Electronic Supplementary Material (ESI) for Dalton Transactions.

1st Row Transition Metal Aluminylene Complexes: Preparation, Properties and Bonding Analysis

Electronic Supporting Information

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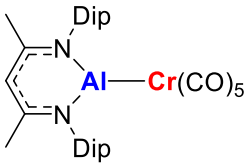
1 General Experimental

All manipulations were carried out using standard Schlenk-line and glovebox techniques under an inert atmosphere of argon or dinitrogen. 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 a 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. C_6D_6 was dried over 3 Å molecular sieves and freeze-pump-thaw degassed thrice before use.

NMR Spectra were recorded on Bruker 400 MHz or 500 MHz at 298 K unless otherwise stated and values recorded in ppm. Data were processed in MestReNova software. Where needed, chemical shifts were assigned with the assistance of 2D NMR (HSQC, HMBC, COSY) spectra. **1**[1], and **2f-h**[2–4] were synthesized according to literature procedures. IR spectra were recorded on an Agilent Cary630 ATR FTIR spectrometer. Photolysis experiments were conducted using a 400W Hg lamp. Chemicals were purchased from Sigma Aldrich, Fluorochem, Alfa Aesar, and VWR. Elemental analyses were performed by Elemental Labs (https://www.elementallab.co.uk/).

2 Synthetic Methods

2.1 – Preparation of compounds



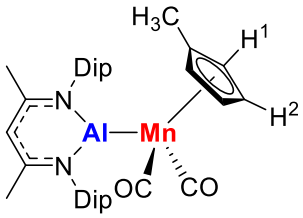
In a glovebox, **1** (18 mg, 0.04 mmol) was suspended in toluene (~ 0.5 mL) in a 20 mL scintillation vial. To this solution, a suspension of [$Cr(CO)_6$] (10 mg, 0.045 mmol) in toluene (~ 0.5 mL) was added at 25°C and the resultant mixture was placed under reduced pressure (static vacuum). The reaction mixture was swirled within the vial and evolution of CO gas was observed during the reaction. The vacuum atmosphere was refreshed periodically to remove the evolved CO gas. Upon dissolution of **1**, the reaction is assumed to be complete and formed a beige suspension of **3a** in toluene. The solvent was partially removed *in vacuo* until approximately 0.1 mL of toluene remained. The resultant crude mixture was diluted with ~2 mL of n-pentane and the solution was agitated to create a suspension of **3a**. The beige solid was collected by suction filtration and the residue was washed thrice with n-pentane. **3a** was transferred to a vial and dried briefly (~2 minutes) *in vacuo*. X-ray quality crystals were obtained from recrystallizing **3a** using a mixture of toluene, n-pentane, and the minimum amount of THF. Yield: 14 mg, 0.22 mmol, 55%.

^{1}H NMR (400 MHz, C_6D_6, 298 K) δ 0.99 (d, $^3J_{HH}$ = 6.8 Hz, 12H, (C***H***$_3$)$_2$CH), 1.43 (s, 6H, {(C***H***$_3$)$_2$C}$_2$CH), 1.46 (d, $^3J_{HH}$ = 6.8 Hz, 12H, (C***H***$_3$)$_2$CH), 3.09 (hept, $^3J_{HH}$ = 6.6 Hz, 4H, 4x (CH$_3$)$_2$C***H***), 5.07 (s, 1H, {(CH$_3$)C}$_2$C***H***), 7.10-7.23 (6H, Ar-***H***).

^{13}C NMR (101 MHz, C_6D_6, 298 K) δ 24.2 (2x (***C***H$_3$)$_2$CH), 24.3 ({(***C***H$_3$)$_2$C}$_2$CH), 24.4 (2x (***C***H$_3$)$_2$CH), 30.2 (4x (CH$_3$)$_2$***C***H)), 100.3 ({(CH$_3$)$_2$C}$_2$***C***H), 144.3 (Ar**C**), 171.1 ({(CH$_3$)$_2$***C***}$_2$CH). **3a** is poorly soluble in C_6D_6 and some quaternary carbon resonances were not observed.

IR (ATR), ν_{CO} (cm^{-1}): 2027, 1946, 1919, 1897, 1887.

Due to the instability of **3a** to vacuum accurate CHN analysis could not be obtained. Anal. Calc. ($C_{34}H_{41}AlCrN_2O_5$): C, 64.40;H, 6.49; N, 4.40. Found: C, 60.13; H, 6.49; N, 4.53.



In a glovebox, **1** (18 mg, 0.04 mmol) was suspended in C_6D_6 (0.6 mL) and transferred to a J-Young NMR tube. To this solution, [(η^5-C_5H_4Me)$Mn(CO)_3$] (7 µL, 9.7 mg, 0.044 mmol) was added *via* micropipette. The J-Young NMR tube was sealed and removed from the glovebox. The reaction mixture was heated at 80°C and shaken to ensure dissolution of **1**. Upon complete dissolution, the homogeneous reaction mixture was heated at 80°C for 16 h. The reaction was complete upon complete consumption of **1** as monitored by ^{1}H NMR spectroscopy. At this point, the NMR tube was returned to the glovebox and the headspace of the NMR tube was evacuated to remove the evolved CO gas. The solution was decanted into a 20 mL scintillation vial and diluted with ~ 2 mL of toluene. The resultant red-orange solution was concentrated *in vacuo* until ~ 0.4 mL of solution remained. The solution was filtered into a 4 mL vial, n-pentane layered on top, and **3b** allowed to crystallise at –35°C. **3b** crystallised as bright yellow crystals. The supernatant was decanted and the crystals were washed with cold (–35°C) n-pentane thrice (3x 0.5 mL) before the solid was dried briefly *in vacuo* (~ 2 minutes). Yield: 11 mg, 0.017 mmol, 43%).

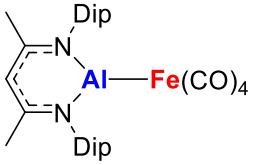
^{1}H NMR (400 MHz, C_6D_6, 298 K) δ 1.05 (d, $^3J_{HH}$ = 6.8 Hz, 12H, 2x (C***H***$_3$)$_2$CH), 1.48 (d, $^3J_{HH}$ = 6.8 Hz, 12H, 2x (C***H***$_3$)$_2$CH), 1.51 (s, 6H, {(C***H***$_3$)$_2$C}$_2$CH), 1.81 (s, 3H, C_5H_4C***H***$_3$), 3.22 (hept, $^3J_{HH}$ = 6.8 Hz, 4H, 4x (CH_3)$_2$C***H***), 3.49 (apparent t, *J* = 2.0 Hz, 2H, Cp'**H**$^2_2$), 3.98 (apparent t, *J* = 2.0 Hz, 2H, Cp'**H**$^1_2$), 5.10 (s, 1H, {(CH_3)C}C***H***), 7.10 – 7.23 (m, 6H, Ar-***H***).

^{13}C NMR (101 MHz, C_6D_6, 298 K) δ 14.2 (***C***$H_3C_5H_4$), 24.2 ({(***C***H_3)$_2$C}$_2$CH), 24.5 (2x (***C***H_3)$_2$CH), 24.5 (2x (***C***H_3)$_2$CH), 29.6 (4x (CH_3)$_2$***C***H), 76.2 (2x **C**H^2), 79.0 (2x **C**H^1), 96.9 (Cp'-**C**CH_3), 101.5 ({(CH_3)$_2$C}$_2$***C***H), 124.9 (Ar-**C**), 128.5 (Ar-**C**), 141.1 (Ar-**C**), 143.7 (Ar-**C**), 170.2 ({(CH_3)$_2$***C***}$_2$CH), 233.3 (Mn(***C***O)$_2$).

IR (ATR), ν_{CO} (cm^{-1}): 1886, 1813.

Anal. Calc. ($C_{38}H_{48}AlMnN_2O_2$): C, 70.02, H, 7.62; N, 4.41. Found: C,69.77; H, 7.60; N, 4.35.

***Synthesis of 3c*:**



In a glovebox, **1** (18 mg, 0.04 mmol) was suspended in toluene (0.6 mL) and transferred to a J-Young NMR tube. To this solution $Fe(CO)_5$ (7.5 µL, 11 mg, 0.055 mmol) was added *via* micropipette. The J-Young NMR tube was sealed and removed from the glovebox. The mixture was heated at 80°C briefly and shaken to ensure the complete dissolution of **1**. The reaction was complete within 5 minutes, and **3c** formed as a bright yellow precipitate. The NMR tube was returned to the glovebox and the headspace of the NMR tube was evacuated to purge the evolved CO gas from the reaction. The contents of the NMR tube were emptied into a 20 mL scintillation vial and the mixture was concentrated *in vacuo* until approximately ~0.5 mL of solvent remained. n-Pentane (2 mL) was added to the resultant crude mixture and the vial was placed in the freezer (–35°C) for 18 h. The supernatant was decanted and the bright yellow powder **3c** was washed with n-pentane thrice (3x 0.5 mL) before being dried *briefly* under vacuum. X-ray quality crystals can be grown from a concentrated toluene solution at –35°C. Yield: 19 mg, 0.31 mmol, 78%.

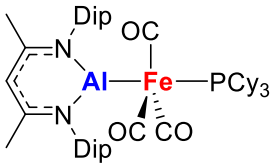
^{1}H NMR (400 MHz, C_6D_6, 298 K) δ 1.05 (d, $^3J_{HH}$ = 6.8 Hz, 12H, 2x (C***H***$_3$)$_2$CH), 1.45 (s overlapping, 6H, {(C***H***$_3$)$_2$C}$_2$CH), 1.46 (d, $^3J_{HH}$ = 6.5 Hz, 12H, 2x (C***H***$_3$)$_2$CH), 3.03 (hept, $^3J_{HH}$ = 6.8 Hz, 4H, 4x (CH$_3$)$_2$C***H***), 5.03 (s, 1H, {(CH$_3$)C}$_2$C***H***), 7.09-7.24 (m, 6H, Ar-***H***).

^{13}C NMR (101 MHz, C_6D_6, 298 K) δ 24.0 ({(***C***H$_3$)$_2$C}$_2$CH), 24.6 (2x (***C***H$_3$)$_2$CH), 24.7 (2x (***C***H$_3$)$_2$CH), 29.5 (4x (CH$_3$)$_2$***C***H), 102.6 ({(CH$_3$)$_2$C}$_2$***C***H), 125.3 (Ar***C***), 129.3 (Ar***C***), 138.3 (Ar***C***), 143.8 (Ar***C***), 172.8 ({(CH$_3$)$_2$ ***C***}$_2$CH), 215.7 (4x Fe***C***O).

IR (ATR), ν_{CO} (cm^{-1}): 2007, 1901, 1873.

Anal. Calc. ($C_{33}H_{41}AlFeN_2O_4$): C, 64.71, H, 6.75; N, 4.57. Found: C, 64.63; H, 6.45; N, 4.20.

Synthesis of 3d



In a glovebox, to a suspension of **3c** (18 mg, 0.029 mmol) in C_6D_6 (0.600 mL), was added PCy_3 (10 mg, 0.035 mmol) as a solid. The mixture was transferred to a borosilicate J-Young NMR tube, removed from the glovebox, and photolyzed at 25°C for 7 hours (400 W, Hg-lamp). The J-Young NMR tube was returned to the glovebox and exposed to vacuum, and refreshed with N_2 at the 2-hour and 4-hour timepoint to remove evolved CO gas. The reaction was monitored by ^{1}H NMR spectroscopy. Upon complete consumption of **3c**, the NMR-tube was returned to the glovebox, diluted with approx. 1 mL of toluene, and decanted into a 4 mL vial. The crude mixture was concentrated *in vacuo* until approximately 0.4 mL of solvent remained. n-Pentane was layered on top of toluene solution and the vial placed in the glovebox freezer at –35°C. **3d** crystallised as orange blocks. The supernatant was decanted, and the crystals were washed thrice with n-pentane (3x 0.5 mL), before the solid was dried briefly *in vacuo* (~ 2 miniutes). Yield: 10 mg, 0.012 mmol, 40%.

^{1}H NMR (400 MHz, C_6D_6, 298 K) δ 1.12 (d, $^3J_{HH}$ = 6.8 Hz, 12H, 2x (C***H***$_3$)$_2$CH), 1.15-1.26 (m, 9H, Cy-***H***), 1.54 (s, 6H, {(C***H***$_3$)$_2$C}$_2$CH), 1.49-1.62 (m overlapping, 9H, Cy-***H***), 1.65 (d, $^3J_{HH}$ = 6.8 Hz, 12H, 2x (C***H***$_3$)$_2$CH), 1.68-1.77 (m, 6H, Cy-***H***), 1.96 – 2.20 (m, 9H, Cy-***H***), 3.29 (hept, $^3J_{HH}$ = 6.7 Hz, 4H, 4x (CH$_3$)$_2$C***H***), 5.13 (s, 1H, {(CH$_3$)C}$_2$C***H***), 7.19 – 7.29 (m, 6H, Ar-***H***).

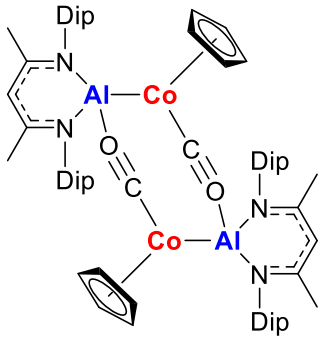
^{13}C NMR (101 MHz, C_6D_6, 298 K) δ 24.3 ({(***C***H$_3$)$_2$C}$_2$CH), 24.7 (2x (***C***H$_3$)$_2$CH), 25.0 (2x (***C***H$_3$)$_2$CH), 27.0 (Cy-***C***H$_2$), 28.3 (d, $^2J_{CP}$ = 9.9 Hz**,** Cy-***C***H$_2$), 29.6 (4x (CH$_3$)$_2$***C***H), 30.1 (Cy-***C***H$_2$), 39.15 (d, $^1J_{CP}$ = 18.1 Hz, Cy-***C***H), 101.9 ({(CH$_3$)$_2$C}$_2$***C***H), 124.9 (Ar-***C***), 128.6 (Ar-***C***), 140.1 (Ar-***C***), 143.9 (Ar-***C***), 171.6 ({(CH$_3$)$_2$***C***}$_2$CH), 216.8 (3x Fe***C***O).

