)2
wB97X
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -3142.276054
Sum of electronic and thermal Energies= -3142.192819
Sum of electronic and thermal Enthalpies= -3142.191875
Sum of electronic and thermal Free Energies= -3142.390599

lowest energy vibrations 22.36 43.79 50.99

0 1

Mg	1.32337000	0.48743600	-0.69911200
F	0.46985600	-1.09792700	0.10018000
N	3.27652800	-0.35484200	-0.82222700
C	4.22305900	0.24136000	-1.55852200
C	4.18903400	1.59231000	-1.95343500
H	5.01005100	1.91590400	-2.58180800
C	5.44299800	-0.54300000	-2.01327700
H	5.94626000	-1.02558800	-1.17054200
H	6.15644700	0.10966100	-2.51913100
H	5.15215200	-1.34083900	-2.70537200
C	3.58688000	-1.67118200	-0.31705300
C	4.16252800	-1.78730900	0.96831400
C	4.54438400	-3.05272600	1.42544100
H	5.00427500	-3.15460200	2.40372100
C	4.33513200	-4.18999600	0.65051200
H	4.63514800	-5.16552900	1.02151900
C	3.72786000	-4.07024100	-0.59497000
H	3.54661300	-4.96087900	-1.19004300
C	3.35978300	-2.81985900	-1.10203100
C	4.39183700	-0.55289000	1.83436500
H	3.61995800	0.17529900	1.55430600
C	4.25625700	-0.84189400	3.33733800
H	3.34820900	-1.41466300	3.55767700
H	4.22108300	0.10205500	3.89582300
H	5.11283100	-1.41094400	3.71747000
C	5.75963600	0.09977000	1.55738300
H	6.56296500	-0.64017500	1.66195500
H	5.94873100	0.90907500	2.27280900
H	5.80725700	0.52831400	0.55174900
C	2.71153000	-2.71863700	-2.47476300
H	2.75128000	-1.66584500	-2.77173400
C	3.43839900	-3.54311600	-3.54852600
H	2.99724200	-3.35029900	-4.53382200

H	3.34641600	-4.61813500	-3.35587700
H	4.50653000	-3.30200200	-3.59756400
C	1.23179600	-3.11985200	-2.39039000
H	1.13277700	-4.18540900	-2.15581800
H	0.72831500	-2.93892100	-3.35138100
H	0.72729900	-2.55739400	-1.59804800
N	2.23287900	2.41119900	-0.76196800
C	3.33705300	2.61404000	-1.49479600
C	3.74480600	4.02518100	-1.88671300
H	3.79246500	4.68788900	-1.01819600
H	4.71934400	4.02313900	-2.37767500
H	3.01206700	4.45985400	-2.57455500
C	1.60848200	3.58685500	-0.20329600
C	1.98597200	4.00119200	1.09486300
C	1.45795700	5.19111100	1.60520100
H	1.75407900	5.52903000	2.59393500
C	0.54784000	5.94631000	0.87034800
H	0.14540700	6.86737100	1.28123200
C	0.14630400	5.50485300	-0.38562800
H	-0.58171500	6.08249800	-0.94889700
C	0.67316900	4.33580800	-0.94572800
C	2.97414800	3.18215900	1.91933300
H	2.87600100	2.14167600	1.58435600
C	2.68034800	3.23247500	3.42690500
H	1.61810500	3.06542900	3.63703900
H	3.26431300	2.46351900	3.94823200
H	2.95946400	4.20069300	3.85911500
C	4.43248100	3.60683600	1.66300900
H	4.55186600	4.68415200	1.83276200
H	5.10919100	3.07863000	2.34538500
H	4.74705900	3.37710000	0.64051800
C	0.20932300	3.89750700	-2.32840900
H	0.84579200	3.06038700	-2.63698200
C	0.32993000	5.01136100	-3.38202400
H	0.07499000	4.62086000	-4.37494100
H	-0.36247800	5.83340300	-3.16647400
H	1.34042300	5.43180300	-3.42967700
C	-1.23723400	3.38715700	-2.25601000
H	-1.92072300	4.19748900	-1.97984800
H	-1.56241800	2.99713200	-3.23150900
H	-1.32506400	2.60159300	-1.49880700
O	0.69684000	0.24821900	-2.63578800
Mg	-1.32345000	-0.48728700	0.69903700
N	-2.23256500	-2.41113700	0.76237100
C	-3.33663200	-2.61410000	1.49531700
C	-4.18885100	-1.59243300	1.95364200
H	-5.00976700	-1.91600900	2.58215200
C	-3.74379400	-4.02522900	1.88792000
H	-3.79098300	-4.68847700	1.01979400
H	-4.71840600	-4.02337900	2.37873500
H	-3.01094000	-4.45913400	2.57615000
C	-1.60786600	-3.58671200	0.20384600
C	-1.98537400	-4.00134300	-1.09421200
C	-1.45698300	-5.19111300	-1.60450500
H	-1.75313700	-5.52925200	-2.59315700
C	-0.54651500	-5.94591200	-0.86967900
H	-0.14378400	-6.86686500	-1.28051000
C	-0.14513100	-5.50427000	0.38628500
H	0.58308200	-6.08165500	0.94956800
C	-0.67236100	-4.33536300	0.94633100
C	-2.97419800	-3.18292500	-1.91851400
H	-2.87700400	-2.14246500	-1.58319700
C	-2.68026100	-3.23252800	-3.42607700
H	-1.61815500	-3.06441600	-3.63604500
H	-3.26492100	-2.46398000	-3.94723200
H	-2.95841100	-4.20088200	-3.85859800
C	-4.43213300	-3.60901200	-1.66228100
H	-4.55053200	-4.68641200	-1.83219100
H	-5.10935700	-3.08132400	-2.34454100
H	-4.74686100	-3.37972400	-0.63972900
C	-0.20885300	-3.89696100	2.32908300
H	-0.84500300	-3.05941400	2.63715200
C	-0.33064600	-5.01046100	3.38292900
H	-0.07608200	-4.61981500	4.37588400
H	0.36145700	-5.83292500	3.16801000
H	-1.34139900	-5.43034700	3.43008700
C	1.23801400	-3.38744700	2.25717400
H	1.92120200	-4.19820700	1.98150500
H	1.56302100	-2.99727800	3.23267600
H	1.32652100	-2.60219700	1.49975500
N	-3.27681600	0.35461600	0.82180100
C	-4.22320700	-0.24161500	1.55827300
C	-5.44343000	0.54252200	2.01265300
H	-5.94713000	1.02411000	1.16959900
H	-6.15643700	-0.11006700	2.51921700
H	-5.15286800	1.34112400	2.70396400
C	-3.58748200	1.67082500	0.31646500
C	-4.16316200	1.78674400	-0.96891900
C	-4.54536000	3.05205300	-1.42606700
H	-5.00529100	3.15379400	-2.40433800
C	-4.33643200	4.18940300	-0.65117000
H	-4.63673900	5.16483700	-1.02220000
C	-3.72898900	4.06987400	0.59424300
H	-3.54787000	4.96059400	1.18923300
C	-3.36055200	2.81961100	1.10132500
C	-4.39196200	0.55224200	-1.83500600
H	-3.61990500	-0.17570200	-1.55479400
C	-4.25613300	0.84124000	-3.33795600
H	-3.34809500	1.41408900	-3.55814400
H	-4.22076200	-0.10271200	-3.89641900
H	-5.11270200	1.41019400	-3.71824400
C	-5.75960900	-0.10088700	-1.55840500
H	-6.56314100	0.63883400	-1.66301000
H	-5.94828000	-0.91008800	-2.27406100
H	-5.80731100	-0.52968000	-0.55288800
C	-2.71192400	2.71865300	2.47388500
H	-2.75124700	1.66585100	2.77089000
C	-3.43870700	3.54300500	3.54781200
H	-2.99705100	3.35052800	4.53295200
H	-3.34724600	4.61802500	3.35493100
H	-4.50671900	3.30148600	3.59738200
C	-1.23236100	3.12034400	2.38905500
H	-1.13373900	4.18590400	2.15434200
H	-0.72850500	2.93967500	3.34990300
H	-0.72793500	2.55792900	1.59663100
F	-0.46999200	1.09828000	-0.10026800
C	1.40140900	0.56116300	-3.88724000
C	-0.69501300	-0.16593700	-2.91365500
C	0.28016100	0.79385600	-4.89331300
H	2.04174800	1.42360000	-3.69699800
H	2.02430600	-0.29881800	-4.15769800
C	-0.79038200	-0.21320700	-4.43856800
H	-0.84821400	-1.13454900	-2.43226900
H	-1.34801500	0.58652300	-2.46601000
H	0.60668000	0.62760900	-5.92294500
H	-0.09821300	1.81959300	-4.81084600
H	-0.54766000	-1.21613700	-4.80888500
H	-1.79240100	0.04436100	-4.79089000
O	-0.69680800	-0.24765800	2.63560300
C	-1.40147300	-0.56005500	3.88710700
C	0.69475000	0.16744400	2.91348300
C	-0.28026800	-0.79263600	4.89322900
H	-2.02418700	0.30014100	4.15735500
H	-2.04200800	-1.42239000	3.69706300
C	0.79024700	0.21445700	4.43843100
H	1.34821300	-0.58447400	2.46558400
H	0.84728400	1.13627000	2.43233200
H	0.09812800	-1.81836600	4.81086700

H	-0.60681100	-0.62628800	5.92283700
H	1.79228600	-0.04323800	4.79060600
H	0.54765200	1.21734700	4.80892900

[Mg]–C_6F_5/C_6F_5–[Mg]
wB97X
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -3932.854015
Sum of electronic and thermal Energies= -3932.765258
Sum of electronic and thermal Enthalpies= -3932.764314
Sum of electronic and thermal Free Energies= -3932.978281

Lowest energy vibrations = 15.33 24.99 28.09 cm^{-1}

0 1

Mg	-2.49868700	-0.19716300	0.45671000
N	-3.43379000	-1.40948700	1.80416600
C	-4.75866600	-1.57434800	1.75301800
C	-5.61022700	-0.96442100	0.80583400
H	-6.66199200	-1.17527600	0.96274100
C	-5.47681200	-2.47309200	2.74451000
H	-4.83062400	-2.81784100	3.55166400
H	-5.87119800	-3.34962000	2.21877500
H	-6.33161900	-1.94500200	3.17714000
C	-2.66218800	-2.03316100	2.85752600
C	-2.09412000	-3.31025000	2.65749600
C	-1.35917100	-3.89105800	3.69720000
H	-0.92848400	-4.87806900	3.55688000
C	-1.17325200	-3.23180400	4.90637700
H	-0.60432000	-3.70035400	5.70309200
C	-1.71807200	-1.96517600	5.08576700
H	-1.56727600	-1.44784400	6.02867000
C	-2.46101700	-1.34415400	4.07632400
C	-2.27846400	-4.08597800	1.35977100
H	-2.69865500	-3.40275200	0.61462300
C	-0.93908500	-4.60767600	0.81659200
H	-0.21309200	-3.79361500	0.71881000
H	-1.08372600	-5.07185100	-0.16469700
H	-0.50210600	-5.36335700	1.47902100
C	-3.26487600	-5.25313800	1.54079600
H	-2.87610900	-5.97752100	2.26696400
H	-3.41969100	-5.77347400	0.58896700
H	-4.23712700	-4.90517600	1.90341400
C	-3.05370200	0.03504700	4.33539400
H	-3.35701400	0.45796800	3.37344200
C	-4.31023000	-0.05045800	5.22119000
H	-4.72271500	0.94978900	5.39495800
H	-4.06485900	-0.49348900	6.19415900
H	-5.08962500	-0.66342200	4.75854700
N	-4.11702600	0.23234900	-0.72925700
C	-5.34120500	-0.14373600	-0.30109400
C	-6.56952500	0.36477900	-1.03512300
H	-6.45607500	0.30953700	-2.11966100
H	-7.45663200	-0.19954700	-0.74394900
H	-6.73815300	1.41733400	-0.78241000
C	-4.04440500	0.99477400	-1.96158500
C	-3.84522000	0.30294500	-3.18250300
C	-3.80078700	1.03483800	-4.37311500
H	-3.65228300	0.51698600	-5.31431700
C	-3.93111900	2.42050200	-4.37612600
H	-3.89272600	2.97008100	-5.31145800
C	-4.10750300	3.09193400	-3.17352400
H	-4.20536400	4.17422700	-3.17307500
C	-4.17325900	2.40137000	-1.95652700
C	-3.67362900	-1.21276800	-3.21272700
H	-3.15135200	-1.49171900	-2.29105400
C	-2.83572900	-1.70053900	-4.40499400
H	-1.88477600	-1.16048200	-4.48825100
H	-2.62068300	-2.76857700	-4.29547200
H	-3.37615400	-1.58038800	-5.35086600
C	-5.01835000	-1.96486200	-3.20815200
H	-5.64346100	-1.63819200	-4.04831300
H	-4.84132800	-3.04127600	-3.31131800
H	-5.57298300	-1.81011500	-2.27932100
C	-4.35418000	3.20819000	-0.67783500
H	-4.45058500	2.50657100	0.15470500
C	-5.61545700	4.08880600	-0.71197800
H	-5.75258300	4.58538300	0.25485000
H	-5.53412500	4.86868500	-1.47831000
H	-6.51749600	3.50670100	-0.92754100
C	-3.11787000	4.08700400	-0.41252100
H	-3.02716500	4.86857600	-1.17785100
H	-3.19710700	4.57637900	0.56487300
H	-2.19391800	3.49850000	-0.43039300
Mg	2.35052600	-0.06944500	-0.63138300
N	4.20597200	-0.81760800	-0.24934800
C	5.16975100	-0.50260100	-1.12473900
C	5.05932400	0.51624000	-2.09790700
H	5.85942900	0.54728800	-2.82801300
C	6.47030300	-1.27996900	-1.12227800
H	6.82821500	-1.46404900	-0.10597700
H	7.24300900	-0.74602200	-1.67749900
H	6.32090300	-2.25639500	-1.59727600
C	4.48301300	-1.72731200	0.83596400
C	4.82550700	-1.17766700	2.09538200
C	5.08357600	-2.04700700	3.15840700
H	5.35036200	-1.64046800	4.12833100
C	4.99399600	-3.42737600	2.99752300
H	5.19757800	-4.08774800	3.83459900
C	4.63300400	-3.95353100	1.76389300
H	4.55086100	-5.03041900	1.64455100
C	4.37259200	-3.12264500	0.66686100
C	4.92106800	0.33253400	2.28652300
H	4.18992400	0.78708600	1.60903400
C	4.57326000	0.78730700	3.71049000
H	3.62561200	0.35597100	4.04895100
H	4.47635900	1.87787000	3.73467500
H	5.35460400	0.50811300	4.42731600
C	6.30710600	0.87222500	1.88688400
H	7.09340100	0.38710600	2.47818500
H	6.36017600	1.95283000	2.07057600
H	6.51822700	0.70562600	0.82591000
C	3.95609000	-3.75962700	-0.65431800
H	3.88301800	-2.96826600	-1.40919900
C	2.57076000	-4.41723300	-0.51958600
H	2.58914500	-5.21543300	0.23192900
H	2.25573100	-4.85897900	-1.47300900
H	1.81765600	-3.68535100	-0.20985600
N	3.05717400	1.67881100	-1.37273500
C	4.12348100	1.55864700	-2.18507000
C	4.32568300	2.56481200	-3.30073800
H	4.02044400	3.57212200	-3.01035400
H	5.36559400	2.58925300	-3.63250300
H	3.70468800	2.26698800	-4.15577000
C	2.33842200	2.92050400	-1.26682100
C	2.79136800	3.91026400	-0.35529600
C	2.00154400	5.05027100	-0.17126000
H	2.32186100	5.81183900	0.53179400
C	0.80190900	5.22363900	-0.86031700
H	0.20103300	6.11173200	-0.69060100
C	0.38595200	4.26107200	-1.77191200
H	-0.54205900	4.40283500	-2.32029600
C	1.14707600	3.10719400	-1.99675000

C	4.10662100	3.75494400	0.40960300
H	4.22384400	2.68697800	0.62892800
C	4.13319400	4.52947600	1.73792500
H	3.22895900	4.37543200	2.33003400
H	4.99246500	4.20096000	2.33474900
H	4.25311100	5.60652400	1.56679200
C	5.32602900	4.19268000	-0.42732500
H	5.18578100	5.21231000	-0.80677600
H	6.22642100	4.18481700	0.19862800
H	5.51134000	3.52843200	-1.27355500
C	0.67214500	2.08937200	-3.02507300
H	1.42228900	1.29125600	-3.08217300
C	0.54785300	2.71316800	-4.42551700
H	0.27627300	1.94722500	-5.16072800
H	-0.23223600	3.48307000	-4.44359300
H	1.48879600	3.17738100	-4.74007600
C	-0.66351900	1.45900300	-2.60780500
H	-1.46905000	2.20122400	-2.61950200
H	-0.94478300	0.65481300	-3.29704500
H	-0.60155800	1.03956200	-1.59601200
C	-2.03432900	0.99469900	4.97345000
H	-1.84940100	0.74359000	6.02436700
H	-1.07330200	0.96265400	4.44801800
H	-2.41537200	2.02238100	4.94274300
C	4.98118000	-4.79498000	-1.14865300
H	5.02614200	-5.65878700	-0.47521900
H	4.70122500	-5.16154000	-2.14247600
H	5.98855200	-4.37048700	-1.21037400
C	1.00523800	-1.41704500	-1.71082400
C	1.62280400	-1.99564600	-2.81066800
C	-0.24616100	-1.93198200	-1.46133800
C	1.08643600	-3.01898100	-3.57812400
C	-0.84181900	-2.97346600	-2.15568500
C	-0.16180400	-3.51779600	-3.23323100
F	2.89336500	-1.54279000	-3.17014800
F	1.75711100	-3.54695300	-4.65088200
F	-0.74186600	-4.52038200	-3.96783800
F	-2.08197500	-3.46890100	-1.82062000
F	-1.04426200	-1.40001300	-0.38866900
C	-1.77995900	2.33079400	1.99794900
C	-1.16231200	1.27456700	1.34223800
C	-1.11975300	3.35407600	2.65992600
C	0.20609900	1.31930300	1.45152800
C	0.26617200	3.32408600	2.72560700
C	0.94377800	2.27507600	2.12800800
F	-3.17447300	2.37521700	2.04249000
F	-1.81181500	4.36617600	3.27493000
F	0.95664200	4.30646400	3.38870700
F	2.31125600	2.18138300	2.21604600
F	1.01204400	0.28911200	0.84759600

[Mg]–[Mg] (3.0 A, torsion = 39°)
wB97XD
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -2477.864422
Sum of electronic and thermal Energies= -2477.794228
Sum of electronic and thermal Enthalpies= -2477.793284
Sum of electronic and thermal Free Energies= -2477.968688

Lowest energy vibrations = 29.99 31.24 36.33 cm^{-1}

0 1

C	-1.21149600	4.28112700	0.39497500
C	1.18183700	4.29284200	-0.42483600
C	-0.01950600	4.89319200	-0.02042600
H	-0.02555200	5.97566700	-0.02245800
C	1.18101300	-4.29306200	0.42519200
C	-1.21232500	-4.28101800	-0.39462400
C	-0.02046100	-4.89324100	0.02092800
H	-0.02672500	-5.97571400	0.02318700
C	2.31382500	5.23227400	-0.79847300
H	3.19757700	5.04344800	-0.17968600
H	2.62041800	5.07944200	-1.83886700
H	2.01638800	6.27414800	-0.67268600
C	-2.34462900	5.21073400	0.78998000
H	-3.25029700	4.99508300	0.21372700
H	-2.60465300	5.07591500	1.84572700
H	-2.06928800	6.25414100	0.63102700
C	2.31276700	-5.23264900	0.79914700
H	3.19681600	-5.04376600	0.18081100
H	2.61886000	-5.08000400	1.83972200
H	2.01530800	-6.27448200	0.67307500
C	-2.34558500	-5.21049300	-0.78956600
H	-3.25134100	-4.99448000	-0.21358700
H	-2.60535500	-5.07594500	-1.84540600
H	-2.07050300	-6.25391000	-0.63023300
C	-2.69045500	-2.48681000	-0.90052000
C	-3.68782200	-2.23506700	0.06667200
C	-2.94256700	-2.29868500	-2.27478900
C	-4.91563700	-1.72221300	-0.36285200
C	-4.19565100	-1.81144700	-2.66235900
C	-5.17057400	-1.50911400	-1.71544700
H	-5.68792100	-1.49930400	0.36414500
H	-4.40932200	-1.65782800	-3.71490500
H	-6.13194000	-1.11746900	-2.03167200
C	2.68678300	-2.51135600	0.89726900
C	2.97074300	-2.32419600	2.26582200
C	3.66250800	-2.26388100	-0.09164200
C	4.23407000	-1.84157100	2.62335900
C	4.90098500	-1.75187600	0.30766000
C	5.18746200	-1.54012900	1.65370800
H	4.47390300	-1.69039000	3.67052000
H	5.65482600	-1.52753800	-0.43850900
H	6.15638000	-1.14997100	1.94795800
C	2.68723900	2.51098200	-0.89728800
C	2.97104700	2.32396200	-2.26591100
C	3.66310000	2.26353700	0.09149700
C	4.23441400	1.84158000	-2.62362300
C	4.90160200	1.75174300	-0.30800100
C	5.18795400	1.54018500	-1.65409600
H	4.47421500	1.69055900	-3.67080600
H	5.65558100	1.52748600	0.43805200
H	6.15691400	1.15024100	-1.94849200
C	-2.69003500	2.48715700	0.90045000
C	-3.68730400	2.23578100	-0.06695500
C	-2.94248600	2.29888100	2.27463100
C	-4.91528500	1.72307000	0.36222000
C	-4.19575200	1.81183400	2.66187700
C	-5.17054200	1.50981900	1.71473800
H	-5.68743900	1.50038200	-0.36498800
H	-4.40962200	1.65808200	3.71436800
H	-6.13203000	1.11827300	2.03071500
Mg	0.00391800	-1.49161400	0.00357200
Mg	0.00423100	1.49155100	-0.00355800
C	1.91982700	-2.63707300	3.32581300
H	1.22326600	-3.36579800	2.89663400
C	3.37280500	-2.59084300	-1.55324900
H	2.60341800	-3.37095200	-1.56458800
C	-3.43280300	-2.56724100	1.53443900
H	-2.73723400	-3.41441000	1.55922900

C	-1.86960200	-2.61205800	-3.31210700
H	-1.16547300	-3.31758500	-2.85724900
C	3.37354300	2.59045000	1.55313800
H	2.60464500	3.37104500	1.56455500
C	1.91988100	2.63684900	-3.32567500
H	1.22380900	3.36609700	-2.89657400
C	-3.43188700	2.56796900	-1.53462800
H	-2.73567000	3.41458900	-1.55930400
C	-1.86969500	2.61175700	3.31225800
H	-1.16495000	3.31677600	2.85756700
N	-1.39822600	2.95347000	0.46888100
N	1.38334300	2.96690400	-0.49196100
N	1.38281400	-2.96715500	0.49206900
N	-1.39879600	-2.95332500	-0.46868400
C	2.80551100	-1.37527300	-2.30333200
H	3.55594800	-0.58303000	-2.37006600
H	2.49730400	-1.65480900	-3.31817100
H	1.93907000	-0.94328100	-1.78785900
C	4.59886000	-3.14939800	-2.29475900
H	5.36701200	-2.38113900	-2.44019100
H	5.05057800	-3.98485400	-1.74895000
H	4.30238500	-3.50643500	-3.28719600
C	2.51300700	-3.26466700	4.59758200
H	3.14228400	-4.12892300	4.35867400
H	3.12131100	-2.54679900	5.15950800
H	1.70693600	-3.59794200	5.26035100
C	1.10019000	-1.38014100	3.66978300
H	0.29129600	-1.61950000	4.36966000
H	1.73894000	-0.61460400	4.12523200
H	0.65505300	-0.94502100	2.76766500
C	-1.07122300	-1.34524100	-3.66999000
H	-0.25185600	-1.58032100	-4.35914100
H	-1.72016400	-0.59913000	-4.14328700
H	-0.64210000	-0.88735500	-2.77132900
C	-2.43262000	-3.27829100	-4.57808700
H	-3.04456700	-4.15212800	-4.32901600
H	-3.05103100	-2.58639600	-5.16113300
H	-1.61125200	-3.60597700	-5.22473300
C	-4.70454500	-2.99968500	2.28276100
H	-5.23627800	-3.79312300	1.74629800
H	-4.44043600	-3.37410100	3.27775700
H	-5.39351200	-2.15866600	2.42262000
C	-2.76066800	-1.40076700	2.27578600
H	-1.85301600	-1.05731600	1.76652300
H	-3.43470500	-0.54197100	2.32513400
H	-2.48904100	-1.69516100	3.29674600
C	1.09952000	1.38015900	-3.66883400
H	0.29043600	1.61964000	-4.36844800
H	1.73774200	0.61418600	-4.12428600
H	0.65454200	0.94548100	-2.76641300
C	2.51276400	3.26353500	-4.59801700
H	3.14266300	4.12753800	-4.35984800
H	3.12033100	2.54503200	-5.15993200
H	1.70652900	3.59696100	-5.26050800
C	2.80549200	1.37514700	2.30308900
H	3.55563000	0.58265600	2.37018200
H	2.49699300	1.65488300	3.31778300
H	1.93910700	0.94335600	1.78736900
C	4.59990600	3.14807400	2.29483500
H	5.36757200	2.37929400	2.44011000
H	5.05218400	3.98339500	1.74927700
H	4.30359400	3.50503300	3.28734700
C	-2.76048400	1.40094200	-2.27576600
H	-3.43541900	0.54288000	-2.32575400
H	-2.48774600	1.69519800	-3.29646700
H	-1.85362900	1.05648200	-1.76573300
C	-4.70318200	3.00152400	-2.28303700
H	-5.39298600	2.16120200	-2.42293200
H	-5.23416400	3.79548800	-1.74660300
H	-4.43867300	3.37567200	-3.27803400
C	-2.43285100	3.27852600	4.57788400
H	-3.04399300	4.15280500	4.32836400
H	-3.05213100	2.58718200	5.16066300
H	-1.61159100	3.60565500	5.22494900
C	-1.07229000	1.34444600	3.67054400
H	-0.25322500	1.57894900	4.36024700
H	-1.72195400	0.59861900	4.14330100
H	-0.64285400	0.88648700	2.77207200

