Supporting information for:

A Combined Experimental and Computational Study on the Reaction of Fluoroarenes with Mg–Mg, Mg–Zn, Mg–Al and Al–Zn Bonds

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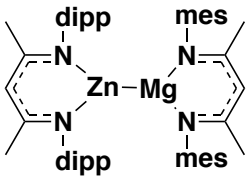
1. General Experimental Section

All manipulations were carried out using standard Schlenk-line and glovebox techniques under an inert atmosphere of argon or dinitrogen. The preparation of all new M–M containing molecules and their reactions with fluoroarenes (and carbodiimides) were carried out in a glovebox. 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 3Å 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, ^{13}C and ^{19}F 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 Topspin 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). C^{IV} refers to quaternary carbons.

Fluorocarbons, where liquids at 25 °C were dried over activated 3Å molecular sieves and freeze-pump-thaw degassed before use. All other chemicals were purchased from Fluorochem, Sigma Aldrich or Alfa Aeser and used without purification unless stated. The β-diketiminate ligands *BDI*H (mes and dipp), *BDI*Mg–Mg*BDI* (**1** = dipp and **2** = mes)[1,2] and [^{dipp}*BDI*Al] (**5**)[3] were prepared by literature procedures. The reagents [^{dipp}*BDI*ZnI], [^{mes}*BDI*ZnI], [^{mes}*BDI*ZnEt] and [^{dipp}*BDI*MgMe] were prepared by modified literature procedures.[4,5]

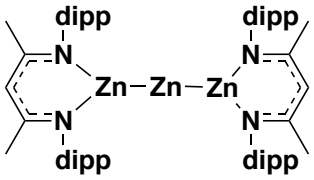
2. Synthetic Procedures

2.1 Preparation of M¹–M² Heterobimetallics



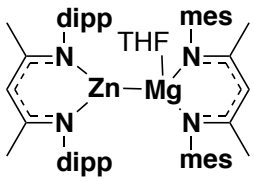
^{dipp}*BDI*Zn-Mg*BDI*^{mes} **(3)**

Synthesis of **3:** To a scintillation vial was added ^{mes}*BDI*Mg–Mg*BDI*^{mes} (**2**, 200 mg, 0.28 mmol) and [^{dipp}*BDI*ZnI] (170 mg, 0.28 mmol) in toluene (10 mL) and the reaction was stirred at 298 K overnight. The vial was transferred to the freezer for 3 hours to ensure all of the [^{mes}*BDI*MgI] was fully precipitated. The residual black precipitate and [^{mes}*BDI*MgI] were removed by filtration, and the supernatant was reduced *in vacuo*. The crude product was extracted into *n*-hexane and recrystallized at –35 °C to yield **3** as a colorless crystalline solid (127 mg, 54 %). ^{1}H NMR (400 MHz, benzene-d_6, 298 K): 0.95 (d, 12H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 1.15 (d, 12H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 1.40 (s, 6H, C(CH_3)CHC(CH_3)^{mes}), 1.68 (s, 6H, C(CH_3)CHC(CH_3)^{dipp}), 1.83 (s, 12H, *o*-CH_3^{mes}), 2.29 (s, 6H, *p*-CH_3^{mes}), 3.09 (sept, 2H, CH(CH$_3$)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 4.81 (s, 1H, C(CH$_3$)CHC(CH$_3$)^{mes}), 4.94 (s, 1H, C(CH$_3$)CHC(CH$_3$)^{dipp}), 6.75 (s, 4H, CH^{mes}), 7.07–7.15 (m, 6H, CH^{dipp}); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 298 K): 18.4 (*o*-*C*H$_3^{mes}$), 20.7 (*p*-*C*H$_3$), 23.0 (C(*C*H$_3$)CHC(*C*H$_3$)^{mes}), 23.1 (CH(*C*H$_3$)$_2$), 23.6 (C(*C*H$_3$)CHC(*C*H$_3$)^{dipp}), 24.0 (CH(*C*H$_3$)$_2$), 28.0 (*C*H(CH$_3$)$_2$), 95.2 (C(CH$_3$)*C*HC(CH$_3$)^{dipp}), 96.0 (C(CH$_3$)*C*HC(CH$_3$)^{mes}), 123.2 (*m*-*C*H^{dipp}), 124.5 (*p*-*C*H^{dipp}), 129.5 (*C*H^{mes}), 131.1 (C^{IV}), 132.5 (C^{IV}), 141.0 (C^{IV}), 145.4 (C^{IV}), 147.1 (C^{IV}), 164.4 (*C*(CH$_3$)CH*C*(CH$_3$) *dipp* or *mes*), 167.8 (*C*(CH$_3$)CH*C*(CH$_3$) *dipp* or *mes*); Anal. Calc. ($MgZnC_{52}H_{70}N_4$): C, 74.28; H, 8.39; N, 6.66. Found: C, 74.25; H, 8.31; N, 6.69.



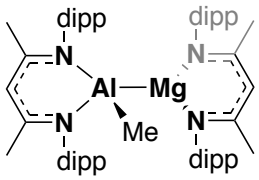
^{dipp}*BDI*Zn-Zn-Zn*BDI*^{dipp} **(4)**

Isolation of ***4****:* From the *n*-hexane filtrate of **3**, a small quantity of yellow crystals (< 10 mg) could be isolated upon prolonged standing at –35 °C (compound **3** crystallises out exclusively first). Single crystal X-ray diffraction revealed the formation of the trizinc compound **4**. The NMR spectra contain traces of *n*-hexanes as prolonged drying at 298 K led to degradation of the product. Attempts to synthesis this product via more rational syntheses have not been successful to date. ^{1}H NMR (400 MHz, benzene-d_6, 298 K): 1.10 (d, 24H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 1.17 (d, 24H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 1.68 (s, 12H, C(CH_3)CHC(CH_3)), 3.08 (sept, 8H, CH(CH$_3$)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 4.89 (s, 2H, C(CH$_3$)CHC(CH$_3$)), 7.08–7.15 (m, 12H, CH); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 298 K): 23.4 ((CH$_3$)CH(*C*H$_3$)), 23.6 (CH(*C*H$_3$)$_2$), 24.9 (CH(*C*H$_3$)$_2$), 28.3 (*C*H(CH$_3$)$_2$), 95.1 (C(CH$_3$)*C*HC(CH$_3$)), 123.5 (*C*H), 125.3 (*C*H), 141.5 (C^{IV}), 145.5 (C^{IV}), 165.3 (*C*(CH$_3$)CH*C*(CH$_3$). The quantity of **4** isolated was too small to run CHN analysis.



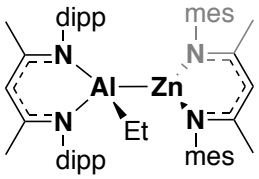
^{dipp}*BDI*Zn-Mg*BDI*^{mes}(THF) **(3.THF)**

Synthesis of **3•THF:** To a solution of compound **3** in benzene-d_6 was added an excess of tetrahydrofuran (THF), ^{1}H NMR analysis revealed quantitative conversion to a new species. The excess solvent was removed *in vacuo*, with ^{1}H NMR analysis showed the coordinaton of one equiv. of THF. Crystals suitable for single crystal X-ray diffraction were grown from *n*-hexane at –35 °C, further confirming the coordination of one equiv. of THF. Characterisation data for **3•THF:** ^{1}H NMR (400 MHz, benzene-d_6, 298 K): 1.08 (d, 12H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.20 (d, 16H, CH(CH_3)$_2$ and O(CH_2)$_2$(CH$_2$)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.47 (s, 6H, C(CH_3)CHC(CH_3)^{mes}), 1.70 (s, 6H, C(CH_3)CHC(CH_3)^{dipp}), 1.96 (s, 12H, *o*-CH_3^{mes}), 2.25 (s, 6H, *p*-CH_3^{mes}), 3.07 (m, 4H, O(CH$_2$)$_2$(CH_2)$_2$), 3.26 (sept, 4H, CH(CH$_3$)$_2$, $^3J_{HH}$ = 6.8 Hz), 4.82 (s, 1H, C(CH$_3$)CHC(CH$_3$)^{mes}), 4.95 (s, 1H, C(CH$_3$)CHC(CH$_3$)^{dipp}), 6.78 (s, 4H, CH^{mes}), 7.05-7.10 (m, 6H, CH^{dipp}); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 298 K): 18.9 (*o*-CH_3^{mes}), 20.7 (*p*-CH_3), 23.1 (C(CH_3)CHC(CH_3)^{mes}), 23.5 (CH(CH_3)$_2$), 23.9 (C(CH_3)CHC(CH_3)^{dipp}), 24.7 (CH(CH_3)$_2$), 25.0 (O(CH$_2$)$_2$(CH_2)$_2$), 28.1 (CH(CH$_3$)$_2$), 67.9 (O(CH_2)$_2$(CH$_2$)$_2$), 95.2 (C(CH$_3$)CHC(CH$_3$)^{dipp}), 95.4 (C(CH$_3$)CHC(CH$_3$)^{mes}), 123.1 (*m*-CH^{dipp}), 124.1 (*p*-CH^{dipp}), 129.2 (CH^{mes}), 131.4 (C^{IV}), 132.3 (C^{IV}), 141.5 (C^{IV}), 146.2 (C^{IV}), 148.0 (C^{IV}), 163.6 (C(CH$_3$)CHC(CH$_3$) *dipp* or *mes*), 166.7 (C(CH$_3$)CHC(CH$_3$) *dipp* or *mes*); Anal. Calc. ($MgZnC_{56}H_{78}N_4O$): C, 73.67; H, 8.61; N, 6.14. Found: C, 73.48; H, 8.28; N, 5.92.



^{dipp}*BDI*(Me)Al-Mg*BDI*^{dipp}(THF) **(6)**

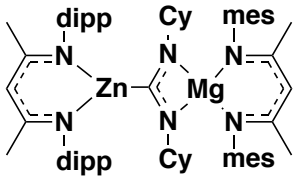
Synthesis of **6:** [^{dipp}*BDI*Al] (104 mg, 0.23 mmol) was dissolved in toluene (2 mL) and [^{dipp}*BDI*MgMe•OEt$_2$] (124 mg, 0.23 mmol) was added at 25 °C. After stirring the reaction mixture for 4 h the solvent was removed *in vacuo*. The resulting residue was extracted into *n*-hexane (2 mL) and recrystallized at –35 °C yielding the product as orange crystals (120 mg, 0.1 mmol, 57 %). ^{1}H NMR (400 MHz, benzene-d_6, 348 K): –1.23 (s, 3H, Al–CH_3), 1.03–1.28 (m, 42H, CH(CH_3)$_2$), 1.31 (d, 6H, CH(CH_3)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.43 (s, 6H, C(CH_3)CHC(CH_3)), 1.67 (s, 6H, C(CH_3)CHC(CH_3)), 3.15–3.43 (m, 6H, CH(CH$_3$)$_2$), 3.62 (sept, 2H, CH(CH$_3$)$_2$, $^3J_{HH}$ = 6.8 Hz), 4.70 (s, 1H, C(CH$_3$)CHC(CH$_3$)), 4.85 (s, 1H, C(CH$_3$)CHC(CH$_3$)), 7.00–7.13 (m, 12H, Ar-*H*); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 348 K): –0.5 (Al – *C*H$_3$), 23.7 (*C*H$_3$), 23.8 (*C*H$_3$), 24.3 (*C*H$_3$), 24.4 (*C*H$_3$), 24.9 (*C*H$_3$ or CH(*C*H$_3$)$_2$), 25.1 (*C*H$_3$), 28.2 (*C*H(CH$_3$)$_2$), 28.6 (*C*H(CH$_3$)$_2$), 28.7 (*C*H(CH$_3$)$_2$), 28.8 (*C*H(CH$_3$)$_2$), 96.2 (C(CH$_3$)*C*HC(CH$_3$)), 97.8 (C(CH$_3$)*C*HC(CH$_3$)), 124.1 (*C*H), 124.2 (*C*H), 124.5 (*C*H), 125.3 (*C*H), 126.7 (*C*H), 142.6 (C^{IV}), 142.7 (C^{IV}), 144.8 (C^{IV}), 145.0 (C^{IV}), 146.0 (C^{IV}), 168.0 (*C*(CH$_3$)CHC(CH$_3$)), 168.2 (*C*(CH$_3$)CHC(CH$_3$)); Anal. Calc. ($AlMgC_{59}H_{85}N_4$): C, 78.60; H, 9.50; N, 6.21. Found: C, 78.49; H, 8.77; N, 6.00. Due to the air sensitive nature of **6**, repeated attempts to acquire more accurate CHN data were unsuccessful.



^{dipp}*BDI*(Et)Al-Zn*BDI*^{mes}(THF) **(7)**

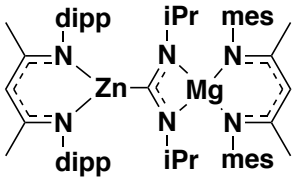
Synthesis of **7:** ^{dipp}BDIAl (15 mg, 0.03 mmol) was dissolved in benzene-d_6 (0.6 mL), [^{mes}*BDI*ZnEt•OEt$_2$] (14.4 mg, 0.03 mmol) was added and the solution was transferred to a Young's tap NMR tube. The reaction was monitored by ^{1}H NMR at 25 °C, with full conversion achieved after 3 days. The solvent was removed *in vacuo* and the resulting residue was extracted into *n*-hexane (1 mL) and recrystallized at –35 °C yielding the product as yellow crystals. ^{1}H NMR (400 MHz, benzene-d$_6$, 298 K): -0.39 – -0.25 (m, 5H, CH$_2$C*H*$_3$ and C*H*$_2$CH$_3$), 1.06 (d, 12H, CH(C*H*$_3$)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.37 (d, 6H, CH(C*H*$_3$)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.41 (d, 6H, CH(C*H*$_3$)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.53 (s, 6H, C(C*H*$_3$)CHC(C*H*$_3$)^{dipp}), 1.59 (s, 3H, C(C*H*$_3$)CHC(CH$_3$)^{mes}), 1.76 (s, 3H, C(CH$_3$)CHC(C*H*$_3$)^{mes}), 1.94 (s, 6H, C*H*$_3^{mes}$), 2.03 (s, 3H, C*H*$_3^{mes}$), 2.25 (s, 3H, C*H*$_3^{mes}$), 2.51 (s, 6H, C*H*$_3^{mes}$), 3.04 (sept, 2H, C*H*(CH$_3$)$_2$, $^3J_{HH}$ = 6.8 Hz), 3.56 (sept, 2H, C*H*(CH$_3$)$_2$, $^3J_{HH}$ = 6.8 Hz), 4.83 (s, 1H, C(CH$_3$)C*H*C(CH$_3$)^{dipp}), 4.98 (s, 1H, C(CH$_3$)C*H*C(CH$_3$)^{mes}), 6.64 (s, 2H, C*H*^{mes}), 6.95 (s, 2H, C*H*^{mes}), 7.05–7.09 (m, 2H, C*H*^{dipp}), 7.10–7.14 (m, 4H, C*H*^{dipp}); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 298 K): 4.1 (*C*H$_2$CH$_3$), 7.6 (CH$_2$*C*H$_3$), 19.4 (*C*H$_3^{mes}$), 19.9 (*C*H$_3^{mes}$), 20.3 (*C*H$_3^{mes}$), 20.6 (*C*H$_3^{mes}$), 22.4 (C(*C*H$_3$)CHC(*C*H$_3$)^{mes}), 23.0 (C(*C*H$_3$)CHC(*C*H$_3$)^{dipp}), 23.2 (C(*C*H$_3$)CHC(*C*H$_3$)^{mes}), 23.4 (CH(*C*H$_3$)$_2$), 24.8 (CH(*C*H$_3$)$_2$), 25.0 (CH(*C*H$_3$)$_2$), 26.0 (CH(*C*H$_3$)$_2$), 28.1 (*C*H(CH$_3$)$_2$), 28.6 (*C*H(CH$_3$)$_2$), 95.2 (C(CH$_3$)*C*HC(CH$_3$))^{mes}, 97.2 (C(CH$_3$)*C*HC(CH$_3$))^{dipp},123.5 (*C*H^{dipp}), 124.5 (*C*H^{dipp}), 126.3 (*C*H^{dipp}), 129.0 (*C*H^{mes}), 130.9 (C^{IV}), 131.7 (C^{IV}), 132.3 (C^{IV}), 132.7 (C^{IV}), 141.1 (C^{IV}), 143.8 (C^{IV}), 144.9 (C^{IV}), 146.2 (C^{IV}), 146.8 (C^{IV}), 164.0 (*C*(CH$_3$)CHC(CH$_3$)), 164.1 (*C*(CH$_3$)CH*C*(CH$_3$)), 168.6 (*C*(CH$_3$)CH*C*(CH$_3$)); Anal. Calc. (AlZnC$_{54}$H$_{75}$N$_4$): C, 74.33; H, 8.66; N, 6.42. Found: C, 74.42; H, 8.76; N, 6.33.

2.2 Trapping and Degradation of the unstable Zn–Mg heterobimetallic 3

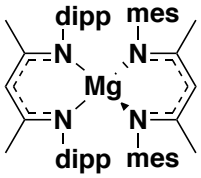


Synthesis of **3•DCC:** To a scintillation vial was added **3** (50 mg, 0.06 mmol) and *N,N'*-dicyclohexylcarbodiimide (12 mg, 0.06 mmol) in toluene (3 mL) and the reaction was stirred at 298 K for 30 minutes. After which time, the solvent was reduced in vacuo and the residues were recrystallised from a toluene/*n*-hexane solution at –35 °C, to yield a colorless crystalline solid. ^{1}H NMR (400 MHz, benzene-d_6, 298 K): 0.88 (bm, 4H, Cy-C*H*$_2$), 1.11–1.35 (bm, 10H, Cy-C*H*$_2$), 1.19 (d, 12H, CH(C*H*$_3$)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.25 (d, 12H, CH(C*H*$_3$)$_2$, $^3J_{HH}$ = 6.8 Hz), 1.49 (bm, 6H, Cy-C*H*$_2$), 1.60 (s, 6H, C(C*H*$_3$)CHC(C*H*$_3$)^{dipp}), 1.69 (s, 6H, C(C*H*$_3$)CHC(C*H*$_3$)^{mes}), 2.19 (s, 12H, *o*-C*H*$_3^{mes}$), 2.27 (s, 6H, *p*-C*H*$_3^{mes}$), 2.63 (m, 2H, Cy-C*H*), 3.25 (sept, 4H, C*H*(CH$_3$)$_2$, $^3J_{HH}$ = 6.8 Hz), 4.83 (s, 1H, C(CH$_3$)C*H*C(CH$_3$) ^{dipp}), 4.92 (s, 1H, C(CH$_3$)C*H*C(CH$_3$) ^{mes}), 6.76 (s, 4H, C*H*^{mes}), 7.14 (bs, 4H, C*H*^{dipp}); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 298 K): 19.1 (*o*-*C*H$_3^{mes}$), 20.6 (*p*-*C*H$_3^{mes}$), 23.0 (C(*C*H$_3$)CHC(*C*H$_3$)^{mes}), 24.1 (C(*C*H$_3$)CHC(*C*H$_3$)^{dipp}), 24.6 (CH(*C*H$_3$)$_2$), 24.9 (CH(*C*H$_3$)$_2$), 25.0 (Cy-*C*H$_2$), 26.4 (Cy-*C*H$_2$), 28.2 (*C*H(CH$_3$)$_2$), 37.1 (Cy-*C*H$_2$), 58.5 (Cy-*C*H), 94.1 (C(CH$_3$)*C*HC(CH$_3$)^{mes}), 96.4

($C(CH_3)CHC(CH_3)^{dipp}$), 124.0 (CH^{dipp}), 125.7 (CH^{dipp}), 128.7 (CH^{mes}), 131.4 (C^{IV}), 131.8 (C^{IV}), 142.2 (C^{IV}), 145.0 (C^{IV}), 145.7 (C^{IV}), 167.4 ($C(CH_3)CHC(CH_3)$ *dipp* or *mes*), 168.0 ($C(CH_3)CHC(CH_3)$ *dipp* or *mes*), 199.3 ($ZnCN_2$). Due to the air sensitive nature of **3•DCC**, repeated attempts to acquire accurate CHN data were unsuccessful.



Synthesis of **3•DIC:** To a YT NMR tube was added **3** (20 mg, 0.02 mmol) and *N,N'*-diisopropylcarbodiimide (3.7 μL, 0.02 mmol) in benzene-d_6 (0.6 mL). A ^{1}H NMR spectrum was aquired after 15 minutes, showing quantitative formation of the insertion product. The solvent was reduced in vacuo and the residues were washed with *n*-hexane to yield **3•DIC** as a colorless solid. Crystals suitable for single crystal X-ray diffraction were grown from *n*-hexane at –35 °C. ^{1}H NMR (400 MHz, benzene-d_6, 298 K): 0.62 (d, 12H, $NCH(CH_3)_2$, $^3J_{HH}$ = 6.2 Hz), 1.11 (d, 12H, $CH(CH_3)_2$, $^3J_{HH}$ = 6.8 Hz), 1.14 (d, 12H, $CH(CH_3)_2$, $^3J_{HH}$ = 6.8 Hz), 1.64 (s, 6H, $C(CH_3)CHC(CH_3)^{dipp}$), 1.66 (s, 6H, $C(CH_3)CHC(CH_3)^{mes}$), 2.19 (s, 12H, *o*-CH_3^{mes}), 2.30 (s, 6H, *p*-CH_3^{mes}), 2.66 (sept, 2H, $NCH(CH_3)_2$, $^3J_{HH}$ = 6.2 Hz), 3.14 (sept, 4H, $CH(CH_3)_2$, $^3J_{HH}$ = 6.8 Hz), 4.89 (s, 1H, $C(CH_3)CHC(CH_3)^{mes}$), 4.95 (s, 1H, $C(CH_3)CHC(CH_3)^{dipp}$), 6.81 (s, 4H, CH^{mes}), 7.12 (bs, 6H, CH^{dipp}); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 298 K): 19.0 (*o*-CH_3^{mes}), 20.7 (*p*-CH_3^{mes}), 22.9 ($C(CH_3)CHC(CH_3)^{mes\ or\ dipp}$), 24.1 ($NCH(CH_3)_2$), 24.2 ($C(CH_3)CHC(CH_3)^{mes\ or\ dipp}$), 24.5 ($CH(CH_3)_2$), 26.5 ($NCH(CH_3)_2$), 28.4 ($CH(CH_3)_2$), 52.6 ($NCH(CH_3)_2$), 94.2 ($C(CH_3)CHC(CH_3)^{mes}$), 96.4 ($(CH_3)CHC(CH_3)^{dipp}$), 124.0 ($CH^{dipp}$), 125.7 ($CH^{dipp}$), 128.9 ($CH^{mes}$), 131.3 ($C^{IV}$), 131.9 ($C^{IV}$), 141.9 ($C^{IV}$), 145.1 ($C^{IV}$), 145.8 ($C^{IV}$), 167.5 ($C(CH_3)CHC(CH_3)$ *dipp* or *mes*), 168.1 ($C(CH_3)CHC(CH_3)$ *dipp* or *mes*), 200.1 ($ZnCN_2$); Anal. Calc. ($MgZnC_{59}H_{84}N_6$): C, 73.28; H, 8.76; N, 8.69. Found: C, 73.09; H, 8.81; N, 8.53.



[Mg(^{dipp}*BDI*)(^{mes}*BDI*)]

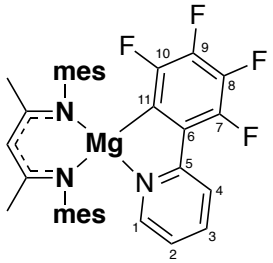
Degradation of **3** *and isolation of* [Mg(^{dipp}*BDI*)(^{mes}*BDI*)]: Compound **3** was found to be unstable at 298 K; after standing in solution overnight formation of a new asymmetric species was observed in the ^{1}H NMR and a black precipitate formed. Heating the benzene-d_6 solution at 323 K for 3 days accelerated the degradation and with full formation of the new asymmetric product. The new product was isolated by filtration and recrystallized from *n*-hexane. ^{1}H NMR (400 MHz, benzene-d_6, 283 K): 0.51 (d, 3H, $CH(CH_3)_2$, $^3J_{HH}$ = 6.8 Hz), 0.54 (d, 3H, $CH(CH_3)_2$, $^3J_{HH}$ = 6.8 Hz), 1.02 (d, 3H, $CH(CH_3)_2$, $^3J_{HH}$ = 6.8 Hz), 1.21 – 1.30 (m, 12H, $CH(CH_3)_2$), 1.31 (s, 6H, $C(CH_3)CHC(CH_3)^{mes}$ and $C(CH_3)CHC(CH_3)^{dipp}$), 1.42 (s, 3H, *o*-CH_3^{mes}), 1.50 (d, 3H, $CH(CH_3)_2$, $^3J_{HH}$ = 6.8 Hz), 1.55 (s, 3H, *o*-CH_3^{mes}), 1.70 (s, 3H, $C(CH_3)CHC(CH_3)^{mes}$), 1.72 (s, 3H, $C(CH_3)CHC(CH_3)^{dipp}$), 2.03 (s, 3H, *p*-CH_3^{mes}), 2.20 (s, 3H, *o*-CH_3^{mes}), 2.27 (s, 3H, *p*-CH_3^{mes}), 2.49 (sept, 1H, $CH(CH_3)_2$, $^3J_{HH}$ = 6.8 Hz), 2.60 (s, 3H, *o*-CH_3^{mes}), 2.65 (sept, 1H, $CH(CH_3)_2$, $^3J_{HH}$ = 6.8 Hz), 3.17 (sept, 1H, $CH(CH_3)_2$, $^3J_{HH}$ = 6.8 Hz), 3.68 (sept, 1H, $CH(CH_3)_2$, $^3J_{HH}$ = 6.8 Hz), 4.82 (s, 1H, $C(CH_3)CHC(CH_3)^{dipp}$), 4.94

(s, 1H, C(CH_3)C*H*C(CH_3)^{mes}), 6.51 (s, 1H, C*H*^{mes}), 6.59 (s, 1H, C*H*^{mes}), 6.86 (s, 1H, C*H*^{mes}), 6.99 (s, 1H, C*H*^{mes}), 7.02 (m, 1H, C*H*^{dipp}), 7.12 – 7.30 (m, 5H, C*H*^{dipp}); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 348 K): 17.8 (*o*-CH_3^{mes}), 17.9 (*o*-CH_3^{mes}), 19.2 (*o*-CH_3^{mes}), 20.5 (*o*-CH_3^{mes}), 20.7 (*p*-CH_3^{mes}), 20.8 (*p*-CH_3^{mes}), 22.6 (CH_3), 23.2 (CH_3), 23.8 (CH_3), 24.1 (CH_3), 25.2 (CH_3), 25.3 (CH_3), 25.5 (CH_3), 25.9 (CH_3), 25.9 (CH_3), 26.2 (CH_3), 27.1 (CH_3), 27.9 (*C*H(CH_3)$_2$), 28.3 (*C*H(CH_3)$_2$), 28.6 (*C*H(CH_3)$_2$), 29.4 (*C*H(CH_3)$_2$), 96.9 (C(CH_3)*C*HC(CH_3)^{dipp}), 99.3 (C(CH_3)*C*HC(CH_3)^{mes}), 123.3 (*C*H^{dipp}), 123.8 (*C*H^{dipp}), 124.1 (*C*H^{dipp}), 124.7 (*C*H^{dipp}), 125.1 (*C*H^{dipp}), 125.3 (*C*H^{dipp}), 129.1 (*C*H^{mes}), 129.3 (*C*H^{mes}), 129.5 (*C*H^{mes}), 129.8 (*C*H^{mes}), 130.7 (C^{IV}), 132.0 (C^{IV}), 132.5 (C^{IV}), 132.8 (C^{IV}), 133.4 (C^{IV}), 133.9 (C^{IV}), 142.4 (C^{IV}), 142.7 (C^{IV}), 143.7 (C^{IV}), 143.8 (C^{IV}), 145.7 (C^{IV}), 147.7 (C^{IV}), 148.0 (C^{IV}), 148.0 (C^{IV}), 169.0 (*C*(CH_3)CHC(CH_3) *dipp* or *mes*), 169.2 (*C*(CH_3)CHC(CH_3) *dipp* or *mes*), 169.7 (*C*(CH_3)CHC(CH_3) *dipp* or *mes*), 170.7 (*C*(CH_3)CHC(CH_3) *dipp* or *mes*); Anal. Calc. ($MgC_{52}H_{70}N_4$): C, 80.54; H, 9.10; N, 7.23. Found: C, 80.45; H, 9.30; N, 7.16.

2.3 C–F bond activation with M–M bimetallics

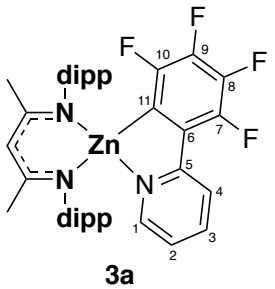
NMR scale: The M–M reagent (0.011 mmol) was dissolved in benzene-d_6 (0.6 mL) and the solution transferred into a Young's tap NMR tube equipped with a capillary tube containing a ferrocene standard solution; a t=0 ^{1}H NMR spectrum was recorded. The fluoroarene (0.11 mmol, 10 equiv.) was added using 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:



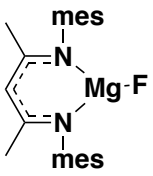
2a

Synthesis of **2a:** ^{mes}*BDI*Mg–Mg*BDI*^{mes} (**2**) (100 mg, 0.1 mmol) was dissolved in toluene (4 mL) and the fluoroarene (34.3 mg, 0.1 mmol) was added at 25 °C. After stirring the reaction mixture at this temperature for 24 h the solvent was removed *in vacuo*. The [*BDI*MgAr^{F}] was extracted into *n*-hexane (3 mL), whereas [{^{mes}*BDI*Mg}$_3$(μ-F)$_3$] remained largely insoluble. The *n*-hexane fraction was transferred to the freezer and crystals of the desired product were isolated after storage of the solution at –35 °C overnight (50 mg, 0.09 mmol, 61 %). ^{1}H NMR (400 MHz, benzene-d_6, 298 K): 1.72 (s, 6H, C(C*H*$_3$)CHC(C*H*$_3$)), 1.92 (s, 6H, *o*- or *p*-C*H*$_3$), 1.98 (s, 6H, *o*- or *p*-C*H*$_3$), 2.48 (s, 6H, *o*- or *p*-C*H*$_3$), 5.03 (s, 1H, C(CH_3)C*H*C(CH_3)), 6.36 (ddd, 1H, Py-C^2*H*), 6.60 (s, 2H, C*H*^{mes}), 6.70 (s, 2H, C*H*^{mes}), 6.75 (ddd, 1H, Py-C^3*H*), 7.49 (dm, 1H, Py-C^4*H*, $^{3}J_{HH}$ = 8.4 Hz), 8.19 (dm, 1H, Py-C^1*H*, $^{3}J_{HH}$ = 5.1 Hz); ^{19}F NMR (376.5 MHz, benzene-d_6, 298 K): -158.4 (t, 1F, *m*^{7}-C_6F_4), -151.6 – -151.4 (m, 1F, *m*^{9} or *p*-C_6F_4), -135.9 – -135.7 (m, 1F, *m*^{9} or *p*-C_6F_4), -107.7 – -107.5 (m, 1F, *o*-C_6F_4); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 298 K): 18.3 (*C*H_3), 18.7 (*C*H_3), 20.6 (*C*H_3), 23.2 (*C*H_3), 94.8 (C(CH_3)*C*HC(CH_3)), 121.8 (Py-*C*^{2}H), 124.6 (d, Py-C^4*H*, $^{4}J_{CF}$ = 22 Hz), 129.0 (*C*H), 129.8 (*C*H), 130.2 (C^{IV}), 132.0 (C^{IV}), 133.5 (C^{IV}), 140.1 (Py-*C*^{3}H), 144.9 (C^{IV}), 147.7 (Py-*C*^{1}H), 169.1 (*C*(CH_3)CH*C*(CH_3)). Due to the air sensitive nature of **2a**, repeated attempts to acquire accurate CHN data were unsuccessful.



3a

Synthesis of **3a:** ^{mes}*BDI*Mg–Zn*BDI*^{dipp} (**3**) (62 mg, 0.07 mmol) was dissolved in toluene (2 mL) and the fluoroarene (18 mg, 0.07 mmol) was added at 25 °C. After stirring the reaction mixture at this temperature for 48 h the solvent was removed *in vacuo*. The [*BDI*ZnAr^{F}] was extracted into *n*-hexane (2 mL), whereas [{^{mes}*BDI*Mg}$_3$(μ-F)$_3$] remained largely insoluble. The *n*-hexane fraction was transferred to the freezer and crystals of the desired product were isolated after storage of the solution at −35 °C overnight (30 mg, 0.04 mmol, 60 %). ^{1}H NMR (400 MHz, benzene-d_6, 298 K): 0.18 (d, 6H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 1.10 (d, 6H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 1.30 (d, 6H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 1.61 (d, 6H, CH(CH_3)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 1.73 (s, 6H, C(CH_3)CHC(CH_3)), 2.86 (sept, 2H, CH(CH$_3$)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 3.79 (sept, 2H, CH(CH$_3$)$_2$, $^{3}J_{HH}$ = 6.8 Hz), 4.89 (s, 1H, C(CH$_3$)CHC(CH$_3$)), 6.46 (ddd, 1H, Py-C^{2}H), 6.86 (m, 2H, CH^{dipp}), 6.98 (m, 3H, ArH and Py-C^{3}H), 7.14 (m, 2H, CH^{dipp}), 7.88 (dm, 1H, Py-C^{4}H, $^{3}J_{HH}$ = 8.4 Hz), 8.54 (dm, 1H, Py-C^{1}H, $^{3}J_{HH}$ = 4.2 Hz); ^{19}F NMR (376.5 MHz, benzene-d_6, 298 K): -157.4 (t, 1F, m^{7}-C$_6$F$_4$), -150.3 – -150.1 (m, 1F, m^{9} or p-C$_6$F$_4$), -138.3 – -138.1 (m, 1F, m^{9} or p-C$_6$F$_4$), -110.6 – -110.4 (m, 1F, o-C$_6$F$_4$); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 298 K): 23.6 (CH(*C*H$_3$)$_2$), 23.8 (*C*H$_3$), 23.9 ((CH$_3$)CH(*C*H$_3$)), 23.9 ((*C*H$_3$)CH(CH$_3$)), 24.3 (CH(*C*H$_3$)$_2$), 24. 8 (CH(*C*H$_3$)$_2$), 27.9 (*C*H(CH$_3$)$_2$), 29.3 (*C*H(CH$_3$)$_2$), 94.3 (C(CH$_3$)*C*HC(CH$_3$)), 122.8 (Py-*C*^{2}H), 123.6 (*C*H), 123.9 (d, Py-C^{4}H, $^{4}J_{CF}$ = 20 Hz) 123.9 (*C*H), 125.8 (*C*H), 139.6 (Py-C^{3}H), 142.2 (C^{IV}), 142.4 (C^{IV}), 145.5 (C^{IV}), 148.2 (Py-*C*^{1}H), 168.3 (*C*(CH$_3$)CH*C*(CH$_3$)); Anal. Calc. (ZnC$_{40}$H$_{45}$F$_4$N$_3$): C, 67.74; H, 6.40; N, 5.93. Found: C, 67.79; H, 6.39; N, 5.61.



[{^{mes}*BDI*Mg}$_3$(μ-F)$_3$] **(2b)**

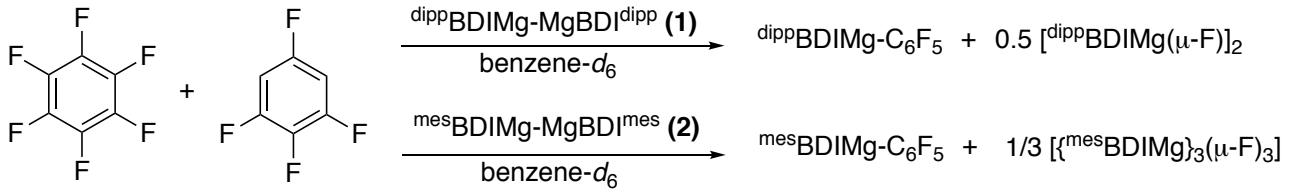
Characterisation of Mg–F by-product [{^{mes}BDIMg}$_3$(μ-F)$_3$]: ^{1}H NMR (400 MHz, benzene-d_6, 298 K): 1.53 (s, 6H, C(CH_3)CHC(CH_3)), 1.89 (s, 12H, *o*-CH_3), 2.31 (s, 6H, *p*-CH_3), 4.88 (s, 1H, C(CH$_3$)CHC(CH$_3$)), 6.79 (s, 4H, *m*-CH); ^{19}F NMR (376.5 MHz, benzene-d_6, 298 K): - 203.5 (s, Mg-F); ^{13}C{^{1}H} NMR (100 MHz, benzene-d_6, 298 K): 18.1 (*C*H$_3$), 20.8 (*C*H$_3$), 23.0 (*C*H$_3$), 94.9 (C(CH$_3$)*C*HC(CH$_3$)), 129.2 (*C*H), 131.5 (C^{IV}), 132.1 (C^{IV}), 145.8 (C^{IV}), 168.4 (*C*(CH$_3$)CH*C*(CH$_3$)).

2.4 Competition reactions

Competition reactions were conducted between compounds **1**, **2** and **3** using a ten-fold excess of the respective metal complexes to fluorocarbon. Competition reactions were also conducted between the fluorinated substrates hexafluorobenzene and 1,2,3,5-tetrafluorobenzene using compounds **1** and **2**; a ten-fold excess of the fluorocarbons was used.

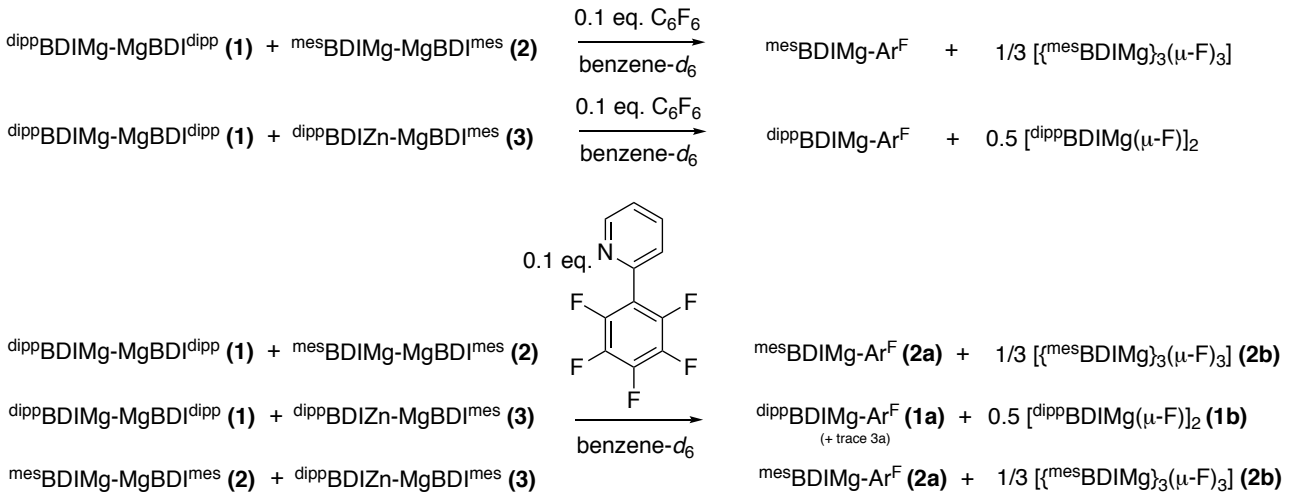
General procedure for competition reactions between fluoroarene substrates: The metal complex (**1** or **2**, 0.011 mmol) was dissolved in 0.5 mL of benzene-d_6 and added to a Young's tap NMR tube. A solution of hexafluorobenzene (11.2 μL, 0.11 mmol) and 1,2,3,5-tetrafluorobenzene (12.1 μL, 0.11 mmol) in 0.1 mL of benzene-d_6 was added and a ^{19}F NMR was immediately recorded. The products were compared against previously synthesised samples.

Figure S1. C–F the activation competition reactions between hexafluorobenzene and 1,2,3,5-tetrafluorobenzene using **1** and **2**.



General procedure for competition reactions between M-M complexes: Compound **1** (10 mg, 0.011 mmol) and compound **2** (8.1 mg, 0.011 mmol) were dissolved in 0.5 mL of benzene-d_6 and added to a Young's tap NMR tube. A 11.3 mM stock solution of the fluorocarbon (0.1 mL, 0.0011 mmol) in benzene-d_6 was added to the solution and a ^{19}F NMR spectrum was immediately recorded.

Figure S2. Competition reactions between **1**, **2** and **3** in the *C–F* the activation of hexafluorobenzene and 2-(2,3,4,5,6-pentafluorophenyl)-pyridine.



3. Kinetic Analysis

3.1 Eyring analysis

Kinetic analysis was conducted using compound **1** at 8.2 mM concentration in toluene-d_8 over a range of temperatures (258, 268, 278 and 288 K). The Young's tap NMR tube was equipped with a capillary tube containing a ferrocene standard solution; a t=0 ^{1}H NMR spectrum was recorded to ensure that the overall concentration of substrate remained consistent throughout the reaction. A ten-fold excess of hexafluorobenzene was added to the Young's tap NMR tube at temperature (−35 °C), and the reaction was maintained at low temperature until inserted to the NMR spectrometer. It is of note that no reaction was observed at −35 °C when monitors for 2 hours. ^{1}H NMR spectra were recorded at regular intervals throughout the reaction, and the data was processed using MNova software.

Figure S3. Plot of ln[**1**] versus time for the reaction of **1** with C_6F_6 at 258 K (blue), 286 K (orange), 278 K (grey) and 288 K (yellow).

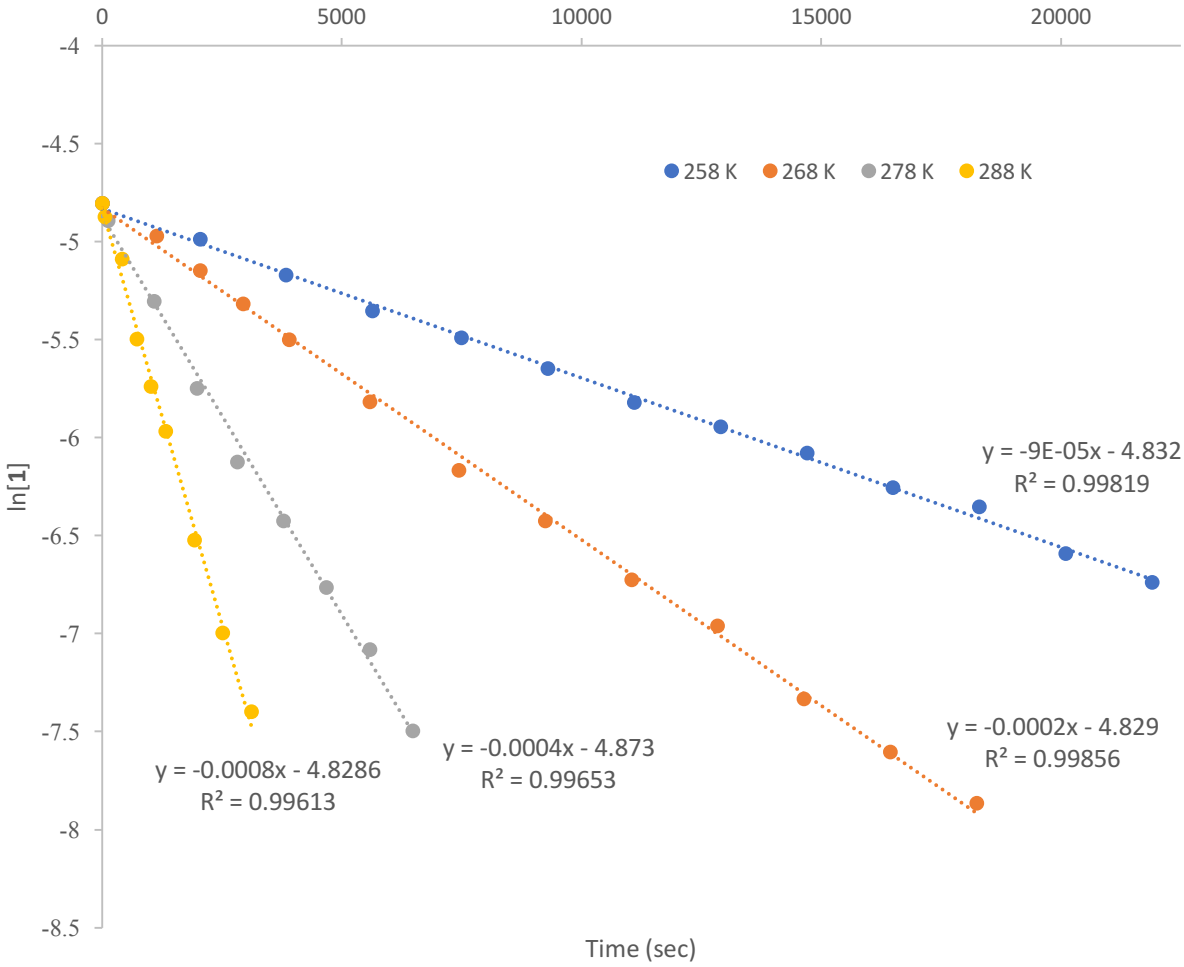
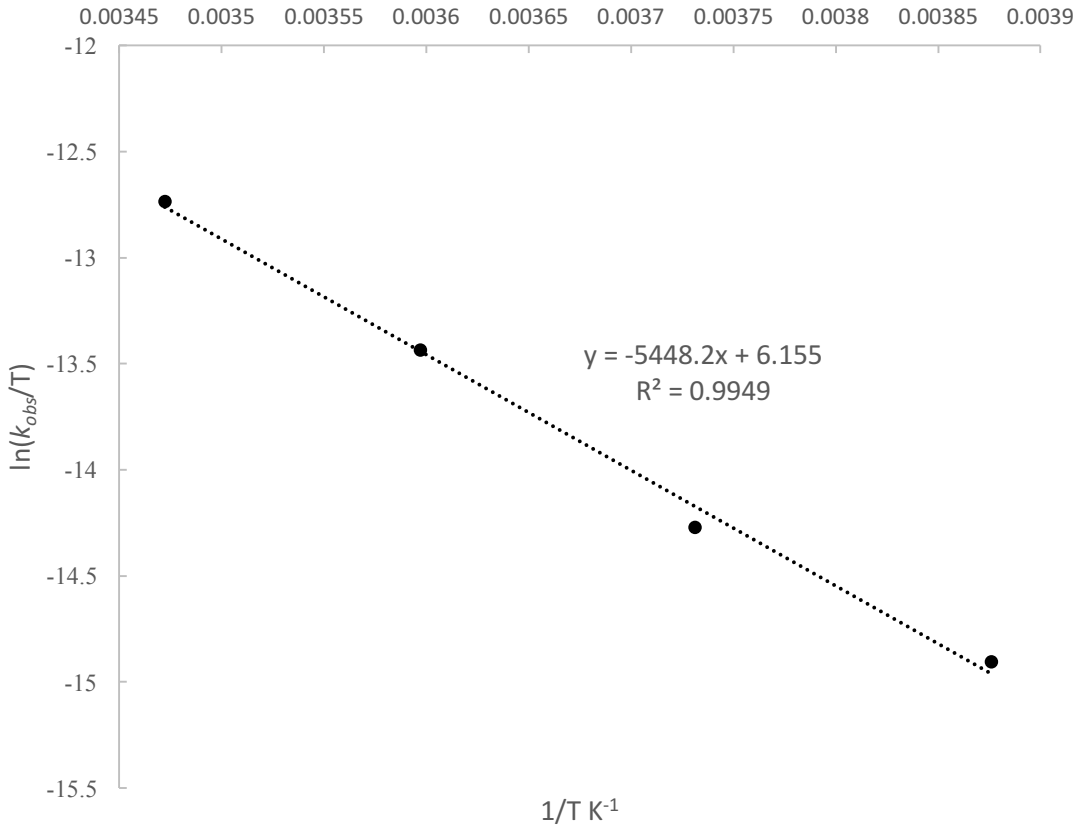


Figure S4. Eyring analysis: ln{k_{obs}/T} versus 1/T.



$\Delta H^{\ddagger}$ = 10.8 kcal mol^{-1}, $\Delta S^{\ddagger}$ = –35.0 cal K^{-1} mol^{-1}, $\Delta G^{\ddagger}_{298K}$ = 21.3 kcal mol^{-1}

3.2 Effect of the *para* substituent of fluoroarenes on the relative rate of reaction

Kinetic analysis was conducted using compound **1** at 8.2 mM concentration in toluene-d_8 at temperatures 288 K using the procedure described in section 3.1 the fluoroarene was varied and the pseudo-first order rate constant measured. The data are presented in Table S1.