^{31}P NMR (162 MHz, C_6D_6) δ 85.46.

IR (ATR), ν_{CO} (cm^{-1}): 1916, 1843, 1806.

Anal. Calc. ($C_{50}H_{74}AlFeN_2O_3P$): C, 69.43, H, 8.62; N, 3.24. Found: C, 69.44; H, 8.55; N, 2.90.

***Synthesis of 3e*:**



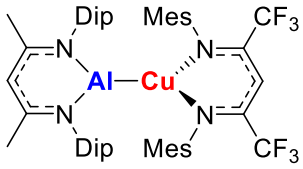
In a glovebox, a solution of **1** (18 mg, 0.040 mmol) and [CoCp(PCyPh$_2$)(CO)] (18 mg, 0.046 mmol) in benzene (~0.6 mL) was transferred to a J-Young NMR tube. n-Hexane was layered on top of this solution and the mixture was allowed to stand at 25°C undisturbed for 18 h. **(3e)$_2$** crystallised directly from the reaction mixture as a bright orange solid. The contents of the NMR tube were emptied into a vial and the crystals collected by decanting the supernatant. The orange solid was washed thrice with n-pentane (3x 1 mL) and dried briefly under vacuum (~ 2 minutes). Yield: 23 mg, 0.019 mmol, 96%.

3e is insoluble in common NMR solvents (toluene, benzene, THF) and so solution-state NMR spectra could not be attained.

IR (ATR), ν_{CO} (cm^{-1}): 1640

Anal. Calc. ($C_{70}H_{92}Al_2Co_2N_4O_2$): C, 70.45, H, 7.77; N 4.69,. Found: C, 70.91; H, 8.12; N, 4.43.

***Synthesis of 3f*:**



In a glovebox, **1** (20 mg, 0.045 mmol) and **2f** (21 mg, 0.038 mmol) were dissolved in toluene (~1 mL) in a 20 mL scintillation vial. The mixture was agitated at 25°C until the total dissolution of **1** was observed. A colour-change of the solution from the characteristic orange-red of **1** to a bright orange was observed. The vial was placed in the glovebox freezer (–35°C) and **3f** was allowed to recrystallise as a bright orange solid over 18 h. n-Pentane (~5 mL) was added to the mixture and the vial was returned to the freezer) for a further 18 h. The supernatant was decanted, and the resultant solid **3f** was washed thrice with n-pentane (3x 2 mL) and dried briefly *in vacuo* (~2 minutes). Yield: 30 mg, 0.031 mmol, 83%.

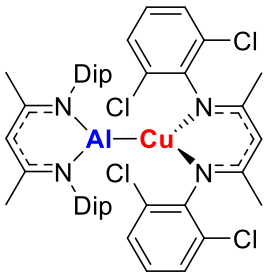
^{1}H NMR (400 MHz, C_6D_6, 298 K) δ 0.93 (d, $^{3}J_{HH}$ = 6.9 Hz, 12H, 2x (C***H***$_3$)$_2$CH), 0.98 (d, $^{3}J_{HH}$ = 6.8 Hz, 12H, 2x (C***H***$_3$)$_2$CH), 1.32 (s, 6H, {(C***H***$_3$)$_2$C}$_2$CH), 1.94 (s, 12H, 4x Mes-C***H***$_3$), 2.23 (s, 6H, 2x Mes-C***H***$_3$), 2.70 (hept, $^{3}J_{HH}$ = 6.8 Hz, 4H, 4x (CH$_3$)$_2$C***H***), 4.96 (s, 1H, {(CH$_3$)C}$_2$C***H***), 6.17 (s, 1H, {(CF$_3$)C}$_2$C***H***), 6.65 (s, 4H, Mes-C***H***), 6.99-7.14 (m, 6H, Ar***H***).

^{13}C NMR (101 MHz, C_6D_6, 298 K) δ 19.1 (4x Mes-***C***H$_3$), 21.1 (2x Mes-***C***H$_3$), 23.3 (2x (***C***H$_3$)$_2$CH), 23.9 ({(***C***H$_3$)$_2$C}$_2$CH), 24.8 (2x (***C***H$_3$)$_2$CH), 29.7 (4x (CH$_3$)$_2$***C***H), 84.6 ({(CF$_3$)$_2$C}$_2$***C***H), 102.5 ({(CH$_3$)$_2$C}$_2$***C***H), 125.3 (Ar***C***), 128.8 (Ar***C***), 130.6 (Ar***C***), 131.5 (Ar***C***), 140.8 (Ar***C***), 143.0 (2x Ar***C***), 147.9 (Ar***C***), 169.6 ({(CH$_3$)$_2$***C***}$_2$CH). Some quaternary carbon resonances cannot be observed due to coupling to ^{19}F.

^{19}F NMR (377 MHz, C_6D_6, 298 K) δ -63.08 .

Anal. Calc. ($C_{52}H_{64}AlCuF_6N_4$): C, 65.77, H, 6.79; N, 5.90. Found: C, 67.03; H, 6.94; N, 5.71.

***Synthesis of 3g*:**



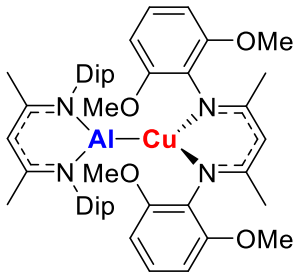
In a glovebox, **1** (20 mg, 0.045 mmol) and **2g** (19 mg, 0.038 mmol) were dissolved in toluene (~1 mL) in a 20 mL scintillation vial. The mixture was agitated at 25°C until the dissolution of **1** was observed. A colour-change of the solution from the characteristic orange-red of **1** to a bright yellow was observed. The solution was concentrated until approximately 0.4 mL remained. The vial was placed in the glovebox freezer (–35°C) and **3f** was allowed to recrystallise as a bright yellow solid over 18 h. The supernatant was decanted, and the resultant solid was washed thrice with n-pentane (3x 2 mL) and dried briefly *in vacuo* (~2 minutes). Yield: 20 mg, 0.022 mmol, 58%.

^{1}H NMR (400 MHz, C_6D_6, 298 K) δ 1.05 (d, $^{3}J_{HH}$ = 6.9 Hz, 12H, 2x (C***H***$_3$)$_2$CH), 1.15 (d, $^{3}J_{HH}$ = 6.8 Hz, 12H, 2x (C***H***$_3$)$_2$CH), 1.39 (s, 6H, {(C***H***$_3$)$_2$C}$_2$CH), 1.62 (s, 6H, {(C***H***$_3$)$_2$C}$_2$CH), 2.86 (hept, $^{3}J_{HH}$ = 6.9 Hz, 4H, 4x (CH$_3$)$_2$C***H***), 4.90 (s, 1H, {(CH$_3$)C}$_2$C***H***), 5.06 (s, 1H, {(CH$_3$)C}$_2$C***H***), 6.42 (apparent t, *J* = 7.9 Hz, 2H, Ar-***H***), 6.90 – 7.32 (m, 10H, Ar-***H***).

^{13}C NMR (101 MHz, C_6D_6, 298 K) δ 23.3 (2x (***C***H$_3$)$_2$CH), 23.6 ({(***C***H$_3$)$_2$C}$_2$CH), 24.0 ({(***C***H$_3$)$_2$C}$_2$CH), 24.8 (2x (***C***H$_3$)$_2$CH), 29.6 (4x (CH$_3$)$_2$***C***H), 96.1 ({(CH$_3$)$_2$C}$_2$***C***H), 102.4 ({(CH$_3$)$_2$C}$_2$***C***H), 122.3 (Ar***C***), 125.2 (Ar***C***), 127.9 (Ar***C***), 128.4 (Ar***C***), 131.4 (Ar***C***), 141.3 (Ar***C***), 142.4 (Ar***C***), 151.1 (Ar***C***), 162.8 ({(CH$_3$)$_2$***C***}$_2$CH), 169.4 ({(CH$_3$)$_2$***C***}$_2$CH).

Anal. Calc. ($C_{46}H_{54}AlCl_4CuN_4$): C, 61.71, H, 6.08; N, 6.26. Found: C, 61.62; H, 5.80; N, 6.13.

***Synthesis of 3h*:**



In a glovebox, **1** (20 mg, 0.045 mmol) and **2h** (18 mg, 0.038 mmol) were suspended in toluene (~0.6 mL) and transferred to a J-Young NMR tube. The NMR tube was removed from the glovebox and heated at 100°C briefly to dissolve the reagents, at which point the reaction is likely complete. The J-Young NMR tube was returned to the glovebox and the reaction mixture was decanted into a 20 mL scintillation vial. The vial was placed in the glovebox freezer (–35°C) and **3h** was allowed to recrystallize as green-brown needles. The supernatant was decanted, and the solid was washed thrice with n-pentane (3x 2 mL) before the crystals were dried briefly *in vacuo* (~2 minutes). Yield: 26 mg, 0.030 mmol, 79%.

^{1}H NMR (400 MHz, C_6D_6, 298 K) δ 1.07 (d, $^{3}J_{HH}$ = 6.8 Hz, 12H, 2x (C***H***$_3$)$_2$CH), 1.11 (d, $^{3}J_{HH}$ = 6.8 Hz, 12H, 2x (C***H***$_3$)$_2$CH), 1.38 (s, 6H, {(C***H***$_3$)$_2$C}$_2$CH), 1.96 (s, 6H, {(C***H***$_3$)$_2$C}$_2$CH), 3.00 (hept, $^{3}J_{HH}$ = 6.8 Hz, 4H, 4x (CH$_3$)$_2$C***H***), 3.33 (s, 12H 4x OC***H***$_3$), 4.91 (s, 1H, {(CH$_3$)C}$_2$C***H***), 5.00 (s, 1H, {(CH$_3$)C}$_2$C***H***), 6.49 (apparent d, *J* = 8.2 Hz, 4H, Ar-***H***), 6.73 – 6.88 (m, 2H, Ar-***H***), 6.97 – 7.18 (m, 6H, Ar-***H***).

^{13}C NMR (101 MHz, C_6D_6, 298 K) δ 23.5 ({(***C***H$_3$)$_2$C}$_2$CH), 23.6 ({(***C***H$_3$)$_2$C}$_2$CH), 24.1 (2x (***C***H$_3$)$_2$CH), 25.4 (2x (***C***H$_3$)$_2$CH), 29.2 (4x (CH$_3$)$_2$***C***H), 56.4 (4x O***C***H$_3$), 96.7 ({(CH$_3$)$_2$C}$_2$***C***H), 101.1 ({(CH$_3$)$_2$C}$_2$***C***H), 108.5 (Ar***C***), 121.1 (Ar***C***), 124.4 (Ar***C***), 127.4 (Ar***C***), 128.3 (Ar***C***), 136.9 (Ar***C***), 140.3 (Ar***C***), 144.2 (Ar***C***), 154.1 (Ar***C***), 162.7 ({(CH$_3$)$_2$***C***}$_2$CH), 167.7 ({(CH$_3$)$_2$***C***}$_2$CH).

Anal. Calc. ($C_{50}H_{66}AlCuN_4O_2$): C, 68.43, H, 7.58; N, 6.38. Found: C, 65.44; H, 7.50; N, 6.12.

3. X-ray Data

The X-ray crystal structure of ***3a***

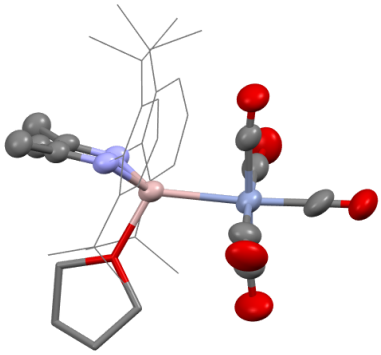


Figure S1: The X-ray crystal structure of **3a**. Hydrogen atoms and included solvent omitted for clarity.

3a was found to crystallise in the space group $P2_1/n$., with an included toluene molecule in the asymmetric unit.

Crystal Data for $C_{45}H_{57}AlCrN_2O_6$, M =800.90, monoclinic, space group $P2_1/n$ (no. 14), a = 10.9861(6) Å, b = 25.9752(14) Å, c = 15.2738(10) Å, β = 99.548(6)°, V = 4298.2(4) Å^3, Z = 4, ρ_{calc}g/cm^3 = 1.238, μ(CuKα) = 2.771 mm^{-1}, T = 173.0(3), yellow needles, F^2 refinement, R_1(obs) = 0.0838, wR_2(all) = 0.2867, 8300 independent observed reflections (R_{int} = 0.1021), 3608 independent measured reflections [$|F_o| > 4\sigma(|F_o|)$, $2\theta_{full}$ = 147.318], 507 parameters. CSD 2071011.

The X-ray crystal structure of ***3b***

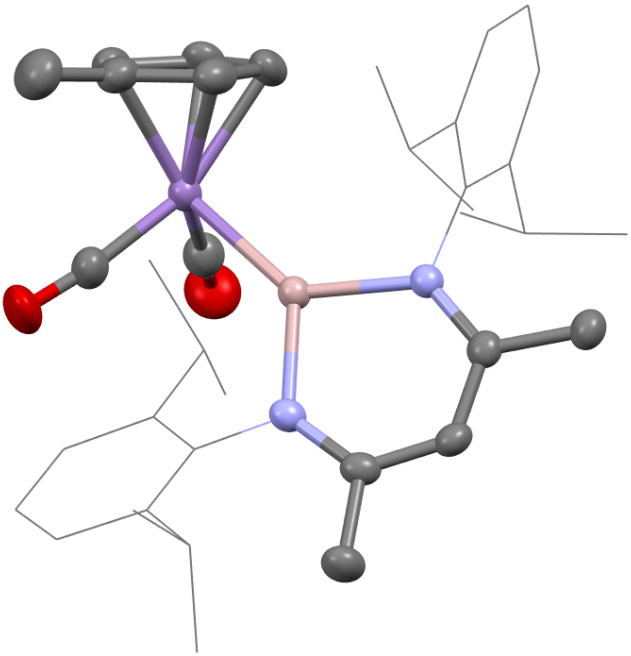


Figure S2: The X-ray crystal structure of **3b**. One of two independent molecules. Hydrogen atoms omitted for clarity.