[Mg]–[Mg] (2.85 A, torsion = 76°)
wB97XD
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -2477.868831
Sum of electronic and thermal Energies= -2477.799215
Sum of electronic and thermal Enthalpies= -2477.798271
Sum of electronic and thermal Free Energies= -2477.971366

Lowest energy vibrations = 24.79 37.89 41.99 cm^{-1}

0 1

Mg	-1.13719800	-0.95353700	0.20844700
N	-2.99628500	-1.25972700	1.03519700
N	-1.29970500	-2.66843600	-0.90527800
C	-4.87956900	-2.63582700	1.85340100
C	-3.60772500	-2.45898500	1.04425700
C	-3.19791100	-3.56938800	0.28822800
C	-2.19689700	-3.63643600	-0.70005800
C	-2.17167000	-4.87408300	-1.57422300
C	-3.71839300	-0.13849300	1.57670000
C	-3.39831800	0.38767900	2.84378500
C	-4.16088700	1.45101700	3.34368700
C	-5.19557300	2.00916300	2.60235000
C	-5.46713000	1.51917700	1.32735400
C	-4.74323800	0.44889800	0.79642400
C	-2.24891800	-0.15822400	3.67972300
C	-1.24164100	0.95610800	4.01858900
C	-2.75416100	-0.85377100	4.95714200
C	-5.02115600	-0.02083700	-0.62792200
C	-4.38284200	0.95597000	-1.63423900
C	-6.51991600	-0.20187600	-0.92305600
C	-0.34289300	-2.76722600	-1.97186300
C	0.85740000	-3.48693700	-1.78419400
C	1.81885800	-3.46294600	-2.79950900
C	1.59944000	-2.76441900	-3.98389400
C	0.40551600	-2.07274300	-4.16318200
C	-0.57506200	-2.05029800	-3.16498100
C	1.13892900	-4.24335900	-0.49186500
C	2.16507900	-3.48607400	0.36586400
C	1.60718900	-5.68783000	-0.74523400
C	-1.86153400	-1.26258300	-3.38751700
C	-1.56939800	0.21446700	-3.69871800
C	-2.72497800	-1.90105700	-4.49133300
H	-4.79685100	-2.15295400	2.83056500
H	-5.10255700	-3.69466600	1.99614700
H	-5.73060400	-2.17334500	1.34100400
H	-3.80303600	-4.46037800	0.40164200
H	-2.21833600	-4.59511900	-2.63196400
H	-3.00995600	-5.53437400	-1.34779500
H	-1.24078000	-5.43291700	-1.43607700
H	-3.93699500	1.84784000	4.32918500
H	-5.77595100	2.83158400	3.00654300

H	-6.25330400	1.97797200	0.73647300
H	-1.72669200	-0.91019600	3.07796900
H	-0.84282000	1.40530900	3.10195700
H	-0.40387100	0.55615900	4.59944700
H	-1.70776100	1.75131900	4.61115800
H	-3.29342400	-0.14905300	5.60093700
H	-1.91436300	-1.26142000	5.53182100
H	-3.43286700	-1.67791400	4.71454600
H	-4.54023700	-0.99352300	-0.76899200
H	-4.83428300	1.95156100	-1.54596800
H	-4.53186000	0.60030600	-2.66037600
H	-3.30668100	1.06356800	-1.45945900
H	-6.99650800	-0.85551600	-0.18480300
H	-6.65510600	-0.64897900	-1.91407800
H	-7.05217100	0.75612000	-0.91849400
H	2.75505200	-3.99377300	-2.65825100
H	2.35562900	-2.75823700	-4.76146100
H	0.23341900	-1.53568100	-5.09105900
H	0.20774800	-4.29168300	0.08183700
H	3.13302100	-3.42208200	-0.14310000
H	2.32198200	-3.98889100	1.32605800
H	1.83076700	-2.46299900	0.56878500
H	0.90767100	-6.23404400	-1.38741500
H	1.69506900	-6.22532800	0.20534600
H	2.59064300	-5.70945300	-1.22839200
H	-2.44045800	-1.30071400	-2.45708900
H	-0.99987700	0.68440400	-2.88968000
H	-2.49888000	0.77784300	-3.82720600
H	-0.98933600	0.32260400	-4.62246800
H	-2.20537900	-1.87785100	-5.45660100
H	-3.66949100	-1.35574200	-4.60136100
H	-2.95720800	-2.94561300	-4.25830500
Mg	1.05036800	0.86345400	0.45535900
N	1.29915000	2.79214300	-0.20520800
N	2.85772100	0.91965000	1.43244300
C	2.08683900	5.13010700	-0.06802700
C	2.12297200	3.67735400	0.36648500
C	3.05615200	3.34272600	1.36629600
C	3.45878000	2.06689500	1.79396000
C	4.70212600	2.01333600	2.66228400
C	0.48113900	3.18282200	-1.31840500
C	0.90537400	2.83078900	-2.62175500
C	0.10129000	3.19998800	-3.70484600
C	-1.11242700	3.85567400	-3.51132400
C	-1.53933700	4.15215400	-2.22172400
C	-0.75251900	3.83319200	-1.10898500
C	2.19971200	2.04714900	-2.83385400
C	3.44878500	2.94792100	-2.76677000
C	2.20341900	1.23480300	-4.13747600
C	-1.26125100	4.15816300	0.29005200
C	-2.41726000	3.22077600	0.67776700
C	-1.69521300	5.62924200	0.43067300
C	3.55724400	-0.30931400	1.69806400
C	4.55899900	-0.72760900	0.79291200
C	5.28993600	-1.88320200	1.08294700
C	5.03434700	-2.62495200	2.23346500
C	4.00516000	-2.23719800	3.08438200
C	3.24340800	-1.09107700	2.82721100
C	4.79743500	0.00971300	-0.52013000
C	4.22504200	-0.81855300	-1.68759400
C	6.27836100	0.34666300	-0.76167400
C	2.08440500	-0.74013400	3.74990100
C	2.55547000	-0.40651000	5.17707600
C	1.04747300	-1.87956900	3.76786300
H	2.02479200	5.21651100	-1.15626900
H	2.97232600	5.66438600	0.27993700
H	1.20243600	5.62742300	0.34502700
H	3.62047800	4.17235200	1.77367200
H	4.58246100	1.30426700	3.48545200
H	4.93333500	2.99867100	3.07030900
H	5.56343200	1.67368000	2.07595500
H	0.40936100	2.94946200	-4.71307000
H	-1.72801800	4.12060200	-4.36435100
H	-2.49739000	4.64043500	-2.07356000
H	2.27967500	1.32878500	-2.00600800
H	3.39553700	3.73190100	-3.53138300
H	4.35216600	2.35291900	-2.94841300
H	3.55411900	3.42185100	-1.78740000
H	1.31034200	0.60920800	-4.21629300
H	3.07546100	0.57425200	-4.16240000
H	2.26003400	1.88491300	-5.01864000
H	-0.44426100	3.98034600	0.99737200
H	-3.26912400	3.34913900	0.00031800
H	-2.76276100	3.42241800	1.69676600
H	-2.10636500	2.17164800	0.62913800
H	-0.91184200	6.31774200	0.09638600
H	-1.92964700	5.85267200	1.47731500
H	-2.59490900	5.83591700	-0.16018600
H	6.06321600	-2.21196500	0.39539600
H	5.61759300	-3.51318100	2.45153000
H	3.78477600	-2.83616600	3.96295800
H	4.24713000	0.95567500	-0.48580400
H	4.71837100	-1.79616600	-1.74967000
H	4.37997100	-0.29883700	-2.63945600
H	3.15088000	-0.99886000	-1.56458900
H	6.69795200	0.91708900	0.07357700
H	6.38285100	0.94709100	-1.67242800
H	6.88278000	-0.55869300	-0.89031800
H	1.59790600	0.15309800	3.34314200
H	3.04002500	-1.27153900	5.64487600
H	1.70286800	-0.11920300	5.80364800
H	3.27097000	0.42207100	5.17552000
H	0.65315800	-2.05908500	2.76138000
H	0.20888800	-1.62992400	4.42673600
H	1.49070900	-2.81409000	4.13009800

[Mg]–F
wB97XD
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -1338.806442
Sum of electronic and thermal Energies= -1338.770789
Sum of electronic and thermal Enthalpies= -1338.769845
Sum of electronic and thermal Free Energies= -1338.873281

Lowest energy vibrations = 31.67 43.77 55.07 cm^{-1}

0 1

Mg	-0.00000100	-0.13001300	-0.71796400
N	1.46544100	0.09235700	0.59739300
C	1.26988800	0.21857900	1.91808800
C	0.00000800	0.28150700	2.52163600
H	0.00001100	0.38131800	3.59956500
C	2.47946700	0.28145800	2.82555100
H	3.09042100	-0.61994700	2.70635900
H	2.18729400	0.37296200	3.87225900
H	3.11803300	1.13187700	2.56316600
C	2.79661800	0.02417000	0.05595200
C	3.36479500	-1.23704300	-0.21051800
C	4.62494700	-1.28356400	-0.81686700

H	5.07655000	-2.24504700	-1.03776500
C	5.30295500	-0.11513600	-1.15059500
H	6.27809300	-0.16951000	-1.62222800
C	4.72193700	1.12481400	-0.89330400
H	5.25173800	2.02884100	-1.17341200
C	3.46344300	1.21717400	-0.29219300
C	2.60245200	-2.52133900	0.09270900
H	1.77062600	-2.26493400	0.75936900
C	2.00372300	-3.10804500	-1.20377600
H	1.36971000	-2.38698000	-1.73334200
H	1.40439900	-3.99806700	-0.97850200
H	2.80504800	-3.40380600	-1.89127000
C	3.46479500	-3.56476200	0.82284800
H	4.27387800	-3.93583700	0.18377200
H	2.85072900	-4.42574900	1.10878000
H	3.91416100	-3.14507600	1.72935100
C	2.78328600	2.56619300	-0.08968100
H	2.03419300	2.45045500	0.70146800
C	2.03384100	2.97169100	-1.37559600
H	2.74126800	3.12036000	-2.19912300
H	1.47414400	3.90159600	-1.22553100
H	1.32906000	2.19446100	-1.69476400
N	-1.46543700	0.09234300	0.59740300
C	-1.26987600	0.21856500	1.91809700
C	-2.47944900	0.28143900	2.82556600
H	-3.09039800	-0.61997100	2.70638100
H	-2.18727100	0.37295000	3.87227200
H	-3.11802200	1.13185300	2.56318100
C	-2.79661700	0.02413400	0.05597100
C	-3.36475800	-1.23709200	-0.21050800
C	-4.62491100	-1.28364500	-0.81685300
H	-5.07648500	-2.24514000	-1.03775900
C	-5.30295500	-0.11523400	-1.15057000
H	-6.27809300	-0.16963400	-1.62219900
C	-4.72197000	1.12472900	-0.89327600
H	-5.25179500	2.02874700	-1.17337100
C	-3.46347700	1.21712100	-0.29217000
C	-2.60237000	-2.52136600	0.09269600
H	-1.77054000	-2.26493800	0.75934200
C	-2.00364200	-3.10804000	-1.20380500
H	-1.36969000	-2.38693400	-1.73338700
H	-1.40426000	-3.99802700	-0.97854600
H	-2.80496800	-3.40384900	-1.89127600
C	-3.46466600	-3.56482200	0.82284300
H	-4.27374800	-3.93591900	0.18377900
H	-2.85056800	-4.42579100	1.10876100
H	-3.91403200	-3.14515700	1.72935600
C	-2.78337800	2.56616800	-0.08966300
H	-2.03432000	2.45049400	0.70152800
C	-3.74860400	3.67790500	0.35062700
H	-3.18747400	4.58546000	0.59837900
H	-4.45754100	3.93889800	-0.44293100
H	-4.32289800	3.37673900	1.23322100
C	-2.03389300	2.97165600	-1.37555800
H	-2.74129100	3.12026700	-2.19912100
H	-1.47424300	3.90159100	-1.22549900
H	-1.32906600	2.19444500	-1.69467100
F	-0.00001300	-0.64868000	-2.42141100
C	3.74843000	3.67796500	0.35070300
H	4.45736400	3.93906800	-0.44282100
H	3.18723300	4.58546300	0.59850700
H	4.32272700	3.37677700	1.23328800

[Mg]–F–[Mg]–C_6F_5
wB97XD
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -3305.212727
Sum of electronic and thermal Energies= -3305.133160
Sum of electronic and thermal Enthalpies= -3305.132216
Sum of electronic and thermal Free Energies= -3305.323081

Lowest energy vibrations = 28.15 32.76 45.19 cm^{-1}

0 1

Mg	-1.28948100	-0.91616400	0.25581100
N	-1.57802500	-2.91862500	0.09013500
C	-1.55713200	-3.76042300	1.13255600
C	-1.57957400	-3.35530600	2.47885000
H	-1.54908700	-4.15459400	3.20881500
C	-1.71965800	-2.05896200	3.00512700
N	-1.70394200	-0.94518300	2.26467400
C	-1.51545200	-5.25505800	0.87759200
H	-2.26042200	-5.55242000	0.13472600
H	-1.69026600	-5.81493400	1.79754700
H	-0.53569000	-5.54050600	0.47942200
C	-1.87098400	-1.95579900	4.51090200
H	-2.15556600	-2.91617500	4.94380500
H	-2.61364100	-1.20508000	4.79150800
H	-0.91934400	-1.64824800	4.95954300
C	-1.73231800	-3.44566600	-1.23776300
C	-3.02804100	-3.47203300	-1.80642400
C	-3.16750300	-3.97366600	-3.10324700
H	-4.14742100	-4.00316300	-3.56444000
C	-2.06251600	-4.41119900	-3.83156500
H	-2.19473900	-4.79078000	-4.83925100
C	-0.79155900	-4.34269400	-3.27263200
H	0.06779800	-4.66508300	-3.85276300
C	-0.60356700	-3.86413800	-1.97062700
C	-4.23147700	-2.93053400	-1.03294500
H	-3.89034500	-2.02079300	-0.52018200
C	-5.40783100	-2.52658900	-1.93652600
H	-5.08308100	-1.86471700	-2.74179900
H	-6.15928600	-1.99838200	-1.33890500
H	-5.89894600	-3.40482000	-2.37297200
C	-4.73549800	-3.90687000	0.05024400
H	-4.97259000	-4.88116900	-0.39368100
H	-5.64904800	-3.51187700	0.51020500
H	-4.00297600	-4.05150100	0.84705400
C	0.80350600	-3.77261000	-1.39067300
H	0.71648300	-3.52219300	-0.32835200
C	1.58087300	-5.09630200	-1.50035400
H	1.02288700	-5.92892900	-1.05920100
H	2.54227700	-5.00651900	-0.98321700
H	1.78630100	-5.35063500	-2.54672100
C	1.59944200	-2.63595200	-2.05834800
H	1.75105800	-2.83870900	-3.12582600
H	2.58172500	-2.54008400	-1.58253000
H	1.06271200	-1.68761600	-1.96647700
C	-2.04649300	0.31525200	2.85718800
C	-1.06690700	1.12188500	3.46924300
C	-1.45024600	2.35984700	3.99351700

H	-0.70646700	2.99351200	4.46810000
C	-2.76306100	2.80846200	3.88575900
H	-3.04215700	3.77598700	4.28853100
C	-3.71266900	2.02311800	3.23540900
H	-4.72625500	2.39433800	3.12859900
C	-3.37532400	0.77307200	2.70853900
C	0.40067000	0.71120900	3.47980600
H	0.45832500	-0.27669800	3.01515700
C	0.99202800	0.61766000	4.89598000
H	0.97765100	1.59499600	5.39204800
H	2.03431300	0.27985800	4.85245800
H	0.42927700	-0.08056000	5.52242300
C	1.24343400	1.67966500	2.62549800
H	0.76494900	1.85688500	1.65614200
H	2.27268200	1.30863000	2.50291200
H	1.32480700	2.66360500	3.10022200
C	-4.41021200	-0.08693400	1.98825400
H	-3.86045500	-0.75942400	1.32047000
C	-5.38027300	0.72557400	1.11688200
H	-6.06205200	1.33504600	1.72114800
H	-5.99262900	0.04577700	0.51396300
H	-4.83926700	1.38960900	0.43684700
C	-5.18608200	-0.97868900	2.97707100
H	-4.51386900	-1.65597200	3.51203700
H	-5.92218900	-1.58912700	2.44144800
H	-5.71747400	-0.36451200	3.71386800
C	-2.23026000	0.67554800	-0.87650300
C	-2.16401000	1.94011900	-0.31922200
F	-1.27834900	2.15059800	0.74016100
C	-2.89906000	3.03711600	-0.73880300
F	-2.83317200	4.25085500	-0.09741300
C	-3.70785500	2.89262700	-1.85734700
C	-3.77148000	1.66627200	-2.50637600
F	-4.54910100	1.53283600	-3.63237200
C	-3.03786000	0.60039600	-1.99793500
F	-3.11393800	-0.59495600	-2.70510600
F	-4.40873700	3.96991700	-2.34186000
F	0.54767600	-0.49235200	0.07633900
Mg	2.04100500	0.52361100	-0.00321700
N	2.39678800	2.41344400	-0.56959600
N	3.89285000	-0.06470100	0.38541200
C	3.61580400	2.91127800	-0.35508000
C	1.35312400	3.15870400	-1.23196900
C	4.77571300	0.89723700	0.73172900
C	4.29455500	-1.44561700	0.35248000
C	4.62901300	2.24814600	0.39309400
C	4.03261300	4.25005000	-0.92631800
C	0.83044900	2.64560100	-2.44235000
C	0.79259000	4.32197400	-0.64846900
C	5.99641600	0.50919000	1.54093000
C	5.05489600	-1.92840000	-0.74527400
C	3.86683800	-2.33059300	1.36482500
H	5.46861100	2.88155700	0.65650900
H	3.27633500	4.67065100	-1.58871300
H	4.96289200	4.12148200	-1.48739400
H	4.23000700	4.96584500	-0.12248500
C	-0.20624400	3.33312200	-3.08033400
C	1.41766300	1.41592100	-3.12283500
C	-0.23178100	4.98171400	-1.33626100
C	1.21704700	4.88599300	0.70625900
H	6.45185500	-0.41372100	1.17764200
H	6.74883600	1.29929700	1.53853500
H	5.68582200	0.33179300	2.57794400
C	5.38238700	-3.28986000	-0.77560400
C	5.55307300	-1.09421700	-1.93136700
C	4.20877600	-3.68578400	1.27733800
C	3.06498500	-1.86642400	2.57298900
H	-0.60894600	2.94880000	-4.01064500
C	-0.72905400	4.50259700	-2.54205700
H	2.00560600	0.84960100	-2.38861200
C	0.35500300	0.45909800	-3.68490800
C	2.41340900	1.85185400	-4.21544100
H	-0.67327700	5.86988100	-0.89949300
H	2.00808500	4.24828600	1.11697700
C	0.04339500	4.87981400	1.70870000
H	5.96292400	-3.66811400	-1.61151500
C	4.96898600	-4.16826000	0.22103700
H	5.85047600	-1.84084900	-2.68018900
C	6.82236300	-0.27125300	-1.62784800
C	4.49868400	-0.21204900	-2.61475400
H	3.87824600	-4.36849600	2.05339000
H	2.88391400	-0.79090400	2.46655700
C	3.86401100	-2.06769700	3.87534200
C	1.70263200	-2.57687300	2.64937300
H	-1.54107200	5.01998900	-3.04098900
H	-0.36921200	0.17285400	-2.91697700
H	0.83302800	-0.44979200	-4.06463900
H	-0.19623500	0.90903900	-4.51690300
H	1.89906500	2.45457900	-4.97219700
H	2.85367700	0.97916000	-4.70879800
H	3.22164800	2.45540400	-3.78854300
H	-0.73269600	5.58850700	1.40090300
H	0.39925800	5.18180100	2.70129100
H	-0.42736200	3.90033500	1.78301400
H	5.22958000	-5.21949200	0.16615900
H	7.56162300	-0.86692200	-1.08239000
H	7.27799200	0.06094000	-2.56775700
H	6.58868400	0.62327300	-1.04382500
H	4.25978200	0.67135100	-2.01741500
H	4.88687400	0.13677300	-3.57821800
H	3.57605400	-0.76996800	-2.80740800
H	3.30685900	-1.67118800	4.73109500
H	4.04813900	-3.13200200	4.06053400
H	4.83456400	-1.56304100	3.82782200
H	1.81984900	-3.66513900	2.69045600
H	1.15804500	-2.27312900	3.54962700
H	1.07963500	-2.33909200	1.78244300
C	1.76236700	6.32523300	0.58568000
H	0.95753900	7.01738200	0.31393100
H	2.17165700	6.65578800	1.54698800
H	2.54369900	6.41509500	-0.17283300

[Mg]–F–[Mg]–F
wB97XD
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -2677.693924
Sum of electronic and thermal Energies= -2677.622551
Sum of electronic and thermal Enthalpies= -2677.621607
Sum of electronic and thermal Free Energies= -2677.795761

Lowest energy vibrations = 32.75 37.83 47.62 cm^{-1}

0 1

Mg	2.02198000	0.23385000	0.36665600
N	3.03593500	-0.28535600	-1.31543700
C	3.41548400	0.59033100	-2.25199500
C	3.18043100	1.97858400	-2.18516000
H	3.51372000	2.54690600	-3.04486600
C	2.65894300	2.74311500	-1.12293800
N	2.19081500	2.22427000	0.01632900
C	4.16235200	0.08143000	-3.46952300
H	5.05133400	-0.48079600	-3.16538300
H	4.47096400	0.90213800	-4.11858500
H	3.53740200	-0.60685400	-4.04936200
C	2.68946600	4.25038900	-1.28470700
H	2.91016700	4.53277200	-2.31535500
H	3.45661800	4.68751000	-0.63482000
H	1.73400200	4.69441200	-0.98901000
C	3.41442000	-1.66833600	-1.41376900
C	4.54120700	-2.11724100	-0.69149500
C	4.86797400	-3.47739000	-0.73393100
H	5.73209500	-3.83192400	-0.18088100
C	4.10498700	-4.38098200	-1.46600400
H	4.37282600	-5.43197900	-1.48664500
C	2.98763800	-3.92971400	-2.16296400
H	2.38308500	-4.63983000	-2.71856500
C	2.62395000	-2.57933400	-2.14846800
C	5.39963800	-1.16550800	0.13383000
H	4.96811000	-0.16210400	0.04468200
C	5.37321700	-1.55215900	1.62414700
H	4.35584700	-1.45360400	2.01499000
H	6.02719000	-0.88631400	2.19873500
H	5.72604100	-2.57973600	1.77339600
C	6.83967800	-1.09823000	-0.40862100
H	7.34311900	-2.06780900	-0.31418900
H	7.42130000	-0.36155100	0.15694700
H	6.85576600	-0.81048700	-1.46591800
C	1.34566700	-2.13808000	-2.85017300
H	1.34509000	-1.04481000	-2.88655100
C	1.23559500	-2.66274100	-4.29046200
H	2.10977700	-2.37706000	-4.88535300
H	0.34070700	-2.25559600	-4.77287200
H	1.15400300	-3.75511600	-4.31751000
C	0.13149800	-2.57136700	-2.00739800
H	0.07372800	-3.66388800	-1.93641600
H	-0.81094500	-2.21245700	-2.43937900
H	0.24360900	-2.17802500	-0.99452300
C	1.87586900	3.07159200	1.13097200
C	0.53401200	3.37881900	1.43325400
C	0.25327900	4.14939300	2.56743200
H	-0.77770700	4.39983000	2.80119300
C	1.27358000	4.59623300	3.39919900
H	1.04200600	5.18791700	4.27836900
C	2.59527500	4.26751600	3.10518400
H	3.38551600	4.59790500	3.77117100
C	2.91993200	3.50676700	1.97907400
C	-0.60716400	2.89047700	0.55311300
H	-0.16160900	2.26915500	-0.22793700
C	-1.35488700	4.04888000	-0.12809600
H	-1.80759100	4.71564400	0.61528700
H	-2.15110800	3.66963000	-0.77712500
H	-0.67139700	4.64534400	-0.74106900
C	-1.59086600	2.01548100	1.35413400
H	-1.07094200	1.19140200	1.86182200
H	-2.40101400	1.65843800	0.69322100
H	-2.09982800	2.58579200	2.13846000
C	4.36214900	3.08627500	1.72320400
H	4.43993000	2.75035000	0.68419700
C	4.71994100	1.88112200	2.61668800
H	4.69646500	2.17126200	3.67453600
H	5.72992700	1.52307300	2.38311900
H	4.01149000	1.05652600	2.47817500
C	5.36549700	4.23641900	1.90997300
H	5.08846900	5.11218700	1.31181000
H	6.36574900	3.91170400	1.60287100
H	5.43139500	4.54941600	2.95832400
F	0.19843800	-0.12621300	0.07007700
Mg	-1.57862900	-0.39646100	-0.07621000
N	-2.36940800	-1.96886600	0.84316900
N	-2.96388800	-0.11891300	-1.48295800
C	-3.19151900	-2.75326500	0.14377700
C	-1.96633500	-2.27886100	2.19385400
C	-3.69374000	-1.20335900	-1.83443000
C	-3.34527000	1.18723400	-1.96328400
C	-3.70126400	-2.42157500	-1.13716900
C	-3.63532200	-4.08880900	0.70184400
C	-0.91952300	-3.18853400	2.45035200
C	-2.59193600	-1.57574000	3.24973600
C	-4.56793500	-1.15815300	-3.07543900
C	-2.65747200	1.84537500	-3.00945500
C	-4.43202100	1.82633800	-1.31109700
H	-4.29910700	-3.20118000	-1.59559100
H	-3.01152500	-4.88411200	0.27808600
H	-4.67281500	-4.29555600	0.43014600
H	-3.53436700	-4.12867200	1.78754100
C	-0.54701900	-3.41707800	3.78012200
C	-0.15444000	-3.89035700	1.33867100
C	-2.18793600	-1.84074400	4.56122400
C	-3.70107100	-0.56765100	2.96733300
H	-4.80102800	-0.13726000	-3.37964100
H	-4.03698600	-1.64102700	-3.90358200
H	-5.50086900	-1.70354100	-2.91739600
C	-3.10367200	3.11698300	-3.39814400
C	-1.44067100	1.30334600	-3.75799500
C	-4.84293100	3.09006000	-1.74794900
C	-5.17893900	1.16749500	-0.15302800
H	0.26315300	-4.10762700	3.98913500
C	-1.17753600	-2.76070300	4.82897700
H	-0.59466600	-3.57920200	0.38737200
C	1.33186400	-3.47447200	1.34340200
C	-0.27577300	-5.42403000	1.42662700
H	-2.65753600	-1.31697000	5.38534600
H	-3.46783200	-0.07913300	2.01248000
C	-3.79890700	0.53895500	4.02886600
H	-2.58287500	3.62526500	-4.20374500
C	-4.18885300	3.73617100	-2.78968300
H	-1.26992400	2.02051100	-4.57256100
C	-1.64902200	-0.05925700	-4.43431600
C	-0.16116000	1.32528300	-2.90706700
H	-5.68557900	3.57410800	-1.26638200
H	-4.56901400	0.33429000	0.21219200
C	-6.52823900	0.57897500	-0.60979900
C	-5.40288400	2.13855300	1.02013700
H	-0.87186200	-2.94830900	5.85226400
H	1.46830100	-2.39724300	1.47844300
H	1.82202200	-3.78709000	0.41441100
H	1.85990500	-3.95721800	2.17499100
H	0.20587000	-5.80148000	2.33589300
H	0.22455500	-5.88798500	0.56905500
H	-1.31990600	-5.75332000	1.44122800
H	-4.19050100	0.15441700	4.97730600
H	-4.48257900	1.32300400	3.68908300
H	-2.82108800	0.99280700	4.22050100
H	-4.51631100	4.71549300	-3.12053500
H	-2.55486200	-0.05910400	-5.04924900
H	-0.79517700	-0.27954100	-5.08450000
H	-1.72708000	-0.86117500	-3.69771200
H	-0.16395800	0.57268500	-2.11431600
H	0.71618500	1.12299000	-3.53017600
H	-0.00980300	2.30543900	-2.44476700

