Molybdenum Carbonyl Assisted Reductive Tetramerization of CO by Activated Magnesium(I) Compounds: Squarate Dianion *vs.* Metallo-Ketene Formation

K. Yuvaraj,[a,¥] Jeremy C. Mullins,[a] Thayalan Rajeshkumar,[b] Iskander Douair,[b] Laurent Maron,*[b] Cameron Jones*[a]

[a] *School of Chemistry, PO Box 23, Monash University, VIC, 3800, Australia.*

[b] *Université de Toulouse et CNRS, INSA, UPS, UMR 5215, LPCNO, 135 Avenue de Rangueil, F-31077 Toulouse, France.*

[¥] *Current address: Department of Chemistry, Indian Institute of Technology Palakkad, Palakkad-678557, Kerala, India.*

Electronic Supplementary Information (52 pages)

Contents

1. Experimental and Spectra

General considerations.

All manipulations were carried out using standard Schlenk and glove box techniques under an atmosphere of high purity dinitrogen. Benzene, *n*-hexane, toluene and THF were distilled over molten potassium. ^{1}H and ^{13}C{^{1}H} NMR spectra were recorded on Bruker Avance Neo 400 or Bruker Avance III 600 spectrometers and were referenced to the resonances of the solvent used or external $SiMe_4$. FTIR spectra were collected for solid samples or Nujol mulls on an Agilent Cary 630 attenuated total reflectance (ATR) spectrometer. Microanalyses were carried out at the Science Centre, London Metropolitan University, or using a PerkinElmer-2400 CHNS/O Series II System. Melting points were determined in sealed glass capillaries under dinitrogen and are uncorrected. The compounds [{(^{Dip}Nacnac)Mg}$_2$],[1] [{(Priso)Mg}$_2$],[2] and :C{N(Me)C(Me)}$_2$ (TMC)[3] were prepared according to literature procedures. CO gas was dried over P_2O_5 prior to use. All other reagents were used as received.

Synthesis of [{(^{Dip}Nacnac)Mg}(C_4O_4){μ-Mg(^{Dip}Nacnac)}]$_2$ 4 and [{(^{Dip}Nacnac)Mg}{μ-(C_4O_4)Mo(CO)$_5$}{Mg(DMAP)(^{Dip}Nacnac)}] 5. [{(^{Dip}Nacnac)Mg}$_2$] (150 mg, 0.170, mmol) and DMAP (21 mg, 0.170 mmol) were dissolved in 5 mL of toluene at room temperature, resulting in an orange-red solution. This reaction mixture was then quickly added to a suspension of $Mo(CO)_6$ (45 mg, 0.170 mmol) in toluene (1 mL) at room temperature, then the reaction vessel placed under vacuum, backfilled with excess CO gas (*ca.* 100 mL), then sealed. The resultant mixture was stirred for 12 h at room temperature, yielding a dark red solution. The mixture was then filtered, and the filtrate was concentrated to *ca.* 3 mL *in vacuo*, then placed at -30 °C for 1 d, after which time orange crystals of **5** had deposited (74 mg, 32 %). These crystals were isolated, the mother liquor concentrated to *ca.* 1 mL, then stored at -30 °C for 1 d, which afforded colourless crystals of **4** (17 mg, 10 %). Data for **4**: M.p. > 260 °C; ^{1}H NMR (400 MHz, 298 K, C_6D_6): δ = 0.43 (v. br., 24H, CH(C*H*$_3$)$_2$), 0.92 (v. br., 24H, CH(C*H*$_3$)$_2$), 1.18 (br., 48H, CH(C*H*$_3$)$_2$), 1.61 (s, 12H, NCC*H*$_3$), 1.66 (s, 12H, NCC*H*$_3$), 2.99-3.07 (br., m, 16H, C*H*(CH$_3$)$_2$), 4.78 (s, 2H, β-C*H*), 4.98 (s, 2H, β-C*H*), 6.96–7.36 (m, 24H, Ar-*H*); N.B. once crystallised, compound **4** has minimal solubility in non-coordinating deuterated solvents such as C_6D_6 and toluene-d_8, which precluded the acquisition of meaningful ^{13}C{^{1}H} NMR spectroscopic data. Further, compound **4** slowly decomposes to protonated ligand, ^{Dip}NacnacH, when dissolved in d_8-THF; IR ν/cm^{-1} (Nujol): 1622

(w), 1512 (w), 1262 (w), 1229 (m), 1176 (m), 1101 (m), 1020 (w), 930 (m), 793 (s); anal. calc. for $C_{124}H_{164}Mg_4N_8O_8$: C 74.77 %, H 8.30 %, N 5.63 %: found: C 73.39 %, H 8.99 %, N 5.56 %.

Data for **5**: M.p. 159-161 °C (decomp.); Accurate integration of the resonances in the ^{1}H NMR spectrum was not possible due to the broad and often overlapping nature of those resonances. Thus, the integrations are estimated. ^{1}H NMR (400 MHz, 298 K, C_6D_6): δ = 0.48 (v. br., 6H, CH(CH_3)$_2$), 0.67 (v. br., 6H, CH(CH_3)$_2$), 0.86 (br., 12H, CH(CH_3)$_2$), 1.10 (br., 12H, CH(CH_3)$_2$), 1.23 (br., 12H, CH(CH_3)$_2$), 1.60 (s, 6H, NCCH_3), 1.64 (s, 6H, NCCH_3), 1.85 (s, 6H, ^{DMAP}N(CH_3)$_2$), 3.03 (br., m, 2H, CH(CH$_3$)$_2$), 3.11 (br., m, 2H, CH(CH$_3$)$_2$), 3.38 (br., m, 2H, CH(CH$_3$)$_2$), 3.44 (br., m, 2H, CH(CH$_3$)$_2$), 4.85 (s, 1H, β-CH), 4.99 (s, 1H, β-CH), 5.61 (d, 2H, ^{DMAP}Ar-H), 6.69 (d, 2H, ^{DMAP}Ar-H), 7.01–7.29 (m, 12H, Ar-H); ^{13}C{^{1}H} NMR (151 MHz, C_6D_6, 298 K): δ = 23.1, 23.4 (NCCH$_3$), 23.7, 23.8, 23.9, 24.1, 24.30, 24.32, 24.50, 24.59, 24.6, 24.7, 24.9, 26.1 (CH(CH$_3$)$_2$), 28.1, 28.3, 28.4, 28.6 (CH(CH$_3$)$_2$), 37.9 (^{DMAP}N(CH$_3$)$_2$), 95.2, 96.6 (β-CH), 106.8, 123.1, 123.4, 123.6, 123.7, 124.4, 124.9, 125.6, 125.8, 136.4, 141.4, 142.4, 142.8, 143.7, 144.0, 145.2, 147.6, 155.0 (Ar-C), 162.1 (NCCH$_3$), 167.4 (C_2O_3), 169.7 (NCCH$_3$), 170.1 (C:C=O), 191.1 (C_2O_3), 207.7, 214.9 (Mo(CO)$_5$), N.B (O=CC:Mo(CO)$_5$) resonance was not observed; IR ν/cm^{-1} (Nujol): 2072 (m), 2042 (m), 1974 (w), 1914 (s), 1876 (s), 1618 (s), 1539 (m), 1515 (m), 1262 (w), 1228 (s), 1175 (m), 1101 (m), 1013 (w), 949 (m), 795 (m); anal. calc. for $C_{74}H_{93}Mg_2MoN_6O_9$: C 65.39 %, H 6.92 %, N 6.20 %: found: C 65.28 %, H 6.79 %, N 6.08 %.

Higher yield synthesis of 4. [{(^{Dip}Nacnac)Mg}$_2$] (150 mg, 0.170, mmol) and DMAP (21 mg, 0.170 mmol) were dissolved in 5 mL of toluene at room temperature, resulting in an orange-red solution. This was then quickly added to a toluene (1 mL) suspension of Mo(CO)$_6$ (45 mg, 0.170 mmol) at room temperature. The reaction vessel was placed under vacuum, backfilled with excess CO gas (*ca.* 100 mL), then sealed. The mixture was placed in a preheated oil bath at 80 °C for 14 h, yielding a dark red solution. The mixture was then cooled to room temperature and left for 1 d, after which time colourless crystals of **4** had deposited. These were isolated by filtration (43 mg, 25 %). N.B A few yellow crystals of *cis*-[Mo(CO)$_4$(DMAP)$_2$] were isolated from the mother liquor, and identified using X-ray crystallography.

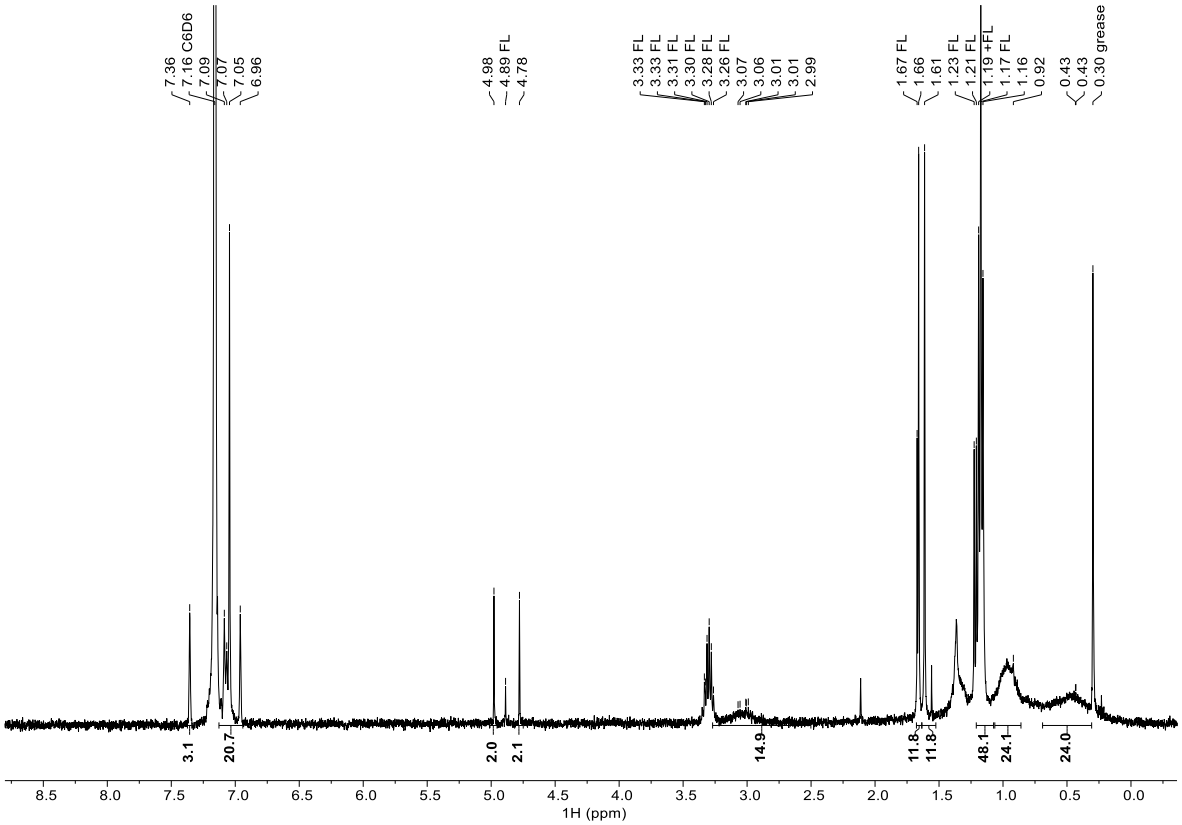


Figure S1. ^{1}H NMR spectrum (400 MHz, 298 K, C_6D_6) of **4**.

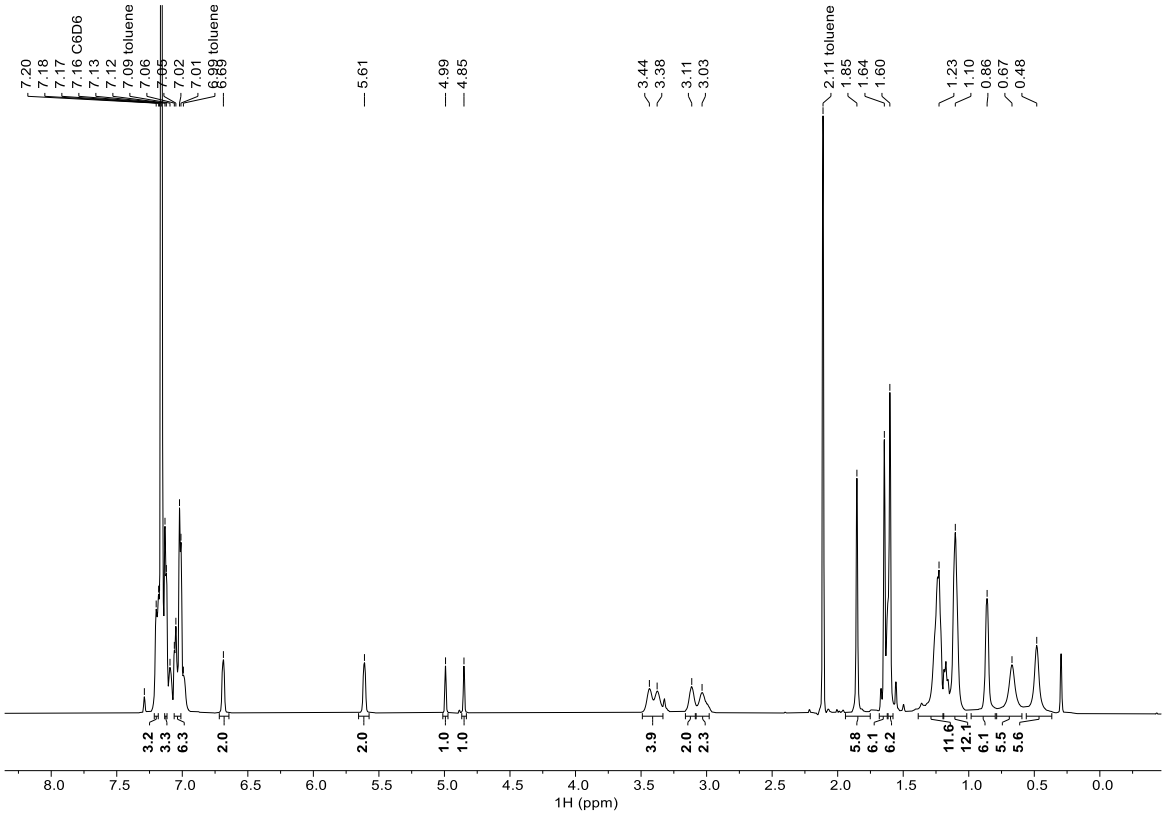


Figure S2. ^{1}H NMR spectrum (400 MHz, 298 K, C_6D_6) of **5**.

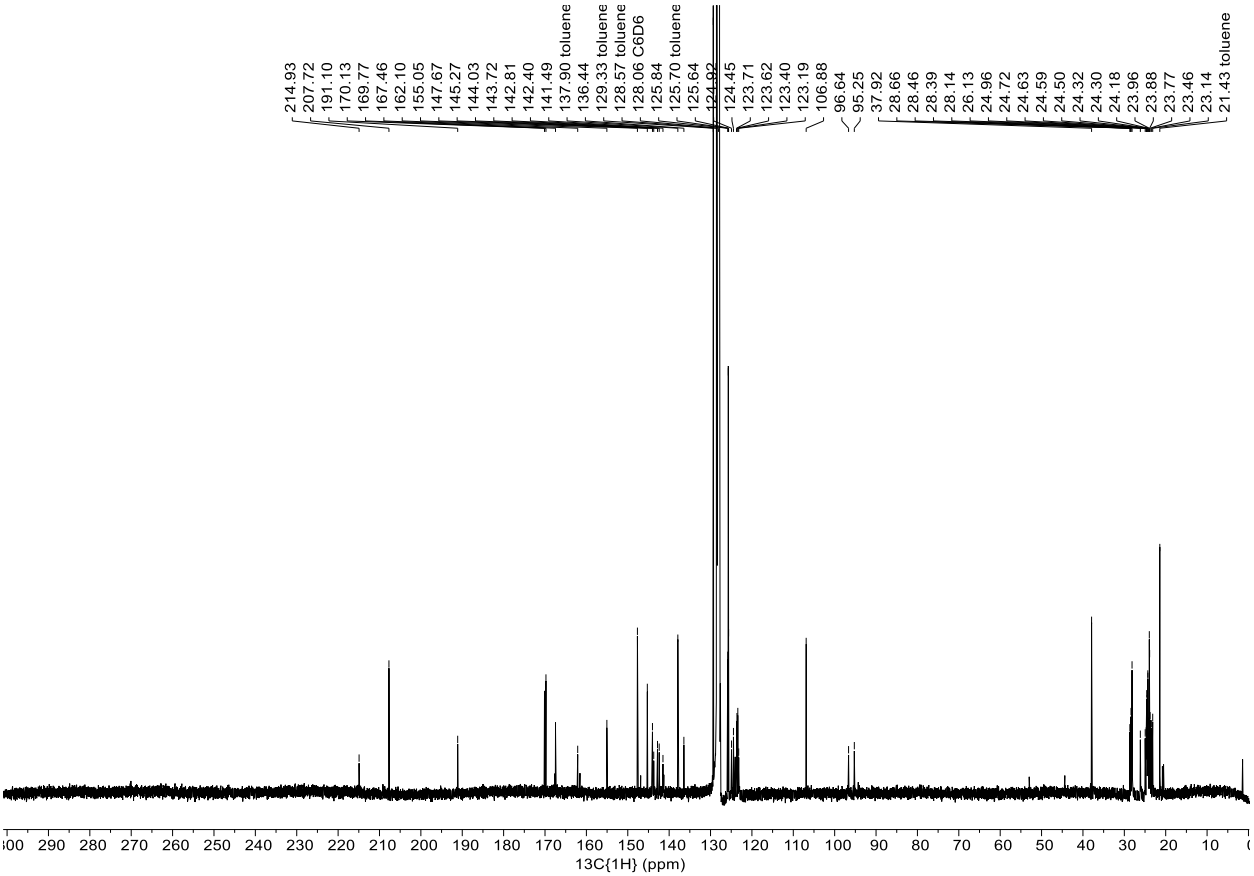


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, 298 K, C_6D_6) of **5**.

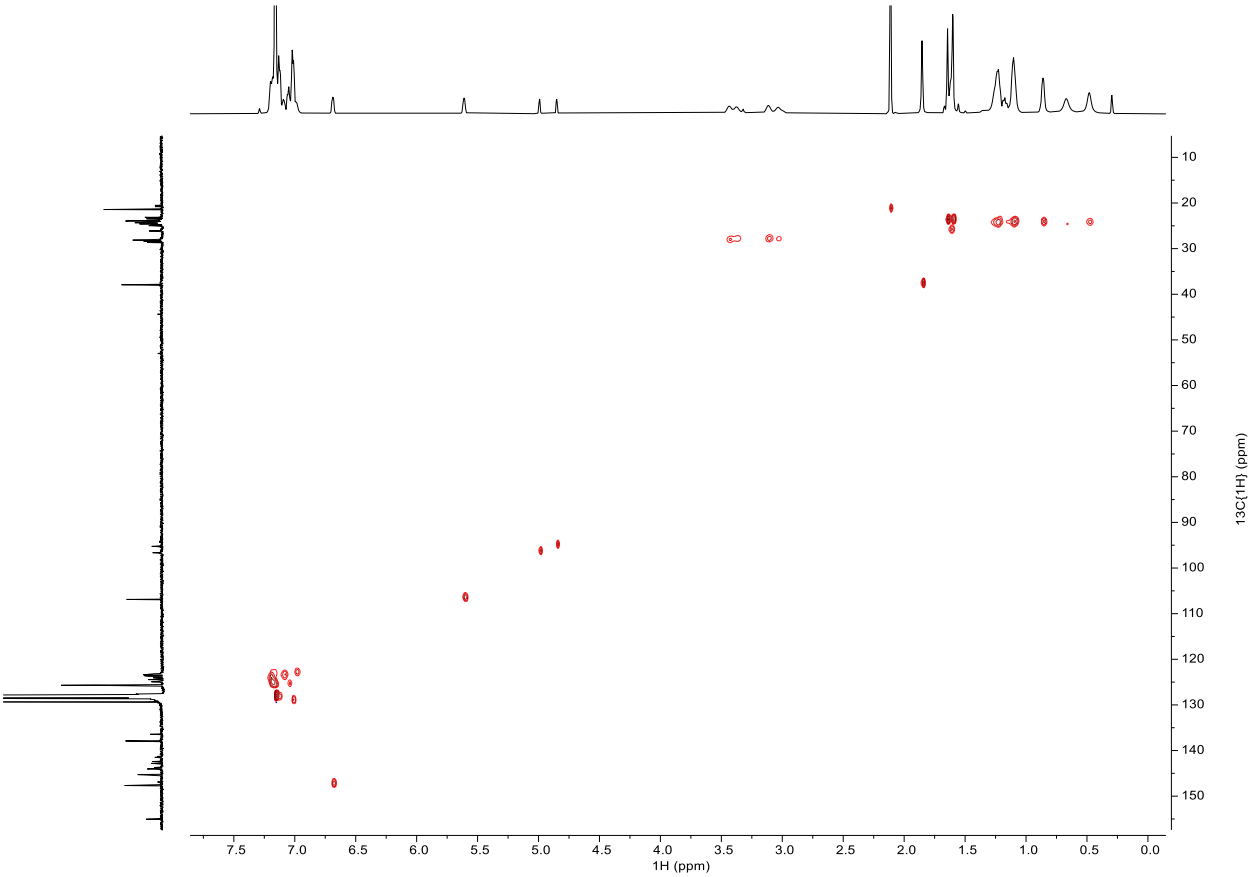


Figure S4. HSQC spectrum (^{1}H: 400 MHz; ^{13}C 101 MHz; 298 K, C_6D_6) of **5**.