3b was found to crystallise in the space group $P2_1/n$.

Crystal Data for $C_{37}H_{48}AlMnN_2O_2$, M =634.69, monoclinic, space group $P2_1/n$ (no. 14), a = 8.86240(19) Å, b = 20.6632(3) Å, c = 18.2680(3) Å, β = 94.2925(17)°, V = 3335.95(10) Å^3, Z = 4, ρ_{calc}g/cm^3 = 1.264, μ(CuKα) = 3.733 mm^{-1}, T = 173.00(14), yellow prisms, F^2 refinement, R_1(obs) = 0.0413, wR_2(all) = 0.1124, 6343 independent observed reflections (R_{int} = 0.0301), 5120 independent measured reflections [$|F_o| > 4\sigma(|F_o|)$, $2\theta_{full}$ = 146.57], 399 parameters. CSD 2071012.

The X-ray crystal structure of ***3c***

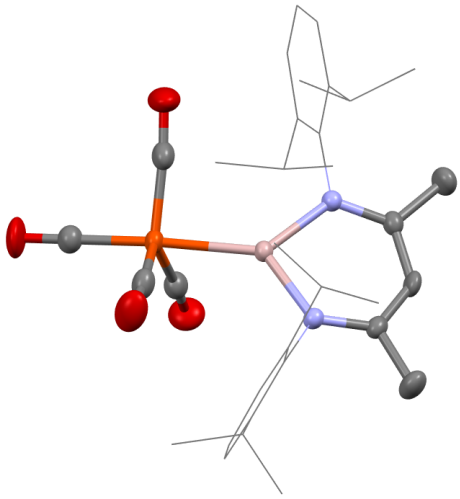


Figure S3: The X-ray crystal structure of **3c**. Hydrogen atoms, disorder, and included solvent omitted for clarity.

3c was found to crystallise in the space group Pnma. The unit cell of the crystal was found to contain four full molecules of **3c**, and four full molecules of toluene. Accordingly, the asymmetric unit of the crystal contains half a molecule of **3c**, and half a molecule of toluene. Both molecules are disordered along a mirror plane defined by the Al1–Fe1–C1 atoms.

The included toluene is disordered over this mirror plane. The toluene is modelled in two orientations in the Part -1 and Part -2 with major and minor occupancies *ca.* 34% and 16%, summing to one half occupancy toluene molecule, with the symmetry element generating the other half. The thermal parameters of adjacent atoms in the major and minor components were restrained to be similar, their geometries optimized, and only the non-hydrogen atoms in the major orientation were refined anisotropically (those in the minor orientation were refined isotropically).

Crystal Data for $C_{40}H_{49}AlFeN_2O_4$, M =704.64, orthorhombic, space group Pnma (no. 62), a = 21.9278(9) Å, b = 16.6105(8) Å, c = 10.6008(6) Å, V = 3861.2(3) Å^3, Z = 4, ρ_{calc}g/cm^3 = 1.212, μ(MoKα) = 0.454 mm^{-1}, T = 173.00(14), yellow plates, F^2 refinement, R_1(obs) = 0.0450, wR_2(all) = 0.1310, 4086 independent observed reflections (R_{int} = 0.0314), 2941 independent measured reflections [|F_o| > 4σ(|F_o|), $2\theta_{full}$ = 56.668], 271 parameters. CSD 2071013.

The X-ray crystal structure of ***3d***

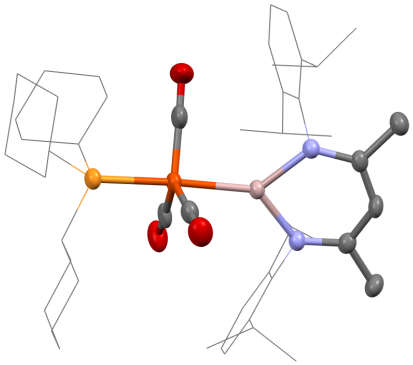


Figure S4: The X-ray crystal structure of **3d**. Hydrogen, included solvent, and disorder omitted for clarity.

3d was found to crystallise in the $P2_1/n$ space group with an included toluene molecule in the asymmetric unit.

The cyclohexyl ring (C39>C44) was modelled as disordered over two sites in *ca.* 77:23 occupancies for the major and minor orientations respectively. The two orientations are related by ring-flip isomerisation of the cyclohexyl group. The carbon atom C39 occupies the same position in both ring conformations and so was not included in the disorder model. The thermal parameters of adjacent atoms in the major and minor components were restrained to be similar, their geometries optimized, and only the non-hydrogen atoms in the major orientation were refined anisotropically (those in the minor orientation were refined isotropically).

The included toluene was found to be disordered over two sites in *ca.* 51:49 occupancies for the major and minor occupancies respectively. The thermal parameters of adjacent atoms in the major and minor components were restrained to be similar, their geometries optimized, and both orientations were refined aniostropically

Crystal Data for $C_{57}H_{82}AlFeN_2O_3P$, M =957.04, monoclinic, space group $P2_1/c$ (no. 14), a = 14.0053(4) Å, b = 16.6674(5) Å, c = 23.4517(10) Å, β = 102.825(4)°, V = 5337.8(3) Å^3, Z = 4, ρ_{calc}g/cm^3 = 1.191, μ(MoKα) = 0.373 mm^{-1}, T = 173.05(10), yellow prisms, F^2 refinement, R_1(obs) = 0.0598, wR_2(all) = 0.1649, 10728 independent observed reflections (R_{int} = 0.0318), 7543 independent measured reflections [$|F_o| > 4\sigma(|F_o|)$, $2\theta_{full}$ = 56.614], 659 parameters. CSD 2071014.

The X-ray crystal structure of ***(3e)*****$_2$**

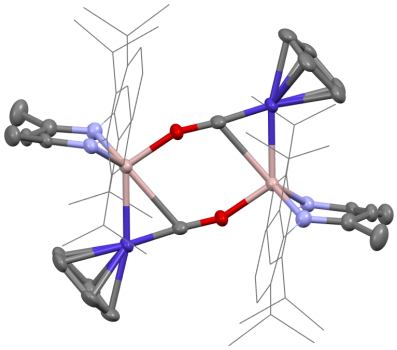


Figure S5: The X-ray crystal structure of **(3e)$_2$**. Hydrogen atoms and included solvent omitted for clarity.

(3e)$_2$ was found to crystallise in the space group $P2_1/c$. The unit cell contains two full molecules of **(3e)$_2$**and four molecules of benzene, corresponding to half a molecule of **(3e)$_2$** and a full benzene molecule in the asymmetric unit. A full molecule of **(3e)$_2$** can be generated from the asymmetric unit by C_2 rotation.

The included benzene molecule (C36–C41) was modelled as disordered over two sites in *ca.* 63:37 ratio for the major and minor components respectively. The thermal parameters of adjacent atoms in the major and minor components were restrained to be similar, their geometries optimized, and only the non-hydrogen atoms in the major orientation were refined anisotropically (those in the minor orientation were refined isotropically).

Crystal Data for $C_{82}H_{104}Al_2Co_2N_4O_2$, M =1349.51, monoclinic, space group $P2_1/c$ (no. 14), a = 13.1004(2) Å, b = 24.5243(3) Å, c = 12.29286(17) Å, β = 111.8523(19)°, V = 3665.66(10) Å^3, Z = 2, ρ_{calc}g/cm^3 = 1.223, μ(CuKα) = 4.145 mm^{-1}, T = 173.00(14), yellow needles, F^2 refinement, R_1(obs) = 0.0428, wR_2(all) = 0.1076, 7023 independent observed reflections (R_{int} = 0.0293), 5595 independent measured reflections [$|F_o| > 4\sigma(|F_o|)$, $2\theta_{full}$ = 146.77], 426 parameters. CSD 2071015.

*The X-ray crystal structure of **3f***

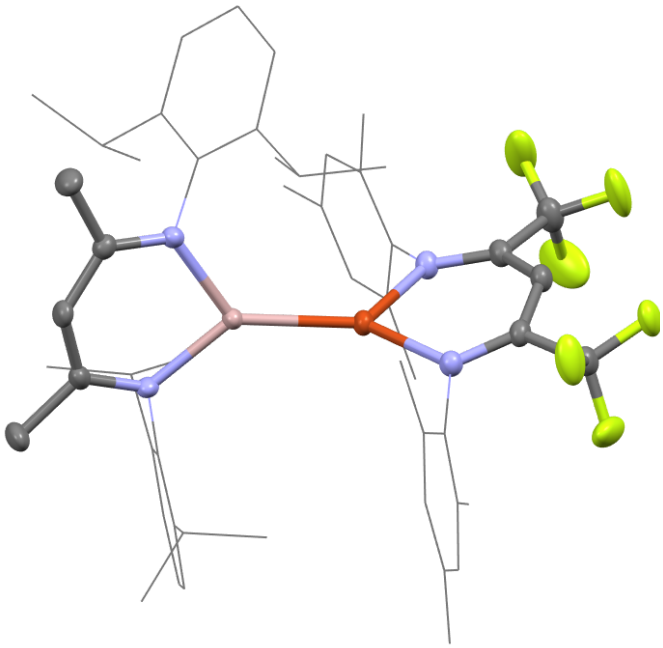


Figure S6: The X-ray crystal structure of **3f**. Hydrogen atoms omitted for clarity.

3f was found to crystallise in the P-1 space group.

Crystal Data for $C_{26}H_{32}Al_{0.5}Cu_{0.5}F_3N_2$, M =474.79, triclinic, space group P-1 (no. 2), a = 11.1165(4) Å, b = 12.5995(5) Å, c = 19.3405(8) Å, α = 88.586(3)°, β = 88.722(3)°, γ = 67.821(4)°, V = 2507.43(18) Å^3, Z = 4, ρ_{calc}g/cm^3 = 1.258, μ(MoKα) = 0.513 mm^{-1}, T = 173.00(14), orange plates, F^2 refinement, R_1(obs) = 0.0412, wR_2(all) = 0.1149, 9920 independent observed reflections (R_{int} = 0.0182), 7902 independent measured reflections [$|F_o| > 4\sigma(|F_o|)$, $2\theta_{full}$ = 56.536], 593 parameters. CSD 2071016.

*The X-ray crystal structure of **3g***

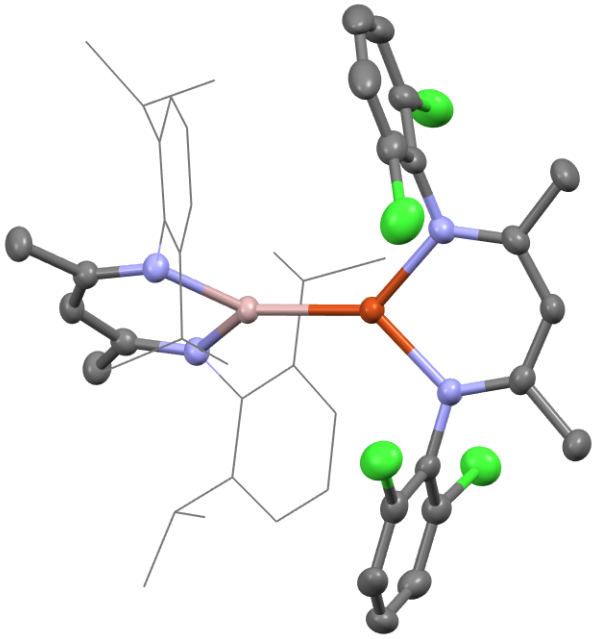


Figure S7: The X-ray crystal structure of **3g**. Hydrogen atoms omitted for clarity.

3g was found to crystallise in the $P2_1/n$ space group.

Crystal Data for $C_{46}H_{54}AlCl_4CuN_4$, M =895.25, monoclinic, space group $P2_1/n$ (no. 14), a = 11.11938(13) Å, b = 20.2656(2) Å, c = 20.5958(2) Å, β = 96.1813(10)°, V = 4614.09(9) Å^3, Z = 4, ρ_{calc}g/cm^3 = 1.289, μ(CuKα) = 3.252 mm^{-1}, T = 173.00(14), yellow needles, F^2 refinement, R_1(obs) = 0.0443, wR_2(all) = 0.1177, 8930 independent observed reflections (R_{int} = 0.0645), 6828 independent measured reflections [$|F_o| > 4\sigma(|F_o|)$, $2\theta_{full}$ = 147.702], 517 parameters. CSD 2071017.

The X-ray crystal structure of ***3h***

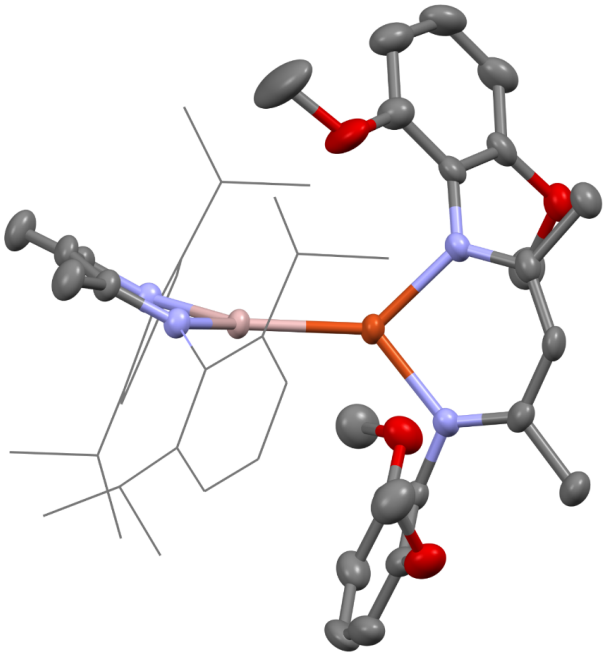


Figure S8: The X-ray crystal structure of **3h**. Hydrogen atoms omitted for clarity.

3h was found to crystallise in the $P2_1/n$ space group. Two toluene molecules were found in the asymmetric unit, for a total of eight within the unit cell.

The included toluene molecule (C58–C64) was modelled as disordered over two sites in *ca.* 71:29 ratio for the major and minor components respectively. The thermal parameters of adjacent atoms in the major and minor components were restrained to be similar, their geometries optimized, and only the non-hydrogen atoms in the major orientation were refined anisotropically (those in the minor orientation were refined isotropically).