H	-7.03395800	0.09410200	0.23286000
H	-7.18265600	1.37054700	-0.99365200
H	-6.39568200	-0.16431600	-1.39953700
H	-6.09972800	2.94032700	0.75349600
H	-5.83749700	1.60177900	1.86954800
H	-4.46593700	2.60006900	1.34649200
F	2.42010100	-0.43592200	2.00163200
C	-5.05992000	-1.27331900	2.78863700
H	-5.31822600	-1.83076200	3.69625300
H	-5.85385500	-0.54211800	2.59758000
H	-5.03762200	-1.97428100	1.94898200

[Mg]–C_6F_5/F–[Mg]
wB97XD
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -3305.234724
Sum of electronic and thermal Energies= -3305.154688
Sum of electronic and thermal Enthalpies= -3305.153743
Sum of electronic and thermal Free Energies= -3305.347955

Lowest energy vibrations = 21.40 29.86 33.62 cm^{-1}

0 1

Mg	1.54578500	-0.91790000	-0.75311000
N	1.45828900	-2.64949900	-1.76271500
C	2.42881700	-3.06854200	-2.58940400
C	3.66885100	-2.42422100	-2.74308200
H	4.34854700	-2.89240000	-3.44376100
C	2.18725400	-4.28429200	-3.46368300
H	1.67191100	-5.08034100	-2.92214100
H	3.12686300	-4.67414900	-3.85842300
H	1.54891100	-4.00943900	-4.31217100
C	0.23950700	-3.40859800	-1.66726600
C	0.08709000	-4.33464100	-0.61130400
C	-1.10636500	-5.06181600	-0.54225300
H	-1.24480900	-5.78971300	0.24883900
C	-2.13662400	-4.84280400	-1.45241600
H	-3.06635000	-5.39427400	-1.36346800
C	-1.98400000	-3.90006900	-2.46334900
H	-2.80452500	-3.71466600	-3.14721700
C	-0.79110700	-3.18444000	-2.60318100
C	1.19596700	-4.54408400	0.41895000
H	1.69295700	-3.57837100	0.56646800
C	0.66894200	-5.00025500	1.78916700
H	-0.13689200	-4.35088700	2.14486900
H	1.47875300	-4.97089300	2.52297200
H	0.28999100	-6.02819300	1.75468800
C	2.26869200	-5.53279000	-0.08148000
H	1.80925800	-6.49122200	-0.35074600
H	3.00800000	-5.71636100	0.70616400
H	2.80067700	-5.14368300	-0.95313400
C	-0.63195800	-2.16777900	-3.72899900
H	0.43616300	-1.96266600	-3.85658000
C	-1.16283000	-2.69082000	-5.07508200
H	-0.90088900	-1.99136300	-5.87634600
H	-2.25443200	-2.78643200	-5.06660700
H	-0.73917800	-3.67127500	-5.31847400
N	3.45137000	-0.50647400	-1.26072100
C	4.15190900	-1.25539200	-2.12998600
C	5.54345500	-0.81143800	-2.54157700
H	6.11891000	-0.43839400	-1.69234300
H	6.09006500	-1.63179900	-3.00897600
H	5.47779700	0.01074300	-3.26455000
C	4.07440700	0.66287200	-0.69564400
C	4.71586400	0.56840700	0.55705000
C	5.32954000	1.71563700	1.07435300
H	5.84650300	1.66100500	2.02654600
C	5.27380600	2.92848500	0.39516100
H	5.74487800	3.80983600	0.81769400
C	4.61106200	3.01162600	-0.82737400
H	4.56651600	3.96336200	-1.34380400
C	4.02002200	1.88365900	-1.40341400
C	4.78226400	-0.74852600	1.32457400
H	4.02284000	-1.41702500	0.90661600
C	4.46988300	-0.57266300	2.81977700
H	3.50852900	-0.07151500	2.96260100
H	4.42261500	-1.54927400	3.30885500
H	5.23951500	0.01866700	3.32819900
C	6.15052900	-1.43559000	1.14386000
H	6.95859800	-0.78309300	1.49542800
H	6.18629600	-2.36643200	1.72066800
H	6.34088200	-1.68195700	0.09521300
C	3.33679000	1.95978600	-2.76475000
H	3.42486700	0.97532900	-3.23739000
C	3.98994600	2.97923200	-3.71215600
H	3.56332300	2.87659900	-4.71569900
H	3.80448000	4.00827300	-3.38384700
H	5.07298100	2.82974600	-3.78009100
C	1.83638700	2.26269600	-2.61944700
H	1.68796500	3.24194400	-2.15743100
H	1.35228000	2.26938300	-3.60278200
H	1.31832800	1.52971600	-1.99568700
Mg	-1.24474100	0.90536300	0.57899200
N	-3.27789100	0.67955200	0.38921100
C	-4.05026900	1.49692400	1.13040500
C	-3.63647300	2.73751000	1.64416900
H	-4.36281900	3.25517200	2.25687200
C	-5.48189800	1.09680100	1.43123300
H	-6.01726600	0.80729900	0.52305100
H	-6.02247400	1.91266500	1.91261000
H	-5.49342900	0.23208600	2.10259800
C	-3.92305200	-0.41415100	-0.28904900
C	-4.39981400	-0.22054700	-1.61010200
C	-5.05650400	-1.28546100	-2.23760300
H	-5.43938200	-1.16224200	-3.24372000
C	-5.22403600	-2.51302800	-1.59905600
H	-5.73456000	-3.32414200	-2.10795400
C	-4.72790100	-2.69555700	-0.31463500
H	-4.84428900	-3.65714400	0.17510100
C	-4.08242500	-1.65479300	0.36141100
C	-4.17915600	1.10436500	-2.34571400
H	-3.14829000	1.41342500	-2.12440700
C	-4.33064800	0.98398200	-3.87293700
H	-3.74527200	0.16178700	-4.29129800
H	-3.99677500	1.91170400	-4.34889000
H	-5.38085400	0.83745800	-4.15286400
C	-5.11106300	2.23935500	-1.86757000
H	-6.16102400	1.93709700	-1.96190300
H	-4.95779400	3.12728000	-2.49316100
H	-4.91936100	2.53183600	-0.83463000
C	-3.55378700	-1.88317800	1.77064600
H	-3.24366500	-0.91415700	2.17076400
C	-2.32201000	-2.80341000	1.73921800
H	-2.60231000	-3.81485500	1.42701700
H	-1.86251700	-2.86454900	2.73370600
H	-1.57134000	-2.44493700	1.02772700
N	-1.40900900	2.93188300	0.71332700
C	-2.46430300	3.45464600	1.35549300
C	-2.43566000	4.91319900	1.76327200
H	-2.48310300	5.56059800	0.88069700
H	-3.27865800	5.15448500	2.41221600
H	-1.50465900	5.15575300	2.28395900

C	-0.38498900	3.81855300	0.24248300
C	-0.56442500	4.48800000	-0.98733500
C	0.44427000	5.34768200	-1.43351300
H	0.32009200	5.87117200	-2.37661700
C	1.61704500	5.52234900	-0.70105300
H	2.39392600	6.18533300	-1.06751500
C	1.79009600	4.83886600	0.49948300
H	2.71037400	4.96455500	1.06116200
C	0.79093400	3.99539000	0.99752100
C	-1.80301100	4.24983200	-1.84387100
H	-2.51766900	3.66968200	-1.25134600
C	-1.44060300	3.40331900	-3.07882700
H	-1.02661400	2.43437200	-2.78011600
H	-2.32859800	3.22468500	-3.69487400
H	-0.69240200	3.91509900	-3.69564700
C	-2.49552800	5.55764200	-2.26288600
H	-1.86202700	6.15446700	-2.92930900
H	-3.42545300	5.33588900	-2.79873700
H	-2.74277900	6.17417600	-1.39230500
C	0.96833900	3.29627000	2.33731200
H	0.03047900	2.77991900	2.56699200
C	1.24297500	4.29248900	3.47846600
H	1.28708800	3.76532200	4.43793100
H	2.20019300	4.80675800	3.33413800
H	0.45797400	5.05297100	3.54228500
C	2.08264700	2.24239800	2.26494800
H	3.05590400	2.70915500	2.08751200
H	2.13543600	1.68073900	3.20494900
H	1.90955200	1.53225100	1.44966000
F	0.06412300	0.21696000	-0.62068600
C	-1.31881900	-0.84279000	-3.35426900
H	-2.37275900	-1.02603600	-3.12620700
H	-0.86366200	-0.39014900	-2.47008700
H	-1.25704100	-0.12366000	-4.17986700
C	-4.61476000	-2.46005300	2.72552200
H	-4.89253900	-3.48208600	2.44293600
H	-4.21872300	-2.49338800	3.74658900
H	-5.52718300	-1.85543000	2.73161000
C	-0.40069900	-0.14582600	2.33705500
C	-1.06837200	-0.04383800	3.54958300
C	0.65701000	-1.01661500	2.38682200
C	-0.73904300	-0.76128500	4.69269700
C	1.06044800	-1.77726500	3.47279000
C	0.33816700	-1.64131800	4.64976100
F	-2.16325300	0.80706200	3.64538600
F	-1.44966800	-0.62573200	5.85735700
F	0.68719200	-2.36445500	5.75953300
F	2.12270100	-2.64490400	3.40780100
F	1.47296900	-1.22155200	1.21254700

[Mg]–C_6F_5
wB97XD
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -1966.321510
Sum of electronic and thermal Energies= -1966.276745
Sum of electronic and thermal Enthalpies= -1966.275801
Sum of electronic and thermal Free Energies= -1966.401948

Lowest energy vibrations = 9.27 13.92 27.27 cm^{-1}

0 1

Mg	0.00001400	-0.31826500	0.00003000
N	-1.46387500	-1.67261700	-0.07967100
C	-1.26481100	-2.99976000	-0.09254100
C	0.00013300	-3.60671300	0.00000000
H	0.00017100	-4.68923100	-0.00000500
C	1.26503300	-2.99967100	0.09254100
N	1.46400500	-1.67251300	0.07969200
C	-2.46681000	-3.91221700	-0.21329100
H	-3.16432400	-3.75173700	0.61562300
H	-2.16889300	-4.96124900	-0.22264100
H	-3.01846400	-3.69453200	-1.13442500
C	2.46710000	-3.91204200	0.21325900
H	2.16925400	-4.96109400	0.22266200
H	3.01879400	-3.69428700	1.13435200
H	3.16455500	-3.75154500	-0.61570300
C	-2.80204800	-1.14410800	-0.13564400
C	-3.51364200	-0.94923900	1.06625600
C	-4.77004700	-0.34258200	1.00132800
H	-5.33327100	-0.17348200	1.91229100
C	-5.30697600	0.06647000	-0.21739900
H	-6.27891800	0.54656100	-0.24716100
C	-4.59220900	-0.13188900	-1.39373500
H	-5.01447500	0.19797900	-2.33744700
C	-3.33339000	-0.74234900	-1.37513600
C	-2.89106000	-1.33420100	2.40440800
H	-2.18429500	-2.15248300	2.22471100
C	-2.08626600	-0.15470100	2.98812400
H	-1.28645900	0.16784500	2.31176800
H	-1.62824700	-0.43452700	3.94338100
H	-2.73532900	0.71244400	3.14720800
C	-3.92001500	-1.83767300	3.42944500
H	-4.57831800	-1.03179800	3.77243100
H	-3.40623700	-2.23687200	4.31044000
H	-4.54549700	-2.63081300	3.00645700
C	-2.54250000	-0.92219200	-2.66551300
H	-1.71122600	-1.60482000	-2.45498900
C	-3.38058200	-1.55864700	-3.78771000
H	-3.83241200	-2.49955600	-3.45654500
H	-2.74990500	-1.76652900	-4.65904100
H	-4.18731100	-0.89329100	-4.11486900
C	-1.94058200	0.42056500	-3.12637600
H	-2.73482400	1.14032500	-3.35512500
H	-1.32968100	0.28381000	-4.02576600
H	-1.31141700	0.86995300	-2.34870500
C	2.80214500	-1.14391700	0.13564200
C	3.51370900	-0.94900500	-1.06626900
C	4.77008600	-0.34228500	-1.00135600
H	5.33329000	-0.17315300	-1.91232600
C	5.30700900	0.06679300	0.21736400
H	6.27892600	0.54693500	0.24711400
C	4.59227300	-0.13161500	1.39371100
H	5.01453900	0.19826700	2.33741800
C	3.33348900	-0.74214600	1.37512900
C	2.89113100	-1.33401000	-2.40441100
H	2.18437600	-2.15229600	-2.22469100
C	3.92009000	-1.83749900	-3.42943700
H	4.57837500	-1.03162400	-3.77245800
H	3.40631300	-2.23674000	-4.31041400
H	4.54558900	-2.63061100	-3.00642300
C	2.08632600	-0.15453500	-2.98816200
H	1.28649900	0.16800800	-2.31182900
H	1.62832800	-0.43438700	-3.94342200
H	2.73537400	0.71262000	-3.14725200
C	2.54263800	-0.92206900	2.66551800

H	1.71142900	-1.60478000	2.45500500
C	1.94059000	0.42062600	3.12639600
H	2.73476300	1.14047100	3.35511600
H	1.32973200	0.28380800	4.02580500
H	1.31135200	0.86994700	2.34874500
C	3.38079800	-1.55844300	3.78770300
H	3.83272000	-2.49930500	3.45652900
H	2.75015300	-1.76639200	4.65904100
H	4.18746300	-0.89300600	4.11485500
C	-0.00008800	1.79877400	0.00002800
C	1.14252500	2.54830700	-0.24469100
F	2.34125700	1.89669000	-0.49674800
C	1.17440300	3.93721700	-0.25132100
F	2.33461300	4.62697900	-0.49969400
C	-0.00020900	4.63388600	0.00000200
C	-1.17476200	3.93712000	0.25133500
F	-2.33503200	4.62678800	0.49968900
C	-1.14276600	2.54821300	0.24473200
F	-2.34144400	1.89649800	0.49678900
F	-0.00026800	6.00410000	-0.00001300

[Mg]–C_6F_5(THF)
wB97XD
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies=
-2198.571855
Sum of electronic and thermal Energies=
-2198.521870
Sum of electronic and thermal Enthalpies=
-2198.520926
Sum of electronic and thermal Free Energies=
-2198.654398

Lowest energy vibrations = 33.86 41.47 48.83 cm^{-1}

0 1

Mg	-0.15934100	-0.46633900	-0.27577100
N	-1.92057100	-0.86498300	0.65468200
C	-2.01769400	-1.88225500	1.53235900
C	-0.92137500	-2.49464500	2.15908100
H	-1.16383600	-3.29020300	2.85353100
C	0.43778900	-2.09708400	2.14876500
N	0.94288600	-1.23360400	1.27002000
C	-3.39492300	-2.41478700	1.88480700
H	-4.05517300	-1.62024300	2.24216400
H	-3.33654700	-3.19252400	2.64774600
H	-3.86888100	-2.83600300	0.99061200
C	1.32497300	-2.71569400	3.21225400
H	0.73921500	-2.99314000	4.09061700
H	2.11775200	-2.02799500	3.51624000
H	1.80697800	-3.62185700	2.82728400
C	-3.09485300	-0.07905200	0.38531100
C	-3.41102200	0.98244300	1.26402700
C	-4.57064800	1.72438700	1.02390200
H	-4.83515800	2.53360100	1.69646900
C	-5.38495800	1.45549800	-0.07383000
H	-6.27974600	2.04411000	-0.24498400
C	-5.03238200	0.44510600	-0.96159500
H	-5.65151100	0.25789600	-1.83389400
C	-3.88962400	-0.33343700	-0.74801800
C	-2.49961700	1.33163700	2.43695500
H	-1.53805900	0.84105500	2.25250100
C	-2.24297800	2.84548900	2.53888100
H	-1.88714600	3.24487900	1.58608400
H	-1.48920200	3.04550400	3.30915200
H	-3.14980900	3.39111200	2.82434300
C	-3.03956400	0.78745100	3.77385800
H	-4.03747100	1.19238400	3.98097400
H	-2.37503900	1.07790800	4.59582600
H	-3.10445500	-0.30465800	3.76662200
C	-3.49414100	-1.39265500	-1.76600100
H	-2.63716600	-1.93234100	-1.35252100
C	-4.61160800	-2.41410800	-2.03589500
H	-4.94181700	-2.89570200	-1.10983000
H	-4.26112800	-3.19310700	-2.72380800
H	-5.48529000	-1.93707400	-2.49395000
C	-3.03736500	-0.71804300	-3.07339500
H	-3.86817500	-0.17801300	-3.54145100
H	-2.67084800	-1.46181500	-3.79217000
H	-2.24198600	0.00920200	-2.87523000
C	2.30376100	-0.78061600	1.33996000
C	3.36418100	-1.58863100	0.88182800
C	4.65986000	-1.06067100	0.88445800
H	5.48382000	-1.66890600	0.52463300
C	4.90741600	0.23542300	1.31976900
H	5.91657600	0.63229700	1.30722500
C	3.85086900	1.03024200	1.75681600
H	4.04989800	2.04530100	2.08020300
C	2.54037900	0.54519600	1.77153500
C	3.13219600	-2.98643800	0.32158700
H	2.09173000	-3.26112000	0.52362500
C	4.03373800	-4.04442200	0.98227400
H	5.08828300	-3.87696400	0.73709800
H	3.76720400	-5.04714500	0.62898100
H	3.93848400	-4.02420200	2.07276600
C	3.31948700	-2.98660300	-1.20757100
H	2.66066000	-2.24600800	-1.66596900
H	3.10150200	-3.97738900	-1.62644000
H	4.34992100	-2.72492800	-1.47175600
C	1.39193000	1.41813000	2.26390000
H	0.50203600	1.15525700	1.68096600
C	1.63213300	2.91924400	2.04908600
H	2.39017100	3.31379500	2.73547500
H	0.70459000	3.47220000	2.22799400
H	1.95782900	3.12145100	1.02348100
C	1.06391200	1.11630400	3.73913600
H	0.75995600	0.07326600	3.87184200
H	0.24283000	1.75316000	4.08732000
H	1.93890400	1.30609400	4.37163200
C	0.56164700	1.34975200	-1.15123200
C	1.86249900	1.44486500	-1.61585800
F	2.63056600	0.28351700	-1.73155400
C	2.47832800	2.63432000	-1.98353000
F	3.77582300	2.66984800	-2.43271400
C	1.74767900	3.81337700	-1.89655000
C	0.43183200	3.77922900	-1.45174300
F	-0.28840400	4.94574800	-1.36799700
C	-0.11888100	2.55376800	-1.09856600
F	-1.43751000	2.56637700	-0.65129800
O	0.01174900	-1.85455200	-1.72276800
C	-0.25805700	-3.27843700	-1.46868400
H	-1.06026800	-3.32778300	-0.73148800
H	0.64773700	-3.73059200	-1.05688600
C	-0.60406300	-3.82472600	-2.84759000
H	-1.64991800	-3.60597500	-3.08926800
H	-0.45098800	-4.90390800	-2.91689300
C	0.34764300	-3.03386200	-3.76880900
H	1.34099100	-3.49385300	-3.76579400
H	-0.00793700	-2.99476700	-4.80076400
C	0.40234300	-1.64020200	-3.13391100
H	1.39141200	-1.18395400	-3.13586300
H	-0.32427800	-0.94966200	-3.56210100
F	2.32176800	5.00573300	-2.25760400

[Mg]–F/F–[Mg]
wB97XD
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -2677.728356
Sum of electronic and thermal Energies= -2677.657152
Sum of electronic and thermal Enthalpies= -2677.656208
Sum of electronic and thermal Free Energies= -2677.830706

Lowest energy vibrations = 23.29 31.28 43.22 cm^{-1}

0 1

Mg	0.04896500	1.43488800	0.48089600
F	-0.03056900	0.42713500	-1.16513600
N	-1.38453000	2.85900900	0.81195400
C	-1.16579500	3.93290000	1.59041900
C	0.06897600	4.24600600	2.18345500
H	0.06137800	5.09643400	2.85253500
C	-2.28526200	4.93107800	1.83138300
H	-2.65093300	5.33492800	0.88184700
H	-1.93727700	5.75875000	2.45027800
H	-3.14456900	4.46545300	2.32310100
C	-2.66664800	2.80128100	0.15404000
C	-2.78481300	3.30053300	-1.15741800
C	-4.05806000	3.35780800	-1.73848100
H	-4.16905900	3.76159100	-2.74004500
C	-5.17903100	2.90264700	-1.05401700
H	-6.15847200	2.95450100	-1.51741000
C	-5.03937800	2.36253200	0.22437400
H	-5.91732200	1.99338500	0.74145100
C	-3.79161400	2.31056500	0.85282600
C	-1.57456500	3.79120000	-1.94429200
H	-0.68109100	3.60694000	-1.33785100
C	-1.41541100	3.00678600	-3.25966500
H	-1.21272700	1.95252800	-3.05120600
H	-0.58176900	3.40651900	-3.84579600
H	-2.31978300	3.07275000	-3.87527000
C	-1.64237700	5.30838100	-2.19860200
H	-2.51206400	5.56817500	-2.81357900
H	-0.74223600	5.64614300	-2.72519800
H	-1.71352900	5.86306200	-1.25692300
C	-3.63466200	1.73369500	2.25533500
H	-2.85813600	2.30764400	2.77375100
C	-4.91508100	1.82137700	3.10011400
H	-4.69201200	1.54883000	4.13699500
H	-5.68026400	1.12452500	2.73835200
H	-5.33841100	2.83202300	3.09401400
N	1.55927600	2.67081800	1.08297100
C	1.33632800	3.72636700	1.88649100
C	2.51924800	4.47929800	2.46272800
H	3.07448900	4.98825700	1.66719200
H	2.19065200	5.22658000	3.18607700
H	3.22108700	3.79870100	2.95182300
C	2.91760700	2.44663800	0.65729600
C	3.40251200	3.14580000	-0.46988500
C	4.71108800	2.89921300	-0.89563800
H	5.09902400	3.42345700	-1.76330500
C	5.52047400	1.97855000	-0.23307800
H	6.52787200	1.78652300	-0.58740300
C	5.03791700	1.31786900	0.89226400
H	5.67520700	0.61239700	1.41551100
C	3.74677200	1.56258200	1.37367000
C	2.53092000	4.15530800	-1.20926300
H	1.65792200	4.36906100	-0.58364200
C	2.00892900	3.57120100	-2.53344000
H	1.40180800	2.67691100	-2.36114200
H	1.39196500	4.31062400	-3.05679900
H	2.84165300	3.29293300	-3.18989900
C	3.25767800	5.48953700	-1.45500500
H	4.07617500	5.37660500	-2.17503500
H	2.55741200	6.22642500	-1.86401700
H	3.67776300	5.89323500	-0.52763800
C	3.27998700	0.92600100	2.67544900
H	2.32859900	1.39320200	2.95040300
C	4.27543400	1.17628500	3.82442900
H	3.86236300	0.79636500	4.76541300
H	5.22582600	0.66028100	3.64634500
H	4.49170200	2.24272100	3.95027500
C	3.02852200	-0.57629200	2.50390000
H	3.94609900	-1.09386400	2.21073700
H	2.67070200	-1.01258000	3.44306000
H	2.27320900	-0.76258900	1.73687600
Mg	-0.10852900	-1.39925600	-0.50352500
N	-1.67127200	-2.69307000	-0.80293400
C	-1.56731500	-3.75799800	-1.61666800
C	-0.37414500	-4.17206500	-2.23521600
H	-0.47092600	-4.99772500	-2.92798800
C	-2.78112300	-4.63568800	-1.87623700
H	-3.23351300	-4.96088200	-0.93471900
H	-2.50008700	-5.51932900	-2.45038200
H	-3.55747900	-4.09713200	-2.42821800
C	-2.93059900	-2.52713000	-0.12220400
C	-3.05379400	-3.00007000	1.20088000
C	-4.31223400	-2.94450300	1.81135900
H	-4.43606800	-3.31792000	2.82141600
C	-5.40676100	-2.39802700	1.14814000
H	-6.37410200	-2.35918600	1.63760200
C	-5.25448000	-1.87958400	-0.13616900
H	-6.10908400	-1.43576000	-0.63339300
C	-4.02286000	-1.94213000	-0.79636200
C	-1.84914200	-3.57331700	1.94220800
H	-0.95948600	-3.05299000	1.56803200
C	-1.91152400	-3.32521500	3.45743000
H	-2.10677900	-2.27090300	3.67475000
H	-0.95668200	-3.59655700	3.91769400
H	-2.68990000	-3.93004100	3.93701300
C	-1.65865400	-5.07485300	1.64819800
H	-2.56472000	-5.63396800	1.91091700
H	-0.82664500	-5.47610200	2.23835800
H	-1.43349300	-5.25202900	0.59231200
C	-3.84973600	-1.37506700	-2.20089900
H	-3.12768000	-2.00032600	-2.73688100
C	-3.25976400	0.04134100	-2.12593100
H	-3.91444600	0.68650400	-1.53749200
H	-3.16284500	0.47358900	-3.12806100
H	-2.26892200	0.05150500	-1.66483800
N	1.26372800	-2.77028500	-1.11699000
C	0.93992500	-3.78463100	-1.93864100
C	2.04493000	-4.62371500	-2.55004400
H	2.63669200	-5.11651700	-1.77249300
H	1.63529200	-5.38763600	-3.21200600
H	2.73605200	-3.99806100	-3.12317900
C	2.62764000	-2.70091500	-0.65994900
C	2.99259900	-3.42860800	0.49326800
C	4.31703800	-3.35484000	0.93616900
H	4.61579100	-3.91110300	1.81970100
C	5.25298100	-2.56376400	0.27454900
H	6.27193000	-2.50348600	0.64267700
C	4.87873300	-1.85469100	-0.86342200
H	5.61136600	-1.24262200	-1.37890700
C	3.57532300	-1.93416800	-1.36546400
C	1.98724100	-4.29796400	1.24290500