Synthesis of [{(^{Dip}Nacnac)Mg}(C_4O_4){μ-Mg(^{Dip}Nacnac)}]$_2$ 4 and [{(^{Dip}Nacnac)Mg}{μ-(C_4O_4)Mo(CO)$_5$}{Mg(TMC)(^{Dip}Nacnac)}] 6. [{(^{Dip}Nacnac)Mg}$_2$] (150 mg, 0.170 mmol) and TMC (21 mg, 0.170 mmol) were dissolved in toluene (50 mL) at -78 °C. This resulted in an immediate solution colour change from yellow to orange red. This mixture was then quickly added to a toluene (1 mL) suspension of $Mo(CO)_6$ (45 mg, 0.170 mmol) at room temperature. The reaction vessel placed under vacuum, backfilled with excess CO gas (*ca.* 100 mL), then sealed. The reaction solution was stirred for 12 h at room temperature, yielding a dark red solution. The mixture was then filtered, the filtrate concentrated to *ca.* 3 mL *in vacuo*, then placed at -30 °C for 1 d, after which time colourless crystals of **4** (14 mg, 8 %) had deposited. The mother liquor was filtered and further concentrated to 1 mL. After 2 days bright yellow crystals of **6** had deposited (37 mg, 16 %). Data for **6**: 165-168 °C (decomp.); ^{1}H NMR (400 MHz, 298 K, C_6D_6): δ = 0.75 (d, 12H, CH(CH_3)$_2$), 1.10 (d, 12H, CH(CH_3)$_2$), 1.15 (d, 12H, CH(CH_3)$_2$), 1.24 (d, 12H, CH(CH_3)$_2$),

1.26 (s, 6H, CCH_3), 1.60 (s, 6H, NCCH_3), 1.63 (s, 6H, NCCH_3), 2.22 (s, 6H, NCH_3), 3.08–3.13 (br., m, 2H, CH(CH_3)$_2$), 3.28–3.33 (br., m, 4H, CH(CH_3)$_2$), 3.41–3.45 (br., m, 2H, CH(CH_3)$_2$), 4.84 (s, 1H, β-CH), 5.01 (s, 1H, β-CH), 6.88–7.13 (m, 12H, Ar-H); N.B. once crystallised, compound **6** has poor solubility in non-coordinating deuterated solvents such as C_6D_6 and toluene-d_8, which precluded the acquisition of meaningful $^{13}C\{^1H\}$ NMR spectroscopic data. Further, compound **6** slowly decomposes to protonated ligand, ^{Dip}NacnacH, when dissolved in d_8-THF; IR ν/cm^{-1} (Nujol): 2070 (m), 2039 (m), 1911 (s), 1875 (s), 1619 (s), 1545 (m), 1229 (s), 1175 (m), 1101 (m), 1010 (w), 924 (m), 830 (w), 790 (m); A satisfactory micro-analysis could not obtained as compound **6** consistently co-crystallizes with small amounts of **4**. The low solubility of both compounds, once crystallised, precluded successful recrystallisations.

Higher yield synthesis of 4. [{(^{Dip}Nacnac)Mg}$_2$] (150 mg, 0.170 mmol) and TMC (21 mg, 0.170 mmol) were dissolved in toluene (5 mL) at -78 °C. This resulted in an immediate solution colour change from yellow to orange red. This mixture was then quickly added to a toluene (1 mL) suspension of $Mo(CO)_6$ (45 mg, 0.170 mmol) at room temperature. The reaction vessel was then placed under vacuum, backfilled with excess CO gas (*ca.* 100 mL), then sealed. The flask was placed in a preheated oil bath at 80 °C for 14 h, yielding a dark red solution. The mixture was then cooled to room temperature and left for 1 d, after which time colourless crystals of **4** had deposited. These were isolated by filtration (51 mg, 31 %). N.B A few yellow crystals of *cis*-[$Mo(CO)_4(TMC)_2$] were isolated from the mother liquor, and identified using X-ray crystallography.

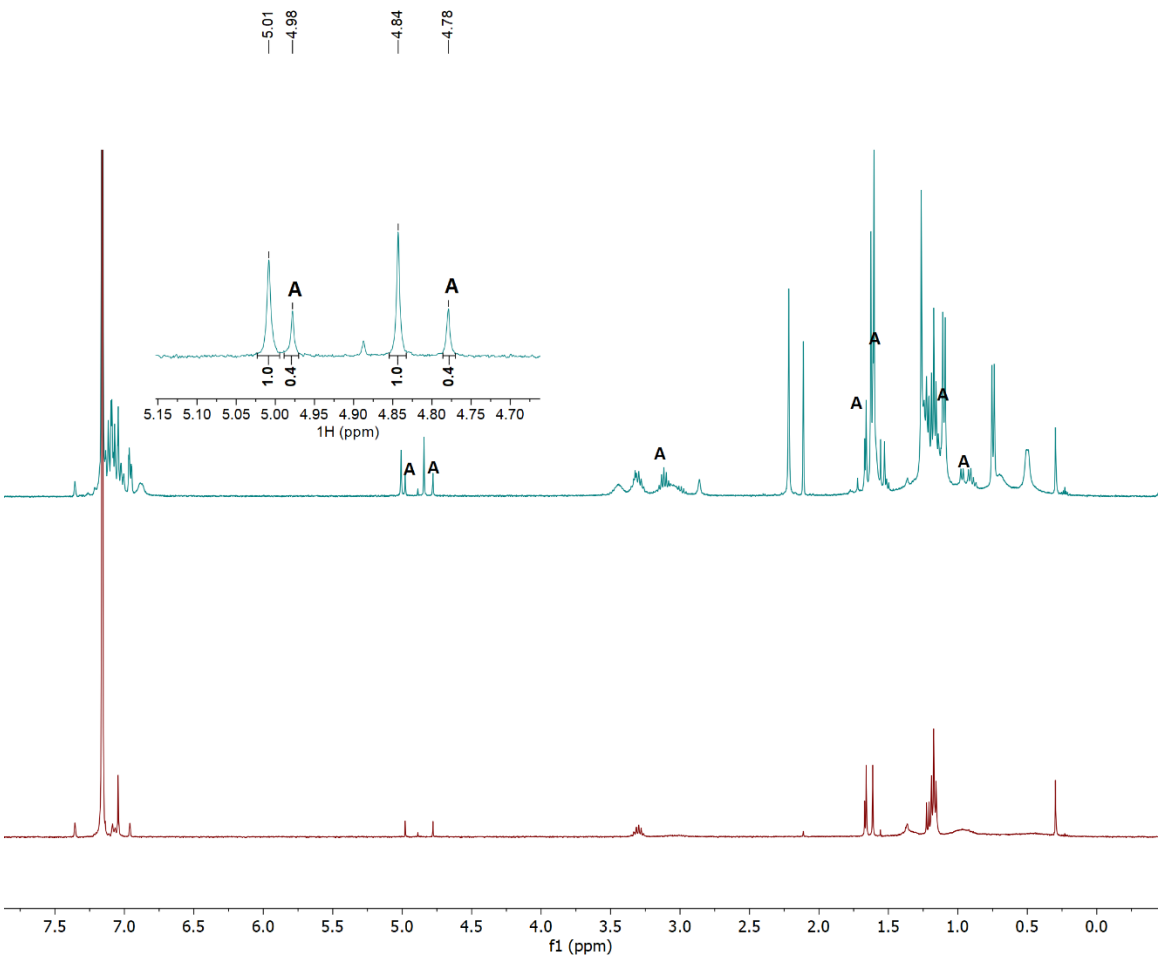


Figure S5. ^{1}H NMR spectra (400 MHz, 298 K, C_6D_6) of **4** (below; red color) and a co-crystallised mixture of **4** and **6** (above; green color, peaks for **4** denoted as **A**).

Synthesis of [{(^{Dip}Nacnac)Mg}{μ-(C_4O_4)Mo(CO)$_5$}{Mg(THF)(^{Dip}Nacnac)}] 7. [{(^{Dip}Nacnac)Mg}$_2$] (150 mg, 0.170 mmol) was dissolved in 5 mL of benzene followed by the addition of 1 mL of tetrahydrofuran (THF) at room temperature, resulting in an orange-red solution. This mixture was then quickly added to a benzene (1 mL) suspension of $Mo(CO)_6$ (45 mg, 0.170 mmol) at room temperature. The reaction vessel was then placed under vacuum, backfilled with excess CO gas (*ca.* 100 mL), then sealed. The solution was stirred for 12 h at room temperature, yielding a dark red solution. The mixture was then filtered, the filtrate concentrated to *ca.* 2 mL *in vacuo*, then placed at 4 °C for 1 d, after which time orange crystals of **7** had deposited. These were washed with cold *n*-hexane, isolated and a second crop obtained from the mother liquor (91 mg, 41 %). M.p. 193-196 °C (decomp.); N.B. accurate integration of the

resonances in the ^{1}H NMR spectrum of the compound was not possible due to the broad and often overlapping nature of those resonances. Thus, the integrations are estimated. ^{1}H NMR (400 MHz, 298 K, C_6D_6): δ = 0.45 (v. br., 6H, CH(C*H*$_3$)$_2$), 1.02 (v. br., 4H, OCH$_2$C*H*$_2$), 1.16–1.17 (d, 24H, CH(C*H*$_3$)$_2$), 1.18–1.19 (d, 12H, CH(C*H*$_3$)$_2$), 1.21–1.23 (d, 6H, CH(C*H*$_3$)$_2$), 1.55 (s, 6H, NCC*H*$_3$), 1.62 (s, 6H, NCC*H*$_3$), 2.96–2.99 (br., m, 4H, OC*H*$_2$CH$_2$), 3.10–3.16 (br., m, 4H, C*H*(CH$_3$)$_2$), 3.24–3.33 (br., m, 4H, C*H*(CH$_3$)$_2$), 4.88 (s, 1H, β-C*H*), 4.91 (s, 1H, β-C*H*), 6.96 – 7.14 (m, 12H, Ar-*H*); ^{1}H NMR (400 MHz, 298 K, toluene-d_8): δ = 0.43 (v. br., 6H, CH(C*H*$_3$)$_2$), 1.11–1.13 (v. br., 16H, OC*H*$_2$CH$_2$ overlapping with C*H*(CH$_3$)$_2$), 1.16–1.18 (d, 24H, CH(C*H*$_3$)$_2$), 1.20–1.22 (d, 12H, CH(C*H*$_3$)$_2$), 1.54 (s, 6H, NCC*H*$_3$), 1.59 (s, 6H, NCC*H*$_3$), 2.93–2.96 (br., m, 4H, OC*H*$_2$CH$_2$), 3.06–3.07 (br., m, 4H, C*H*(CH$_3$)$_2$), 3.14–3.29 (br., m, 4H, C*H*(CH$_3$)$_2$), 4.82 (s, 1H, β-C*H*), 4.87 (s, 1H, β-C*H*), 6.98–7.10 (m, 12H, Ar-*H*); ^{13}C{^{1}H} NMR (151 MHz, C_6D_6, 298 K): δ = 20.5 (CH(*C*H$_3$)$_2$), 23.1, 23.7 (NC*C*H$_3$), 23.91, 23.94, 24.41 (CH(*C*H$_3$)$_2$), 24.45 (OCH$_2$C*H*$_2$), 28.1, 28.31, 28.32, 28.4, (*C*H(CH$_3$)$_2$), 69.8 (O*C*H$_2$CH$_2$), 95.3, 96.7 (β-*C*H), 123.4, 124.0, 125.8, 127.6, 136.4, 143.9, 144.4, 146.8 (Ar-*C*), 162.3 (N*C*CH$_3$), 167.4 (*C*$_2$O$_3$), 167.6 (N*C*CH$_3$), 170.3 (C:*C*=O), 190.2 (*C*$_2$O$_3$), 207.5, 214.6 (Mo(*C*O)$_5$), N.B (O=C*C*:Mo(CO)$_5$) resonance was not observed; N.B. THF-d_8 solutions of the compound presented broad and complex ^{1}H and ^{13}C{^{1}H} NMR spectra, showing the presence of significant quantities of ^{Dip}NacnacH, suggesting the compound slowly decomposes in THF-d_8; IR ν/cm^{-1} (Nujol): 2075 (s), 2046 (s), 1979 (s), 1919 (s), 1887 (s), 1626 (s), 1547 (m), 1523 (m), 1263 (m), 1176 (m), 1102 (m), 1021 (w), 934 (m), 797 (s); anal. calc. for $C_{71}H_{91}Mg_2MoN_4O_{10}$: C 65.34 %, H 7.03 %, N 4.29 %: found: C 65.77 %, H 7.36 %, N 4.41 %.

Synthesis of 7 using ^{13}CO. [{(^{Dip}Nacnac)Mg}$_2$] (80 mg, 0.091 mmol) was dissolved in 3 mL of benzene at room temperature, followed by the addition of 0.5 mL of THF, resulting in an orange-red solution. This mixture was then quickly added to a benzene (0.5 mL) suspension of Mo(CO)$_6$ (24 mg, 0.091 mmol) at room temperature. The reaction vessel was then placed under vacuum, backfilled with excess ^{13}CO gas (*ca.* 20 mL), then sealed. The resultant solution was stirred for 12 h at room temperature, yielding a dark red solution. The mixture was then filtered, the filtrate concentrated to *ca.* 1 mL *in vacuo*, then placed at 4 °C for 1 d, after which time orange crystals of **7** had deposited (30 mg, 25 %). ^{13}CO enriched ^{13}C{^{1}H} NMR (151 MHz, C_6D_6, 298 K): δ = 167.4 (d, *J* = 61 Hz, *C*$_2$O$_3$), 170.3 (s, C:*C*=O), 190.2 (d, *J* = 61 Hz, *C*$_2$O$_3$), 207.5, 214.6 (Mo(*C*O)$_5$), N.B. O=C*C*:(Mo(CO)$_5$) resonance was not observed.

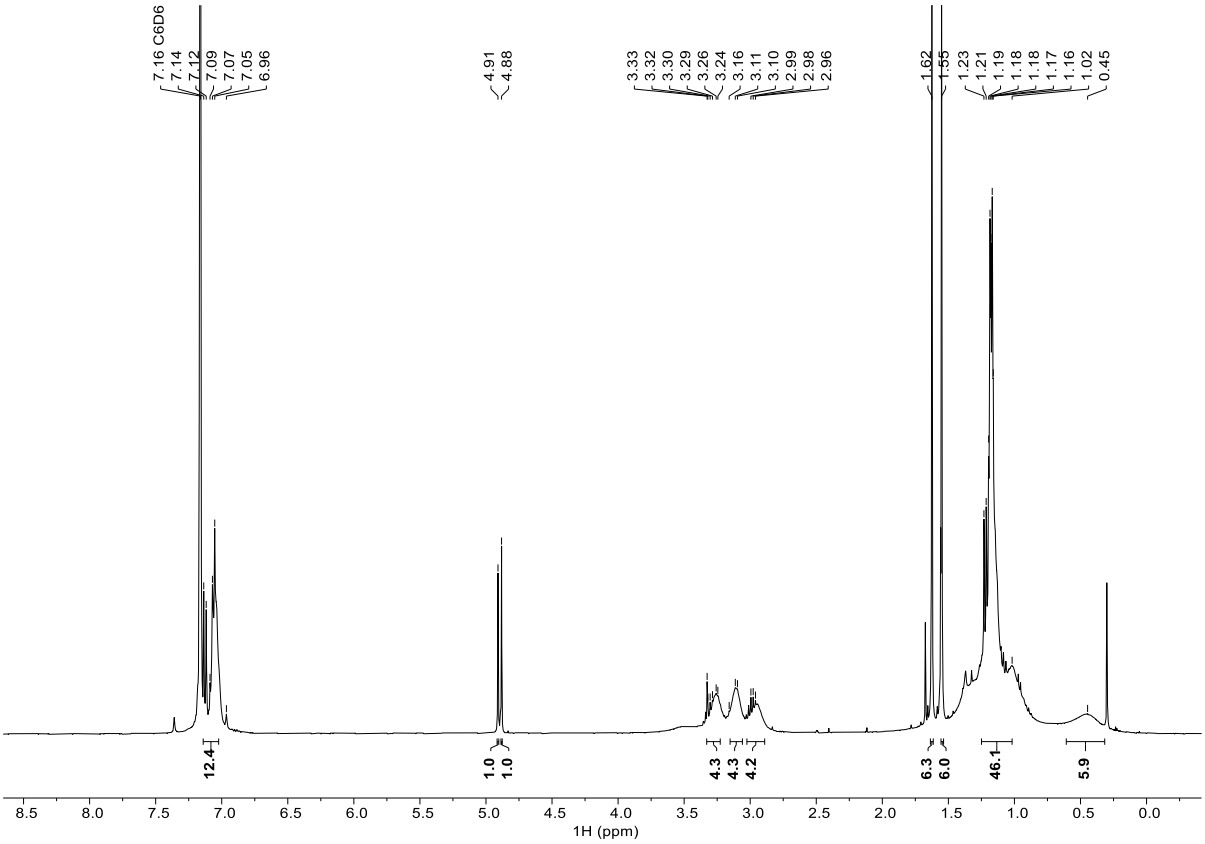


Figure S6. ^{1}H NMR spectrum (400 MHz, 298 K, C_6D_6) of **7**.