Crystal Data for $C_{64}H_{82}AlCuN_4O_4$, M =1061.85, monoclinic, space group $P2_1/n$ (no. 14), a = 12.1523(2) Å, b = 27.1205(6) Å, c = 17.9897(4) Å, β = 97.1641(19)°, V = 5882.7(2) Å^3, Z = 4, ρ_{calc}g/cm^3 = 1.199, μ(CuKα) = 1.048 mm^{-1}, T = 173.0(3), yellow needles, F^2 refinement, R_1(obs) = 0.0573, wR_2(all) = 0.1284, 10285 independent observed reflections (R_{int} = 0.0532), 6665 independent measured reflections [$|F_o| > 4\sigma(|F_o|)$, $2\theta_{full}$ = 133.186], 691 parameters.

4. Density Functional Theory Calculations

4.1 Computational Methods

DFT calculations were run using Gaussian 09 (Revision D.01)[5] using the M06l Minnesota functional.[6] Al and Mg centres were described with Stuttgart SDDAll ECP and associated basis sets, and the 6-31G** basis sets were used for all other atoms. M06l has been previously benchmarked against other functionals (ωB97x, B3PW91, M062x) to provide the best agreement with experimental data for closely related systems.[7,8] Geometry optimisation calculations were performed without symmetry constraints. 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). Single point solvent corrections (benzene, ε = 2.2706) were applied using the polarizable continuum model (PCM) to free energies reported in the main text. Single point dispersion corrections were applied to the free energies to the Minnesota functional (M06l) energies using Grimme's D3 correction.[9]

ETS-NOCV calculations were performed in the Orca 4.2.1 quantum chemistry software package[10–12] with optimised geometries attained above. The calculations were run using the M06l Minnesota functional with the def2-tzvpp basis set. Calculations were performed with the resolution of identity approximation for the Coulomb integrals, and chain of spheres approximation for the exchange integrals (RIJCOSX) with the def2/j auxiliary basis set.[13]

LED calculations were performed in the Orca 4.2.1 quantum chemistry software with optimized geometries attained above.[14,15] The calculations were performed at the DLPNO-CCSD(T)[16] level with the def2-tzvpp basis set, def2/jk, and def2-tzvpp/c auxiliary basis sets. TightPNO settings were used for the DLPNO-CCSD(T) calculations. The Foster-Boys method was used to localize orbitals. Calculations were performed with the resolution of identity approximation for the Coulomb integrals, and chain of spheres approximation for the exchange integrals (RIJCOSX) with the def2/j auxiliary basis set. Dispersion interaction density plots were generated as described by Pollice and Chen[17] and as implemented in Orca 4.2.1. The perturbative triples correction was decomposed to dispersive and non-dispersive components using the scheme recommended by Bistoni and co-workers.[14]

4.2 ETS-NOCV Deformation Density Plots

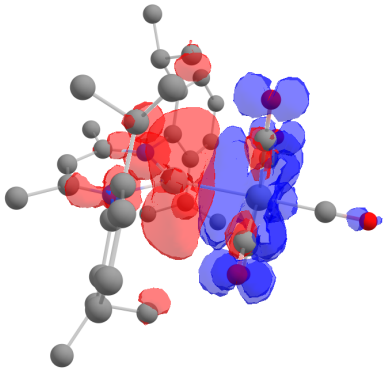
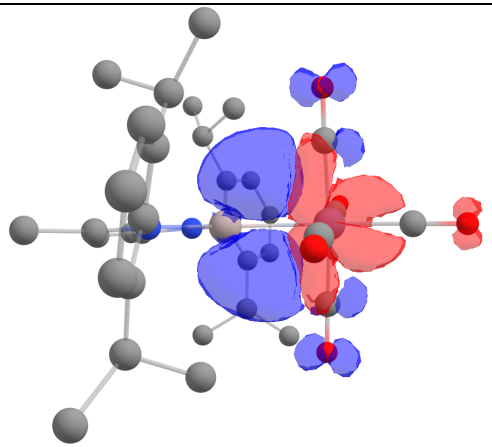
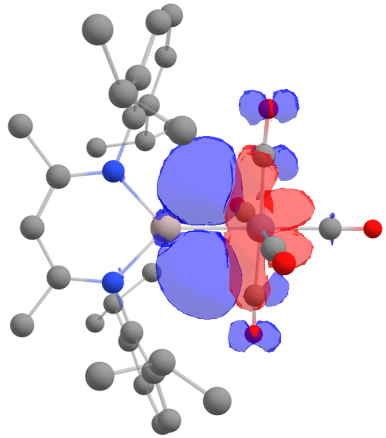
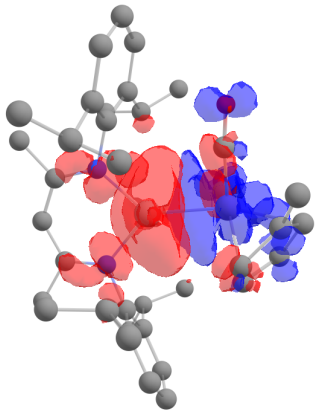
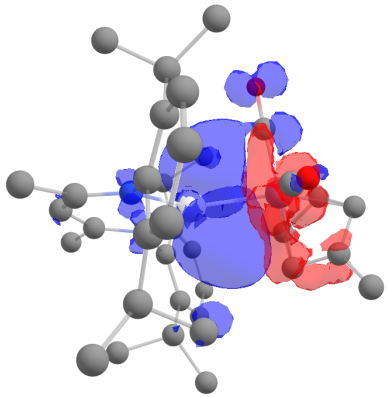
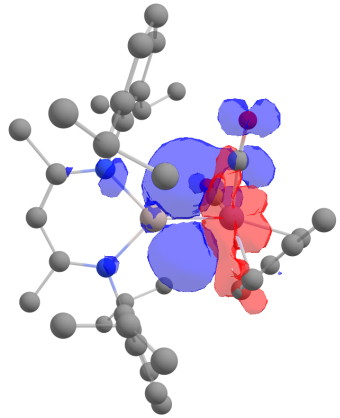
	ΔE_{orb}	$\Delta\rho_1$	$\Delta\rho_2$	$\Delta\rho_3$
3a	–84.4			
		–64.6	–7.1	–5.9
3b	–93.3			
		–64.2	–13.0	–8.5

Table S1: Deformation densities of the first three contributions. Energies in kcal mol^{-1}, charge flow from red to blue.

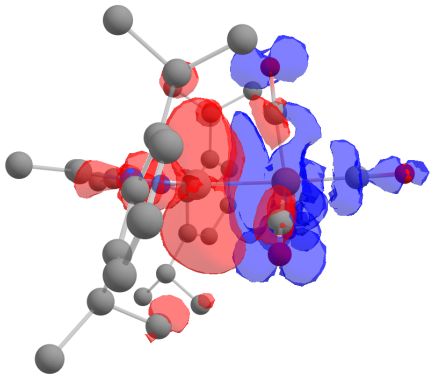
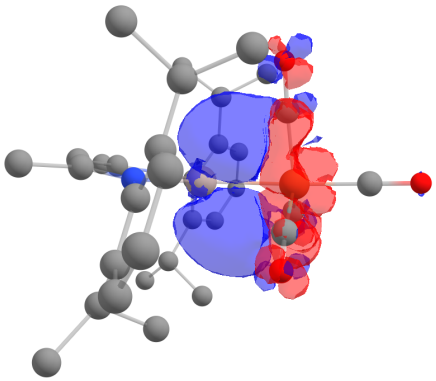
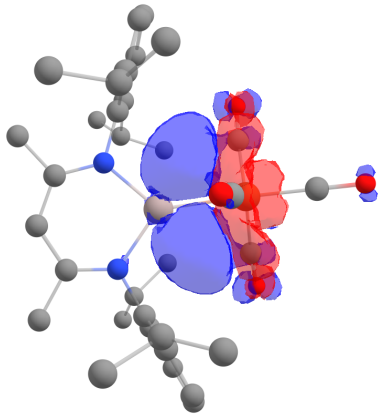
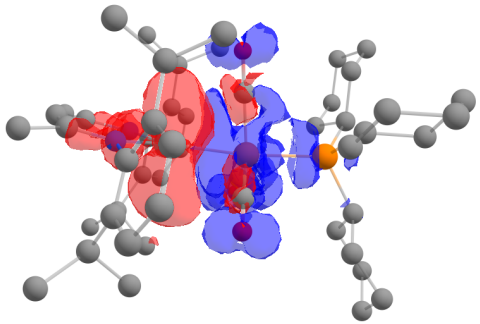
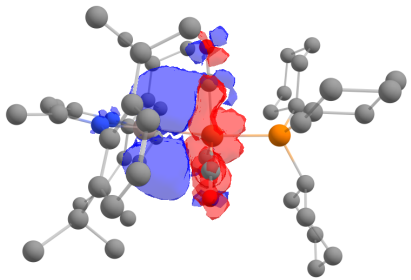
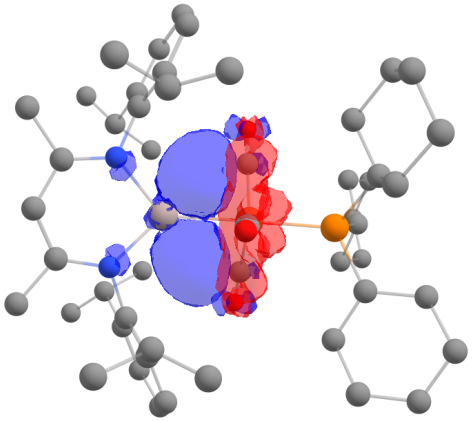
	ΔE_{orb}	$\Delta\rho_1$	$\Delta\rho_2$	$\Delta\rho_3$
3c	−128.1	 −103.0	 −9.7	 −7.8
3d	−129.7	 −102.1	 −10.9	 −8.8

Table S2: Deformation densities of the first three contributions. Energies in kcal mol^{-1}, charge flow from red to blue.

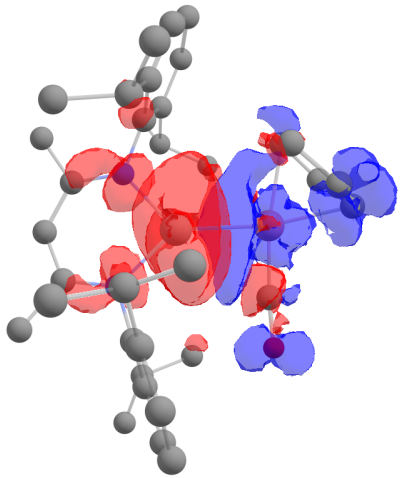
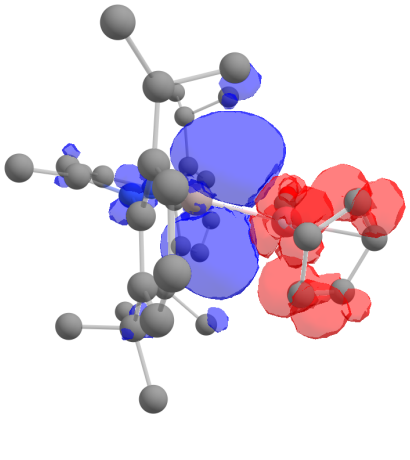
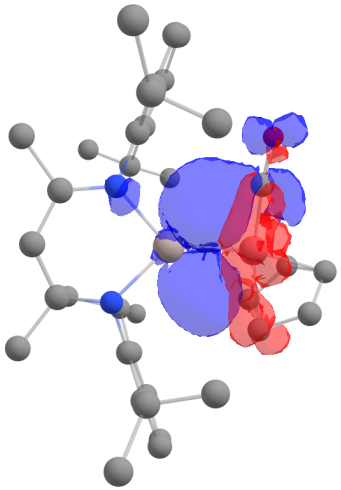
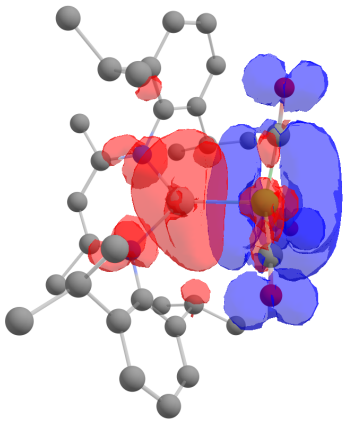
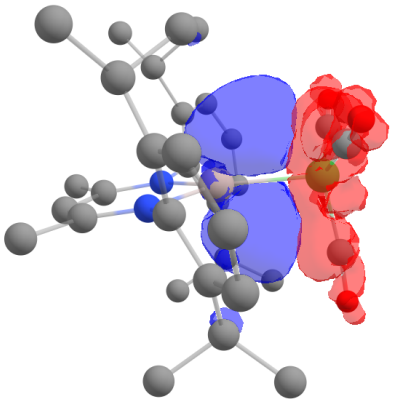
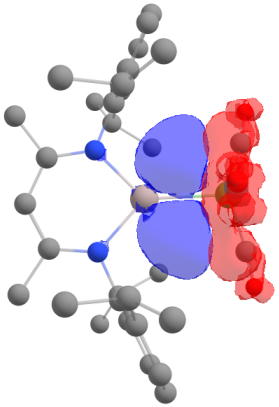
	ΔE_{orb}	$\Delta\rho_1$	$\Delta\rho_2$	$\Delta\rho_3$
3e	–86.1	 –55.3	 –16.4	 –7.1
[Ni(CO)$_3$1]	–65.5	 –46.1	 –7.2	 –5.7

Table S3: Deformation densities of the first three contributions. Energies in kcal mol^{-1}, charge flow from red to blue.