H	1.03709600	-4.25855100	0.70029100
C	1.72853800	-3.76323600	2.66297800
H	1.25480900	-2.77761600	2.63085500
H	1.06897400	-4.44576000	3.21063700
H	2.66326700	-3.67228200	3.22815400
C	2.43226900	-5.77153100	1.29069900
H	3.35569600	-5.89013100	1.86921000
H	1.65711200	-6.38412900	1.76506600
H	2.61072100	-6.16793000	0.28588200
C	3.20292800	-1.23281600	-2.66397100
H	2.23570600	-1.63137800	-2.98863600
C	4.22174300	-1.50374700	-3.78608700
H	3.85285800	-1.09195800	-4.73194300
H	5.18596400	-1.02823600	-3.57333100
H	4.39899600	-2.57620600	-3.92238200
C	3.03183100	0.27606900	-2.44765500
H	3.96853800	0.72708200	-2.10946300
H	2.72700800	0.76465600	-3.37980700
H	2.26490400	0.48266800	-1.69747800
F	0.00009000	-0.39260300	1.13638700
C	-3.15587400	0.27506600	2.17579900
H	-3.86385800	-0.31591000	1.59170000
H	-2.17055800	0.18431200	1.71254300
H	-3.08963000	-0.16213500	3.17877100
C	-5.14789900	-1.36711400	-3.02260300
H	-5.85666200	-0.62106800	-2.64462600
H	-4.92463300	-1.10521600	-4.06217100
H	-5.64022400	-2.34603400	-3.01246100

[Mg]–F/F–[Mg] (THF)2
wB97XD
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -3142.204316
Sum of electronic and thermal Energies= -3142.123297
Sum of electronic and thermal Enthalpies= -3142.122353
Sum of electronic and thermal Free Energies= -3142.313204

Lowest energy vibrations = 35.92 48.11 53.70 cm^{-1}

0 1

Mg	-1.27766000	0.55082300	0.69802500
F	-0.52483700	-1.07487400	-0.09054300
N	-3.25848200	-0.16868200	0.83840400
C	-4.17192300	0.46884200	1.58385100
C	-4.06280100	1.81131000	1.98803600
H	-4.85893600	2.17681200	2.62434700
C	-5.42952200	-0.25760700	2.03210600
H	-5.93963400	-0.73001500	1.18806200
H	-6.12282500	0.42915100	2.52018900
H	-5.17884100	-1.05682400	2.73754800
C	-3.63665700	-1.45955500	0.32645100
C	-4.22360400	-1.53244000	-0.95564400
C	-4.69131300	-2.76874900	-1.41207600
H	-5.16418800	-2.83992600	-2.38562100
C	-4.54328900	-3.92027100	-0.64271900
H	-4.90588400	-4.87290700	-1.01480800
C	-3.90952800	-3.84621200	0.59373600
H	-3.76903800	-4.74978000	1.17812900
C	-3.46471200	-2.62215100	1.10295600
C	-4.36330700	-0.27794400	-1.81023100
H	-3.52996100	0.38012600	-1.53540800
C	-4.27248700	-0.56471100	-3.31777600
H	-3.42094300	-1.21140000	-3.55302300
H	-4.16231900	0.37752700	-3.86731900
H	-5.18008900	-1.05338500	-3.69066700
C	-5.66690800	0.48835400	-1.50617600
H	-6.53005400	-0.18349700	-1.58534200
H	-5.80349500	1.30483300	-2.22413100
H	-5.65167600	0.92570900	-0.50454600
C	-2.79841600	-2.55097300	2.46744300
H	-2.78701400	-1.49742000	2.75919500
C	-3.55115000	-3.33736700	3.55389700
H	-3.09666600	-3.15075100	4.53415600
H	-3.50005700	-4.41690200	3.37170100
H	-4.60868900	-3.05542400	3.60489000
C	-1.33827500	-3.01694400	2.36970700
H	-1.28829400	-4.08639400	2.14492200
H	-0.81919300	-2.84655400	3.32293400
H	-0.82070900	-2.48376200	1.56785900
N	-2.06729800	2.50544300	0.79289000
C	-3.15173700	2.77972300	1.53314500
C	-3.45650100	4.21377000	1.93390600
H	-3.43776000	4.88574700	1.07183800
H	-4.43484400	4.28496800	2.41177800
H	-2.70078900	4.58098400	2.63525100
C	-1.37136200	3.63386700	0.23420500
C	-1.74503100	4.08542000	-1.05118400
C	-1.15240700	5.24681100	-1.55609300
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H	1.41343400	0.47827600	2.42066100
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C	-0.71896700	0.22790600	-2.87336100
C	0.17607400	-0.78581000	-4.86130000
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H	1.89475300	-1.53746700	-3.67370000
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H	-0.81238000	1.19481800	-2.37747700
H	-0.27353200	-1.78078100	-4.77229200
H	0.50431400	-0.64266300	-5.89333000
H	-1.83446200	0.11820700	-4.74767400
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[Mg]−C_6F_5/C_6F_5−[Mg]
wB97XD
6,31G+(d,p) / Lanl2DZ

Sum of electronic and zero-point Energies= -3932.706595
Sum of electronic and thermal Energies= -3932.618671
Sum of electronic and thermal Enthalpies= -3932.617726
Sum of electronic and thermal Free Energies= -3932.827056

Lowest energy vibrations = 23.50 28.96 34.17 cm^{-1}

0 1

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C	4.02685000	1.46177600	-2.31845900
C	4.16585000	2.33254200	-3.55133800
H	3.82293800	3.35377800	-3.37404600
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C	2.20650800	2.85606600	-1.52421900
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C	1.81510700	5.07588300	-0.65301900
H	2.12044300	5.92074400	-0.04685100
C	0.58361500	5.12100500	-1.30692400
H	-0.05145700	5.99471300	-1.20712800
C	0.17831600	4.04839300	-2.09304000
H	-0.77208200	4.09220400	-2.61599000
C	0.98346400	2.91036800	-2.22241600
C	3.98937900	3.91901400	-0.00758100
H	4.13884600	2.88481800	0.32382300
C	4.03656400	4.83791200	1.22667900
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H	4.91596000	4.58797000	1.83109400
H	4.13486400	5.89042400	0.93354300
C	5.17856600	4.28503400	-0.92308600
H	4.99999600	5.24618100	-1.41968300
H	6.09095500	4.37675700	-0.32247700
H	5.36509300	3.52722100	-1.68460500
C	0.52907400	1.76037700	-3.11125400
H	1.31770700	0.99962000	-3.10720600
C	0.32830600	2.21047500	-4.56986300
H	0.06735700	1.35162000	-5.19830200
H	-0.48684500	2.93895100	-4.64684100
H	1.23672000	2.67265000	-4.96956000
C	-0.75719500	1.11696600	-2.57408600
H	-1.60107500	1.80901100	-2.64988200
H	-1.01111300	0.21866600	-3.14501400
H	-0.64114900	0.83802200	-1.52166000
C	-2.30087000	1.82667400	4.68828300
H	-2.19022100	1.79888700	5.77836000
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C	5.29875200	-4.57454200	-0.70286800
H	5.38116700	-5.38904600	0.02633300
H	5.18854700	-5.02271900	-1.69653400
H	6.23585900	-4.01136300	-0.67872700
C	1.05149400	-1.54256700	-1.54994800
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C	-0.13661300	-2.12376900	-1.17912900
C	1.24151500	-3.39259300	-3.15579300
C	-0.64384400	-3.31421800	-1.67400600
C	0.06590800	-3.95535700	-2.67769800
F	2.89577900	-1.70182600	-3.06142000
F	1.94230800	-4.02826800	-4.14646100
F	-0.41523800	-5.12100800	-3.21247400
F	-1.81828200	-3.86408800	-1.21938200
F	-0.94848700	-1.49267600	-0.17821800
C	-1.93051400	2.57173700	1.56112200
C	-1.25372600	1.44804600	1.10888600
C	-1.32493800	3.72533100	2.03659500
C	0.10635400	1.56460200	1.23980300
C	0.05912000	3.76134900	2.13994300
C	0.79039100	2.64783700	1.75924500
F	-3.32224100	2.55659000	1.59373800
F	-2.06854000	4.80227300	2.44295300
F	0.69406000	4.86912700	2.63433200
F	2.14972400	2.61534300	1.91655500
F	0.95988000	0.47717100	0.83202500

7. Multinuclear NMR Data

Figure S20: ^{1}H NMR spectrum of compound **2a**; solvent peak marked with asterisk.

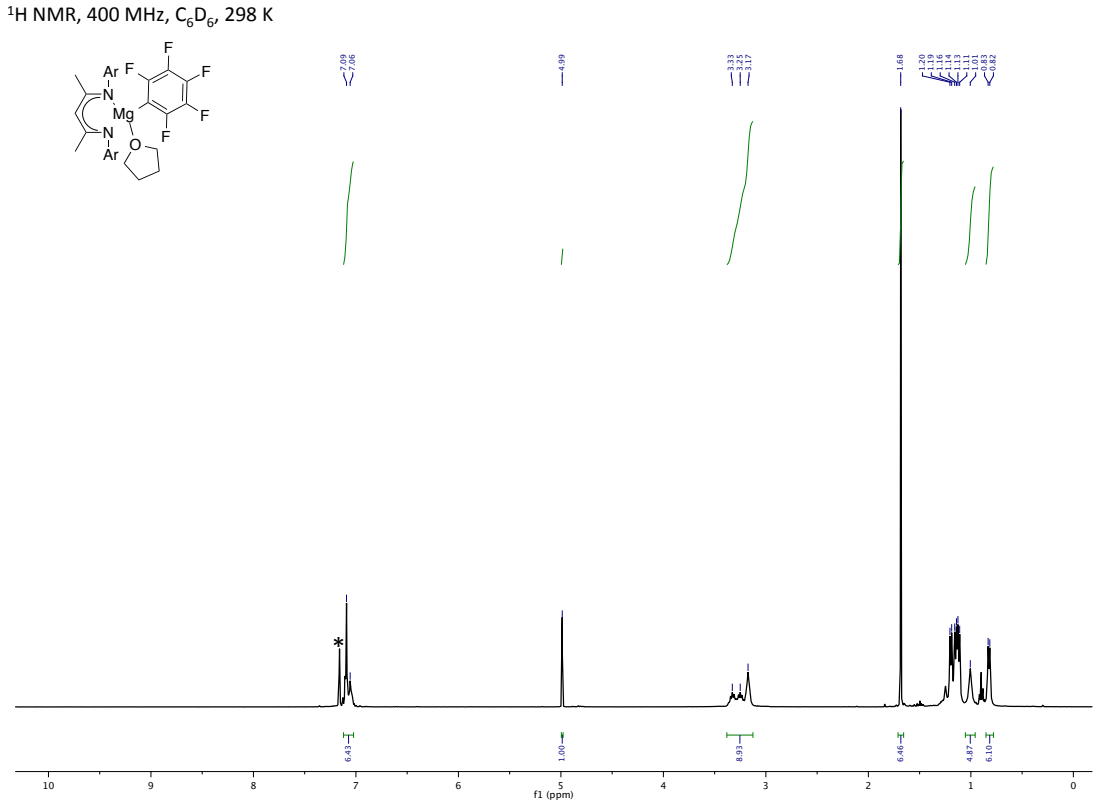


Figure S21: ^{19}F NMR spectrum of compound **2a**.

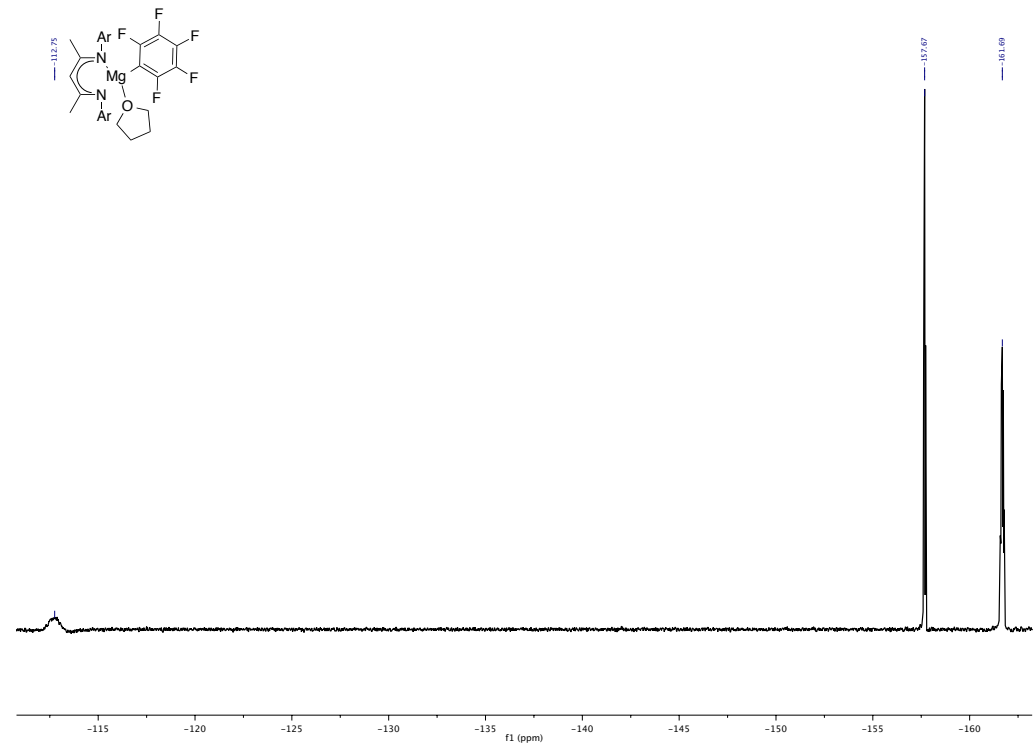


Figure S22: $^{13}C\{^{1}H\}$ NMR spectrum of compound **2a**.

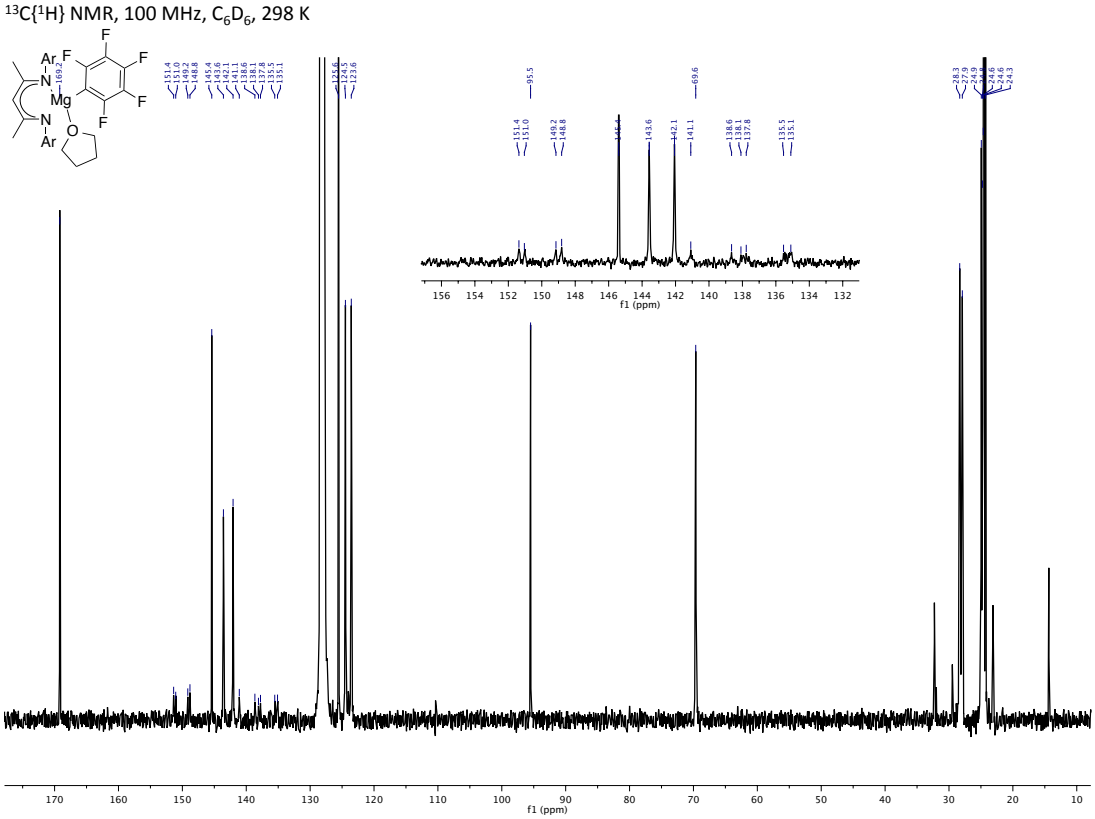


Figure S23: ^{1}H NMR spectrum of compound **2b**; solvent peak marked with asterisk.

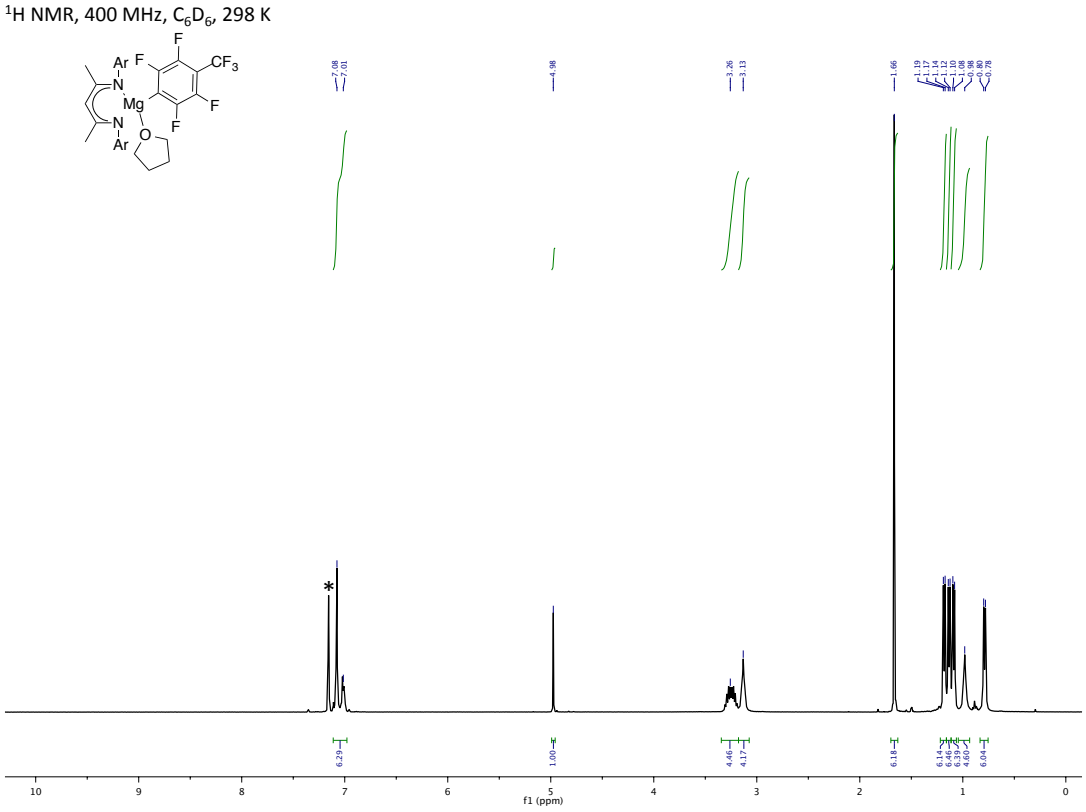


Figure S24: ^{19}F NMR spectrum of compound **2b**.

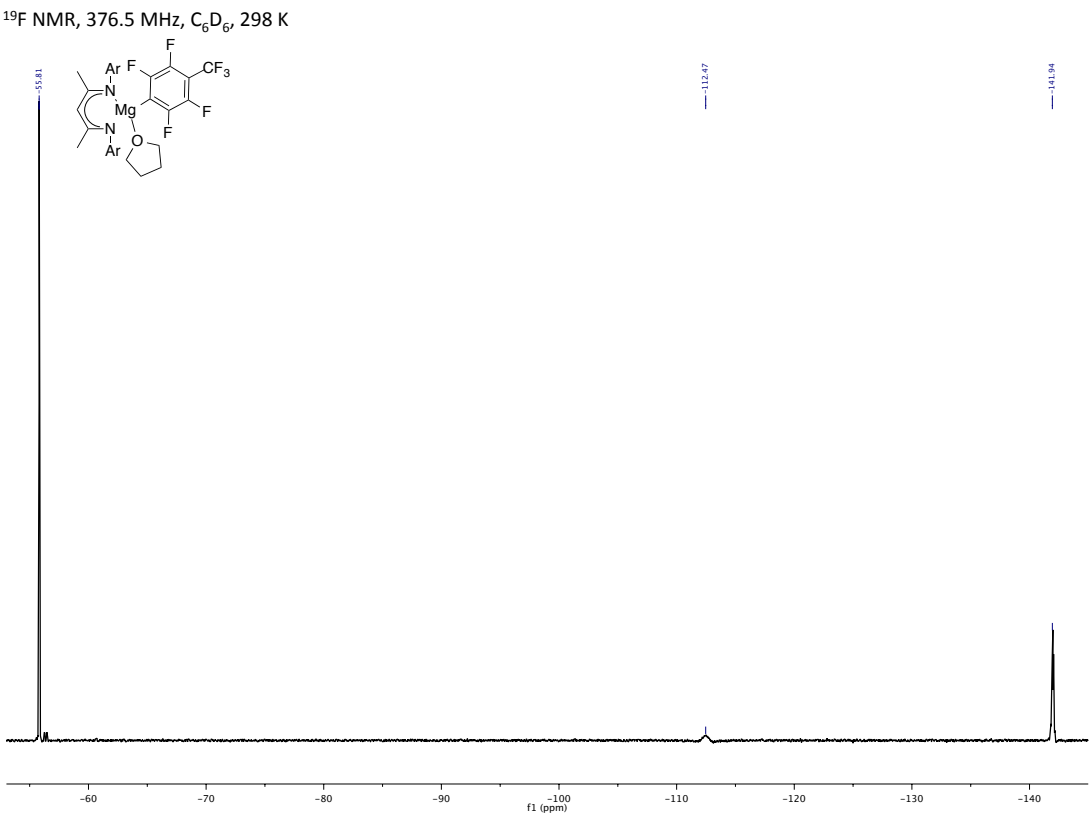


Figure S25: $^{13}C\{^{1}H\}$ NMR spectrum of compound **2b**.