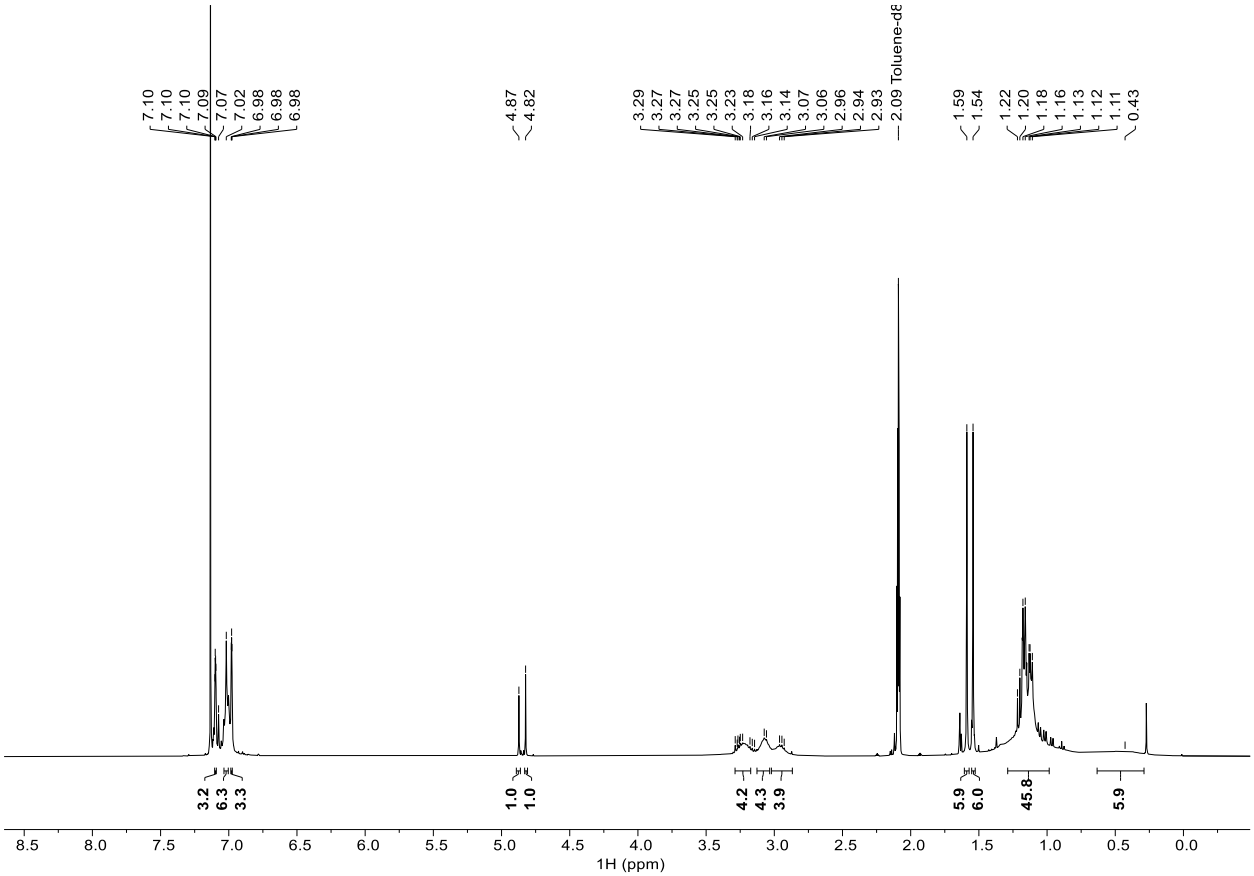


Figure S7. ^{1}H NMR spectrum (400 MHz, 298 K, toluene-d_8) of **7**.

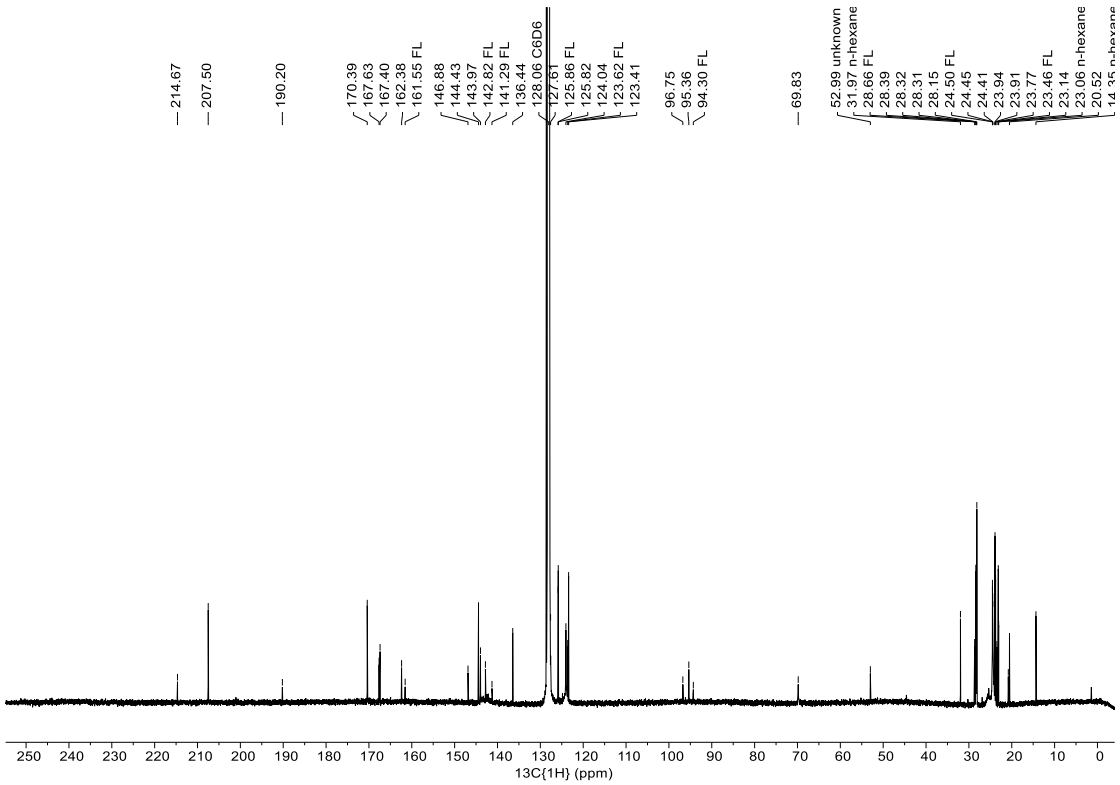


Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, 298 K, C_6D_6) of **7**, (FL = ^{Dip}NacnacH).

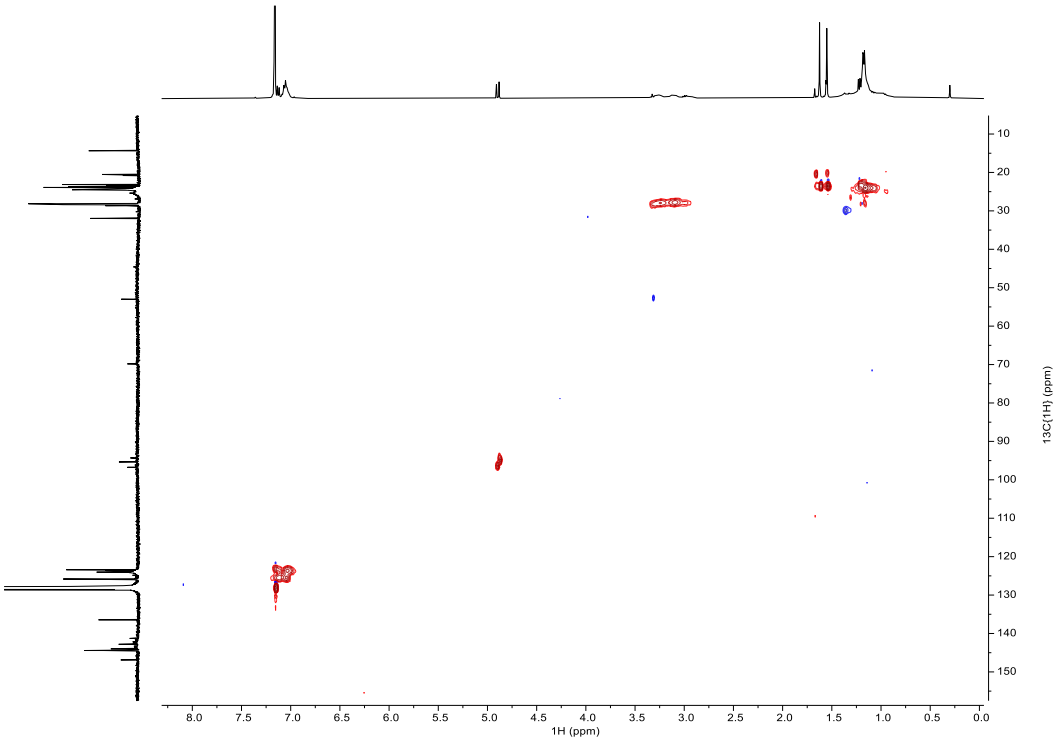


Figure S9. HSQC spectrum (^{1}H: 400 MHz; ^{13}C 101 MHz; 298 K, C_6D_6) of **7**.

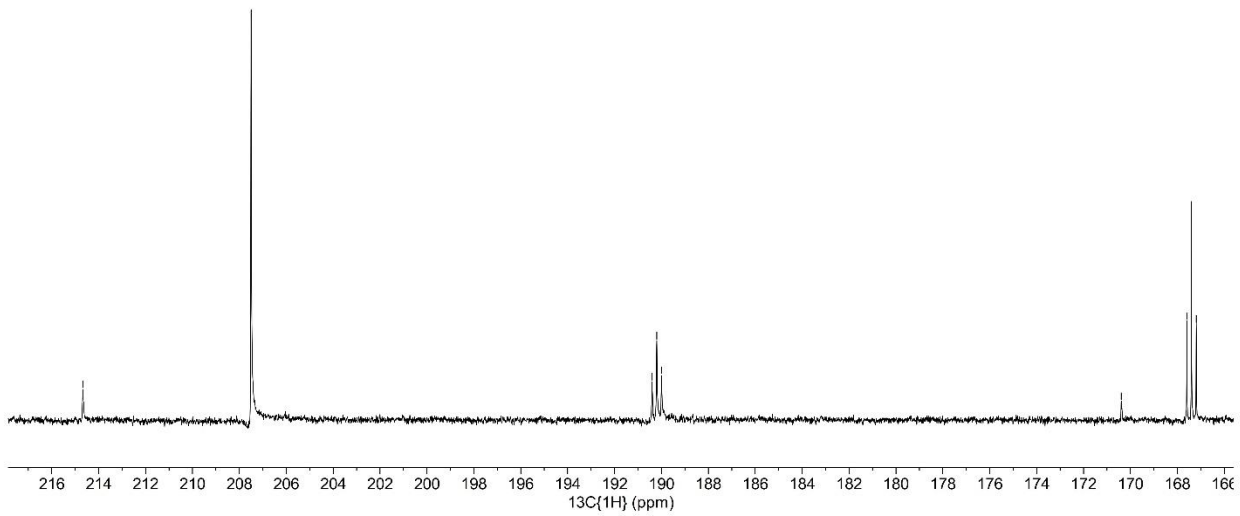


Figure S10. Low field region of the ^{13}CO enriched $^{13}C\{^1H\}$ NMR spectrum (151 MHz, 298 K, C_6D_6) of **7** after 254 scans. N.B. The apparent triplet resonances were confirmed to be doublet resonances superimposed on singlet resonances, using 1D- and 2D-INADEQUATE NMR experiments.

Synthesis of [{(Priso)(THF)Mg}(C_4O_4){μ-Mg(THF)(Priso)}]$_2$ 8. [{(Priso)Mg}$_2$] (150 mg, 0.154 mmol) was dissolved in 3 mL of benzene, followed by the addition of THF (0.2 mL), yielding a pale-yellow solution, which was quickly transferred into a 1 mL benzene suspension of $Mo(CO)_6$ (41 mg, 0.154 mmol). The head space above the mixture was evacuated, and backfilled with excess CO gas (*ca.* 100 mL), then the reaction flask sealed. The mixture was then stirred for 14 h, at 80 °C, yielding a dark green solution. The reaction mixture was then kept at room temperature overnight, after which time colorless crystals of **8**, had formed (32 mg, 17 %); M.p. = 151-156 °C; ^{1}H NMR (600 MHz, C_6D_6, 298 K) δ = 0.95–0.97 (dd, *J* = 7.1, 5.0 Hz, 48H, CH(C*H*$_3$)$_2$), 1.08 (d, *J* = 6.7 Hz, 24H, NCH(C*H*$_3$)$_2$), 1.18–1.23 (v. br., 16H, OC*H*$_2$CH$_2$, overlapping with FL), 1.38 (d, 24H, *J* = 6.8 Hz, NCH(C*H*$_3$)$_2$), 1.46–1.48 (dd, *J* = 7.1, 5.0 Hz, 48H, CH(C*H*$_3$)$_2$), 3.44–3.51 (br. m, 16H, OC*H*$_2$CH$_2$, overlapping with FL), 3.84–3.89 (m, 8H, C*H*(CH$_3$)$_2$), 3.92–3.97 (m, 8H, C*H*(CH$_3$)$_2$), 4.16–4.21 (m, 4H, NC*H*(CH$_3$)$_2$), 4.23–4.26 (m, 4H, NC*H*(CH$_3$)$_2$), 6.99–7.22 (m, 24H, Ar-*H*); $^{13}C\{^1H\}$ NMR (151 MHz, C_6D_6, 298 K) δ = 21.8, 22.0 (NCH(*C*H$_3$)$_2$), 23.51, 23.59, 24.4, 25.1, 25.3, 25.8 (CH(*C*H$_3$)$_2$), 28.1, 28.2, 28.4, 30.2 (*C*H(CH$_3$)$_2$), 49.8, 50.0 (N*C*H(CH$_3$)$_2$), 123.1, 123.3, 123.6, 123.9, 127.90, 127.98, 128.2, 128.3, 128.5, 142.9, 143.7, 145.3 (Ar-*C*), 166.7, 166.8

(CN_3), THF and $(C_4O_4)^{2-}$ resonances were not observed. N.B. Compound **8** has poor solubility in C_6D_6 and tolunene-d_8. IR ν/cm^{-1} (Nujol): 1625 (s), 1562 (s), 1275 (s), 1238 (s), 1204 (s), 1176 (s), 1124 (m), 1027 (m), 934 (m), 919 (m), 871 (m), 801 (s), 755 (s), 726 (s); a satisfactory micro-analysis could not obtained as the compound consistently co-crystallizes with small amounts of PrisoH (FL), which could not be removed after repeated recrystallizations.

Synthesis of 8 using ^{13}CO. [{(Priso)Mg}$_2$] (10 mg, 0.010 mmol) and $Mo(CO)_6$ (3 mg, 0.010 mmol) were dissolved in 0.4 mL of C_6D_6, followed by the addition of THF-d_8 (0.1 mL), yielding a pale-yellow solution. The head space above the mixture was evacuated and backfilled with excess ^{13}CO gas (*ca.* 20 mL), and the reaction flask sealed. The mixture was placed in an oil bath at 80 °C for 14 h, yielding a dark green solution. A $^{13}C\{^1H\}$ NMR spectrum of an aliquot of the reaction mixture was then taken. ^{13}CO enriched $^{13}C\{^1H\}$ NMR (151 MHz, C_6D_6, 298 K): δ = 231.4 (s, C_4O_4), 237.7 (s, C_4O_4).

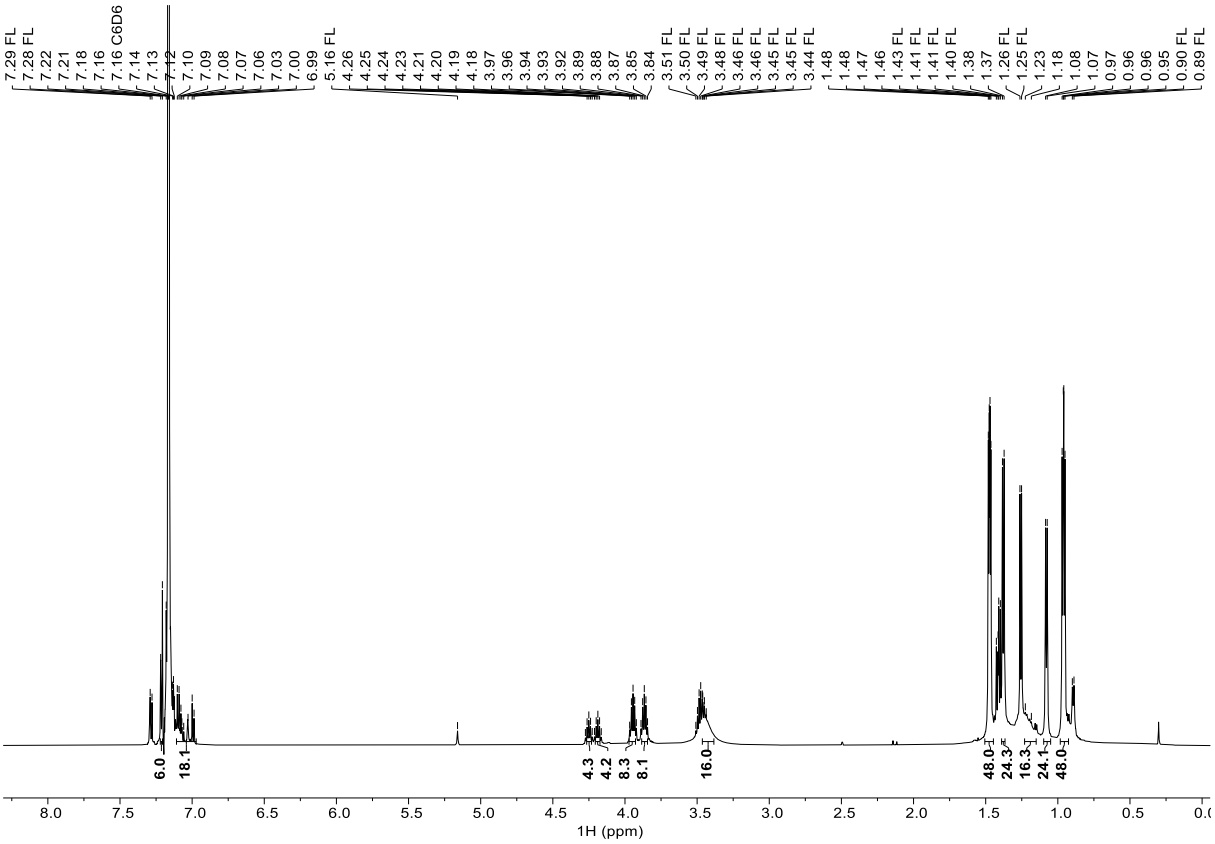


Figure S11. ^{1}H NMR spectrum (600 MHz, 298 K, C_6D_6) of **8**, (FL = PrisoH).

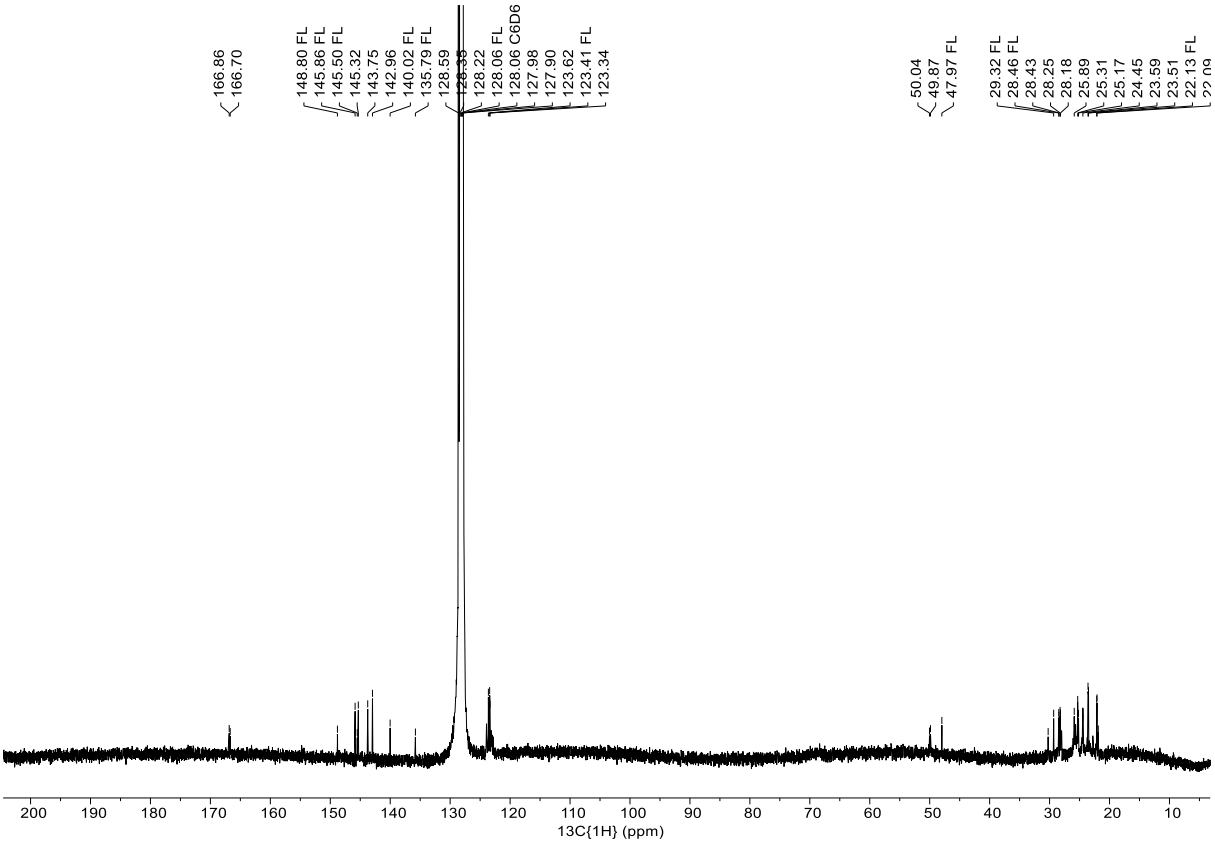


Figure S12. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, 298 K, C_6D_6) of **8**, (FL = PrisoH).