Table S1. Relative rates of reaction of **1** with fluoroarenes

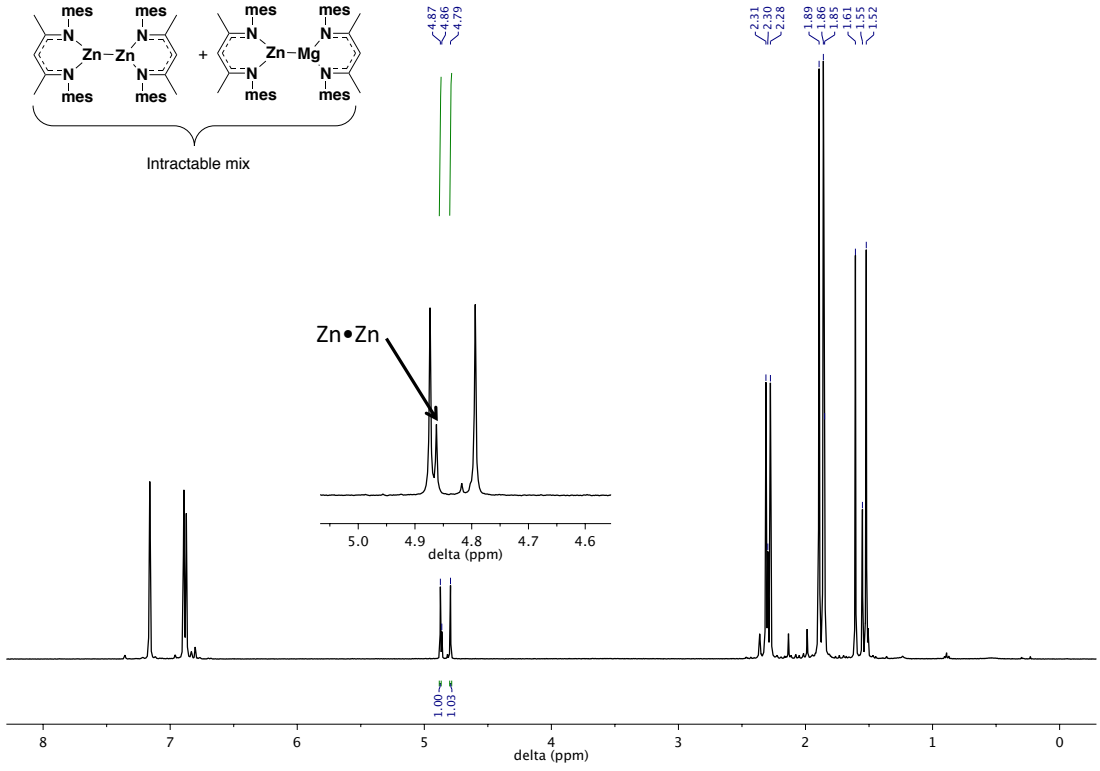
Substrate	σ_p	k_{obs} (s^{-1} x 10^{-3})	Relative Rate
p-$C_6F_5CH_3$	**–0.17**	**0.06**	**0.1**
C_6F_6	**0.06**	**0.85**	**1**
C_6F_5–C_6F_5	**0.27**	**0.16**	**0.2**
p-$C_6F_5CF_3$	**0.54**	**1.8**	**2.2**

4. Supporting Figures

Further reactivity of compound 3 and synthesis of ^{mes}*BDI*Mg–Zn*BDI*^{mes}: Compound **3**, ^{mes}*BDI*Mg–Zn*BDI*^{dipp}, does not undergo further reaction with [^{dipp}*BDI*ZnI], and the known compound ^{dipp}*BDI*Zn–Zn*BDI*^{dipp} was not observed. This is in contrast to the stoichiometric reduction of [^{mes}*BDI*ZnI] using ^{mes}*BDI*Mg–Mg*BDI*^{mes} (**2**), which resulted in the formation of a new asymmetic species ^{mes}*BDI*Mg–Zn*BDI*^{mes} along with ^{mes}*BDI*Zn–Zn*BDI*^{mes}, presumably formed by ^{mes}*BDI*Mg–Zn*BDI*^{mes} premoting the further reduction of unreacted [^{mes}*BDI*ZnI].[6] It was not possible to seperate the two products, which co-crystalise with one another, inhibiting full characterisation. However, the clear formation of a new asymmetric product is observed in the ^{1}H NMR spectrum, with the β-diketiminate ligand occupying two different coordination environments (product observed in the presence of ^{mes}*BDI*Zn–Zn*BDI*^{mes}, Figure S5). Crystals suitable for single crystal X-ray diffraction were grown from a toluene/*n*-hexane solution at –35 °C (Figure S26).

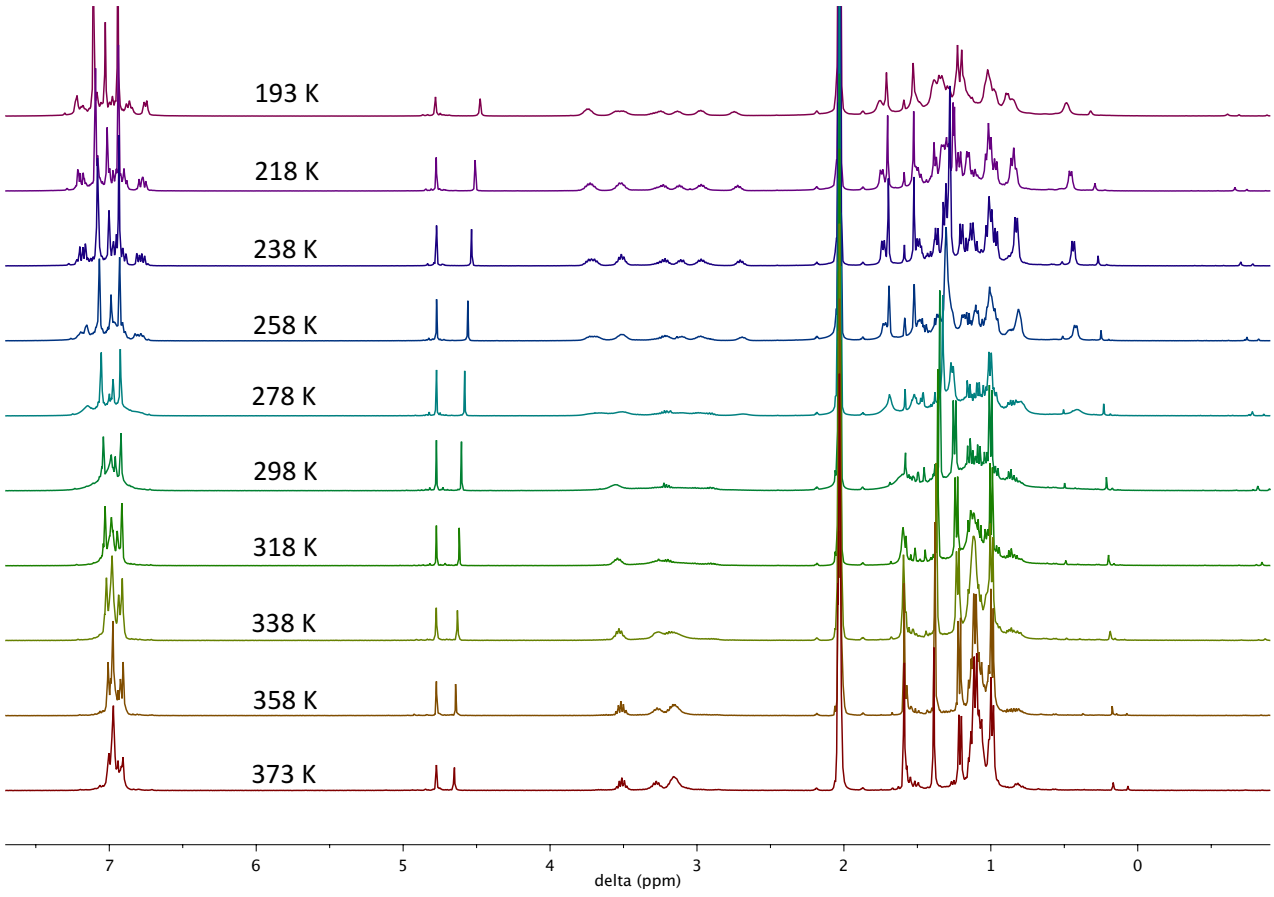
Synthesis of **^{mes}*BDI*Mg–Zn*BDI*^{mes}:** To a scintillation vial was added ^{mes}*BDI*Mg–Mg*BDI*^{mes} (**2**, 50 mg, 0.07 mmol) and [^{dipp}*BDI*ZnI] (73.5 mg, 0.14 mmol) in toluene (5 mL) and the reaction was stirred at 298 K overnight. The residual black precipitate and [^{mes}*BDI*MgI] were removed by filtration, and the supernatant was reduced *in vacuo*. The crude product was recrystallised from *n*-hexane at -35 °C, yielding clear crystals. ^{1}H NMR analysis revealed the presence of a new heterobimetallic species, in addition to ^{mes}*BDI*Zn–Zn*BDI*^{mes}. The novel heterobimetallic species could be enriched by fractional recrystallistion (~80% purity, Figure S5). ^{1}H NMR (400 MHz, benzene-d_6, 298 K): 1.52 (s, 6H, CH_3), 1.61 (s, 6H, CH_3), 1.86 (s, 12H, CH_3), 1.89 (s, 12H, CH_3), 2.28 (s, 6H, CH_3), 2.31 (s, 6H, CH_3), 4.79 (s, 1H, C(CH$_3$)C*H*C(CH$_3$)), 4.87 (s, 1H, C(CH$_3$)C*H*C(CH$_3$)), 6.87 (s, 4H, C*H*), 6.89 (s, 4H, C*H*).

Figure S5. ^{1}H NMR of **Mg•Zn**, in the presence of **Zn•Zn** in benzene-d_6.



NMR spectra discussion of compounds 6 and 7: Variable temperature ^{1}H NMR spectra of **6** in toluene-d_8 shows a fast-exchange regime above 358 K, and slow-exchange regime at temperatures lower than 258 K. Below the coalescence temperature the resonances of the isopropyl groups are chemically and magnetic inequivalent. Conversely, compound **7** has a well-defined ^{1}H NMR spectrum at 298 K. Both the CH_2 and CH_3 of the ethyl group of **7** resonate as overlapping signals at $\delta \approx -0.3$ ppm (Figure S47). Analysis of the single crystal X-ray structure (Figures 7 and S25) shows that the CH_3 group sits in between two of the phenyl rings of the β-diketiminate ligands, shielding the protons and resulting in a more up-field resonance in the ^{1}H NMR spectrum than expected.

Figure S6. Variable temperature ^{1}H NMR of compound **6** in toluene-d_8.



C–F activation of C_6F_6 using 2: Evidence for the C–F bond activation is clear but isolation and separation of the reaction products was hindered by the complex Schlenk equilibria which persisted even in the presence of a strongly coordinating co-ligand such as pyridine.

Figure S7. ^{1}H NMR of the reaction of **2** with C_6F_6 (bottom). Addition of pyridine (top) in benzene-d_6.

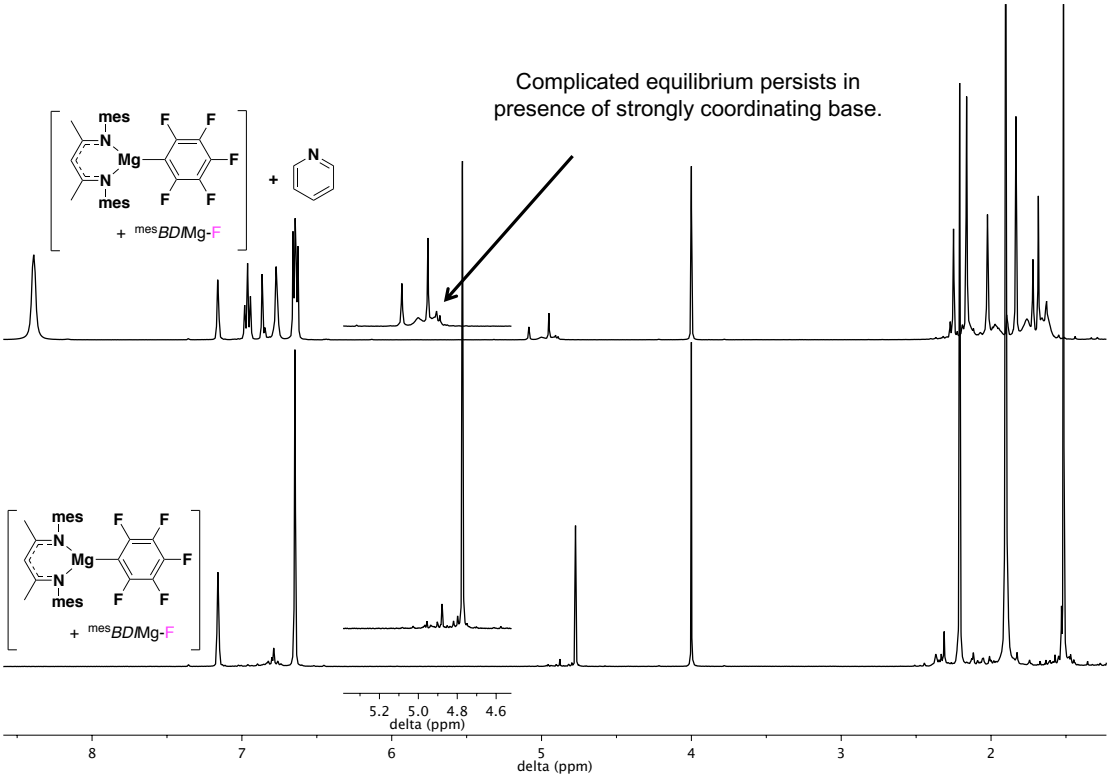
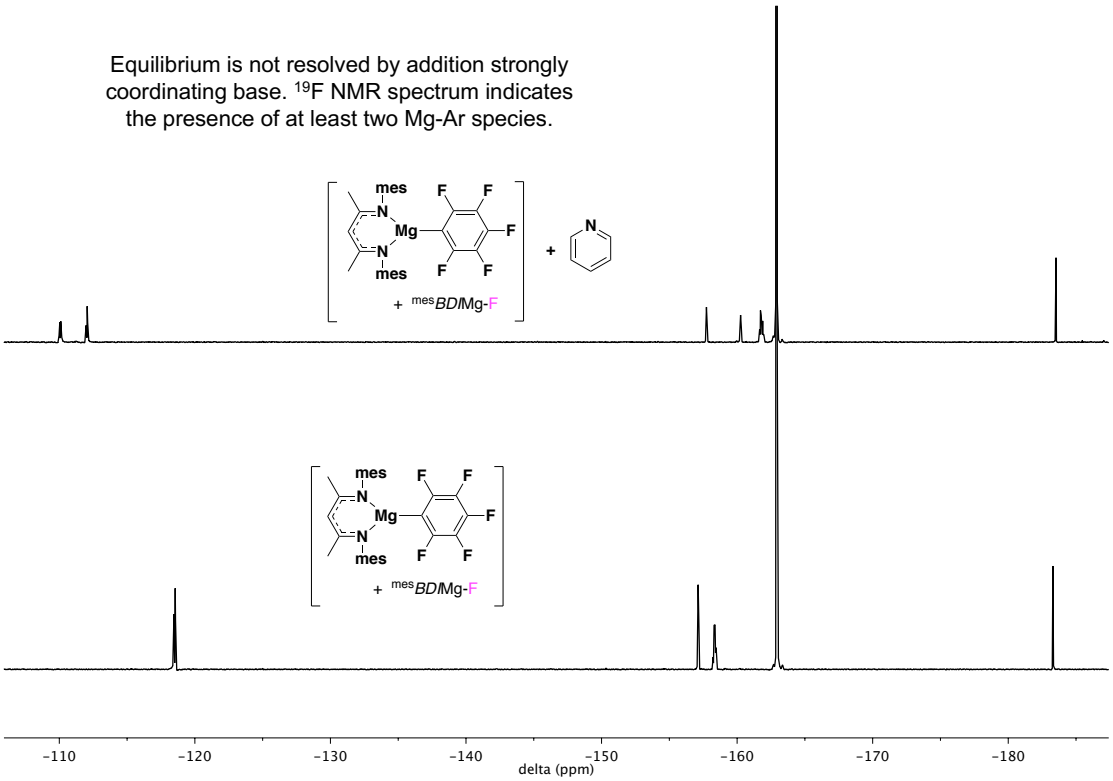


Figure S8. ^{19}F NMR of the reaction of **2** with C_6F_6 (bottom). Addition of pyridine (top) in benzene-d_6.



***C–F* activation of 1,2,3,5-tetrafluorobenzen using 2:** Compound **2** appears to be more reactive toward fluoroarenes. The reaction with 1,2,3,5-tetrafluorobenzene occurs significantly faster (hours versus days) than with **1** and results in only one regioisomeric product.

Figure S9. ^{1}H NMR of the reaction of **2** with 1,2,3,5-tetrafluorobenzene in benzene-d_6.

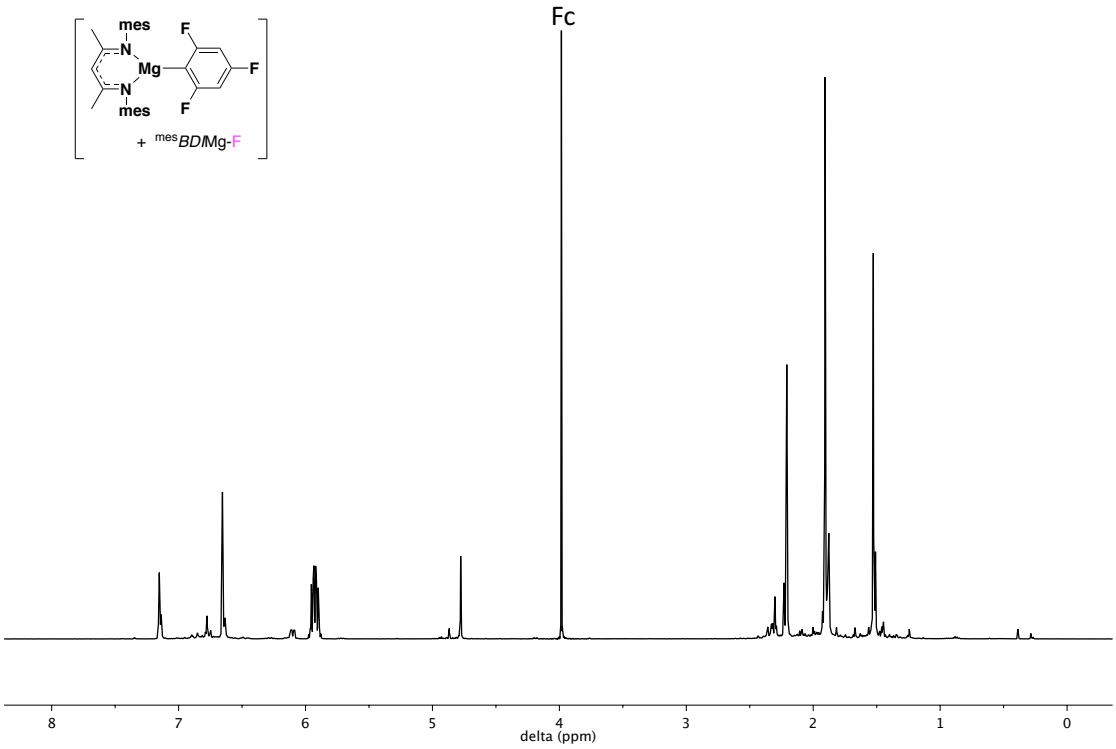
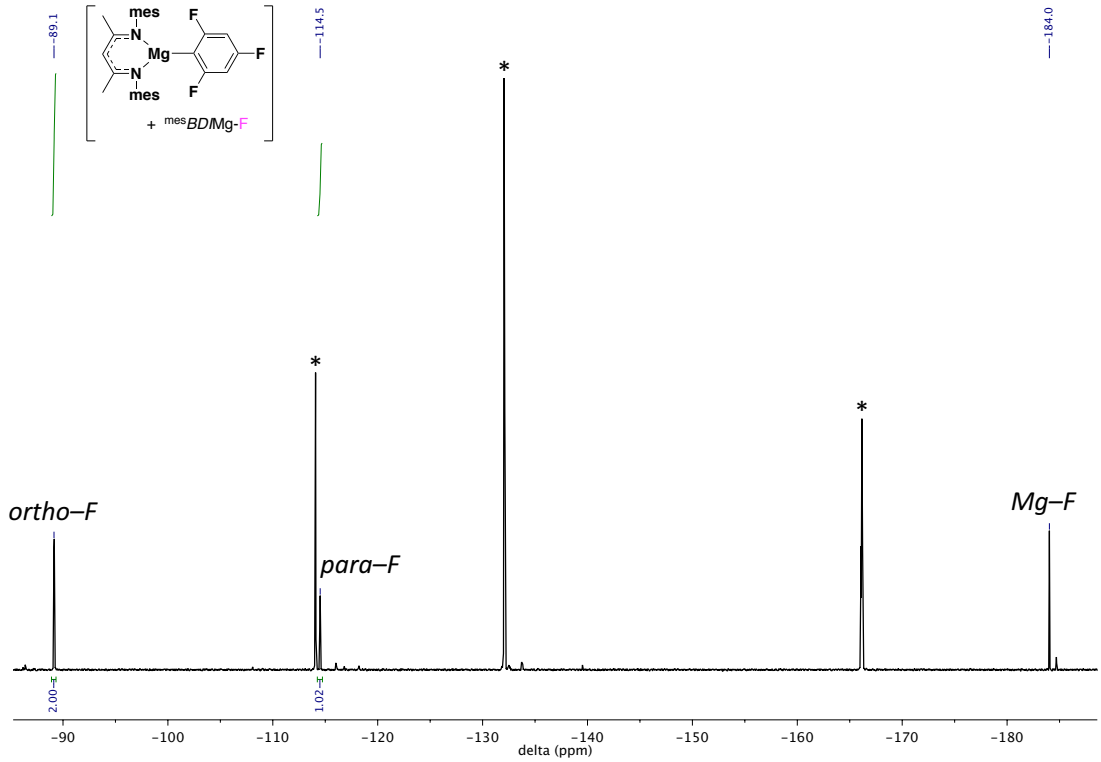


Figure S10. ^{19}F NMR of the reaction of **2** with excess 1,2,3,5-tetrafluorobenzene (asterisks) in benzene-d_6.



***C–F* activation of C_6F_6 using 3:** Whilst compound **3** reacts slowly with C_6F_6 over several days, the reaction is competitive with decomposition of the Mg–Zn reagent. The organozinc product [^{dipp}*BDI*Zn(C_6F_5)] is a known species.[7]

Figure S11. ^{1}H NMR of the reaction of **3** with C_6F_6 (bottom); degradation product of **3** (top) in benzene-d_6.

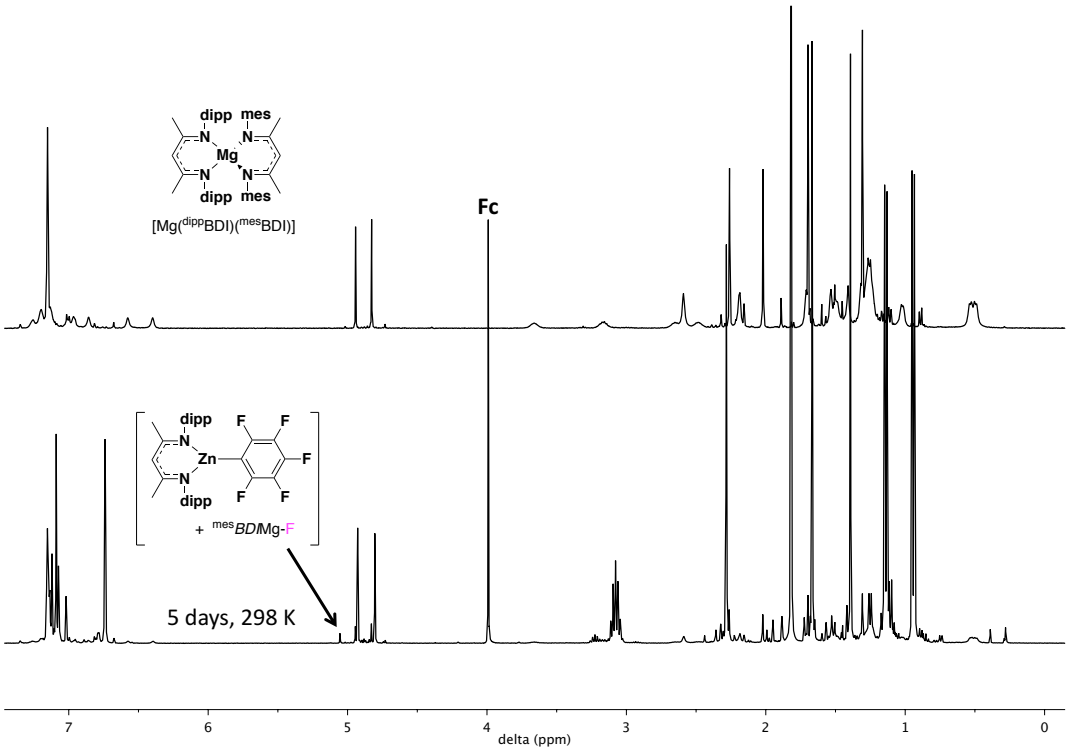
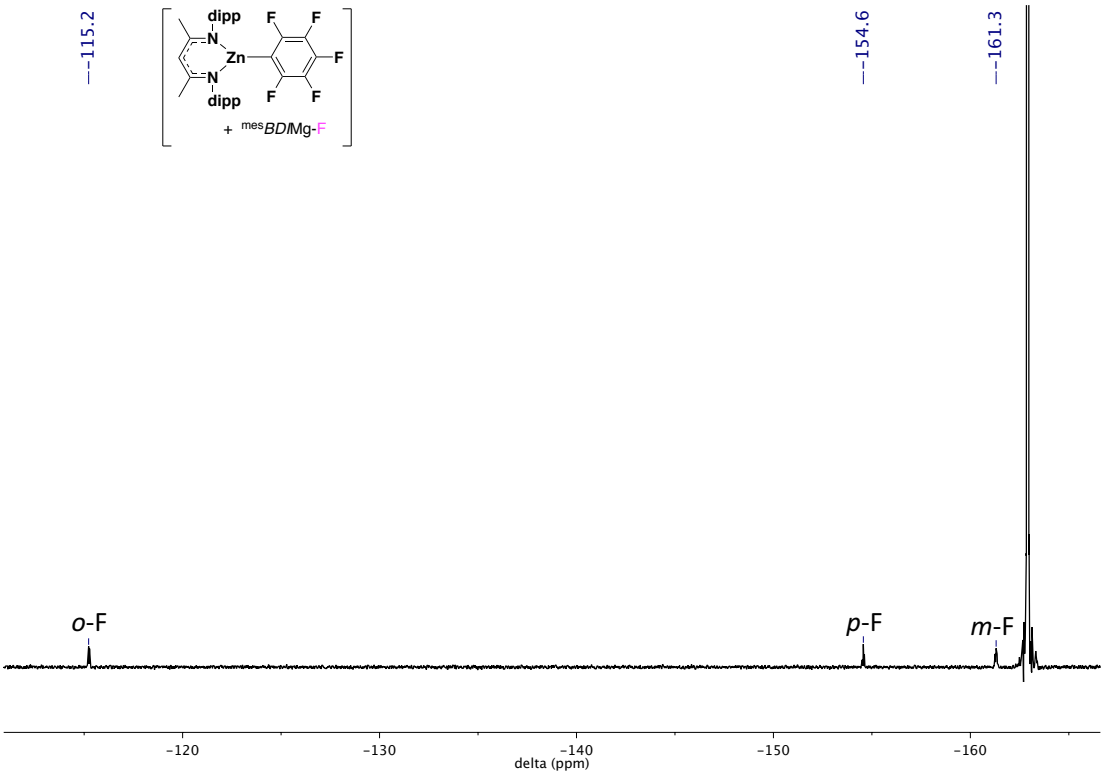
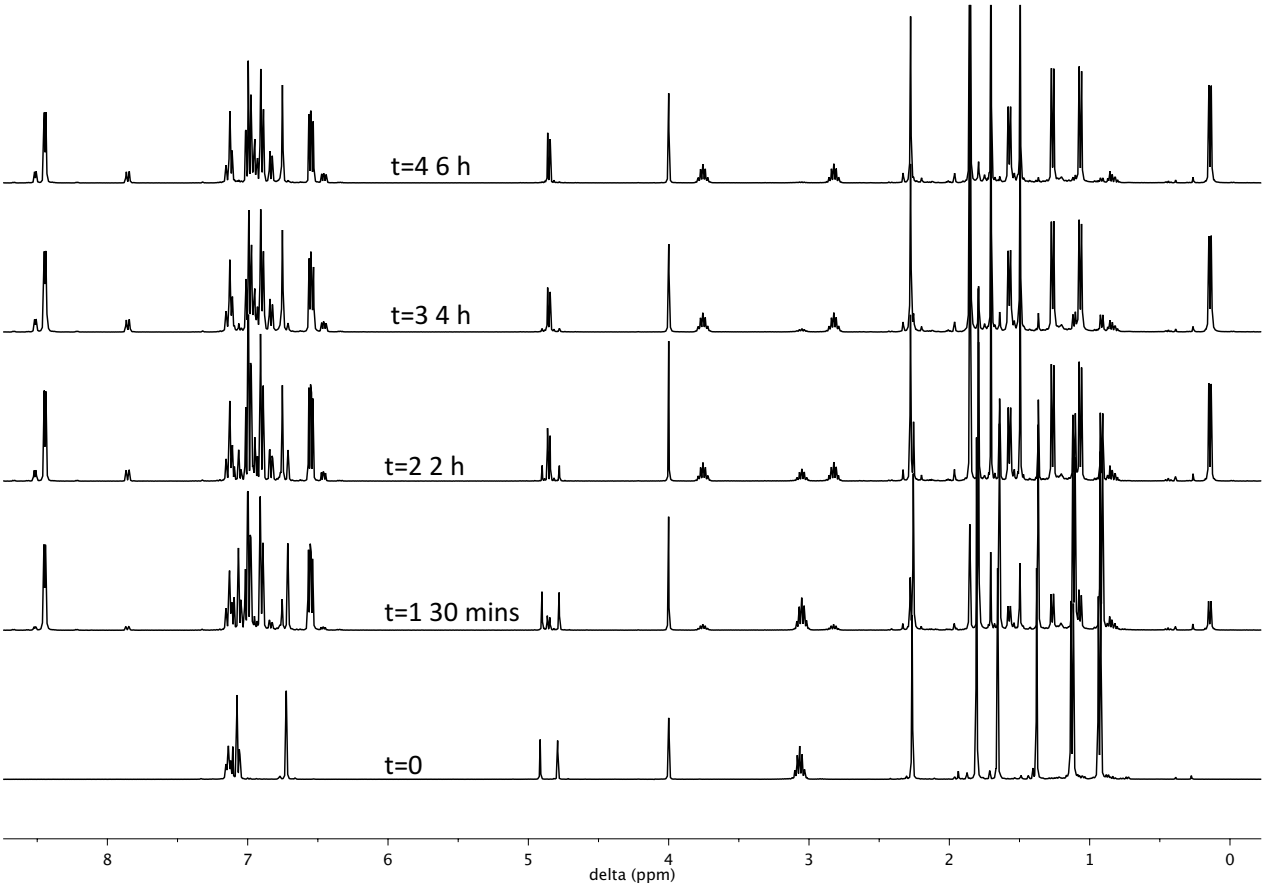


Figure S12. ^{19}F NMR of the reaction of **3** with C_6F_6.



***C–F* activation of 2-Py-C_6F_5 using 3:** Compound **3** reacts cleanly with 2-Py-C_6F_5 to form **3a** and [{^{mes}*BDI*Mg}$_3$(μ-F)$_3$], with no evidence for the formation of the degradation product [Mg(^{dipp}*BDI*)(^{mes}*BDI*)].

Figure S13. ^{1}H NMR stack plot showing the reaction of **3** with 2-Py-C_6F_5 in benzene-d_6.



5. X-ray Crystallographic Data

The X-ray crystal structure of 2a

The crystal structure of **2a**, which was refined as a two-component inversion twin [Flack parameter x = +0.38(6)], was found to contain two independent molecules, **2a-A** and **2a-B**, in the asymmetric unit.

The C6-based mesityl group in molecule **2a-B** was found to be disordered. Two orientations were identified of *ca*. 78 and 22% occupancy, their geometries 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 2a-hexane

The asymmetric unit for the crystal structure of the hexane solvate **2a-hexane** was found to contain two independent molecules, **2a-hexane-A** and **2a-hexane-B**, as well as a hexane molecule disordered across a centre of symmetry (and so of only 50% occupancy in the asymmetric unit). Two orientations were identified of *ca*. 30 and 20% occupancy (with two further orientations of the same occupancies being generated by operation of the adjacent centre of symmetry), their geometries were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and all of the atoms were refined isotropically.

The X-ray crystal structure of 2b

The crystal of **2b** that was studied was found to be a two-component twin in a *ca*. 56:44 ratio, with the two lattices related by the approximate twin law [0.01 –0.99 0.03 –1.01 –0.01 –0.03 0.00 0.00 –1.00]. The C101-based included hexane solvent molecule was found to be disordered. Two orientations were identified of *ca*. 55 and 45% occupancy, their geometries 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 3

Both the toluene and hexane included solvent molecules in the structure of **3** were found to be disordered over independent centres of symmetry. In both cases one unique 50% occupancy orientation was identified, (with a second 50% occupancy orientation being generated in each case by operation of the adjacent centre of symmetry), its geometry optimised, and all of the non-hydrogen atoms were refined anisotropically.

The X-ray crystal structure of 3·THF

The C24-based isopropyl group in the structure of **3·THF** 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 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 3·DIC

The structure of **3·DIC** was found to sit across a C_2 axis that passes through C2, Zn1, C42, Mg1 and C22.

The X-ray crystal structure of 3a

Both the toluene and hexane included solvent molecules in the structure of **3a** were found to be disordered over independent centres of symmetry. Two unique orientations of *ca*. 30 and 20% occupancy were identified for both solvent molecules, with two further orientations of the same occupancies being generated in each case by operation of the adjacent centre of symmetry. The geometries of each pair of orientations were optimised, the thermal parameters of adjacent atoms were restrained to be similar, and all of the atoms were refined isotropically.

The X-ray crystal structure of 4

The structure of **4** was found to sit on a centre of symmetry at the Zn2 site.

The X-ray crystal structure of 6

The included solvent in the structure of **6** was found to be highly disordered, and the best approach to handling this diffuse electron density was found to be the SQUEEZE routine of PLATON.[8] This suggested a total of 498 electrons per unit cell, equivalent to 62.3 electrons per asymmetric unit. Before the use of SQUEEZE the solvent clearly resembled dichloromethane (CH_2Cl_2, 42 electrons), and 1.5 dichloromethane molecules corresponds to 63 electrons, so this was used as the solvent present. As a result, the atom list for the asymmetric unit is low by 1.5(CH_2Cl_2) = $C_{1.5}H_3Cl_3$ (and that for the unit cell low by $C_{12}H_{24}Cl_{24}$) compared to what is actually presumed to be present.

The X-ray crystal structure of 7

The absolute structure of **7** was determined by use of the Flack parameter [x = –0.036(16)].

The X-ray crystal structure of ^{mes}*BDI*Mg-Zn*BDI*^{mes}

The structure of ^{mes}***BDI*Mg-Zn*BDI*^{mes}** was found to sit across a C_2 axis that passes through the middle of the metal–metal bond and bisects the N1···N1A and N3···N3A vectors. As a consequence the metal site is inherently disordered between magnesium and zinc, and when refined the occupancy ratio settled at *ca*. 53:47 Mg:Zn; for simplicity (and to match what the compound was expected to be) the ratio was set to exactly 50:50. Both metal atoms were refined anisotropically.

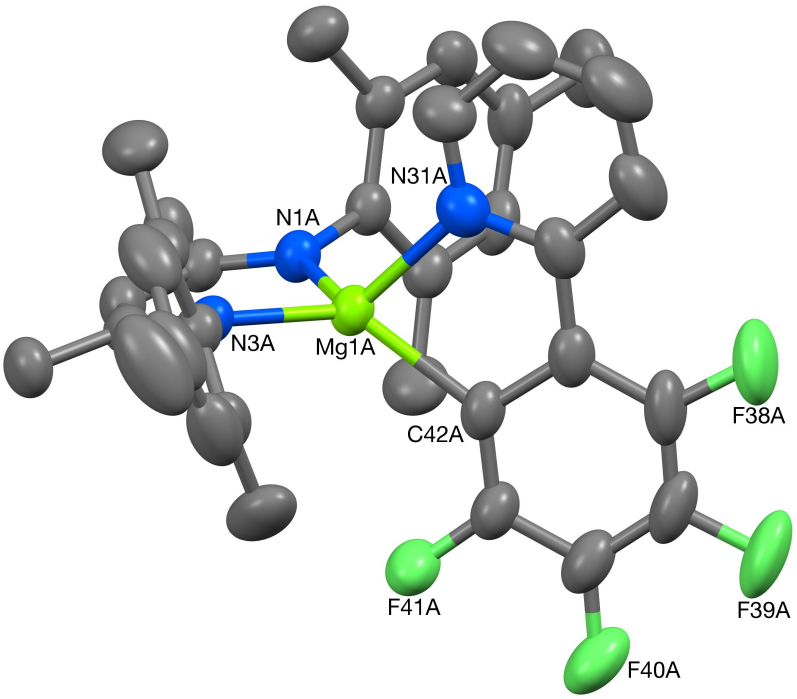


Figure S14. The crystal structure of one (**2a-A**) of the two independent complexes present in the crystal of **2a** (50% probability ellipsoids).

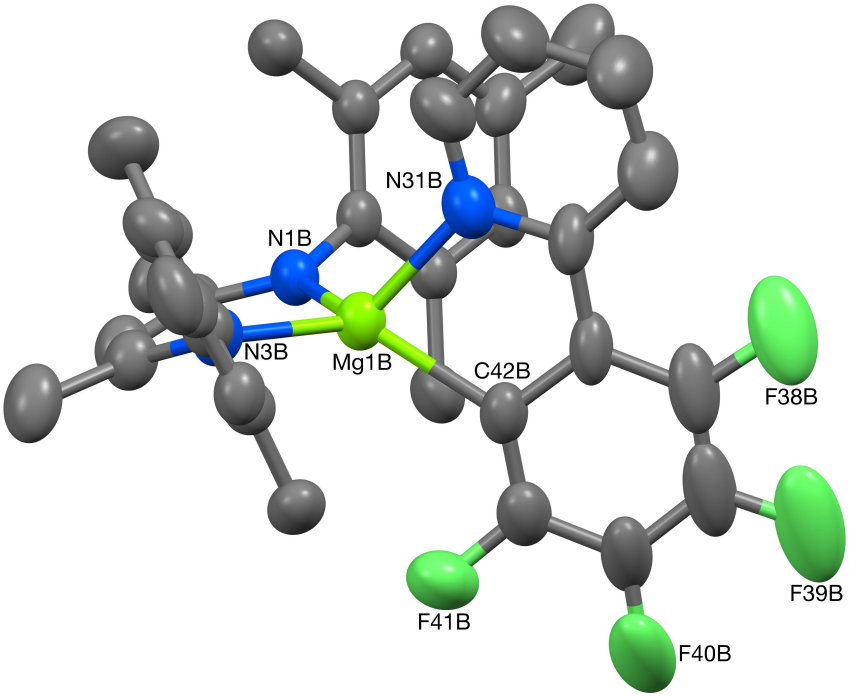


Figure S15. The crystal structure of one (**2a-B**) of the two independent complexes present in the crystal of **2a** (50% probability ellipsoids).

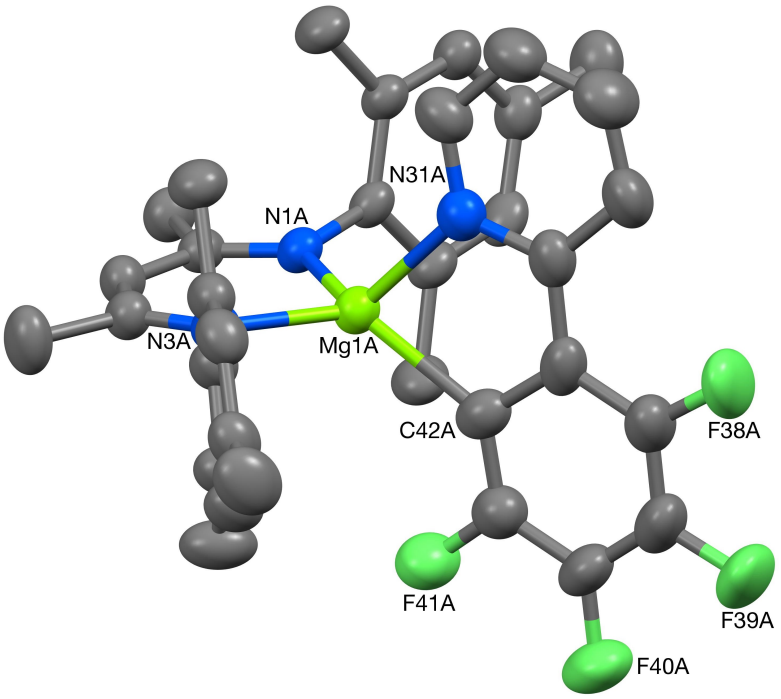


Figure S16. The crystal structure of one (**2a-hexane-A**) of the two independent complexes present in the crystal of **2a-hexane** (50% probability ellipsoids).

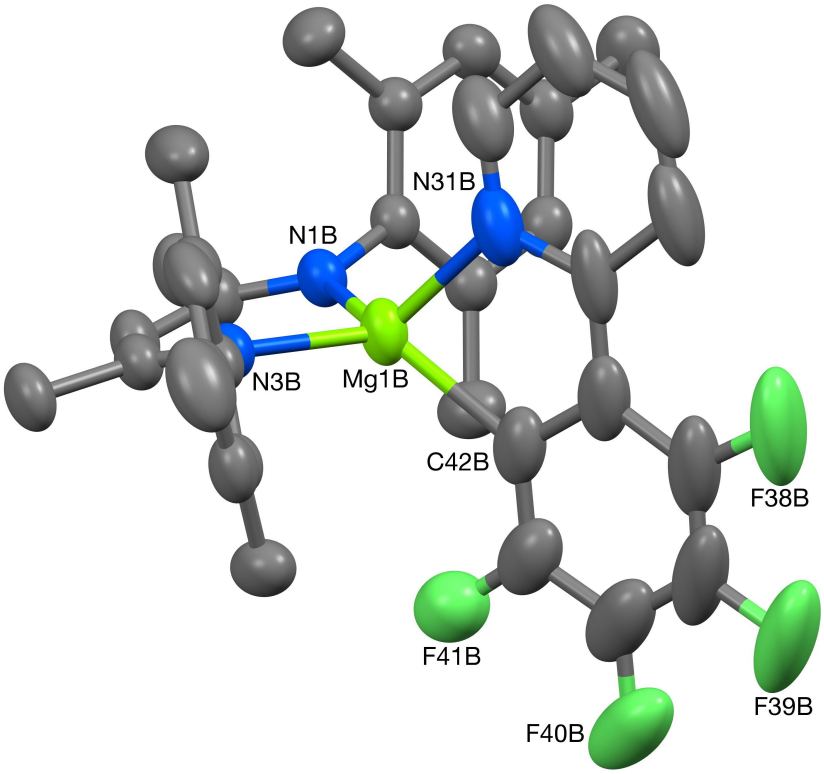


Figure S17. The crystal structure of one (**2a-hexane-B**) of the two independent complexes present in the crystal of **2a-hexane** (50% probability ellipsoids).

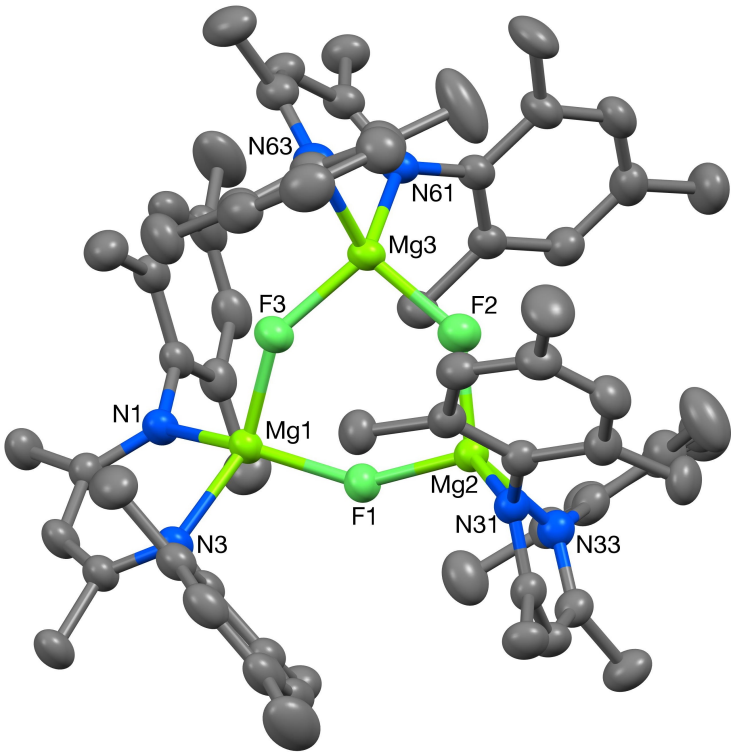


Figure S18. The crystal structure of **2b** (50% probability ellipsoids).

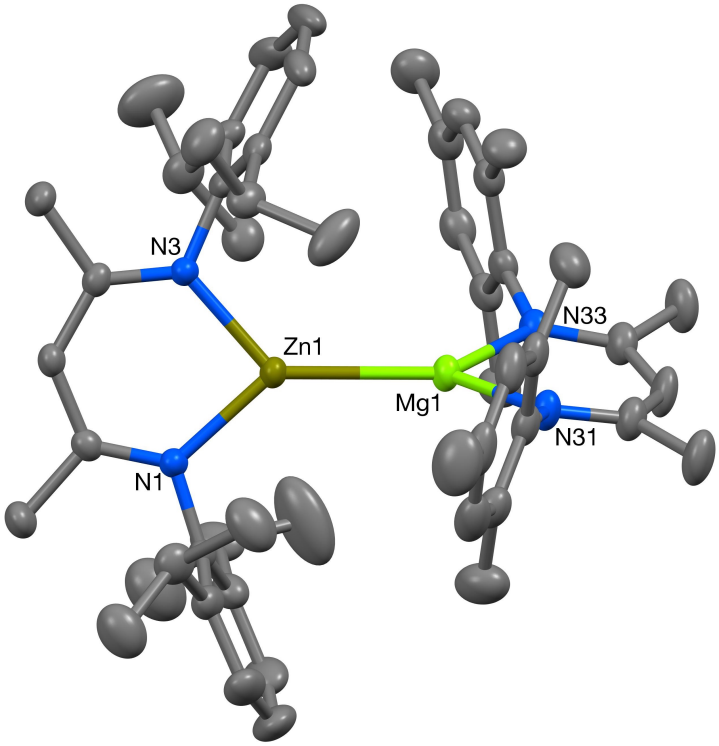


Figure S19. The crystal structure of **3** (50% probability ellipsoids).

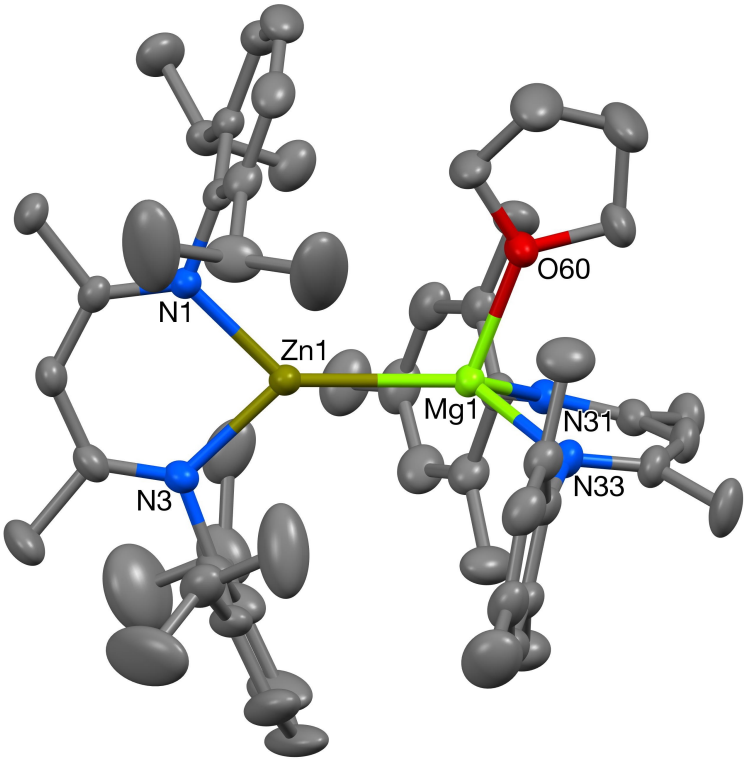


Figure S20. The crystal structure of **3·THF** (50% probability ellipsoids).