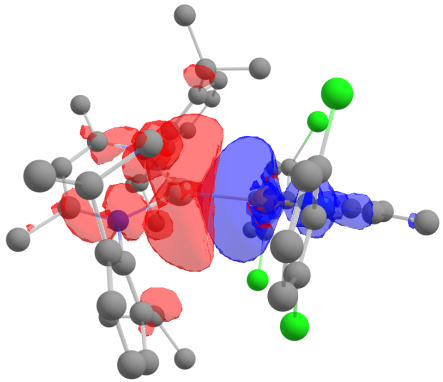
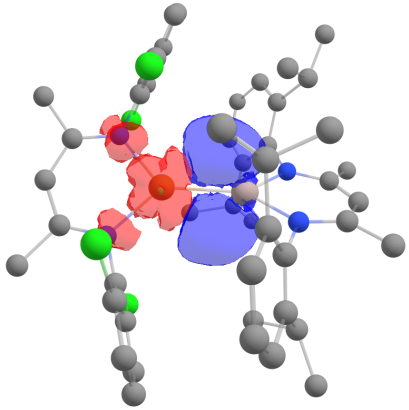
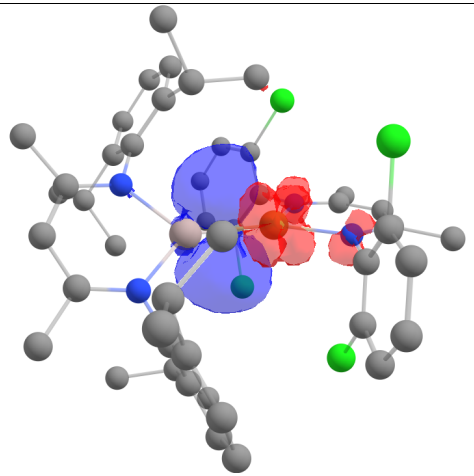
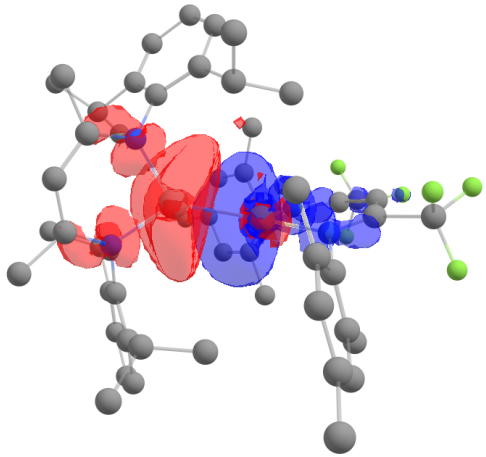
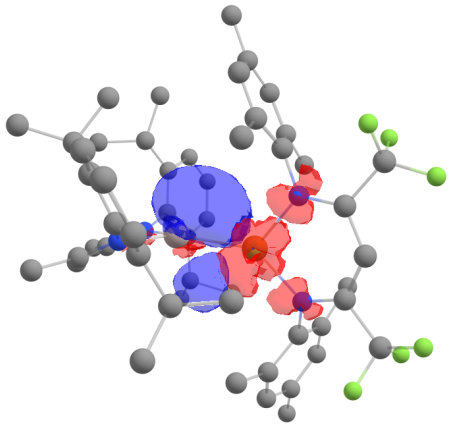
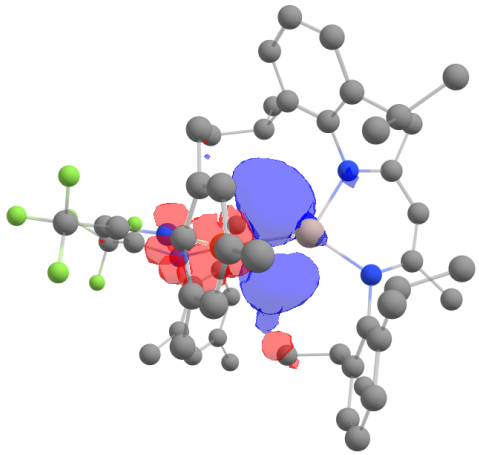
	ΔE_{orb}	$\Delta\rho_1$	$\Delta\rho_2$	$\Delta\rho_3$
3f	−47.5	 −22.5	 −8.0	 −4.1
3g	−43.4	 −21.3	 −7.0	 −4.1

Table S4: Deformation densities of the first three contributions. Energies in kcal mol^{-1}, charge flow from red to blue.

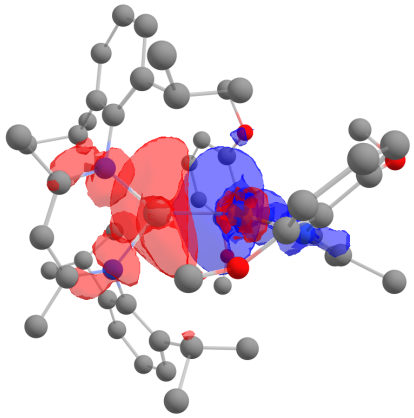
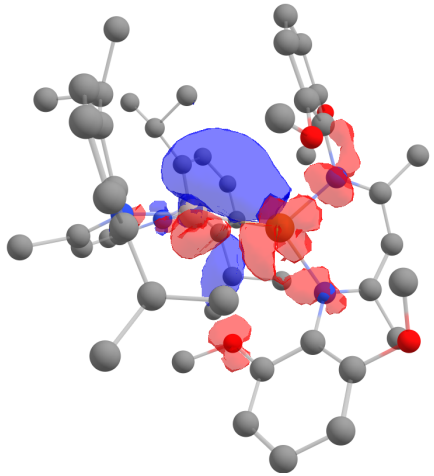
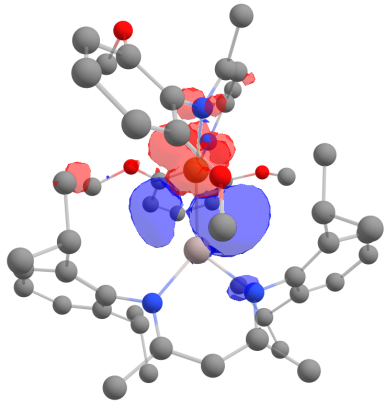
	ΔE_{orb}	$\Delta\rho_1$	$\Delta\rho_2$	$\Delta\rho_3$
3h	–47.4	 –18.6	 –9.9	 –4.9

Table S5: Deformation densities of the first three contributions. Energies in kcal mol^{-1}, charge flow from red to blue.

4.3 Local energy decomposition calculations

4.3.1 Local energy decomposition components

	ΔE_{int}	ΔE_{int}^{HF}	E_{elstat}^{HF}	$E_{exchange}^{HF}$	$\Delta E_{el-prep}^{HF}$	ΔE_{int}^{C}	$E_{disp}^{C-CCSD(T)}$	$\Delta E_{non-disp}^{C-CCSD(T)}$
3a	–77.2	–27.4	–719.4	–155.1	+847.1	–49.7	–38.5	–11.2
3b	–78.5	–5.5	–905.4	–173.4	+1073.3	–73.0	–42.7	–30.3
3c	–95.7	–20.0	–1056.1	–187.8	+1224.0	–75.6	–42.1	–33.6
3d	–95.5	–12.3	–1108.1	–197.3	+1293.1	–83.3	–44.8	–38.5
3e	–78.6	–5.5	–855.8	–144.9	+995.2	–73.1	–40.5	–32.7
[Ni(CO)$_3$1]	–54.1	–18.3	–791.7	–163.3	+936.7	–35.8	–27.5	–8.3
3f	–61.6	–8.1	–450.6	–79.2	+521.1	–53.5	–42.5	–11.3
3g	–62.3	–8.7	–431.7	–75.8	+499.4	–53.6	–42.3	–11.1
3h	–63.0	–0.2	–460.3	–85.2	+545.3	–62.8	–50.3	–12.6

Table S6: Local energy decomposition results. All energies in kcal mol^{-1}.

4.3.2 Dispersion interaction density plots

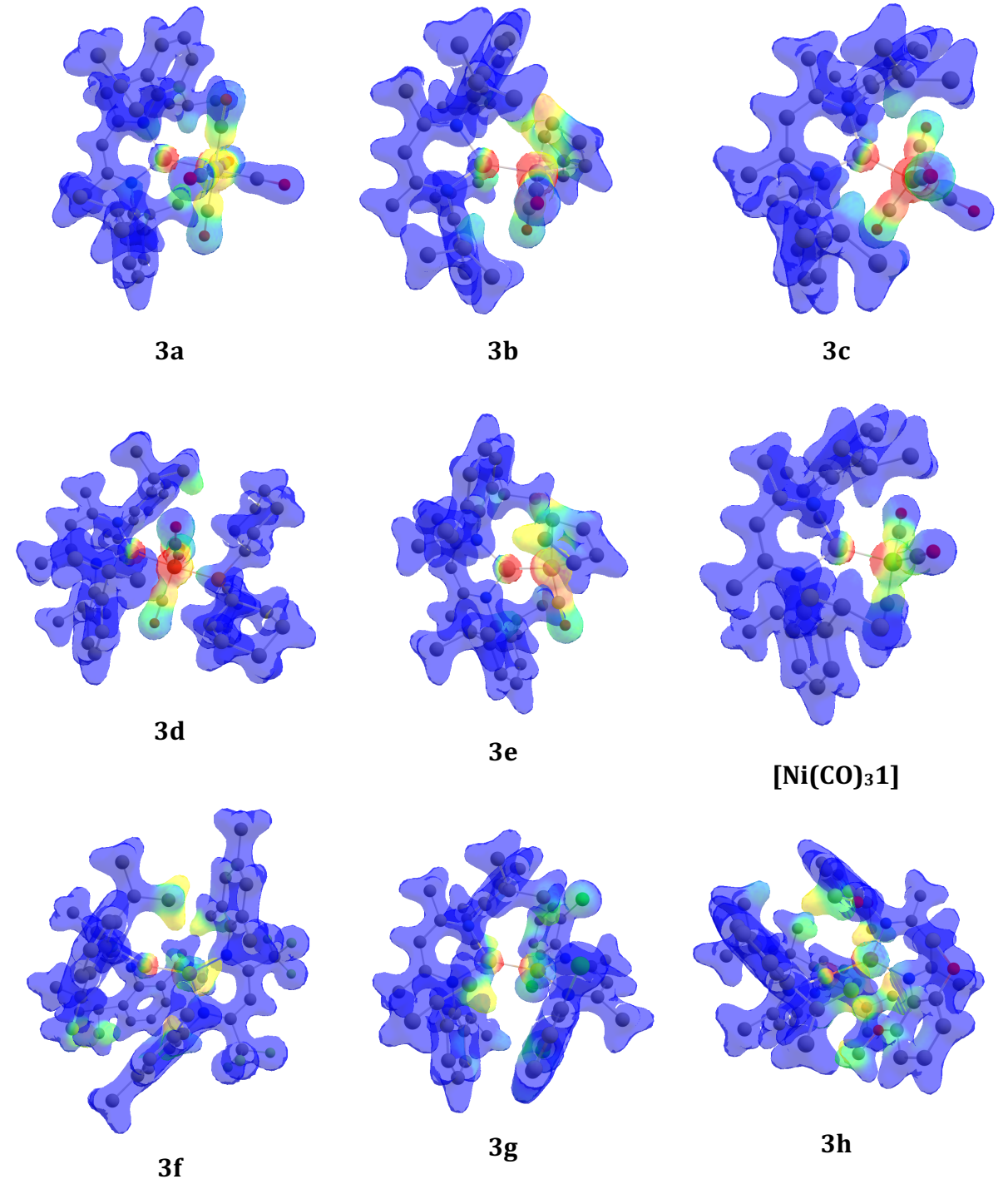


Figure S9: Dispersion interaction density plots for complexes explored computationally.

4.4 Comparison of calculated DFT M–M bond lengths to XRD data

Complex	XRD	DFT
3a·THF	2.557(2)	2.46*
3b	2.3094(7)	2.30
3c	2.2762(10)	2.30
3d	2.2547(9)	2.25
(3e)$_2$	2.3152(7)	2.31
3f	2.3021(7)	2.32
3g	2.3132(7)	2.34
3h	2.2670(9)	2.28

Table S7: Comparison of DFT calculated Al–M bond lengths to the XRD data. All values in the Å. *Compared to the solvent free calculated structure of **3a**.

4.5 Computational Coordinates

3a.log

SCF (m06l) = -1895.06560092
E(SCF)+ZPE(0 K)= -1894.381086
H(298 K)= -1894.333229
G(298 K)= -1894.458599
Lowest Frequency = 21.1450cm-1

Cr	4.365857	21.512426	5.284143
Al	6.761991	21.333567	5.821616
N	7.967845	19.838105	5.975550
O	5.075349	21.364272	2.321687
N	8.122389	22.634194	6.242378
O	3.869220	21.685754	8.291664
C	7.038008	24.642693	7.149016
C	7.436340	18.548668	5.606840
O	1.410550	21.727737	4.686080
C	9.258904	19.885525	6.350661
C	6.748919	26.003306	7.017506
H	6.195638	26.508030	7.803831
C	9.391970	22.374023	6.602212
O	4.094872	18.477485	5.470187
C	7.757699	23.291265	2.932638
H	7.172137	22.578097	3.523659
H	8.213150	22.737989	2.103900
H	7.040132	24.005846	2.514352
C	4.813081	21.395910	3.457859
C	7.298864	18.245175	4.238213
C	4.565931	23.383991	5.125341
C	2.548215	21.644498	4.914913
C	7.066517	17.639059	6.615816
C	10.070255	18.623639	6.390327
H	9.716184	17.941010	7.169095
H	11.121492	18.843802	6.578321
H	9.984125	18.076099	5.446825
C	10.329958	23.507169	6.900123
H	10.623193	24.019872	5.977222
H	11.235692	23.142405	7.386057
H	9.860714	24.265439	7.532327
C	9.908690	21.077621	6.681650
H	10.945903	20.992147	6.983413
C	4.067870	21.634237	7.143229
C	6.813862	16.978730	3.900770
H	6.695114	16.714145	2.854675
C	7.664140	19.254110	3.161561
H	7.279102	20.235140	3.489252
C	6.586998	23.865325	8.371839
H	6.321131	22.851221	8.034284
C	8.807936	24.000578	3.787248
H	9.465039	23.221406	4.199480
C	7.755332	24.023141	6.110001
C	8.132418	24.717287	4.943644
C	7.810394	26.072157	4.859070
H	8.088529	26.633322	3.971590
C	6.588566	16.388574	6.222759
H	6.295750	15.667045	6.980060
C	7.120306	18.027509	8.082311
H	7.976327	18.699795	8.228056
C	6.471244	16.056060	4.879731
H	6.095867	15.077646	4.593953
C	7.010363	18.961358	1.817520
H	7.453868	18.080206	1.340121
H	7.152626	19.808383	1.141163
H	5.934517	18.794099	1.913539
C	7.137619	26.714366	5.891185
H	6.899829	27.770981	5.808189
C	9.176334	19.404706	2.979026
H	9.673147	19.810204	3.864925
H	9.392733	20.082498	2.146790
H	9.636544	18.437838	2.744390
C	5.868808	18.819051	8.460205
H	5.750575	19.704111	7.826596
H	5.906525	19.155851	9.501197
H	4.965569	18.214253	8.326387
C	7.704707	23.712940	9.404612
H	8.554661	23.143144	9.017486
H	7.337218	23.190307	10.293396
H	8.074545	24.694138	9.724362
C	7.312445	16.842542	9.020987
H	6.429238	16.195926	9.045092
H	7.476746	17.192396	10.044079
H	8.168697	16.223721	8.733050
C	9.674274	24.911628	2.926121
H	10.233936	24.322017	2.194511
H	10.393527	25.480026	3.524650
H	9.071716	25.630130	2.360922
C	5.340731	24.453078	9.021985
H	5.556832	25.402132	9.524913
H	4.949571	23.765330	9.775421
H	4.548017	24.630676	8.289079
C	4.236389	19.630534	5.398214
O	4.636055	24.535149	4.967432