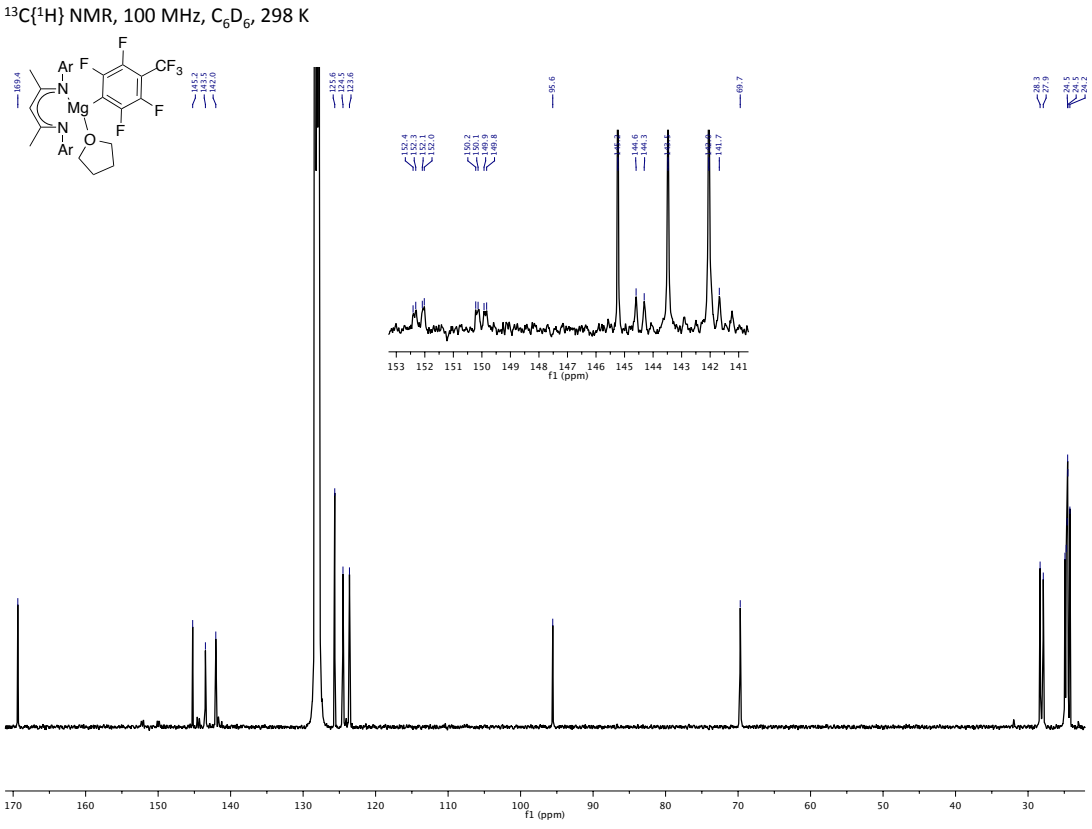


Figure S26: ^{1}H NMR spectrum of compound **2c**; solvent peak marked with asterisk.

^{1}H NMR, 400 MHz, C_6D_6, 298 K

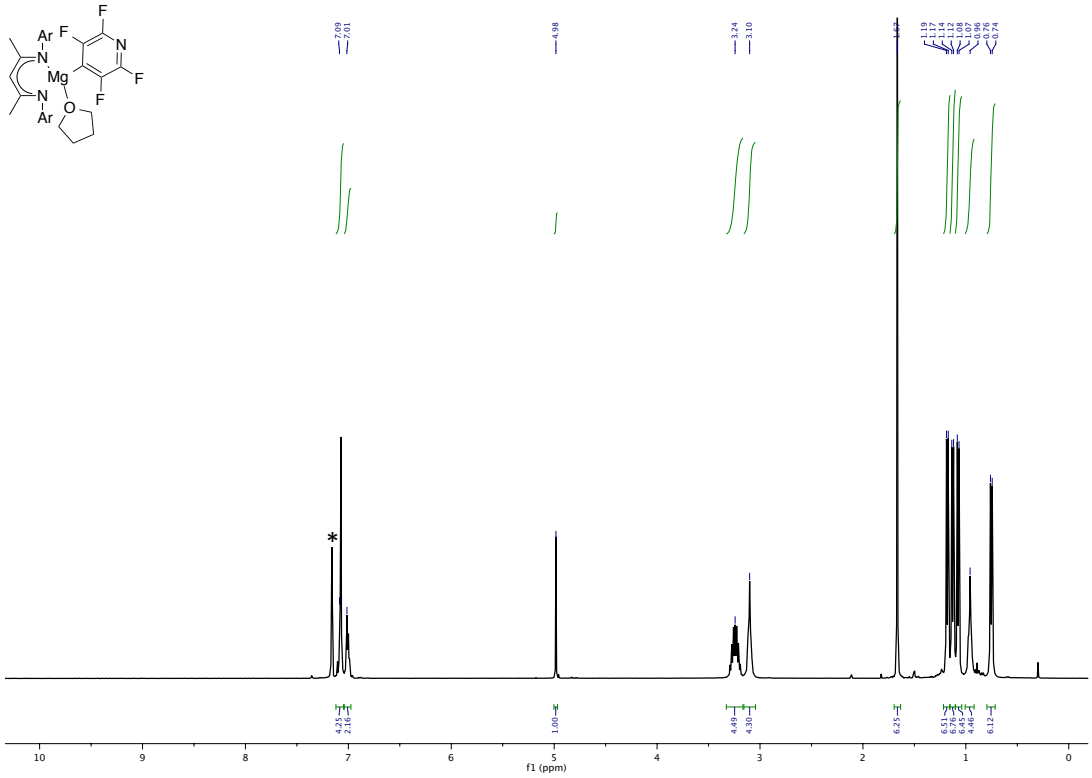


Figure S27: ^{19}F NMR spectrum of compound **2c**.

^{19}F NMR, 376.5 MHz, C_6D_6, 298 K

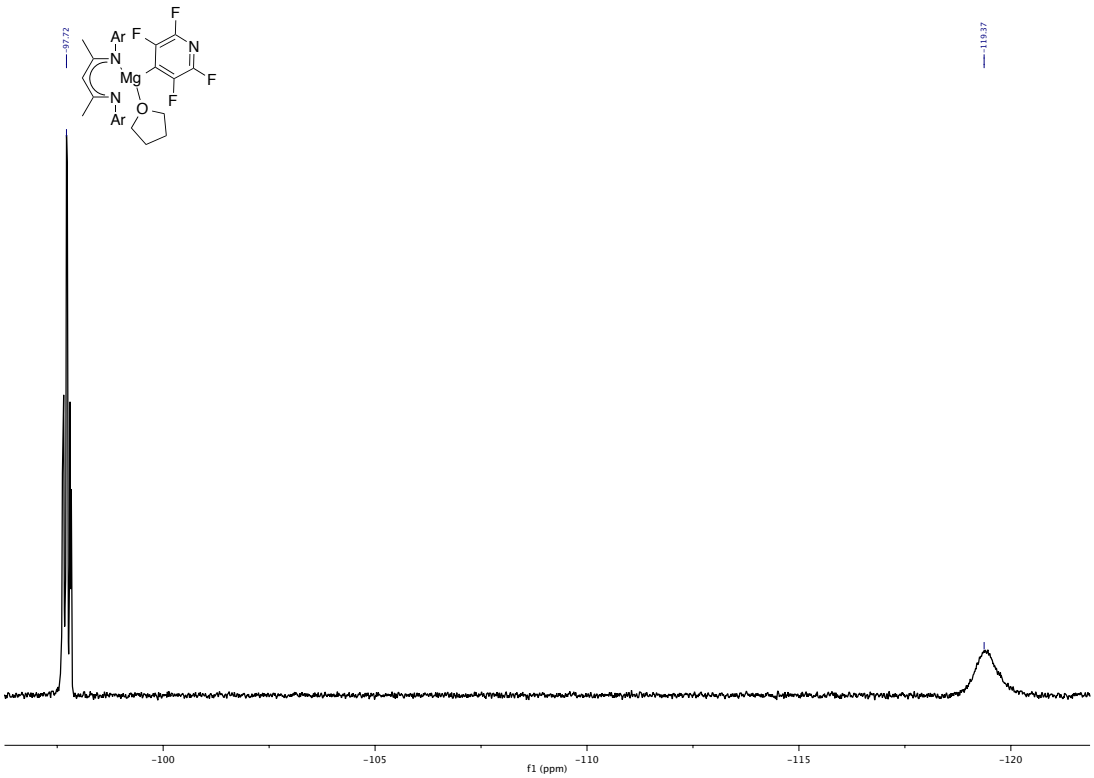


Figure S28: $^{13}C\{^{1}H\}$ NMR spectrum of compound **2c**.

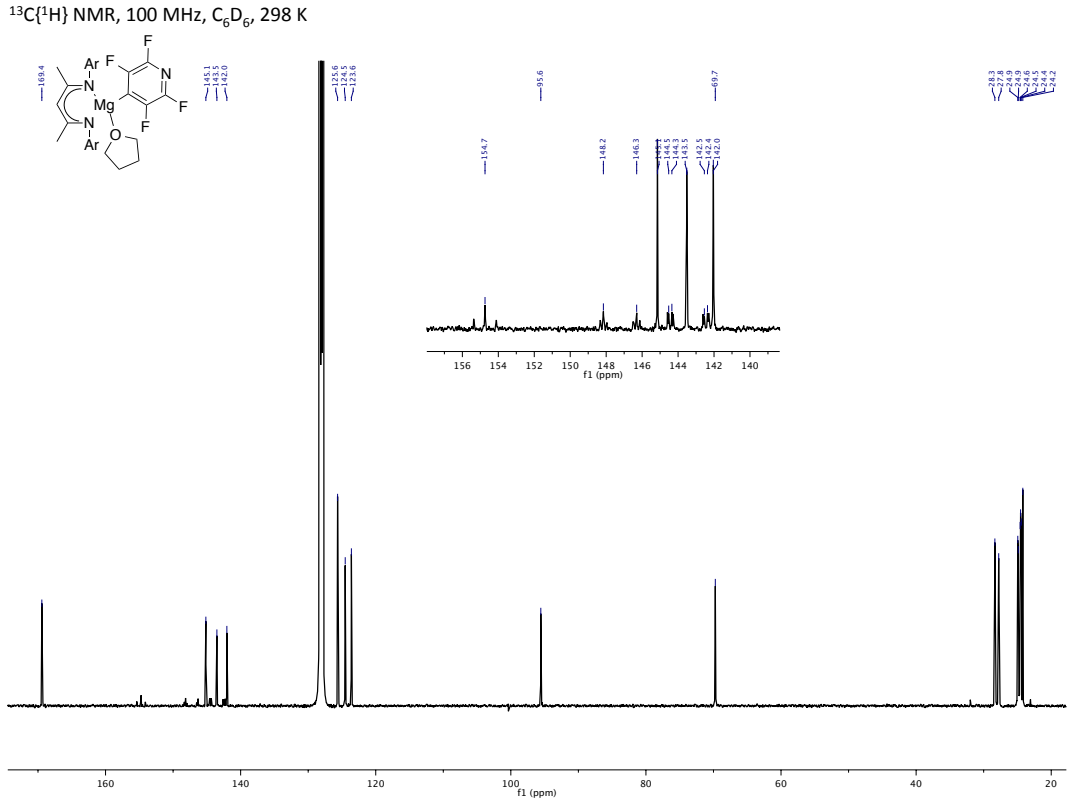


Figure S29: ^{1}H NMR spectrum of compound **2d**; solvent peak marked with asterisk.

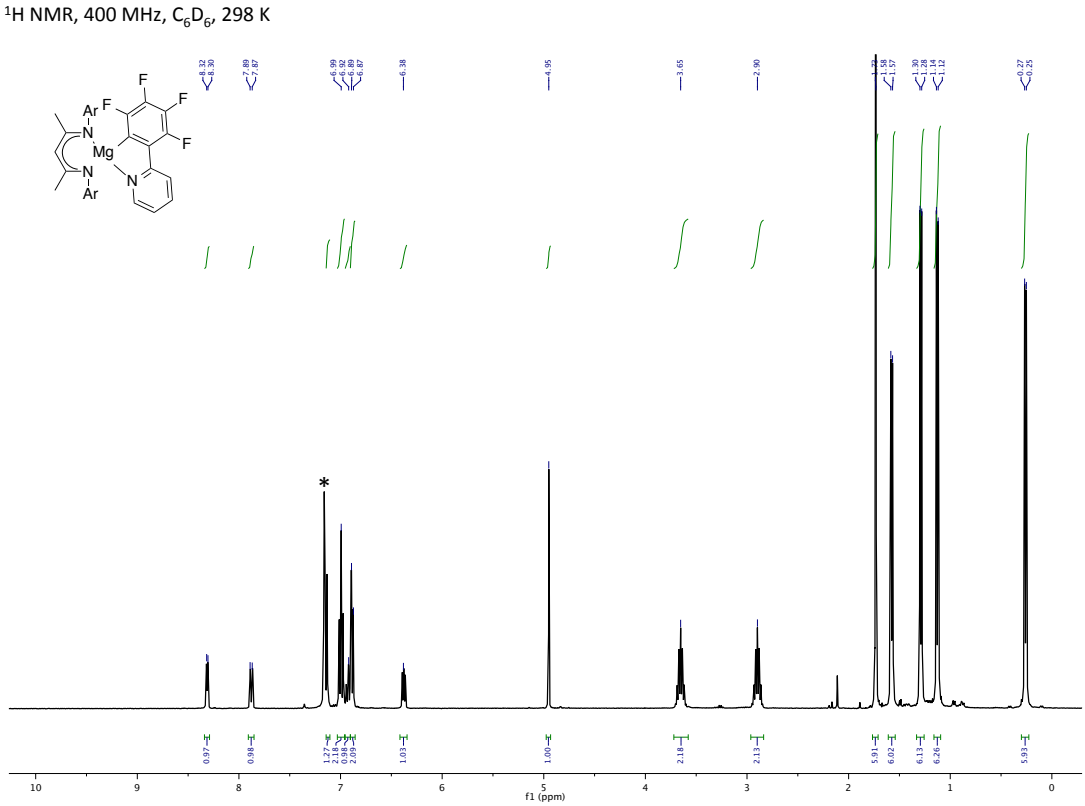


Figure S30: ^{19}F NMR spectrum of compound **2d**.

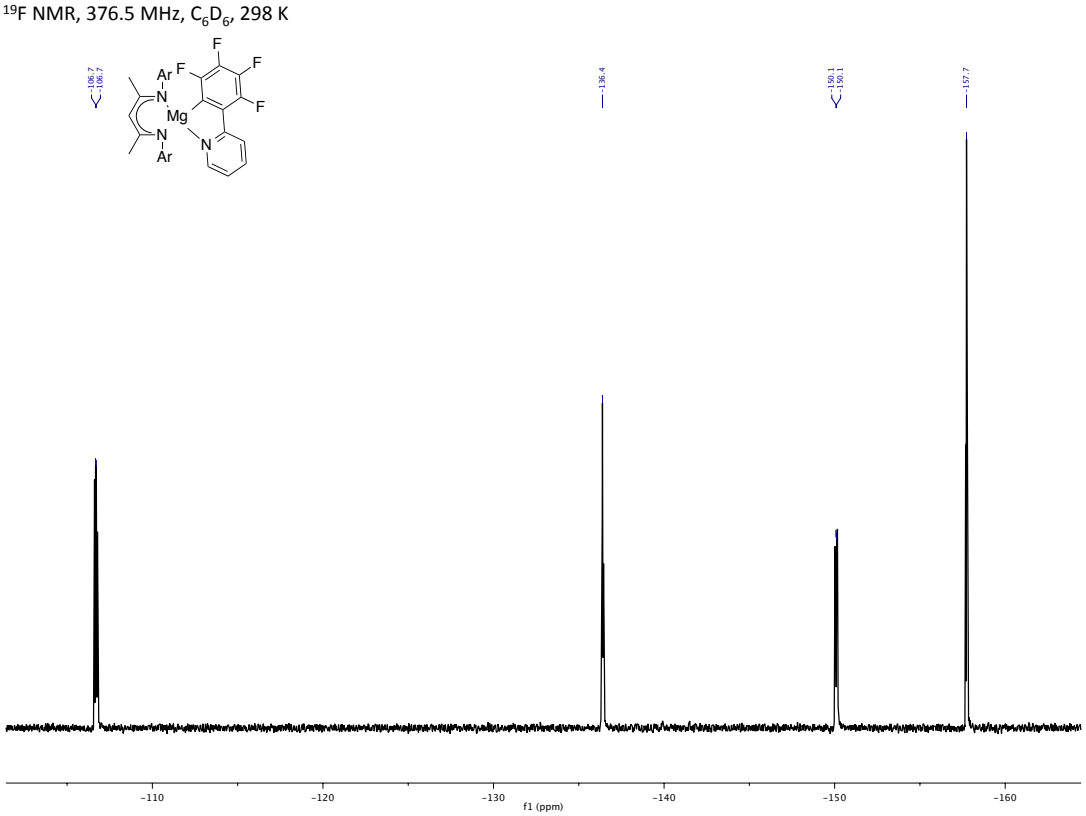


Figure S31: $^{13}C\{^{1}H\}$ NMR spectrum of compound **2d**.

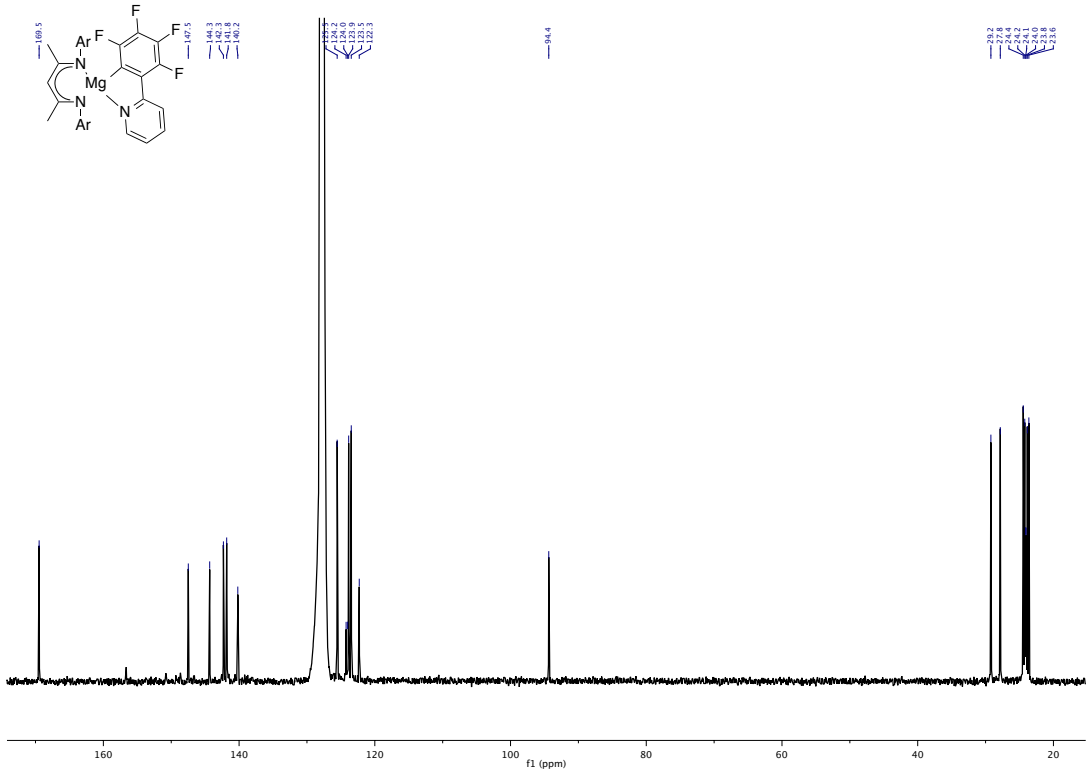


Figure S32: ^{1}H NMR spectrum of compound **2e**; solvent peak marked with asterisk.

^{1}H NMR, 400 MHz, C_6D_6, 298 K

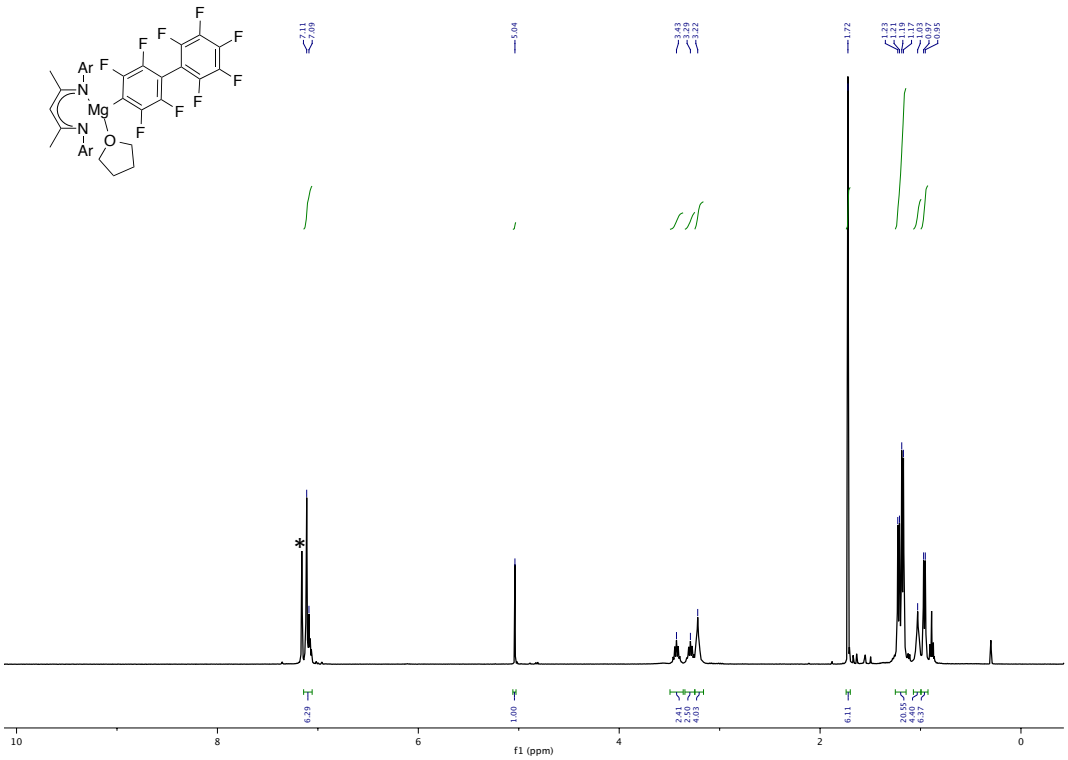


Figure S33: ^{19}F NMR spectrum of compound **2e**.

^{19}F NMR, 376.5 MHz, C_6D_6, 298 K .

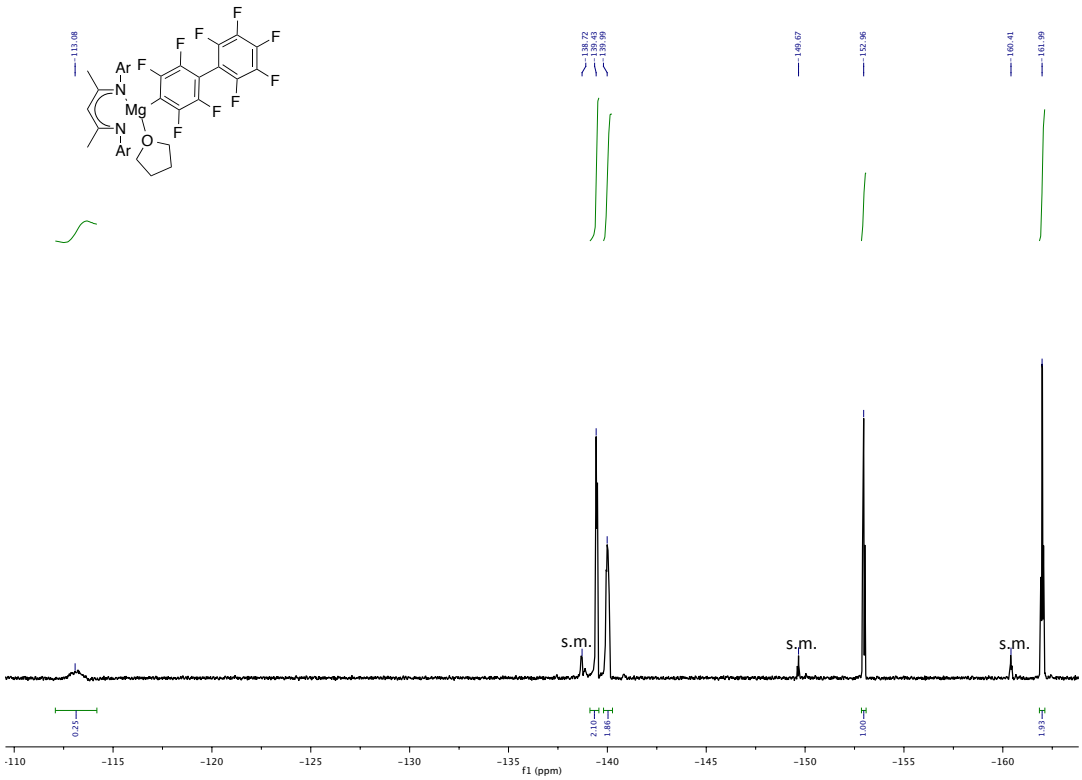


Figure S34: $^{13}C\{^{1}H\}$ NMR spectrum of compound **2e**.