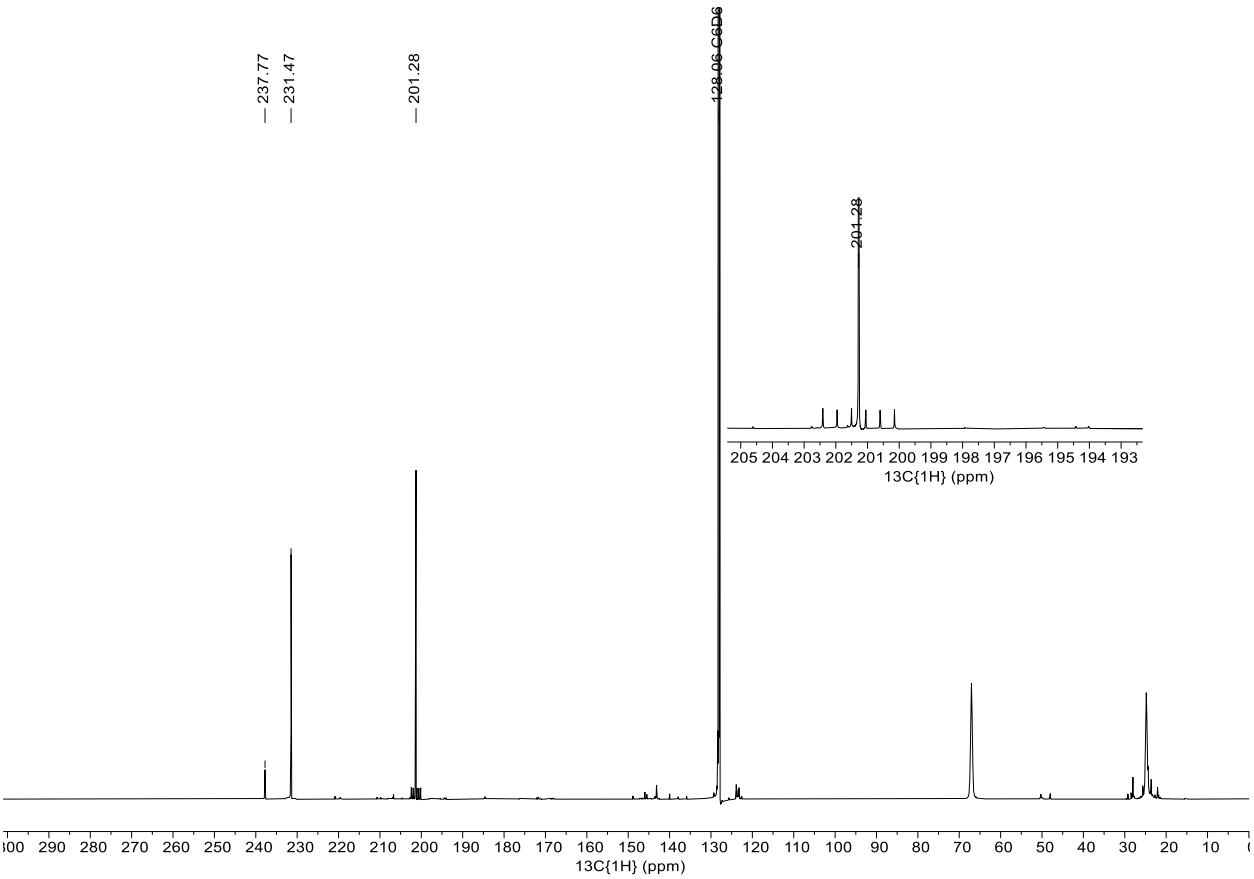


Figure S13. $^{13}C\{^{1}H\}$ NMR spectrum (151 MHz, 298 K, C_6D_6) of an aliquot of the ^{13}CO enriched reaction mixture that gave **8** (254 scans). The signal at δ 201 ppm is associated with $Mo(CO)_6$ in the mixture.

Synthesis of *cis*-[Mo(CO)$_4$(TMC)$_2$]

TMC (188 mg, 1.52 mmol) and $Mo(CO)_6$ (200 mg, 0.757 mmol) were suspended in 10 mL of toluene at room temperature, then the reaction mixture placed in an oil bath at 80 °C overnight. After this time, a pale yellow solid precipitated. This was isolated and washed with hexane, then dried under vacuum to give the title compound (242 mg, 70 %). N.B. the compound has poor solubility in aromatic solvents such as C_6D_6 and toluene-d_8. M.p 141-144 °C; ^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 1.33 (s, 12H, CCH_3), 3.26 (s, 12H, NCH_3); ^{1}H NMR (400 MHz, $CDCl_3$, 298 K): δ = 2.06 (s, 12H, CCH_3), 3.51(s, 12H, NCH_3); $^{13}C\{^{1}H\}$ NMR (101 MHz, $CDCl_3$, 298 K): δ = 9.8 (CCH$_3$), 36.0 (NCH$_3$), 124.7 (CCH$_3$), 193.1, 211.6 (MoC:); IR ν/cm^{-1} (Nujol): 1988 (s), 1914

(s), 1850 (s), 1798 (s), 1069 (m), 844 (m), 670 (m); anal. calc. for $C_{18}H_{24}MoN_4O_4$: C 47.37 %, H 5.30 %, N 12.28 %: found: C 47.28 %, H 5.50 %, N 12.03 %.

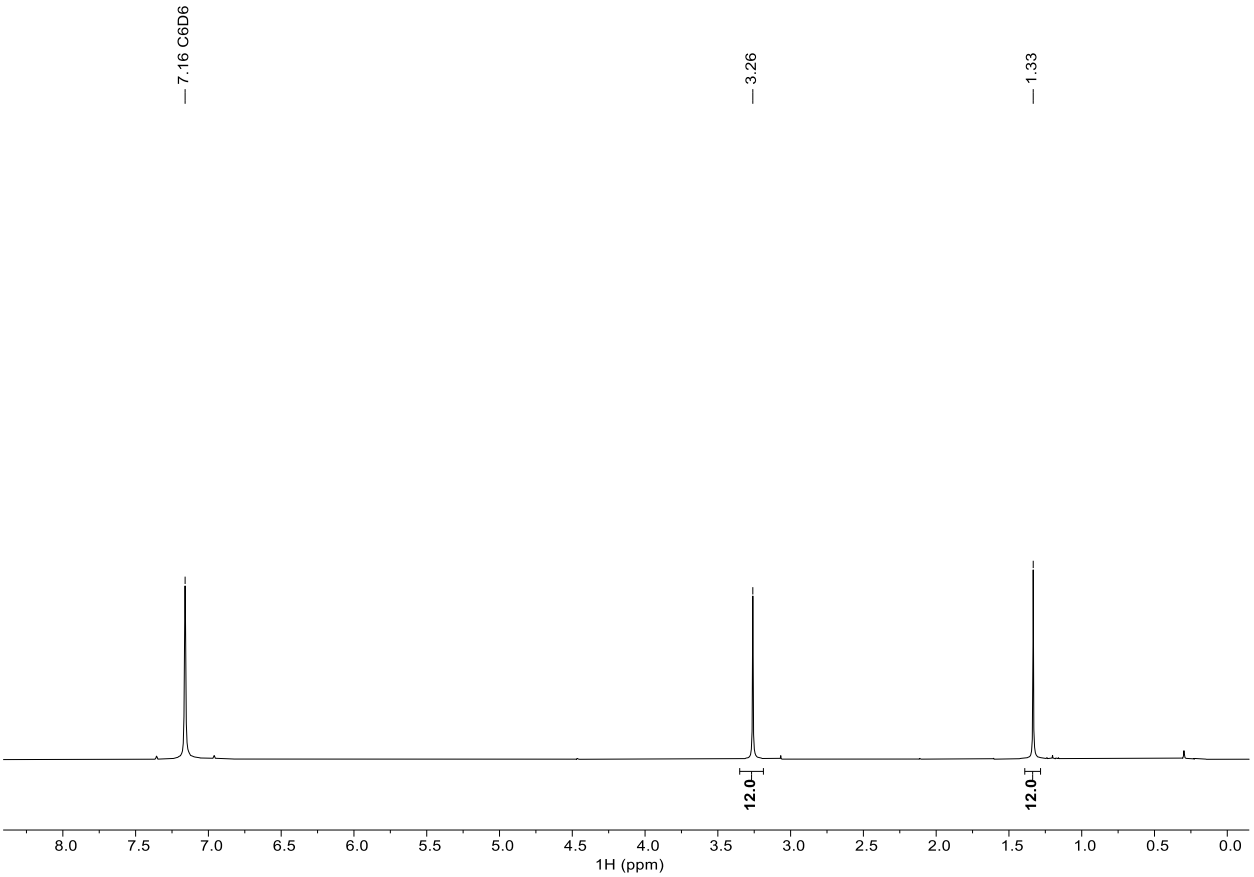


Figure S14. ^{1}H NMR spectrum (400 MHz, 298 K, C_6D_6) of *cis*-[$Mo(CO)_4(TMC)_2$].

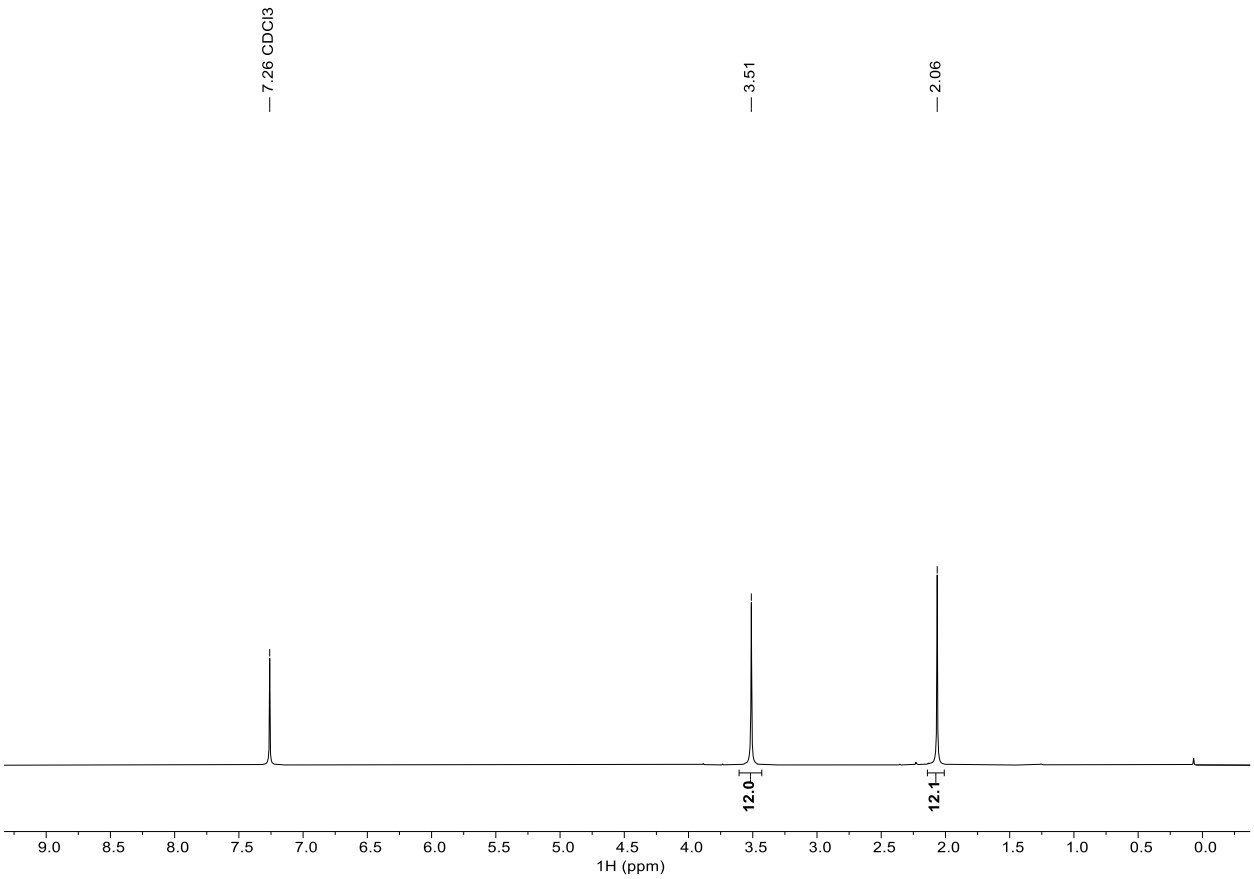


Figure S15. ^{1}H NMR spectrum (400 MHz, 298 K, $CDCl_3$) of *cis*-$[Mo(CO)_4(TMC)_2]$.

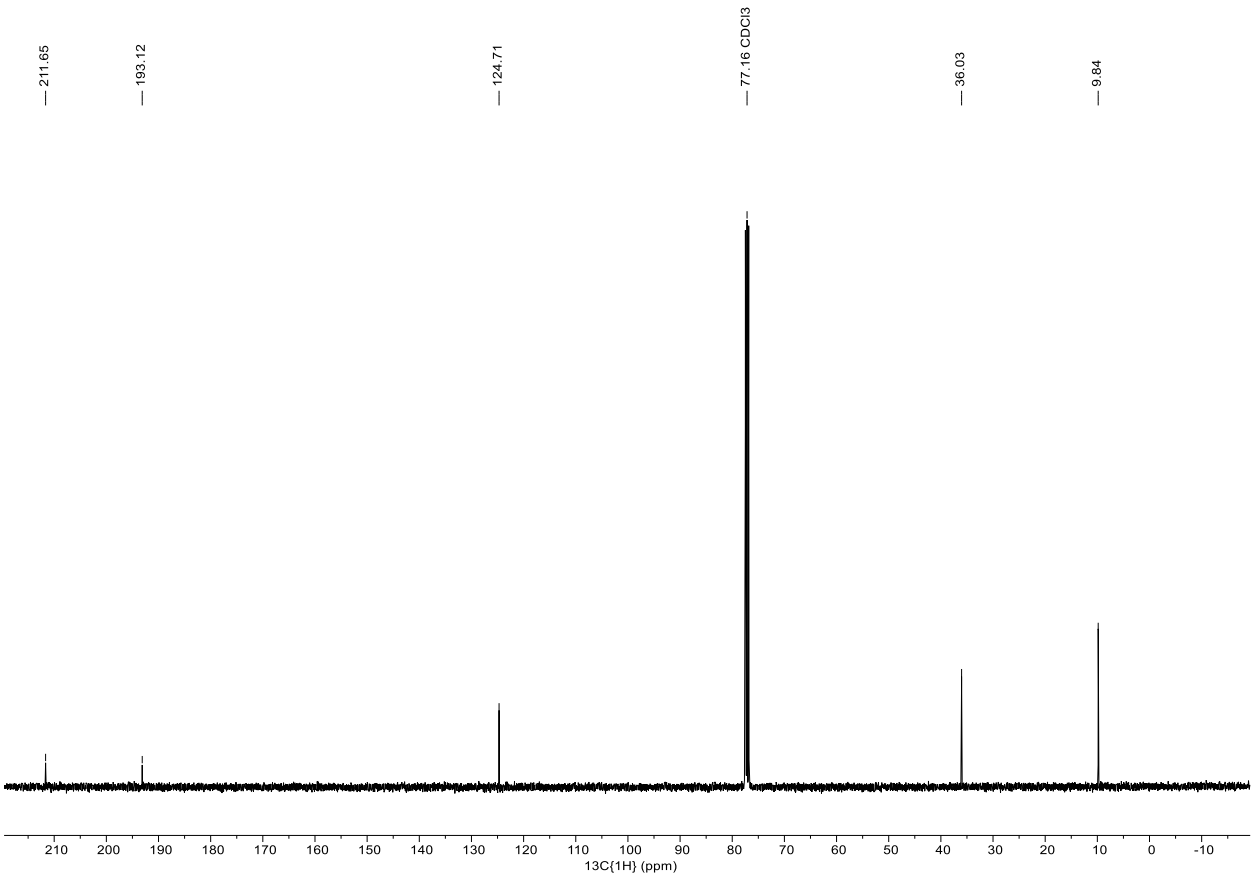


Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum (101 MHz, 298 K, $CDCl_3$) of *cis*-$[Mo(CO)_4(TMC)_2]$.

2. X-Ray Crystallographic Studies

Crystals suitable for X-ray structural determination were mounted in silicone oil. Crystallographic measurements were made using either a Rigaku Xtalab Synergy Dualflex diffractometer with a graphite monochromator with Mo Kα radiation (λ = 0.71073 Å) or Cu Kα radiation (1.54180 Å); or the MX1 beamline of the Australian Synchrotron (λ = 0.71090 Å). The software package Blu-Ice[4] was used for synchrotron data acquisition, while the program XDS[5] was employed for synchrotron data reduction. All structures were solved by direct methods and refined on F^2 by full matrix least squares (SHELX-16[6]) using all unique data. Hydrogen atoms are typically included in calculated positions (riding model). Crystal data, details of data collections and refinements for all structures can be found in their CIF files and are summarized in Table S1.

Table S1. Crystal data for compounds **4-8**, *cis*-[Mo(CO)$_4$(DMAP)] **1S** and *cis*-[Mo(CO)$_4$(TMC)] **2S**.

	4·(benzene)	**5**·(toluene)$_2$	**6**·(toluene)	**7**·(benzene)$_{1.5}$
empirical formula	$C_{130}H_{170}Mg_4N_8O_8$	$C_{88}H_{108}Mg_2MoN_6O_9$	$C_{81}H_{102}Mg_2MoN_6O_9$	$C_{89}H_{108}Mg_2MoN_4O_{10}$
formula weight	2069.97	1538.36	1448.24	1538.35
crystal system	triclinic	monoclinic	monoclinic	monoclinic
space group	*P*-1	$P2_1/n$	$P2_1/n$	$P2_1/m$
a (Å)	12.5268(3)	12.471(3)	13.040(3)	12.6201(3)
b (Å)	15.3082(4)	23.565(5)	48.660(10)	23.4471(5)
c (Å)	17.5288(4)	29.107(6)	13.390(3)	14.4084(3)
α (º)	83.714(2)	90	90	90
β (º)	89.854(2)	91.73(3)	113.04(3)	96.396(2)
γ (º)	65.992(3)	90	90	90
V (Å^3)	3048.85(14)	8550(3)	7819(3)	4236.98(16)
Z	1	4	4	2
T (K)	123(2)	100(2)	100(2)	123(2)
ρ_{calcd} (g·cm^3)	1.127	1.195	1.230	1.206
μ (mm^{-1})	0.723	0.225	0.242	0.228
F(000)	1118	3264	3072	1632
reflns collected	43967	102482	542177	42901
unique reflns	11073	16565	15187	8083
R_{int}	0.0797	0.0259	0.0869	0.0424
R1 [I > 2σ(I)]	0.0792	0.0388	0.0451	0.0321
wR2 (all data)	0.2118	0.1113	0.1256	0.0839
largest peak and hole (e·Å^{-3})	0.655, -0.281	1.933, -0.561	0.553, -0.742	0.538, -0.541
CCDC no.	2250280	2250281	2250283	2250278

Table S1 (contd.). Crystal data for compounds **4-8**, *cis*-[Mo(CO)$_4$(DMAP)] **1S** and *cis*-[Mo(CO)$_4$(TMC)] **2S**.