3b.log

SCF (m06l) = -1805.23965386
E(SCF)+ZPE(0 K)= -1804.468435
H(298 K)= -1804.421230
G(298 K)= -1804.545131
Lowest Frequency = 19.2388cm-1

Mn	1.209133	15.667263	4.754936
Al	2.451264	15.443200	6.673364
O	0.270485	12.893901	4.908336
N	3.279600	16.718973	7.886633
N	3.114642	13.926540	7.680145

O	3.650393	15.056903	3.233643
C	2.498705	12.655262	7.388827
C	3.104644	20.291321	6.831626
H	3.669819	21.004864	6.236302
C	2.838836	18.078934	7.739343
C	3.591882	18.988928	6.974977
C	0.837643	17.357784	3.528734
H	1.520784	17.669756	2.748647
C	1.909180	20.680100	7.418815
H	1.545330	21.696079	7.294847
C	2.993688	11.881976	6.324024
C	1.406994	12.232756	8.169140
C	1.374042	10.169274	6.898530
H	0.940277	9.190953	6.711636
C	1.607477	18.447392	8.326184
C	1.167320	19.761640	8.152950
H	0.223547	20.071658	8.591218
C	4.851408	18.577462	6.237574
H	5.186116	17.613610	6.640470
C	0.777686	17.443173	9.111265
H	0.779552	16.503553	8.532033
C	2.420758	10.626856	6.109597
H	2.787742	10.008405	5.295470
C	0.773262	13.141708	9.205731
H	1.516257	13.891920	9.510480
C	4.002119	13.958891	8.684517
C	-0.848701	16.255307	4.656661
C	4.218639	16.448825	8.808357
C	4.353560	12.693475	9.410516
H	3.530126	12.402818	10.073454
H	5.245939	12.829953	10.023018
H	4.504723	11.854005	8.727526
C	4.588533	15.144948	9.146361
H	5.339580	15.041472	9.920755
C	4.095888	12.401264	5.421656
H	3.982999	13.493187	5.368830
C	0.880007	17.780102	4.883119
H	1.558802	18.508298	5.307355
C	0.859328	10.976598	7.904364
H	0.012125	10.630243	8.491292
C	1.371191	17.126312	10.486211
H	2.359154	16.663918	10.426475
H	0.720267	16.431569	11.029026
H	1.456653	18.037836	11.088993
C	-0.161212	17.092198	5.578159
H	-0.409435	17.199269	6.626478
C	4.870083	17.575546	9.553756
H	5.448200	18.212045	8.875594
H	5.539156	17.200436	10.328824
H	4.120426	18.225696	10.016130
C	4.538280	18.366994	4.754812
H	3.743821	17.626267	4.617978
H	5.421437	18.020932	4.208769
H	4.202678	19.304819	4.295302
C	0.712301	13.985216	4.882843
C	5.992075	19.576413	6.414477
H	5.765072	20.537050	5.940120
H	6.907206	19.198684	5.949054
H	6.208300	19.777752	7.469341
C	-0.218126	16.414441	3.383351
H	-0.499224	15.899511	2.474145
C	-0.679365	17.859128	9.283122
H	-0.776321	18.703011	9.975462
H	-1.258137	17.032227	9.704951
H	-1.150196	18.150970	8.339658
C	3.982900	11.879096	3.994240
H	4.243680	10.816608	3.927891
H	4.665745	12.427379	3.340691
H	2.970183	12.006660	3.600876
C	-2.035760	15.404602	4.956519
H	-2.051580	14.502624	4.339684
H	-2.966245	15.952805	4.769304
H	-2.043871	15.088275	6.004015
C	-0.404619	13.891561	8.575539
H	-0.095377	14.468540	7.693429
H	-0.865221	14.580344	9.294138
H	-1.173222	13.186547	8.238323
C	5.487416	12.118497	5.988750
H	5.655872	12.622393	6.945561
H	6.262123	12.462625	5.296252
H	5.633605	11.043044	6.145202
C	2.682992	15.277901	3.872294
C	0.328597	12.407703	10.466562
H	-0.503331	11.724092	10.267775
H	-0.018369	13.120340	11.221568
H	1.139940	11.818658	10.906165

3c.log

SCF (m06l) = -1818.65433413
E(SCF)+ZPE(0 K)= -1817.978399
H(298 K)= -1817.932552
G(298 K)= -1818.054653
Lowest Frequency = 25.7566cm-1

Fe	5.456569	4.136094	8.363229
Al	7.611042	4.142815	9.169596
N	8.857154	2.738054	9.507364
O	2.754364	4.023287	7.216408
C	10.765560	4.166771	9.867469
H	11.831291	4.176022	10.063931
O	6.789995	4.179699	5.743547
C	8.329531	1.395858	9.582555
C	8.111853	0.832048	10.855918
C	5.255630	2.623050	9.277060
C	10.170596	2.907221	9.746130
C	11.047315	1.706854	9.944079
H	10.889560	1.271509	10.937100

H	12.100286	1.978172	9.859758
H	10.816467	0.915779	9.226296
O	5.042965	1.633475	9.862722
C	3.822016	4.068995	7.673048
C	6.283014	4.158666	6.802799
C	8.343050	1.632119	12.125224
H	9.167824	2.336244	11.950753
C	8.249018	1.303916	7.027252
H	8.261841	2.396321	7.133639
C	8.020799	0.702893	8.399551
C	7.516152	-0.595528	8.519252
H	7.274501	-1.153325	7.618641
C	7.603354	-0.464704	10.918316
H	7.422687	-0.920996	11.887462
C	7.313628	-1.177841	9.761319
H	6.918076	-2.187107	9.830658
C	7.130757	0.966567	6.047436
H	7.132833	-0.094819	5.777184
H	7.252990	1.540130	5.125257
H	6.149578	1.211132	6.466015
C	9.608880	0.892532	6.461309
H	10.437700	1.232304	7.091003
H	9.756772	1.316755	5.463336
H	9.681287	-0.197785	6.375665
C	8.734097	0.772650	13.322394
H	7.903595	0.145358	13.661877
H	9.019015	1.405731	14.167631
H	9.576524	0.111527	13.094946
C	7.105364	2.467992	12.452017
H	6.839724	3.151171	11.634761
H	7.264750	3.072571	13.351077
H	6.232634	1.827477	12.613960
N	8.823525	5.559370	9.562649
C	8.264774	6.889341	9.621582
C	7.932435	7.440654	10.871568
C	10.130295	5.412403	9.843054
C	10.950810	6.617248	10.190458
H	10.703980	6.960598	11.201950
H	12.016107	6.385477	10.163339
H	10.743481	7.459071	9.525021
C	8.049045	6.652709	12.162835
H	8.708397	5.789892	11.992033
C	8.374057	6.968700	7.072488
H	8.263242	5.880012	7.165100
C	8.037028	7.581833	8.417357
C	7.506623	8.871017	8.498539
H	7.323103	9.427145	7.583633
C	7.399569	8.730597	10.895939
H	7.124001	9.173045	11.850104
C	7.197783	9.446159	9.724077
H	6.781616	10.448676	9.764070
C	7.427370	7.410404	5.963569
H	7.579029	8.460770	5.691839
H	7.597772	6.812074	5.065062
H	6.381299	7.281426	6.257215
C	9.828812	7.236374	6.684341
H	10.533374	6.793259	7.395445
H	10.049230	6.816397	5.698005
H	10.028947	8.313278	6.642153
C	8.653398	7.468795	13.302584
H	7.992196	8.285093	13.610703
H	8.814439	6.838741	14.182431
H	9.614614	7.914820	13.025806
C	6.674328	6.109784	12.558178
H	6.258672	5.451332	11.787220
H	6.727242	5.545875	13.495270
H	5.959647	6.928760	12.691575
C	5.192327	5.693527	9.181506
O	4.933493	6.712891	9.690753

3d.log

SCF (m06l) = -2752.45161086
E(SCF)+ZPE(0 K)= -2751.296646
H(298 K)= -2751.232793
G(298 K)= -2751.391803
Lowest Frequency = 12.8830cm-1

Fe	2.171956	9.093484	6.063447
P	0.395919	7.836637	6.523847
Al	3.825596	10.626545	5.799107
O	0.379157	11.414931	6.208732
N	4.558165	11.530154	4.278052
N	4.908104	11.597049	7.064614
C	5.483161	12.505269	4.296519
C	5.783244	10.269724	8.933876
C	2.830838	11.479612	2.542420
C	5.762709	12.592993	6.786477
C	6.526805	13.263342	7.892394
H	5.961458	13.288380	8.825805
H	6.799552	14.281074	7.607139
H	7.456575	12.722726	8.102796
C	4.092513	11.051859	3.000232
C	4.876299	10.135642	2.277690
C	4.385868	9.679943	1.052519
H	4.969533	8.963369	0.479811
C	6.012577	13.028680	5.479893
H	6.727217	13.836633	5.371444
C	4.788465	11.121826	8.418609
C	3.628549	11.449288	9.147625
C	1.991783	12.457287	3.344286
H	2.132507	12.220401	4.408784
C	6.174201	9.576298	2.830026
H	6.535604	10.246845	3.621822
C	7.000593	9.882720	8.111578
H	7.233239	10.710371	7.430862
C	5.586965	9.739944	10.210344
H	6.333190	9.070988	10.629949

C	3.475042	10.878203	10.413226
H	2.582139	11.098363	10.992738
C	2.609995	12.432288	8.600991
H	2.533686	12.268856	7.517198
C	6.005807	13.050676	3.000890
H	6.677631	12.325115	2.527873
H	6.564778	13.973357	3.162047
H	5.202034	13.233934	2.283120
C	8.243453	9.644146	8.962710
H	8.441771	10.481396	9.639891
H	9.121404	9.508220	8.324222
H	8.151826	8.739572	9.572669
C	2.385560	10.989988	1.312960
H	1.414386	11.299580	0.937509
C	3.157072	10.105934	0.569057
H	2.789999	9.735066	-0.383808
C	7.274674	9.481586	1.776723
H	7.040727	8.733144	1.012599
H	8.221081	9.181851	2.236856
H	7.435451	10.434768	1.261682
C	0.498949	12.337772	3.069492
H	0.238068	12.701742	2.069056
H	-0.063569	12.932021	3.793949
H	0.157581	11.302673	3.156418
C	1.212236	12.237796	9.167824
H	0.885084	11.199542	9.059241
H	0.496788	12.864452	8.629365
H	1.158690	12.507619	10.229140
C	3.068492	13.877968	8.803125
H	3.247129	14.086794	9.864326
H	2.302790	14.575729	8.449489
H	3.990130	14.100200	8.257979
C	5.923462	8.210926	3.473364
H	5.192144	8.271587	4.287616
H	6.851340	7.792469	3.877709
H	5.518111	7.506179	2.739774
C	4.440879	10.029249	10.939102
H	4.298455	9.590155	11.922828
C	2.454602	13.900931	3.139208
H	3.478798	14.063140	3.487637
H	1.808816	14.593092	3.688956
H	2.412513	14.176110	2.078739
C	6.714661	8.667646	7.229789
H	6.457612	7.792317	7.832804
H	7.586431	8.425740	6.612066
H	5.865295	8.839066	6.556704
O	3.834254	7.850045	8.152276
O	2.577673	8.042250	3.347319
C	1.134235	10.501162	6.181264
C	3.174304	8.373744	7.328119
C	2.428964	8.470027	4.432887
C	-0.320614	7.988058	8.264063
H	-0.823234	7.022954	8.457059
C	0.507507	5.975951	6.379845
H	-0.525461	5.615948	6.522745
C	-1.364199	9.098318	8.440485
H	-0.905489	10.068187	8.196347
H	-2.201351	8.971471	7.745915
C	-1.081619	8.272157	5.464674
H	-1.390592	9.236137	5.897477
C	-1.914545	9.126695	9.865207
H	-2.648499	9.935195	9.961950
H	-2.463627	8.190570	10.049081
C	-2.263954	7.305693	5.574751
H	-2.477324	7.055441	6.623110
H	-2.000703	6.357884	5.080480
C	0.785891	8.171807	9.311502
H	1.300367	9.121574	9.105612
H	1.560182	7.407156	9.214351
C	-0.815051	9.268725	10.908715
H	-1.239169	9.244348	11.919379
H	-0.335651	10.252534	10.797374
C	1.848534	3.371073	5.938339
H	2.894326	3.677506	5.791271
H	1.830137	2.278555	5.850930
C	-2.017140	9.164633	3.319454
H	-2.247719	10.132129	3.792210
H	-1.804103	9.381013	2.265620
C	0.234447	8.181146	10.731547
H	-0.214081	7.201117	10.957143
H	1.056795	8.313373	11.445324
C	-0.782865	8.574240	3.993918
H	-0.479176	7.660069	3.465164
H	0.065075	9.262175	3.920709
C	-3.223753	8.241093	3.444321
H	-3.024900	7.314337	2.885774
H	-4.108820	8.693933	2.982852
C	-3.502914	7.889652	4.901379
H	-4.343177	7.189454	4.976105
H	-3.807542	8.797918	5.442935
C	0.986941	5.533723	4.996530
H	2.004638	5.913774	4.839486
H	0.372342	5.984710	4.209037
C	1.367520	5.325362	7.467480
H	0.990831	5.584609	8.462963
H	2.390926	5.721104	7.407302
C	0.986266	4.015135	4.861068
H	-0.045530	3.641350	4.949583
H	1.333532	3.728273	3.862023
C	1.389538	3.805280	7.323659
H	2.028417	3.368237	8.099658
H	0.376312	3.415024	7.503572