$^{13}C\{^{1}H\}$ NMR, 100 MHz, C_6D_6, 298 K

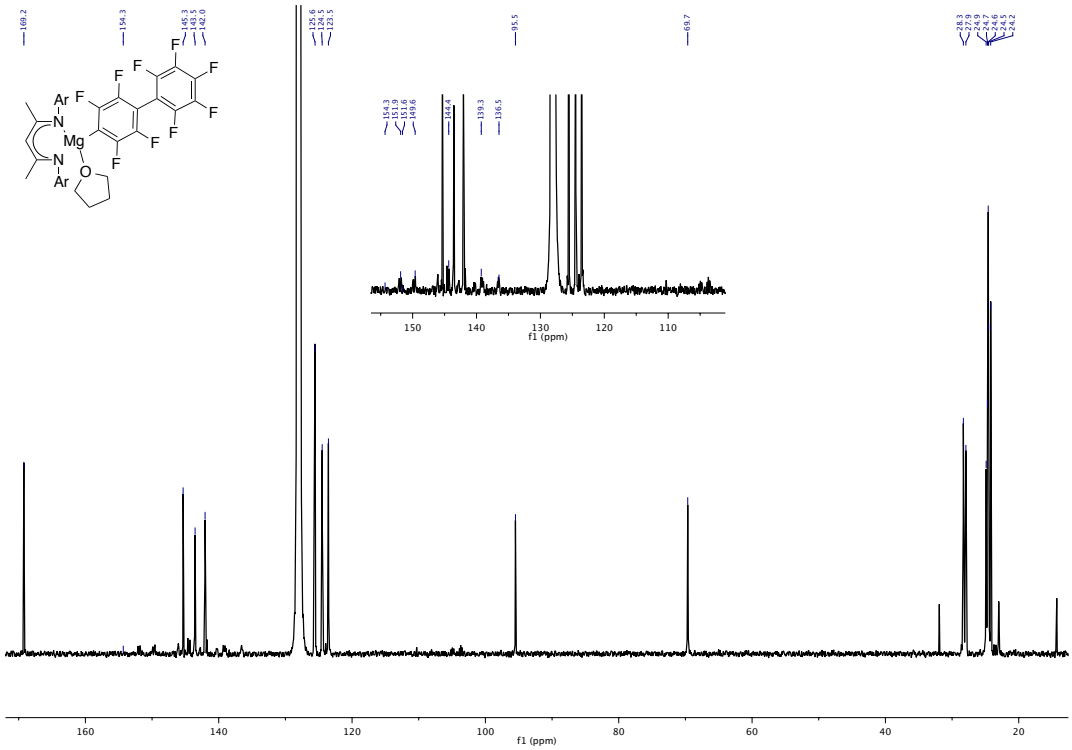


Figure S35: ^{1}H NMR spectrum of compound **2f**; solvent peak marked with asterisk.

^{1}H NMR, 400 MHz, C_6D_6, 298 K

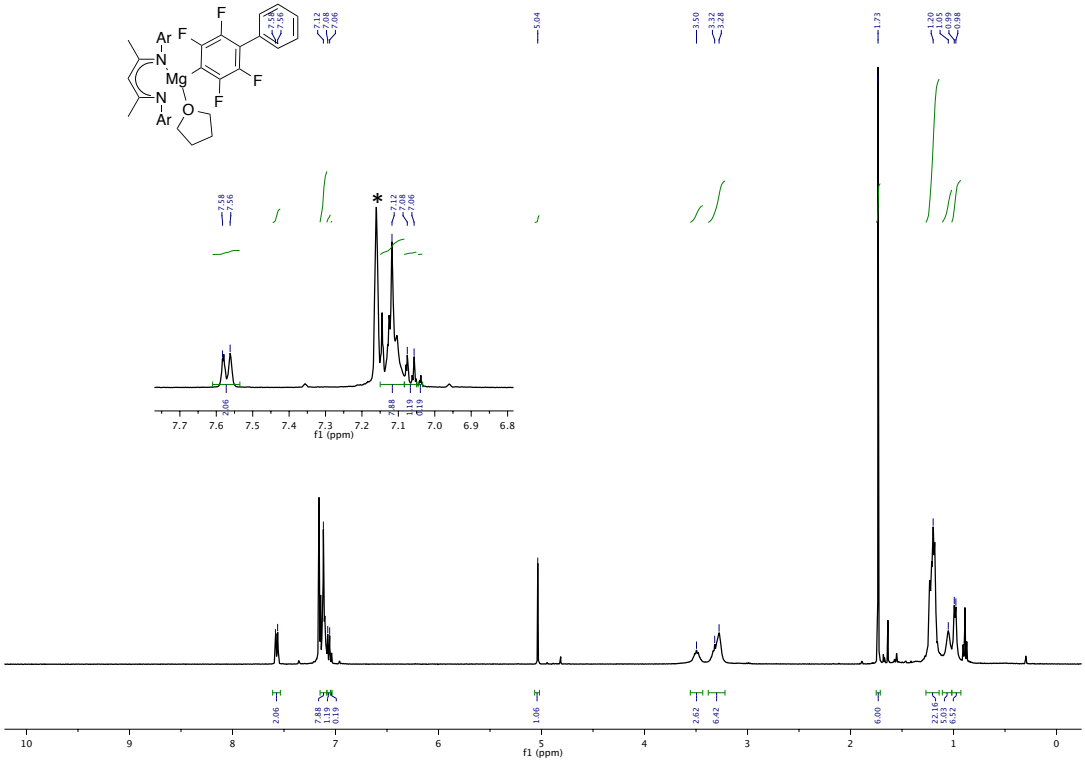


Figure S36: ^{19}F NMR spectrum of compound **2f**.

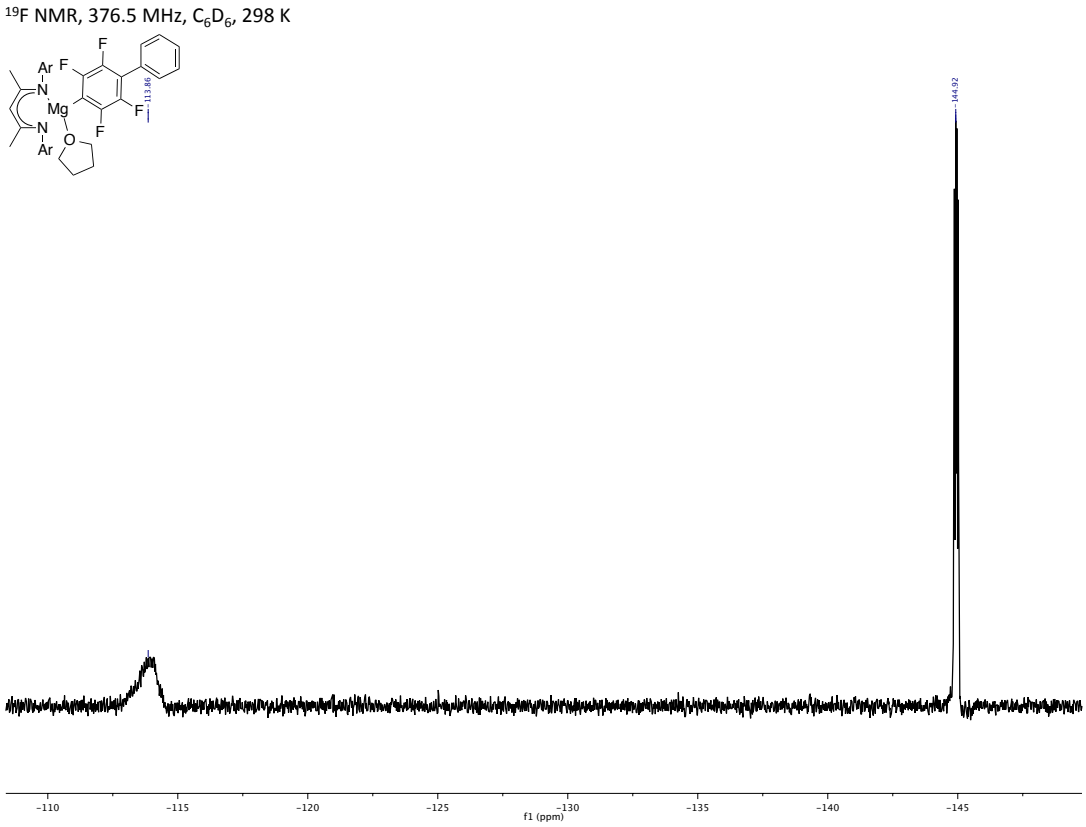


Figure S37: $^{13}C\{^{1}H\}$ NMR spectrum of compound **2f**.

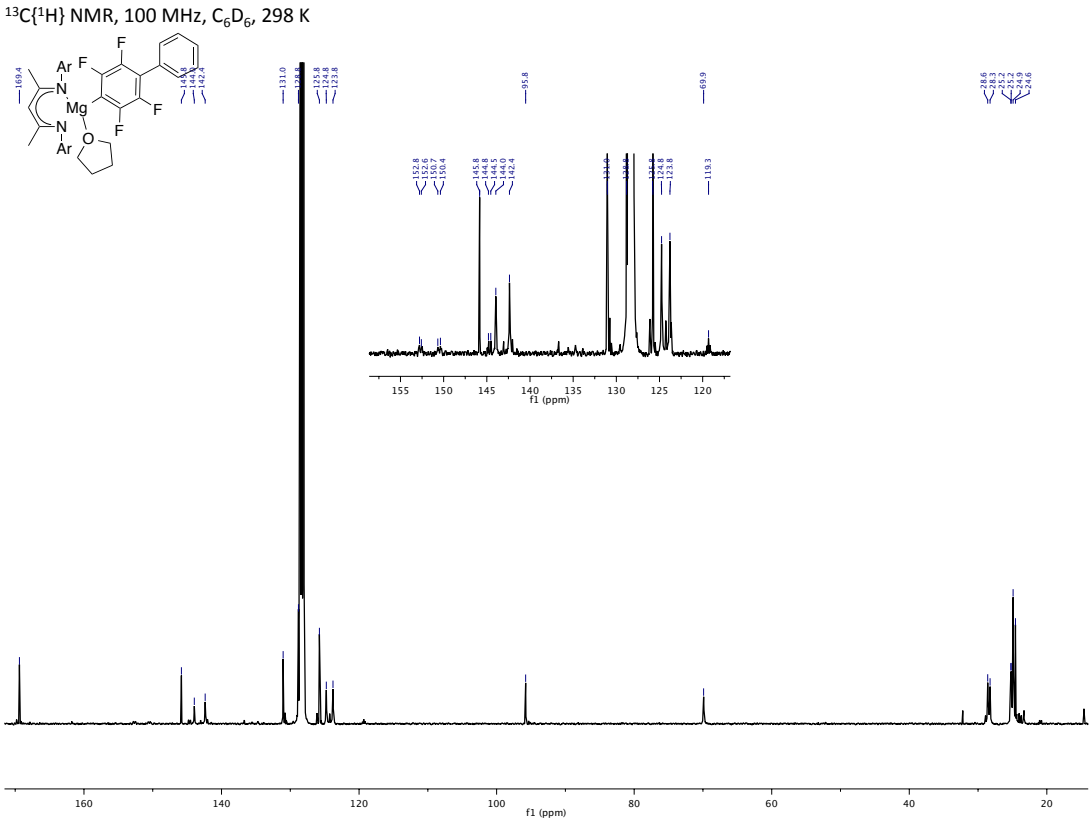


Figure S38: ^{1}H NMR spectrum of compound **2g**; solvent peak marked with asterisk.

^{1}H NMR, 400 MHz, C_6D_6, 298 K

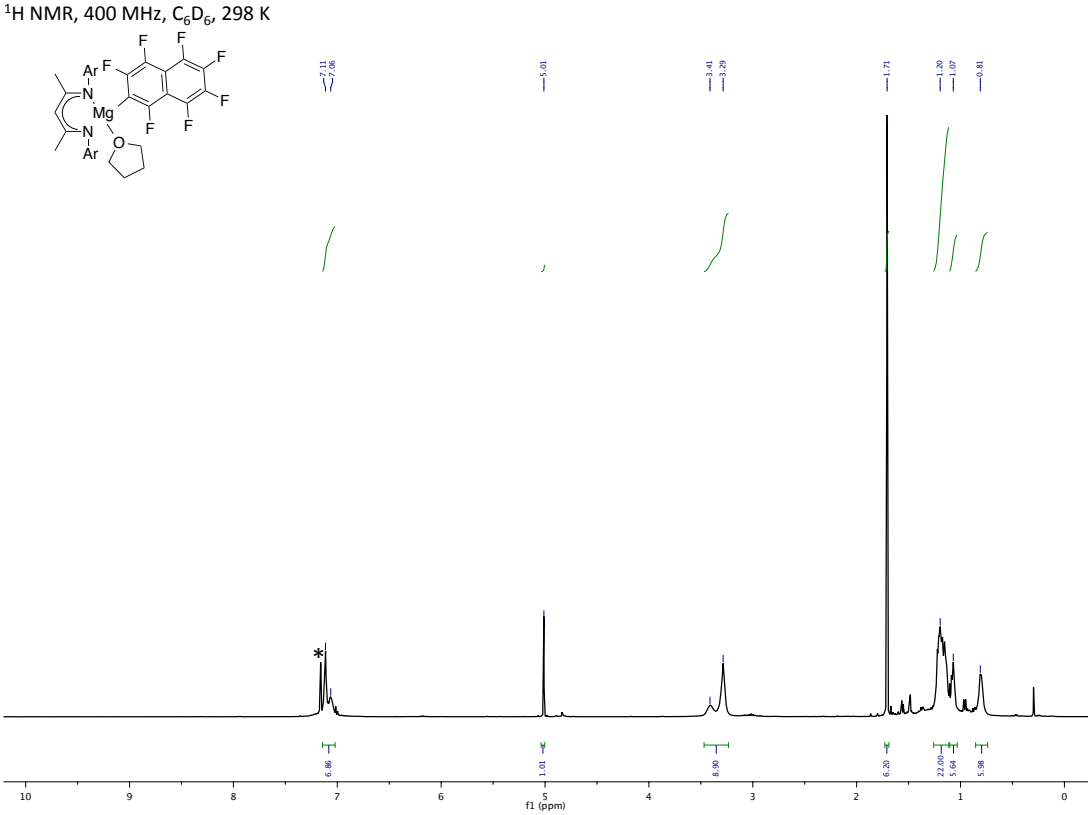


Figure S39: ^{19}F NMR spectrum of compound **2g**.

^{19}F NMR, 376.5 MHz, C_6D_6, 298 K

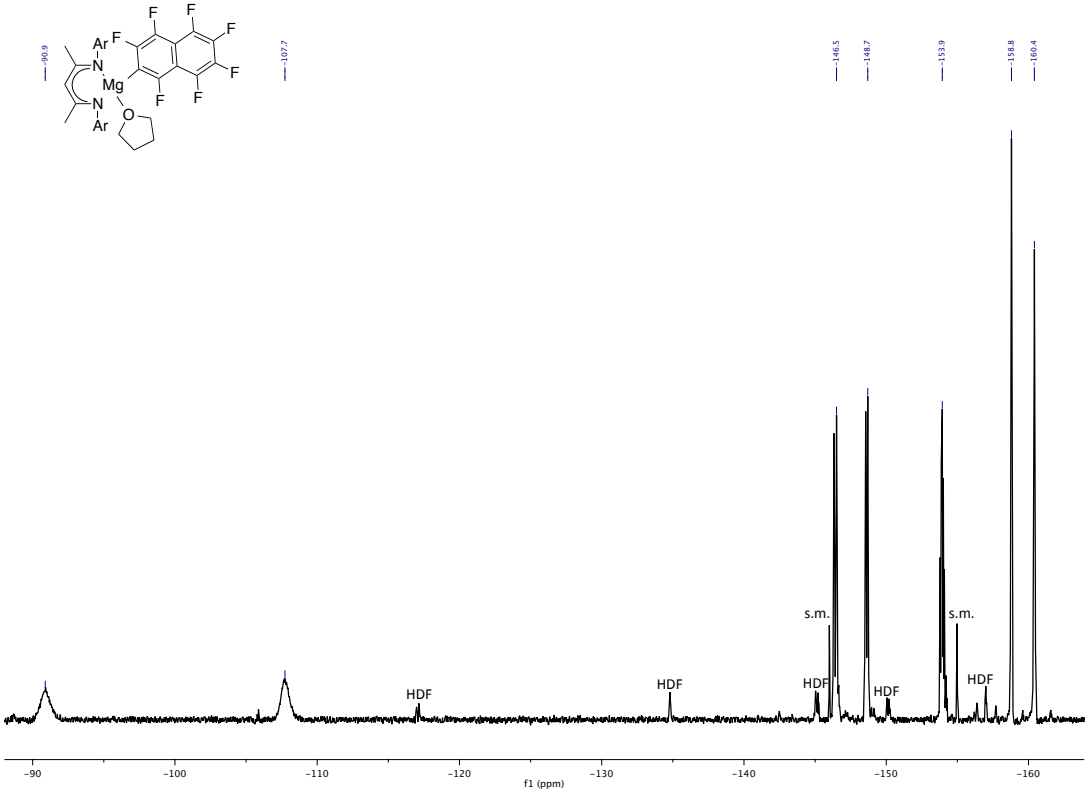


Figure S40: $^{13}C\{^{1}H\}$ NMR spectrum of compound **2g**.

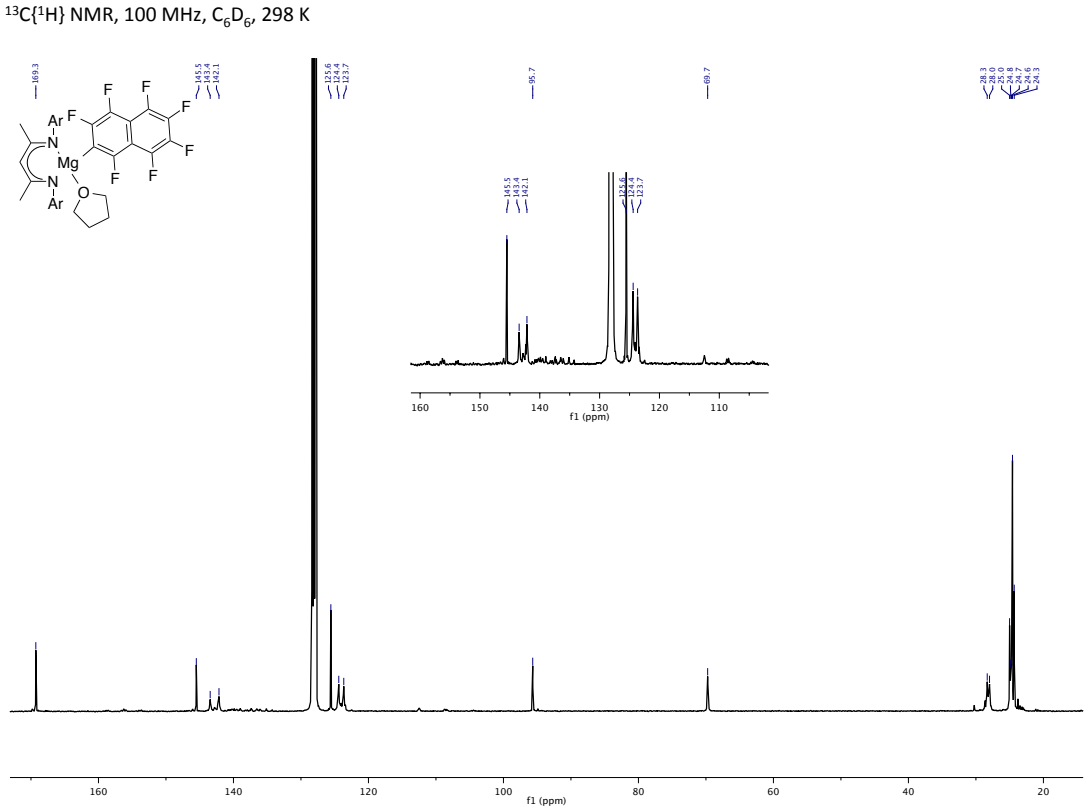


Figure S41: ^{1}H NMR spectrum of compounds **2h** and **2h'**; solvent peak marked with asterisk.

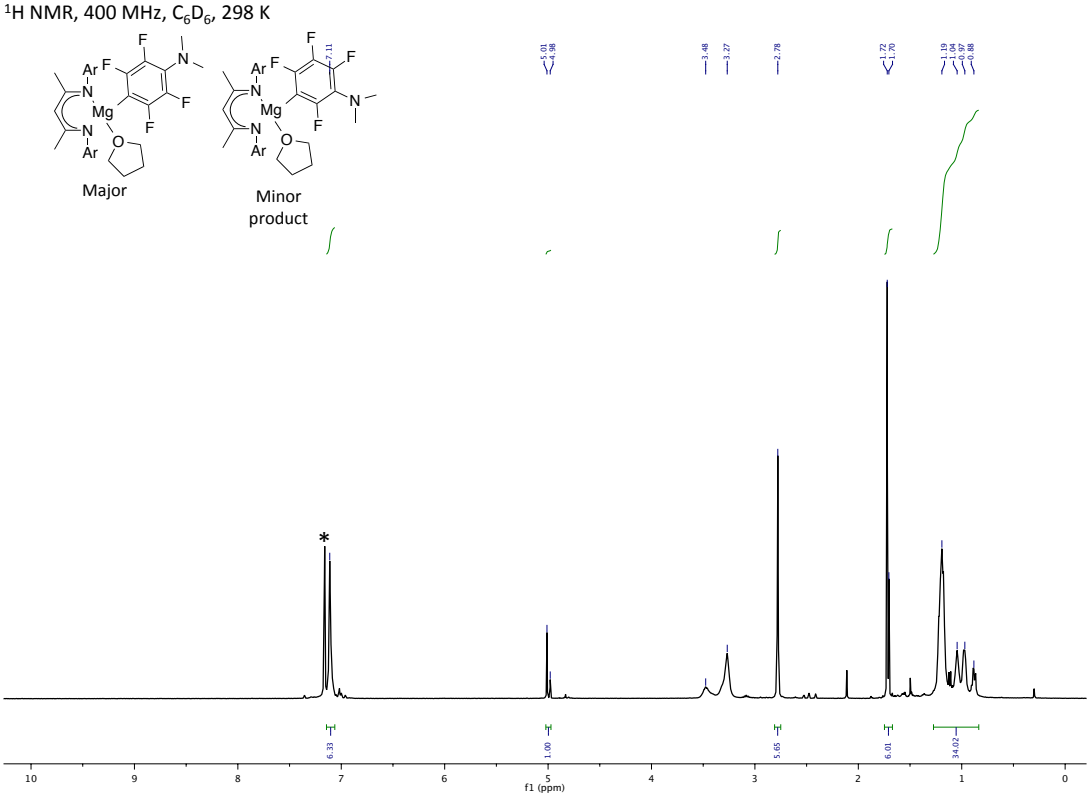


Figure S42: ^{19}F NMR spectrum of compounds **2h** and **2h'**.

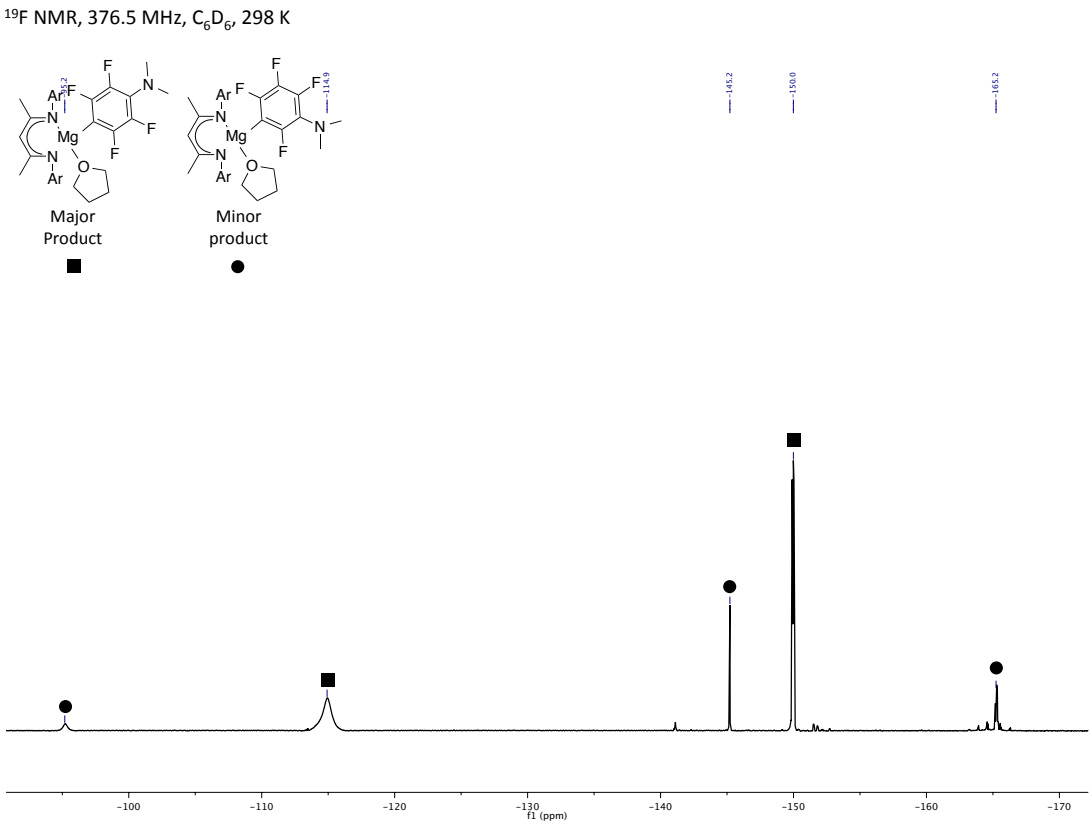


Figure S43: ^{19}F NMR spectrum of protonated **2h** and **2h'**.