	8·(benzene)$_5$	**1S**	**2S**
empirical formula	$C_{178}H_{254}Mg_4N_{12}O_{12}$	$C_{18}H_{20}MoN_4O_4$	$C_{18}H_{24}MoN_4O_4$
formula weight	2851.16	452.32	456.35
crystal system	triclinic	monoclinic	monoclinic
space group	*P*-1	*C*2/*c*	$P2_1/c$
a (Å)	12.180(2)	29.705(6)	16.1752(2)
b (Å)	17.740(4)	9.751(2)	8.34020(10)
c (Å)	19.440(4)	14.098(3)	16.1713(2)
α (º)	87.54(3)	90	90
β (º)	87.79(3)	105.68(3)	112.5330(10)
γ (º)	87.49(3)	90	90
V (Å^3)	4189.7(14)	3931.5(15)	2015.03(4)
Z	1	8	4
T (K)	100(2)	123(2)	123(2)
ρ_{calcd} (g·cm^3)	1.130	1.528	1.504
μ (mm^{-1})	0.083	0.698	5.586
F(000)	1550	1840	936
reflns collected	101217	19999	20009
unique reflns	15340	3646	3653
R_{int}	0.0360	0.0389	0.0391
R1 [I > 2σ(I)]	0.0437	0.0280	0.0238
wR2 (all data)	0.1182	0.0730	0.0640
largest peak and hole (e·Å^{-3})	0.729, -0.392	0.543, -0.545	0.367, -0.758
CCDC no.	2250282	2250279	2250277

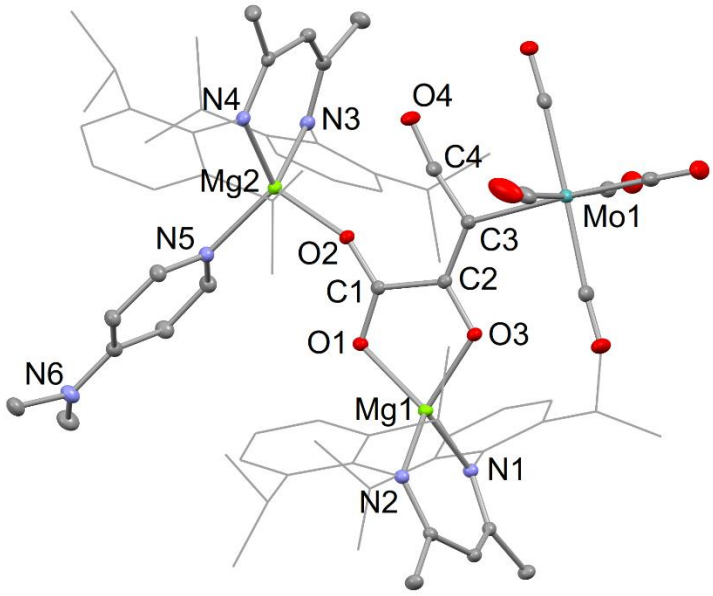


Figure S17. Molecular structure of **5** (25% thermal ellipsoids; hydrogen atoms omitted; Dip substituents shown as wire-frame for sake of clarity). Selected bond lengths (Å) and angles (°):Mo(1)-C(3) 2.3222(19), Mg(1)-O(3) 1.9707(14), Mg(1)-O(1) 1.9957(14), O(1)-C(1) 1.258(2), C(1)-O(2) 1.250(2), C(1)-C(2) 1.546(2), Mg(2)-O(2) 1.9380(13), Mg(2)-N(5) 2.0769(17), C(2)-O(3) 1.268(2), C(2)-C(3) 1.386(2), C(3)-C(4) 1.323(3), O(4)-C(4) 1.158(2), O(3)-C(2)-C(3) 124.43(16), O(3)-C(2)-C(1) 114.24(14), C(3)-C(2)-C(1) 121.33(15), C(4)-C(3)-C(2) 120.44(17), C(4)-C(3)-Mo(1) 109.76(13), C(2)-C(3)-Mo(1) 129.79(13), O(4)-C(4)-C(3) 170.7(2).

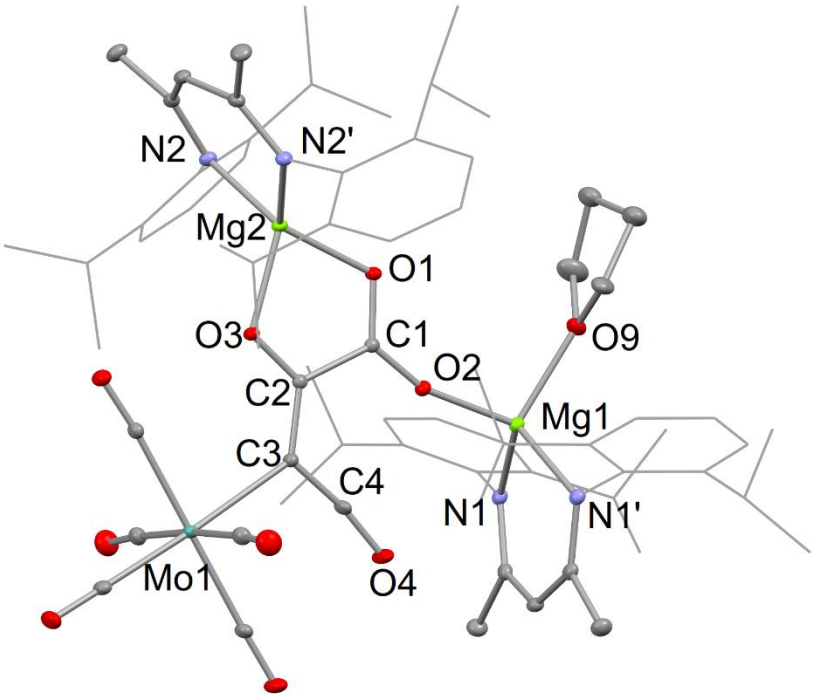


Figure S18. Molecular structure of **7** (25% thermal ellipsoids are shown; hydrogen atoms omitted; Dip substituents shown as wireframe for clarity). Selected bond lengths (Å) and angles (°): Mo(1)-C(3) 2.333(2), O(1)-C(1) 1.255(3), C(1)-O(2) 1.251(3), C(1)-C(2) 1.548(3), C(2)-O(3) 1.265(3), C(2)-C(3) 1.386(3), C(3)-C(4) 1.316(3), O(4)-C(4) 1.159(3), Mo(1)-C(3) 2.333(2), O(1)-C(1) 1.255(3), C(1)-O(2) 1.251(3), C(1)-C(2) 1.548(3), C(2)-O(3) 1.265(3), C(2)-C(3) 1.386(3), C(3)-C(4) 1.316(3), O(4)-C(4) 1.159(3), O(2)-C(1)-O(1) 125.8(2), O(2)-C(1)-C(2) 118.55(19), O(1)-C(1)-C(2) 115.62(18), O(3)-C(2)-C(3) 124.2(2), O(3)-C(2)-C(1) 114.01(19), C(3)-C(2)-C(1) 121.77(19), C(4)-C(3)-C(2) 121.6(2), C(4)-C(3)-Mo(1) 108.43(16), C(2)-C(3)-Mo(1) 129.95(16), O(4)-C(4)-C(3) 171.4(3).

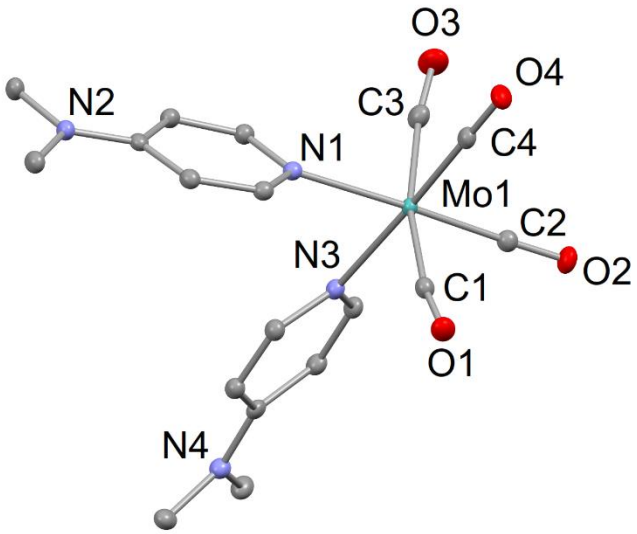


Figure S19. Molecular structure of **1S** (25% thermal ellipsoids are shown; hydrogen atoms omitted). Selected bond lengths (Å) and angles (°): Mo(1)-N(1) 2.230(2), Mo(1)-N(3) 2.298(2), N(1)-Mo(1)-N(3) 82.07(8).

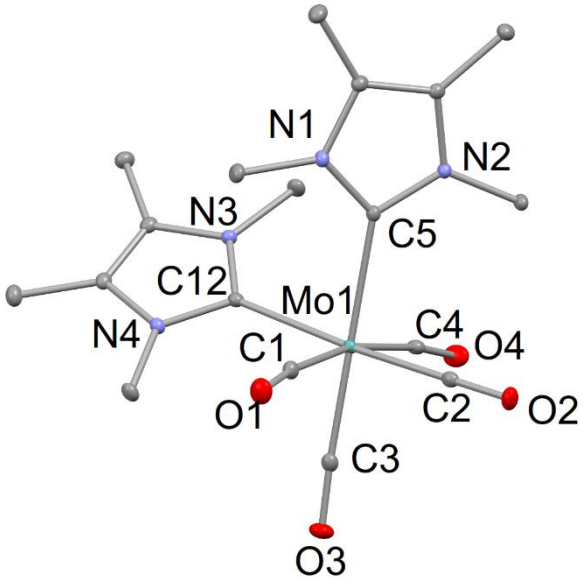


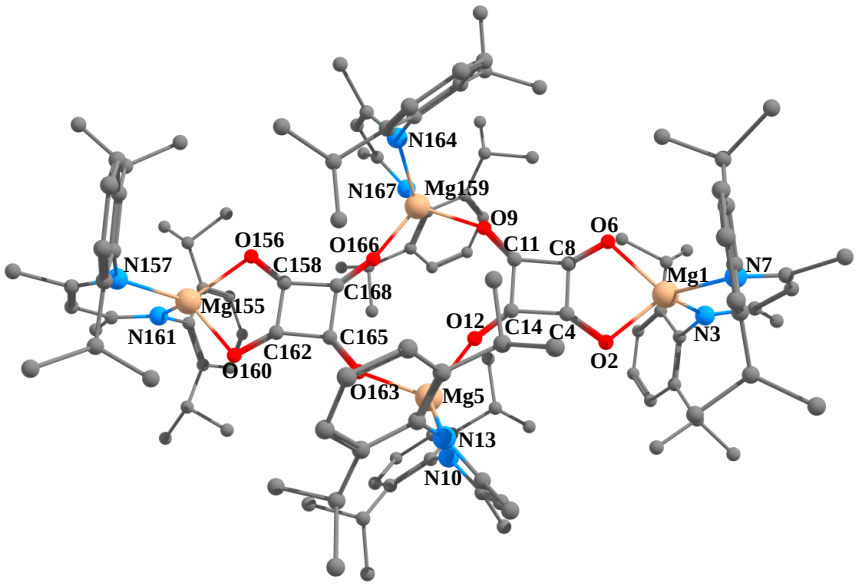
Figure S20. Molecular structure of **2S** (25% thermal ellipsoids are shown; hydrogen atoms omitted). Selected bond lengths (Å) and angles (°): Mo(1)-C(12) 2.2893(18), Mo(1)-C(5) 2.2894(17), C(12)-Mo(1)-C(5) 85.94(6).

3. Computational Studies

The optimizations were carried out by employing DFT hybrid functional (B3PW91)[7] along with small core pseudopotential Stuttgart basis set along with additional polarization functions for the molybdenum atom.[8] Pople basis sets (6-311+G** for Mg atom and 6-31G** for carbon, nitrogen, oxygen and hydrogen atoms) were employed for the rest of the atoms.[9] Frequency calculations were performed to locate minima for the optimized structures. All the calculations were performed using Gaussian 09 suite of programs.[10] NBO analysis were carried out using NBO 6.0 version as implemented in the Gaussian program.[11]

Table S2: Computed natural charges for **4**

Atom label	Natural charges
Mg1	1.74139
N3	-0.80320
N7	-0.80387
Mg5	1.76229
N10	-0.79402
N13	-0.79117
Mg155	1.74139
N157	-0.80320
N161	-0.80387
Mg159	1.76229
N164	-0.79402
N167	-0.79117
O2	-0.77900
C4	0.33373
O6	-0.77613
C8	0.33440
O9	-0.80745
C11	0.38689
O12	-0.80868
C14	0.38579
O156	-0.77900



C158	0.33373	
O160	-0.77613	
C162	0.33440	
O163	-0.80745	
C165	0.38689	
O166	-0.80868	
C168	0.38579	

Table S3: Computed Wiberg bond indices (WBI) for **4**

	WBI		WBI		WBI		WBI		WBI		WBI		WBI		WBI
Mg1	0.00	Mg5	0.00	Mg155	0.00	Mg159	0.00	O2	1.40	O6	1.40	O9	1.39	O12	1.39
N3	0.10	N10	0.09	N157	0.10	N164	0.09	C4	0.00	C4	1.10	C4	0.11	C4	1.08
N7	0.10	N13	0.09	N161	0.10	N167	0.09	C8	1.10	C8	0.00	C8	1.08	C8	0.11
O2	0.10	O12	0.08	O156	0.10	O9	0.09	C11	0.11	C11	1.08	C11	0.00	C11	1.06
O6	0.10	O163	0.09	O160	0.10	O166	0.08	C14	1.08	C14	0.11	C14	1.06	C14	0.00

Table S4. NBO analysis of bonding orbitals in squarate-core of **4**

(1.99608) BD (1) O 2- C 4

(65.46%) 0.8091* O 2 s(40.22%)p 1.48(59.56%)d 0.01(0.22%)

(34.54%) 0.5877* C 4 s(32.57%)p 2.06(67.26%)d 0.01(0.17%)

(1.98184) BD (2) O 2- C 4

(75.88%) 0.8711* O 2 s(0.00%)p 1.00(99.81%)d 0.00(0.19%)

(24.12%) 0.4912* C 4 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)

(1.96410) BD (1) C 4- C 8

(50.04%) 0.7074* C 4 s(31.56%)p 2.17(68.35%)d 0.00(0.09%)

(49.96%) 0.7068* C 8 s(31.57%)p 2.16(68.34%)d 0.00(0.09%)

(1.97027) BD (1) C 4- C 14

(50.77%) 0.7125* C 4 s(35.40%)p 1.82(64.53%)d 0.00(0.07%)

(49.23%) 0.7017* C 14 s(34.03%)p 1.94(65.89%)d 0.00(0.07%)

(1.99608) BD (1) O 6- C 8

(65.37%) 0.8085* O 6 s(40.15%)p 1.48(59.62%)d 0.01(0.23%)

(34.63%) 0.5885* C 8 s(32.47%)p 2.07(67.36%)d 0.01(0.17%)

(1.97981) BD (2) O 6- C 8

(75.80%) 0.8706* O 6 s(0.00%)p 1.00(99.80%)d 0.00(0.20%)

(24.20%)   0.4920* C 8 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)

(1.96887) BD (1) C 8- C 11

(50.82%)   0.7129* C 8 s(35.47%)p 1.82(64.46%)d 0.00(0.07%)

(49.18%)   0.7013* C 11 s(33.72%)p 1.96(66.21%)d 0.00(0.07%)

(1.99666) BD (1) O 9- C 11

(66.33%)   0.8144* O 9 s(44.66%)p 1.24(55.16%)d 0.00(0.17%)

(33.67%)   0.5803* C 11 s(32.79%)p 2.04(67.03%)d 0.01(0.18%)

(1.98642) BD (2) O 9- C 11

(76.38%)   0.8739* O 9 s(0.00%)p 1.00(99.87%)d 0.00(0.13%)

(23.62%)   0.4860* C 11 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)

(1.95959) BD (1) C 11- C 14

(50.10%)   0.7078* C 11 s(32.94%)p 2.03(66.99%)d 0.00(0.08%)

(49.90%)   0.7064* C 14 s(32.66%)p 2.06(67.26%)d 0.00(0.08%)

(1.99659) BD (1) O 12- C 14

(66.43%)   0.8151* O 12 s(45.90%)p 1.18(53.94%)d 0.00(0.17%)

(33.57%)   0.5794* C 14 s(32.76%)p 2.05(67.06%)d 0.01(0.18%)

(1.98522) BD (2) O 12- C 14

(76.26%)   0.8733* O 12 s(0.00%)p 1.00(99.88%)d 0.00(0.12%)

(23.74%)   0.4873* C 14 s(0.00%)p 1.00(99.73%)d 0.00(0.26%)

(1.99608) BD (1) O156- C158

(65.46%)   0.8091* O156 s(40.22%)p 1.48(59.56%)d 0.01(0.22%)

(34.54%)   0.5877* C158 s(32.57%)p 2.06(67.26%)d 0.01(0.17%)

(1.98184) BD (2) O156- C158

(75.88%)   0.8711* O156 s(0.00%)p 1.00(99.81%)d 0.00(0.19%)

(24.12%)   0.4912* C158 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)

(1.96410) BD (1) C158- C162

(50.04%)   0.7074* C158 s(31.56%)p 2.17(68.35%)d 0.00(0.09%)

(49.96%)   0.7068* C162 s(31.57%)p 2.16(68.34%)d 0.00(0.09%)

(1.97027) BD (1) C158- C168

(50.77%)   0.7125* C158 s(35.40%)p 1.82(64.53%)d 0.00(0.07%)

(49.23%)   0.7017* C168 s(34.03%)p 1.94(65.89%)d 0.00(0.07%)

(1.99608) BD (1) O160- C162

(65.37%)   0.8085* O160 s(40.15%)p 1.48(59.62%)d 0.01(0.23%)

(34.63%)   0.5885* C162 s(32.47%)p 2.07(67.36%)d 0.01(0.17%)

(1.97981) BD (2) O160- C162

(75.80%)   0.8706* O160 s(0.00%)p 1.00(99.80%)d 0.00(0.20%)

(24.20%)   0.4920* C162 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)

(1.96887) BD (1) C162- C165

(50.82%) 0.7129* C162 s(35.47%)p 1.82(64.46%)d 0.00(0.07%)

(49.18%) 0.7013* C165 s(33.72%)p 1.96(66.21%)d 0.00(0.07%)

(1.99666) BD (1) O163- C165

(66.33%) 0.8144* O163 s(44.66%)p 1.24(55.16%)d 0.00(0.17%)

(33.67%) 0.5803* C165 s(32.79%)p 2.04(67.03%)d 0.01(0.18%)

(1.98642) BD (2) O163- C165

(76.38%) 0.8739* O163 s(0.00%)p 1.00(99.87%)d 0.00(0.13%)

(23.62%) 0.4860* C165 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)

(1.95959) BD (1) C165- C168

(50.10%) 0.7078* C165 s(32.94%)p 2.03(66.99%)d 0.00(0.08%)

(49.90%) 0.7064* C168 s(32.66%)p 2.06(67.26%)d 0.00(0.08%)

(1.99659) BD (1) O166- C168

(66.43%) 0.8151* O166 s(45.90%)p 1.18(53.94%)d 0.00(0.17%)

(33.57%) 0.5794* C168 s(32.76%)p 2.05(67.06%)d 0.01(0.18%)

(1.98522) BD (2) O166- C168

(76.26%) 0.8733* O166 s(0.00%)p 1.00(99.88%)d 0.00(0.12%)

(23.74%) 0.4873* C168 s(0.00%)p 1.00(99.73%)d 0.00(0.26%)