3e_dimer.log

SCF (m06l) = -3388.19127909
E(SCF)+ZPE(0 K)= -3386.722416
H(298 K)= -3386.635323

G(298 K)= -3386.838458
Lowest Frequency = 22.2885cm-1

Co	2.726686	1.197846	7.936191
Al	4.416966	0.649727	3.665569
O	3.772801	1.330149	5.265916
N	2.803026	0.595268	2.584461
N	5.073118	2.325684	2.963144
C	4.919929	2.534391	1.647763
C	1.750190	0.642367	9.711193
H	1.639771	-0.365724	10.093828
C	5.761572	3.330118	3.733003
C	2.837759	1.524951	10.008684
H	3.683871	1.287524	10.642866
C	0.505438	0.794025	3.426974
C	3.996802	1.818035	0.868649
H	4.009738	2.031900	-0.194020
C	1.546889	-0.024882	2.940982
C	5.724853	5.484105	4.822845
H	5.175212	6.370777	5.133320
C	2.457583	-2.370342	2.434622
H	3.384431	-1.797384	2.342090
C	-0.775624	0.246948	3.530815
H	-1.593706	0.875740	3.871844
C	2.610393	2.747078	9.323930
H	3.263407	3.610438	9.320470
C	0.747242	2.230751	3.845913
H	1.809080	2.314879	4.104744
C	5.741421	3.588702	0.967486
H	5.505653	4.586701	1.349955
H	5.580120	3.584054	-0.110923
H	6.806655	3.435629	1.172620
C	2.923472	1.024640	1.317757
C	9.089589	2.251669	2.779959
H	9.815665	2.926188	3.248589
H	8.763569	2.722461	1.845942
H	9.621350	1.330518	2.517259
C	3.303996	1.229075	6.412172
C	7.919484	1.951448	3.714611
H	7.248000	1.250932	3.212250
C	3.556443	4.638192	3.901079
H	3.184690	3.726020	3.420247
C	0.845345	1.322050	8.851510
H	-0.070949	0.920417	8.438162
C	5.041846	4.470530	4.147327
C	-1.021713	-1.084327	3.222229
H	-2.028190	-1.487065	3.300353
C	2.635648	-3.322115	3.618244
H	2.803662	-2.777852	4.554730
H	3.496493	-3.983672	3.467847
H	1.749149	-3.951354	3.759398
C	0.038905	-1.906528	2.875868
H	-0.129453	-2.968888	2.708285
C	1.335503	-1.402962	2.735382
C	2.807521	4.809185	5.222690
H	2.924655	3.934759	5.873368
H	1.738137	4.959275	5.038302
H	3.165754	5.686542	5.773455
C	1.388295	2.616056	8.594704
H	0.956281	3.367092	7.945611
C	8.406214	1.269107	4.988608
H	8.947609	0.343719	4.761274
H	7.572045	1.003691	5.649628
H	9.083742	1.915607	5.556860
C	-0.049293	2.587799	5.098897
H	-1.129633	2.593709	4.918165
H	0.218432	3.589062	5.447832
H	0.164040	1.883996	5.911721
C	1.864096	0.680834	0.311235
H	1.740678	-0.403834	0.226786
H	2.106035	1.088440	-0.670593
H	0.887249	1.067682	0.620184
C	7.079417	5.379861	5.107084
H	7.593819	6.181892	5.629747
C	7.125018	3.190182	4.056094
C	0.467746	3.218984	2.714104
H	1.152797	3.079563	1.869575
H	0.587589	4.251035	3.064213
H	-0.557593	3.113205	2.339823
C	3.267013	5.812093	2.965797
H	3.644219	6.753588	3.381270
H	2.189485	5.930346	2.809809
H	3.728289	5.677444	1.982001
C	2.242719	-3.154819	1.142532
H	3.089164	-3.823922	0.953046
H	2.140798	-2.500751	0.269561
H	1.341843	-3.777455	1.191229
C	7.761682	4.229825	4.739837
H	8.816705	4.123744	4.986355
Co	5.798125	-1.197845	3.473379
Al	4.107846	-0.649727	7.744004
O	4.752021	-1.330147	6.143659
N	5.721783	-0.595269	8.825116
N	3.451692	-2.325681	8.446434
C	3.604883	-2.534391	9.761814
C	6.774621	-0.642370	1.698376
H	6.885042	0.365721	1.315742
C	2.763239	-3.330116	7.676574
C	5.687050	-1.524952	1.400886
H	4.840938	-1.287523	0.766703
C	8.019371	-0.794025	7.982600
C	4.528013	-1.818039	10.540928
H	4.515078	-2.031906	11.603597
C	6.977919	0.024882	8.468592
C	2.799960	-5.484103	6.586732
H	3.349602	-6.370776	6.276259
C	6.067224	2.370341	8.974950
H	5.140376	1.797382	9.067476

C	9.300432	-0.246947	7.878757
H	10.118514	-0.875740	7.537728
C	5.914414	-2.747078	2.085641
H	5.261398	-3.610437	2.089102
C	7.777568	-2.230751	7.563661
H	6.715729	-2.314881	7.304835
C	2.783390	-3.588702	10.442090
H	3.019164	-4.586702	10.059627
H	2.944685	-3.584049	11.520500
H	1.718157	-3.435633	10.236949
C	5.601342	-1.024644	10.091820
C	-0.564772	-2.251668	8.629621
H	-1.290843	-2.926198	8.161000
H	-0.238746	-2.722446	9.563643
H	-1.096540	-1.330518	8.892313
C	5.220818	-1.229073	4.997401
C	0.605327	-1.951446	7.694961
H	1.276812	-1.250927	8.197316
C	4.968369	-4.638189	7.508501
H	5.340121	-3.726016	7.989331
C	7.679464	-1.322054	2.558060
H	8.595758	-0.920421	2.971410
C	3.482966	-4.470527	7.262251
C	9.546521	1.084328	8.187342
H	10.552998	1.487066	8.109218
C	5.889162	3.322119	7.791332
H	5.721147	2.777859	6.854844
H	5.028319	3.983678	7.941731
H	6.775663	3.951357	7.650181
C	8.485902	1.906529	8.533702
H	8.654259	2.968889	8.701283
C	7.189305	1.402962	8.674190
C	5.717292	-4.809184	6.186891
H	5.600158	-3.934758	5.536213
H	6.786676	-4.959274	6.371280
H	5.359061	-5.686541	5.636126
C	7.136511	-2.616059	2.814868
H	7.568522	-3.367096	3.463962
C	0.118587	-1.269111	6.420966
H	-0.422798	-0.343717	6.648302
H	0.952749	-1.003705	5.759932
H	-0.558954	-1.915608	5.852726
C	8.574098	-2.587794	6.310672
H	9.654439	-2.593697	6.491397
H	8.306376	-3.589060	5.961740
H	8.360756	-1.883994	5.497848
C	6.660720	-0.680840	11.098339
H	6.784143	0.403828	11.182786
H	6.418782	-1.088444	12.080168
H	7.637565	-1.067691	10.789389
C	1.445397	-5.379859	6.302489
H	0.930996	-6.181890	5.779824
C	1.399794	-3.190180	7.353479
C	8.057072	-3.218984	8.695467
H	7.372025	-3.079568	9.539999
H	7.937232	-4.251036	8.345356
H	9.082413	-3.113202	9.069743
C	5.257798	-5.812089	8.443786
H	4.880586	-6.753583	8.028317
H	6.335325	-5.930346	8.599770
H	4.796527	-5.677434	9.427583
C	6.282084	3.154812	10.267045
H	5.435637	3.823911	10.456533
H	6.384006	2.500739	11.140013
H	7.182958	3.777450	10.218353
C	0.763131	-4.229823	6.669735
H	-0.291891	-4.123741	6.423214

3e.log

SCF (m06l) = -1694.05852525
E(SCF)+ZPE(0 K)= -1693.325445
H(298 K)= -1693.281444
G(298 K)= -1693.399826
Lowest Frequency = 17.9102cm-1

Co	4.322645	-0.001902	6.063017
O	6.910838	1.220531	6.261761
C	2.571231	-0.906910	5.410388
H	2.181470	-1.874959	5.697333
C	2.262286	0.339659	6.055279
H	1.637517	0.460736	6.930316
C	2.937244	1.367827	5.357089
H	2.936542	2.420973	5.605336
C	5.862933	0.683984	6.229871
C	3.408020	-0.642647	4.290203
H	3.802581	-1.375511	3.599321
C	3.661265	0.757238	4.276783
H	4.298020	1.280393	3.575060
Al	4.758684	-1.237327	7.874554
N	6.077940	-1.176672	9.297704
N	3.756460	-2.654308	8.750583
C	4.171938	-3.401785	9.786391
C	2.463010	-2.931392	8.189961
C	8.238608	-0.079282	8.852255
C	5.342467	-3.126689	10.498667
H	5.560480	-3.777971	11.336910
C	6.903711	0.002720	9.291457
C	1.047238	-4.209892	6.722817
H	0.913269	-5.019113	6.008870
C	4.890818	1.332978	10.169773
H	4.404885	0.356077	10.034502
C	8.995130	1.092284	8.843037
H	10.026760	1.056560	8.503432
C	8.821624	-1.381443	8.336404
H	8.295703	-2.209883	8.828160
C	3.323839	-4.545347	10.258789
H	3.237720	-5.319454	9.489046

H	3.740163	-4.998373	11.159079
H	2.302768	-4.211113	10.469316
C	6.189037	-2.022436	10.329468
C	1.820223	-1.298221	10.910964
H	0.991614	-1.909977	11.286530
H	2.748170	-1.856783	11.052062
H	1.881535	-0.406580	11.544361
C	1.575336	-0.891575	9.455347
H	2.473854	-0.354755	9.101302
C	3.487406	-4.832293	6.818387
H	4.303318	-4.707875	7.540799
C	2.310892	-3.992708	7.278591
C	8.449042	2.306261	9.242564
H	9.055785	3.207167	9.223034
C	4.089517	2.350114	9.360480
H	4.093283	2.090864	8.295218
H	3.048564	2.375160	9.703848
H	4.495094	3.361795	9.471266
C	7.126271	2.367707	9.655146
H	6.698228	3.319987	9.961903
C	6.325463	1.223056	9.685834
C	3.996216	-4.320721	5.468625
H	4.304784	-3.269334	5.525713
H	4.852107	-4.910282	5.123953
H	3.209789	-4.392730	4.707470
C	0.420966	0.104119	9.416300
H	0.680548	0.997395	9.991684
H	0.168065	0.422625	8.400869
H	-0.485841	-0.315428	9.867094
C	8.568754	-1.523806	6.834605
H	9.022659	-0.693942	6.283849
H	8.991322	-2.461785	6.458736
H	7.498757	-1.511699	6.597414
C	7.226727	-1.776188	11.385019
H	7.129100	-0.764881	11.792238
H	7.136150	-2.495258	12.199671
H	8.240642	-1.838103	10.977558
C	-0.029514	-3.399519	7.052905
H	-1.004680	-3.580797	6.609988
C	1.386507	-2.078216	8.521456
C	10.306355	-1.538398	8.648519
H	10.523851	-1.376094	9.709619
H	10.646757	-2.543590	8.382724
H	10.918846	-0.834857	8.075088
C	3.160006	-6.321268	6.746687
H	2.430417	-6.539801	5.959867
H	4.059469	-6.900072	6.516860
H	2.747200	-6.698758	7.688541
C	4.838041	1.650363	11.663982
H	3.801959	1.726397	12.010942
H	5.335919	0.879676	12.262303
H	5.330228	2.605182	11.880669
C	0.144459	-2.342120	7.938481
H	-0.701880	-1.703617	8.171432

3f.log

SCF (m06l) = -3037.46377478
E(SCF)+ZPE(0 K)= -3036.405027
H(298 K)= -3036.336480
G(298 K)= -3036.505431
Lowest Frequency = -33.9481cm-1

Cu	5.603211	1.087239	4.775865
Al	6.027412	3.363474	4.635989
F	6.289640	-3.919566	3.453759
N	6.549617	-0.654864	4.940994
F	8.061745	-2.737225	3.800776
F	2.221908	-2.803569	3.532850
C	4.684386	-1.858878	3.915891
H	4.417363	-2.824687	3.518295
F	1.503575	-1.344802	4.961834
C	5.991824	-1.735417	4.397222
N	6.416942	4.791687	5.881715
F	1.558442	-0.867643	2.845214
C	9.968250	-0.501873	6.425133
H	10.972512	-0.186690	6.141649
N	6.561207	4.437752	3.102686
C	7.972571	6.061805	1.916541
H	8.240535	5.291826	1.187290
H	8.842894	6.686365	2.121686
H	7.214294	6.686494	1.433033
F	7.000500	-3.627956	5.472590
N	3.782646	0.348210	4.323085
C	2.230139	-1.491656	3.834173
C	7.438806	5.452146	3.178048
C	6.337604	3.039155	1.069743
C	7.774009	3.435633	8.115003
H	8.225256	3.769075	7.171576
C	2.692531	1.244298	4.477177
C	7.649148	-0.797956	5.836490
C	1.173063	2.867942	3.553583
H	0.793981	3.410380	2.687225
C	7.388566	-1.270592	7.139734
C	5.958010	4.167679	1.821850
C	7.724756	6.657847	6.791390
H	6.850184	7.102226	7.276907
H	8.383733	7.455871	6.448125
H	8.244616	6.085108	7.566762
C	3.635736	-0.928292	4.029664
C	2.218128	1.963646	3.365521
C	6.403437	4.066435	8.240411
C	7.322178	2.004106	1.569508
H	7.607950	2.276286	2.593029
C	3.786379	5.032846	8.495970
H	2.767153	5.389473	8.605196
C	7.311176	5.765374	5.661179
C	4.952427	5.042202	1.354166