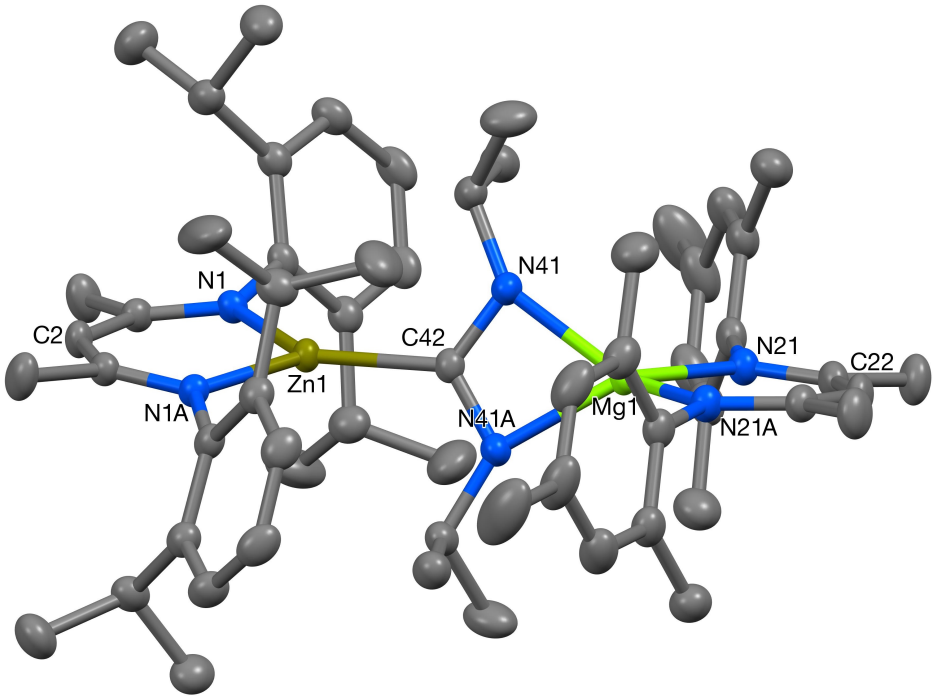


Figure S21. The crystal structure of the C_2-symmetric complex **3·DIC** (50% probability ellipsoids). The C_2 axis passes through C2, Zn1, C42, Mg1 and C22.

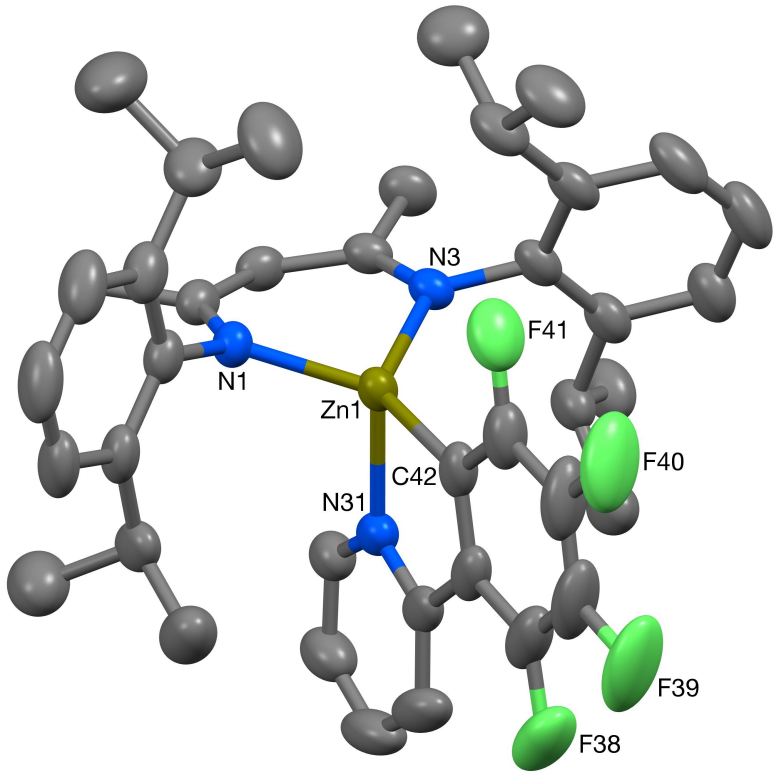


Figure S22. The crystal structure of **3a** (50% probability ellipsoids).

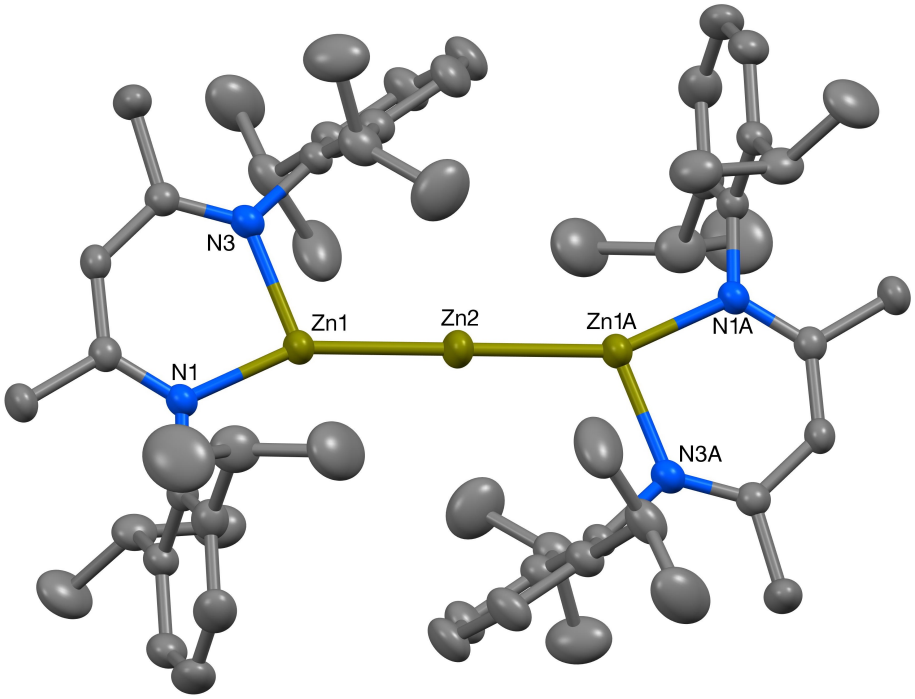


Figure S23. The crystal structure of the C_i-symmetric complex **4** (50% probability ellipsoids).

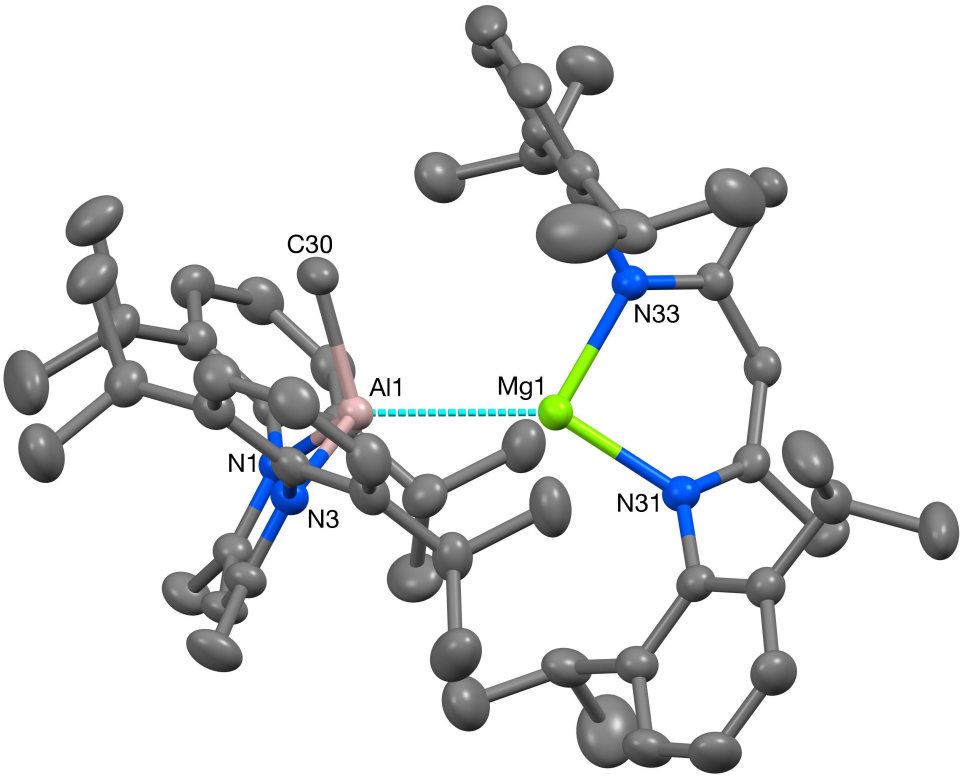


Figure S24. The crystal structure of **6** (50% probability ellipsoids).

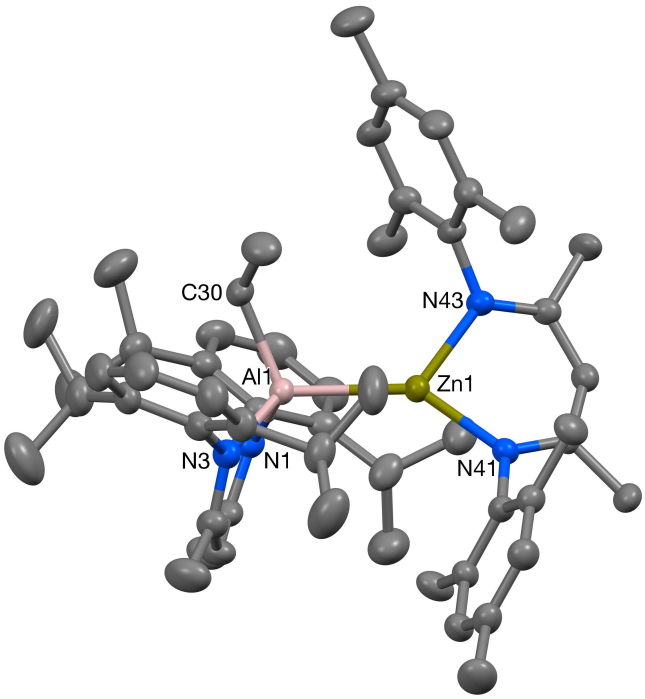


Figure S25. The crystal structure of **7** (50% probability ellipsoids).

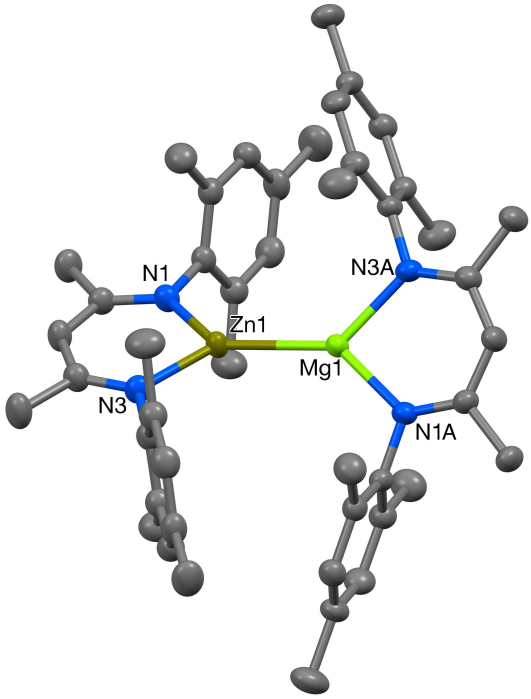


Figure S26. The crystal structure of ^{mes}***BDI***Mg–Zn***BDI***^{mes} (50% probability ellipsoids). The complex is disordered about a C_2 axis that passes through the middle of the metal–metal bond and bisects the N1···N1A and N3···N3A vectors.

Table S2. Crystal Data, Data Collection and Refinement Parameters for the structures of **2a**, **2a-hexane**, **2b**, **3**, **3·THF**, **3·DIC**, **3a**, **4**, **6**, **7** and ^{mes}***BDI***Mg–Zn***BDI***^{mes}.

data	2a	2a-hexane	2b	3
formula	$C_{34}H_{33}F_4MgN_3$	$C_{34}H_{33}F_4MgN_3$	$C_{69}H_{87}F_3Mg_3N_6$	$C_{52}H_{70}MgN_4Zn$
solvent	—	$0.25(C_6H_{14})$	$2(C_6H_{14})$	$0.5(C_7H_8)\cdot 0.5(C_6H_{14})$
formula weight	583.94	605.48	1302.71	929.95
colour, habit	colourless	pale yellow	colourless	colourless blocks
temperature / K	173	173	173	173
crystal system	orthorhombic	triclinic	triclinic	triclinic
space group	*Pca*2$_1$ (no. 29)	*P*-1 (no. 2)	*P*-1 (no. 2)	*P*-1 (no. 2)
***a* / Å**	24.8934(3)	11.8799(7)	14.5708(8)	11.7887(7)
***b* / Å**	13.45834(18)	16.0457(8)	14.6964(8)	12.0703(6)
***c* / Å**	18.5282(3)	17.2413(8)	18.2421(7)	21.6822(7)
α / deg	90	83.738(4)	91.379(4)	80.152(3)
β / deg	90	85.661(4)	93.348(4)	74.593(4)
γ / deg	90	88.935(4)	91.651(4)	66.945(5)
***V* / Å^3**	6207.38(14)	3257.4(3)	3896.7(3)	2729.0(3)
Z	8 [b]	4 [b]	2	2
***D*$_c$ / g cm^{-3}**	1.250	1.235	1.110	1.132
radiation used	Cu-Kα	Cu-Kα	Cu-Kα	Mo-Kα
μ / mm^{-1}	0.928	0.901	0.755	0.500
2θ max / deg	148	148	149	56
no. of unique reflns				
measured (*R*$_{int}$)	8638 (0.0309)	12455 (0.0397)	26000 (0.0452)	10726 (0.0208)
obs, $\|F_o\| > 4\sigma(\|F_o\|)$	7633	7949	15998	8567
no. of variables	790	822	890	647
***R*$_1$(obs), *wR*$_2$(all)** [a]	0.0414, 0.1073	0.0640, 0.2005	0.0490, 0.1262	0.0460, 0.1071

[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] There are two crystallographically independent molecules. [c] The molecule has crystallographic C_2 symmetry. [d] The molecule has crystallographic C_i symmetry.

Table S2. part 2…

data	3·THF	3·DIC	3a	4
formula	$C_{56}H_{78}MgN_4OZn$	$C_{59}H_{84}MgN_6Zn$	$C_{40}H_{45}F_4N_3Zn$	$C_{58}H_{82}N_4Zn_3$
solvent	—	—	$0.5(C_7H_8)\cdot0.5(C_6H_{14})$	—
formula weight	912.90	967.00	798.31	1031.38
colour, habit	pale yellow blocks	colourless plates	colourless blocks	yellow needles
temperature / K	173	173	173	173
crystal system	monoclinic	monoclinic	monoclinic	monoclinic
space group	$P2_1/n$ (no. 14)	$C2/c$ (no. 15)	$I2/a$ (no. 15)	$P2_1/n$ (no. 14)
***a* / Å**	12.3877(6)	10.18598(12)	15.6052(4)	12.7429(2)
***b* / Å**	22.4084(10)	24.1833(3)	24.2499(5)	17.3446(4)
***c* / Å**	19.0461(7)	23.1663(3)	23.5838(5)	13.0260(3)
α / deg	90	90	90	90
β / deg	90.149(4)	99.0832(12)	102.230(2)	101.313(2)
γ / deg	90	90	90	90
***V* / Å^3**	5287.0(4)	5635.01(13)	8722.1(3)	2823.07(10)
Z	4	4 [c]	8	2 [d]
D_c / g cm^{-3}	1.147	1.140	1.216	1.213
radiation used	Mo-Kα	Cu-Kα	Mo-Kα	Cu-Kα
μ / mm^{-1}	0.517	1.015	0.614	1.759
2θ max / deg	57	148	57	147
no. of unique reflns				
measured (R_{int})	10807 (0.0281)	5435 (0.0201)	8797 (0.0171)	5434 (0.0352)
obs, $\|F_o\| > 4\sigma(\|F_o\|)$	8207	4744	6650	4192
no. of variables	597	316	525	305
R_1(obs), wR_2(all) [a]	0.0462, 0.1178	0.0329, 0.0907	0.0442, 0.1384	0.0382, 0.0984

Table S2. part3…

data	6	7	^{mes}***BDI*Mg–Zn*BDI*^{mes}**
formula	$C_{59}H_{85}AlMgN_4$	$C_{54}H_{75}AlN_4Zn$	$C_{46}H_{58}MgN_4Zn$
solvent	C_6H_{14}	—	—
formula weight	987.77	872.53	756.64
colour, habit	colourless blocky needles	orange blocks	colourless tabular needles
temperature / K	173	173	173
crystal system	monoclinic	orthorhombic	monoclinic
space group	*I*2/*a* (no. 15)	$P2_12_12_1$ (no. 19)	*P*2/*n* (no. 13)
***a* / Å**	21.9257(3)	13.75991(19)	13.4443(3)
***b* / Å**	15.7003(2)	13.8927(2)	8.2978(2)
***c* / Å**	37.0659(6)	26.7330(4)	19.6313(5)
α / deg	90	90	90
β / deg	97.8995(14)	90	102.544(2)
γ / deg	90	90	90
***V* / Å^3**	12638.5(3)	5110.34(13)	2137.77(9)
Z	8	4	2 [c]
***D*$_c$ / g cm^{-3}**	1.038	1.134	1.175
radiation used	Cu-Kα	Cu-Kα	Cu-Kα
μ / mm^{-1}	0.660	1.104	1.194
2θ max / deg	148	148	148
no. of unique reflns			
measured (*R*$_{int}$)	12130 (0.0178)	8375 (0.0286)	4100 (0.0322)
obs, $\|F_o\| > 4\sigma(\|F_o\|)$	10359	7388	3275
no. of variables	608	561	248
***R*$_1$(obs), *wR*$_2$(all)** [a]	0.0377, 0.1075	0.0352, 0.0867	0.0402, 0.1132

Table S2 provides a summary of the crystallographic data for the structures of **2a**, **2a-hexane**, **2b**, **3**, **3·THF**, **3·DIC**, **3a**, **4**, **6**, **7** and ^{mes}***BDI*Mg–Zn*BDI*^{mes}. Data were collected using Agilent Xcalibur 3 E (**3**, **3·THF** and **3a**) and Xcalibur PX Ultra A (**2a**, **2a-hexane**, **2b**, **3·DIC**, **4**, **6**, **7** and ^{mes}***BDI*Mg–Zn*BDI*^{mes}) diffractometers, and the structures were refined using the SHELXTL and SHELX-2013 program systems.[9,10] The structure of **2a** was refined as a two component inversion twin [Flack parameter x = +0.38(6)], and the absolute structure of **7** was determined by use of the Flack parameter [x = −0.036(16)]. CCDC 1575549 (**2a**), 1575550 (**2a-hexane**), 1575551 (**2b**), 1575552 (**3**), 1575553 (**3·THF**), 1577209 (**3·DIC**), 1575554 (**3a**), 1575555 (**4**), 1575556 (**6**), 1575557 (**7**), and 1575558 (^{mes}***BDI*Mg–Zn*BDI*^{mes}).

6. Computational Details

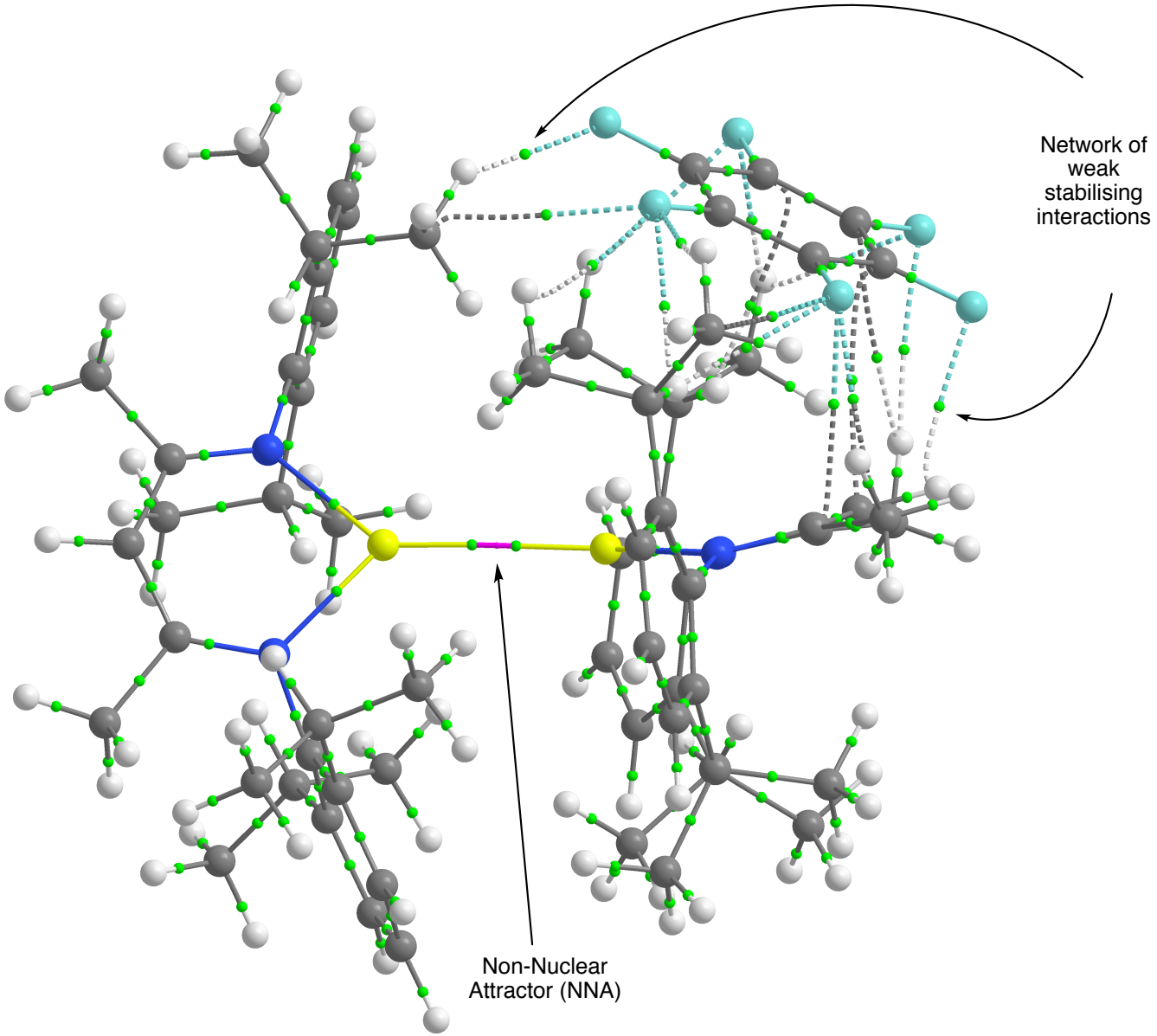
Full Computational Details

DFT calculations were run using Gaussian 09 (Revision D.01)[11] using the ωB97X density functional.[12] Mg and Zn centers were described with Stuttgart SDDAll RECPs and associated basis sets whereas 6-31G** basis sets was used for all other atoms.[13-15]

Geometry optimisation calculations were performed without symmetry constraints. The Gaussian 09 default optimisation criteria were tightened to 10^{-9} on the density matrix and 10^{-7} on the energy matrix. The default numerical integration grid was also improved using a pruned grid with 99 radial shells and 590 angular points per shell. Frequency analyses for all stationary points were performed using the enhanced criteria to confirm the nature of the structures as either minima (no imaginary frequency) or transition states (only one imaginary frequency). Intrinsic reaction coordinate (IRC) calculations were used to connect transition states and minima located on the potential energy surface allowing a full energy profile (calculated at 298.15 K, 1 atm) of the reaction to be constructed.[16,17] Free energies reported within the main text are corrected for the effects of benzene solvent (ε=2.2706) using the using the polarizable continuum model (PCM).[18] In addition, single point dispersion corrections were applied to the ωB97X optimised geometries employing dispersion corrected ωB97X-D functional.[19]

The graphical user interface used to visualise the various properties of the intermediates and transition states was GaussView 5.0.9.[20] Natural Bond Orbital analysis was carried out using NBO 5.9.[21,22] The topology of the electron density for selected systems within the QTAIM framework was carried out using the AIMALL software.[23-25] Weak interactions were identified using the Non Covalent Interaction (NCI) approach.[26] The analysis was carried out with the NCIplot software and visualized using the VMD interface.[27,28]

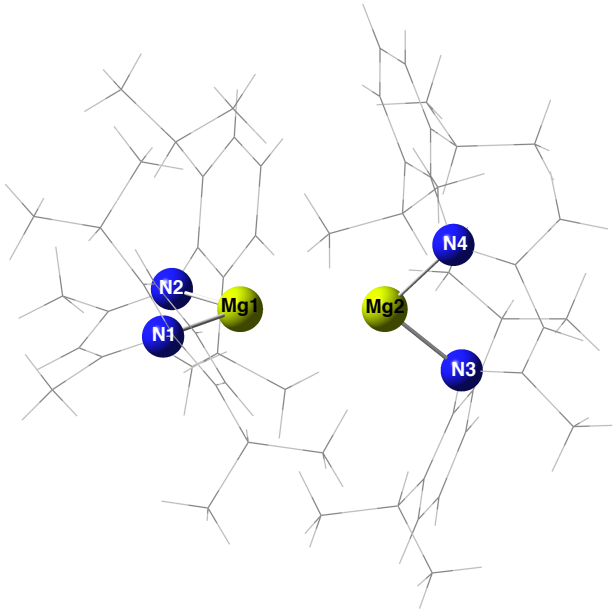
Figure S27. QTAIM molecular graph depicting network of stabilizing interactions between substrate and dimer in **Int-A**.



Assessment of DFT Functionals

We performed a series of benchmark calculations assessing the performance of functionals in describing key bond lengths in **1**, activation energy associated with **TS-1** and recovery of the experimental reactivity trend, **TS-2** > **TS-1** > **TS-3**. The functionals include the hybrid GGA functional, B3PW91[29-32]; Minnesota meta and hybrid-meta functionals , M06-L[33] and M06-2X[34] respectively; long range-corrected functional, ωB97X[12] and with Grimme's D2 dispersion correction, ωB97X-D[19] whilst maintaining the same basis set and pseudopotential combination. The final functional of choice, ωB97X, was based on the ability to accurately describe various bond distances in **1**. While we recognize that ωB97X-derived enthalpy and free energy barriers do not correlate as well as other functionals with data from the Eyring analysis, ωB97X does correctly describe the experimental reactivity trend (**TS-2** > **TS-1** > **TS-3**).

Table S3. Selected bond distances (in angstroms) using different DFT methods. The notation exp corresponds to the X-ray derived values taken from Green *et. al.*[1]



	Mg1–Mg2	**Mg1–N1**	**Mg1–N2**	**Mg2–N3**	**Mg2–N4**
			(Å)		
exp	2.8457(8)	2.0643(13)	2.0547(13)	2.0571(13)	2.0656(12)
B3PW91	2.96	2.11	2.10	2.10	2.11
M06L	2.82	2.07	2.07	2.06	2.07
M062X	2.85	2.07	2.06	2.06	2.07
ωB97X	**2.87**	**2.08**	**2.07**	**2.07**	**2.08**
ωB97X-D	2.83	2.07	2.06	2.06	2.07

Table S4. Relative free energies (kcal mol^{-1}) of **Int-A** and **TS-1** using specified density functionals. All values single point corrected for solvent. Dispersion single point correction using D3 for B3PW91, D2 single point correction for ωB97X. **ΔG in bold** and ΔH in parenthesis.

	Int A	**TS-1**	**ΔΔG (ΔΔH)**
exp			**21.3** (10.8)
B3PW91	**-0.4** (-10.7)	**19.1** (0.4)	**19.5** (11.2)
M06L	**5.0** (-11.5)	**22.7** (4.7)	**22.7** (16.2)
M062X	**2.0** (-12.3)	**23.8** (6.2)	**21.8** (18.5)
ωB97X	**1.1** (-13.7)	**25.7** (7.3)	**25.7** (21.0)
ωB97XD	**1.4** (-13.6)	**25.1** (6.6)	**25.1** (20.2)

Table S5. Relative free energies of key C–F transition states, **TS-1**, **TS-2** and **TS-3** using specified density functionals. All values single point corrected for solvent. Dispersion single point correction using -D2 correction for ωB97X.

	TS-1	**TS-2**	**TS-3**
ωB97X	**25.7**	**23.0**	**26.4**
M06L	22.7	19.0	21.4
M062X	23.8	24.8	21.8

Table S6. NPA Charges for **Int-A'** and **TS-1**.

	Mg	Mg'	C_i	C_o	C_m	C_p	C'_m	C'_o	F_i	F_o	F_m	F_p	F'_m	F'_o
Int-A'	0.95	0.91	0.31	0.32	0.31	0.31	0.32	0.32	-0.31	-0.31	-0.31	-0.31	-0.31	-0.31
TS-1	1.28	1.10	0.04	0.28	0.32	0.28	0.33	0.27	-0.39	-0.36	-0.31	-0.32	-0.31	-0.33
ΔNPA Charge	0.33	0.19	-0.27	-0.04	0.02	-0.03	0.01	-0.05	-0.08	-0.05	0.00	-0.01	0.00	-0.02

Figure S28. Transition state, **TS-1**, depicting key bond lengths (in Å) and dihedral angles designated χ and ϕ (a) and full QTAIM molecular graph (b).

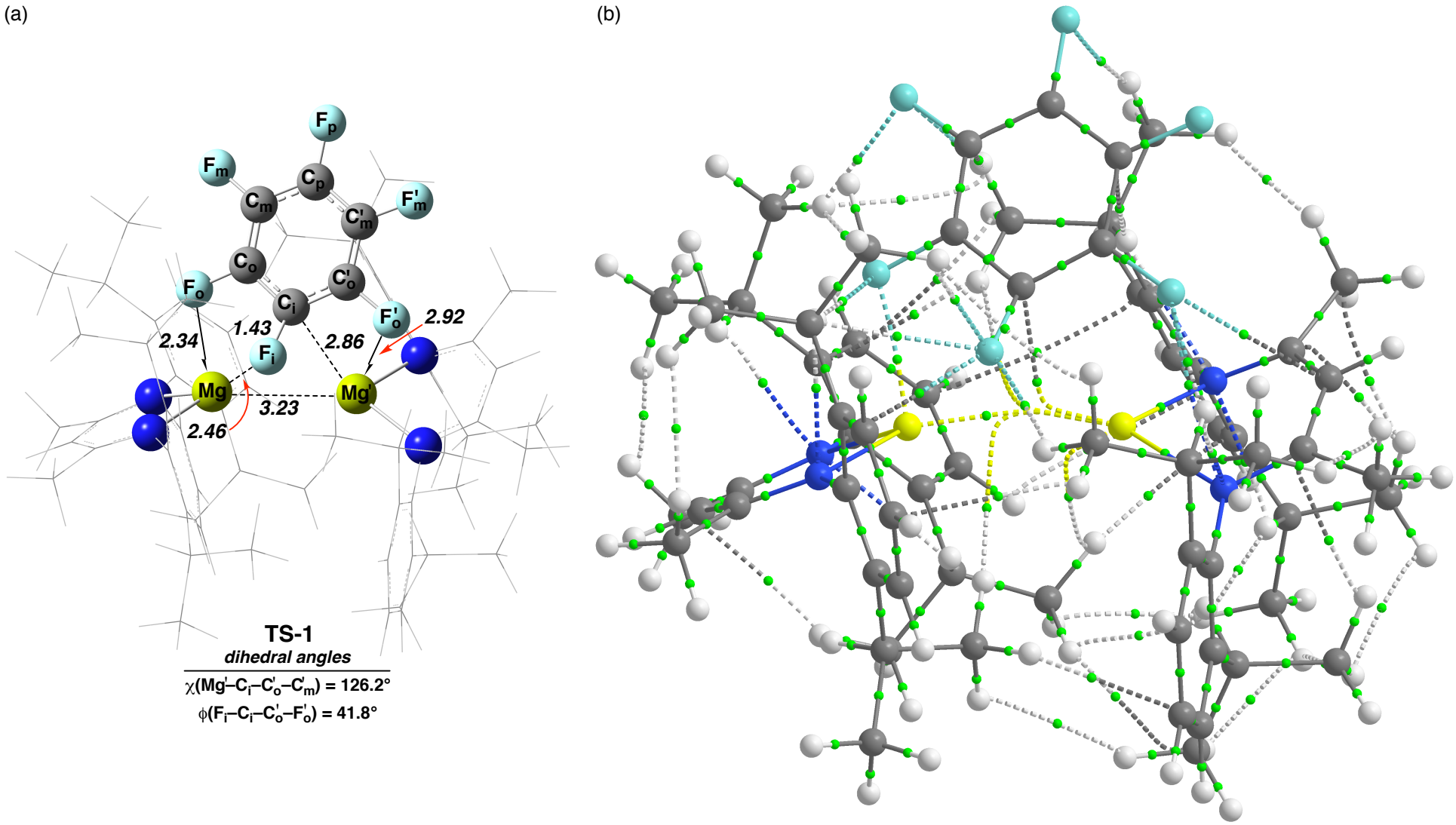
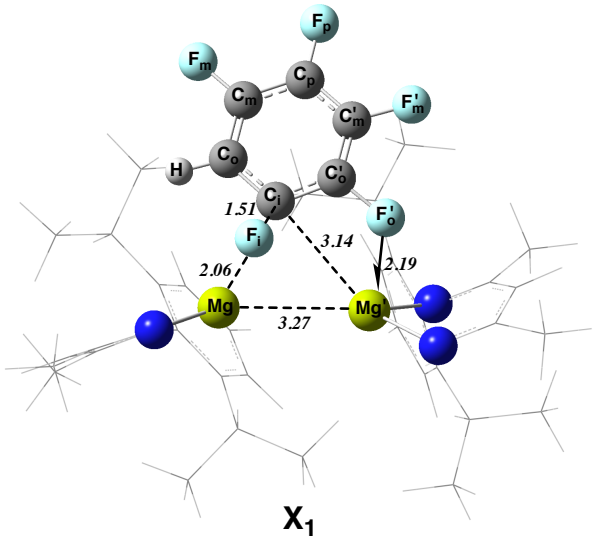
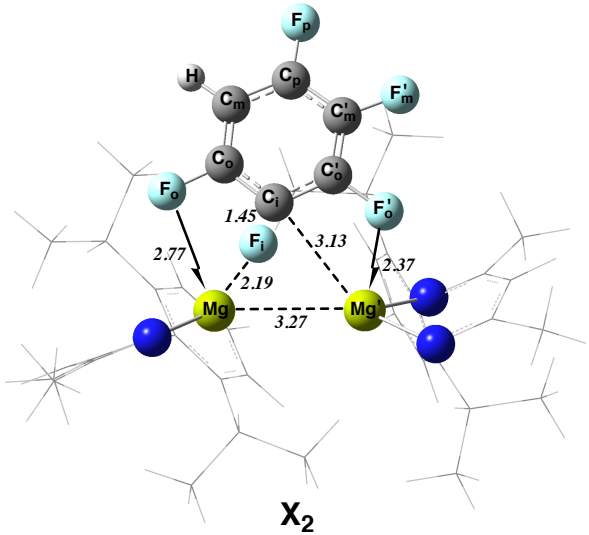


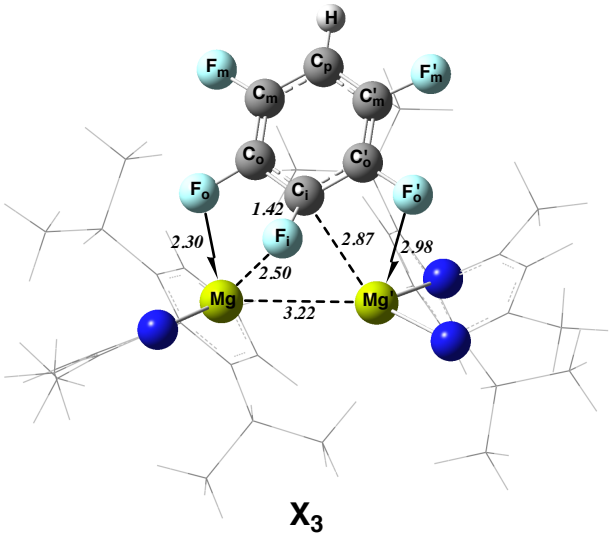
Figure S29. Transition states for C–F activation of C_6F_5H depicting key bond lengths (in Å).



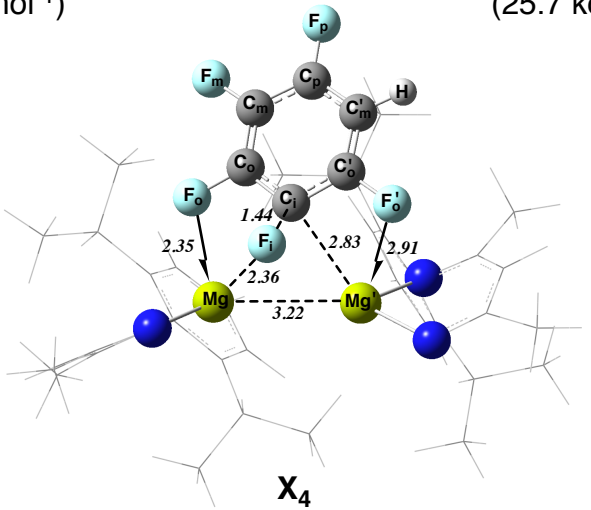
X_1
(30.7 kcal mol^{-1})



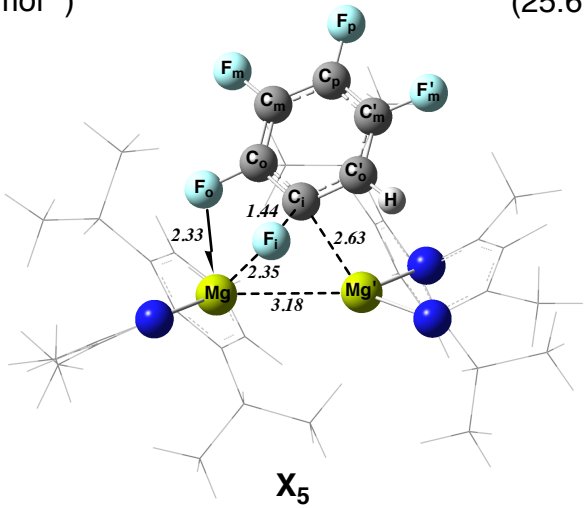
X_2
(25.7 kcal mol^{-1})



X_3
(25.6 kcal mol^{-1})



X_4
(28.5 kcal mol^{-1})



X_5
(27.5 kcal mol^{-1})

Figure S30. Transition state for C–F activation of double *ortho*-substituted $C_6F_4H_2$.

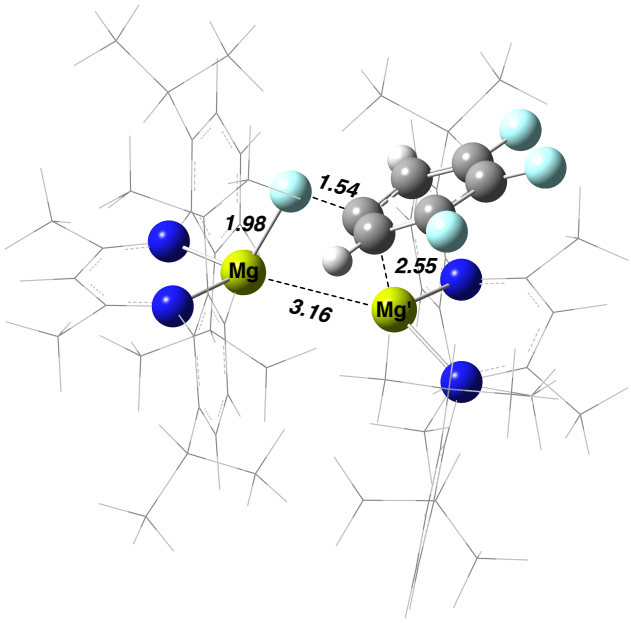


Figure S31. Transition state, **TS-2**, depicting key bond lengths in Å (a) and QTAIM molecular graph (b).

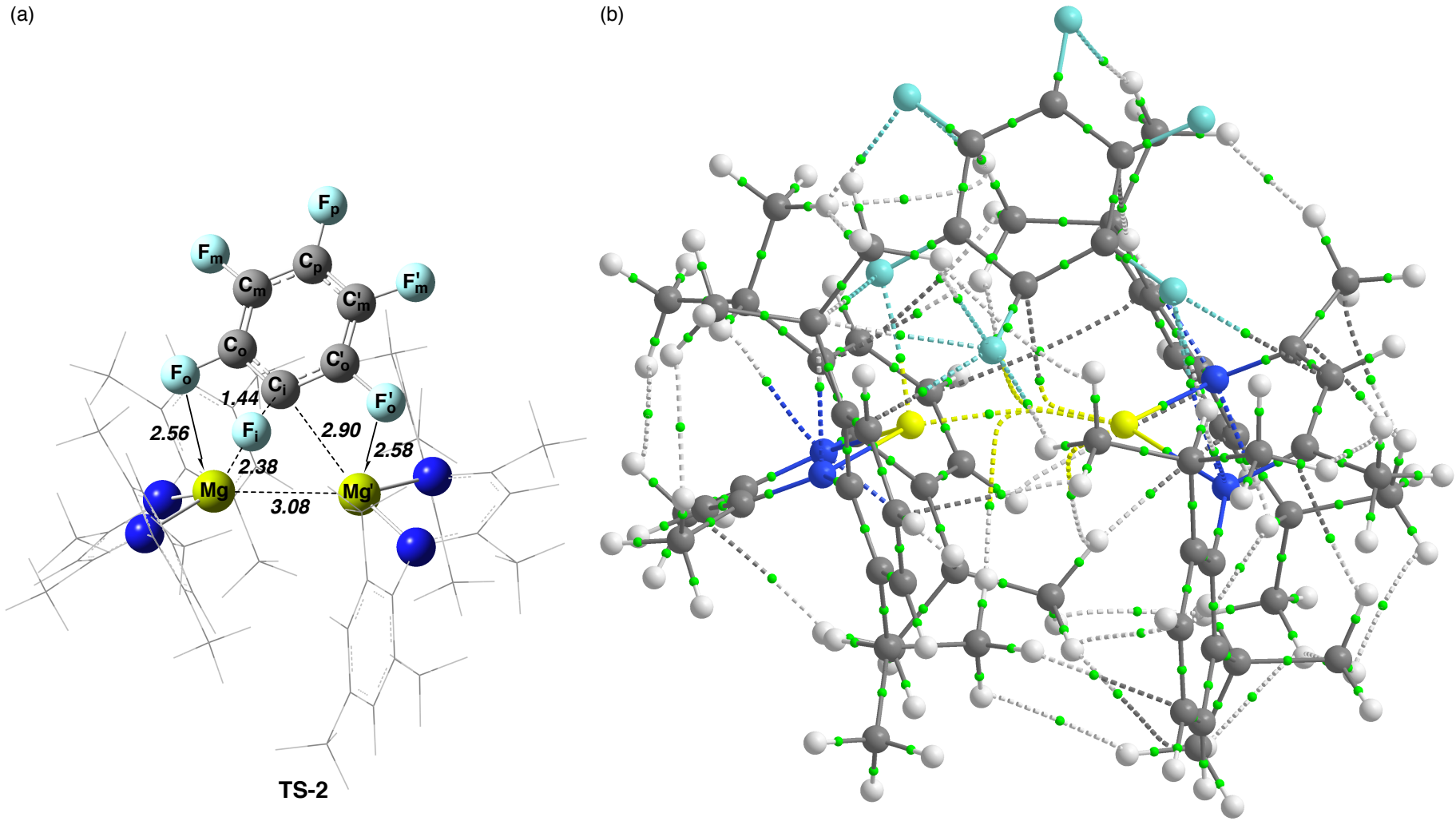


Figure S32. Transition state, **TS-3**, depicting key bond lengths in Å (a) and QTAIM molecular graph (b).

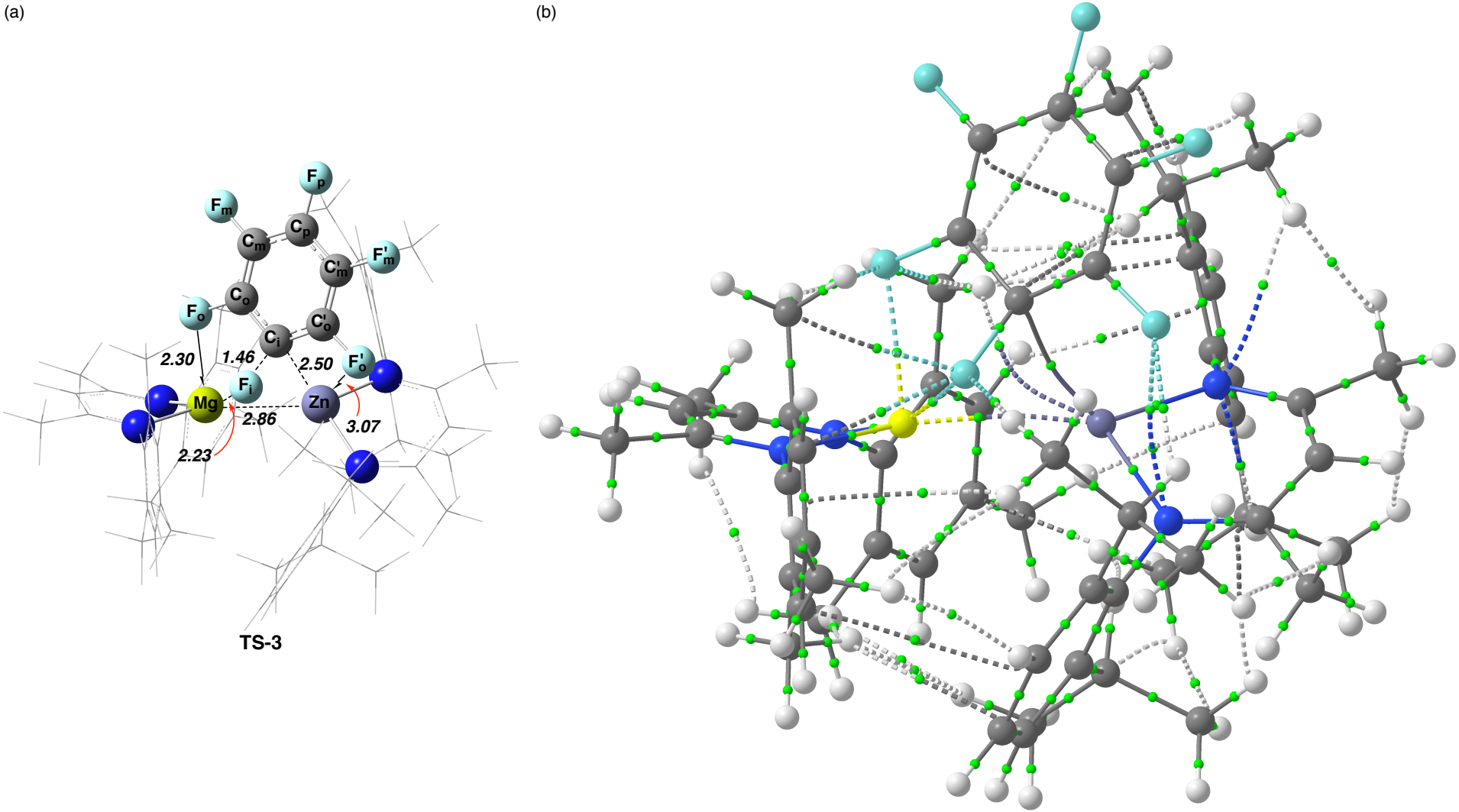


Table S7. Bonding characteristics of metal dimers.

Dimer	$r_{(M-M)}$ (Å)	NPA		Wiberg Bond Index	QTAIM Analysis of M1–M2 BCP	
		M	M		$\rho_{(r)}$ ()	$\nabla^2\rho$ ()
1	2.87	0.94	0.93	0.82	-	-
2	2.83	0.92	0.92	0.82	-	-
3	2.61	0.62 (Zn)	1.19 (Mg)	0.70	0.0347	+0.0404
6	2.77	1.42 (Mg)	0.84 (Al)	0.63	0.0337	+0.0206
7	2.49	1.07 (Zn)	1.14 (Al)	0.80	0.0513	+0.0081

Figure S33. Transition states, **TS-4** and **TS-5**, depicting key bond lengths in Å.