Table S5: Second order perturbation analysis for **4**

Donor NBO	Acceptor NBO	E(2) kcal/mol
(1.96420) LP (1) O 2 s(54.40%)p 0.84(45.54%)d 0.00(0.06%)	(0.22072) LV (1)Mg 1 s(99.76%)p 0.00(0.14%)d 0.00(0.10%)	8.67
(1.86968) LP (2) O 2 s(5.37%)p17.61(94.50%)d 0.03(0.14%)	(0.22072) LV (1)Mg 1 s(99.76%)p 0.00(0.14%)d 0.00(0.10%)	17.92
(1.96585) LP (1) O 6 s(54.39%)p 0.84(45.55%)d 0.00(0.06%)	(0.22072) LV (1)Mg 1 s(99.76%)p 0.00(0.14%)d 0.00(0.10%)	8.78
(1.86963) LP (2) O 6 s(5.44%)p17.36(94.42%)d 0.03(0.14%)	(0.22072) LV (1)Mg 1 s(99.76%)p 0.00(0.14%)d 0.00(0.10%)	17.94
(1.99608) BD (1) O 2- C 4 (65.46%) 0.8091* O 2 s(40.22%)p 1.48(59.56%)d 0.01(0.22%) (34.54%) 0.5877* C 4 s(32.57%)p 2.06(67.26%)d 0.01(0.17%)	(0.22072) LV (1)Mg 1 s(99.76%)p 0.00(0.14%)d 0.00(0.10%)	2.09
(1.99608) BD (1) O 6- C 8 (65.37%) 0.8085* O 6 s(40.15%)p 1.48(59.62%)d 0.01(0.23%) (34.63%) 0.5885* C 8 s(32.47%)p 2.07(67.36%)d 0.01(0.17%)	(0.22072) LV (1)Mg 1 s(99.76%)p 0.00(0.14%)d 0.00(0.10%)	2.24
(1.96420) LP (1) O 2 s(54.40%)p 0.84(45.54%)d 0.00(0.06%)	(0.08070) BD*(1) C 4- C 8 (49.96%) 0.7068* C 4 s(31.56%)p 2.17(68.35%)d 0.00(0.09%)	4.79

	(50.04%) -0.7074* C 8 s(31.57%)p 2.16(68.34%)d 0.00(0.09%)	
(1.86968) LP (2) O 2 s(5.37%)p17.61(94.50%)d 0.03(0.14%)	(0.08070) BD*(1) C 4- C 8 (49.96%) 0.7068* C 4 s(31.56%)p 2.17(68.35%)d 0.00(0.09%) (50.04%) -0.7074* C 8 s(31.57%)p 2.16(68.34%)d 0.00(0.09%)	10.08
(1.86968) LP (2) O 2 s(5.37%)p17.61(94.50%)d 0.03(0.14%)	(0.09921) BD*(1) C 4- C 14 (49.23%) 0.7017* C 4 s(35.40%)p 1.82(64.53%)d 0.00(0.07%) (50.77%) -0.7125* C 14 s(34.03%)p 1.94(65.89%)d 0.00(0.07%)	20.50
(1.96585) LP (1) O 6 s(54.39%)p 0.84(45.55%)d 0.00(0.06%)	(0.08070) BD*(1) C 4- C 8 (49.96%) 0.7068* C 4 s(31.56%)p 2.17(68.35%)d 0.00(0.09%) (50.04%) -0.7074* C 8 s(31.57%)p 2.16(68.34%)d 0.00(0.09%)	4.93
(1.86963) LP (2) O 6 s(5.44%)p17.36(94.42%)d 0.03(0.14%)	(0.08070) BD*(1) C 4- C 8 (49.96%) 0.7068* C 4 s(31.56%)p 2.17(68.35%)d 0.00(0.09%) (50.04%) -0.7074* C 8 s(31.57%)p 2.16(68.34%)d 0.00(0.09%)	10.04
(1.86963) LP (2) O 6 s(5.44%)p17.36(94.42%)d 0.03(0.14%)	(0.09598) BD*(1) C 8- C 11 (49.18%) 0.7013* C 8 s(35.47%)p 1.82(64.46%)d 0.00(0.07%) (50.82%) -0.7129* C 11 s(33.72%)p 1.96(66.21%)d 0.00(0.07%)	20.39
(1.88723) LP (2) O 9 s(1.70%)p57.85(98.24%)d 0.04(0.06%)	(0.09598) BD*(1) C 8- C 11 (49.18%) 0.7013* C 8 s(35.47%)p 1.82(64.46%)d 0.00(0.07%) (50.82%) -0.7129* C 11 s(33.72%)p 1.96(66.21%)d 0.00(0.07%)	19.56
(1.88723) LP (2) O 9 s(1.70%)p57.85(98.24%)d 0.04(0.06%)	(0.09785) BD*(1) C 11- C 14 (49.90%) 0.7064* C 11 s(32.94%)p 2.03(66.99%)d 0.00(0.08%) (50.10%) -0.7078* C 14 s(32.66%)p 2.06(67.26%)d 0.00(0.08%)	13.60
(1.94396) LP (1) O 12 s(53.85%)p 0.86(46.14%)d 0.00(0.01%)	(0.09921) BD*(1) C 4- C 14 (49.23%) 0.7017* C 4 s(35.40%)p 1.82(64.53%)d 0.00(0.07%) (50.77%) -0.7125* C 14 s(34.03%)p 1.94(65.89%)d 0.00(0.07%)	3.84
(1.89003) LP (2) O 12 s(0.19%)p99.99(99.74%)d 0.37(0.07%)	(0.09921) BD*(1) C 4- C 14 (49.23%) 0.7017* C 4 s(35.40%)p 1.82(64.53%)d 0.00(0.07%) (50.77%) -0.7125* C 14 s(34.03%)p 1.94(65.89%)d 0.00(0.07%)	16.80
(1.89003) LP (2) O 12 s(0.19%)p99.99(99.74%)d 0.37(0.07%)	(0.09785) BD*(1) C 11- C 14 (49.90%) 0.7064* C 11 s(32.94%)p 2.03(66.99%)d 0.00(0.08%) (50.10%) -0.7078* C 14 s(32.66%)p 2.06(67.26%)d 0.00(0.08%)	19.29
(1.98184) BD (2) O 2- C 4	(0.50038) BD*(2) O 6- C 8	7.25

(75.88%) 0.8711* O 2 s(0.00%)p 1.00(99.81%)d 0.00(0.19%) (24.12%) 0.4912* C 4 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	(24.20%) 0.4920* O 6 s(0.00%)p 1.00(99.80%)d 0.00(0.20%) (75.80%) -0.8706* C 8 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	
(1.98184) BD (2) O 2- C 4 (75.88%) 0.8711* O 2 s(0.00%)p 1.00(99.81%)d 0.00(0.19%) (24.12%) 0.4912* C 4 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	(0.49858) BD*(2) O 12- C 14 (23.74%) 0.4873* O 12 s(0.00%)p 1.00(99.88%)d 0.00(0.12%) (76.26%) -0.8733* C 14 s(0.00%)p 1.00(99.73%)d 0.00(0.26%)	5.21
(1.96410) BD (1) C 4- C 8 (50.04%) 0.7074* C 4 s(31.56%)p 2.17(68.35%)d 0.00(0.09%) (49.96%) 0.7068* C 8 s(31.57%)p 2.16(68.34%)d 0.00(0.09%)	(0.02501) BD*(1) O 9- C 11 (33.67%) 0.5803* O 9 s(44.66%)p 1.24(55.16%)d 0.00(0.17%) (66.33%) -0.8144* C 11 s(32.79%)p 2.04(67.03%)d 0.01(0.18%)	8.87
(1.96410) BD (1) C 4- C 8 (50.04%) 0.7074* C 4 s(31.56%)p 2.17(68.35%)d 0.00(0.09%) (49.96%) 0.7068* C 8 s(31.57%)p 2.16(68.34%)d 0.00(0.09%)	(0.02620) BD*(1) O 12- C 14 (33.57%) 0.5794* O 12 s(45.90%)p 1.18(53.94%)d 0.00(0.17%) (66.43%) -0.8151* C 14 s(32.76%)p 2.05(67.06%)d 0.01(0.18%)	9.11
(1.97027) BD (1) C 4- C 14 (50.77%) 0.7125* C 4 s(35.40%)p 1.82(64.53%)d 0.00(0.07%) (49.23%) 0.7017* C 14 s(34.03%)p 1.94(65.89%)d 0.00(0.07%)	(0.02558) BD*(1) O 6- C 8 (34.63%) 0.5885* O 6 s(40.15%)p 1.48(59.62%)d 0.01(0.23%) (65.37%) -0.8085* C 8 s(32.47%)p 2.07(67.36%)d 0.01(0.17%)	6.50
(1.97027) BD (1) C 4- C 14 (50.77%) 0.7125* C 4 s(35.40%)p 1.82(64.53%)d 0.00(0.07%) (49.23%) 0.7017* C 14 s(34.03%)p 1.94(65.89%)d 0.00(0.07%)	(0.02501) BD*(1) O 9- C 11 (33.67%) 0.5803* O 9 s(44.66%)p 1.24(55.16%)d 0.00(0.17%) (66.33%) -0.8144* C 11 s(32.79%)p 2.04(67.03%)d 0.01(0.18%)	6.68
(1.97981) BD (2) O 6- C 8 (75.80%) 0.8706* O 6 s(0.00%)p 1.00(99.80%)d 0.00(0.20%) (24.20%) 0.4920* C 8 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	(0.49681) BD*(2) O 9- C 11 (23.62%) 0.4860* O 9 s(0.00%)p 1.00(99.87%)d 0.00(0.13%) (76.38%) -0.8739* C 11 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	5.31
(1.96887) BD (1) C 8- C 11 (50.82%) 0.7129* C 8 s(35.47%)p 1.82(64.46%)d 0.00(0.07%) (49.18%) 0.7013* C 11 s(33.72%)p 1.96(66.21%)d 0.00(0.07%)	(0.02536) BD*(1) O 2- C 4 (34.54%) 0.5877* O 2 s(40.22%)p 1.48(59.56%)d 0.01(0.22%) (65.46%) -0.8091* C 4 s(32.57%)p 2.06(67.26%)d 0.01(0.17%)	6.45
(1.96887) BD (1) C 8- C 11 (50.82%) 0.7129* C 8 s(35.47%)p 1.82(64.46%)d 0.00(0.07%) (49.18%) 0.7013* C 11 s(33.72%)p 1.96(66.21%)d 0.00(0.07%)	(0.02620) BD*(1) O 12- C 14 (33.57%) 0.5794* O 12 s(45.90%)p 1.18(53.94%)d 0.00(0.17%) (66.43%) -0.8151* C 14 s(32.76%)p 2.05(67.06%)d 0.01(0.18%)	6.68
(1.98642) BD (2) O 9- C 11 (76.38%) 0.8739* O 9 s(0.00%)p 1.00(99.87%)d 0.00(0.13%) (23.62%) 0.4860* C 11 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	(0.50038) BD*(2) O 6- C 8 (24.20%) 0.4920* O 6 s(0.00%)p 1.00(99.80%)d 0.00(0.20%) (75.80%) -0.8706* C 8 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	5.64
(1.98642) BD (2) O 9- C 11 (76.38%) 0.8739* O 9 s(0.00%)p 1.00(99.87%)d 0.00(0.13%) (23.62%) 0.4860* C 11 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	(0.49858) BD*(2) O 12- C 14 (23.74%) 0.4873* O 12 s(0.00%)p 1.00(99.88%)d 0.00(0.12%) (76.26%) -0.8733* C 14 s(0.00%)p 1.00(99.73%)d 0.00(0.26%)	5.15

(1.95959) BD (1) C 11- C 14 (50.10%) 0.7078* C 11 s(32.94%)p 2.03(66.99%)d 0.00(0.08%) (49.90%) 0.7064* C 14 s(32.66%)p 2.06(67.26%)d 0.00(0.08%)	(0.02536) BD*(1) O 2- C 4 (34.54%) 0.5877* O 2 s(40.22%)p 1.48(59.56%)d 0.01(0.22%) (65.46%) -0.8091* C 4 s(32.57%)p 2.06(67.26%)d 0.01(0.17%)	9.99
(1.95959) BD (1) C 11- C 14 (50.10%) 0.7078* C 11 s(32.94%)p 2.03(66.99%)d 0.00(0.08%) (49.90%) 0.7064* C 14 s(32.66%)p 2.06(67.26%)d 0.00(0.08%)	(0.02558) BD*(1) O 6- C 8 (34.63%) 0.5885* O 6 s(40.15%)p 1.48(59.62%)d 0.01(0.23%) (65.37%) -0.8085* C 8 s(32.47%)p 2.07(67.36%)d 0.01(0.17%)	10.15
(1.98522) BD (2) O 12- C 14 (76.26%) 0.8733* O 12 s(0.00%)p 1.00(99.88%)d 0.00(0.12%) (23.74%) 0.4873* C 14 s(0.00%)p 1.00(99.73%)d 0.00(0.26%)	(0.49681) BD*(2) O 9- C 11 (23.62%) 0.4860* O 9 s(0.00%)p 1.00(99.87%)d 0.00(0.13%) (76.38%) -0.8739* C 11 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	5.17
(1.94396) LP (1) O 12 s(53.85%)p 0.86(46.14%)d 0.00(0.01%)	(0.20045) LV (1)Mg 5 s(99.94%)p 0.00(0.04%)d 0.00(0.02%)	25.24
(1.99659) BD (1) O 12- C 14 (66.43%) 0.8151* O 12 s(45.90%)p 1.18(53.94%)d 0.00(0.17%) (33.57%) 0.5794* C 14 s(32.76%)p 2.05(67.06%)d 0.01(0.18%)	(0.20045) LV (1)Mg 5 s(99.94%)p 0.00(0.04%)d 0.00(0.02%)	3.02
(1.94652) LP (1) O 9 s(53.58%)p 0.87(46.39%)d 0.00(0.03%)	(0.20045) LV (1)Mg159 s(99.94%)p 0.00(0.04%)d 0.00(0.02%)	22.21
(1.88723) LP (2) O 9 s(1.70%)p57.85(98.24%)d 0.04(0.06%)	(0.20045) LV (1)Mg159 s(99.94%)p 0.00(0.04%)d 0.00(0.02%)	7.84
(1.99666) BD (1) O 9- C 11 (66.33%) 0.8144* O 9 s(44.66%)p 1.24(55.16%)d 0.00(0.17%) (33.67%) 0.5803* C 11 s(32.79%)p 2.04(67.03%)d 0.01(0.18%)	(0.20045) LV (1)Mg159 s(99.94%)p 0.00(0.04%)d 0.00(0.02%)	2.57
(1.88723) LP (2) O 9 s(1.70%)p57.85(98.24%)d 0.04(0.06%)	(0.22072) LV (1)Mg 1 s(99.76%)p 0.00(0.14%)d 0.00(0.10%)	25.40
(1.86845) LP (1) N 7 s(27.08%)p 2.69(72.92%)d 0.00(0.01%)	(0.22072) LV (1)Mg 1 s(99.76%)p 0.00(0.14%)d 0.00(0.10%)	25.39
(1.86556) LP (1) N 10 s(26.68%)p 2.75(73.31%)d 0.00(0.01%)	(0.20045) LV (1)Mg 5 s(99.94%)p 0.00(0.04%)d 0.00(0.02%)	25.13
(1.86553) LP (1) N 13 s(26.60%)p 2.76(73.40%)d 0.00(0.01%)	(0.20045) LV (1)Mg 5 s(99.94%)p 0.00(0.04%)d 0.00(0.02%)	25.05
(1.94652) LP (1) O163 s(53.58%)p 0.87(46.39%)d 0.00(0.03%)	(0.20045) LV (1)Mg 5 s(99.94%)p 0.00(0.04%)d 0.00(0.02%)	22.21
(1.88723) LP (2) O163 s(1.70%)p57.85(98.24%)d 0.04(0.06%)	(0.20045) LV (1)Mg 5 s(99.94%)p 0.00(0.04%)d 0.00(0.02%)	7.84
(1.99666) BD (1) O163- C165 (66.33%) 0.8144* O163 s(44.66%)p 1.24(55.16%)d 0.00(0.17%) (33.67%) 0.5803* C165 s(32.79%)p 2.04(67.03%)d 0.01(0.18%)	(0.20045) LV (1)Mg 5 s(99.94%)p 0.00(0.04%)d 0.00(0.02%)	2.57
(1.96420) LP (1) O156 s(54.40%)p 0.84(45.54%)d 0.00(0.06%)	(0.22072) LV (1)Mg155 s(99.76%)p 0.00(0.14%)d 0.00(0.10%)	8.67
(1.86968) LP (2) O156 s(5.37%)p17.61(94.50%)d 0.03(0.14%)	(0.22072) LV (1)Mg155 s(99.76%)p 0.00(0.14%)d 0.00(0.10%)	17.92
(1.96585) LP (1) O160 s(54.39%)p 0.84(45.55%)d 0.00(0.06%)	(0.22072) LV (1)Mg155 s(99.76%)p 0.00(0.14%)d 0.00(0.10%)	8.78

(1.86963) LP (2) O160 s(5.44%)p17.36(94.42%)d 0.03(0.14%)	(0.22072) LV (1)Mg155 s(99.76%)p 0.00(0.14%)d 0.00(0.10%)	17.94
(1.98184) BD (2) O156- C158 (75.88%) 0.8711* O156 s(0.00%)p 1.00(99.81%)d 0.00(0.19%) (24.12%) 0.4912* C158 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	(0.22072) LV (1)Mg155 s(99.76%)p 0.00(0.14%)d 0.00(0.10%)	2.09
(1.99608) BD (1) O160- C162 (65.37%) 0.8085* O160 s(40.15%)p 1.48(59.62%)d 0.01(0.23%) (34.63%) 0.5885* C162 s(32.47%)p 2.07(67.36%)d 0.01(0.17%)	(0.22072) LV (1)Mg155 s(99.76%)p 0.00(0.14%)d 0.00(0.10%)	2.24
(1.96420) LP (1) O156 s(54.40%)p 0.84(45.54%)d 0.00(0.06%)	(0.08070) BD*(1) C158- C162 (49.96%) 0.7068* C158 s(31.56%)p 2.17(68.35%)d 0.00(0.09%) (50.04%) -0.7074* C162 s(31.57%)p 2.16(68.34%)d 0.00(0.09%)	4.79
(1.86968) LP (2) O156 s(5.37%)p17.61(94.50%)d 0.03(0.14%)	(0.08070) BD*(1) C158- C162 (49.96%) 0.7068* C158 s(31.56%)p 2.17(68.35%)d 0.00(0.09%) (50.04%) -0.7074* C162 s(31.57%)p 2.16(68.34%)d 0.00(0.09%)	10.08
(1.86968) LP (2) O156 s(5.37%)p17.61(94.50%)d 0.03(0.14%)	(0.09921) BD*(1) C158- C168 (49.23%) 0.7017* C158 s(35.40%)p 1.82(64.53%)d 0.00(0.07%) (50.77%) -0.7125* C168 s(34.03%)p 1.94(65.89%)d 0.00(0.07%)	20.50
(1.96585) LP (1) O160 s(54.39%)p 0.84(45.55%)d 0.00(0.06%)	(0.08070) BD*(1) C158- C162 (49.96%) 0.7068* C158 s(31.56%)p 2.17(68.35%)d 0.00(0.09%) (50.04%) -0.7074* C162 s(31.57%)p 2.16(68.34%)d 0.00(0.09%)	4.93
(1.86963) LP (2) O160 s(5.44%)p17.36(94.42%)d 0.03(0.14%)	(0.08070) BD*(1) C158- C162 (49.96%) 0.7068* C158 s(31.56%)p 2.17(68.35%)d 0.00(0.09%) (50.04%) -0.7074* C162 s(31.57%)p 2.16(68.34%)d 0.00(0.09%)	10.04
(1.86963) LP (2) O160 s(5.44%)p17.36(94.42%)d 0.03(0.14%)	(0.09598) BD*(1) C162- C165 (49.18%) 0.7013* C162 s(35.47%)p 1.82(64.46%)d 0.00(0.07%) (50.82%) -0.7129* C165 s(33.72%)p 1.96(66.21%)d 0.00(0.07%)	20.39
(1.94652) LP (1) O163 s(53.58%)p 0.87(46.39%)d 0.00(0.03%	(0.09785) BD*(1) C165- C168 (49.90%) 0.7064* C165 s(32.94%)p 2.03(66.99%)d 0.00(0.08%) (50.10%) -0.7078* C168 s(32.66%)p 2.06(67.26%)d 0.00(0.08%)	5.31
(1.88723) LP (2) O163 s(1.70%)p57.85(98.24%)d 0.04(0.06%)	(0.09598) BD*(1) C162- C165 (49.18%) 0.7013* C162 s(35.47%)p 1.82(64.46%)d 0.00(0.07%) (50.82%) -0.7129* C165 s(33.72%)p 1.96(66.21%)d 0.00(0.07%)	19.56
(1.88723) LP (2) O163 s(1.70%)p57.85(98.24%)d 0.04(0.06%)	(0.09785) BD*(1) C165- C168	13.60