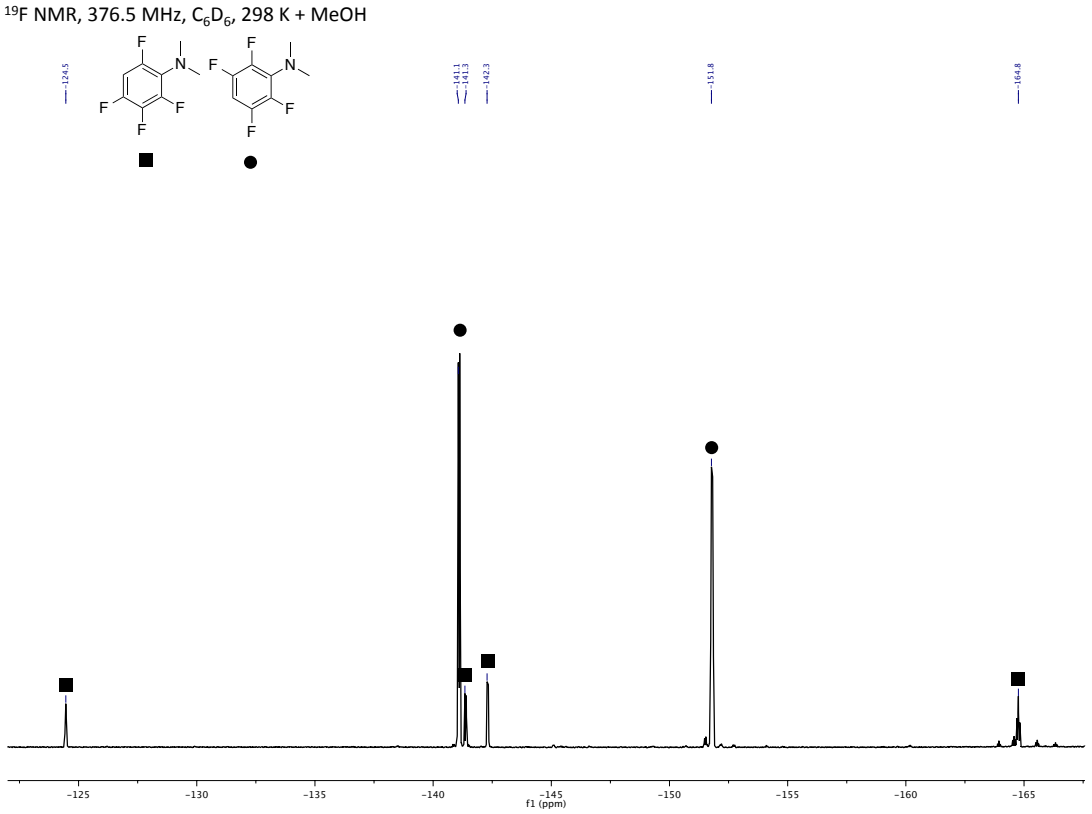


Figure S44: ^{1}H NMR spectrum of compound **2i**; solvent peak marked with asterisk.

^{1}H NMR, 400 MHz, C_6D_6, 298 K

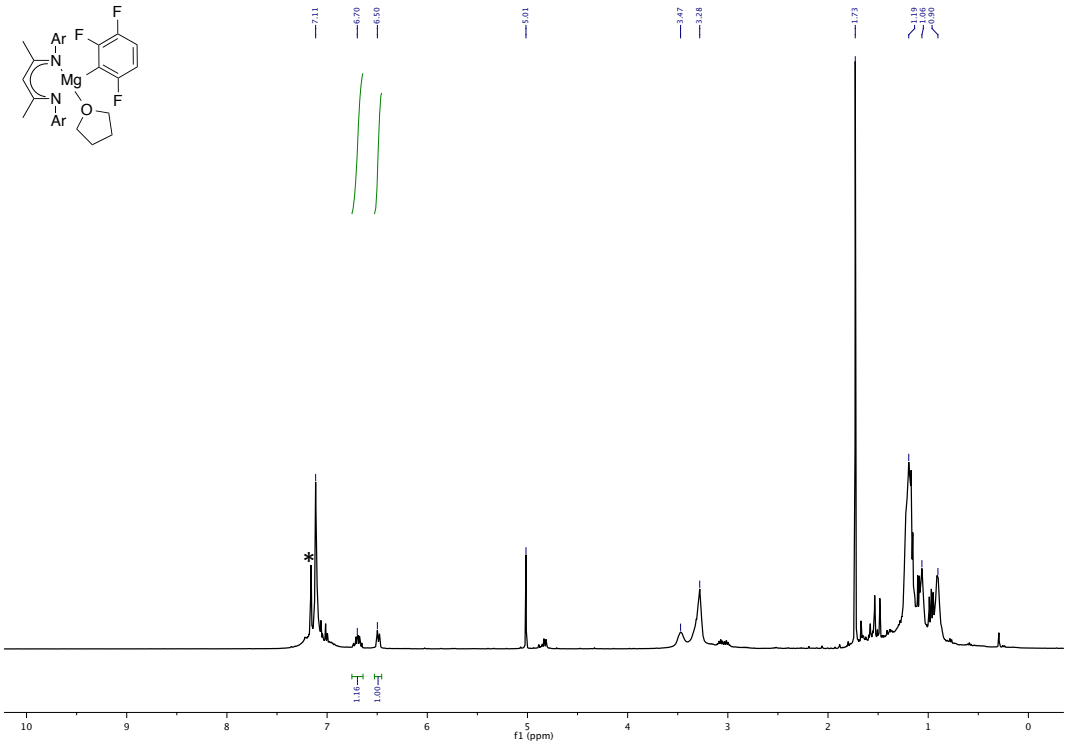


Figure S45: ^{19}F NMR spectrum of compound **2i**.

^{19}F NMR, 376.5 MHz, C_6D_6, 298 K

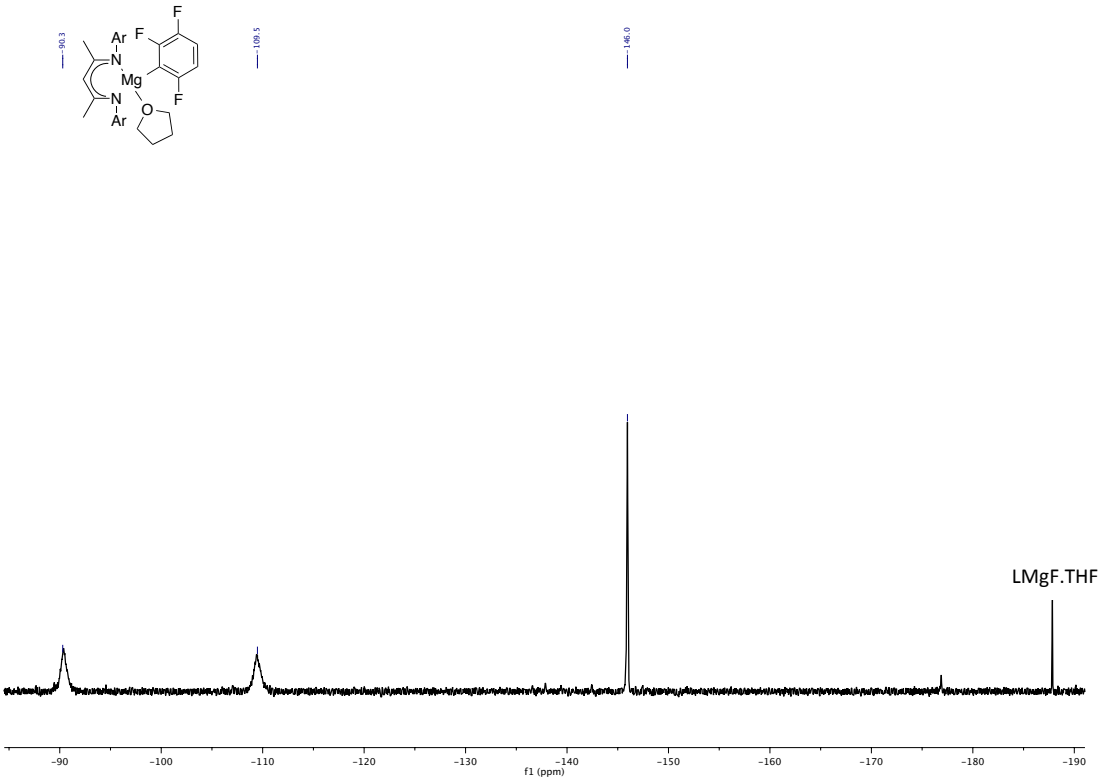


Figure S46: $^{13}C\{^{1}H\}$ NMR spectrum of compound **2i**.

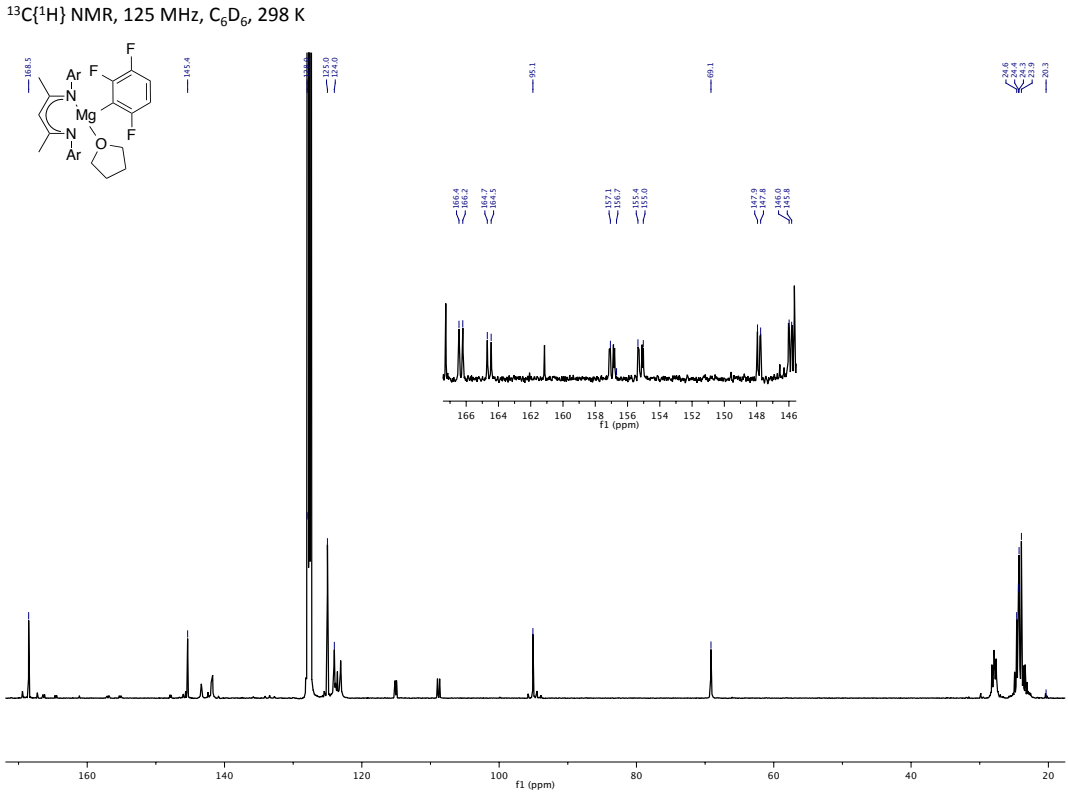


Figure S47: ^{1}H NMR spectrum of the NMR scale formation of compounds **2j, 2j'** and **2a**; solvent peak marked with asterisk.

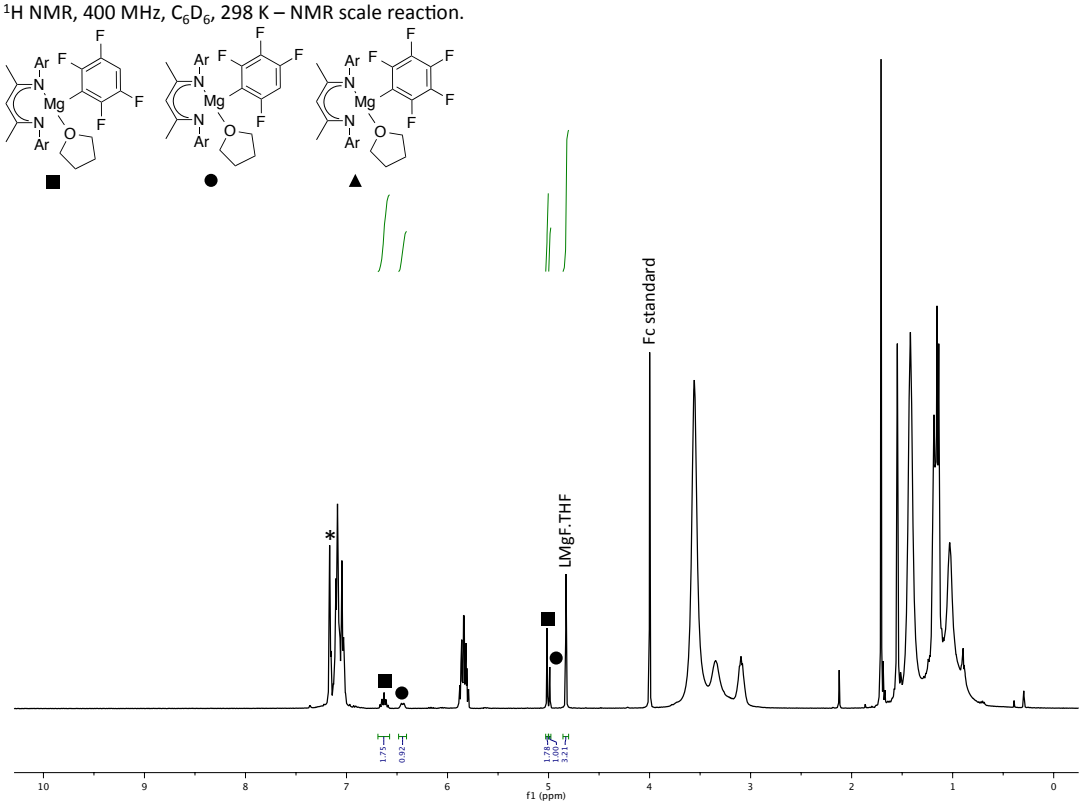


Figure S48: ^{19}F NMR spectrum of the NMR scale formation of compounds **2j, 2j'** and **2a**.

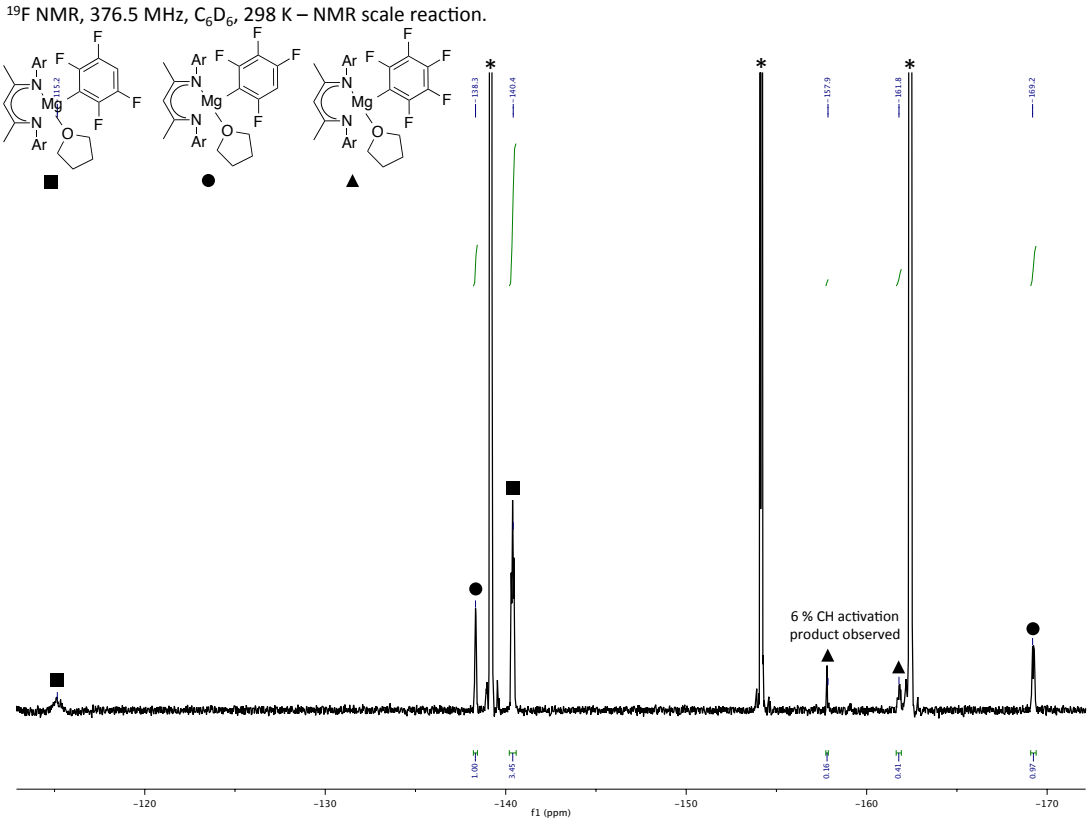


Figure S49: ^{19}F NMR spectrum of the NMR scale formation of compounds **2j**, **2j'** and **2a** protonated with MeOH.

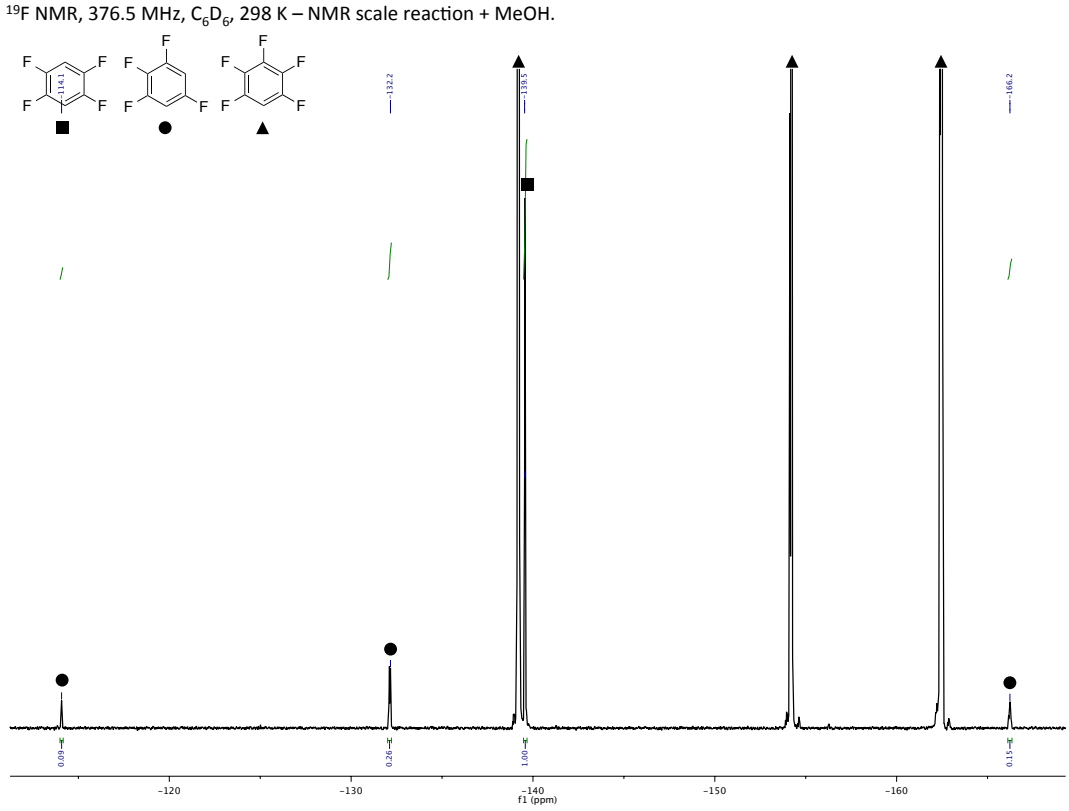


Figure S50: ^{1}H NMR spectrum of isolated compounds **2j, 2j'** and **2a**; solvent peak marked with asterisk.

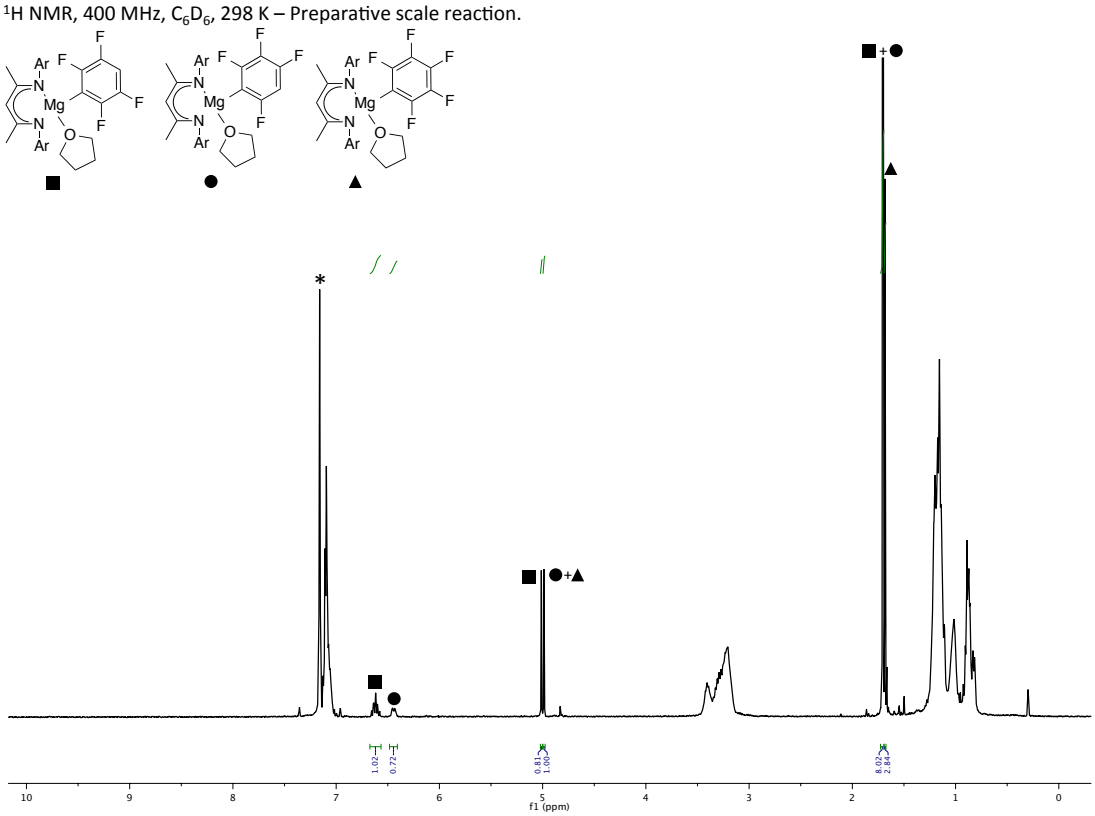


Figure S51: ^{19}F NMR spectrum of isolated compounds **2j**, **2j'** and **2a**.

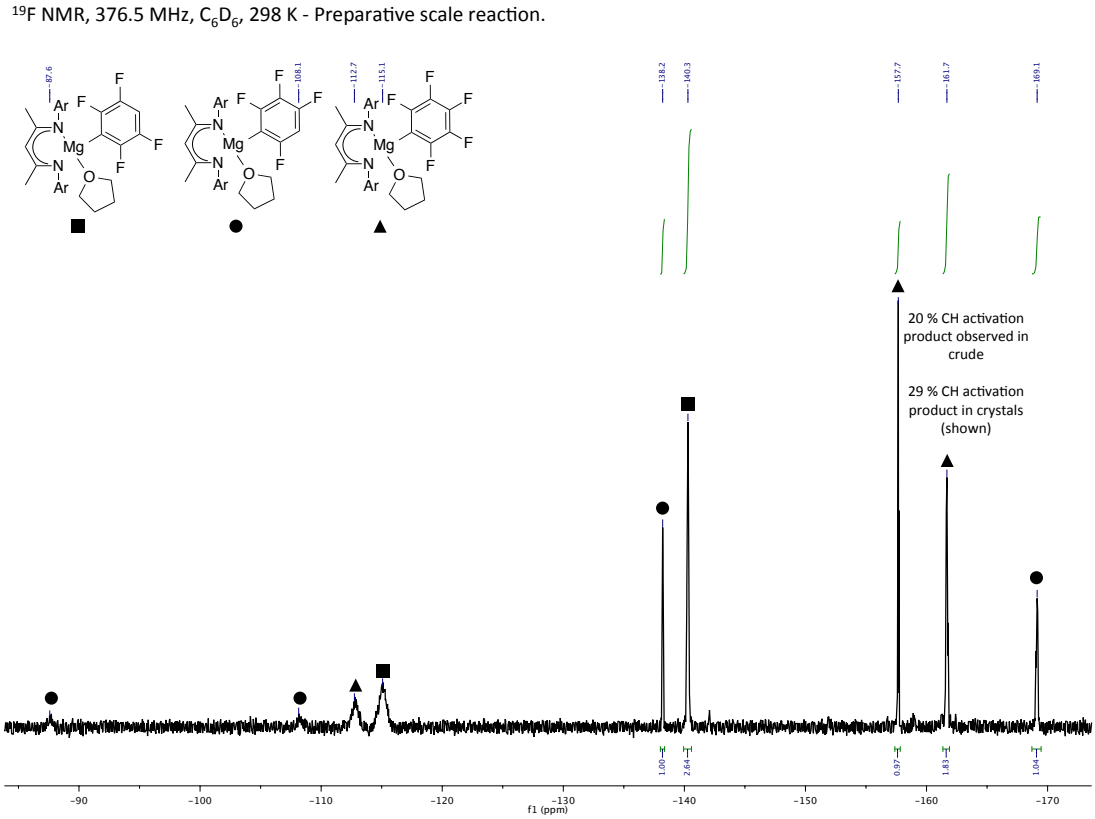


Figure S52: ^{19}F NMR spectrum protonated **2j**, **2j'** and **2a**.