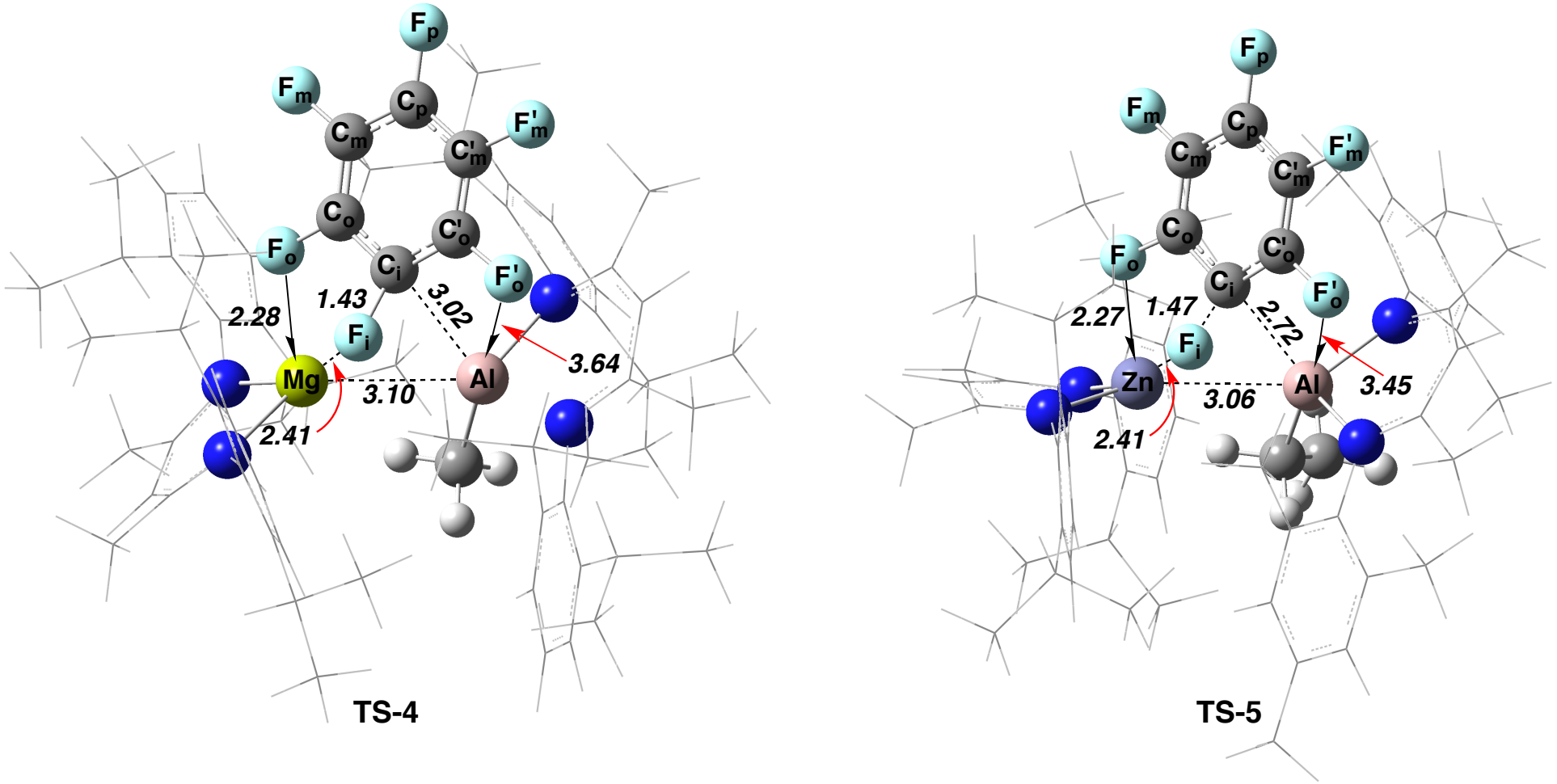
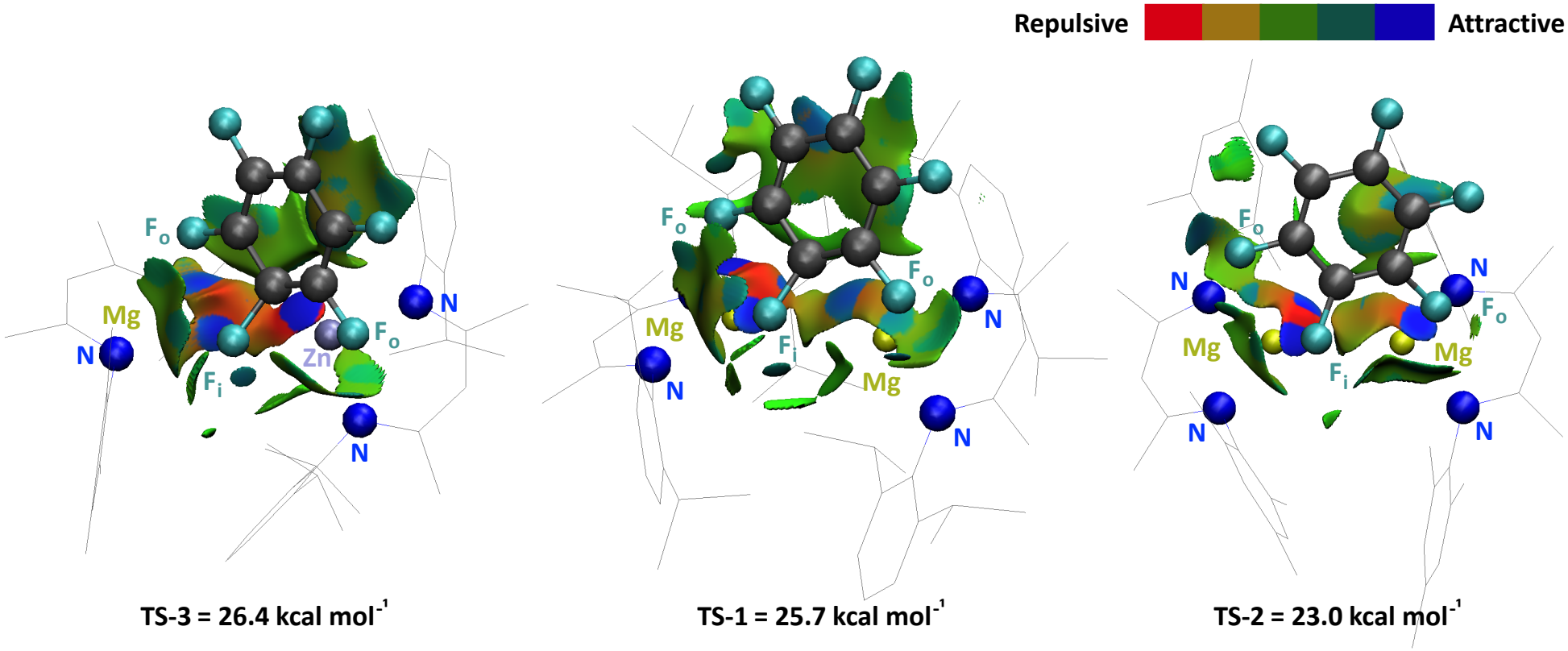


Figure S34. Non-covalent Interaction plots of **TS-1-3**.



7. Multinuclear NMR Data

Figure S35: ^{1}H NMR spectrum of compound **3**; solvent peak marked with asterisk.

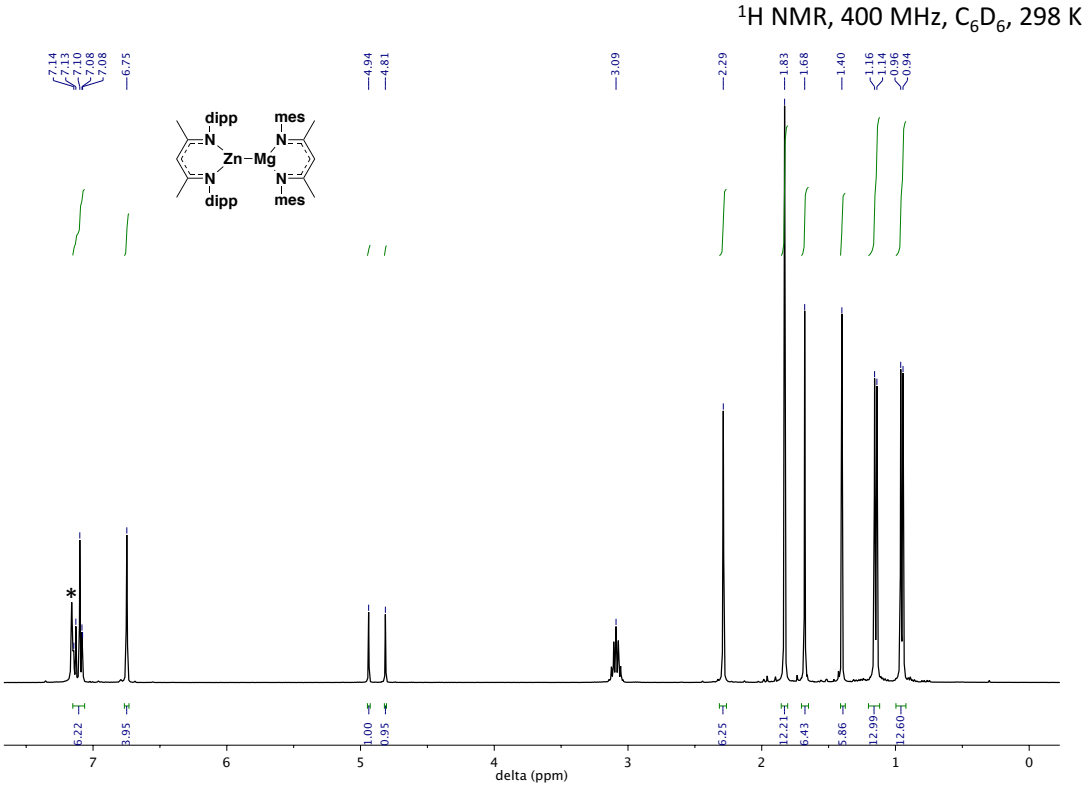


Figure S36: $^{13}C\{^{1}H\}$ NMR spectrum of compound **3**.

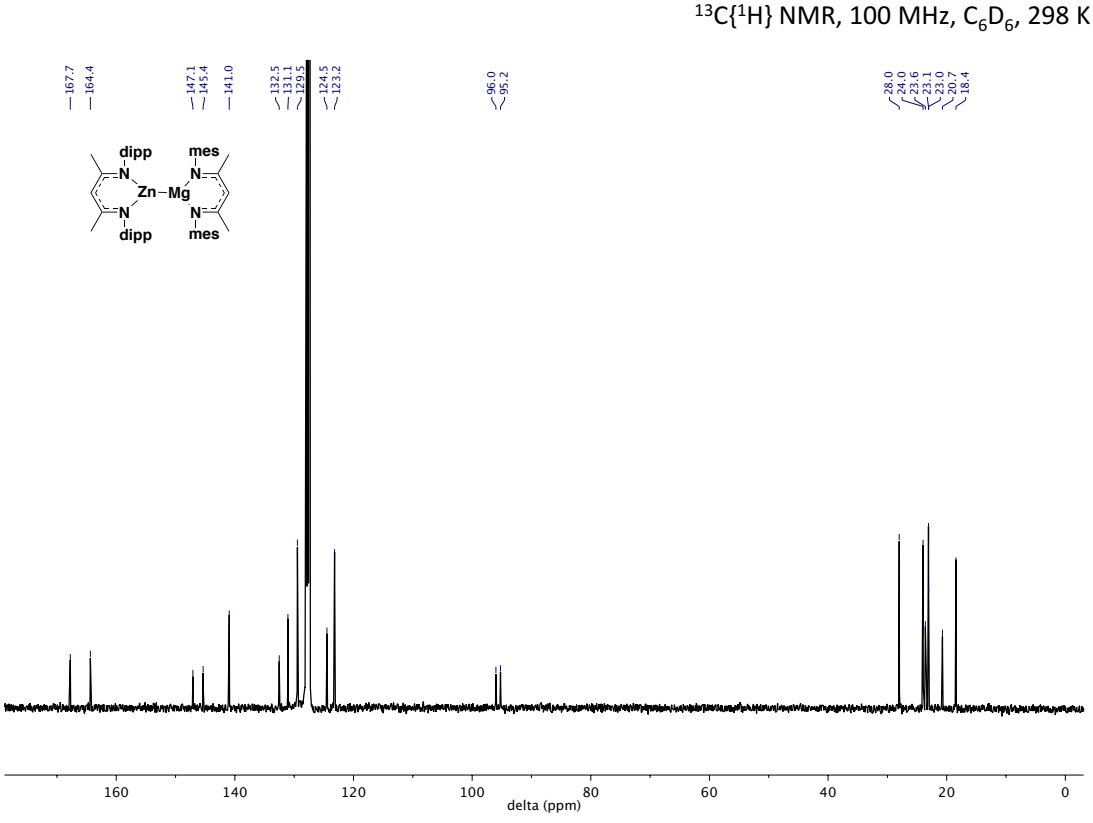


Figure S37: ^{1}H NMR spectrum of compound **4**; residual hexane and solvent peaks marked with asterisk.

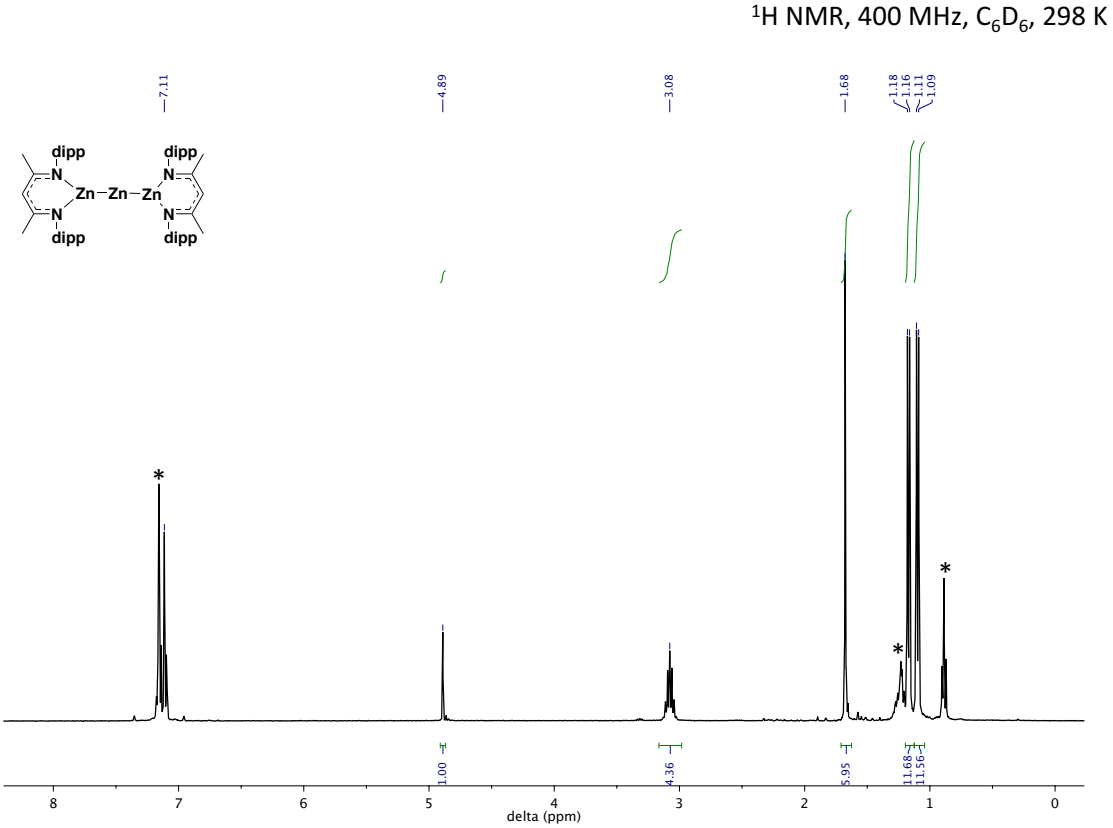


Figure S38: ^{13}C{^{1}H} NMR spectrum of compound **4**.

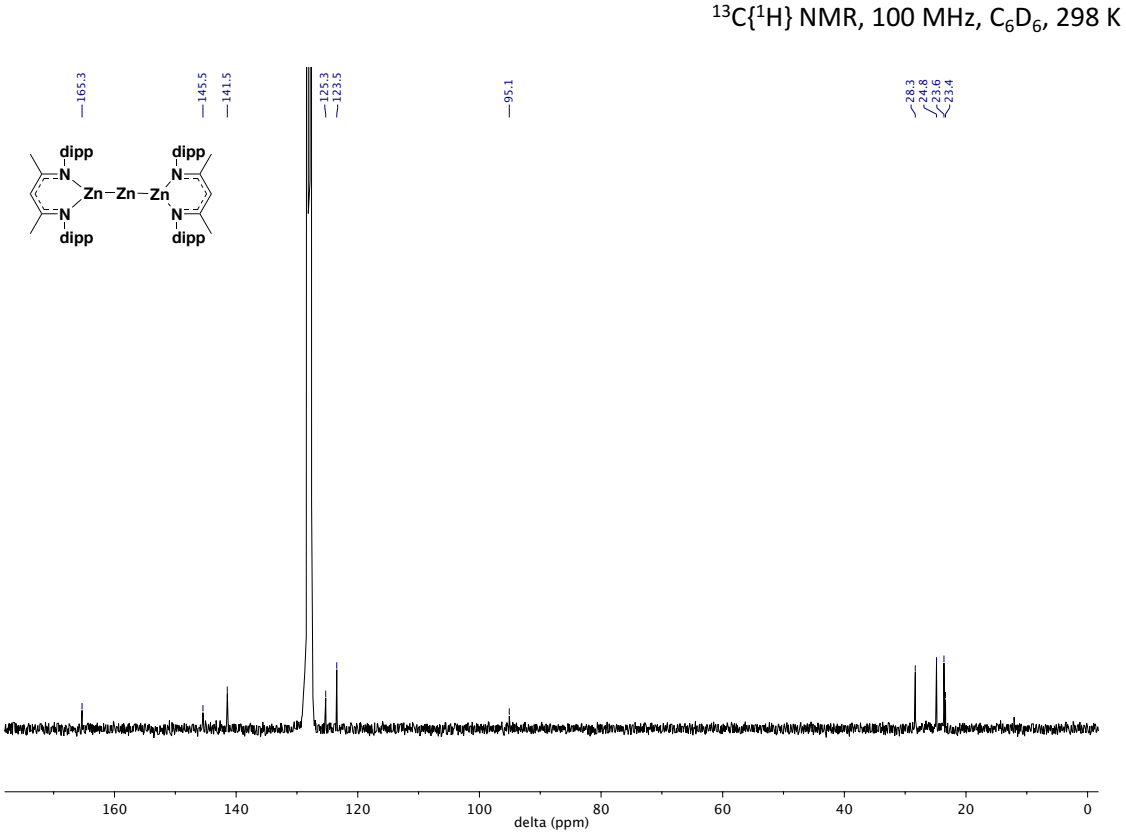


Figure S39: ^{1}H NMR spectrum of compound **3•THF**; solvent peak marked with asterisk.

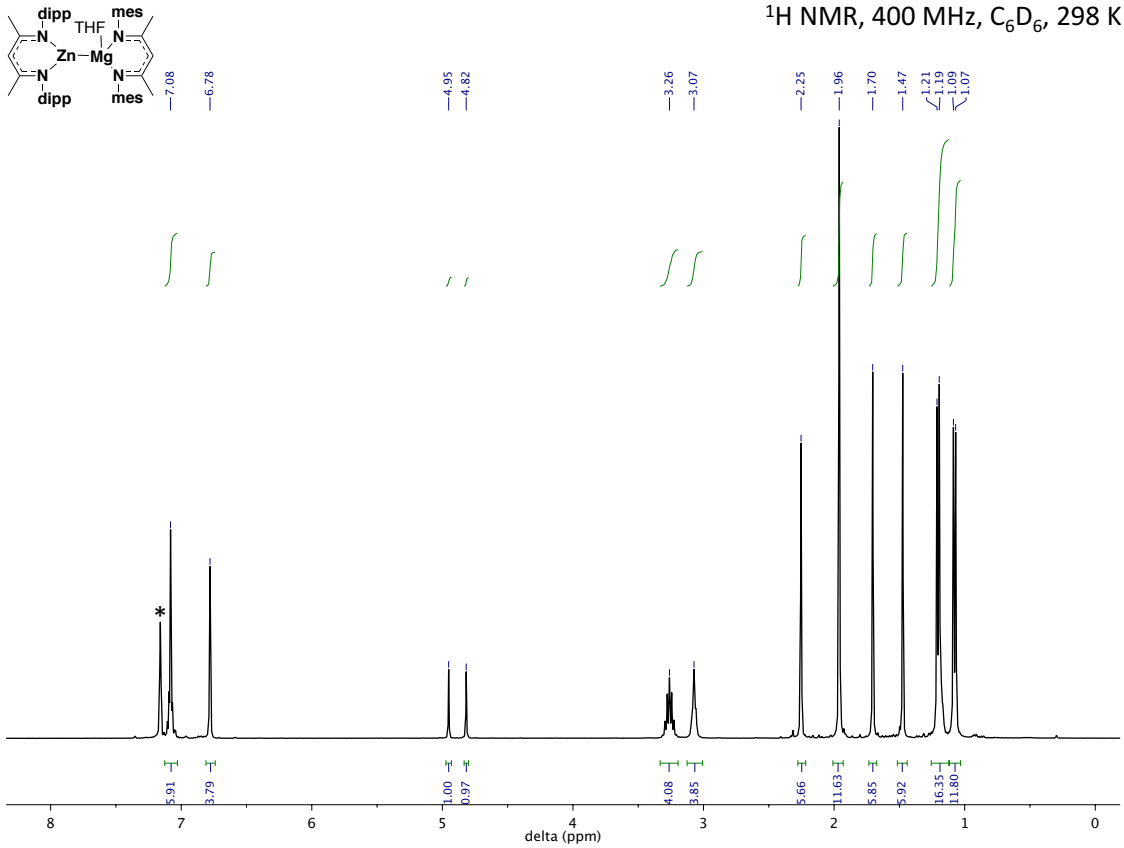


Figure S40: ^{13}C{^{1}H} NMR spectrum of compound **3•THF**.

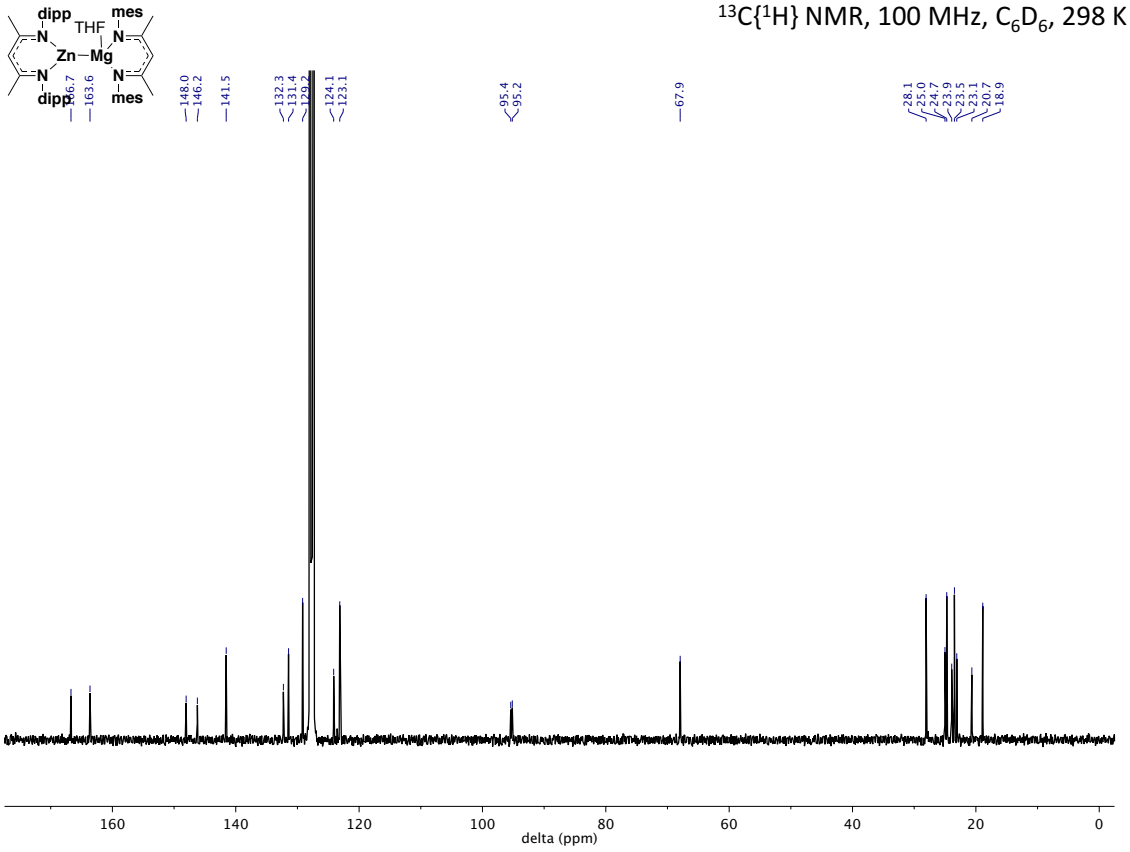


Figure S41: ^{1}H NMR spectrum of compound **3•DCC**; solvent peak marked with asterisk.

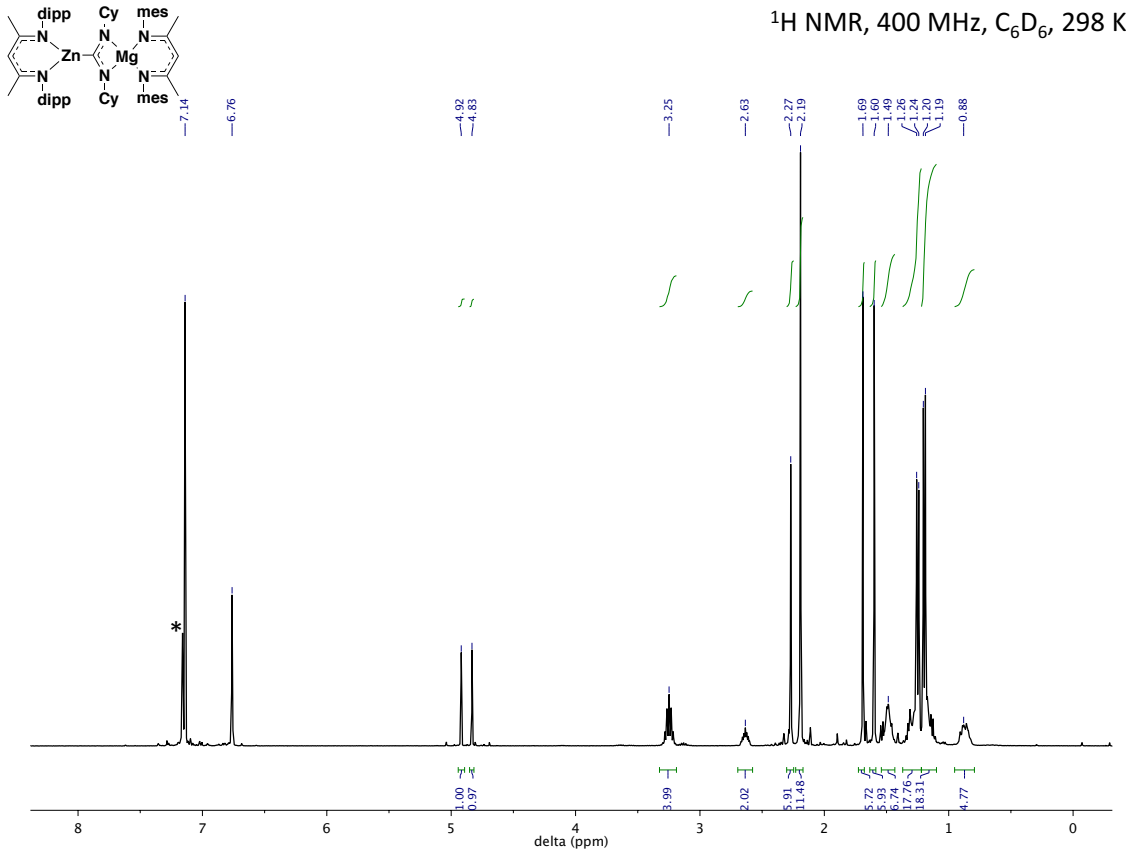


Figure S42: ^{13}C{^{1}H} NMR spectrum of compound **3•DCC**.

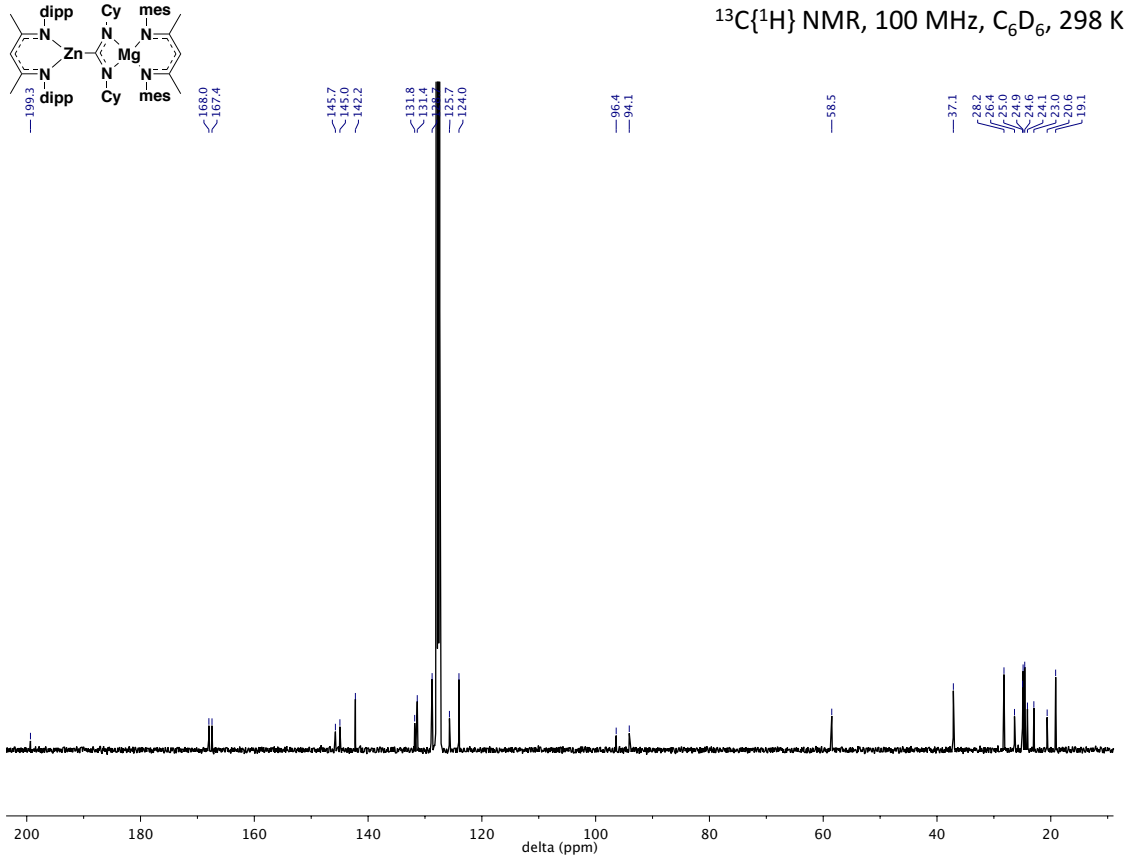


Figure S43: ^{1}H NMR spectrum of compound **3•DIC**; solvent peak marked with asterisk.

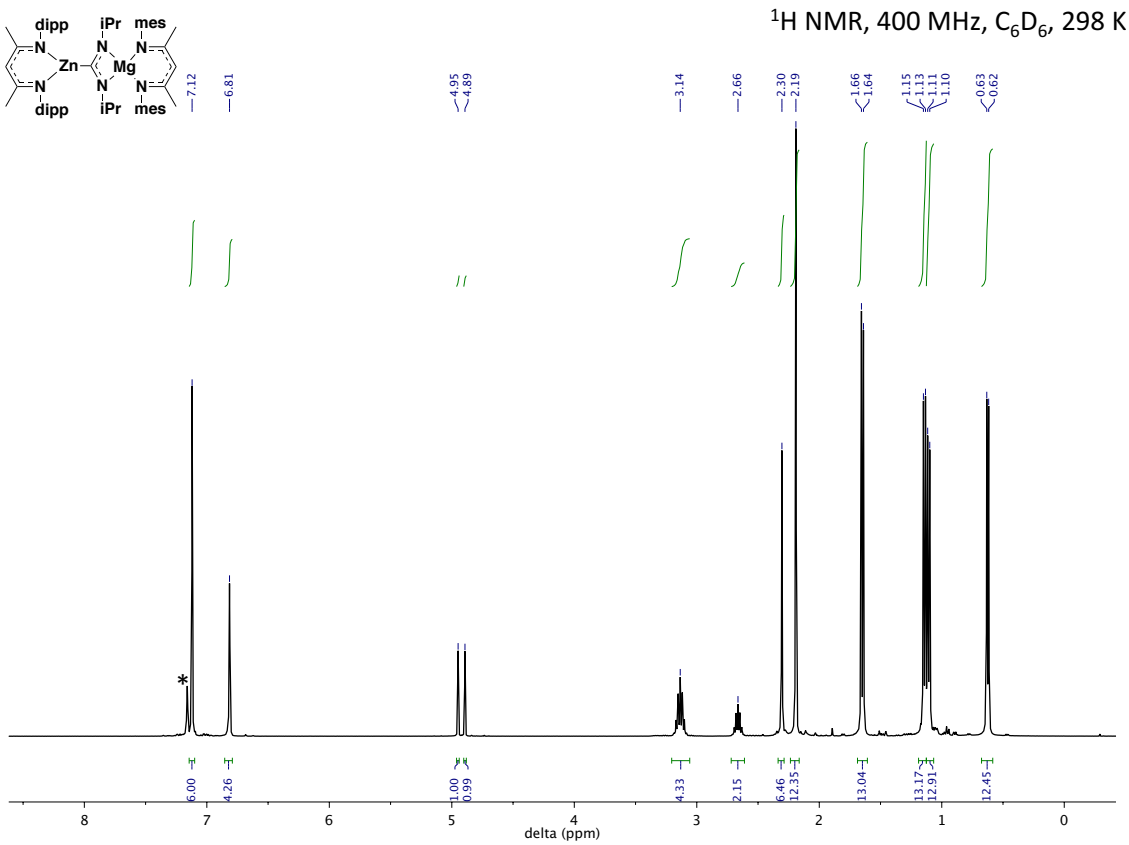


Figure S44: ^{13}C{^{1}H} NMR spectrum of compound **3•DIC**.

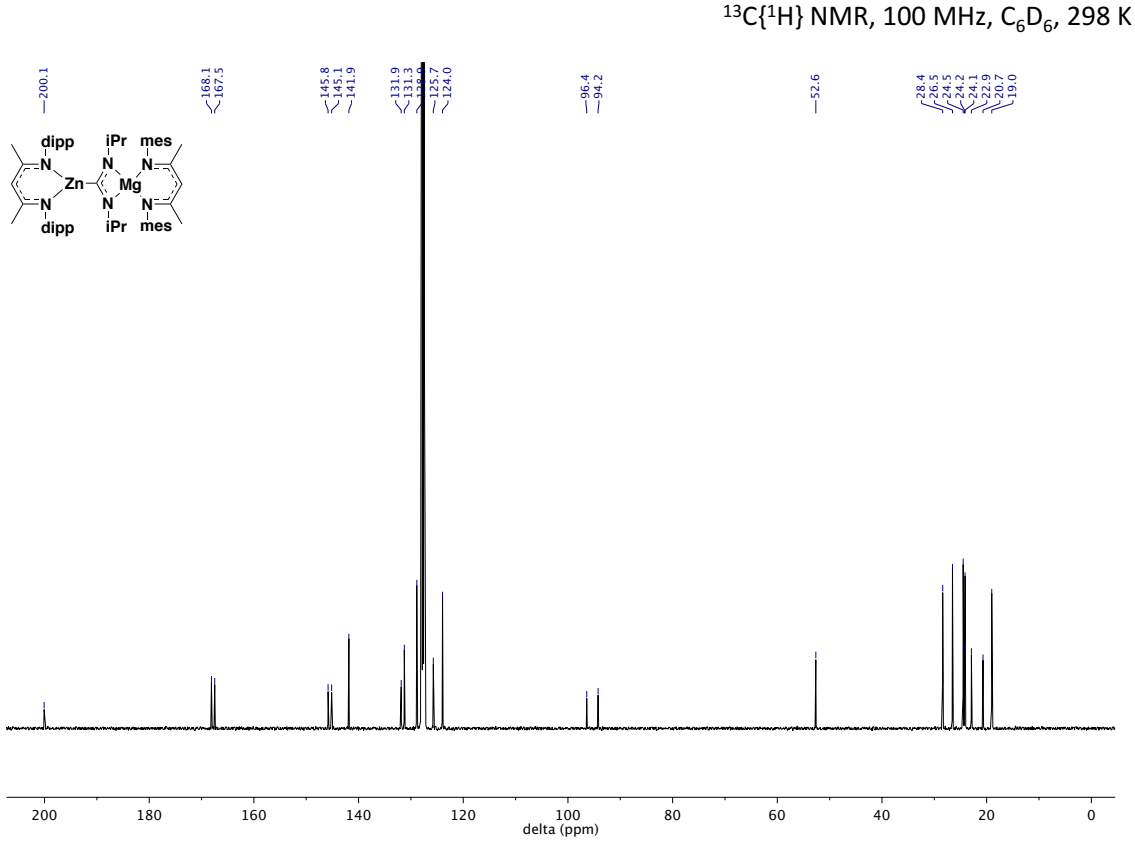


Figure S45: ^{1}H NMR spectrum of compound [Mg(dipp*BDI*)(mes*BDI*)]; solvent peak marked with asterisk.

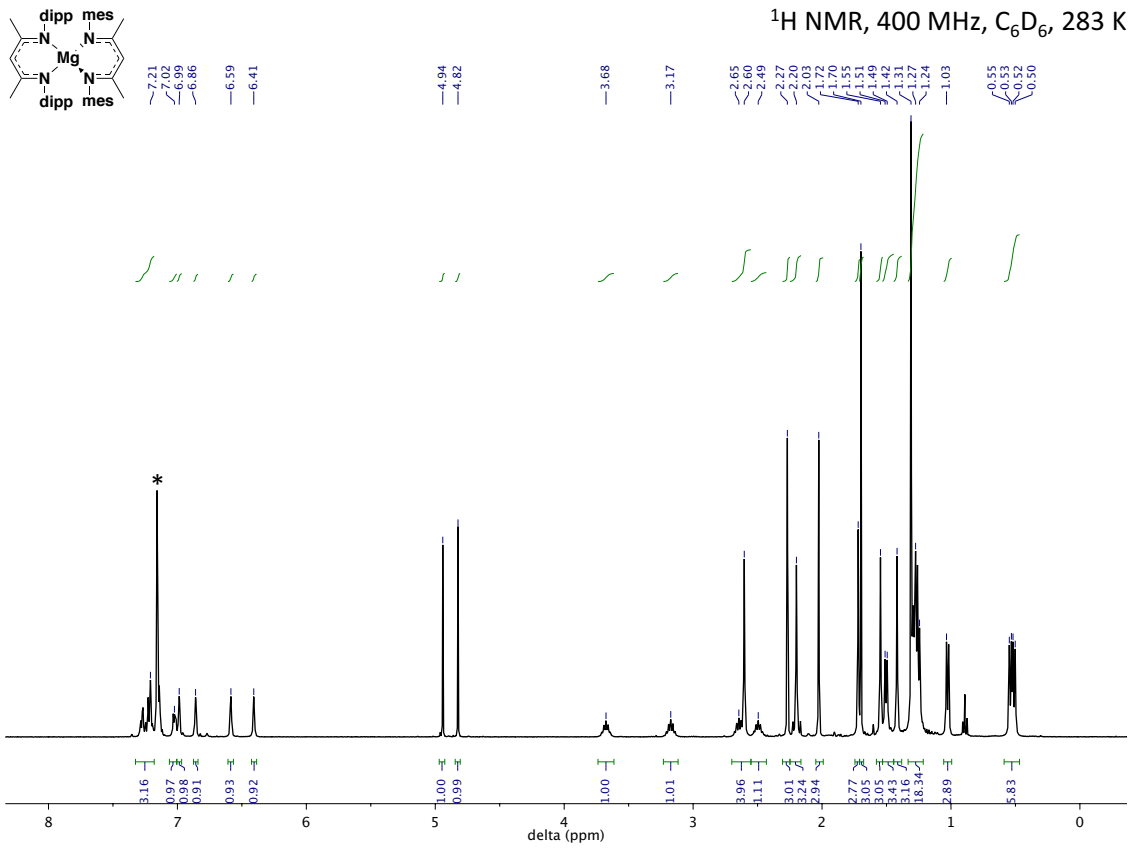


Figure S46: ^{13}C{^{1}H} NMR spectrum of compound [Mg(dipp*BDI*)(mes*BDI*)].

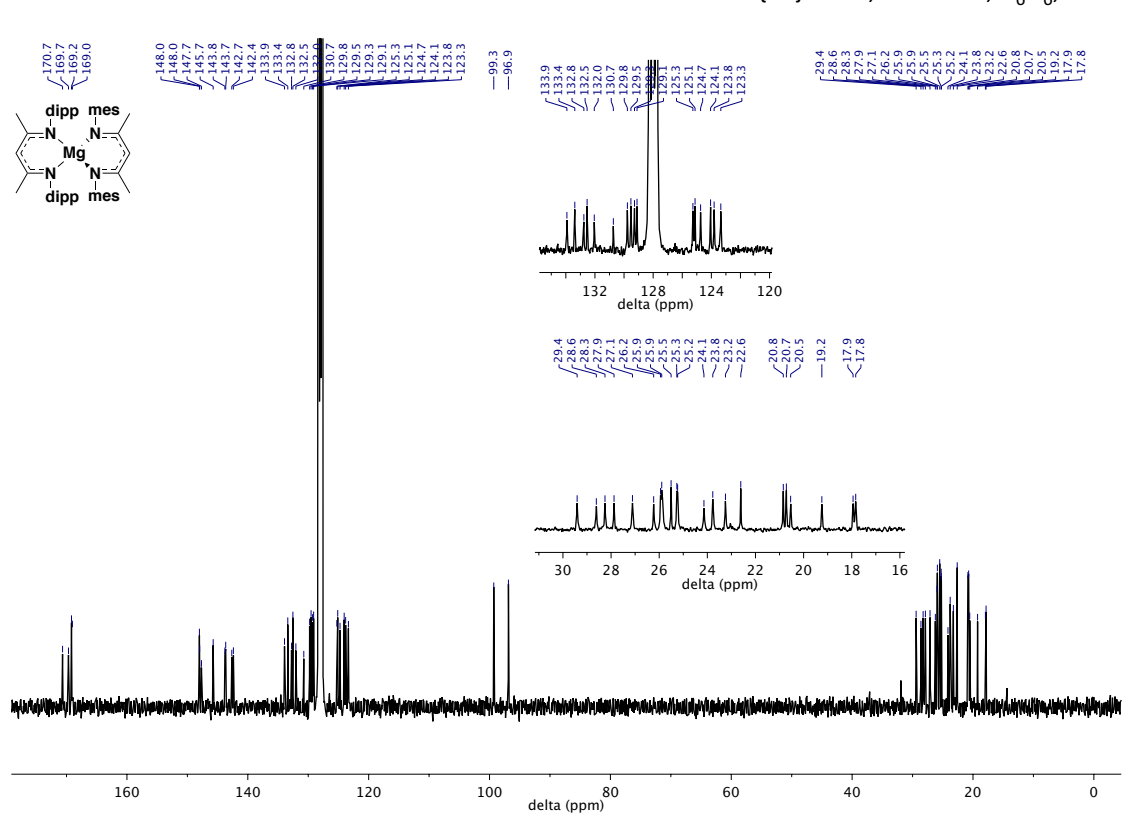


Figure S47: ^{1}H NMR spectrum of compound **6**; solvent peak marked with asterisk.

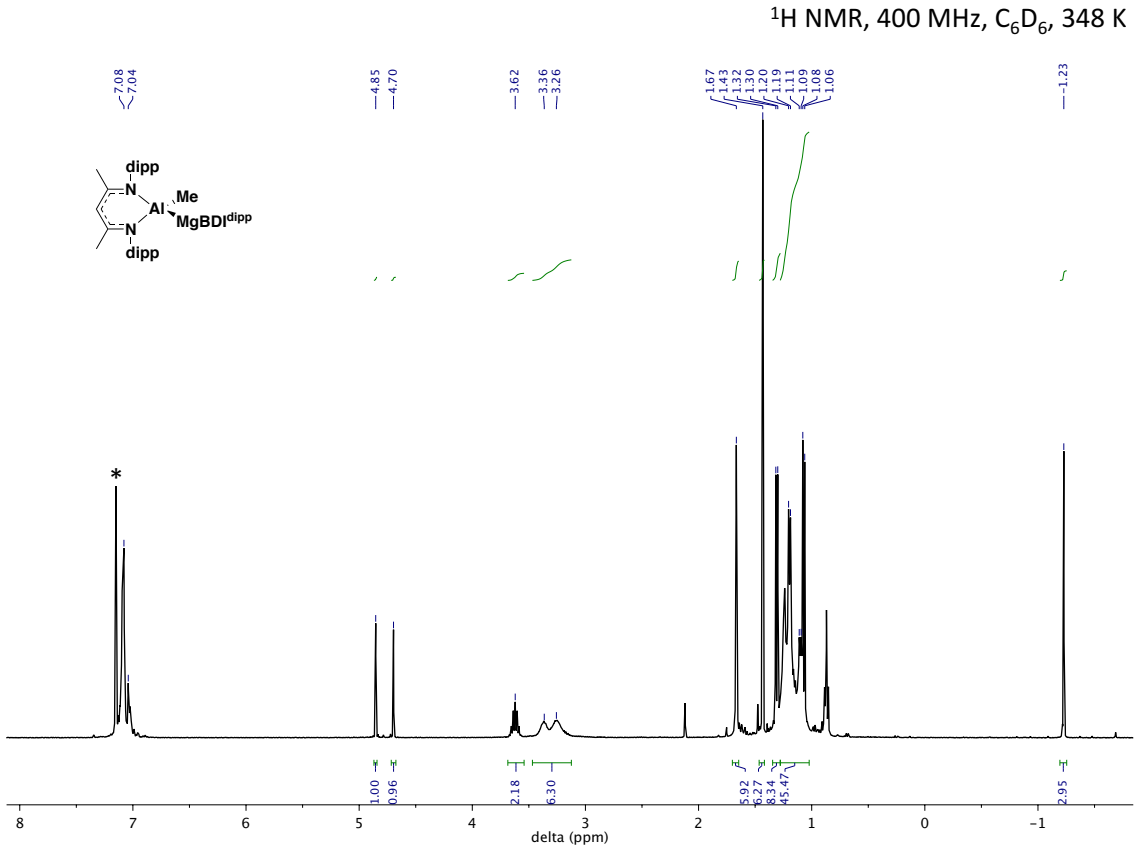


Figure S48: ^{13}C{^{1}H} NMR spectrum of compound **6**.