C	2.207453	1.525745	5.766883
C	2.876850	1.815717	2.031685
H	3.930057	2.126048	2.091020
H	2.390905	2.438963	1.275568
H	2.881922	0.781598	1.674764
C	8.715747	3.835324	9.248819
H	8.817121	4.921806	9.345957
H	9.712773	3.416291	9.082294
H	8.365327	3.454868	10.214147
C	4.390611	6.174037	2.195159
H	4.989034	6.266171	3.110550
C	9.210610	0.204996	4.138806
H	10.210814	0.644002	4.083851
H	8.471648	0.982442	3.906239
H	9.127978	-0.547557	3.347541
C	5.761522	4.699010	7.160941
C	6.832111	-3.008947	4.285969
C	7.862873	6.003298	4.394603
H	8.609643	6.786519	4.333635
C	4.436150	5.177437	7.268393
C	1.166186	2.443371	5.904906
H	0.780928	2.647816	6.904579
C	3.731468	5.828234	6.089410
H	3.925010	5.196682	5.203971
C	8.941652	-0.374801	5.487557
C	5.706425	3.946466	9.445978
H	6.187614	3.449749	10.285475
C	4.800483	3.728728	-0.681951
H	4.360731	3.564805	-1.661623
C	5.986250	-1.579495	7.562929
H	5.322233	-0.732071	7.346439
H	5.936139	-1.790669	8.634230
H	5.566345	-2.439079	7.030746
C	5.751756	2.850309	-0.185769
H	6.050822	1.987800	-0.777509
C	8.445913	-1.386114	8.039223
H	8.237179	-1.755547	9.043322
C	6.665555	0.623239	1.622189
H	5.748173	0.635282	2.224183
H	7.338700	-0.117733	2.064459
H	6.396987	0.273676	0.618674
C	10.860442	-1.107980	8.703953
H	10.784933	-2.012010	9.315755
H	10.845249	-0.256980	9.397162
H	11.841769	-1.110538	8.221452
C	9.749816	-1.018504	7.701807
C	4.423609	7.522405	1.478767
H	5.431205	7.797125	1.151046
H	4.060981	8.316992	2.138826
H	3.781875	7.520247	0.591049
C	2.958963	5.832178	2.611739
H	2.312076	5.726043	1.732516
H	2.532781	6.621870	3.241387
H	2.905751	4.887787	3.165214
C	0.613975	3.109047	4.809013
C	4.394648	4.804362	0.097021
H	3.617105	5.472273	-0.268594
C	2.841716	0.890412	6.963103
H	2.849229	-0.202529	6.897343
H	2.330836	1.177724	7.885875
H	3.893793	1.206071	7.052851
C	8.596320	1.972500	0.728617
H	8.377339	1.701634	-0.310560
H	9.300007	1.231457	1.121493
H	9.102562	2.943329	0.716435
C	4.413905	4.428527	9.579190
H	3.886073	4.323603	10.522920
C	7.634564	1.916528	8.044847
H	7.203179	1.520031	8.972397
H	8.604224	1.433290	7.890461
H	6.978520	1.612031	7.219668
C	2.220374	5.907669	6.260876
H	1.785971	4.939147	6.519875
H	1.754019	6.239234	5.328527
H	1.943799	6.632439	7.035289
C	-0.531420	4.061876	4.969728
H	-0.447078	4.912801	4.284664
H	-0.590483	4.458036	5.988299
H	-1.492894	3.579327	4.757448
C	4.275281	7.226738	5.783014
H	4.187430	7.873370	6.663908
H	3.696557	7.691555	4.976604
H	5.321956	7.221661	5.468849

3g.log

SCF (m06l) = -2263.74373791
E(SCF)+ZPE(0 K)= -2262.844953
H(298 K)= -2262.783644
G(298 K)= -2262.941605
Lowest Frequency = 8.0103cm-1

Cu	-1.391690	18.098680	6.597840
Al	0.595983	16.862405	6.473327
Cl	-3.101649	18.017138	10.644862
Cl	-3.399944	15.337223	5.816812
Cl	-2.242396	18.806133	3.079603
Cl	-0.161343	22.101983	6.978539
N	-1.958506	19.883560	5.870491
N	1.619658	15.947293	7.855387
N	-3.124844	17.776844	7.584400
N	1.907164	16.391931	5.112340
C	2.853314	15.433573	7.758752
C	-3.159281	20.428147	6.081920
C	-3.437414	15.346229	7.629524
C	3.036767	15.680545	5.275649
C	3.447773	18.681793	4.302083
H	3.946526	17.893700	4.879645

C	2.224090	18.510897	2.081834
H	2.811092	19.350856	1.720481
C	-5.498249	18.171571	8.103158
H	-5.795198	17.189884	7.717860
H	-6.285468	18.885917	7.859410
H	-5.446836	18.084190	9.192592
C	0.517263	21.774969	2.996553
H	1.143366	22.260844	2.254416
C	-3.280793	16.582472	8.279625
C	3.501656	15.273847	6.529710
H	4.466393	14.779546	6.550711
C	-1.126288	20.504231	4.942460
C	-3.509485	21.730930	5.412324
H	-2.807861	22.523197	5.693344
H	-4.515701	22.055753	5.679507
H	-3.459831	21.636327	4.321800
C	2.437455	18.027564	3.372642
C	1.263391	17.942027	1.253276
H	1.113475	18.331168	0.249303
C	0.653334	16.366016	2.995289
C	-4.160775	19.836700	6.862359
H	-5.091687	20.390801	6.907769
C	-3.676566	14.127020	9.675325
H	-3.834658	13.193423	10.206265
C	0.940681	15.820632	9.114949
C	1.660017	16.929604	3.801518
C	-3.497311	15.311385	10.383113
H	-3.506733	15.326104	11.467039
C	-4.178722	18.596097	7.511942
C	0.479158	16.893275	1.712186
H	-0.292172	16.483758	1.067398
C	-3.300329	16.490857	9.684205
C	0.572266	13.358526	8.528906
H	1.608421	13.349855	8.163832
C	3.580330	14.999478	8.998502
H	3.572151	15.802928	9.742107
H	4.614258	14.734809	8.773844
H	3.101029	14.141797	9.480292
C	0.785872	16.940676	9.946727
C	0.131915	16.763255	11.170695
H	0.005293	17.618527	11.830574
C	0.552102	22.197896	4.322325
H	1.198235	23.009086	4.638649
C	-0.317761	20.724562	2.623589
H	-0.364365	20.376535	1.598387
C	-0.246913	21.553022	5.253865
C	1.328134	18.311191	9.592890
H	1.743780	18.267820	8.576398
C	-0.360910	15.525091	11.546157
H	-0.868180	15.408480	12.500555
C	-1.497259	15.038950	2.709391
H	-2.066634	15.970396	2.652412
H	-2.125799	14.287244	3.194248
H	-1.306617	14.689689	1.687963
C	-1.107603	20.123336	3.588709
C	4.538368	19.451621	3.566781
H	5.033476	18.840567	2.804844
H	5.300234	19.795917	4.271967
H	4.138027	20.343063	3.070729
C	0.416708	14.552579	9.461445
C	-0.225104	14.432946	10.693243
H	-0.634899	13.472936	10.993243
C	-3.646497	14.142551	8.283864
H	-3.788351	13.235393	7.706625
C	-0.203200	15.213789	3.493004
H	-0.498498	15.450101	4.530156
C	2.756242	19.598718	5.311173
H	2.310926	20.458245	4.803460
H	3.466815	19.972956	6.056140
H	1.939457	19.098834	5.847699
C	-0.320770	13.447236	7.290724
H	-1.376670	13.404074	7.568840
H	-0.112196	12.617248	6.607511
H	-0.179154	14.376715	6.725939
C	0.339149	12.020892	9.221326
H	0.955063	11.907620	10.119075
H	0.576603	11.196996	8.542387
H	-0.709365	11.900568	9.517913
C	0.230959	19.372146	9.596834
H	-0.587828	19.114106	8.913041
H	0.633559	20.340141	9.285490
H	-0.204299	19.492752	10.595007
C	0.564394	13.890673	3.525699
H	0.952471	13.642272	2.530694
H	-0.098834	13.075967	3.834901
H	1.406015	13.908979	4.224047
C	3.869372	15.309238	4.080642
H	3.240759	14.941477	3.264663
H	4.598661	14.541572	4.343230
H	4.414071	16.170213	3.679855
C	2.468468	18.708671	10.530435
H	2.116965	18.778190	11.566082
H	2.875866	19.686211	10.253762
H	3.289365	17.983838	10.510883

3h.log

SCF (m06l) = -2664.24375395
E(SCF)+ZPE(0 K)= -2663.175678
H(298 K)= -2663.109943
G(298 K)= -2663.272354
Lowest Frequency = 17.0283cm-1

Cu	4.688885	17.378493	14.643531
Al	6.955952	17.445060	14.900821
N	8.484805	18.158483	13.944445
N	8.078461	16.206934	15.915305
N	3.456865	16.237407	13.583954

O	1.763819	17.223481	11.561904
N	3.318639	18.096164	15.909774
O	4.093832	20.226458	14.579287
O	3.609105	18.142185	18.856015
C	9.644005	17.512628	13.747700
C	2.260421	15.901367	14.091866
C	2.118120	17.550305	16.041891
C	8.313051	19.452915	13.343300
C	9.996901	16.365499	14.468996
H	10.958107	15.923873	14.231846
C	10.620767	18.041538	12.740119
H	10.160067	18.090695	11.747747
H	11.513037	17.417005	12.684404
H	10.922297	19.066137	12.981069
C	9.313045	15.820325	15.566703
C	1.700588	16.451685	15.256471
H	0.728888	16.045899	15.523491
C	3.762737	19.191597	16.657150
O	5.729093	14.871874	12.800636
C	3.720619	15.979978	12.235279
C	1.428358	14.851179	13.399503
H	0.775361	15.303520	12.647042
H	0.796026	14.328774	14.121408
H	2.057683	14.116668	12.888600
C	7.764795	19.580616	12.055479
C	7.543785	15.697517	17.153240
C	7.163624	18.415606	11.295086
H	7.308658	17.500878	11.886560
C	10.033925	14.794905	16.390778
H	9.383906	13.954889	16.651804
H	10.358928	15.231758	17.341747
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C	3.931975	19.206379	18.053894
C	4.452615	20.329206	18.706425
H	4.549161	20.289173	19.786956
C	7.698558	20.859691	11.492462
H	7.287594	20.971987	10.490981
C	7.922619	16.317371	18.362044
C	8.661614	20.589168	14.108397
C	6.234132	14.086368	18.369845
H	5.555503	13.235997	18.373087
C	6.645111	14.615431	17.142044
C	4.892756	15.309585	11.808643
C	6.099775	14.032535	15.857854
H	6.369926	14.709307	15.041954
C	8.128905	21.978352	12.189394
H	8.081134	22.961557	11.729476
C	2.881554	16.494972	11.222489
C	4.237432	20.317402	15.935998
C	2.062284	18.523399	12.062342
H	2.719433	18.489180	12.941903
H	1.109380	18.970964	12.349831
H	2.532322	19.140501	11.282049
C	8.579704	21.842515	13.498297
H	8.855613	22.729092	14.061924
C	8.661750	17.640985	18.370603
H	9.203540	17.747778	17.420338
C	6.667600	14.629145	19.570933
H	6.345075	14.197561	20.514611
C	1.138621	18.089719	17.047917
H	0.124747	17.739741	16.845492
H	1.142346	19.184213	17.039057
H	1.414181	17.793533	18.065832
C	4.788793	21.420205	16.581217
H	5.129851	22.277254	16.010348
C	7.480220	15.757009	19.561246
H	7.766465	16.220529	20.502057
C	4.875604	21.426690	17.975415
H	5.298110	22.289654	18.482708
C	3.136795	16.280934	9.869667
H	2.442725	16.691556	9.142874
C	4.270221	15.576702	9.485889
H	4.479211	15.401592	8.434686
C	4.779820	21.186091	13.803423
H	4.640939	20.891718	12.761301
H	5.855160	21.195560	14.034679
H	4.373938	22.196386	13.948392
C	5.159358	15.109207	10.453627
H	6.050426	14.571557	10.148042
C	9.066930	20.459558	15.566813
H	8.491681	19.616362	15.981194
C	5.656377	18.627641	11.149336
H	5.162160	18.626493	12.130528
H	5.206560	17.836041	10.544624
H	5.441425	19.585695	10.659726
C	7.805649	18.198435	9.926887
H	7.652071	19.063177	9.271622
H	7.354924	17.331052	9.432872
H	8.885580	18.027159	9.993020
C	4.574960	13.980258	15.873621
H	4.195647	13.278734	16.626226
H	4.200551	13.667001	14.894407
H	4.146808	14.968766	16.078622
C	4.078393	16.858496	18.454471
H	3.300303	16.284188	17.934127
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H	4.953087	16.933866	17.793702
C	9.680293	17.776036	19.496755
H	10.398032	16.949560	19.504313
H	9.199945	17.806005	20.480342
H	10.242476	18.709248	19.391183
C	8.702704	21.691346	16.387841
H	7.644744	21.950548	16.278309
H	9.303398	22.563572	16.107901
H	8.892122	21.507453	17.449873
C	7.006927	14.425851	12.405455
H	7.573663	14.261317	13.326194
H	7.529325	15.175626	11.791637

H	6.962162	13.482927	11.843511
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H	7.789136	12.698294	15.459608
H	6.293657	12.262911	14.616712
H	6.462010	11.941166	16.347630
C	7.617775	18.759849	18.446361
H	6.908490	18.724749	17.606117
H	8.083394	19.751456	18.448229
H	7.019751	18.667189	19.360714
C	10.547470	20.122496	15.749681
H	10.813843	19.156592	15.311309
H	10.798977	20.075625	16.815316
H	11.182171	20.890582	15.292297

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