^{19}F NMR, 376.5 MHz, C_6D_6, 298 K – Preparative scale reaction + MeOH.

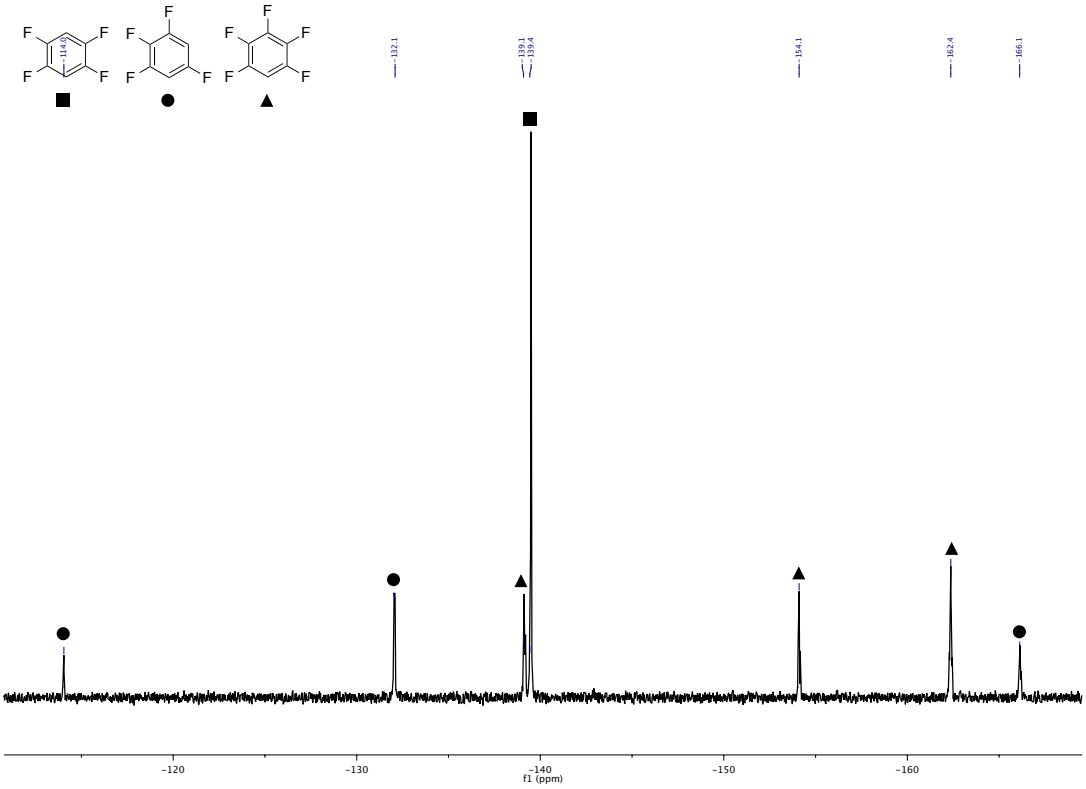


Figure S53: ^{1}H NMR spectrum of the NMR scale formation of compounds **2k**, **2k'** and **2j'**; solvent peak marked with asterisk.

^{1}H NMR, 400 MHz, C_6D_6, 298 K – NMR scale reaction.

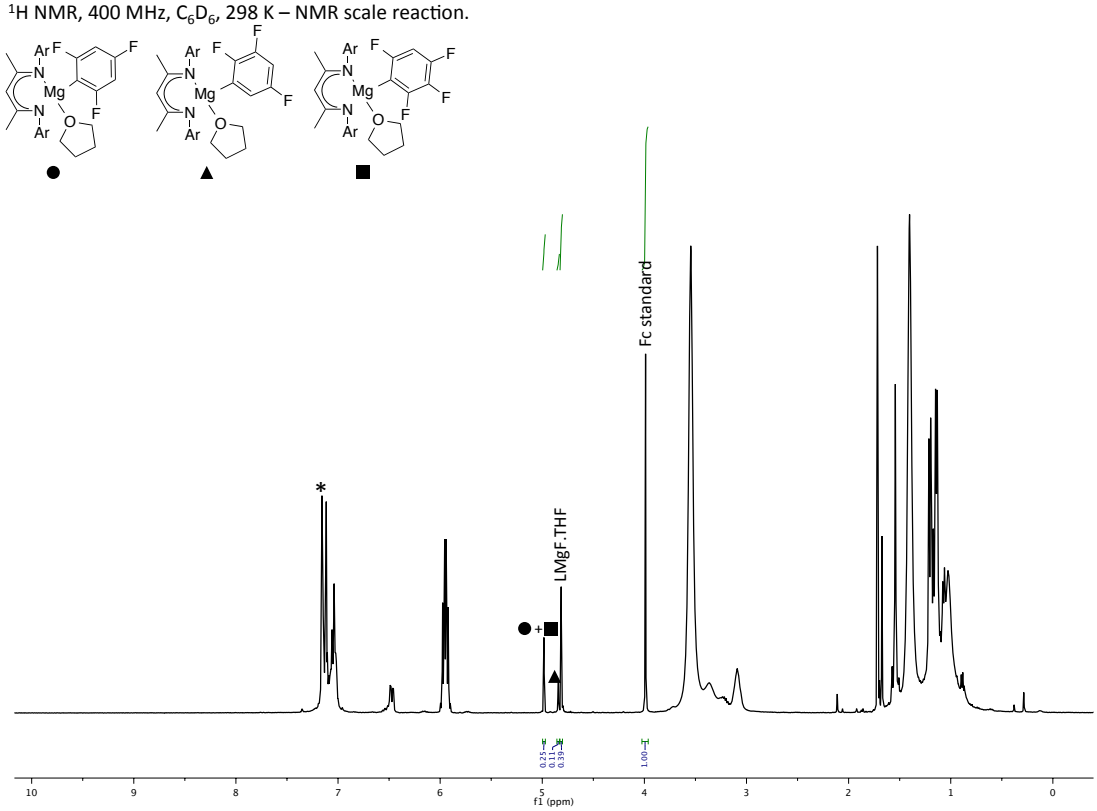


Figure S54: ^{19}F NMR spectrum of the NMR scale formation of compounds **2k**, **2k'** and **2j'**.

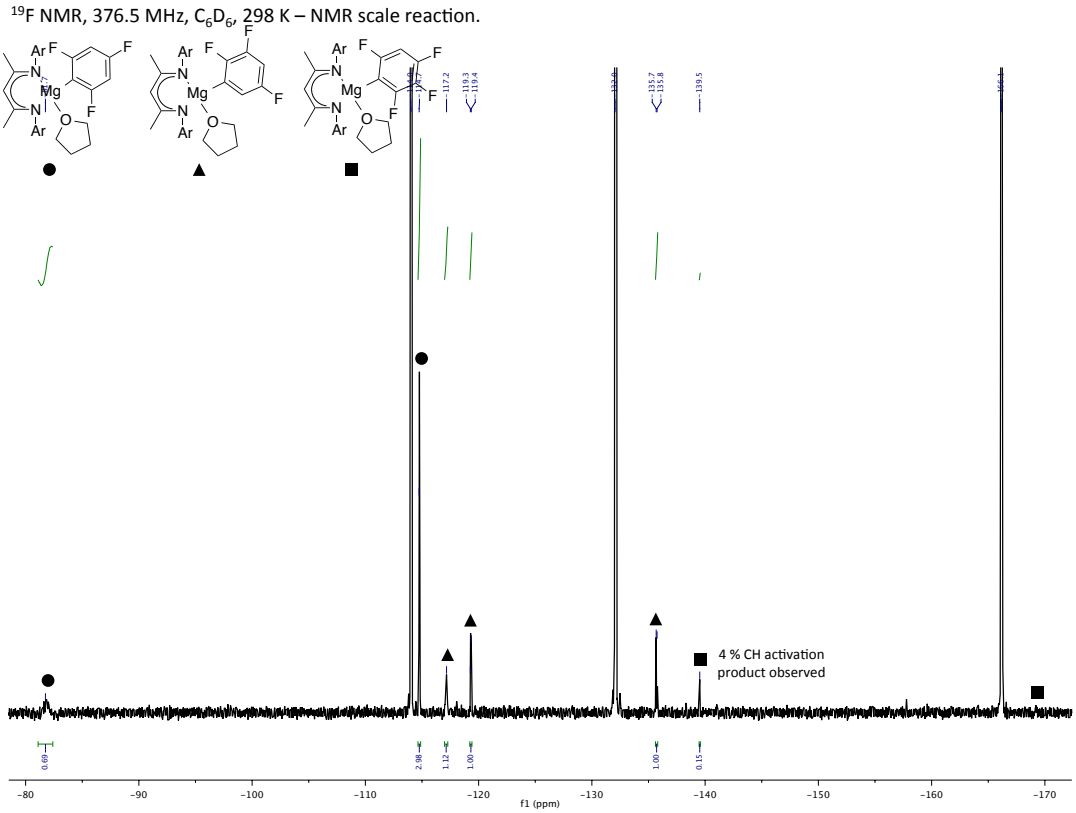


Figure S55: ^{1}H NMR spectrum of isolated compounds **2k, 2k'** and **2j'**; solvent peak marked with asterisk.

^{1}H NMR, 400 MHz, C_6D_6, 298 K - Preparative scale reaction. Note: product ratios not representative of crude material.

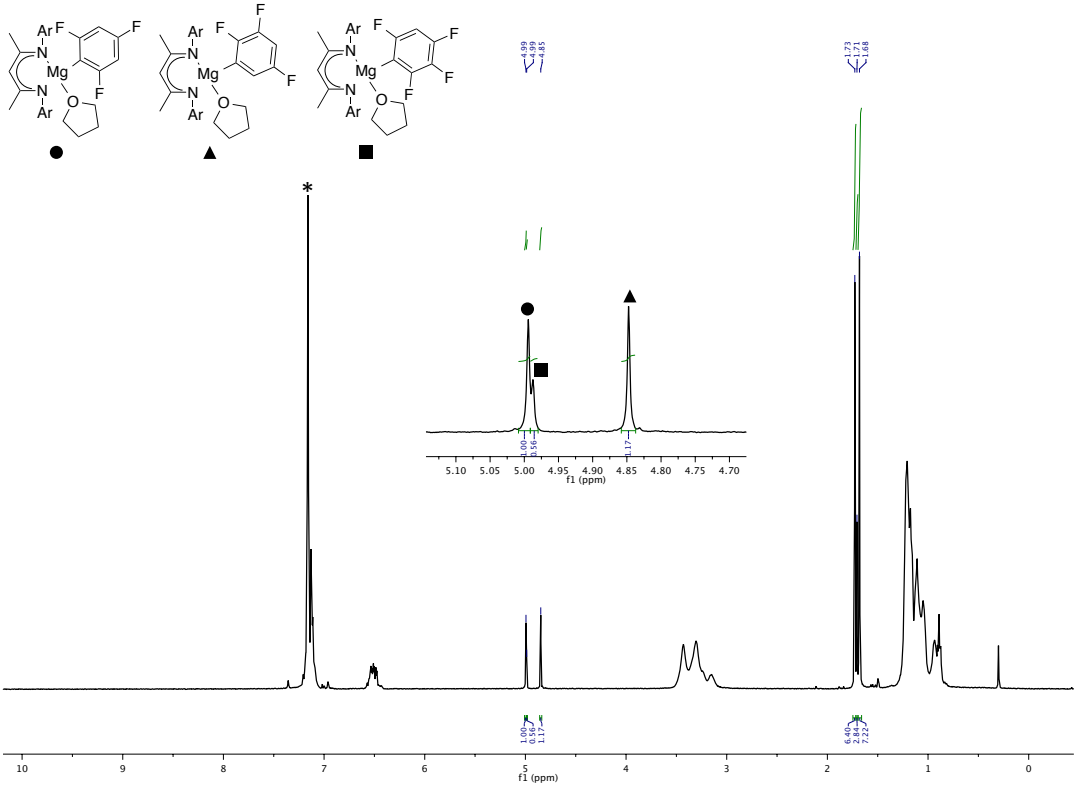


Figure S56: ^{19}F NMR spectrum of isolated compounds **2k**, **2k'** and **2j'**.

^{19}F NMR, 376.5 MHz, C_6D_6, 298 K - Preparative scale reaction. Note: product ratios not representative of crude material.

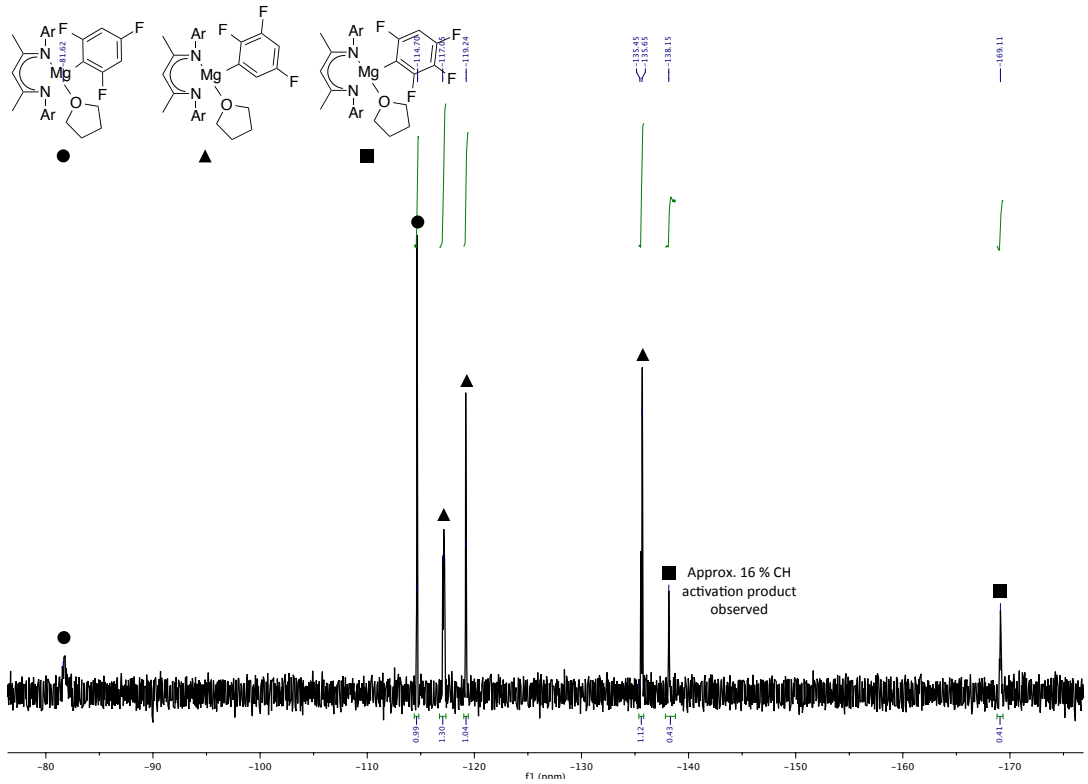


Figure S57: ^{19}F NMR spectrum protonated **2k**, **2k'** and **2j'**.

^{19}F NMR, 376.5 MHz, C_6D_6, 298 K – Preparative scale reaction + MeOH.

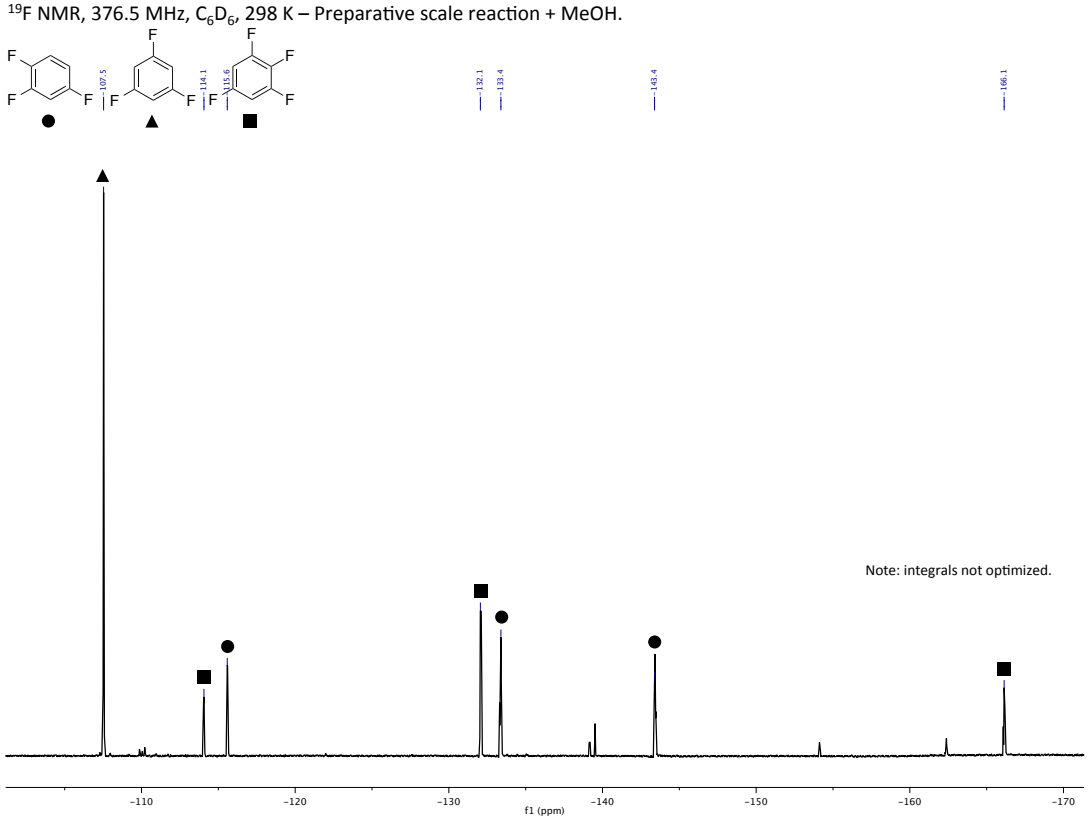


Figure S58: ^{1}H NMR spectrum of compound **4**; solvent peak marked with asterisk.

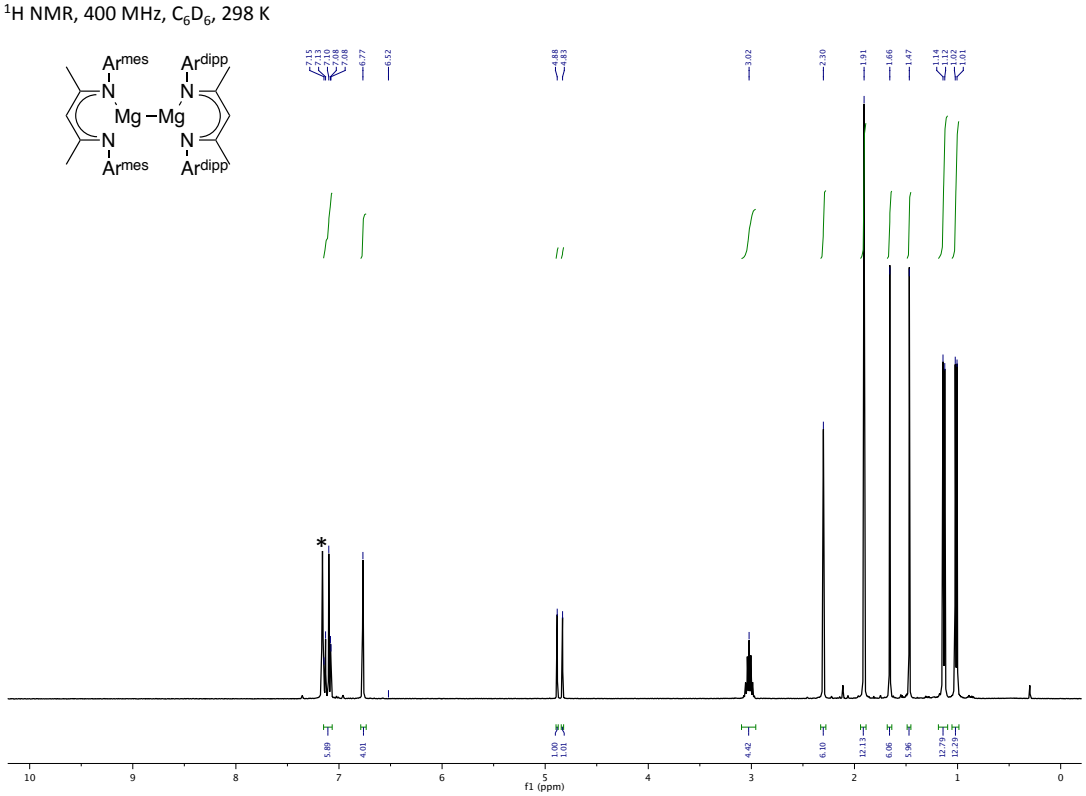
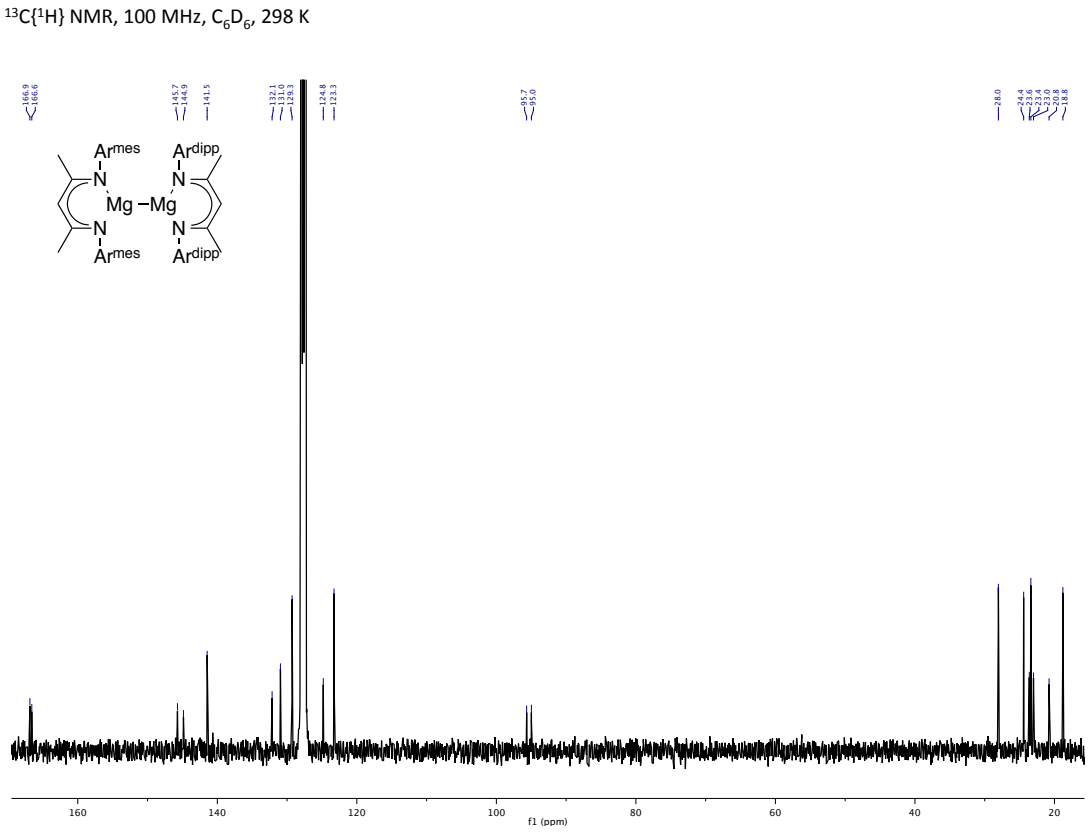


Figure S59: ^{13}C{^{1}H} NMR spectrum of compound **4**.



[i] Feldman, J.; McLain, S.J.; Parthasarathy, A.; Marshall, W. J.; Calabrese, J. C.; Arthur, S .D. *Organometallics*, **1997**, 16, 1514-1515.

[ii] Green, S. P.; S. J.; Jones, C.; Nembenna, S.; Stasch, A. *Science*, **2007**, 318, 1754-1757.

[iii] Bonyhady, S. J.; Jones, C.; Nembenna, S.; Stasch, A.; Edwards, A. J.; McIntyre, G. J. *Chem. Eur. J.*, **2010**, 16, 938-955.

[iv] Roberts, K. M.; Jones, J.P. *Chem. Eur. J.*, **2010**, 8096-8107.

[v] Hao, H.; Roesky, H. W.; Ding, Y.; Cui, C.; Schormann, M.; Schmidt, H.G.; Noltemeyer, M.; Zemva, B. *J. Fluorine Chem.*, **2002**, 115, 143-147.

[vi] Recrystallized yield.

[vii] *J* coupling presumed to arise from a through space interaction with the *ortho*-fluorine.

[viii] Recrystallized yield.

[ix] Product could not be isolated in high purity, due to high solubility in apolar solvents. For this reason only the NMR scale yield is recorded in Table S1.

[x] Based on C–F activation products, but C–H activation product **2a** was also observed; 6 % for NMR scale reaction, 20% for preparative scale reaction in either silylated or non-silylated glassware.

[xi] Based on C–F activation products, but C–H activation product **2j'** was also observed, 4% for NMR scale reaction, 16% for preparative scale reaction in non-silylated glassware.

[xii] S.P. Green, C. Jones and A. Stasch, *Angew. Chem., Int. Ed.*, **2008**, 47, 9079.

[xiii] H. Hao, H.W. Roesky, Y. Ding, C. Cui, M. Schormann, H.-G. Schmidt, M. Noltemeyer and B. Zemva, *J. Fluorine Chem.*, **2002**, 115, 143.

[xiv] (a) SHELXTL, Bruker AXS, Madison, WI; (b) SHELX-97, G.M. Sheldrick, *Acta Cryst.*, **2008**, A64, 112-122; (c) SHELX-2013, G.M. Sheldrick, *Acta Cryst.*, **2015**, C71, 3-8.