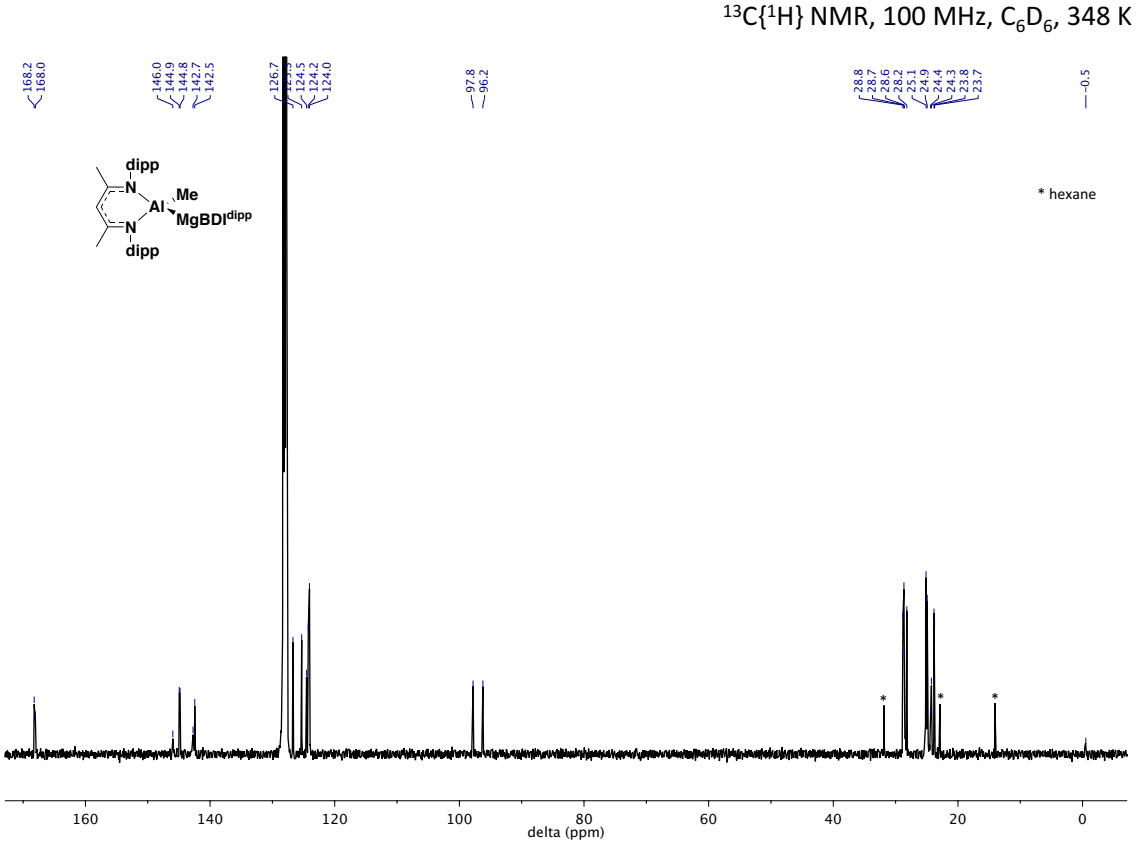


Figure S49: ^{1}H NMR spectrum of compound **7**; solvent peak marked with asterisk.

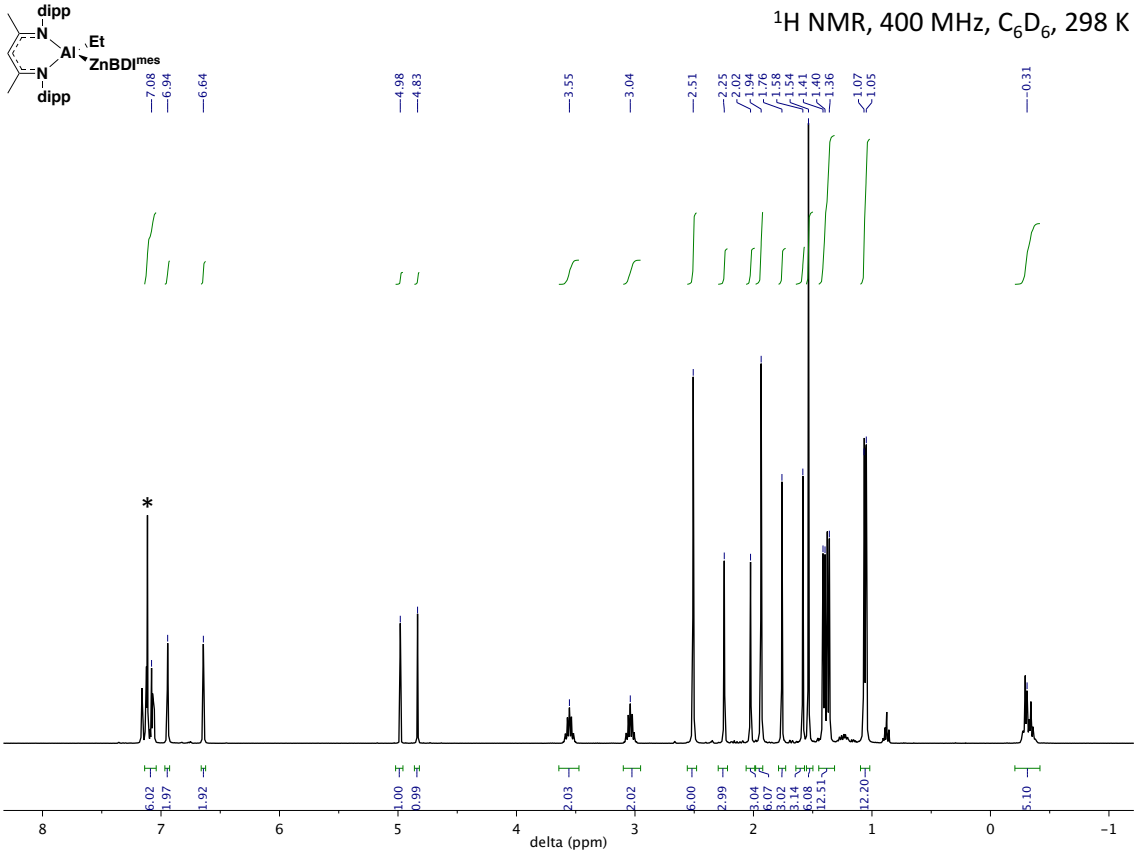


Figure S50: ^{13}C{^{1}H} NMR spectrum of compound **7**.

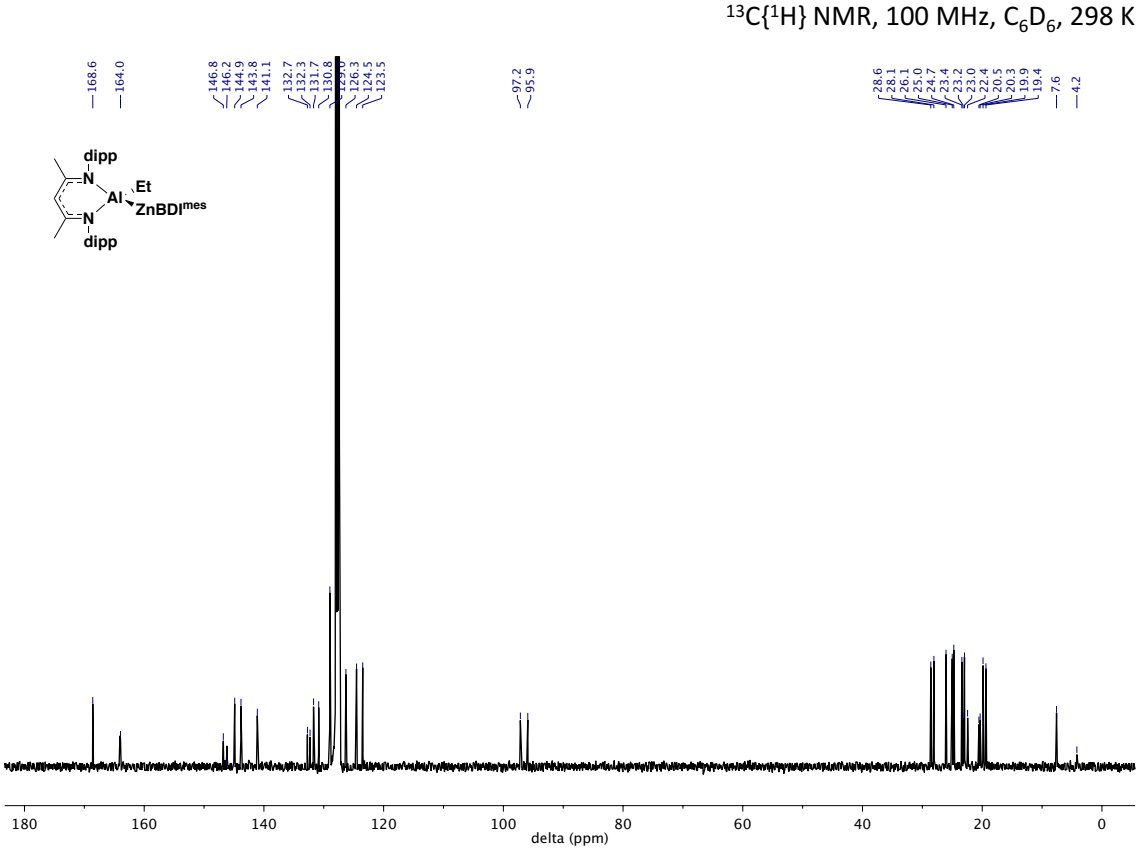


Figure S51: ^{1}H NMR spectrum of compound **2a**; solvent peak marked with asterisk.

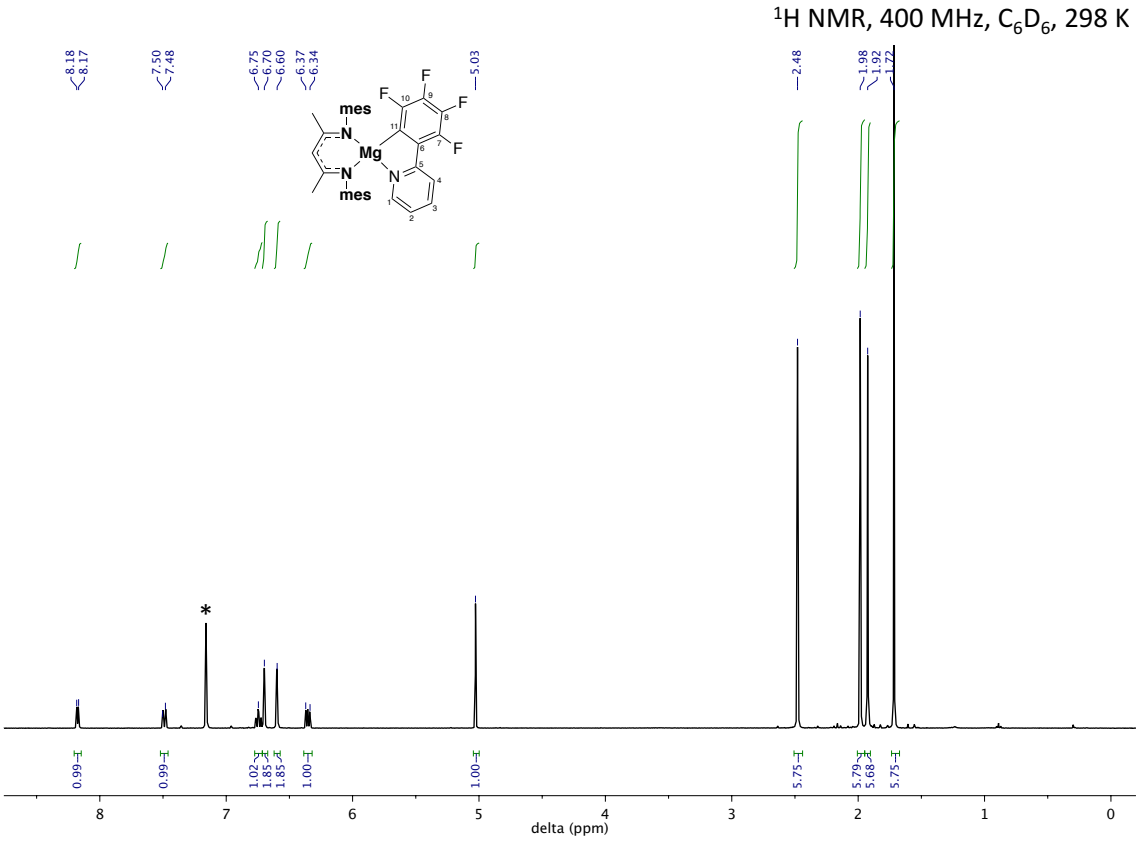


Figure S52: ^{19}F NMR spectrum of compound **2a**.

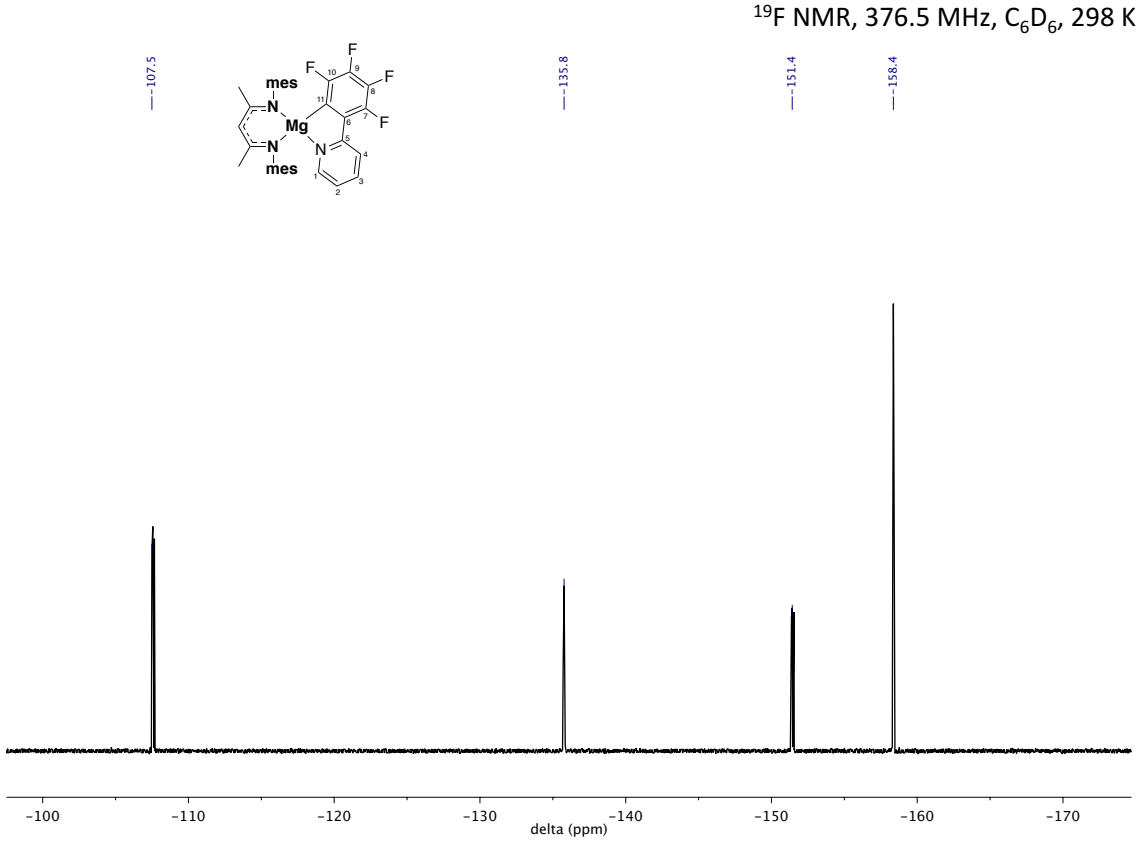


Figure S53: $^{13}C\{^{1}H\}$ NMR spectrum of compound **2a**.

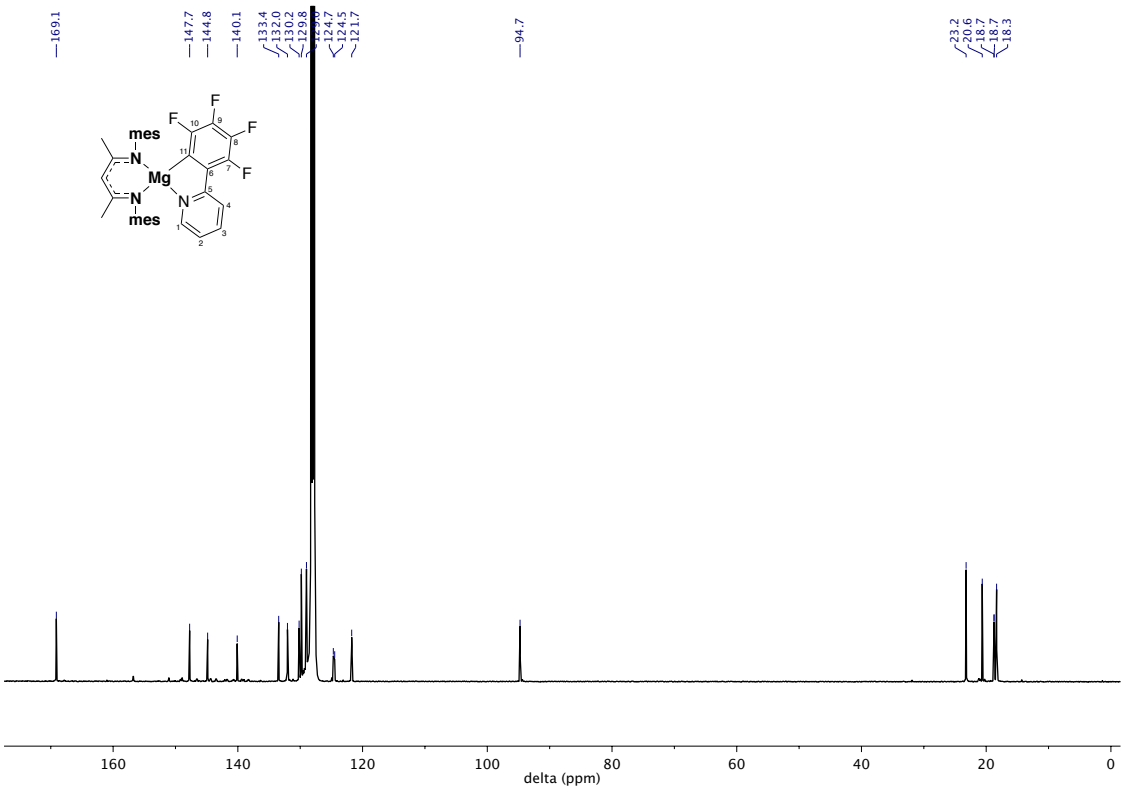


Figure S54: ^{1}H NMR spectrum of compound [{^{mes}*BDI*Mg}$_3$(μ-F)$_3$] **2b**; solvent peak marked with asterisk.

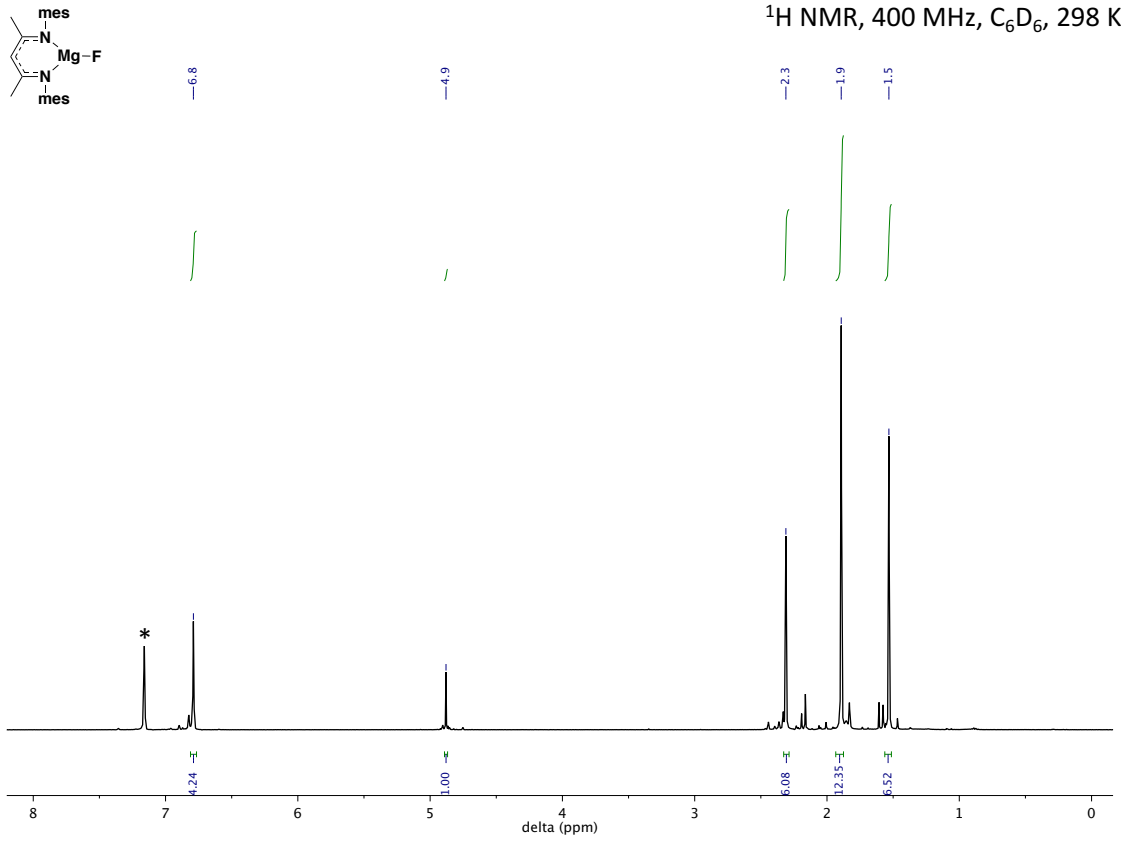


Figure S55: $^{13}C\{^{1}H\}$ NMR spectrum of compound [{^{mes}BDIMg}$_3$(μ-F)$_3$] **2b**.

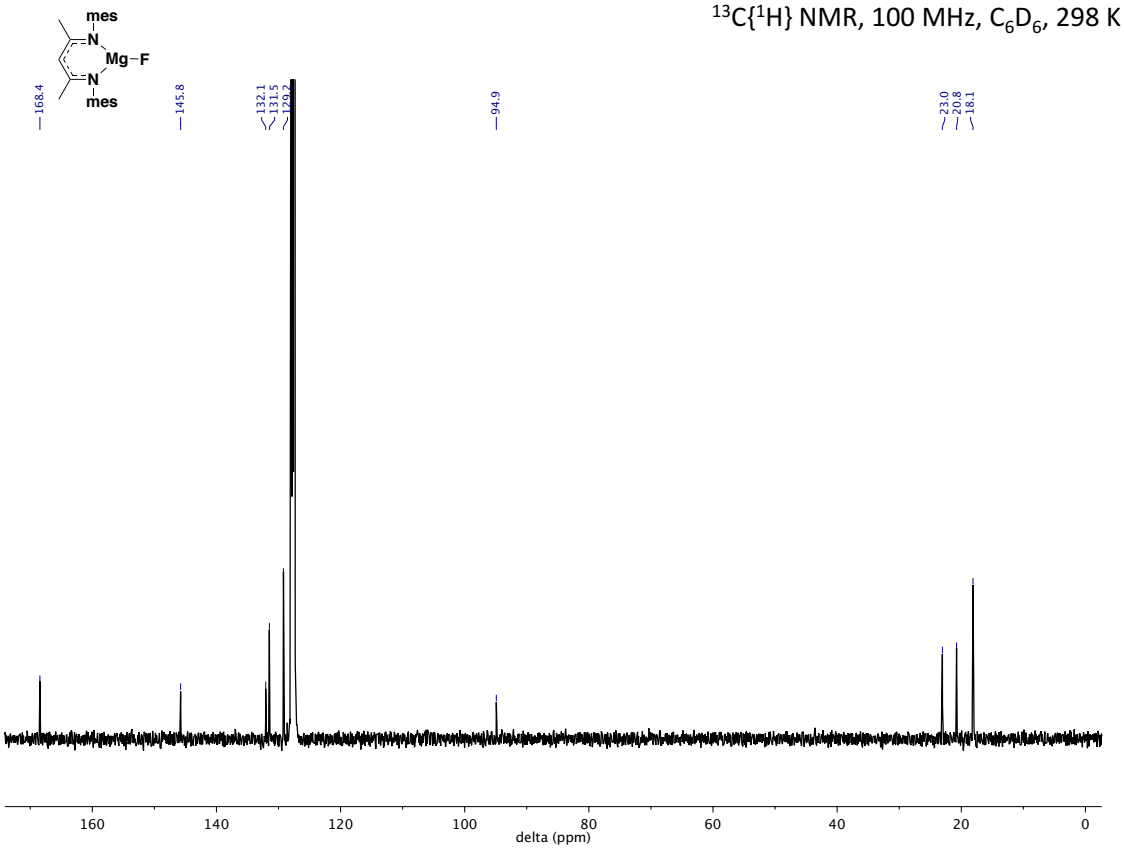


Figure S56: ^{1}H NMR spectrum of compound **3a**; solvent peak marked with asterisk.

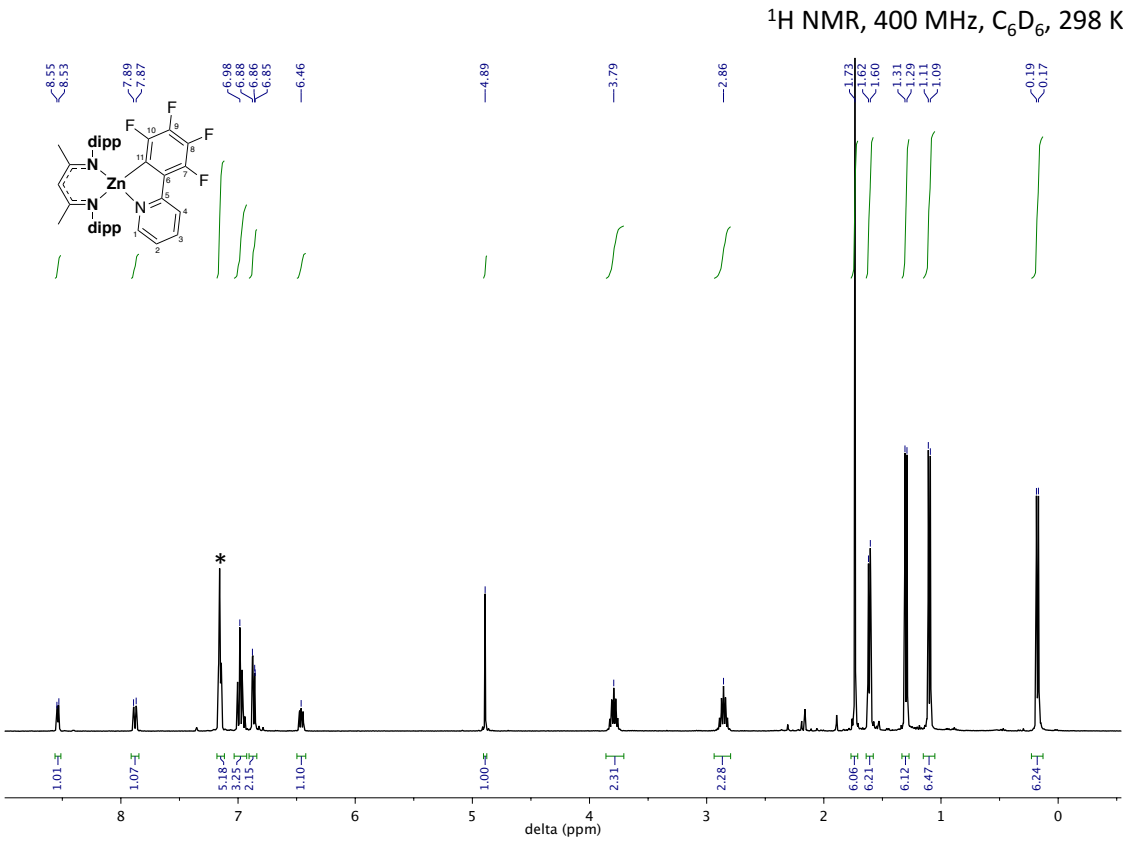


Figure S57: ^{19}F NMR spectrum of compound **3a**.

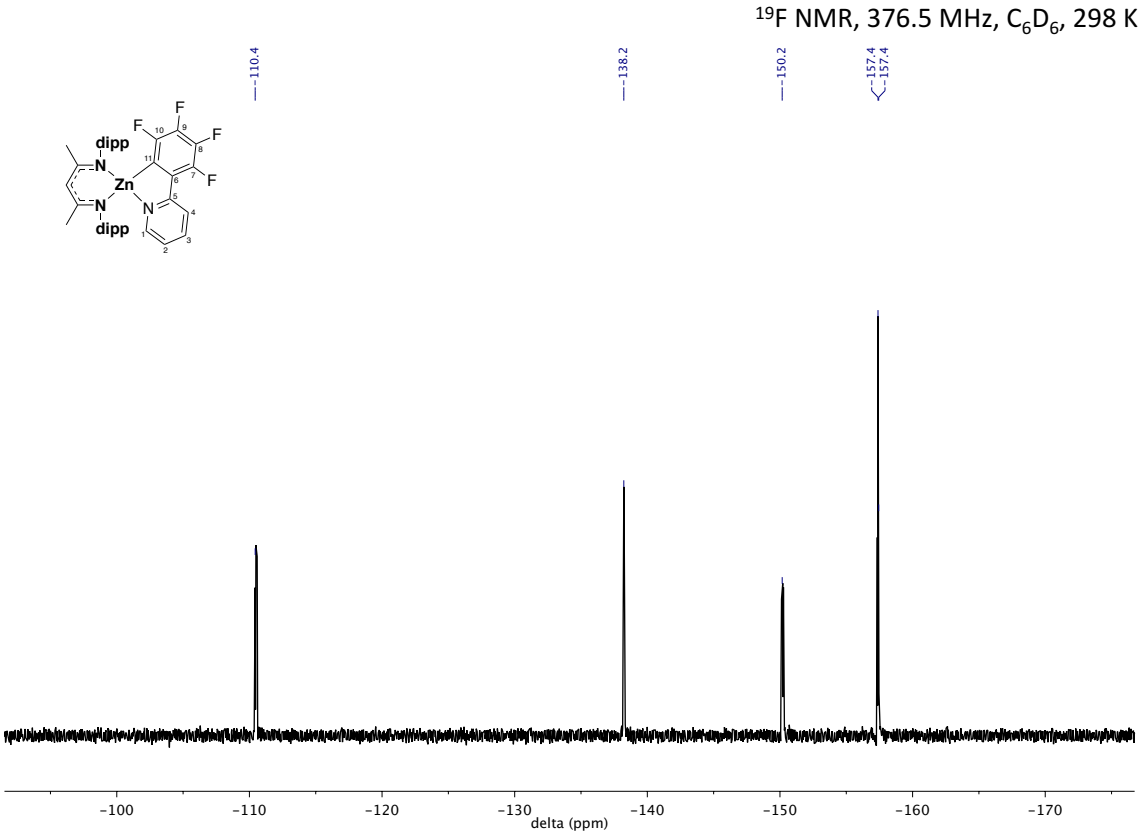
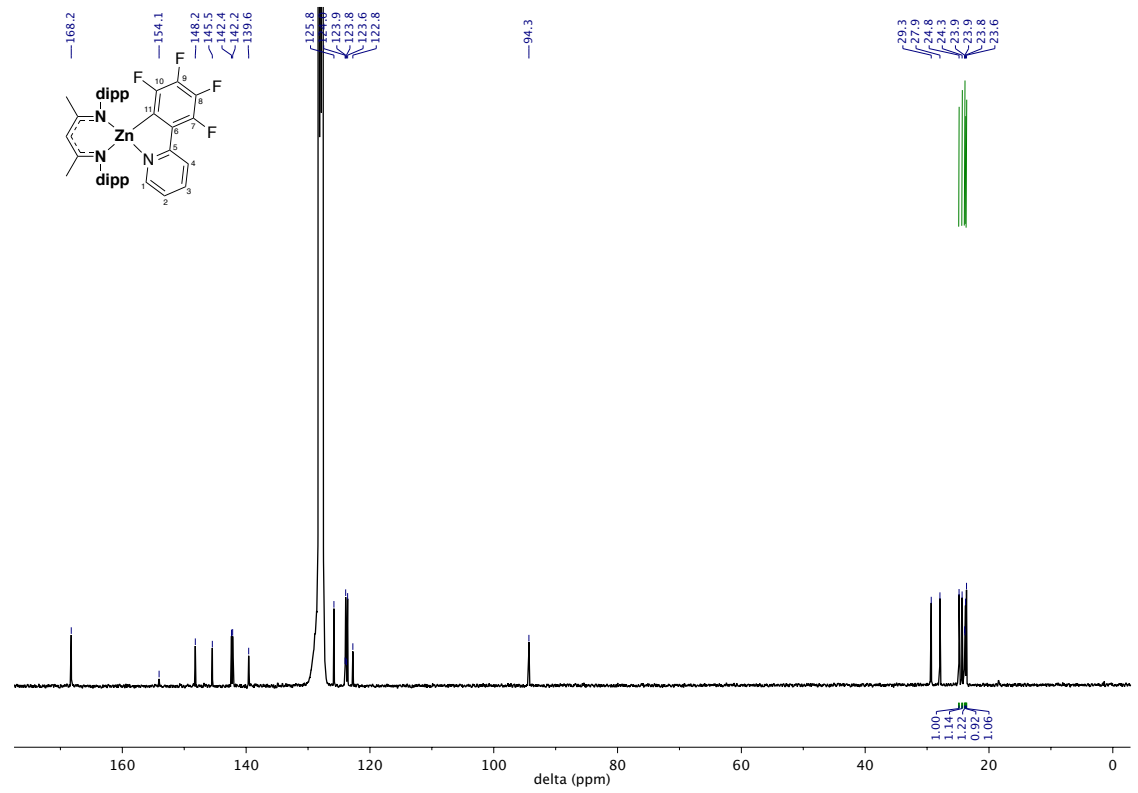


Figure S58: $^{13}C\{^{1}H\}$ NMR spectrum of compound **3a**.



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9. XYZ Coordinates

C–F Activation of C_6F_6 with **1**

1
SCF (wB97X) = -2479.92989036
H(0 K)= -2478.636629
H(298 K)= -2478.564920
G(298 K)= -2478.743585
Lowest Frequency = 17.3440cm-1
PCM (Benzene) Energy = -2479.94003839
wB97XD Corr = -0.1995925865

Mg	1.739740	5.790802	10.118521
Mg	3.556975	3.773877	11.056232
N	1.590527	7.864214	10.148350
N	-0.111343	5.627880	9.200358
N	5.406679	3.150412	10.352354
N	3.685211	2.458818	12.662618
C	0.375599	10.008052	10.222772
C	0.430749	8.507151	10.012901
C	-0.779246	7.910345	9.615514
C	-1.003639	6.604766	9.132189
C	-2.352705	6.347455	8.494929
C	2.776155	8.661864	10.262330
C	3.411759	8.840655	11.505812
C	4.549096	9.650367	11.569726
C	5.076957	10.247163	10.435525
C	4.473924	10.021689	9.204825
C	3.327693	9.236384	9.094619
C	2.906280	8.187242	12.784208
C	4.019419	7.383717	13.468348
C	2.307861	9.217921	13.748802
C	2.736441	8.971268	7.715082
C	3.576140	7.920780	6.976316
C	2.598616	10.240505	6.867348
C	-0.393045	4.354614	8.609079
C	-1.103419	3.373889	9.331624
C	-1.249776	2.103778	8.771728
C	-0.726734	1.800159	7.522021
C	-0.045068	2.778881	6.812264
C	0.141924	4.058539	7.338381
C	-1.694760	3.649018	10.707859
C	-0.943908	2.876899	11.796825
C	-3.192493	3.321556	10.767235
C	0.902292	5.093723	6.517944
C	2.305036	4.603641	6.143582
C	0.113212	5.496875	5.266164
C	7.711661	2.302586	10.571848
C	6.314298	2.546583	11.105797
C	6.073367	2.095669	12.420579
C	4.846469	1.968876	13.095869
C	4.886401	1.152903	14.373200
C	5.696139	3.458888	8.985540
C	5.167055	2.616082	7.981294
C	5.399163	2.943650	6.645431
C	6.104047	4.089108	6.295931
C	6.591862	4.922886	7.290412
C	6.406108	4.625779	8.642670
C	4.365364	1.370166	8.346872
C	5.279380	0.186858	8.691471
C	3.353305	0.959001	7.274855
C	6.956681	5.583397	9.691114
C	6.191372	6.910707	9.684478
C	8.457812	5.840161	9.504119
C	2.495307	1.990177	13.309621
C	1.948014	0.750818	12.910600
C	0.813418	0.271765	13.564218
C	0.212623	0.994173	14.586714
C	0.727785	2.233332	14.935945
C	1.856099	2.758706	14.301273
C	2.526377	-0.046580	11.747903
C	1.589583	0.040471	10.534866
C	2.804891	-1.509647	12.109106
C	2.336382	4.149102	14.692228
C	2.847788	4.198441	16.136692
C	1.223365	5.183451	14.477079
H	0.968781	10.312612	11.088806
H	-0.654786	10.341865	10.355941
H	0.792935	10.528549	9.353689
H	-1.629074	8.580717	9.554718
H	-2.229217	5.897734	7.505030
H	-2.926164	7.270152	8.396753
H	-2.932692	5.638201	9.093618
H	5.030654	9.814504	12.531365
H	5.961761	10.874380	10.506353
H	4.903986	10.466953	8.310490
H	2.106435	7.489382	12.511451
H	4.438411	6.634919	12.786118
H	3.637832	6.864564	14.354411
H	4.839545	8.030912	13.797646
H	3.059531	9.955662	14.052742
H	1.932612	8.728801	14.655215
H	1.474032	9.758880	13.289383
H	1.732375	8.555565	7.845806
H	4.598247	8.283819	6.813500
H	3.137905	7.693217	5.997235
H	3.648595	6.984557	7.542955
H	2.036588	11.019475	7.393619
H	2.072524	10.015176	5.933670
H	3.574537	10.659185	6.597712
H	-1.784062	1.336422	9.328379
H	-0.852920	0.805874	7.101581
H	0.356085	2.543933	5.828140
H	-1.575879	4.717161	10.918345
H	-1.036934	1.794349	11.650431
H	-1.341743	3.112105	12.790261
H	0.125248	3.116031	11.797913
H	-3.757266	3.831044	9.979259
H	-3.609087	3.622298	11.734457
H	-3.369244	2.246062	10.654371
H	1.017266	5.993082	7.134268
H	2.894885	4.352230	7.032376
H	2.851279	5.373263	5.587723
H	2.263282	3.709749	5.509822
H	-0.032237	4.639691	4.598551
H	0.649486	6.271086	4.705847
H	-0.876009	5.889784	5.524454
H	7.693513	2.015198	9.517770
H	8.218471	1.525431	11.146403
H	8.303331	3.221307	10.647283
H	6.929546	1.663098	12.925822

H	4.301881	1.625615	15.166763
H	5.913464	1.016048	14.715131
H	4.445680	0.164344	14.204802
H	5.005561	2.305032	5.859836
H	6.264283	4.332730	5.248882
H	7.131393	5.826637	7.014470
H	3.794296	1.605134	9.254944
H	5.913904	-0.071218	7.835329
H	4.681155	-0.696182	8.947477
H	5.928025	0.407092	9.544230
H	2.695709	1.789641	7.000047
H	2.722284	0.147348	7.651143
H	3.846681	0.589432	6.368503
H	6.812793	5.125609	10.675643
H	6.295769	7.421559	8.719803
H	6.569083	7.585734	10.460167
H	5.121132	6.760905	9.864484
H	9.030813	4.908390	9.454832
H	8.847787	6.439762	10.333582
H	8.653543	6.394768	8.579562
H	0.390090	-0.684961	13.264967
H	-0.663555	0.600824	15.095496
H	0.242231	2.811379	15.719743
H	3.481429	0.407886	11.463575
H	0.608206	-0.391125	10.766732
H	2.005747	-0.512180	9.684323
H	1.422810	1.077864	10.219205
H	3.461386	-1.592019	12.981756
H	3.292312	-2.020194	11.271153
H	1.881669	-2.055555	12.333718
H	3.173566	4.410576	14.035179
H	2.052341	3.945370	16.847106
H	3.208578	5.203491	16.384094
H	3.673449	3.497127	16.295532
H	0.878719	5.179012	13.436525
H	1.574545	6.193394	14.717072
H	0.357414	4.976843	15.115704

Int-A

SCF (wB97X) = -3307.36138787
H(0 K)= -3306.012489
H(298 K)= -3305.929949
G(298 K)= -3306.130637
Lowest Frequency = 18.2379cm-1
PCM (Benzene) Energy = -3307.37257599
wB97XD Corr = -0.2275746825

H	-4.331596	2.303731	-3.290628
H	-3.982734	3.803801	-2.429978
C	-4.140324	2.727269	-2.300634
H	-5.039923	2.595419	-1.690703
H	1.009590	4.528389	2.373834
H	0.464780	3.666518	3.821134
H	0.953633	5.542463	0.301202
H	-1.805508	1.900806	-3.519679
H	0.953160	5.895380	-1.424258
H	-0.868860	-5.469054	-2.375506
C	1.022481	3.557768	2.883261
H	3.246468	5.110467	3.407931
H	2.747908	4.344696	4.922268
C	0.896026	5.082425	-0.691239
H	0.470813	2.845165	2.258391
H	-0.082313	4.600119	-0.779334
H	-1.437811	3.360001	-2.598007
H	3.419264	5.414790	0.144141
C	3.223576	4.159915	3.952403
C	-1.664747	2.292002	-2.505316
H	-5.138572	1.360779	0.715477
C	-2.915993	2.066575	-1.651546
H	-3.096101	0.986393	-1.610176
H	1.129123	-3.940818	-2.168171
H	1.607955	2.463931	5.635582
C	-0.792367	-5.652483	-1.298666
H	-1.777734	-5.967696	-0.941529
H	3.541231	5.454673	-1.624427
H	-0.101877	-6.490537	-1.150643
C	2.461884	3.101347	3.145410
H	-5.399393	0.411808	-0.753921
C	3.388036	4.796431	-0.760796
H	-2.596602	4.615220	-0.809157
H	4.257533	3.852947	4.142638
H	-0.782051	1.806803	-2.072900
H	0.954090	4.816000	-3.257662
C	-5.175834	0.344732	0.318563
H	-4.970919	-2.191593	0.319258
H	-0.967656	-3.569484	-0.877768
C	2.036628	4.076340	-0.864113
C	2.035133	1.599879	5.129854
C	1.112904	-4.032693	-1.077307
H	2.963593	3.009441	2.175658
C	-0.297656	-4.385627	-0.590828
H	1.830468	-4.810328	-0.790473
H	-2.983162	-4.858075	0.379698
C	-2.728109	2.552727	-0.221661
H	1.980941	3.376161	-0.020445
H	1.720644	0.289731	6.807759
C	-2.594678	3.919466	0.027890
H	4.225071	4.094921	-0.708673
H	-5.999566	-0.195047	0.790223
C	-3.977697	-1.804833	0.512709
C	2.511348	1.737390	3.824686
C	-3.869674	-0.400655	0.517281
H	-3.400013	-4.542239	2.054672
H	1.455533	-3.084107	-0.648114
C	1.320181	3.793154	-3.279975
C	2.099218	0.381926	5.793014
C	-3.535909	-4.178293	1.031922
C	1.915680	3.249942	-2.141911
C	-3.017963	-2.759539	0.891984
N	-2.725663	0.249202	0.671646
C	-2.722623	1.665779	0.871697
Mg	-0.834718	-0.649750	0.738865
H	0.681523	3.481553	-5.310789
C	-2.468483	4.409633	1.321450
H	-2.359656	5.477353	1.493233
C	1.160189	3.043212	-4.438932
C	-0.317140	-4.497826	0.926404
N	-1.739350	-2.490348	1.155382
H	-4.595012	-4.232575	0.776819
Mg	1.867129	0.470607	0.421306
C	3.046503	0.605783	3.176443
H	0.864277	-6.293826	0.920189

C	2.665079	-0.715481	5.156086
H	5.761983	0.159463	3.171229
N	3.416547	0.709935	1.797504
C	0.361809	-5.553394	1.539527
C	2.404930	1.925226	-2.204441
C	-0.970937	-3.552197	1.737781
C	-2.634315	2.152698	2.192415
H	-4.922689	1.352933	3.478966
C	-2.504492	3.527803	2.393160
N	3.047354	1.383007	-1.043707
H	2.735682	-1.663224	5.686690
C	3.146268	-0.628584	3.849132
C	1.599773	1.728738	-4.470144
C	4.677253	0.986138	1.490864
H	4.746648	2.856765	-2.617215
C	5.712389	1.085301	2.591331
C	4.373088	1.493096	-0.970351
H	1.891586	-2.523576	2.268760
C	2.237765	1.153139	-3.368920
H	-2.434502	3.914068	3.408336
H	-4.094158	2.479782	4.564136
C	5.133876	1.238588	0.183921
C	-4.060199	1.467629	4.144358
H	1.455053	1.137153	-5.371604
H	5.439697	1.881326	3.292459
C	0.396845	-5.679038	2.919449
H	-2.778316	0.194061	3.018377
C	-2.744735	1.222183	3.394360
H	6.701237	1.301538	2.184865
C	5.160783	1.941122	-2.187040
C	-0.874381	-3.623445	3.146089
H	-1.345832	-1.582386	3.487468
H	2.254190	-3.301014	3.811397
H	6.203517	1.377929	0.080321
H	0.956400	-1.145361	-2.498981
C	2.704079	-2.920311	2.887731
H	0.913019	-6.516882	3.380950
C	3.762960	-1.855925	3.190149
H	6.208330	2.111074	-1.934171
H	-4.171028	0.756449	4.970961
H	4.197416	-1.538823	2.236461
C	-0.207316	-4.709846	3.711731
H	0.860773	-1.084072	-4.265312
H	5.113659	1.174270	-2.967048
C	-1.460331	-2.527952	4.034327
C	1.536206	-1.258645	-3.422594
H	0.368959	-2.267529	5.200679
C	2.720114	-0.287600	-3.457226
H	3.340977	-0.487349	-2.577048
H	-3.558573	-2.647591	3.397467
H	3.145310	-3.773762	2.360479
H	4.503399	-2.872138	4.978476
C	-1.545932	1.328798	4.341606
H	-1.451274	2.336809	4.762915
C	4.888899	-2.460255	4.039093
H	5.655341	-1.720492	4.293873
H	-0.602287	1.091542	3.836923
C	-0.708792	-2.370285	5.359034
H	-0.139509	-4.794413	4.792724
C	-2.958853	-2.712368	4.309193
H	1.886321	-2.295121	-3.478395
H	-1.056015	-1.470806	5.878484
H	-3.315140	-1.932612	4.993501
H	2.980426	-0.466177	-5.620601
H	-1.661245	0.632551	5.180511
H	4.402971	0.168505	-4.787430
C	3.575735	-0.544123	-4.704085
H	-0.885082	-3.218222	6.030974
H	5.374053	-3.279192	3.497393
H	-3.147260	-3.684126	4.781480
H	3.997411	-1.554414	-4.673537
C	-2.364451	-0.994858	-4.237306
C	-3.550928	-0.275289	-4.267224
C	-2.274959	-2.151013	-3.471375
C	-4.641627	-0.697983	-3.519589
C	-3.374010	-2.586780	-2.741527
C	-4.558793	-1.862161	-2.767511
F	-1.326977	-0.571866	-4.957295
F	-3.631942	0.831836	-5.005307
F	-5.767820	0.014164	-3.517324
F	-5.621267	-2.279245	-2.083688
F	-3.291144	-3.710198	-2.031764
F	-1.142011	-2.854837	-3.444575

Int-A'

SCF (wB97X) = -3307.35575875
H(0 K)= -3306.006215
H(298 K)= -3305.923799
G(298 K)= -3306.124057
Lowest Frequency = 14.7935cm-1
PCM (Benzene) Energy = -3307.36692519
wB97XD Corr = -0.2291001763

H	-4.155251	3.188385	-2.462170
H	-4.015310	4.409198	-1.200425
C	-4.140641	3.335892	-1.379138
H	-5.119146	3.048436	-0.979757
H	2.068659	2.774733	-3.695568
H	0.743988	3.815771	-3.145847
H	2.054945	0.471248	-4.349471
H	-1.597395	2.873218	-2.361745
H	2.936575	-1.006338	-4.734496
H	-1.142238	-5.163683	-3.063911
C	1.509400	3.105163	-2.811924
H	3.871588	4.468399	-3.268034
H	2.615239	5.646062	-2.871113
C	2.415242	-0.474285	-3.930793
H	0.989780	2.234600	-2.395993
H	1.541404	-1.065323	-3.638530
H	-1.474078	4.050565	-1.043110
H	4.277187	1.493686	-3.728364
C	3.264927	4.870953	-2.449289
C	-1.648324	2.994744	-1.273165
H	-5.521284	0.727217	1.445869
C	-3.002364	2.533289	-0.733678
H	-3.126913	1.480245	-1.010680
H	0.818570	-3.537352	-2.840885
H	0.739707	5.838044	-1.628981
C	-0.923488	-5.471075	-2.035733
H	-1.827466	-5.926985	-1.618955
H	5.209072	-0.012420	-3.829706
H	-0.154401	-6.250294	-2.083491