	(49.90%) 0.7064* C165 s(32.94%)p 2.03(66.99%)d 0.00(0.08%) (50.10%) -0.7078* C168 s(32.66%)p 2.06(67.26%)d 0.00(0.08%)	
(1.89003) LP (2) O166 s(0.19%)p99.99(99.74%)d 0.37(0.07%)	(0.09921) BD*(1) C158- C168 (49.23%) 0.7017* C158 s(35.40%)p 1.82(64.53%)d 0.00(0.07%) (50.77%) -0.7125* C168 s(34.03%)p 1.94(65.89%)d 0.00(0.07%)	16.80
(1.89003) LP (2) O166 s(0.19%)p99.99(99.74%)d 0.37(0.07%)	(0.09785) BD*(1) C165- C168 (49.90%) 0.7064* C165 s(32.94%)p 2.03(66.99%)d 0.00(0.08%) (50.10%) -0.7078* C168 s(32.66%)p 2.06(67.26%)d 0.00(0.08%)	19.29
(1.98184) BD (2) O156- C158 (75.88%) 0.8711* O156 s(0.00%)p 1.00(99.81%)d 0.00(0.19%) (24.12%) 0.4912* C158 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	(0.50038) BD*(2) O160- C162 (24.20%) 0.4920* O160 s(0.00%)p 1.00(99.80%)d 0.00(0.20%) (75.80%) -0.8706* C162 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	7.25
(1.98184) BD (2) O156- C158 (75.88%) 0.8711* O156 s(0.00%)p 1.00(99.81%)d 0.00(0.19%) (24.12%) 0.4912* C158 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	(0.49858) BD*(2) O166- C168 (23.74%) 0.4873* O166 s(0.00%)p 1.00(99.88%)d 0.00(0.12%) (76.26%) -0.8733* C168 s(0.00%)p 1.00(99.73%)d 0.00(0.26%)	5.21
(1.96410) BD (1) C158- C162 (50.04%) 0.7074* C158 s(31.56%)p 2.17(68.35%)d 0.00(0.09%) (49.96%) 0.7068* C162 s(31.57%)p 2.16(68.34%)d 0.00(0.09%)	(0.02501) BD*(1) O163- C165 (33.67%) 0.5803* O163 s(44.66%)p 1.24(55.16%)d 0.00(0.17%) (66.33%) -0.8144* C165 s(32.79%)p 2.04(67.03%)d 0.01(0.18%)	8.87
(1.96410) BD (1) C158- C162 (50.04%) 0.7074* C158 s(31.56%)p 2.17(68.35%)d 0.00(0.09%) (49.96%) 0.7068* C162 s(31.57%)p 2.16(68.34%)d 0.00(0.09%)	(0.02620) BD*(1) O166- C168 (33.57%) 0.5794* O166 s(45.90%)p 1.18(53.94%)d 0.00(0.17%) (66.43%) -0.8151* C168 s(32.76%)p 2.05(67.06%)d 0.01(0.18%)	9.11
(1.97027) BD (1) C158- C168 (50.77%) 0.7125* C158 s(35.40%)p 1.82(64.53%)d 0.00(0.07%) (49.23%) 0.7017* C168 s(34.03%)p 1.94(65.89%)d 0.00(0.07%)	(0.02558) BD*(1) O160- C162 (34.63%) 0.5885* O160 s(40.15%)p 1.48(59.62%)d 0.01(0.23%) (65.37%) -0.8085* C162 s(32.47%)p 2.07(67.36%)d 0.01(0.17%)	6.50
(1.97027) BD (1) C158- C168 (50.77%) 0.7125* C158 s(35.40%)p 1.82(64.53%)d 0.00(0.07%) (49.23%) 0.7017* C168 s(34.03%)p 1.94(65.89%)d 0.00(0.07%)	(0.02501) BD*(1) O163- C165 (33.67%) 0.5803* O163 s(44.66%)p 1.24(55.16%)d 0.00(0.17%) (66.33%) -0.8144* C165 s(32.79%)p 2.04(67.03%)d 0.01(0.18%)	6.68
(1.97981) BD (2) O160- C162 (75.80%) 0.8706* O160 s(0.00%)p 1.00(99.80%)d 0.00(0.20%) (24.20%) 0.4920* C162 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	(0.49681) BD*(2) O163- C165 (23.62%) 0.4860* O163 s(0.00%)p 1.00(99.87%)d 0.00(0.13%) (76.38%) -0.8739* C165 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	5.31
(1.97981) BD (2) O160- C162 (75.80%) 0.8706* O160 s(0.00%)p 1.00(99.80%)d 0.00(0.20%) (24.20%) 0.4920* C162 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	(0.02536) BD*(1) O156- C158 (34.54%) 0.5877* O156 s(40.22%)p 1.48(59.56%)d 0.01(0.22%) (65.46%) -0.8091* C158 s(32.57%)p 2.06(67.26%)d 0.01(0.17%)	6.45

(1.96887) BD (1) C162- C165 (50.82%) 0.7129* C162 s(35.47%)p 1.82(64.46%)d 0.00(0.07%) (49.18%) 0.7013* C165 s(33.72%)p 1.96(66.21%)d 0.00(0.07%)	(0.02620) BD*(1) O166- C168 (33.57%) 0.5794* O166 s(45.90%)p 1.18(53.94%)d 0.00(0.17%) (66.43%) -0.8151* C168 s(32.76%)p 2.05(67.06%)d 0.01(0.18%)	6.68
(1.98642) BD (2) O163- C165 (76.38%) 0.8739* O163 s(0.00%)p 1.00(99.87%)d 0.00(0.13%) (23.62%) 0.4860* C165 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	(0.50038) BD*(2) O160- C162 (24.20%) 0.4920* O160 s(0.00%)p 1.00(99.80%)d 0.00(0.20%) (75.80%) -0.8706* C162 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	5.64
(1.98642) BD (2) O163- C165 (76.38%) 0.8739* O163 s(0.00%)p 1.00(99.87%)d 0.00(0.13%) (23.62%) 0.4860* C165 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	(0.49858) BD*(2) O166- C168 (23.74%) 0.4873* O166 s(0.00%)p 1.00(99.88%)d 0.00(0.12%) (76.26%) -0.8733* C168 s(0.00%)p 1.00(99.73%)d 0.00(0.26%)	5.15
(1.95959) BD (1) C165- C168 (50.10%) 0.7078* C165 s(32.94%)p 2.03(66.99%)d 0.00(0.08%) (49.90%) 0.7064* C168 s(32.66%)p 2.06(67.26%)d 0.00(0.08%)	(0.02536) BD*(1) O156- C158 (34.54%) 0.5877* O156 s(40.22%)p 1.48(59.56%)d 0.01(0.22%) (65.46%) -0.8091* C158 s(32.57%)p 2.06(67.26%)d 0.01(0.17%)	9.99
(1.95959) BD (1) C165- C168 (50.10%) 0.7078* C165 s(32.94%)p 2.03(66.99%)d 0.00(0.08%) (49.90%) 0.7064* C168 s(32.66%)p 2.06(67.26%)d 0.00(0.08%)	(0.02558) BD*(1) O160- C162 (34.63%) 0.5885* O160 s(40.15%)p 1.48(59.62%)d 0.01(0.23%) (65.37%) -0.8085* C162 s(32.47%)p 2.07(67.36%)d 0.01(0.17%)	10.15
(1.98522) BD (2) O166- C168 (76.26%) 0.8733* O166 s(0.00%)p 1.00(99.88%)d 0.00(0.12%) (23.74%) 0.4873* C168 s(0.00%)p 1.00(99.73%)d 0.00(0.26%)	(0.49681) BD*(2) O163- C165 (23.62%) 0.4860* O163 s(0.00%)p 1.00(99.87%)d 0.00(0.13%) (76.38%) -0.8739* C165 s(0.00%)p 1.00(99.73%)d 0.00(0.27%)	5.17
(1.94396) LP (1) O166 s(53.85%)p 0.86(46.14%)d 0.00(0.01%)	(0.20045) LV (1)Mg159 s(99.94%)p 0.00(0.04%)d 0.00(0.02%)	25.24
(1.99659) BD (1) O166- C168 (66.43%) 0.8151* O166 s(45.90%)p 1.18(53.94%)d 0.00(0.17%) (33.57%) 0.5794* C168 s(32.76%)p 2.05(67.06%)d 0.01(0.18%)	(0.20045) LV (1)Mg159 s(99.94%)p 0.00(0.04%)d 0.00(0.02%)	3.02
(1.86856) LP (1) N157 s(27.09%)p 2.69(72.91%)d 0.00(0.01%)	(0.22072) LV (1)Mg155 s(99.76%)p 0.00(0.14%)d 0.00(0.10%)	25.40
(1.86845) LP (1) N161 s(27.08%)p 2.69(72.92%)d 0.00(0.01%)	(0.22072) LV (1)Mg155 s(99.76%)p 0.00(0.14%)d 0.00(0.10%)	25.39
(1.86556) LP (1) N164 s(26.68%)p 2.75(73.31%)d 0.00(0.01%)	(0.20045) LV (1)Mg159 s(99.94%)p 0.00(0.04%)d 0.00(0.02%)	25.13
(1.86553) LP (1) N167 s(26.60%)p 2.76(73.40%)d 0.00(0.01%)	(0.20045) LV (1)Mg159 s(99.94%)p 0.00(0.04%)d 0.00(0.02%)	25.05

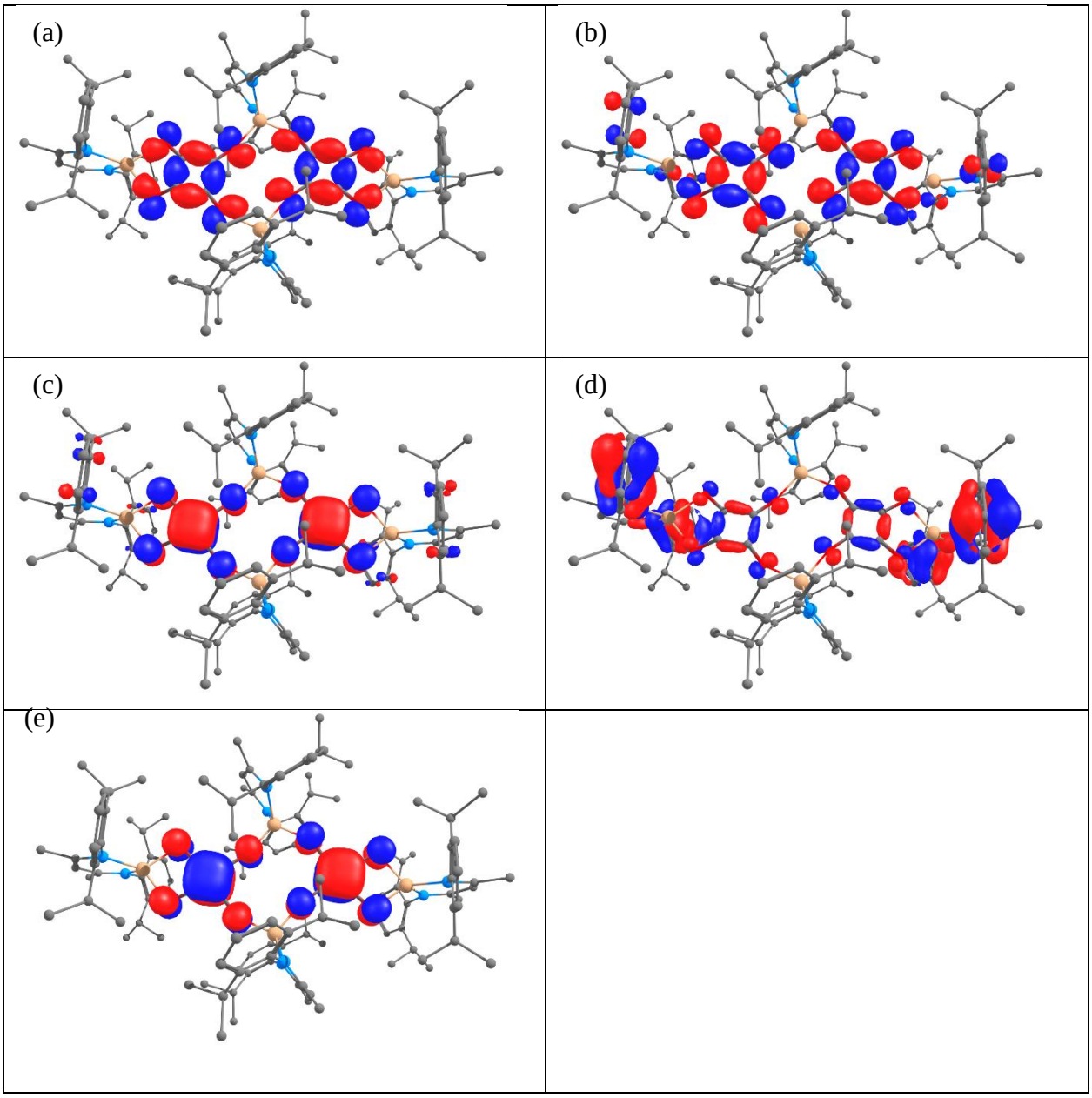


Figure S21. DFT computed MOs for **4**. (a) HOMO-23 (b) HOMO-22 (c) HOMO-17 (d) HOMO-15 (e) HOMO-14.

Table S6: Computed natural charges for **6**.

Atom label	Natural charges
Mo1	-1.00558
C12	-0.53637
C18	0.61276
C21	0.61946
C23	0.60972
C25	0.59282
C27	0.61741
Mg2	1.70102
O3	-0.84087
C5	0.81015
Mg6	1.77560
O7	-0.83004
C9	0.38088
O10	-0.79937
N11	-0.81100
C12	-0.53637
O13	-0.44318
N14	-0.78618
N17	-0.81015
N20	-0.79767
C28	-0.06609
O16	-0.46211
O19	-0.46277
O22	-0.46439
O24	-0.45552
O26	-0.47689

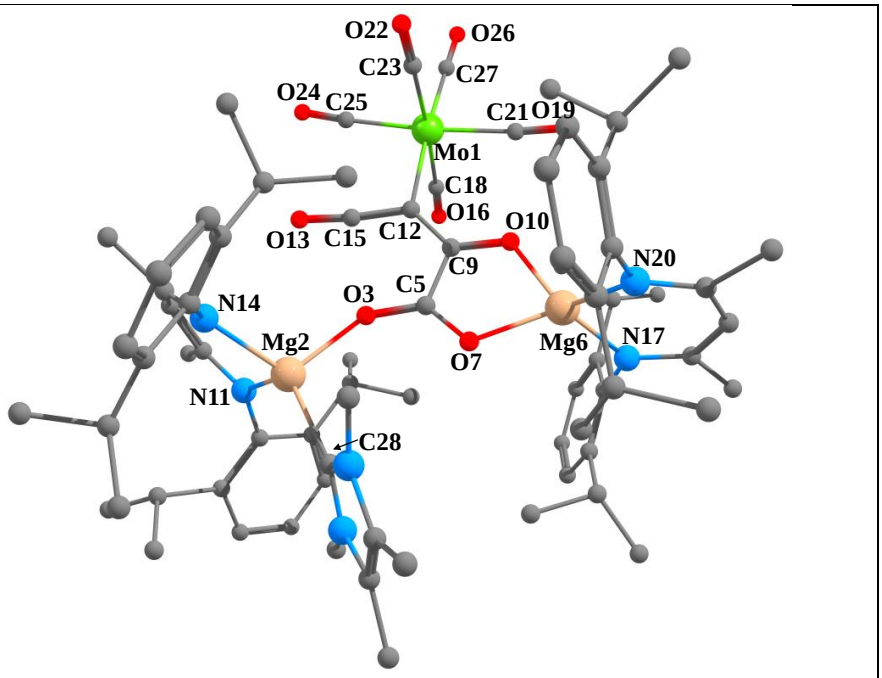


Table S7: Computed Wiberg bond index (WBI) for **6**.

	WBI		WBI		WBI		WBI		WBI		WBI		WBI
Mo1	0.00	Mg2	0.00	Mg6	0.00	O3	1.37	C5	0.92	Mo1	0.29	C12	1.62
C12	0.29	O3	0.08	O7	0.08	C5	0.00	C9	0.00	C9	1.37	O13	1.94
C18	0.80	N11	0.09	O10	0.08	O7	1.40	O10	1.37	C12	0.00	C15	0.00
C21	0.78	N14	0.08	N17	0.09	C9	0.92	C12	1.37	C15	1.62		
C23	0.81	C28	0.18	N20	0.08								
C25	0.83												
C27	1.04												

Table S8. NBO analysis of bonding orbitals in ketene-core of **6**.

(1.69432) BD (1)Mo 1- C 12
(45.51%) 0.6746*Mo 1 s(3.95%)p 0.06(0.23%)d24.27(95.82%)
(54.49%) 0.7382* C 12 s(27.35%)p 2.66(72.62%)d 0.00(0.04%)
(1.94396) BD (1)Mo 1- C 21
(27.85%) 0.5277*Mo 1 s(34.71%)p 0.00(0.08%)d 1.88(65.21%)
(72.15%) 0.8494* C 21 s(68.27%)p 0.46(31.73%)d 0.00(0.00%)
(1.95025) BD (1)Mo 1- C 23
(28.80%) 0.5366*Mo 1 s(32.98%)p 0.00(0.11%)d 2.03(66.91%)

(71.20%) 0.8438* C 23 s(68.26%)p 0.46(31.74%)d 0.00(0.00%)
(1.90237) BD (1)Mo 1- C 27
(33.10%) 0.5753*Mo 1 s(25.37%)p 0.01(0.31%)d 2.93(74.32%)
(66.90%) 0.8179* C 27 s(67.27%)p 0.49(32.73%)d 0.00(0.00%)
(1.99504) BD (1) O 3- C 5
(67.53%) 0.8217* O 3 s(43.30%)p 1.31(56.52%)d 0.00(0.19%)
(32.47%) 0.5699* C 5 s(32.09%)p 2.11(67.70%)d 0.01(0.21%)
(1.99500) BD (1) C 5- O 7
(32.84%) 0.5731* C 5 s(31.46%)p 2.17(68.34%)d 0.01(0.20%)
(67.16%) 0.8195* O 7 s(40.51%)p 1.46(59.26%)d 0.01(0.23%)
(1.98298) BD (2) C 5- O 7
(22.52%) 0.4745* C 5 s(0.00%)p 1.00(99.66%)d 0.00(0.34%)
(77.48%) 0.8803* O 7 s(0.00%)p 1.00(99.81%)d 0.00(0.19%)
(1.97569) BD (1) C 5- C 9
(49.06%) 0.7005* C 5 s(36.33%)p 1.75(63.59%)d 0.00(0.08%)
(50.94%) 0.7137* C 9 s(31.15%)p 2.21(68.77%)d 0.00(0.08%)
(1.99377) BD (1) C 9- O 10
(33.85%) 0.5818* C 9 s(28.51%)p 2.50(71.30%)d 0.01(0.18%)
(66.15%) 0.8133* O 10 s(41.24%)p 1.42(58.56%)d 0.01(0.21%)
(1.97177) BD (2) C 9- O 10
(24.22%) 0.4922* C 9 s(0.00%)p 1.00(99.71%)d 0.00(0.29%)
(75.78%) 0.8705* O 10 s(0.00%)p 1.00(99.83%)d 0.00(0.17%)
(1.96443) BD (1) C 9- C 12
(49.57%) 0.7040* C 9 s(40.09%)p 1.49(59.85%)d 0.00(0.06%)
(50.43%) 0.7102* C 12 s(40.12%)p 1.49(59.80%)d 0.00(0.07%)
(1.98073) BD (1) C 12- C 15
(49.63%) 0.7045* C 12 s(32.52%)p 2.07(67.39%)d 0.00(0.10%)
(50.37%) 0.7097* C 15 s(59.52%)p 0.68(40.45%)d 0.00(0.03%)
(1.99624) BD (1) O 13- C 15
(66.29%) 0.8142* O 13 s(43.67%)p 1.28(56.00%)d 0.01(0.34%)
(33.71%) 0.5806* C 15 s(40.02%)p 1.49(59.82%)d 0.00(0.17%)
(1.99233) BD (2) O 13- C 15
(74.64%) 0.8640* O 13 s(0.51%)p99.99(99.16%)d 0.63(0.32%)
(25.36%) 0.5036* C 15 s(0.36%)p99.99(99.29%)d 0.98(0.35%)
(1.98702) BD (3) O 13- C 15
(73.79%) 0.8590* O 13 s(0.00%)p 1.00(99.67%)d 0.00(0.33%)
(26.21%) 0.5119* C 15 s(0.00%)p 1.00(99.67%)d 0.00(0.33%)