C	2.453354	3.749507	-1.789270
H	-5.255714	0.932515	-0.278344
C	4.571993	0.593831	-3.174774
H	-3.141944	4.755259	0.796564
H	3.939625	5.355067	-1.735476
H	-0.827796	2.427110	-0.820784
H	3.871394	-2.673943	-3.751374
C	-5.284439	0.187630	0.524804
H	-4.928362	-2.287821	0.020718
H	-1.182892	-3.464650	-1.350351
C	3.334741	-0.200250	-2.737289
C	0.852350	5.344374	-0.665513
C	0.891982	-3.763203	-1.771597
H	3.162612	2.980191	-1.465192
C	-0.446879	-4.261395	-1.222178
H	1.669065	-4.523069	-1.641944
H	-3.064956	-4.772285	-0.416052
C	-3.061065	2.608230	0.783928
H	2.778141	0.442079	-2.043343
H	-0.517279	6.675240	0.326999
C	-3.169163	3.853866	1.404847
H	5.170009	0.912615	-2.314806
H	-6.088447	-0.517384	0.310396
C	-3.969499	-1.894202	0.335870
C	1.696466	4.238750	-0.558455
C	-3.949116	-0.523776	0.631882
H	-3.101566	-4.892041	1.339141
H	1.232036	-2.860227	-1.252628
C	3.958694	-2.655080	-2.668106
C	0.144308	5.818721	0.431454
C	-3.453678	-4.300168	0.490467
C	3.718994	-1.465585	-1.978269
C	-2.973767	-2.864032	0.579765
N	-2.862306	0.149963	1.006760
C	-3.058547	1.449344	1.583068
Mg	-0.914144	-0.634843	0.829449
H	4.488038	-4.735590	-2.546727
C	-3.334451	3.962729	2.778355
H	-3.435852	4.940753	3.242296
C	4.300784	-3.818986	-1.992997
C	-0.316599	-4.549780	0.265039
N	-1.707450	-2.593456	0.878737
H	-4.543107	-4.340831	0.457347
Mg	1.841948	0.544464	0.584023
C	1.835678	3.613689	0.698652
H	0.843146	-6.324916	-0.075248
C	0.295274	5.198859	1.664360
H	3.877112	4.516216	2.185429
N	2.679105	2.459526	0.809070
C	0.411886	-5.667707	0.676782
C	3.871733	-1.457566	-0.576550
C	-0.879904	-3.710286	1.245287
C	-3.236791	1.547607	2.979703
H	-5.491135	0.134822	3.740589
C	-3.386488	2.811220	3.552001
N	3.748292	-0.210065	0.119305
H	-0.253865	5.576176	2.524684
C	1.153336	4.109669	1.826010
C	4.372269	-3.814523	-0.606421
C	3.971566	2.682875	1.036607
H	6.280635	-0.634516	-0.876356
C	4.448125	4.085047	1.358866
C	4.888543	0.410097	0.414037
H	-0.206715	2.011693	2.984564
C	4.161945	-2.644581	0.124218
H	-3.537893	2.894560	4.626727
H	-4.930927	1.020855	5.166746
C	4.977244	1.708150	0.948209
C	-4.707737	0.176400	4.504491
H	4.606544	-4.737480	-0.081521
H	4.300973	4.745461	0.498016
C	0.587200	-5.959301	2.020961
H	-3.154117	-0.566902	3.245346
C	-3.316649	0.315374	3.873182
H	5.507215	4.087017	1.619897
C	6.220485	-0.270517	0.153272
C	-0.649813	-3.959117	2.615773
H	-1.257185	-2.024333	3.263113
H	-0.731957	3.472857	3.815845
H	5.978573	2.048610	1.183089
H	2.060375	-2.541620	1.901267
C	0.108476	2.780976	3.698040
H	1.141250	-6.844279	2.323378
C	1.360585	3.512292	3.210919
H	7.047307	0.417982	0.332246
H	-4.769380	-0.741698	5.099856
H	2.170778	2.779153	3.135491
C	0.070866	-5.097158	2.979581
H	2.685579	-4.189990	1.889804
H	6.348039	-1.141344	0.803487
C	-1.204352	-3.033482	3.692017
C	2.899329	-3.169078	2.223320
H	0.734961	-2.743475	4.651238
C	4.229156	-2.672221	1.645684
H	4.377199	-1.644640	1.993434
H	-3.322644	-3.356544	3.243167
H	0.291443	2.301762	4.667260
H	0.986744	5.302403	4.408137
C	-2.232089	0.323548	4.956093
H	-2.306494	1.211743	5.593939
C	1.784911	4.571626	4.236391
H	2.674161	5.123492	3.913989
H	-1.228095	0.315016	4.517071
C	-0.304405	-2.949702	4.928241
H	0.236624	-5.313365	4.031342
C	-2.632535	-3.428197	4.089977
H	2.926430	-3.169726	3.320005
H	-0.647481	-2.147095	5.588698
H	-3.009229	-2.772648	4.884407
H	5.239929	-4.582547	1.990356
H	-2.330223	-0.556289	5.602539
H	6.348377	-3.227519	1.736080
C	5.390651	-3.514794	2.183911
H	-0.323493	-3.877237	5.511177
H	2.010341	4.098923	5.198415
H	-2.654614	-4.458618	4.463967
H	5.472161	-3.392069	3.268963
C	-1.943683	0.227847	-3.768607
C	-3.118632	0.960478	-3.856394
C	-1.982692	-1.082949	-3.311030
C	-4.321334	0.403011	-3.439299
C	-3.187584	-1.653277	-2.922348

C	-4.355584	-0.902470	-2.966437
F	-0.785782	0.778240	-4.128483
F	-3.085317	2.211408	-4.316584
F	-5.440588	1.122448	-3.487886
F	-5.508539	-1.434709	-2.568982
F	-3.223253	-2.922345	-2.521183
F	-0.858679	-1.798173	-3.252681

TS-1

SCF (wB97X) = -3307.32024094
H(0 K)= -3305.971951
H(298 K)= -3305.890690
G(298 K)= -3306.085679
Lowest Frequency = -133.2245cm-1
PCM (Benzene) Energy = -3307.32838652
wB97XD Corr = -0.2390382786

H	-3.919357	2.858688	-2.894982
H	-4.310303	4.129710	-1.728861
C	-4.109640	3.057304	-1.833904
H	-5.019609	2.523162	-1.544308
H	1.850897	5.306386	-3.430379
H	0.472027	5.700069	-2.391412
H	2.028534	-0.604858	-5.444423
H	-1.529050	3.515974	-2.436512
H	2.735745	-2.219430	-5.407283
H	-1.349859	-5.870946	-2.128278
C	1.304176	5.000041	-2.531458
H	3.545924	6.568424	-2.057114
H	2.177436	7.175060	-1.121768
C	2.338309	-1.416486	-4.776308
H	0.883546	4.010216	-2.715897
H	1.452340	-1.794582	-4.258586
H	-1.812127	4.526361	-1.023868
H	4.409074	0.230592	-5.326664
C	2.917660	6.369421	-1.182126
C	-1.682668	3.490393	-1.353888
H	-5.518517	0.940759	0.980948
C	-2.900885	2.638850	-0.984911
H	-2.675680	1.590337	-1.213291
H	0.509162	-4.162684	-2.664669
H	0.326003	6.416290	-0.076233
C	-1.016553	-5.858698	-1.084871
H	-1.867577	-6.124713	-0.450935
H	5.157981	-1.335837	-4.969056
H	-0.263543	-6.647049	-0.972900
C	2.236337	4.999798	-1.314486
H	-5.247854	0.561112	-0.718089
C	4.654716	-0.470678	-4.521393
H	-3.516522	4.855141	0.376495
H	3.544574	6.431697	-0.287426
H	-0.771941	3.114806	-0.873817
H	3.806547	-3.567725	-4.060754
C	-5.272326	0.132119	0.290001
H	-4.803496	-2.370720	0.266720
H	-1.185237	-3.725242	-0.959285
C	3.383987	-0.904138	-3.779059
C	0.529888	5.492488	0.461651
C	0.791710	-4.201911	-1.605955
H	3.012929	4.251640	-1.502109
C	-0.433426	-4.483294	-0.731179
H	1.543405	-4.990394	-1.492366
H	-3.422558	-4.670527	0.129884
C	-3.185050	2.736505	0.506073
H	2.971668	-0.014321	-3.295190
H	-0.961727	5.879088	1.962796
C	-3.491281	3.992008	1.038395
H	5.364708	0.026099	-3.853172
H	-6.065729	-0.616499	0.321136
C	-3.866839	-1.883581	0.515960
C	1.498296	4.616237	-0.036195
C	-3.919479	-0.487703	0.586328
H	-2.606878	-4.797959	1.696461
H	1.268781	-3.253970	-1.346406
C	3.890358	-3.260351	-3.021049
C	-0.190669	5.200201	1.608227
C	-3.302587	-4.197112	1.110562
C	3.694052	-1.918205	-2.685012
C	-2.833201	-2.767190	0.913812
N	-2.875325	0.298878	0.880952
C	-3.165346	1.620306	1.362349
Mg	-1.002103	-0.484015	0.435781
H	4.349379	-5.244992	-2.336281
C	-3.767508	4.160212	2.384700
H	-4.010421	5.144200	2.777942
C	4.195410	-4.206371	-2.054327
C	-0.086921	-4.376141	0.746791
N	-1.569138	-2.416716	1.098032
H	-4.279878	-4.203611	1.598692
Mg	1.841826	0.665060	-0.569074
C	1.750305	3.423488	0.671426
H	1.252477	-6.050210	0.631434
C	0.072833	4.026873	2.304495
H	3.786220	4.446900	1.503419
N	2.666232	2.441393	0.171618
C	0.814149	-5.299328	1.285316
C	3.831962	-1.537391	-1.337448
C	-0.646304	-3.401039	1.597399
C	-3.437094	1.783008	2.744300
H	-5.200675	-0.449820	2.875612
C	-3.733651	3.056873	3.228281
N	3.705809	-0.158268	-0.958370
H	-0.502641	3.805078	3.198979
C	1.052217	3.136698	1.866346
C	4.288959	-3.824897	-0.721090
C	3.970718	2.667689	0.246446
H	6.145721	-0.756383	-1.987197
C	4.518598	3.934813	0.878239
C	4.851334	0.501294	-0.766876
H	-0.659041	1.301386	3.008024
C	4.113026	-2.495903	-0.338588
H	-3.951198	3.189955	4.284778
H	-5.584762	0.736725	4.138566
C	4.964411	1.795087	-0.238323
C	-4.858207	-0.020356	3.820185
H	4.512457	-4.575957	0.031536
H	4.841831	4.627352	0.093875
C	1.149372	-5.285067	2.630109
H	-2.796824	-0.171495	3.281049
C	-3.455584	0.595648	3.702853
H	5.397385	3.694264	1.481662
C	6.177118	-0.179532	-1.061094

C	-0.297597	-3.367521	2.966082
H	-1.078170	-1.425853	3.339249
H	0.074559	2.095071	4.407112
H	5.979480	2.161650	-0.130202
H	2.147591	-1.375519	1.248535
C	0.273703	1.409266	3.575445
H	1.843519	-6.018811	3.031716
C	1.416352	1.914010	2.698100
H	6.979457	0.557192	-1.124714
H	-4.858897	-0.823863	4.565842
H	1.672114	1.098319	2.008832
C	0.591066	-4.321874	3.460841
H	2.373116	-3.043904	1.772157
H	6.425486	-0.884422	-0.259645
C	-0.926529	-2.351280	3.908877
C	2.830962	-2.050252	1.780083
H	0.975657	-1.759740	4.814261
C	4.217639	-2.087943	1.128476
H	4.626827	-1.072754	1.170299
H	-3.012089	-2.927660	3.556041
H	0.534938	0.439569	4.012210
H	2.480156	3.013072	4.244155
C	-2.945349	0.947315	5.105453
H	-3.663902	1.566605	5.654275
C	2.660786	2.179926	3.555069
H	3.529676	2.429890	2.939827
H	-1.992698	1.483452	5.074642
C	-0.048489	-2.008069	5.115173
H	0.857223	-4.311515	4.513889
C	-2.304282	-2.833343	4.385067
H	2.895335	-1.707832	2.820803
H	-0.467823	-1.147094	5.647413
H	-2.732323	-2.131820	5.110229
H	4.726596	-3.985098	2.091346
H	-2.803597	0.033198	5.692780
H	6.130223	-3.095340	1.470957
C	5.150176	-2.984627	1.947472
H	0.002362	-2.836296	5.830948
H	2.913227	1.294424	4.149735
H	-2.215927	-3.810946	4.873043
H	5.301695	-2.553515	2.942379
C	0.088525	0.995094	-3.006738
C	-0.759870	1.628321	-3.886727
C	-0.254160	-0.168110	-2.308211
C	-2.000078	1.063963	-4.167641
C	-1.485427	-0.740505	-2.660105
C	-2.365958	-0.112936	-3.523105
F	1.250671	1.612572	-2.619480
F	-0.419523	2.792004	-4.444912
F	-2.840589	1.665685	-5.015036
F	-3.571905	-0.637146	-3.740203
F	-1.904906	-1.833218	-1.990153
F	0.840646	-1.038853	-2.038883

Int-B

SCF (wB97X) = -3307.54641615
H(0 K)= -3306.196568
H(298 K)= -3306.115143
G(298 K)= -3306.311933
Lowest Frequency = 10.7565cm-1
PCM (Benzene) Energy = -3307.55379173
wB97XD Corr = -0.2346051681

H	-4.762741	2.956156	-1.990295
H	-4.684878	4.143716	-0.680518
C	-4.664709	3.071242	-0.905391
H	-5.544559	2.617049	-0.438178
H	1.138936	3.699848	-4.159813
H	0.310680	5.071515	-3.417205
H	2.498814	-0.574243	-5.028177
H	-2.235356	2.907717	-2.204679
H	3.412222	-2.078433	-4.892802
H	-1.872113	-4.909626	-3.369839
C	0.716289	4.072529	-3.222422
H	3.301365	4.797638	-3.534490
H	2.570578	6.087895	-2.563450
C	2.747013	-1.396385	-4.351238
H	-0.116900	3.420273	-2.944579
H	1.822956	-1.936113	-4.118871
H	-2.104501	4.134520	-0.930183
H	4.617141	0.498008	-4.303231
C	2.926015	5.051057	-2.537078
C	-2.161508	3.057271	-1.120669
H	-5.649653	0.140642	2.644867
C	-3.362608	2.424755	-0.415287
H	-3.394601	1.366286	-0.693058
H	-0.142032	-3.008494	-3.329175
H	0.061048	6.093290	-1.520750
C	-1.490703	-5.235602	-2.396197
H	-2.297836	-5.757505	-1.872271
H	5.479733	-0.951021	-3.758234
H	-0.693821	-5.964580	-2.581986
C	1.792822	4.098459	-2.132775
H	-5.651702	1.020974	1.123513
C	4.751177	-0.187811	-3.459609
H	-3.234051	4.654634	1.107938
H	3.769293	5.001101	-1.841595
H	-1.215362	2.621692	-0.780759
H	3.626120	-3.552407	-3.325448
C	-5.573574	0.021316	1.558563
H	-5.337967	-2.389381	0.723210
H	-1.785823	-3.302064	-1.534065
C	3.411622	-0.838987	-3.088431
C	0.346152	5.530511	-0.634955
C	0.189766	-3.374189	-2.349082
H	2.216255	3.091025	-2.067791
C	-0.973135	-4.031120	-1.599322
H	1.006919	-4.086111	-2.507614
H	-3.546437	-4.705912	-0.454011
C	-3.233170	2.505682	1.098763
H	2.761198	-0.042451	-2.706971
H	-0.884311	6.714897	0.671657
C	-3.207285	3.755510	1.720503
H	5.174081	0.386855	-2.631360
H	-6.416497	-0.584198	1.222452
C	-4.335259	-1.992029	0.827290
C	1.230217	4.457011	-0.761293
C	-4.258614	-0.637343	1.197092
H	-3.206001	-5.053864	1.237925
H	0.603976	-2.527422	-1.790951
C	3.651927	-3.235779	-2.286669
C	-0.186906	5.884139	0.596897

C	-3.747885	-4.378784	0.571635
C	3.560855	-1.877194	-1.978949
C	-3.298627	-2.940327	0.738442
N	-3.126512	0.055513	1.287402
C	-3.177487	1.348163	1.899023
Mg	-1.445410	-0.701911	0.353944
H	3.794340	-5.250975	-1.551102
C	-3.160388	3.869893	3.102851
H	-3.150722	4.850959	3.571508
C	3.743248	-4.197156	-1.288741
C	-0.563616	-4.407465	-0.182666
N	-1.999753	-2.651840	0.794823
H	-4.818024	-4.478704	0.758503
Mg	1.745684	0.782513	-0.014340
C	1.603037	3.759179	0.405506
H	0.769699	-5.953635	-0.855650
C	0.176916	5.175522	1.734361
H	4.053485	4.399466	1.948854
N	2.500477	2.643186	0.301084
C	0.351961	-5.444565	0.010598
C	3.618877	-1.498773	-0.621359
C	-1.080775	-3.741412	0.944295
C	-3.141530	1.451267	3.305479
H	-5.168500	0.398387	4.873162
C	-3.138586	2.720898	3.883968
N	3.551211	-0.106895	-0.275307
H	-0.248637	5.452988	2.695500
C	1.088275	4.121681	1.665652
C	3.755957	-3.810587	0.043709
C	3.802398	2.862627	0.471413
H	6.055321	-0.894968	-0.944897
C	4.283238	4.237601	0.889020
C	4.696248	0.527438	-0.023187
H	0.337718	1.577468	2.547674
C	3.714980	-2.462395	0.401219
H	-3.110364	2.812225	4.968030
H	-3.989148	1.049359	6.018071
C	4.804105	1.884671	0.330436
C	-4.168327	0.247581	5.292876
H	3.804340	-4.570041	0.819890
H	3.781250	5.032176	0.333781
C	0.726184	-5.842960	1.284216
H	-3.274970	-0.662266	3.578142
C	-3.091941	0.219410	4.201332
H	5.361817	4.331710	0.755644
C	6.005021	-0.236664	-0.075011
C	-0.687495	-4.119448	2.249027
H	-1.283796	-2.317282	3.195898
H	-0.499326	2.791289	3.518988
H	5.813743	2.231930	0.515101
H	1.638188	-1.513471	2.003782
C	0.476827	2.331497	3.330465
H	1.426478	-6.663735	1.418548
C	1.510231	3.389835	2.932940
H	6.852950	0.449362	-0.096320
H	-4.171948	-0.698718	5.844934
H	2.449115	2.867761	2.720354
C	0.201523	-5.185445	2.391415
H	1.994215	-3.186019	2.444793
H	6.101724	-0.872737	0.812040
C	-1.211164	-3.376419	3.476775
C	2.368572	-2.158422	2.504568
H	0.752956	-3.224306	4.441493
C	3.759663	-2.059855	1.870009
H	4.071217	-1.012003	1.925295
H	-3.374136	-3.605064	3.141436
H	0.791456	1.812255	4.243487
H	0.855301	4.813837	4.460919
C	-1.702919	0.053687	4.828144
H	-1.441206	0.925572	5.439551
C	1.777415	4.343871	4.102019
H	2.473061	5.142439	3.821779
H	-0.929166	-0.059859	4.060584
C	-0.280366	-3.481312	4.689212
H	0.507714	-5.499481	3.385309
C	-2.617423	-3.832028	3.895647
H	2.409146	-1.864282	3.560483
H	-0.618974	-2.800355	5.476593
H	-2.915361	-3.322528	4.820376
H	4.458930	-3.920914	2.785752
H	-1.676112	-0.831174	5.474665
H	5.763684	-2.873526	2.208742
C	4.773528	-2.877260	2.677632
H	-0.288514	-4.491020	5.116169
H	2.209209	3.793683	4.944551
H	-2.631153	-4.911409	4.089348
H	4.871576	-2.462881	3.686415
C	-0.256631	0.386695	-2.488315
C	-0.129054	0.527884	-3.861339
C	-1.246375	-0.271681	-1.809697
C	-1.111297	-0.046269	-4.654947
C	-2.202081	-0.804419	-2.660432
C	-2.167270	-0.717606	-4.047143
F	0.782978	1.030864	-1.771556
F	0.899920	1.179679	-4.418822
F	-1.046502	0.052166	-5.983431
F	-3.120776	-1.262618	-4.806779
F	-3.252760	-1.480591	-2.134730
F	0.292719	-0.028882	0.837254

C–F Activation TSs with C_6F_5H

X1

SCF (wB97X) = -3208.11265052
H(0 K)= -3206.757292
H(298 K)= -3206.676782
G(298 K)= -3206.871078
Lowest Frequency = -241.3459cm-1
wB97XD Corr = -0.2373104054

H	-4.682135	2.173697	-2.791799
H	-4.891152	3.646828	-1.836716
C	-4.733547	2.564475	-1.769173
H	-5.613351	2.132014	-1.282171
H	0.824779	4.620398	-4.374620
H	-0.429518	5.208802	-3.271751
H	2.174270	-1.369227	-5.413030
H	-2.213722	2.716351	-2.746122
H	2.811674	-2.959762	-4.988192
H	-1.089681	-5.895831	-1.634686
C	0.410182	4.510246	-3.366475
H	2.504101	6.322482	-3.461016

H	1.203940	6.952225	-2.446814
C	2.469677	-2.005626	-4.571190
H	0.009667	3.499303	-3.270026
H	1.585182	-2.194123	-3.957924
H	-2.342111	4.030267	-1.568929
H	4.568229	-0.602799	-5.549746
C	2.017147	6.218899	-2.485267
C	-2.253353	2.943548	-1.676093
H	-5.565850	0.735919	1.578690
C	-3.438228	2.234615	-1.016723
H	-3.281321	1.152675	-1.095298
H	0.507037	-4.046894	-2.386958
H	-0.433483	6.201953	-1.063789
C	-0.648827	-5.805968	-0.636204
H	-1.375253	-6.177120	0.093583
H	5.262528	-2.093772	-4.892963
H	0.219351	-6.473637	-0.601997
C	1.479798	4.791924	-2.304762
H	-5.476309	0.286640	-0.121071
C	4.822826	-1.126800	-4.621809
H	-4.030349	4.630580	0.052847
H	2.739453	6.490291	-1.709906
H	-1.301879	2.649467	-1.218403
H	4.119554	-3.950450	-3.495428
C	-5.341223	-0.088850	0.899418
H	-4.689912	-2.548006	1.011848
H	-1.108199	-3.711575	-0.547373
C	3.571610	-1.319772	-3.754544
C	-0.061619	5.407185	-0.419969
C	0.857063	-3.936028	-1.353300
H	2.305214	4.091791	-2.473528
C	-0.238293	-4.351287	-0.367217
H	1.749868	-4.558465	-1.233421
H	-2.765910	-4.830255	0.913092
C	-3.506421	2.587137	0.460122
H	3.206799	-0.328335	-3.469007
H	-1.406872	5.893802	1.186458
C	-3.831149	3.894368	0.829035
H	5.591203	-0.540393	-4.108827
H	-6.060612	-0.892198	1.065488
C	-3.768915	-1.982487	1.094639
C	0.943584	4.561270	-0.896457
C	-3.917461	-0.588921	1.055415
H	-2.266983	-4.557774	2.581556
H	1.159091	-2.896008	-1.211420
C	4.158223	-3.445356	-2.532733
C	-0.606552	5.244139	0.843035
C	-2.923122	-4.192570	1.788992
C	3.891630	-2.075246	-2.469843
C	-2.628931	-2.748703	1.428770
N	-2.909038	0.284733	1.142969
C	-3.247338	1.640769	1.467150
Mg	-1.063095	-0.429416	0.493583
H	4.670286	-5.239843	-1.465395
C	-3.906964	4.268562	2.161250
H	-4.167972	5.288929	2.431136
C	4.468897	-4.173843	-1.394004
C	0.213152	-4.141089	1.072546
N	-1.384936	-2.287050	1.433144
H	-3.961234	-4.303782	2.105775
Mg	1.768332	0.623606	-0.768931
C	1.418130	3.539056	-0.050884
H	1.669856	-5.715246	0.945343
C	-0.130255	4.235260	1.671451
H	3.350254	4.919582	0.426141
N	2.408460	2.598243	-0.490612
C	1.218756	-4.963183	1.589061
C	3.969098	-1.435601	-1.217488
C	-0.349543	-3.158759	1.910723
C	-3.324984	2.009136	2.831416
H	-4.796048	-0.353209	3.494505
C	-3.653125	3.326893	3.151555
N	3.723852	-0.025748	-1.100099
H	-0.572934	4.110702	2.655943
C	0.892818	3.385506	1.253125
C	4.520328	-3.535280	-0.160708
C	3.681128	2.983189	-0.533004
H	6.200320	-0.582999	-2.070630
C	4.082291	4.409521	-0.201268
C	4.792249	0.768217	-1.105683
H	-0.472849	1.605988	2.849319
C	4.287557	-2.164875	-0.051552
H	-3.721521	3.622864	4.195128
H	-5.199283	0.999152	4.572576
C	4.762295	2.153020	-0.877843
C	-4.423168	0.270045	4.310892
H	4.761106	-4.112247	0.728165
H	4.191459	4.983045	-1.127696
C	1.637767	-4.852194	2.906282
H	-2.423975	0.227260	3.558445
C	-3.113815	0.986583	3.944182
H	5.051022	4.416227	0.303143
C	6.177956	0.177761	-1.288652
C	0.100404	-3.006676	3.240856
H	-0.718384	-1.067923	3.499588
H	0.315496	2.661336	4.028769
H	5.727903	2.646113	-0.898008
H	2.238491	-0.973584	1.355455
C	0.497474	1.881938	3.280172
H	2.405376	-5.516350	3.295369
C	1.480490	2.356926	2.212200
H	6.902871	0.958315	-1.524683
H	-4.269248	-0.383538	5.177112
H	1.764508	1.470636	1.629537
C	1.075495	-3.878925	3.723960
H	2.668993	-2.444779	2.219340
H	6.496601	-0.314957	-0.362557
C	-0.482525	-1.925749	4.142103
C	3.010272	-1.431629	1.989089
H	1.472700	-1.188214	4.791211
C	4.378044	-1.465983	1.301170
H	4.684133	-0.429358	1.124626
H	-2.580051	-2.562026	4.060644
H	0.905432	1.013569	3.809774
H	2.553315	3.794263	3.441396
C	-2.502782	1.587032	5.215068
H	-3.227770	2.201844	5.760822
C	2.761957	2.879473	2.874717
H	3.538021	3.104442	2.138003
H	-1.628693	2.207677	4.999630
C	0.493387	-1.435978	5.215617
H	1.418090	-3.785672	4.750803

C	-1.792608	-2.382028	4.798720
H	3.055067	-0.858269	2.924309
H	0.092332	-0.538220	5.699416
H	-2.159364	-1.618477	5.494990
H	5.104050	-3.080584	2.587901
H	-2.192401	0.784246	5.893829
H	6.390912	-2.192157	1.752416
C	5.415366	-2.089414	2.239493
H	0.646043	-2.184869	6.001132
H	3.165109	2.133380	3.569349
H	-1.633464	-3.306369	5.366465
H	5.541636	-1.460922	3.127194
C	0.172009	0.908458	-3.561610
C	-0.791803	1.182848	-4.511189
C	-0.119874	0.070974	-2.460785
C	-2.063328	0.620734	-4.451965
C	-1.371109	-0.549031	-2.470997
C	-2.349897	-0.229010	-3.390350
F	-0.511707	2.010889	-5.524254
F	-2.995939	0.898877	-5.369294
F	-3.584868	-0.713587	-3.245914
F	-1.765985	-1.298653	-1.384738
F	1.088413	-0.768340	-2.122261
H	1.151243	1.364958	-3.677109

X2

SCF (wB97X) = -3208.12226819
H(0 K)= -3206.766943
H(298 K)= -3206.686295
G(298 K)= -3206.880649
Lowest Frequency = -243.3762cm-1
PCM (Benzene) Energy = -3208.13075197
wB97XD Corr = -0.2381916558

H	-4.258174	2.833238	-2.748059
H	-4.434336	4.186569	-1.623003
C	-4.365155	3.094849	-1.688993
H	-5.312998	2.681326	-1.330124
H	1.473774	5.047591	-3.535288
H	0.155879	5.516635	-2.446718
H	2.352453	-0.898709	-5.414490
H	-1.767696	3.165830	-2.445725
H	2.884983	-2.563377	-5.170458
H	-1.463132	-5.452912	-2.487683
C	0.982274	4.809563	-2.584722
H	3.162177	6.501628	-2.300359
H	1.827456	7.071768	-1.294939
C	2.565111	-1.653941	-4.649036
H	0.553721	3.808021	-2.659250
H	1.636347	-1.874410	-4.116395
H	-1.898169	4.315505	-1.106836
H	4.778348	-0.251435	-5.319294
C	2.601513	6.300974	-1.380836
C	-1.881290	3.249570	-1.360092
H	-5.606875	0.887862	1.342596
C	-3.166338	2.561822	-0.894376
H	-3.082828	1.490039	-1.107899
H	0.476075	-3.824751	-2.880993
H	0.080024	6.263905	-0.111089
C	-1.160006	-5.534890	-1.438230
H	-2.046516	-5.776195	-0.845188
H	5.368937	-1.846225	-4.822501
H	-0.468689	-6.381889	-1.359821
C	1.982714	4.897095	-1.426883
H	-5.401454	0.718874	-0.397004
C	4.953386	-0.900748	-4.454227
H	-3.679693	4.834865	0.452618
H	3.280415	6.422250	-0.531409
H	-0.996631	2.817306	-0.878067
H	4.029628	-3.814376	-3.743936
C	-5.379633	0.170490	0.551164
H	-4.913828	-2.331031	0.362519
H	-1.188679	-3.411419	-1.134630
C	3.644798	-1.139070	-3.689159
C	0.354724	5.361526	0.431967
C	0.755522	-3.966088	-1.829919
H	2.780909	4.177699	-1.634841
C	-0.486172	-4.235555	-0.975762
H	1.456242	-4.806415	-1.785063
H	-3.695200	-4.562129	0.068459
C	-3.330902	2.720362	0.608076
H	3.307756	-0.175698	-3.298589
H	-1.063973	5.716085	2.009530
C	-3.593161	3.988307	1.130976
H	5.711420	-0.421155	-3.827601
H	-6.162817	-0.588808	0.525144
C	-3.964667	-1.852382	0.578988
C	1.334319	4.518758	-0.100092
C	-4.011692	-0.461720	0.727750
H	-2.596400	-4.846442	1.432113
H	1.291915	-3.074255	-1.497177
C	4.041998	-3.435803	-2.724126
C	-0.285589	5.063481	1.623898
C	-3.369102	-4.184309	1.043382
C	3.852243	-2.069766	-2.500709
C	-2.909795	-2.745069	0.884383
N	-2.951968	0.307511	1.003042
C	-3.217606	1.630047	1.488947
Mg	-1.098780	-0.443111	0.405040
H	4.381139	-5.378472	-1.867979
C	-3.747268	4.186454	2.494017
H	-3.958409	5.179035	2.884362
C	4.240703	-4.318177	-1.672615
C	-0.135634	-4.277073	0.505581
N	-1.642131	-2.390233	1.030151
H	-4.235483	-4.220951	1.709181
Mg	1.842909	0.592150	-0.586028
C	1.680478	3.355760	0.615369
H	1.204556	-5.935388	0.241366
C	0.066597	3.916328	2.325086
H	3.695342	4.482772	1.376310
N	2.622577	2.411130	0.093291
C	0.761399	-5.248262	0.959194
C	3.897247	-1.594666	-1.175646
C	-0.699193	-3.390375	1.443153
C	-3.372515	1.819667	2.882833
H	-5.035959	-0.498730	3.118368
C	-3.634307	3.104676	3.359313
N	3.745175	-0.194690	-0.895154
H	-0.449639	3.688543	3.253676
C	1.057373	3.058939	1.849006
C	4.254949	-3.841596	-0.367452

C	3.918734	2.691668	0.145405
H	6.225364	-0.830222	-1.799699
C	4.416074	4.011968	0.706263
C	4.871193	0.499428	-0.728082
H	-0.531444	1.182773	3.086711
C	4.101408	-2.482282	-0.096774
H	-3.761300	3.263997	4.426971
H	-5.433502	0.726802	4.341065
C	4.942529	1.832144	-0.295043
C	-4.687269	-0.015990	4.034618
H	4.404339	-4.538838	0.452777
H	4.617375	4.707041	-0.115897
C	1.082012	-5.362975	2.303452
H	-2.645164	-0.104478	3.414059
C	-3.311538	0.645508	3.855508
H	5.355386	3.859105	1.242420
C	6.215756	-0.176975	-0.925791
C	-0.341428	-3.464491	2.806741
H	-1.046048	-1.524792	3.293633
H	0.251297	1.993015	4.450827
H	5.945189	2.235740	-0.206308
H	2.040731	-1.394049	1.374925
C	0.425558	1.316826	3.605928
H	1.765994	-6.137917	2.640059
C	1.506049	1.857830	2.672159
H	7.009749	0.565206	-1.022491
H	-4.640164	-0.786468	4.812738
H	1.757319	1.047108	1.976142
C	0.531955	-4.471409	3.217057
H	2.373935	-2.986846	2.049338
H	6.444019	-0.808114	-0.058834
C	-0.914222	-2.480036	3.817721
C	2.763114	-1.967374	1.971145
H	1.035163	-1.994530	4.684048
C	4.157744	-1.967289	1.337980
H	4.505750	-0.929374	1.310418
H	-3.033819	-2.947624	3.513099
H	0.735312	0.351724	4.022375
H	2.605524	3.006370	4.156835
C	-2.758410	1.025409	5.233432
H	-3.480754	1.613852	5.810939
C	2.779772	2.171898	3.467648
H	3.611937	2.440335	2.810835
H	-1.832982	1.603459	5.161338
C	0.013544	-2.221894	5.008176
H	0.801861	-4.552674	4.266378
C	-2.294847	-2.923913	4.319365
H	2.789849	-1.527561	2.976926
H	-0.358495	-1.371834	5.591140
H	-2.664117	-2.235198	5.088623
H	4.778450	-3.762762	2.426369
H	-2.550319	0.119059	5.813801
H	6.125880	-2.821901	1.762609
C	5.134872	-2.746766	2.223101
H	0.058098	-3.082792	5.685000
H	3.086502	1.300947	4.058558
H	-2.236407	-3.924913	4.762518
H	5.245121	-2.244656	3.189943
C	0.431478	1.179621	-3.354320
C	-0.351030	1.767035	-4.323535
C	-0.024985	0.204613	-2.457851
C	-1.669108	1.343719	-4.443189
C	-1.341908	-0.209408	-2.648825
C	-2.178517	0.382054	-3.577748
F	1.704416	1.617049	-3.153153
F	-2.477937	1.875800	-5.367385
F	-3.470967	0.049768	-3.621333
F	-1.899789	-1.054898	-1.734799
F	1.006643	-0.756200	-2.100946
H	0.044345	2.544443	-4.967584

X3

SCF (wB97X) = -3208.12441794
H(0 K)= -3206.768305
H(298 K)= -3206.687924
G(298 K)= -3206.881313
Lowest Frequency = -223.0728cm-1
PCM (Benzene) Energy = -3208.13274974
wB97XD Corr = -0.2381423653

H	-3.970943	2.920311	-2.848652
H	-4.310823	4.180879	-1.655568
C	-4.137616	3.106026	-1.781428
H	-5.053752	2.587833	-1.482144
H	1.811262	5.290005	-3.437904
H	0.435210	5.678116	-2.392837
H	2.024090	-0.635086	-5.435605
H	-1.549604	3.472191	-2.444985
H	2.746755	-2.243048	-5.392319
H	-1.351170	-5.855122	-2.157206
C	1.272566	4.984416	-2.533835
H	3.507797	6.570608	-2.085356
H	2.141839	7.176638	-1.145906
C	2.340035	-1.442013	-4.764747
H	0.859855	3.989775	-2.710439
H	1.456045	-1.826810	-4.248546
H	-1.788872	4.505164	-1.036835
H	4.399330	0.218131	-5.316007
C	2.886122	6.374624	-1.204976
C	-1.688703	3.463504	-1.359922
H	-5.515093	0.947157	1.006884
C	-2.921330	2.644559	-0.967134
H	-2.731559	1.592300	-1.211592
H	0.528089	-4.161737	-2.679837
H	0.307629	6.418433	-0.073979
C	-1.027237	-5.846546	-1.110789
H	-1.887429	-6.101011	-0.484712
H	5.160447	-1.339864	-4.947172
H	-0.285517	-6.644520	-0.991215
C	2.212084	5.000139	-1.322710
H	-5.245561	0.592943	-0.697721
C	4.648034	-0.476664	-4.506054
H	-3.475942	4.865025	0.412473
H	3.518317	6.446956	-0.314678
H	-0.780847	3.069827	-0.888783
H	3.816742	-3.579470	-4.033061
C	-5.271150	0.148393	0.303596
H	-4.806763	-2.356790	0.250948
H	-1.168270	-3.710336	-0.985206
C	3.378226	-0.917007	-3.766214
C	0.518734	5.497335	0.465821
C	0.805456	-4.214441	-1.620344

H	2.992121	4.255411	-1.509471
C	-0.428652	-4.478819	-0.752943
H	1.541629	-5.018034	-1.510021
H	-3.443338	-4.654251	0.097003
C	-3.173777	2.741084	0.529761
H	2.957371	-0.028417	-3.287861
H	-0.957792	5.887893	1.980580
C	-3.456305	3.998635	1.070320
H	5.351093	0.029930	-3.837859
H	-6.066310	-0.598772	0.323666
C	-3.869278	-1.873474	0.504606
C	1.485012	4.621480	-0.036761
C	-3.919743	-0.478486	0.591186
H	-2.610333	-4.802231	1.653034
H	1.299430	-3.278029	-1.351384
C	3.896341	-3.266276	-2.994755
C	-0.189507	5.208514	1.620953
C	-3.309734	-4.192192	1.081299
C	3.692066	-1.923482	-2.666361
C	-2.836390	-2.762324	0.893610
N	-2.873761	0.301884	0.893629
C	-3.154716	1.622000	1.382170
Mg	-1.002663	-0.477027	0.427712
H	4.362335	-5.245196	-2.297996
C	-3.715737	4.165230	2.420128
H	-3.940231	5.150990	2.819946
C	4.202738	-4.205788	-2.022094
C	-0.089430	-4.376704	0.726843
N	-1.571506	-2.415929	1.078863
H	-4.281482	-4.199319	1.580507
Mg	1.831385	0.678956	-0.568229
C	1.746325	3.432811	0.673854
H	1.247132	-6.052855	0.611879
C	0.082682	4.038457	2.319502
H	3.785864	4.459144	1.496494
N	2.661258	2.452142	0.170496
C	0.807417	-5.303398	1.266477
C	3.824915	-1.534436	-1.320583
C	-0.651367	-3.403346	1.577803
C	-3.413315	1.782444	2.766895
H	-5.190624	-0.440444	2.887684
C	-3.689950	3.057848	3.258595
N	3.696467	-0.153005	-0.950245
H	-0.484261	3.818786	3.219955
C	1.058878	3.148017	1.875337
C	4.289558	-3.816859	-0.690636
C	3.965532	2.679796	0.239846
H	6.137190	-0.760370	-1.973955
C	4.513745	3.951208	0.862615
C	4.842345	0.507478	-0.763602
H	-0.641293	1.304929	3.020252
C	4.107150	-2.486439	-0.315918
H	-3.896691	3.189259	4.317437
H	-5.568471	0.745965	4.152847
C	4.957503	1.804883	-0.243946
C	-4.846768	-0.015495	3.833809
H	4.513463	-4.562848	0.066910
H	4.821011	4.645097	0.072964
C	1.136387	-5.294673	2.612768
H	-2.786849	-0.178732	3.293353
C	-3.439637	0.590826	3.719699
H	5.402165	3.718031	1.454612
C	6.168108	-0.176111	-1.052519
C	-0.307505	-3.374695	2.947937
H	-1.084194	-1.432215	3.323050
H	0.091517	2.100892	4.418737
H	5.973041	2.171484	-0.140698
H	2.130842	-1.375185	1.261762
C	0.291882	1.416620	3.586025
H	1.827007	-6.031322	3.015166
C	1.430275	1.926696	2.705994
H	6.970586	0.559990	-1.121614
H	-4.854420	-0.820748	4.577517
H	1.687506	1.112451	2.015779
C	0.576492	-4.332739	3.443821
H	2.369639	-3.039013	1.794701
H	6.416014	-0.874485	-0.245214
C	-0.935670	-2.358842	3.891448
C	2.818739	-2.041285	1.798233
H	0.966656	-1.773349	4.799993
C	4.206761	-2.070320	1.149096
H	4.607279	-1.051497	1.186232
H	-3.021989	-2.929737	3.534715
H	0.558244	0.447443	4.021168
H	2.494263	3.029846	4.249181
C	-2.926453	0.931072	5.123929
H	-3.638954	1.555063	5.675355
C	2.676170	2.197649	3.559247
H	3.542073	2.451494	2.941277
H	-1.968278	1.457542	5.095796
C	-0.058514	-2.019126	5.099418
H	0.838151	-4.325825	4.498034
C	-2.314832	-2.839591	4.364796
H	2.878525	-1.692952	2.837354
H	-0.476234	-1.157405	5.631703
H	-2.742222	-2.139947	5.092100
H	4.731187	-3.958467	2.121550
H	-2.794235	0.012985	5.707214
H	6.127622	-3.059493	1.498482
C	5.146091	-2.955001	1.973403
H	-0.010890	-2.848066	5.814624
H	2.934331	1.313062	4.152818
H	-2.228650	-3.819083	4.849377
H	5.292745	-2.517886	2.966439
C	0.101935	0.967150	-3.018500
C	-0.731776	1.585007	-3.921738
C	-0.254846	-0.199089	-2.330669
C	-1.962462	1.030423	-4.251173
C	-1.484466	-0.766796	-2.697633
C	-2.328514	-0.138359	-3.595528
F	1.262215	1.581053	-2.610688
F	-0.354002	2.746986	-4.470002
F	-3.522189	-0.689963	-3.836893
F	-1.913822	-1.864312	-2.040970
F	0.821045	-1.072583	-2.034889
H	-2.613826	1.497041	-4.979090

X4

SCF (wB97X) = -3208.12162157
H(0 K)= -3206.765153
H(298 K)= -3206.685001
G(298 K)= -3206.877154

Lowest Frequency = -233.4508cm-1
PCM (Benzene) Energy = -3208.12976985
wB97XD Corr = -0.2379090079

H	-3.896251	2.865023	-2.916237
H	-4.300330	4.131679	-1.750025
C	-4.101174	3.059192	-1.857030
H	-5.017531	2.527338	-1.582966
H	1.867115	5.321185	-3.428261
H	0.495463	5.733269	-2.387918
H	2.002323	-0.537076	-5.421401
H	-1.516292	3.511702	-2.430421
H	2.685448	-2.162801	-5.407307
H	-1.354921	-5.920772	-2.095436
C	1.313062	5.017317	-2.532971
H	3.576683	6.545463	-2.043993
H	2.215065	7.162346	-1.104775
C	2.310199	-1.358518	-4.764476
H	0.872387	4.038450	-2.727469
H	1.426721	-1.727059	-4.235681
H	-1.811613	4.517833	-1.016908
H	4.401435	0.260729	-5.331553
C	2.945074	6.347811	-1.171060
C	-1.680392	3.482938	-1.349550
H	-5.547802	0.890096	1.025428
C	-2.904242	2.632555	-0.995353
H	-2.680909	1.584096	-1.226160
H	0.451855	-4.172310	-2.658255
H	0.329356	6.407724	-0.092997
C	-1.001738	-5.899603	-1.058685
H	-1.830678	-6.195631	-0.408372
H	5.125886	-1.323269	-5.001859
H	-0.221188	-6.662998	-0.964866
C	2.244189	4.988895	-1.315237
H	-5.236283	0.626748	-0.685623
C	4.646078	-0.453594	-4.537515
H	-3.542310	4.846903	0.356388
H	3.571735	6.395151	-0.275496
H	-0.775127	3.104326	-0.861766
H	3.778009	-3.532734	-4.094333
C	-5.276864	0.129812	0.289852
H	-4.807204	-2.375893	0.263407
H	-1.239548	-3.774106	-0.932691
C	3.379167	-0.870769	-3.779594
C	0.530999	5.486918	0.450887
C	0.743895	-4.181068	-1.601354
H	3.009325	4.230181	-1.508424
C	-0.460116	-4.505560	-0.712421
H	1.532971	-4.930882	-1.480448
H	-3.365011	-4.698960	0.143212
C	-3.200786	2.730367	0.493758
H	2.989196	0.022161	-3.282903
H	-0.966075	5.882263	1.944468
C	-3.515115	3.986118	1.021240
H	5.375819	0.022334	-3.875330
H	-6.061596	-0.627833	0.257270
C	-3.870156	-1.888151	0.509985
C	1.500670	4.607653	-0.039290
C	-3.923560	-0.491603	0.581222
H	-2.631998	-4.780055	1.751142
H	1.176496	-3.206885	-1.361385
C	3.870981	-3.238541	-3.051532
C	-0.193520	5.201571	1.596580
C	-3.303944	-4.200845	1.117120
C	3.688252	-1.898874	-2.698464
C	-2.837826	-2.770211	0.916635
N	-2.881912	0.295100	0.879811
C	-3.177425	1.617739	1.354780
Mg	-0.999470	-0.481198	0.448549
H	4.317961	-5.234935	-2.393129
C	-3.795397	4.158116	2.366126
H	-4.044389	5.142339	2.754949
C	4.174493	-4.198417	-2.098123
C	-0.101267	-4.385008	0.761637
N	-1.575658	-2.418066	1.106805
H	-4.304688	-4.209513	1.554537
Mg	1.845081	0.649329	-0.554347
C	1.751162	3.418690	0.675905
H	1.238226	-6.059123	0.649631
C	0.068689	4.032738	2.300682
H	3.781451	4.451622	1.502490
N	2.668450	2.433004	0.184762
C	0.804332	-5.303336	1.300756
C	3.837008	-1.534753	-1.347375
C	-0.653286	-3.401788	1.608019
C	-3.450823	1.784676	2.736053
H	-5.182260	-0.483373	2.880673
C	-3.755920	3.058576	3.214415
N	3.714363	-0.160705	-0.950445
H	-0.508771	3.816356	3.195197
C	1.050045	3.140410	1.871216
C	4.281218	-3.832906	-0.761353
C	3.972595	2.659578	0.262998
H	6.152111	-0.736437	-1.998784
C	4.520052	3.926568	0.895855
C	4.859122	0.498305	-0.756151
H	-0.661789	1.312228	3.022372
C	4.118094	-2.507221	-0.362139
H	-3.974674	3.194987	4.270218
H	-5.592356	0.719902	4.120370
C	4.969422	1.788458	-0.218888
C	-4.852803	-0.031830	3.819601
H	4.504644	-4.594344	-0.019175
H	4.867440	4.608244	0.112429
C	1.149628	-5.278404	2.642802
H	-2.788581	-0.158931	3.285440
C	-3.458156	0.602161	3.701109
H	5.383994	3.681166	1.518719
C	6.184661	-0.177745	-1.061470
C	-0.295978	-3.359055	2.974313
H	-1.072588	-1.414486	3.342735
H	0.065828	2.119763	4.417098
H	5.983583	2.156625	-0.107143
H	2.174067	-1.384112	1.254302
C	0.268651	1.426810	3.592227
H	1.847472	-6.008366	3.044891
C	1.413484	1.925274	2.714099
H	6.987945	0.558997	-1.111174
H	-4.847121	-0.822205	4.579101
H	1.672769	1.104750	2.032090
C	0.596176	-4.309630	3.470130
H	2.382895	-3.064230	1.746494

H	6.432124	-0.898882	-0.274396
C	-0.921991	-2.338706	3.914628
C	2.852419	-2.076261	1.769327
H	0.980884	-1.745548	4.817479
C	4.234758	-2.117998	1.109055
H	4.652706	-1.106861	1.160675
H	-3.008834	-2.912809	3.564869
H	0.529594	0.461491	4.038610
H	2.469422	3.040285	4.254324
C	-2.955692	0.968199	5.102931
H	-3.685543	1.577254	5.648356
C	2.654121	2.201245	3.573471
H	3.524892	2.447309	2.959407
H	-2.012397	1.520493	5.070964
C	-0.042999	-1.993476	5.119554
H	0.869045	-4.291844	4.521324
C	-2.300118	-2.817481	4.393094
H	2.926599	-1.753356	2.815517
H	-0.462008	-1.131574	5.650556
H	-2.726356	-2.113505	5.116937
H	4.733071	-4.030633	2.046629
H	-2.798935	0.058918	5.694006
H	6.140534	-3.146170	1.427292
C	5.164599	-3.032316	1.911471
H	0.008180	-2.820442	5.836781
H	2.905927	1.321647	4.177075
H	-2.212667	-3.793949	4.883555
H	5.326320	-2.614109	2.910280
C	0.075794	1.027985	-2.968258
C	-0.763328	1.622613	-3.884293
C	-0.243751	-0.134796	-2.260065
C	-1.974439	1.005276	-4.180296
C	-1.446103	-0.744549	-2.650305
C	-2.328692	-0.177686	-3.548045
F	1.219398	1.671929	-2.575352
F	-0.438412	2.788911	-4.449768
F	-2.800150	1.587106	-5.061333
F	-1.816527	-1.861682	-1.983858
F	0.898458	-0.967426	-1.981070
H	-3.282293	-0.650398	-3.754625

X5

SCF (wB97X) = -3208.12111782
H(0 K)= -3206.765005
H(298 K)= -3206.684738
G(298 K)= -3206.877746
Lowest Frequency = -244.7395cm-1
PCM (Benzene) Energy = -3208.12881356
wB97XD Corr = -0.2380395143

H	-4.041527	3.210447	-2.521503
H	-4.288172	4.409581	-1.243069
C	-4.165578	3.338322	-1.440008
H	-5.094089	2.841442	-1.142623
H	1.781915	5.416989	-3.260006
H	0.479927	5.822638	-2.131743
H	1.651251	0.085557	-5.575188
H	-1.587214	3.716110	-2.117908
H	2.304096	-1.535587	-5.809829
H	-1.654644	-5.723350	-2.905736
C	1.268353	5.092064	-2.348085
H	3.589586	6.551917	-1.922719
H	2.294116	7.158541	-0.888110
C	1.991180	-0.812914	-5.047772
H	0.789819	4.132934	-2.554085
H	1.141442	-1.236303	-4.504070
H	-1.777001	4.611630	-0.613323
H	4.067536	0.852592	-5.557782
C	3.000760	6.332351	-1.025494
C	-1.703102	3.604705	-1.036840
H	-5.283675	0.795972	-0.574154
C	-2.945092	2.776814	-0.697233
H	-2.785652	1.749715	-1.046678
H	0.177513	-4.004709	-3.437470
H	0.453573	6.403998	0.200561
C	-1.241260	-5.795081	-1.893909
H	-2.037874	-6.123750	-1.219823
H	4.781512	-0.768617	-5.488635
H	-0.477083	-6.579811	-1.909373
C	2.262897	4.994873	-1.184366
H	-6.075008	-0.508906	0.322093
C	4.353873	0.038686	-4.882396
H	-3.437736	4.854213	0.919369
H	3.674903	6.330629	-0.163777
H	-0.793288	3.152827	-0.625362
H	3.467550	-3.063755	-4.763893
C	-5.270998	0.227641	0.362516
H	-4.854702	-2.239049	-0.070644
H	-1.421661	-3.689843	-1.585056
C	3.137215	-0.459912	-4.092378
C	0.659076	5.454856	0.691767
C	0.522051	-4.082199	-2.399157
H	3.000124	4.229690	-1.448004
C	-0.640153	-4.446960	-1.470565
H	1.301942	-4.850505	-2.363826
H	-3.504904	-4.568678	-0.554649
C	-3.150778	2.728327	0.807787
H	2.798502	0.367175	-3.461811
H	-0.747056	5.817764	2.278803
C	-3.395865	3.925713	1.485041
H	5.138765	0.416200	-4.219623
H	-5.471648	0.931692	1.172267
C	-3.894405	-1.813055	0.199412
C	1.579588	4.576575	0.113611
C	-3.917990	-0.443721	0.504742
H	-2.689742	-4.870264	0.986142
H	0.983901	-3.133033	-2.121013
C	3.635438	-2.903947	-3.701399
C	-0.013319	5.133991	1.859864
C	-3.374650	-4.198199	0.468219
C	3.505617	-1.617206	-3.172991
C	-2.873740	-2.765109	0.426514
N	-2.857731	0.266402	0.900389
C	-3.104357	1.529019	1.540756
Mg	-0.977858	-0.438436	0.352843
H	4.072864	-4.974894	-3.326234
C	-3.587502	3.953815	2.856333
H	-3.781966	4.894477	3.365404
C	3.974198	-3.981163	-2.896315
C	-0.204140	-4.450575	-0.011599
N	-1.589728	-2.470430	0.586771
H	-4.350260	-4.236926	0.957220

Mg	1.840436	0.656841	-0.625886
C	1.839293	3.352171	0.763375
H	1.065628	-6.151031	-0.337311
C	0.251244	3.926433	2.493847
H	3.914096	4.294087	1.581837
N	2.718664	2.379473	0.184667
C	0.690203	-5.443706	0.398804
C	3.751206	-1.425970	-1.800374
C	-0.679750	-3.528118	0.943465
C	-3.293993	1.546278	2.944161
H	-5.055280	-0.682061	2.864487
C	-3.531696	2.766647	3.576200
N	3.673558	-0.111246	-1.228640
H	-0.287671	3.680450	3.404658
C	1.187437	3.032175	1.975905
C	4.175143	-3.786821	-1.535136
C	4.028239	2.585266	0.220941
H	6.040507	-0.563342	-2.484242
C	4.619266	3.801332	0.911706
C	4.835431	0.515300	-1.029743
H	-0.515541	1.158998	3.067272
C	4.074102	-2.517810	-0.965906
H	-3.683773	2.791161	4.651913
H	-5.406804	0.354430	4.261610
C	4.990641	1.741774	-0.368093
C	-4.690607	-0.363365	3.844376
H	4.426548	-4.638182	-0.908488
H	4.942991	4.528791	0.159945
C	1.091968	-5.557714	1.719759
H	-2.644783	-0.454157	3.240207
C	-3.288986	0.260319	3.764255
H	5.505385	3.505807	1.479349
C	6.132034	-0.131094	-1.485664
C	-0.262180	-3.628539	2.290404
H	-0.981663	-1.714138	2.884646
H	0.243387	1.890488	4.486398
H	6.014228	2.086996	-0.270076
H	2.253773	-1.627686	0.928661
C	0.426143	1.238786	3.623854
H	1.777243	-6.345931	2.020391
C	1.557012	1.771606	2.746364
H	6.945269	0.596228	-1.483765
H	-4.679397	-1.245894	4.494380
H	1.790638	0.985935	2.016408
C	0.610015	-4.653045	2.656472
H	2.487673	-3.362249	1.142179
H	6.406026	-0.951238	-0.812755
C	-0.813146	-2.690928	3.355481
C	2.962482	-2.386780	1.283298
H	1.142178	-2.182070	4.190182
C	4.295279	-2.320572	0.530577
H	4.709224	-1.318520	0.684260
H	-2.921806	-3.214800	3.069733
H	0.687875	0.249611	4.015100
H	2.659166	2.800154	4.314526
C	-2.737158	0.447754	5.181924
H	-3.431052	1.011155	5.816039
C	2.819851	1.994568	3.588621
H	3.677525	2.265206	2.966197
H	-1.776644	0.971322	5.183169
C	0.139830	-2.464509	4.531598
H	0.924651	-4.744325	3.692020
C	-2.169376	-3.199076	3.864502
H	3.111197	-2.228109	2.358788
H	-0.244896	-1.661895	5.170557
H	-2.547602	-2.560241	4.670438
H	4.876951	-4.331601	1.169309
H	-2.594653	-0.527721	5.660460
H	6.226361	-3.349073	0.571915
C	5.288278	-3.316398	1.136594
H	0.234378	-3.357393	5.159560
H	3.078989	1.084510	4.141579
H	-2.067282	-4.216453	4.259501
H	5.520654	-3.030150	2.167516
C	-0.168086	1.100305	-2.821483
C	-1.117015	1.700789	-3.609705
C	-0.373688	-0.136017	-2.187608
C	-2.324537	1.044891	-3.854126
C	-1.554489	-0.833743	-2.518449
C	-2.519609	-0.211676	-3.295422
F	0.971774	1.778480	-2.474497
F	-0.905113	2.910931	-4.131983
F	-3.260341	1.626614	-4.613838
F	-3.673673	-0.838867	-3.543206
F	0.845730	-0.894917	-2.079706
H	-1.745934	-1.829394	-2.135148

C–F Activation TS with $C_6F_4H_2$

SCF (wB97X) = -3108.91355441
H(0 K)= -3107.548079
H(298 K)= -3107.469127
G(298 K)= -3107.659407
Lowest Frequency = -340.8747cm-1
PCM (Benzene) Energy = -3108.92270876
wB97XD Corr = -0.2353414336

H	-5.023059	3.667429	-1.857721
H	-4.812555	4.808269	-0.524874
C	-4.806742	3.744631	-0.786675
H	-5.622526	3.263704	-0.238495
H	1.055988	4.459605	-4.090471
H	-0.140609	5.050579	-2.924428
H	1.992732	-0.122082	-6.018451
H	-2.472829	3.818092	-2.289754
H	3.030257	-1.538772	-6.168455
H	-1.656300	-5.109704	-3.099659
C	0.711828	4.372708	-3.053662
H	2.832775	6.138205	-3.404124
H	1.613208	6.882545	-2.368558
C	2.379711	-0.990976	-5.476810
H	0.361499	3.348215	-2.897448
H	1.530320	-1.636370	-5.229934
H	-2.320532	4.905848	-0.898675
H	4.098768	1.030208	-5.415708
C	2.400552	6.121101	-2.397986
C	-2.332851	3.853136	-1.202442
H	-5.977697	-0.210492	0.960004
C	-3.450851	3.095029	-0.478108
H	-3.496699	2.075689	-0.866036
H	0.567924	-3.974540	-3.260369
H	0.158141	6.369503	-0.760234

C	-1.494884	-5.306186	-2.034738
H	-2.475804	-5.352826	-1.552694
H	5.122949	-0.387805	-5.134740
H	-1.026366	-6.292753	-1.939866
C	1.844394	4.727077	-2.081439
H	-5.249771	1.317709	1.493928
C	4.381031	0.275241	-4.673543
H	-3.461445	5.132053	1.216766
H	3.176360	6.422212	-1.686247
H	-1.341652	3.450892	-0.964343
H	3.514815	-3.158855	-4.819534
C	-5.200261	0.524636	0.746568
H	-4.873926	-1.870712	0.135321
H	-1.110715	-3.251644	-1.581225
C	3.143851	-0.520966	-4.233409
C	0.496050	5.556959	-0.120095
C	0.730879	-4.162746	-2.195709
H	2.648255	4.001128	-2.241861
C	-0.601411	-4.209157	-1.441612
H	1.268512	-5.113211	-2.108648
H	-3.630061	-4.049618	1.838899
C	-3.174267	3.014925	1.014483
H	2.487804	0.167891	-3.690216
H	-0.685521	6.206491	1.555779
C	-3.252557	4.204009	1.744471
H	4.854884	0.796596	-3.837964
H	-5.418100	0.967057	-0.231989
C	-3.876411	-1.500155	0.340993
C	1.383897	4.608644	-0.633470
C	-3.833608	-0.136974	0.692162
H	-4.495526	-3.968247	0.299698
H	1.389686	-3.384909	-1.796308
C	3.661676	-2.959356	-3.761993
C	0.021584	5.471317	1.179901
C	-3.508315	-3.896506	0.759363
C	3.501851	-1.658465	-3.278217
C	-2.914271	-2.518819	0.540427
N	-2.727340	0.551544	0.989729
C	-2.884171	1.809267	1.686893
Mg	-0.949177	-0.360550	0.243449
H	4.133271	-5.009622	-3.318880
C	-3.085213	4.224273	3.117098
H	-3.152623	5.158374	3.669013
C	4.008327	-4.006771	-2.918708
C	-0.345084	-4.379216	0.047526
N	-1.604502	-2.321388	0.638719
H	-2.876019	-4.703299	0.392321
Mg	1.814141	0.748086	-0.821226
C	1.812185	3.566819	0.211703
H	0.715720	-6.215766	-0.278035
C	0.443523	4.433135	2.001207
H	3.943205	4.653101	0.801248
N	2.689661	2.543593	-0.271380
C	0.384741	-5.494516	0.465774
C	3.713858	-1.425255	-1.900610
C	-0.797312	-3.458109	1.015344
C	-2.759414	1.817387	3.100043
H	-4.272844	-0.594120	3.045094
C	-2.854765	3.029272	3.784709
N	3.637306	-0.084124	-1.392392
H	0.050812	4.366444	3.012055
C	1.348449	3.476314	1.542498
C	4.171468	-3.771072	-1.561465
C	3.990344	2.793593	-0.339564
H	6.046207	-0.706587	-2.513292
C	4.534436	4.161181	0.027071
C	4.801422	0.553382	-1.244413
H	-0.095024	1.680343	3.068296
C	4.026314	-2.489185	-1.028992
H	-2.752060	3.042809	4.865167
H	-4.658799	0.361605	4.489581
C	4.957097	1.867444	-0.774135
C	-3.891435	-0.258489	4.011574
H	4.416192	-4.599562	-0.901288
H	4.517526	4.806241	-0.858774
C	0.696759	-5.701442	1.800431
H	-1.867374	-0.091983	3.325909
C	-2.575139	0.525797	3.889056
H	5.571225	4.083650	0.360498
C	6.102033	-0.161097	-1.568843
C	-0.478332	-3.659861	2.374335
H	-1.681701	-2.038575	3.021505
H	0.661456	2.741552	4.263747
H	5.979083	2.226910	-0.742822
H	2.044165	-2.051563	0.834702
C	0.860281	1.952637	3.528664
H	1.266174	-6.575936	2.104197
C	1.876716	2.395686	2.478624
H	6.929488	0.548202	-1.616604
H	-3.745198	-1.149814	4.633433
H	2.115457	1.514203	1.869490
C	0.275914	-4.774600	2.742080
H	2.642005	-3.695807	1.065421
H	6.328166	-0.896719	-0.789133
C	-0.905640	-2.677961	3.451454
C	2.893552	-2.638145	1.205990
H	0.678752	-1.240836	2.989650
C	4.188185	-2.270898	0.470603
H	4.370162	-1.204145	0.637823
H	-2.342053	-4.022245	4.397501
H	1.243129	1.085175	4.077673
H	3.017068	3.761543	3.729892
C	-2.002667	0.731852	5.295092
H	-2.725127	1.226586	5.954111
C	3.178835	2.840087	3.158309
H	3.974833	3.025963	2.431931
H	-1.082970	1.324703	5.290681
C	0.284759	-1.795876	3.850750
H	0.527229	-4.924872	3.789349
C	-1.514947	-3.362238	4.679460
H	2.988844	-2.451496	2.282233
H	0.005341	-1.071404	4.623163
H	-1.902100	-2.612033	5.378411
H	5.204812	-4.118857	1.059070
H	-1.778632	-0.239929	5.747901
H	6.302638	-2.841452	0.516900
C	5.374811	-3.036697	1.065618
H	1.102876	-2.411804	4.242896
H	3.532416	2.068483	3.851217
H	-0.778109	-3.961780	5.224930
H	5.527517	-2.740220	2.108562
C	-1.720968	0.637351	-2.267919

C	-2.768832	0.007870	-2.915843
C	-0.448295	0.030150	-2.230276
C	-2.592202	-1.166781	-3.630557
C	-0.236082	-1.127304	-3.015127
C	-1.302619	-1.692200	-3.681456
F	-3.994838	0.548840	-2.855508
F	-1.117077	-2.808588	-4.405596
F	0.688177	1.044504	-2.427147
H	0.736421	-1.601089	-3.072805
F	-3.614010	-1.777397	-4.242538
H	-1.891867	1.583058	-1.780112

C–F Activation of C_6F_6 with **2**

2

SCF (wB97X) = -2008.27258150
H(0 K)= -2007.329881
H(298 K)= -2007.271929
G(298 K)= -2007.427928
Lowest Frequency = -2.6965cm-1
PCM (Benzene) Energy = -2008.28243030
wB97XD Corr = -0.1260211221

C	-1.105161	-0.125192	-0.602701
C	-0.677586	0.024551	0.724932
C	0.685523	0.209374	1.012157
C	1.597367	0.267966	-0.040035
C	1.194198	0.143811	-1.369030
C	-0.160811	-0.046503	-1.626679
N	-1.610317	-0.112717	1.798584
C	-2.196697	0.967030	2.301534
C	-1.896292	2.321082	1.692182
C	1.154082	0.323059	2.440553
C	2.201778	0.174491	-2.490747
C	-2.552490	-0.400283	-0.920701
Mg	-1.910787	-2.039932	2.446435
N	-3.216940	-1.410372	3.902540
C	-3.771207	-2.453333	4.706603
C	-3.072621	-2.922483	5.828013
C	-3.603473	-3.988781	6.555473
C	-4.787764	-4.618207	6.184561
C	-5.450989	-4.150733	5.049606
C	-4.963771	-3.079872	4.303941
C	-1.747820	-2.320676	6.221021
C	-5.342542	-5.771891	6.982168
C	-5.686568	-2.614577	3.065538
C	-3.564861	-0.149486	4.130075
C	-3.099417	0.950221	3.382911
C	-4.519953	0.158826	5.264815
Mg	-0.926737	-4.570695	1.649609
N	-0.069414	-6.156946	2.635181
C	0.112119	-5.968645	4.039947
C	1.306661	-5.399971	4.513275
C	1.445062	-5.153271	5.877969
C	0.429004	-5.451555	6.784882
C	-0.748071	-6.006699	6.289584
C	-0.933769	-6.256205	4.929706
C	2.413734	-5.044981	3.553489
C	0.584566	-5.144538	8.253219
C	-2.249796	-6.792048	4.427031
N	-0.801740	-5.546368	-0.155193
C	-1.326474	-4.824042	-1.270780
C	-0.521251	-3.899135	-1.952020
C	-1.079440	-3.159488	-2.994799
C	-2.416657	-3.290477	-3.359857
C	-3.204135	-4.195475	-2.649177
C	-2.682684	-4.964902	-1.610755
C	0.910536	-3.670704	-1.540205
C	-2.994989	-2.484257	-4.495824
C	-3.565262	-5.915238	-0.842240
C	-0.292801	-6.758779	-0.339133
C	0.218810	-7.570645	0.692066
C	0.316914	-7.294490	2.069943
C	0.902937	-8.388464	2.938777
C	-0.241549	-7.332588	-1.740247
H	-1.245679	-7.391796	-2.172339
H	0.203706	-8.328500	-1.745894
H	0.342775	-6.680100	-2.397427
H	0.588625	-8.541452	0.382561
H	1.793119	-8.030576	3.465922
H	1.172220	-9.264527	2.347054
H	0.184619	-8.688906	3.708698
H	-0.447183	-2.450038	-3.527379
H	-4.257388	-4.303638	-2.906396
H	1.438921	-3.073845	-2.289611
H	1.453526	-4.610395	-1.397092
H	0.956393	-3.117214	-0.592368
H	-2.432082	-1.558524	-4.652741
H	-4.038617	-2.217016	-4.302794
H	-2.969370	-3.046948	-5.436192
H	-4.579608	-5.921365	-1.250312
H	-3.627073	-5.627928	0.214906
H	-3.181910	-6.941209	-0.864757
H	2.373680	-4.714570	6.241824
H	-1.555868	-6.249162	6.979222
H	2.749016	-5.911729	2.973454
H	3.276561	-4.637648	4.087406
H	2.079310	-4.293618	2.827261
H	0.288312	-4.111259	8.472676
H	1.622631	-5.261370	8.578949
H	-0.039287	-5.802135	8.866037
H	-2.879232	-7.120457	5.259348
H	-2.116780	-7.631738	3.737165
H	-2.804690	-6.011119	3.889542
H	-5.469479	-0.368305	5.127002
H	-4.718298	1.229094	5.337892
H	-4.105142	-0.189735	6.216399
H	-3.485894	1.917133	3.684171
H	-0.826005	2.543709	1.750820
H	-2.449321	3.115210	2.195821
H	-2.158012	2.326971	0.628961
H	-3.062099	-4.342433	7.432043
H	-6.372784	-4.637099	4.731564
H	-1.440448	-2.672835	7.210231
H	-1.779156	-1.226488	6.235389
H	-0.962917	-2.616843	5.511854
H	-5.673948	-6.584293	6.326958
H	-6.206738	-5.463356	7.581422
H	-4.592458	-6.176630	7.668672
H	-6.605969	-3.186281	2.912827
H	-5.059040	-2.737680	2.173910
H	-5.949329	-1.552393	3.117920

H	2.653199	0.413773	0.186195
H	-0.499747	-0.144594	-2.657415
H	0.657716	1.142241	2.972185
H	2.233352	0.492532	2.484230
H	0.932452	-0.593303	3.001817
H	2.647716	-0.815721	-2.645998
H	3.019537	0.869094	-2.275589
H	1.738435	0.478052	-3.434279
H	-2.736248	-0.322486	-1.996278
H	-3.226721	0.288089	-0.400745
H	-2.828056	-1.419403	-0.617699

Int-C

SCF (wB97X) = -2835.70442277
H(0 K)= -2834.706896
H(298 K)= -2834.637052
G(298 K)= -2834.817895
Lowest Frequency = 6.5507cm-1
PCM (Benzene) Energy = -2835.71388996
wB97XD Corr = -0.1541992440

C	-0.472643	-0.140636	-0.636265
C	-0.047029	0.085814	0.683383
C	1.294832	0.396639	0.950407
C	2.189218	0.496566	-0.116615
C	1.795550	0.263182	-1.433616
C	0.458557	-0.054417	-1.670922
N	-0.974201	-0.086778	1.755585
C	-1.671750	0.959287	2.185928
C	-1.410013	2.322614	1.578435
C	1.766500	0.593809	2.369458
C	2.791517	0.335684	-2.565290
C	-1.915598	-0.470291	-0.922642
Mg	-1.177939	-2.024579	2.436240
N	-2.786593	-1.480956	3.610823
C	-3.500484	-2.563082	4.210793
C	-3.096133	-3.076332	5.450994
C	-3.797691	-4.152708	5.996866
C	-4.866836	-4.747729	5.334146
C	-5.223111	-4.246998	4.081404
C	-4.557592	-3.166608	3.505660
C	-1.905929	-2.497046	6.170843
C	-5.613796	-5.909835	5.939215
C	-4.950320	-2.663891	2.138931
C	-3.219272	-0.241022	3.800800
C	-2.673300	0.895717	3.172071
C	-4.391871	0.001278	4.729370
Mg	-0.332010	-4.673521	1.842161
N	0.151217	-6.438179	2.793923
C	0.211123	-6.386163	4.221787
C	1.413459	-6.089126	4.879592
C	1.407979	-5.955014	6.268659
C	0.244180	-6.103591	7.018637
C	-0.935632	-6.411680	6.343052
C	-0.975029	-6.551733	4.957278
C	2.691899	-5.910502	4.101968
C	0.249477	-5.913661	8.514813
C	-2.275332	-6.852849	4.256327
N	-0.913797	-5.692480	0.145594
C	-1.749093	-4.978461	-0.767223
C	-1.191007	-4.187385	-1.783405
C	-2.038953	-3.473878	-2.629245
C	-3.423101	-3.491785	-2.473422
C	-3.953973	-4.260883	-1.439716
C	-3.142200	-5.005245	-0.583285
C	0.302154	-4.072331	-1.934042
C	-4.312271	-2.665554	-3.368052
C	-3.751270	-5.806764	0.539596
C	-0.611954	-6.960485	-0.105542
C	0.031568	-7.819130	0.808125
C	0.282624	-7.606926	2.179270
C	0.671345	-8.829177	2.986289
C	-1.012225	-7.567811	-1.434576
H	-2.103616	-7.599279	-1.523033
H	-0.624971	-8.582385	-1.539793
H	-0.648069	-6.957974	-2.267181
H	0.233670	-8.820602	0.445386
H	1.548418	-8.632139	3.609438
H	0.878193	-9.681481	2.337187
H	-0.142546	-9.101905	3.667237
H	-1.599111	-2.872865	-3.425401
H	-5.033537	-4.286290	-1.293680
H	0.569171	-3.681363	-2.920351
H	0.807304	-5.030009	-1.790397
H	0.701387	-3.372037	-1.186365
H	-4.373697	-1.630078	-3.011178
H	-5.330813	-3.063522	-3.397000
H	-3.930144	-2.636143	-4.393121
H	-4.842760	-5.811483	0.465838
H	-3.486551	-5.381649	1.517118
H	-3.400911	-6.844421	0.542513
H	2.344090	-5.726440	6.777031
H	-1.857039	-6.546647	6.909443
H	2.881677	-6.754530	3.430285
H	3.545098	-5.813066	4.779177
H	2.652159	-5.013085	3.477941
H	-0.100293	-4.910072	8.785046
H	1.254895	-6.033353	8.928862
H	-0.409292	-6.633440	9.010716
H	-3.042260	-7.154607	4.975441
H	-2.167170	-7.646086	3.509349
H	-2.653013	-5.963659	3.734622
H	-5.291563	-0.491610	4.345933
H	-4.597101	1.067160	4.839024
H	-4.198231	-0.427663	5.717560
H	-3.131120	1.841987	3.436537
H	-0.357021	2.602365	1.682852
H	-2.027582	3.090146	2.047033
H	-1.624004	2.307747	0.504426
H	-3.486117	-4.541680	6.965622
H	-6.042149	-4.712507	3.533409
H	-1.780486	-2.963534	7.152182
H	-1.995122	-1.414241	6.309659
H	-0.985277	-2.674753	5.600432
H	-5.724123	-6.728235	5.219515
H	-6.621164	-5.615385	6.254382
H	-5.093075	-6.301931	6.818262
H	-5.827705	-3.200313	1.765755
H	-4.139256	-2.807536	1.412337
H	-5.180538	-1.592967	2.145834
H	3.226257	0.760315	0.090096
H	0.125098	-0.231822	-2.693203

H	1.088619	1.234645	2.940810
H	2.765224	1.035784	2.392059
H	1.817174	-0.366264	2.899182
H	3.275611	-0.632404	-2.742545
H	3.584480	1.058077	-2.351049
H	2.306892	0.630200	-3.500786
H	-2.098355	-0.511533	-2.000325
H	-2.593396	0.270553	-0.484703
H	-2.194302	-1.447329	-0.507699
C	3.523626	-3.814746	-0.736329
C	3.060430	-3.820452	0.572245
C	3.399060	-2.789765	1.438894
C	4.199703	-1.749259	0.990907
C	4.635243	-1.723768	-0.325998
C	4.298276	-2.755084	-1.189983
F	5.350123	-0.690147	-0.765582
F	4.703599	-2.720328	-2.458648
F	3.225378	-4.816463	-1.559578
F	2.292531	-4.832991	0.999242
F	2.962722	-2.793089	2.697667
F	4.523758	-0.752965	1.812538

Int-C'

SCF (wB97X) = -2835.69555996
H(0 K)= -2834.697738
H(298 K)= -2834.628042
G(298 K)= -2834.807596
Lowest Frequency = 6.7231cm-1
PCM (Benzene) Energy = -2835.70551320
wB97XD Corr = -0.1540634224

H	-5.123364	0.677337	3.288404
H	0.118421	5.498021	-2.410985
H	-5.532283	0.658110	1.583206
H	-4.097273	4.085617	-0.147488
H	4.190455	-3.430067	-2.966077
C	-5.205925	0.024529	2.413307
H	-4.804104	-2.496110	2.434258
C	0.230496	5.089860	-1.406437
H	-2.795224	-4.996601	1.450279
C	-3.453050	2.211387	0.673671
C	-3.741863	3.575695	0.747640
H	-5.974655	-0.724360	2.607982
C	-3.854487	-2.034162	2.191656
C	1.200795	4.108575	-1.187480
C	-3.871640	-0.631228	2.109155
H	-2.518960	-4.761017	3.166180
C	4.036277	-3.178676	-1.917070
C	-0.584942	5.561305	-0.385870
C	-3.085626	-4.383483	2.308880
C	3.882618	-1.839326	-1.561959
C	-2.770331	-2.920276	2.062014
N	-2.819376	0.126754	1.807423
C	-3.028208	1.542387	1.828749
Mg	-0.930723	-0.612272	1.319633
C	-3.611205	4.289779	1.934445
C	4.008831	-4.197483	-0.967935
C	-0.264774	-4.282754	0.551847
N	-1.526682	-2.557684	1.760723
H	-4.149368	-4.528077	2.502081
Mg	1.579380	0.581137	0.412574
C	1.346339	3.574726	0.100814
H	0.856046	-5.873261	-0.347572
C	-0.411442	5.024960	0.891258
H	3.247926	4.872245	1.338072
N	2.291630	2.532335	0.353221
C	0.649512	-5.334769	0.577026
C	3.687602	-1.511754	-0.210809
C	-0.542405	-3.596343	1.743004
C	-2.820029	2.256723	3.021094
C	-3.124256	3.615033	3.055413
N	3.513246	-0.143107	0.165724
H	-1.031049	5.382423	1.711301
C	0.529378	4.034990	1.150874
C	3.816953	-3.846076	0.366396
C	3.556862	2.870563	0.570377
H	6.194550	-0.493058	-0.586407
C	3.930994	4.335520	0.673242
C	4.606387	0.570030	0.420640
C	3.640564	-2.521585	0.762348
H	-2.992602	4.160050	3.990303
C	4.616819	1.951893	0.683845
H	3.799087	-4.624992	1.126396
H	3.857891	4.814481	-0.309120
C	1.301508	-5.714272	1.748231
H	4.952892	4.453399	1.037263
C	5.960333	-0.113146	0.413398
C	0.145761	-3.919664	2.922118
H	5.588504	2.381667	0.898051
H	6.749167	0.576816	0.716507
C	1.052514	-4.978691	2.905524
H	5.966530	-0.977589	1.084274
H	1.573433	-5.239575	3.826670
C	-0.110694	0.359537	-2.721882
C	-1.167099	1.188238	-3.067488
C	-0.181298	-1.008748	-2.941380
C	-2.310464	0.638271	-3.633199
C	-1.328199	-1.555521	-3.502161
C	-2.393934	-0.731664	-3.845020
F	0.992621	0.886303	-2.165257
F	-1.098766	2.495665	-2.841426
F	-3.338182	1.425403	-3.945362
F	-3.493921	-1.256164	-4.377172
F	-1.411736	-2.868719	-3.703208
F	0.839054	-1.791536	-2.604277
C	-0.956257	-3.893607	-0.728145
H	-2.039204	-4.056430	-0.674343
H	-0.804039	-2.828881	-0.935639
H	-0.565171	-4.460454	-1.576416
C	-0.102982	-3.140319	4.188202
H	0.136459	-2.078327	4.050778
H	-1.153043	-3.186864	4.498064
H	0.512515	-3.520819	5.007875
C	2.242580	-6.892930	1.768497
H	2.677605	-7.072993	0.780530
H	3.063012	-6.737661	2.477078
H	1.720737	-7.808331	2.070597
C	-3.649170	1.457866	-0.615939
H	-2.831497	0.747704	-0.780111
H	-4.574414	0.867907	-0.604341
H	-3.696580	2.139760	-1.469563
C	-3.972540	5.751827	2.018317

H	-3.084566	6.379550	2.160146
H	-4.472767	6.091303	1.106626
H	-4.643182	5.943825	2.862310
C	-2.308284	1.551551	4.251067
H	-2.971336	0.735429	4.559329
H	-1.323198	1.104189	4.068315
H	-2.210514	2.248437	5.087993
C	0.693168	3.483809	2.544005
H	0.493999	2.404946	2.566146
H	1.712966	3.627084	2.919466
H	-0.004231	3.965310	3.235405
C	-1.643309	6.601688	-0.650188
H	-2.635230	6.139388	-0.724173
H	-1.689175	7.340770	0.156493
H	-1.454415	7.133861	-1.587134
C	2.082257	3.685273	-2.337764
H	2.778649	4.488116	-2.608658
H	2.672092	2.798870	-2.096488
H	1.477251	3.468735	-3.224094
C	3.421647	-2.179080	2.213758
H	4.178832	-1.480636	2.588115
H	2.444735	-1.700579	2.358171
H	3.442494	-3.080652	2.832106
C	3.943594	-0.759714	-2.612623
H	3.024342	-0.167488	-2.625798
H	4.765841	-0.058489	-2.429093
H	4.086444	-1.194560	-3.605931
C	4.152106	-5.642292	-1.375368
H	4.708084	-5.741044	-2.312563
H	4.674532	-6.223211	-0.608426
H	3.169512	-6.107083	-1.527040

TS-2

SCF (wB97X) = -2835.66642517
H(0 K)= -2834.670375
H(298 K)= -2834.601337
G(298 K)= -2834.777344
Lowest Frequency = -236.1663cm-1
PCM (Benzene) Energy = -2835.67511077
wB97XD Corr = -0.1586577955

H	-5.259978	0.574847	2.314215
H	0.354458	6.115502	-2.088690
H	-5.368739	0.828584	0.579836
H	-3.857238	4.619995	-0.163472
H	4.218725	-3.456358	-3.825874
C	-5.163207	0.074295	1.344956
H	-4.629335	-2.425577	1.300369
C	0.439003	5.458209	-1.223325
H	-2.250991	-4.843611	1.214035
C	-3.262163	2.615659	0.302878
C	-3.594881	3.929032	0.637011
H	-5.918499	-0.710512	1.285215
C	-3.681809	-1.903863	1.235392
C	1.380027	4.425120	-1.261185
C	-3.770642	-0.502601	1.181773
H	-2.461161	-4.306589	2.872136
C	4.107354	-3.202340	-2.772350
C	-0.370638	5.683093	-0.118033
C	-2.802802	-4.140802	1.844782
C	3.978598	-1.861064	-2.413969
C	-2.538317	-2.707132	1.430401
N	-2.730640	0.323722	1.042538
C	-2.973538	1.705959	1.327488
Mg	-0.930780	-0.449574	0.418283
C	-3.612333	4.372266	1.956259
C	4.105644	-4.220229	-1.821063
C	0.353847	-4.048006	0.830841
N	-1.287466	-2.275990	1.314349
H	-3.867180	-4.373396	1.792025
Mg	1.775644	0.615599	-0.586334
C	1.507873	3.585993	-0.144193
H	1.757758	-5.646878	0.602715
C	-0.232110	4.829708	0.978603
H	3.426230	4.591154	1.300989
N	2.452148	2.508609	-0.140176
C	1.314206	-4.941081	1.303951
C	3.834673	-1.532068	-1.057770
C	-0.246908	-3.162515	1.738855
C	-2.938543	2.140361	2.664187
C	-3.259182	3.464636	2.955274
N	3.671336	-0.163089	-0.670099
H	-0.857172	4.980071	1.857458
C	0.688199	3.787080	0.984132
C	3.969186	-3.865144	-0.480882
C	3.720201	2.791925	0.136743
H	6.306819	-0.548862	-1.403502
C	4.099423	4.205396	0.529737
C	4.764434	0.521570	-0.338356
C	3.815274	-2.538503	-0.080779
H	-3.250636	3.791722	3.994789
C	4.779690	1.866930	0.069295
H	3.978668	-4.642976	0.281592
H	4.011953	4.876986	-0.330866
C	1.723983	-4.952448	2.635495
H	5.125864	4.247273	0.896990
C	6.113531	-0.167201	-0.395937
C	0.163743	-3.137727	3.081358
H	5.755298	2.262029	0.327013
H	6.916331	0.517326	-0.119231
C	1.144105	-4.033343	3.507149
H	6.139424	-1.031780	0.274583
H	1.455073	-4.016517	4.551122
C	0.178343	0.966496	-3.172272
C	-0.709152	1.576654	-4.031188
C	-0.161073	-0.121602	-2.359623
C	-1.985309	1.039215	-4.187477
C	-1.442906	-0.647157	-2.555471
C	-2.353691	-0.054847	-3.411479
F	1.408074	1.506751	-2.961302
F	-0.346063	2.658090	-4.722663
F	-2.851597	1.587398	-5.043337
F	-3.606078	-0.510725	-3.466950
F	-1.880451	-1.594972	-1.685614
F	0.942800	-1.005860	-2.113121
C	-0.027614	-4.042152	-0.626539
H	-1.107796	-4.151656	-0.770844
H	0.265527	-3.099949	-1.101618
H	0.477714	-4.852612	-1.159211
C	-0.450969	-2.158264	4.048712
H	-0.232053	-1.125413	3.751512
H	-1.542455	-2.246503	4.086230

H	-0.058722	-2.308417	5.058099
C	2.798627	-5.901254	3.103433
H	2.732675	-6.863887	2.587208
H	3.798510	-5.493292	2.906585
H	2.728176	-6.086737	4.179181
C	-3.211233	2.184122	-1.137665
H	-2.173096	1.985059	-1.431554
H	-3.784491	1.268342	-1.319220
H	-3.594574	2.966691	-1.798427
C	-3.967196	5.796850	2.301438
H	-3.067844	6.394508	2.494361
H	-4.512431	6.280440	1.485432
H	-4.589674	5.844526	3.200354
C	-2.570291	1.181913	3.768004
H	-3.228838	0.306318	3.792145
H	-1.551672	0.800429	3.628378
H	-2.617437	1.673762	4.743387
C	0.835813	2.915862	2.205468
H	0.682007	1.856664	1.960058
H	1.839867	2.993222	2.638728
H	0.103371	3.193439	2.969106
C	-1.366864	6.814154	-0.098649
H	-2.391981	6.439591	-0.197752
H	-1.315632	7.372846	0.842031
H	-1.186995	7.516183	-0.917924
C	2.241278	4.285434	-2.494694
H	2.737173	5.235657	-2.721988
H	3.008668	3.518065	-2.379607
H	1.631193	4.019322	-3.363948
C	3.621722	-2.196586	1.374646
H	4.264855	-1.370729	1.694930
H	2.583612	-1.894579	1.569191
H	3.826051	-3.062807	2.009044
C	4.004123	-0.780635	-3.464205
H	3.073381	-0.205138	-3.460731
H	4.817543	-0.066483	-3.291744
H	4.135605	-1.210604	-4.460877
C	4.218463	-5.668350	-2.227179
H	4.705763	-5.773889	-3.200888
H	4.794104	-6.243753	-1.495455
H	3.228202	-6.133500	-2.303774

Int-D

SCF (wB97X) = -2835.89641905
H(0 K)= -2834.898171
H(298 K)= -2834.829620
G(298 K)= -2835.002448
Lowest Frequency = 15.9709cm-1
PCM (Benzene) Energy = -2835.90300492
wB97XD Corr = -0.1693564459

H	-5.109132	0.736911	2.168507
H	-0.071372	6.519477	0.092795
H	-5.632336	-0.080925	0.702612
H	-3.625329	2.661016	-2.353925
H	2.219041	-2.282862	-4.234131
C	-5.233191	-0.248919	1.708470
H	-4.735458	-2.595369	2.693230
C	0.253551	5.768949	0.812884
H	-2.556571	-5.179587	2.828094
C	-3.406119	1.185603	-0.813215
C	-3.311811	2.482426	-1.325272
H	-5.962832	-0.819983	2.284362
C	-3.818486	-2.236299	2.240398
C	1.049050	4.714083	0.371103
C	-3.902667	-0.965066	1.631157
H	-2.311504	-4.167282	4.241237
C	2.350199	-2.290005	-3.152118
C	-0.147041	5.883320	2.144617
C	-2.898204	-4.264792	3.321470
C	2.757086	-1.118544	-2.517134
C	-2.689620	-3.053775	2.433330
N	-2.889261	-0.377935	1.022461
C	-2.990050	0.948136	0.505290
Mg	-1.060343	-1.231631	0.721839
C	-2.819777	3.541600	-0.569615
C	2.065355	-3.455443	-2.439784
C	-0.023122	-4.801966	1.657990
N	-1.474325	-2.828044	1.929694
H	-3.948967	-4.378746	3.590841
Mg	1.421023	0.936810	0.345827
C	1.482639	3.757767	1.304737
H	1.323975	-6.468551	1.570291
C	0.263922	4.899491	3.041013
H	3.879633	4.324108	2.382665
N	2.298658	2.664730	0.872667
C	1.047484	-5.569891	2.121279
C	2.894419	-1.124216	-1.119003
C	-0.394751	-3.655455	2.376221
C	-2.510306	2.009510	1.296869
C	-2.435711	3.286451	0.747982
N	3.089883	0.109032	-0.420696
H	-0.046872	4.962991	4.083323
C	1.069916	3.831171	2.642268
C	2.260241	-3.447051	-1.060616
C	3.624202	2.817440	0.855341
H	5.481885	-0.338437	-1.759280
C	4.213413	4.117626	1.360900
C	4.299102	0.611661	-0.224513
C	2.674858	-2.298415	-0.384157
H	-2.051398	4.100082	1.361159
C	4.542980	1.857220	0.392763
H	2.066224	-4.350616	-0.483107
H	3.873314	4.956805	0.745313
C	1.761810	-5.226396	3.267260
H	5.303448	4.090473	1.342588
C	5.505492	-0.180702	-0.676734
C	0.325293	-3.275223	3.522377
H	5.587157	2.132125	0.484851
H	6.435764	0.325818	-0.416359
C	1.385112	-4.071666	3.952202
H	5.499447	-1.173403	-0.214935
H	1.933946	-3.778942	4.846732
C	-0.331069	0.260136	-1.964663
C	-0.285201	0.608406	-3.303450
C	-0.675571	-0.951193	-1.426700
C	-0.612136	-0.376781	-4.223834
C	-1.001408	-1.882346	-2.397656
C	-0.975673	-1.638222	-3.764643
F	0.056893	1.313713	-1.094934
F	0.096679	1.825495	-3.707440
F	-0.559084	-0.122309	-5.533118

F	-1.274756	-2.598343	-4.646051
F	-1.389859	-3.130856	-2.036852
F	0.339247	-0.120318	1.415646
C	-0.764966	-5.201481	0.409256
H	-1.840090	-5.307613	0.590453
H	-0.654095	-4.448904	-0.377634
H	-0.389232	-6.153785	0.023393
C	-0.034469	-2.011270	4.262273
H	0.120498	-1.134929	3.621193
H	-1.086596	-1.999329	4.567461
H	0.583561	-1.895762	5.156962
C	2.931753	-6.056124	3.733887
H	2.856364	-7.087188	3.376436
H	3.878249	-5.646740	3.361854
H	2.992747	-6.079112	4.826169
C	-3.948007	0.080986	-1.686549
H	-3.709381	-0.905646	-1.283582
H	-5.038825	0.152364	-1.776668
H	-3.533885	0.146907	-2.698707
C	-2.671692	4.919869	-1.163762
H	-2.771264	5.695754	-0.397912
H	-1.683679	5.041608	-1.624966
H	-3.422250	5.104662	-1.938219
C	-2.073712	1.760244	2.719100
H	-2.877354	1.316244	3.317389
H	-1.231302	1.060309	2.750574
H	-1.761696	2.694278	3.195452
C	1.491529	2.771629	3.628926
H	1.137466	1.779544	3.321903
H	2.582010	2.705902	3.714432
H	1.083480	2.979597	4.621655
C	-1.039670	7.017298	2.582840
H	-2.077222	6.842729	2.273091
H	-1.035244	7.131223	3.670486
H	-0.723059	7.966904	2.140512
C	1.424344	4.589852	-1.084390
H	1.069502	5.455350	-1.651067
H	2.507889	4.512115	-1.225202
H	0.980624	3.691260	-1.530278
C	2.856738	-2.313077	1.113023
H	3.840778	-1.927731	1.402982
H	2.109465	-1.686827	1.614411
H	2.751085	-3.326640	1.507852
C	3.004184	0.138735	-3.313233
H	2.434972	0.987898	-2.919996
H	4.059356	0.435211	-3.292650
H	2.719558	-0.002867	-4.359775
C	1.492750	-4.660608	-3.141125
H	0.422386	-4.510849	-3.325881
H	1.975809	-4.833390	-4.107814
H	1.602038	-5.565106	-2.535560

<u>C–F Activation of C_6F_6 with **3**</u>

3

SCF (wB97X) = -2470.38936414
H(0 K)= -2469.271294
H(298 K)= -2469.205933
G(298 K)= -2469.374243
Lowest Frequency = 6.8906cm-1
PCM (Benzene) Energy = -2470.39819744
wB97XD Corr = -0.1675841395

H	-0.378903	0.830217	-3.519623
H	-1.498219	2.054758	-2.892048
H	2.423386	-1.416508	-3.327193
H	1.958781	-2.773663	-2.278271
C	-0.561323	1.522327	-2.689455
H	1.049598	2.607676	-4.650530
H	-0.037449	3.883284	-4.084138
C	2.457112	-1.799419	-2.300254
H	-0.700120	0.929482	-1.778101
H	1.875870	-1.121409	-1.665442
H	4.751973	-2.340937	-3.767259
C	0.842620	3.287344	-3.816760
H	-4.013026	0.066106	4.354368
H	-1.330543	4.351727	-2.202433
H	4.238566	-3.792103	-2.909662
C	0.610617	2.496586	-2.523534
H	-4.680056	0.823874	2.920104
C	4.706439	-2.809023	-2.778533
H	-2.675100	4.578912	2.451334
H	1.690736	3.973529	-3.720847
H	4.150057	-4.478175	-0.875375
C	-4.340505	-0.133007	3.329503
H	-4.370996	-2.431584	2.208383
C	3.907322	-1.923119	-1.818534
C	-0.664833	4.322919	-1.341660
H	1.510082	1.902205	-2.331391
H	-3.256123	-4.198364	-0.360908
C	-2.418034	2.456593	2.307239
H	4.349868	-0.922060	-1.861792
H	-1.718563	5.882750	-0.302148
C	-2.372445	3.676887	2.981656
H	5.732063	-2.967972	-2.428204
H	-5.185321	-0.822270	3.358414
C	-3.428261	-1.968914	1.941371
C	0.399664	3.417730	-1.329749
C	-3.207829	-0.693953	2.491827
H	-2.418719	-4.878503	1.021985
C	4.092238	-3.752525	-0.068174
C	-0.885799	5.183838	-0.277479
C	-3.130760	-4.102970	0.721873
C	3.968651	-2.397583	-0.370081
C	-2.604585	-2.730191	1.093326
N	-2.100661	0.025440	2.322808
C	-2.035165	1.291924	2.987906
Mg	-0.518167	-0.544265	1.122624
H	4.247381	-5.258471	1.462475
C	-1.949172	3.770878	4.305121
C	4.145813	-4.197063	1.248685
C	-1.023267	-3.197743	-1.643438
N	-1.428355	-2.329274	0.616352
H	-4.088699	-4.299543	1.204938
C	1.252507	3.393974	-0.211489
H	-0.592823	-4.084216	-3.547500
C	-0.031550	5.154778	0.819813
H	3.142877	4.374223	-1.890193
N	2.307390	2.433174	-0.135860
C	-0.366277	-4.096916	-2.481846
C	3.889912	-1.474865	0.696448
C	-0.741706	-3.222129	-0.267900

C	-1.575643	1.363010	4.312972
C	-1.552727	2.601205	4.952702
N	3.692098	-0.090731	0.402015
H	-0.209804	5.835415	1.648281
C	1.046201	4.272794	0.874724
C	4.075998	-3.279334	2.285638
C	3.538300	2.806286	-0.464086
H	6.309508	-0.368146	1.171125
C	3.772454	4.200102	-1.011704
C	4.746452	0.654390	0.092492
H	1.470137	2.199014	2.664262
C	3.946270	-1.911204	2.032419
H	-1.206124	2.653953	5.984302
C	4.674810	1.991581	-0.331192
H	4.123563	-3.628681	3.315505
H	4.817048	4.340082	-1.293484
C	0.577594	-5.000717	-1.995305
H	3.501881	4.964312	-0.276029
C	6.134411	0.050851	0.175181
C	0.218555	-4.107080	0.243255
H	0.530200	3.439819	3.494544
H	5.619218	2.453719	-0.594127
H	1.724035	-1.085146	3.443890
C	1.525329	3.199373	3.107702
C	1.974973	4.248591	2.084486
H	6.248671	-0.773631	-0.536046
H	2.970969	3.955246	1.735370
C	0.858368	-4.985459	-0.631272
H	2.635803	-2.174557	4.504588
H	6.900120	0.799742	-0.032286
C	2.629605	-1.174616	4.054817
C	3.880861	-0.937712	3.201233
H	3.813333	0.074341	2.788356
H	2.224319	3.159542	3.951547
H	1.198233	5.916200	3.271418
C	2.120943	5.614381	2.761454
H	2.381508	6.399525	2.043433
H	1.600530	-5.674421	-0.230049
H	2.565841	-0.439693	4.865515
H	5.256368	-1.988855	4.535780
H	6.046923	-0.814973	3.475612
C	5.144874	-1.004475	4.066979
H	2.908151	5.571476	3.521203
H	5.101982	-0.257928	4.867476
C	-2.023390	-2.218745	-2.204096
H	-1.712708	-1.184610	-2.013302
H	-2.125862	-2.344470	-3.285385
H	-3.014456	-2.336415	-1.751967
C	0.545613	-4.116454	1.714362
H	1.044174	-3.185046	2.012287
H	-0.354558	-4.217916	2.330463
H	1.228237	-4.935185	1.955715
C	1.318419	-5.925357	-2.928003
H	0.702930	-6.204700	-3.788385
H	2.224416	-5.443078	-3.317263
H	1.628101	-6.842697	-2.418528
C	-1.118002	0.120201	5.033415
H	-1.904280	-0.641106	5.084449
H	-0.266612	-0.342140	4.519574
H	-0.806063	0.355832	6.054523
C	-2.881076	2.389338	0.874631
H	-3.240898	3.364250	0.536096
H	-2.057311	2.102619	0.208133
H	-3.682277	1.654345	0.740314
C	-1.861934	5.107554	4.997513
H	-0.867645	5.552635	4.862673
H	-2.594935	5.813835	4.596490
H	-2.033171	5.013484	6.074082
Zn	1.755793	0.563455	0.486840

Int-E

SCF (wB97X) = -3297.81844237
H(0 K)= -3296.645861
H(298 K)= -3296.569219
G(298 K)= -3296.762112
Lowest Frequency = 11.8390cm-1
PCM (Benzene) Energy = -3297.82784588
wB97XD Corr = -0.1935507302

H	-2.127272	1.032802	-3.115625
H	-2.931857	2.454677	-2.447806
H	2.298632	-2.703457	-3.349396
H	2.206616	-3.988478	-2.133877
C	-2.122321	1.736844	-2.275697
H	-0.482366	2.546484	-4.304764
H	-1.142796	4.026693	-3.591417
C	2.260846	-2.902825	-2.270009
H	-2.361637	1.174319	-1.366802
H	1.335261	-2.478931	-1.867075
H	4.849114	-2.623907	-3.249962
C	-0.432535	3.207633	-3.429916
H	-4.302628	-0.417604	5.010561
H	-2.503901	4.384785	-1.444905
H	4.781478	-4.004667	-2.152629
C	-0.763600	2.434600	-2.146961
H	-5.134004	0.416264	3.710674
C	4.775214	-2.909725	-2.194843
H	-3.128210	4.215997	3.282897
H	0.573295	3.639146	-3.391095
H	3.783379	-4.676209	-0.277939
C	-4.747019	-0.559804	4.021039
H	-4.915147	-2.780339	2.760190
C	3.498132	-2.330187	-1.573376
C	-1.703479	4.286218	-0.714242
H	-0.000981	1.661406	-2.015541
H	-4.132989	-4.316828	-0.067400
C	-2.928754	2.106904	2.964987
H	3.496460	-1.252738	-1.752194
H	-2.482264	5.845063	0.545689
C	-2.781250	3.276094	3.710562
H	5.674913	-2.555626	-1.680926
H	-5.581652	-1.256582	4.107967
C	-4.007738	-2.296595	2.418338
C	-0.704590	3.330076	-0.916906
C	-3.720433	-1.060069	3.023235
H	-3.141548	-5.121898	1.135261
C	3.610108	-3.861348	0.422153
C	-1.696107	5.107609	0.402729
C	-3.876679	-4.322685	0.996525
C	3.435946	-2.565485	-0.069735
C	-3.295596	-2.988912	1.422305
N	-2.640826	-0.322665	2.771363

C	-2.486601	0.893132	3.511838
Mg	-1.215048	-0.800447	1.348517
H	3.715419	-5.141931	2.146826
C	-2.198738	3.273682	4.975972
C	3.571122	-4.128029	1.782176
C	-2.052362	-3.144054	-1.522268
N	-2.178607	-2.550898	0.848799
H	-4.771474	-4.563404	1.571998
C	0.337789	3.231351	0.023583
H	-1.839877	-3.763753	-3.563125
C	-0.678166	4.980123	1.341571
H	1.920736	4.381442	-1.720356
N	1.372218	2.259436	-0.137854
C	-1.504384	-3.925747	-2.539182
C	3.199543	-1.521771	0.846129
C	-1.617892	-3.342513	-0.203179
C	-1.872836	0.867824	4.774428
C	-1.747516	2.058536	5.488797
N	2.922799	-0.198265	0.384683
H	-0.685607	5.617542	2.222256
C	0.350234	4.055084	1.172424
C	3.345908	-3.089345	2.677968
C	2.565718	2.669148	-0.558450
H	5.521072	-0.658693	0.735550
C	2.736074	4.093443	-1.051276
C	3.906352	0.579348	-0.042037
H	0.756907	1.929785	2.844434
C	3.149199	-1.781511	2.234368
H	-1.278458	2.035190	6.471945
C	3.728329	1.886567	-0.535379
H	3.317016	-3.304538	3.742554
H	3.686775	4.211170	-1.574002
C	-0.546515	-4.902557	-2.276267
H	2.717098	4.796367	-0.210940
C	5.339449	0.079926	-0.047695
C	-0.618746	-4.286103	0.081405
H	0.165334	3.243428	3.857615
H	4.628098	2.371661	-0.898004
H	1.419710	-1.757856	4.368685
C	1.034643	2.890076	3.293888
C	1.443221	3.913407	2.227438
H	5.565519	-0.393970	-1.009293
H	2.342472	3.527024	1.737750
C	-0.115117	-5.063430	-0.960246
H	2.999188	-1.669685	5.166251
H	6.031269	0.915151	0.080395
C	2.288390	-1.113568	4.543772
C	2.919202	-0.650800	3.229045
H	2.216486	0.051534	2.765498
H	1.856868	2.714805	3.999099
H	1.022429	5.630455	3.521460
C	1.826550	5.242167	2.885410
H	2.066904	6.009782	2.141598
H	0.647763	-5.808718	-0.735549
H	1.956954	-0.245034	5.123560
H	4.979150	-0.542009	3.924417
H	4.614447	0.584005	2.602046
C	4.213198	0.124125	3.509672
H	2.703294	5.102177	3.526266
H	4.029832	0.924480	4.235983
C	1.359588	0.109204	-3.897688
C	1.843371	0.474959	-5.146659
C	0.117842	-0.500884	-3.782304
C	1.079904	0.231913	-6.282185
C	-0.646113	-0.739485	-4.916014
C	-0.165037	-0.373537	-6.167149
F	2.077944	0.361235	-2.805227
F	3.033149	1.058821	-5.257315
F	1.541684	0.579248	-7.480838
F	-0.896617	-0.603569	-7.254560
F	-1.848984	-1.305700	-4.807901
F	-0.349224	-0.828297	-2.579352
C	-3.101871	-2.107663	-1.831339
H	-2.804025	-1.121894	-1.457254
H	-3.260834	-2.022902	-2.908519
H	-4.061841	-2.346297	-1.359151
C	-0.100217	-4.453719	1.486496
H	0.451534	-3.560920	1.809882
H	-0.911141	-4.614687	2.205200
H	0.592125	-5.297556	1.548213
C	0.045799	-5.727547	-3.391066
H	-0.659011	-5.842971	-4.219848
H	0.951125	-5.254385	-3.791346
H	0.325898	-6.726211	-3.042373
C	-1.371295	-0.430256	5.352954
H	-2.188504	-1.131453	5.558924
H	-0.695092	-0.936514	4.655723
H	-0.830039	-0.258326	6.287518
C	-3.558763	2.145804	1.597086
H	-3.952213	3.141522	1.377180
H	-2.817980	1.915728	0.820982
H	-4.371836	1.417920	1.501590
C	-2.005492	4.559281	5.740067
H	-1.055287	5.036576	5.467524
H	-2.804635	5.275264	5.525904
H	-1.985061	4.384561	6.819858
Zn	0.943545	0.360339	0.472462

TS-3

SCF (wB97X) = -3297.78014916
H(0 K)= -3296.607549
H(298 K)= -3296.532819
G(298 K)= -3296.714955
Lowest Frequency = -241.3331cm-1
PCM (Benzene) Energy = -3297.78840891
wB97XD Corr = -0.2080480433

H	-1.802346	3.630966	-3.598692
H	-1.688664	5.225436	-2.878223
H	3.004847	-2.915390	-3.747390
H	2.866895	-4.104058	-2.440757
C	-1.588691	4.155620	-2.663689
H	0.549626	3.840546	-4.221000
H	0.892087	5.325018	-3.317962
C	2.842318	-3.031909	-2.669726
H	-2.358718	3.880201	-1.935503
H	1.842645	-2.668713	-2.425917
H	5.498760	-2.653075	-3.337080
C	0.841858	4.232406	-3.240204
H	-4.150560	-0.185999	3.768217
H	-1.381679	5.925569	-0.928288
H	5.370927	-3.900341	-2.093609

C	-0.178521	3.815347	-2.170710
H	-4.581835	0.797999	2.379987
C	5.308016	-2.820710	-2.271353
H	-2.039000	4.272726	2.436666
H	1.843061	3.854492	-3.020157
H	3.975485	-4.483113	-0.383608
C	-4.423268	-0.233372	2.709356
H	-4.640277	-2.512619	1.560867
C	3.923492	-2.277566	-1.887367
C	-0.587352	5.501584	-0.322220
H	-0.110591	2.725226	-2.062650
H	-3.345236	-4.744624	-0.523100
C	-2.109289	2.172118	2.028813
H	3.872261	-1.228324	-2.186496
H	-0.885818	6.927034	1.261242
C	-1.903494	3.276257	2.854110
H	6.112443	-2.346538	-1.701200
H	-5.360709	-0.783847	2.618564
C	-3.636197	-2.156642	1.362363
C	0.137448	4.408117	-0.800480
C	-3.326889	-0.893644	1.896194
H	-2.705467	-5.216737	1.043087
C	3.785782	-3.605874	0.231663
C	-0.313939	6.069238	0.916073
C	-3.336405	-4.478082	0.538258
C	3.692815	-2.355143	-0.383519
C	-2.778629	-3.084318	0.738929
N	-2.156588	-0.272771	1.750546
C	-1.927553	0.884890	2.558561
Mg	-0.816557	-0.887345	0.318967
H	3.725789	-4.737968	2.058444
C	-1.519044	3.138490	4.186157
C	3.643494	-3.754737	1.601388
C	-0.786845	-4.235331	-1.533450
N	-1.539738	-2.814957	0.343117
H	-4.351435	-4.555888	0.929697
C	1.172362	3.883585	0.004926
H	0.014680	-5.525466	-3.046779
C	0.685915	5.528257	1.708430
H	2.818491	5.127322	-1.415961
N	1.971098	2.782913	-0.453953
C	0.043918	-5.261297	-1.989685
C	3.429091	-1.226940	0.421741
C	-0.746762	-3.888790	-0.175993
C	-1.510906	0.720818	3.890121
C	-1.314310	1.852808	4.681663
N	3.262247	0.080324	-0.142822
H	0.889989	5.962200	2.685455
C	1.437650	4.434078	1.276700
C	3.398890	-2.636633	2.387295
C	3.222948	3.059489	-0.837006
H	5.786696	-0.673859	0.154251
C	3.642370	4.499381	-1.074969
C	4.312184	0.787056	-0.522529
H	1.115393	2.375760	3.064524
C	3.281205	-1.367156	1.821007
H	-0.993653	1.722304	5.715013
C	4.251992	2.123323	-0.977180
H	3.296874	-2.755598	3.462335
H	4.448370	4.533292	-1.811461
C	0.905276	-5.947570	-1.140662
H	4.024288	4.934409	-0.145699
C	5.712901	0.205697	-0.486376
C	0.116409	-4.566910	0.702496
H	1.222050	3.875071	3.988332
H	5.198511	2.528627	-1.319626
H	1.421242	-1.042171	3.816998
C	1.805268	3.158592	3.399166
C	2.488601	3.856732	2.218584
H	6.010532	-0.083138	-1.500287
H	3.068623	3.103186	1.676113
C	0.921053	-5.588288	0.207105
H	2.948823	-1.037965	4.715529
H	6.421910	0.960826	-0.138901
C	2.331793	-0.466432	4.012709
C	3.085708	-0.151328	2.718526
H	2.489282	0.584072	2.164243
H	2.550301	2.708256	4.065385
H	2.974252	5.642053	3.386984
C	3.471436	4.915088	2.735021
H	3.944306	5.472594	1.920297
H	1.585040	-6.114079	0.892545
H	2.038797	0.461282	4.514588
H	5.100067	-0.215285	3.534219
H	4.941305	0.848743	2.125063
C	4.439052	0.501834	3.033463
H	4.263442	4.437885	3.322518
H	4.311589	1.365138	3.696604
C	0.878070	0.275711	-3.221069
C	0.423709	1.008596	-4.305640
C	0.020719	-0.092006	-2.168197
C	-0.924173	1.309570	-4.449268
C	-1.338177	0.191315	-2.386404
C	-1.814990	0.909410	-3.457906
F	2.196938	0.046219	-3.117780
F	1.290531	1.436481	-5.223671
F	-1.350858	2.041754	-5.484125
F	-3.104634	1.230886	-3.547064
F	-2.191176	-0.177335	-1.382212
F	0.214069	-1.417440	-1.582488
C	-1.707406	-3.546468	-2.511613
H	-2.198000	-2.678391	-2.067652
H	-1.150808	-3.211476	-3.393078
H	-2.488640	-4.231536	-2.861973
C	0.162169	-4.191014	2.161634
H	0.557249	-3.175722	2.294622
H	-0.833061	-4.213077	2.619305
H	0.815568	-4.869172	2.717384
C	1.827397	-7.019649	-1.664383
H	1.435431	-7.472362	-2.579821
H	2.815951	-6.605795	-1.901576
H	1.975176	-7.814980	-0.927405
C	-1.320902	-0.658148	4.471061
H	-2.280940	-1.120895	4.732501
H	-0.840253	-1.332535	3.754916
H	-0.713725	-0.618661	5.379939
C	-2.546443	2.365799	0.599598
H	-2.787596	3.415908	0.413118
H	-1.747311	2.085051	-0.098065
H	-3.420156	1.752836	0.353863
C	-1.334671	4.352849	5.061135
H	-0.948498	5.198578	4.482055

H	-2.285210	4.668373	5.506563
H	-0.637424	4.153075	5.880824
Zn	1.357607	0.865290	-0.279848

Int-F

SCF (wB97X) = -3297.96548519
H(0 K)= -3296.792853
H(298 K)= -3296.717072
G(298 K)= -3296.904673
Lowest Frequency = 14.1342cm-1
PCM (Benzene) Energy = -3297.97210680
wB97XD Corr = -0.2000320338

H	-0.684655	2.950136	-4.481349
H	-1.566896	4.237193	-3.662328
H	2.011527	-2.559892	-3.896103
H	2.119130	-3.966690	-2.819677
C	-0.975034	3.330083	-3.495637
H	1.306181	4.507771	-4.345635
H	0.532496	5.686409	-3.269336
C	2.101141	-2.870756	-2.848566
H	-1.624307	2.589355	-3.019006
H	1.202540	-2.546496	-2.312800
H	4.580154	-2.532432	-4.009350
C	1.088592	4.741885	-3.297699
H	-4.867362	-0.338452	4.425602
H	-1.737508	5.172257	-1.703865
H	4.668903	-3.908915	-2.905530
C	0.272210	3.612677	-2.652930
H	-5.492211	0.545026	3.043858
C	4.612981	-2.815224	-2.951796
H	-3.415753	4.315026	2.892212
H	2.042793	4.896978	-2.785761
H	3.727162	-4.663401	-0.996057
C	-5.188346	-0.449233	3.385146
H	-5.181403	-2.754453	2.295671
C	3.372786	-2.284168	-2.223158
C	-1.114331	4.791046	-0.898522
H	0.894488	2.713022	-2.659100
H	-3.940904	-4.772757	0.022266
C	-3.217070	2.212125	2.531310
H	3.337780	-1.200996	-2.365392
H	-2.222926	5.828984	0.625561
C	-3.134580	3.356229	3.326570
H	5.540568	-2.419160	-2.524999
H	-6.052083	-1.114469	3.356706
C	-4.248189	-2.281857	2.013639
C	-0.050342	3.939183	-1.200522
C	-4.062208	-0.985303	2.524242
H	-3.035786	-5.214371	1.460302
C	3.598264	-3.861535	-0.271137
C	-1.386711	5.167745	0.410256
C	-3.806234	-4.535336	1.081126
C	3.413548	-2.556231	-0.727052
C	-3.371437	-3.096691	1.269054
N	-2.981501	-0.228277	2.323532
C	-2.872423	0.975750	3.093069
Mg	-1.571047	-0.784613	0.988017
H	3.788610	-5.175694	1.422841
C	-2.704456	3.305752	4.649901
C	3.628970	-4.154073	1.085416
C	-1.671433	-3.918481	-1.318351
N	-2.213263	-2.694429	0.754093
H	-4.740745	-4.734687	1.606519
C	0.747869	3.459791	-0.140904
H	-1.053735	-5.047087	-3.034207
C	-0.574491	4.710974	1.439007
H	2.605791	5.005890	-0.672427
N	1.778061	2.503610	-0.405007
C	-0.862736	-4.846113	-1.980485
C	3.257871	-1.524609	0.220379
C	-1.422679	-3.651671	0.035362
C	-2.397943	0.901177	4.413696
C	-2.335592	2.066788	5.173869
N	3.083035	-0.168700	-0.208585
H	-0.784414	5.014538	2.462285
C	0.504967	3.863117	1.187151
C	3.453556	-3.132459	2.008588
C	3.045271	2.878940	-0.465573
H	5.669052	-0.565718	0.675488
C	3.415144	4.344496	-0.360467
C	4.160525	0.601124	-0.349762
H	0.380041	1.487461	2.622654
C	3.260188	-1.810894	1.601594
H	-1.976050	2.007231	6.200499
C	4.135953	1.989499	-0.555175
H	3.475270	-3.363410	3.072049
H	4.305146	4.552839	-0.958884
C	0.168626	-5.517827	-1.334780
H	3.655012	4.583266	0.682373
C	5.533195	-0.034381	-0.270530
C	-0.371531	-4.303166	0.705254
H	-0.262290	2.794439	3.636546
H	5.105938	2.461659	-0.662312
H	0.984306	-1.012371	3.024497
C	0.652497	2.370333	3.209985
C	1.381193	3.402417	2.345068
H	5.652221	-0.776645	-1.066117
H	2.267787	2.912441	1.930692
C	0.398734	-5.229788	0.010813
H	2.021556	-1.987677	4.096447
H	6.318578	0.715658	-0.370601
C	1.917346	-1.018333	3.595111
C	3.098448	-0.726960	2.662438
H	2.883608	0.216518	2.149726
H	1.293168	2.046456	4.039619
H	1.034989	5.057662	3.733702
C	1.864636	4.580874	3.198880
H	2.352164	5.349979	2.589801
H	1.210879	-5.731857	0.533526
H	1.842029	-0.248421	4.371103
H	4.649281	-1.454661	4.018186
H	5.236755	-0.282635	2.829676
C	4.388477	-0.540623	3.471963
H	2.580910	4.234219	3.951532
H	4.266737	0.264223	4.205388
C	0.508511	0.052916	-3.383047
C	-0.262815	-0.169538	-4.515727
C	-0.000335	0.135170	-2.094724
C	-1.640768	-0.303177	-4.382598
C	-1.364973	-0.002300	-2.043783
C	-2.212160	-0.204213	-3.123569

F	1.834863	0.212494	-3.586038
F	0.292690	-0.256189	-5.726163
F	-2.404870	-0.517852	-5.453845
F	-3.534586	-0.317822	-2.968015
F	-2.034126	0.096287	-0.813319
F	0.149695	-0.143445	1.005301
C	-2.810715	-3.266992	-2.060419
H	-3.092399	-2.306989	-1.624714
H	-2.550763	-3.110132	-3.111838
H	-3.707513	-3.899128	-2.044895
C	-0.098080	-4.015631	2.159069
H	0.221637	-2.977598	2.306237
H	-0.988476	-4.172475	2.778473
H	0.705238	-4.654377	2.535232
C	1.018903	-6.531888	-2.057248
H	0.860513	-6.487376	-3.138667
H	2.084178	-6.362578	-1.864092
H	0.787222	-7.550782	-1.727176
C	-1.945046	-0.416157	4.991698
H	-2.740652	-1.169530	4.987499
H	-1.114388	-0.833078	4.408354
H	-1.601961	-0.289909	6.021946
C	-3.668824	2.310651	1.096755
H	-4.036897	3.315494	0.874207
H	-2.840643	2.112116	0.405615
H	-4.462047	1.590446	0.869235
C	-2.580101	4.562887	5.473307
H	-3.288453	5.328391	5.143152
H	-2.761100	4.366233	6.534216
H	-1.571970	4.987568	5.387410
Zn	1.271645	0.559859	-0.569047

C–F Activation of C_6F_6 with **6**

6

SCF (wB97X) = -2521.00632192
H(0 K)= -2519.674840
H(298 K)= -2519.601481
G(298 K)= -2519.781533
Lowest Frequency = 15.9482cm-1
PCM (Benzene) Energy = -2521.01223744
wB97XD Corr = -0.2188555261

Al	7.555182	8.175132	5.039345
N	5.782048	7.219562	4.998628
C	5.133235	6.933060	3.871052
C	5.689910	7.052280	2.590484
H	5.033869	6.821920	1.758792
C	7.036140	7.292125	2.260626
N	7.961648	7.628293	3.147299
C	3.698534	6.452859	3.925438
H	3.557354	5.673212	4.677204
H	3.380899	6.073221	2.953377
H	3.041275	7.283309	4.202639
C	7.370600	7.158411	0.790062
H	7.042222	8.068982	0.275779
H	6.825019	6.319752	0.351256
H	8.437380	7.030535	0.605365
C	5.148462	6.872786	6.243216
C	5.432688	5.615012	6.817121
C	4.780804	5.253672	7.996537
H	4.982586	4.281500	8.439691
C	3.873425	6.107318	8.609537
H	3.368156	5.804768	9.523105
C	3.626558	7.353196	8.053476
H	2.930160	8.029644	8.545084
C	4.257996	7.762324	6.876862
C	6.396734	4.635081	6.161937
H	6.996280	5.201484	5.445087
C	7.360192	4.004842	7.173038
H	7.853237	4.769756	7.780510
H	8.136331	3.436938	6.647246
H	6.848130	3.307429	7.846033
C	5.649147	3.546054	5.381921
H	4.983878	2.976799	6.042124
H	6.359895	2.843524	4.931800
H	5.043914	3.969004	4.573691
C	3.975715	9.161979	6.348120
H	4.522784	9.277420	5.405979
C	2.486768	9.404282	6.071594
H	2.069816	8.674500	5.370734
H	2.338800	10.404194	5.647898
H	1.896567	9.348456	6.993140
C	4.491536	10.223104	7.330283
H	3.937791	10.187474	8.276052
H	4.378655	11.234342	6.920339
H	5.547520	10.063471	7.577679
C	9.344724	7.678052	2.755029
C	9.896195	8.863518	2.236337
C	11.257041	8.882711	1.918420
H	11.694677	9.793131	1.514078
C	12.054111	7.763134	2.099102
H	13.110297	7.796424	1.844734
C	11.493119	6.594942	2.599616
H	12.119687	5.716360	2.730063
C	10.141883	6.527865	2.936982
C	9.062793	10.109878	1.977889
H	8.043141	9.917237	2.328779
C	8.994188	10.453605	0.483882
H	9.983542	10.724955	0.097387
H	8.326666	11.308784	0.327184
H	8.626612	9.613607	-0.113178
C	9.593688	11.314947	2.755706
H	9.644140	11.097148	3.829546
H	8.944214	12.182502	2.602408
H	10.605031	11.590503	2.432108
C	9.545079	5.214949	3.425963
H	8.620900	5.456821	3.958496
C	10.459386	4.464224	4.398735
H	11.344678	4.058063	3.895934
H	9.920549	3.615068	4.834911
H	10.793195	5.111372	5.214817
C	9.176509	4.309041	2.243029
H	8.449911	4.784397	1.577029
H	8.739179	3.370027	2.600991
H	10.065985	4.064441	1.650278
C	8.859184	7.201826	6.208913
H	9.866340	7.590420	5.991896
H	8.912639	6.111812	6.119924
H	8.685066	7.432565	7.268505
Mg	7.445468	10.831990	5.810525
N	6.760472	12.755553	5.436028

C	6.337148	13.526036	6.444077
C	6.665182	13.332506	7.791234
H	6.259142	14.066291	8.480442
C	7.619640	12.445559	8.355009
N	8.105709	11.396346	7.721343
C	5.478141	14.738055	6.143069
H	6.093456	15.572290	5.792919
H	4.946140	15.064476	7.038594
H	4.753460	14.519540	5.354154
C	8.048254	12.791130	9.767386
H	7.256968	12.508794	10.470869
H	8.197502	13.869838	9.858567
H	8.964053	12.275622	10.060740
C	6.688352	13.264325	4.100030
C	7.614714	14.246591	3.673536
C	7.618942	14.633867	2.333098
H	8.336436	15.380611	1.999154
C	6.739289	14.078658	1.413667
H	6.764942	14.387466	0.371950
C	5.813814	13.140708	1.845833
H	5.101522	12.726583	1.135149
C	5.761030	12.730272	3.180149
C	8.632638	14.892995	4.610137
H	8.436865	14.549278	5.630734
C	10.066104	14.478076	4.254988
H	10.209332	13.398847	4.360312
H	10.783957	14.983925	4.910857
H	10.310647	14.748071	3.221010
C	8.524793	16.424707	4.598376
H	8.833372	16.838326	3.631718
H	9.178040	16.857346	5.363576
H	7.503390	16.769019	4.789206
C	4.654434	11.772614	3.600289
H	4.817953	11.515426	4.652680
C	3.284518	12.458514	3.501206
H	3.237529	13.359897	4.121375
H	2.487235	11.780306	3.826055
H	3.068349	12.754978	2.468487
C	4.662052	10.473632	2.789188
H	4.479858	10.661670	1.724897
H	3.874237	9.795692	3.140173
H	5.616837	9.946774	2.882364
C	9.111578	10.562256	8.311450
C	8.794872	9.623540	9.313515
C	9.801878	8.772198	9.774778
H	9.564423	8.041244	10.544756
C	11.089352	8.829786	9.266413
H	11.855487	8.152913	9.634695
C	11.391803	9.758867	8.280431
H	12.403129	9.805395	7.886173
C	10.421693	10.630872	7.788732
C	7.400486	9.477739	9.908372
H	6.757791	10.250602	9.473776
C	7.407095	9.676153	11.430379
H	7.962731	8.875368	11.930912
H	6.383859	9.658745	11.821442
H	7.867992	10.626467	11.717299
C	6.788744	8.116081	9.559259
H	6.734248	7.958916	8.477353
H	5.773237	8.032062	9.960668
H	7.384890	7.298512	9.981463
C	10.804530	11.690032	6.764455
H	9.902822	11.957580	6.198156
C	11.859282	11.221140	5.758897
H	12.837299	11.078934	6.231546
H	11.989958	11.975091	4.974466
H	11.572291	10.278183	5.279929
C	11.263557	12.966432	7.482532
H	10.475566	13.360907	8.133387
H	11.532455	13.746046	6.761367
H	12.141750	12.758903	8.104877

TS-4

SCF (wB97X) = -3348.37705116
H(0 K)= -3346.989993
H(298 K)= -3346.907139
G(298 K)= -3347.103395
Lowest Frequency = -255.3991cm-1
PCM (Benzene) Energy = -3348.38229481
wB97XD Corr = -0.2542931363

H	-3.334813	3.109191	-3.334925
H	-3.767572	4.388631	-2.197820
C	-3.641396	3.305112	-2.301248
H	-4.622494	2.845512	-2.146209
H	3.328867	3.106229	-4.632754
H	2.826512	4.768270	-4.340968
H	2.468872	0.406403	-5.305159
H	-0.972294	3.646436	-2.516219
H	3.180547	-1.178208	-5.611878
H	-1.316595	-6.005424	-2.053458
C	2.733884	3.742423	-3.966590
H	5.318258	3.682443	-3.196074
H	4.697104	5.239863	-2.615058
C	2.684816	-0.566859	-4.849607
H	1.686835	3.442808	-4.052984
H	1.733791	-1.044458	-4.592587
H	-1.435336	4.611758	-1.120076
H	4.806573	1.131785	-4.563215
C	4.682408	4.157619	-2.439844
C	-1.292345	3.585908	-1.473868
H	-5.386333	1.012876	0.232127
C	-2.583336	2.776350	-1.321607
H	-2.378115	1.728792	-1.570068
H	0.518270	-4.343835	-2.662458
H	1.930817	5.962588	-2.771428
C	-0.989998	-5.930749	-1.010481
H	-1.837152	-6.189589	-0.368215
H	5.497239	-0.503044	-4.590052
H	-0.215905	-6.690818	-0.856834
C	3.249692	3.612698	-2.529882
H	-4.755749	0.909774	-1.407754
C	4.925147	0.208437	-3.983392
H	-3.443448	4.930136	0.000791
H	5.130386	3.964945	-1.460498
H	-0.475810	3.158068	-0.885341
H	3.791173	-2.939836	-4.496164
C	-4.979826	0.323215	-0.511391
H	-4.587972	-2.210740	-0.519459
H	-1.211102	-3.802798	-1.027696
C	3.558243	-0.376238	-3.607057
C	1.776450	5.521509	-1.789878

C	0.780165	-4.262058	-1.601541
H	3.302752	2.547001	-2.287412
C	-0.449522	-4.520072	-0.730171
H	1.566710	-4.995668	-1.395462
H	-3.447402	-4.495852	-0.301749
C	-3.047489	2.822781	0.124208
H	3.059712	0.370270	-2.982841
H	0.593858	7.176845	-1.087448
C	-3.459294	4.053260	0.644078
H	5.514956	0.443102	-3.091234
H	-5.742685	-0.414171	-0.764524
C	-3.702369	-1.743431	-0.104208
C	2.346972	4.283236	-1.497595
C	-3.718516	-0.356513	-0.025112
H	-2.715014	-4.670619	1.304614
H	1.198776	-3.267820	-1.433500
C	3.850719	-2.881943	-3.412472
C	1.028103	6.210577	-0.843721
C	-3.339298	-4.030171	0.683468
C	3.722041	-1.643529	-2.780018
C	-2.788622	-2.629279	0.512047
N	-2.711431	0.378348	0.477927
C	-3.070947	1.692068	0.959912
H	4.177577	-4.992910	-3.182581
C	-3.890123	4.177247	1.954073
H	-4.212072	5.141914	2.337769
C	4.068894	-4.036223	-2.678230
C	-0.156936	-4.319892	0.750562
N	-1.578545	-2.287932	0.925795
H	-4.337917	-3.969034	1.124081
Mg	1.829039	0.626436	-0.554127
C	2.138148	3.720061	-0.215654
H	1.176093	-6.001010	0.761068
C	0.850575	5.661302	0.416069
H	4.255158	4.624712	0.644236
N	2.733302	2.435199	0.046896
C	0.705150	-5.230625	1.367944
C	3.810486	-1.588968	-1.378363
C	-0.749775	-3.307629	1.538504
C	-3.513835	1.806431	2.297717
H	-5.406159	-0.254840	2.235497
C	-3.912910	3.055273	2.771914
N	3.705454	-0.317830	-0.722179
H	0.274499	6.206791	1.160609
C	1.398592	4.421442	0.756524
C	4.141347	-3.970326	-1.291303
C	3.970978	2.463884	0.554892
H	6.709472	-0.497346	0.547688
C	4.499621	3.725644	1.213358
C	4.814656	0.195524	-0.206721
H	-0.685466	2.869005	1.728840
C	4.000736	-2.761484	-0.609805
H	-4.261751	3.150629	3.796944
H	-5.771326	0.831799	3.589064
C	4.882842	1.403820	0.515054
C	-5.077539	0.062379	3.230097
H	4.304603	-4.886918	-0.733469
H	5.581569	3.672935	1.342462
C	0.964672	-5.178293	2.727509
H	-3.007844	-0.195860	2.789817
C	-3.637084	0.593119	3.209089
H	4.044854	3.833736	2.202992
C	6.177565	-0.451074	-0.406757
C	-0.553353	-3.295603	2.937587
H	-1.587040	-1.475763	3.291862
H	-0.898235	4.497581	2.372292
H	5.854036	1.613431	0.949426
H	2.598000	-1.179919	1.351982
C	-0.284744	3.592262	2.442854
H	1.644932	-5.891426	3.186144
C	1.190152	3.905582	2.174043
H	6.137863	-1.448188	-0.841235
H	-5.156135	-0.803638	3.897589
H	1.762260	2.976563	2.279967
C	0.318513	-4.226672	3.503614
H	1.951531	-2.829579	1.246627
H	6.768886	0.189527	-1.069699
C	-1.358227	-2.382753	3.850974
C	2.802681	-2.229203	1.577369
H	0.387485	-1.578658	4.892080
C	4.102644	-2.705711	0.917091
H	4.880107	-1.973744	1.170133
H	-3.300472	-3.249191	3.326906
H	-0.413895	3.175729	3.448558
H	1.072814	5.803627	3.246096
C	-3.157883	0.872370	4.636905
H	-3.819634	1.570822	5.160851
C	1.696176	4.902658	3.227247
H	2.725621	5.222395	3.040128
H	-2.146558	1.292823	4.649367
C	-0.609961	-1.966527	5.120354
H	0.483532	-4.215554	4.576996
C	-2.692514	-3.049554	4.215327
H	2.871003	-2.317434	2.667369
H	-1.165258	-1.178119	5.638501
H	-3.276752	-2.404682	4.882696
H	3.764393	-4.802870	1.419151
H	-3.150317	-0.056375	5.218044
H	5.473124	-4.404509	1.127157
C	4.533474	-4.032188	1.547985
H	-0.502747	-2.799907	5.824082
H	1.651652	4.453972	4.225470
H	-2.522999	-4.002555	4.729961
H	4.678208	-3.894299	2.624022
C	-0.009540	0.902726	-2.963861
C	-0.821215	1.471171	-3.920695
C	-0.271098	-0.321326	-2.338947
C	-1.960043	0.791104	-4.332234
C	-1.370935	-1.023348	-2.853188
C	-2.239003	-0.448216	-3.766965
F	1.056855	1.606939	-2.464270
F	-0.534290	2.662148	-4.458791
F	-2.768322	1.323705	-5.254624
F	-3.329200	-1.114977	-4.149412
F	-1.671704	-2.241001	-2.387046
F	0.915099	-1.047143	-2.023807
Al	-0.871054	-0.357428	0.619893
C	0.019111	0.179107	2.349299
H	0.732161	0.998551	2.189941
H	-0.650572	0.509441	3.153313
H	0.604881	-0.665088	2.737207

C–F Activation of C_6F_6 with **7**

7

SCF (wB97X) = -2550.77347080
H(0 K)= -2549.587824
H(298 K)= -2549.519607
G(298 K)= -2549.689592
Lowest Frequency = 17.7193cm-1
PCM (Benzene) Energy = -2550.77855609
wB97XD Corr = -0.1943275628

Al	9.369332	6.468373	9.584221
Zn	11.341635	7.978007	9.348435
N	9.766877	5.043271	10.951203
C	9.417474	5.191679	12.220217
C	8.609670	6.248291	12.696502
H	8.487963	6.296780	13.773348
C	7.796149	7.099721	11.940026
N	7.825334	7.141092	10.608605
C	9.869172	4.213888	13.283202
H	9.013554	3.917551	13.895696
H	10.587921	4.709158	13.945209
H	10.337483	3.321453	12.867681
C	6.861424	8.010561	12.702403
H	7.319833	9.005851	12.757552
H	6.701840	7.650595	13.720392
H	5.896808	8.122710	12.203562
C	10.597606	3.942875	10.532230
C	9.998951	2.871789	9.833711
C	10.815760	1.857672	9.335496
H	10.367771	1.030068	8.792968
C	12.191836	1.883024	9.522540
H	12.812773	1.085026	9.123961
C	12.764629	2.924827	10.233803
H	13.840488	2.935349	10.394660
C	11.990927	3.967419	10.751583
C	8.487436	2.777588	9.686496
H	8.099417	3.798094	9.673480
C	8.040304	2.103477	8.387639
H	8.516309	2.563457	7.516233
H	6.956098	2.204098	8.271501
H	8.267068	1.031074	8.381598
C	7.871943	2.069013	10.900583
H	8.244594	1.041064	10.981693
H	6.779890	2.027869	10.808825
H	8.110422	2.588432	11.834544
C	12.695693	5.054746	11.553403
H	11.945554	5.785082	11.868578
C	13.361023	4.479467	12.812461
H	12.662577	3.900480	13.423098
H	13.767150	5.288596	13.430057
H	14.193332	3.817637	12.547150
C	13.743748	5.803073	10.722319
H	14.559472	5.135903	10.419064
H	14.184861	6.620849	11.303095
H	13.316993	6.232929	9.812253
C	6.724147	7.717911	9.886872
C	6.749870	9.060815	9.475297
C	5.679726	9.547158	8.719015
H	5.690498	10.584224	8.390435
C	4.606815	8.736690	8.383802
H	3.783570	9.133737	7.795698
C	4.588656	7.413169	8.806096
H	3.742747	6.782333	8.544875
C	5.637504	6.879695	9.553235
C	7.890675	10.004198	9.825151
H	8.606419	9.462778	10.454943
C	7.392295	11.218093	10.620087
H	6.715442	11.837304	10.020059
H	8.239766	11.840275	10.926255
H	6.847997	10.911930	11.520285
C	8.632810	10.457444	8.562253
H	9.006118	9.598022	7.992789
H	9.481515	11.096311	8.830239
H	7.974064	11.031932	7.900310
C	5.572561	5.433368	10.027472
H	6.592854	5.125571	10.276393
C	5.045359	4.474492	8.955670
H	3.983152	4.641477	8.744213
H	5.144179	3.438881	9.301829
H	5.598127	4.576867	8.016179
C	4.731223	5.307541	11.305127
H	5.146078	5.901505	12.125363
H	4.690464	4.263468	11.636044
H	3.703976	5.647682	11.128207
C	8.693920	5.690865	7.861300
H	9.443557	4.976717	7.483361
H	7.779618	5.100749	8.012891
C	8.424774	6.743861	6.774754
H	8.141073	6.290249	5.815726
H	9.310963	7.360791	6.578685
H	7.610596	7.421591	7.064525
N	12.459898	9.341879	10.339292
C	13.772795	9.472625	10.155279
C	14.485114	8.901857	9.090793
H	15.555708	9.072510	9.089318
C	13.955188	8.291375	7.933841
N	12.689565	7.928025	7.808927
C	14.573558	10.298870	11.142052
H	14.337534	11.363608	11.050294
H	15.644659	10.169775	10.977558
H	14.332755	10.009693	12.169997
C	14.910306	8.076009	6.778741
H	14.846307	7.050355	6.403192
H	15.939114	8.285890	7.075892
H	14.649720	8.734304	5.942936
C	11.794781	10.223161	11.244116
C	11.506401	11.537603	10.830946
C	10.786841	12.372867	11.683602
H	10.565492	13.389542	11.359012
C	10.332807	11.940705	12.929282
C	10.639579	10.640186	13.319921
H	10.311274	10.285399	14.296467
C	11.366057	9.773267	12.501850
C	11.969762	12.044806	9.487792
H	13.044713	12.262090	9.481914
H	11.445624	12.966557	9.219484
H	11.800214	11.301965	8.701996
C	9.503964	12.845334	13.805510
H	9.846031	13.883100	13.745843
H	9.545280	12.533701	14.853269
H	8.451483	12.829408	13.496870

C	11.677162	8.376422	12.970099
H	11.018808	7.651230	12.477937
H	11.522518	8.285032	14.049304
H	12.709681	8.092731	12.739695
C	12.204153	7.488459	6.538114
C	12.116356	6.119702	6.241983
C	11.564139	5.731264	5.021768
H	11.494442	4.667997	4.795008
C	11.095628	6.658075	4.093418
C	11.200065	8.010808	4.408939
H	10.839508	8.753995	3.698630
C	11.738371	8.443360	5.619871
C	12.592558	5.081896	7.224034
H	13.629159	5.254378	7.535663
H	12.527168	4.077728	6.795968
H	11.983622	5.090145	8.135136
C	10.456355	6.208469	2.804139
H	10.890177	5.268565	2.449730
H	10.576991	6.957630	2.015910
H	9.381195	6.043719	2.940805
C	11.783211	9.914033	5.950465
H	11.101825	10.146833	6.778475
H	11.479845	10.514675	5.088660
H	12.781134	10.241037	6.262456

TS-5

SCF (wB97X) = -3378.10419124
H(0 K)= -3376.863483
H(298 K)= -3376.785601
G(298 K)= -3376.974327
Lowest Frequency = -241.3374cm-1
PCM (Benzene) Energy = -3378.11021748
wB97XD Corr = -0.2213986630

H	-0.653364	3.989570	-2.027974
H	-1.236790	4.486877	-0.417686
H	1.169132	-1.690438	-5.226090
H	1.947496	-3.254520	-4.980456
C	-0.461083	3.924420	-0.950803
H	0.886260	6.076263	-2.065455
H	0.268144	6.542331	-0.480830
C	1.635618	-2.334650	-4.472098
H	-0.556833	2.875394	-0.650366
H	0.880106	-2.587926	-3.725541
H	3.498696	-0.912677	-5.779422
C	1.033839	5.945373	-0.988389
H	-5.761356	-0.014634	0.588612
H	0.149594	5.841952	1.582044
H	4.352541	-2.354353	-5.206354
C	0.931973	4.460986	-0.621725
H	-5.246992	0.496859	-1.012462
C	3.921128	-1.396509	-4.891960
H	-3.984802	4.544977	-0.488451
H	2.010284	6.366503	-0.725106
H	3.385399	-4.241825	-3.616504
C	-5.241490	-0.344532	-0.316182
H	-4.420738	-2.784671	-0.337019
C	2.828424	-1.610021	-3.834732
C	0.788147	5.001415	1.842972
H	1.638941	3.914432	-1.252109
H	-1.870766	-4.850082	0.103206
C	-3.487290	2.481166	-0.197006
H	2.483985	-0.627000	-3.502184
H	0.726416	5.434054	3.947728
C	-3.954072	3.725853	0.229266
H	4.734942	-0.763788	-4.526638
H	-5.805238	-1.169680	-0.753478
C	-3.601430	-2.159758	-0.004853
C	1.283681	4.176902	0.831050
C	-3.830675	-0.786211	0.005335
H	-2.456005	-4.602497	1.742681
C	3.603497	-3.718222	-2.688689
C	1.110502	4.775947	3.172728
C	-2.619473	-4.319348	0.698573
C	3.363856	-2.345108	-2.610113
C	-2.481293	-2.825605	0.516997
N	-2.911463	0.131580	0.344212
C	-3.432717	1.425168	0.721388
H	4.276429	-5.501197	-1.690298
C	-4.393608	3.940569	1.531645
C	4.105720	-4.430904	-1.606741
C	0.536071	-3.818665	0.890510
N	-1.353923	-2.215657	0.876642
H	-3.612091	-4.652494	0.393944
C	2.100911	3.089163	1.188701
H	2.138169	-5.224152	1.081341
C	1.921756	3.700481	3.512167
H	4.388461	4.210678	0.979985
N	2.647419	2.232215	0.174253
C	1.422051	-4.610781	1.627768
C	3.667928	-1.686181	-1.400473
C	-0.386680	-3.024446	1.583052
C	-3.945853	1.595866	2.020064
C	-4.401928	2.854179	2.405025
N	3.475148	-0.269026	-1.271055
H	2.158535	3.526613	4.558031
C	2.419350	2.832807	2.539462
C	4.394318	-3.767434	-0.422273
C	3.781651	2.647274	-0.398367
H	5.676891	-1.000476	-2.621626
C	4.308408	4.038878	-0.096329
C	4.519016	0.507102	-1.529435
H	1.872605	0.887335	4.430092
C	4.199097	-2.389885	-0.301901
H	-4.783086	2.986050	3.416954
C	4.580313	1.886964	-1.260400
H	4.796717	-4.324635	0.421520
H	3.629010	4.800891	-0.489500
C	1.416421	-4.636513	3.015739
H	5.289317	4.184636	-0.550166
C	5.814237	-0.080369	-2.055907
C	-0.447443	-3.068939	2.990436
H	3.242994	1.783658	5.120010
H	5.471646	2.383882	-1.624287
H	2.601984	-1.774495	1.898299
C	2.943031	1.090571	4.325788
C	3.280248	1.635662	2.935154
H	6.333280	0.654263	-2.675749
H	3.068292	0.837099	2.213490
C	0.464767	-3.861700	3.680191
H	3.673547	-3.092684	2.370288
H	6.465350	-0.311162	-1.204463

C	3.643036	-2.022493	2.139576
C	4.598087	-1.685115	0.990849
H	4.539844	-0.605035	0.821224
H	3.483322	0.154210	4.499908
H	5.047251	2.789088	3.483614
C	4.782560	1.938079	2.844634
H	5.096559	2.163571	1.821524
H	0.414595	-3.894136	4.767698
H	3.925755	-1.473284	3.045111
H	6.162500	-3.053392	1.678432
H	6.745266	-1.798944	0.577175
C	6.043884	-2.001991	1.393252
H	5.363143	1.070945	3.182890
H	6.338544	-1.392913	2.255215
C	-0.020889	0.896672	-2.827947
C	-0.739203	1.433859	-3.876515
C	-0.365895	-0.272950	-2.111860
C	-1.843592	0.758140	-4.375252
C	-1.452428	-0.953628	-2.721438
C	-2.194329	-0.444832	-3.769560
F	1.043772	1.634089	-2.371493
F	-0.380297	2.614486	-4.394554
F	-2.543590	1.240951	-5.410313
F	-3.241258	-1.134433	-4.234685
F	-1.813386	-2.158609	-2.236208
F	0.745638	-1.200208	-1.854246
C	0.576296	-3.913628	-0.612652
H	0.503412	-4.963670	-0.919173
H	-0.221572	-3.350386	-1.093413
H	1.525289	-3.531699	-0.995965
C	-1.528140	-2.342451	3.750507
H	-1.478497	-2.587498	4.814696
H	-1.439414	-1.257305	3.649997
H	-2.525058	-2.618910	3.387114
C	2.415493	-5.461790	3.785433
H	1.981681	-5.856641	4.709105
H	2.778262	-6.305131	3.190627
H	3.286313	-4.856653	4.066574
C	-4.089244	0.432782	2.969426
H	-5.043670	-0.083835	2.804464
H	-3.299464	-0.307976	2.834874
H	-4.079416	0.772863	4.008870
C	-3.145832	2.263450	-1.644659
H	-2.327722	1.554507	-1.759303
H	-4.004724	1.850298	-2.188880
H	-2.872279	3.200471	-2.135686
C	-4.848933	5.303463	1.986771
H	-5.194530	5.909970	1.144658
H	-5.665364	5.229285	2.711417
H	-4.029355	5.846548	2.470923
Zn	1.763316	0.533252	-0.519158
Al	-0.983643	-0.291547	0.541543
C	-0.101173	0.478882	2.187669
H	0.284017	-0.385495	2.752858
H	0.803415	0.988113	1.839067
C	-0.810757	1.457624	3.132417
H	-0.137595	1.815494	3.920938
H	-1.167155	2.345144	2.597218
H	-1.676096	1.007528	3.627867

Substrates

C_6F_6

SCF (wB97X) = -827.413804701
H(0 K)= -827.360908
H(298 K)= -827.351329
G(298 K)= -827.395947
Lowest Frequency = 139.1309cm-1
PCM (Benzene) Energy = -827.414769740
wB97XD Corr = -0.0052457324

C	-3.233027	-0.308482	0.000084
C	-1.844013	-0.308552	0.000548
C	-1.149531	0.894316	0.000002
C	-1.843918	2.097320	-0.001010
C	-3.232864	2.097391	-0.001471
C	-3.927379	0.894462	-0.000930
F	-3.898413	3.249862	-0.002457
F	-1.178246	3.249719	-0.001548
F	0.181283	0.894321	0.000435
F	-1.178592	-1.461099	0.001503
F	-3.898569	-1.460955	0.000595
F	-5.258194	0.894607	-0.001388

C_6F_5H

SCF (wB97X) = -728.218165047
H(0 K)= -728.157082
H(298 K)= -728.148515
G(298 K)= -728.190885
Lowest Frequency = 135.8804cm-1
PCM (Benzene) Energy = -728.219319323
wB97XD Corr = -0.0050771270

C	-3.231079	-0.297081	0.000064
C	-1.842221	-0.311117	0.000549
C	-1.151615	0.894332	0.000005
C	-1.842103	2.099861	-0.001011
C	-3.230953	2.085969	-0.001477
C	-3.937898	0.894475	-0.000951
F	-3.880430	3.252446	-0.002468
F	-1.170862	3.251259	-0.001534
F	0.178674	0.894277	0.000455
F	-1.171119	-1.462596	0.001519
F	-3.880658	-1.463502	0.000586
H	-5.021199	0.894540	-0.001327

$C_6F_4H_2$

SCF (wB97X) = -629.021618702
H(0 K)= -628.952350
H(298 K)= -628.944763
G(298 K)= -628.984913
Lowest Frequency = 143.9116cm-1
PCM (Benzene) Energy = -629.022812527
wB97XD Corr = -0.0049184253

C	-3.230945	-0.295742	0.000069
C	-1.841907	-0.312224	0.000548
C	-1.161589	0.898925	-0.000021
C	-1.835005	2.110077	-0.001041
C	-3.221105	2.076925	-0.001481
C	-3.942975	0.893147	-0.000951
F	-3.890902	3.237157	-0.002485

F	0.172878	0.876116	0.000442
F	-1.174409	-1.468280	0.001530
F	-3.878558	-1.462769	0.000611
H	-5.026065	0.890469	-0.001318
H	-1.290973	3.046627	-0.001477