Table S9: Second order perturbation analysis for **6**

Donor NBO	Acceptor NBO	E(2) kcal/mol
(1.88339) LP (2) O 3 s(0.02%)p99.99(99.91%)d 3.19(0.07%)	(0.04945) BD*(1) C 5- O 7 (67.16%) 0.8195* C 5 s(31.46%)p 2.17(68.34%)d 0.01(0.20%) (32.84%) -0.5731* O 7 s(40.51%)p 1.46(59.26%)d 0.01(0.23%)	18.68
(1.88339) LP (2) O 3 s(0.02%)p99.99(99.91%)d 3.19(0.07%)	(0.12062) BD*(1) C 5- C 9 (50.94%) 0.7137* C 5 s(36.33%)p 1.75(63.59%)d 0.00(0.08%) (49.06%) -0.7005* C 9 s(31.15%)p 2.21(68.77%)d 0.00(0.08%)	16.22
(1.64498) LP (3) O 3 s(0.00%)p 1.00(99.87%)d 0.00(0.12%)	(0.38632) BD*(2) C 5- O 7	99.98

	(77.48%) 0.8803* C 5 s(0.00%)p 1.00(99.66%)d 0.00(0.34%) (22.52%) -0.4745* O 7 s(0.00%)p 1.00(99.81%)d 0.00(0.19%)	
(1.89296) LP (2) O 7 s(2.31%)p42.31(97.58%)d 0.05(0.11%)	(0.05117) BD*(1) O 3- C 5 (32.47%) 0.5699* O 3 s(43.30%)p 1.31(56.52%)d 0.00(0.19%) (67.53%) -0.8217* C 5 s(32.09%)p 2.11(67.70%)d 0.01(0.21%)	21.02
(1.89296) LP (2) O 7 s(2.31%)p42.31(97.58%)d 0.05(0.11%)	(0.12062) BD*(1) C 5- C 9 (50.94%) 0.7137* C 5 s(36.33%)p 1.75(63.59%)d 0.00(0.08%) (49.06%) -0.7005* C 9 s(31.15%)p 2.21(68.77%)d 0.00(0.08%)	11.07
(1.95608) LP (1) O 10 s(55.41%)p 0.80(44.54%)d 0.00(0.06%)	(0.12062) BD*(1) C 5- C 9 (50.94%) 0.7137* C 5 s(36.33%)p 1.75(63.59%)d 0.00(0.08%) (49.06%) -0.7005* C 9 s(31.15%)p 2.21(68.77%)d 0.00(0.08%)	3.55
(1.90129) LP (2) O 10 s(3.33%)p28.99(96.57%)d 0.03(0.10%)	(0.12062) BD*(1) C 5- C 9 (50.94%) 0.7137* C 5 s(36.33%)p 1.75(63.59%)d 0.00(0.08%) (49.06%) -0.7005* C 9 s(31.15%)p 2.21(68.77%)d 0.00(0.08%)	11.74
(1.90129) LP (2) O 10 s(3.33%)p28.99(96.57%)d 0.03(0.10%)	(0.04038) BD*(1) C 9- C 12 (50.43%) 0.7102* C 9 s(40.09%)p 1.49(59.85%)d 0.00(0.06%) (49.57%) -0.7040* C 12 s(40.12%)p 1.49(59.80%)d 0.00(0.07%)	13.53
(1.13107) LP (1) C 12 s(0.00%)p 1.00(99.88%)d 0.00(0.12%)	(0.47772) BD*(2) C 9- O 10 (75.78%) 0.8705* C 9 s(0.00%)p 1.00(99.71%)d 0.00(0.29%) (24.22%) -0.4922* O 10 s(0.00%)p 1.00(99.83%)d 0.00(0.17%)	288.87
(1.13107) LP (1) C 12 s(0.00%)p 1.00(99.88%)d 0.00(0.12%)	(0.39419) BD*(3) O 13- C 15 (26.21%) 0.5119* O 13 s(0.00%)p 1.00(99.67%)d 0.00(0.33%) (73.79%) -0.8590* C 15 s(0.00%)p 1.00(99.67%)d 0.00(0.33%)	247.68
(1.97452) LP (1) O 13 s(55.81%)p 0.79(44.12%)d 0.00(0.07%)	(0.01941) BD*(1) C 12- C 15 (50.37%) 0.7097* C 12 s(32.52%)p 2.07(67.39%)d 0.00(0.10%) (49.63%) -0.7045* C 15 s(59.52%)p 0.68(40.45%)d 0.00(0.03%)	10.39
(1.69432) BD (1)Mo 1- C 12 (45.51%) 0.6746*Mo 1 s(3.95%)p 0.06(0.23%)d24.27(95.82%) (54.49%) 0.7382* C 12 s(27.35%)p 2.66(72.62%)d 0.00(0.04%)	(0.30690) BD*(2) O 13- C 15 (25.36%) 0.5036* O 13 s(0.51%)p99.99(99.16%)d 0.63(0.32%) (74.64%) -0.8640* C 15 s(0.36%)p99.99(99.29%)d 0.98(0.35%)	24.48
(1.98298) BD (2) C 5- O 7 (22.52%) 0.4745* C 5 s(0.00%)p 1.00(99.66%)d 0.00(0.34%) (77.48%) 0.8803* O 7 s(0.00%)p 1.00(99.81%)d 0.00(0.19%)	(0.47772) BD*(2) C 9- O 10 (75.78%) 0.8705* C 9 s(0.00%)p 1.00(99.71%)d 0.00(0.29%) (24.22%) -0.4922* O 10 s(0.00%)p 1.00(99.83%)d 0.00(0.17%)	4.72

(1.97177) BD (2) C 9- O 10 (24.22%) 0.4922* C 9 s(0.00%)p 1.00(99.71%)d 0.00(0.29%) (75.78%) 0.8705* O 10 s(0.00%)p 1.00(99.83%)d 0.00(0.17%)	(0.38632) BD*(2) C 5- O 7 (77.48%) 0.8803* C 5 s(0.00%)p 1.00(99.66%)d 0.00(0.34%) (22.52%) -0.4745* O 7 s(0.00%)p 1.00(99.81%)d 0.00(0.19%)	5.54
(1.96443) BD (1) C 9- C 12 (49.57%) 0.7040* C 9 s(40.09%)p 1.49(59.85%)d 0.00(0.06%) (50.43%) 0.7102* C 12 s(40.12%)p 1.49(59.80%)d 0.00(0.07%)	(0.01941) BD*(1) C 12- C 15 (50.37%) 0.7097* C 12 s(32.52%)p 2.07(67.39%)d 0.00(0.10%) (49.63%) -0.7045* C 15 s(59.52%)p 0.68(40.45%)d 0.00(0.03%)	4.50
(1.96443) BD (1) C 9- C 12 (49.57%) 0.7040* C 9 s(40.09%)p 1.49(59.85%)d 0.00(0.06%) (50.43%) 0.7102* C 12 s(40.12%)p 1.49(59.80%)d 0.00(0.07%)	(0.02075) BD*(1) O 13- C 15 (33.71%) 0.5806* O 13 s(43.67%)p 1.28(56.00%)d 0.01(0.34%) (66.29%) -0.8142* C 15 s(40.02%)p 1.49(59.82%)d 0.00(0.17%)	6.64
(1.94462) LP (1) O 3 s(56.62%)p 0.77(43.35%)d 0.00(0.03%)	(0.25817) LV (1)Mg 2 s(99.75%)p 0.00(0.23%)d 0.00(0.02%)	23.25
131. BD (1) O 3- C 5	(0.25817) LV (1)Mg 2 s(99.75%)p 0.00(0.23%)d 0.00(0.02%)	3.77
(1.95413) LP (1) O 7 s(57.15%)p 0.75(42.79%)d 0.00(0.05%)	(0.18661) LV (1)Mg 6 s(99.94%)p 0.00(0.03%)d 0.00(0.03%)	13.86
(1.89296) LP (2) O 7 s(2.31%)p42.31(97.58%)d 0.05(0.11%)	(0.18661) LV (1)Mg 6 s(99.94%)p 0.00(0.03%)d 0.00(0.03%)	11.41
(1.95608) LP (1) O 10 s(55.41%)p 0.80(44.54%)d 0.00(0.06%)	(0.18661) LV (1)Mg 6 s(99.94%)p 0.00(0.03%)d 0.00(0.03%)	14.13
(1.90129) LP (2) O 10 s(3.33%)p28.99(96.57%)d 0.03(0.10%)	(0.18661) LV (1)Mg 6 s(99.94%)p 0.00(0.03%)d 0.00(0.03%)	13.06
(1.99500) BD (1) C 5- O 7 (32.84%) 0.5731* C 5 s(31.46%)p 2.17(68.34%)d 0.01(0.20%) (67.16%) 0.8195* O 7 s(40.51%)p 1.46(59.26%)d 0.01(0.23%)	(0.18661) LV (1)Mg 6 s(99.94%)p 0.00(0.03%)d 0.00(0.03%)	2.81
(1.99377) BD (1) C 9- O 10 (33.85%) 0.5818* C 9 s(28.51%)p 2.50(71.30%)d 0.01(0.18%) (66.15%) 0.8133* O 10 s(41.24%)p 1.42(58.56%)d 0.01(0.21%)	(0.18661) LV (1)Mg 6 s(99.94%)p 0.00(0.03%)d 0.00(0.03%)	2.94
(1.85266) LP (1) C 28 s(43.68%)p 1.29(56.31%)d 0.00(0.02%)	(0.25817) LV (1)Mg 2 s(99.75%)p 0.00(0.23%)d 0.00(0.02%)	43.01
(1.86962) LP (1) N 11 s(27.27%)p 2.67(72.73%)d 0.00(0.01%)	(0.25817) LV (1)Mg 2 s(99.75%)p 0.00(0.23%)d 0.00(0.02%)	23.54
(1.86975) LP (1) N 14 s(26.60%)p 2.76(73.39%)d 0.00(0.01%)	(0.25817) LV (1)Mg 2 s(99.75%)p 0.00(0.23%)d 0.00(0.02%)	22.19
(1.87580) LP (1) N 17 s(27.02%)p 2.70(72.98%)d 0.00(0.01%)	(0.18661) LV (1)Mg 6 s(99.94%)p 0.00(0.03%)d 0.00(0.03%)	21.40
(1.87316) LP (1) N 20 s(26.36%)p 2.79(73.63%)d 0.00(0.01%)	(0.18661) LV (1)Mg 6 s(99.94%)p 0.00(0.03%)d 0.00(0.03%)	20.38
170. BD (1) O 24- C 25	(0.46911) BD*(1)Mo 1- C 21 (72.15%) 0.8494*Mo 1 s(34.71%)p 0.00(0.08%)d 1.88(65.21%) (27.85%) -0.5277* C 21 s(68.27%)p 0.46(31.73%)d 0.00(0.00%)	6.47
(1.47834) LP (1)Mo 1 s(0.00%)p 0.00(0.00%)d 1.00(100.00%)	(0.14909) BD*(2) O 16- C 18	38.93

	(24.76%) 0.4976* O 16 s(0.03%)p99.99(99.60%)d10.66(0.37%) (75.24%) -0.8674* C 18 s(0.01%)p 1.00(99.59%)d 0.00(0.41%)	
(1.47834) LP (1)Mo 1 s(0.00%)p 0.00(0.00%)d 1.00(100.00%)	(0.14263) BD*(3) O 19- C 21 (24.87%) 0.4987* O 19 s(0.00%)p 1.00(99.63%)d 0.00(0.37%) (75.13%) -0.8668* C 21 s(0.00%)p 1.00(99.59%)d 0.00(0.41%)	36.65
(1.47834) LP (1)Mo 1 s(0.00%)p 0.00(0.00%)d 1.00(100.00%)	(0.15078) BD*(2) O 22- C 23 (24.74%) 0.4974* O 22 s(0.04%)p99.99(99.59%)d 8.99(0.37%) (75.26%) -0.8675* C 23 s(0.02%)p99.99(99.58%)d25.09(0.41%)	38.61
(1.47834) LP (1)Mo 1 s(0.00%)p 0.00(0.00%)d 1.00(100.00%)	(0.15039) BD*(2) O 24- C 25 (25.11%) 0.5011* O 24 s(0.02%)p99.99(99.61%)d15.87(0.37%) (74.89%) -0.8654* C 25 s(0.02%)p99.99(99.59%)d26.13(0.40%)	38.51

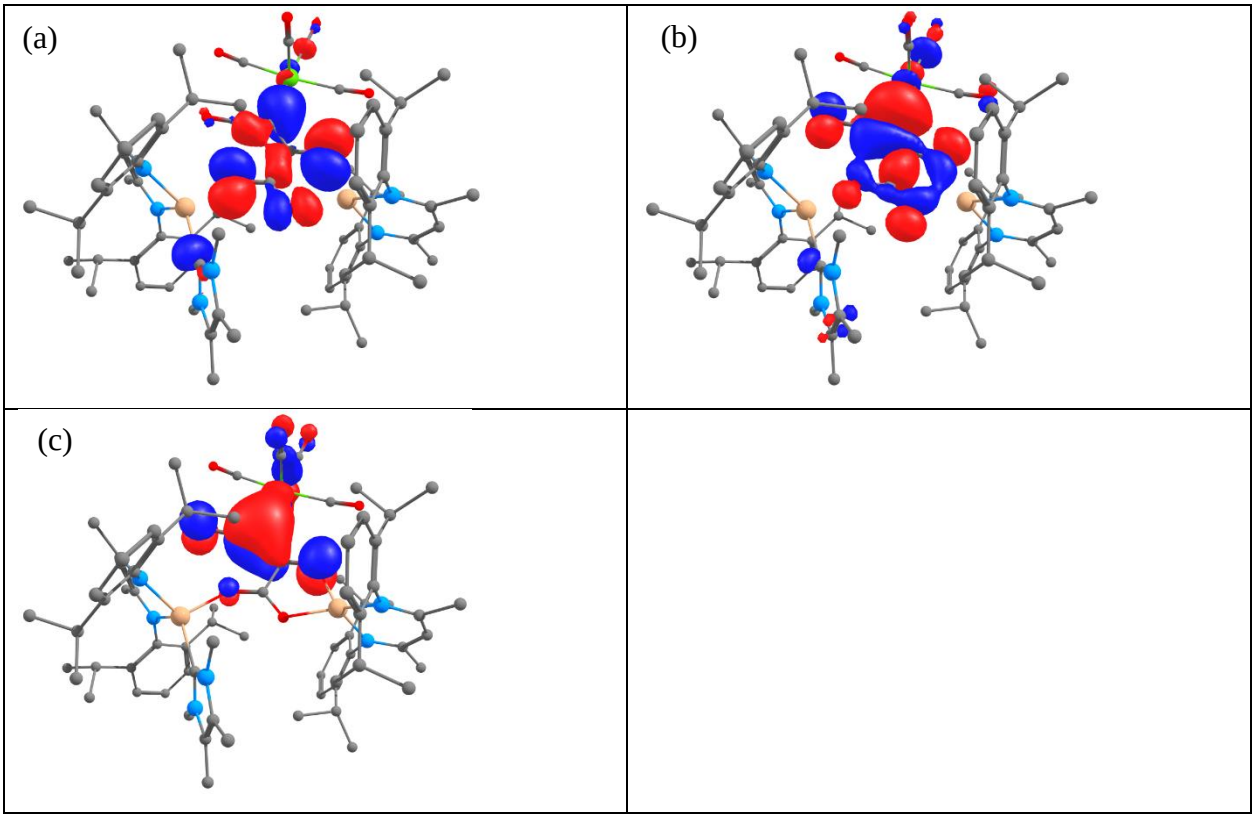


Figure S22. DFT computed MOs for **6**. (a) HOMO-16 (b) HOMO-14 (c) HOMO-13

Table S10. Optimised geometries (xyz coordinates) of calculated molecules.

4

Mg	1.112390000	-2.639326000	5.787831000
O	1.068546000	-3.112605000	3.736710000
N	2.838982000	-2.930022000	6.881613000
C	0.748479000	-2.007820000	3.210816000
Mg	0.550101000	-2.477838000	-1.042334000
O	0.581176000	-0.691909000	5.203863000
N	-0.100692000	-3.664519000	7.106351000
C	0.504320000	-0.796571000	3.946101000
O	-0.099037000	1.100739000	2.398899000
N	2.359014000	-3.440010000	-1.317358000
C	0.220255000	-0.068507000	2.707456000
O	0.442942000	-1.592643000	0.727845000
N	-0.589279000	-4.202925000	-1.105774000
C	0.473097000	-1.320274000	1.943830000
C	4.097632000	-3.543731000	8.905928000
H	4.830509000	-4.148944000	8.364817000
H	3.925486000	-3.994543000	9.884102000
H	4.554769000	-2.560683000	9.050168000
C	2.809554000	-3.427634000	8.121513000
C	1.652029000	-3.884504000	8.778228000
H	1.816600000	-4.233469000	9.790313000
C	0.334976000	-4.046691000	8.310352000
C	-0.621311000	-4.726863000	9.264604000
H	-1.466386000	-4.073951000	9.500319000
H	-0.122835000	-5.001476000	10.195090000
H	-1.044384000	-5.629315000	8.814147000
C	4.113653000	-2.610541000	6.306873000
C	4.793103000	-3.590356000	5.543638000
C	6.009233000	-3.247754000	4.944505000
H	6.541000000	-3.994575000	4.360315000
C	6.551590000	-1.975161000	5.081294000
H	7.495785000	-1.728008000	4.603748000
C	5.879265000	-1.024400000	5.838787000
H	6.308150000	-0.031990000	5.951985000
C	4.666100000	-1.318210000	6.469739000
C	4.255778000	-5.004867000	5.369238000
H	3.332893000	-5.083253000	5.952782000
C	5.232588000	-6.059573000	5.911200000
H	6.169362000	-6.069412000	5.343189000
H	4.791914000	-7.059856000	5.836282000
H	5.484996000	-5.881886000	6.961290000
C	3.905484000	-5.302181000	3.903958000
H	3.156987000	-4.603848000	3.520165000
H	3.501971000	-6.316386000	3.806826000
H	4.793415000	-5.236679000	3.265207000
C	3.996782000	-0.245377000	7.317396000
H	3.132552000	-0.701986000	7.811161000
C	3.478029000	0.912464000	6.454729000
H	4.296522000	1.397898000	5.911600000
H	2.996226000	1.669413000	7.083015000
H	2.740802000	0.570267000	5.725165000
C	4.929942000	0.291795000	8.413836000

H	5.340079000	-0.508773000	9.037590000
H	4.386953000	0.983624000	9.066857000
H	5.776570000	0.841053000	7.987626000
C	-1.443180000	-4.000158000	6.729577000
C	-2.506845000	-3.110912000	7.011893000
C	-3.791379000	-3.441574000	6.568177000
H	-4.613937000	-2.761352000	6.773947000
C	-4.039494000	-4.623308000	5.881381000
H	-5.045953000	-4.863765000	5.549933000
C	-2.990242000	-5.499216000	5.627636000
H	-3.187043000	-6.429323000	5.100337000
C	-1.684743000	-5.211351000	6.037587000
C	-2.305727000	-1.820341000	7.793875000
H	-1.267416000	-1.799882000	8.141284000
C	-2.521929000	-0.584748000	6.910314000
H	-1.822849000	-0.563251000	6.071487000
H	-2.369412000	0.330605000	7.492360000
H	-3.540415000	-0.560615000	6.506984000
C	-3.213235000	-1.747144000	9.031918000
H	-4.269902000	-1.675884000	8.751779000
H	-2.971792000	-0.858949000	9.625815000
H	-3.104455000	-2.624184000	9.677790000
C	-0.578351000	-6.215827000	5.742615000
H	0.344650000	-5.832865000	6.189589000
C	-0.863276000	-7.585084000	6.378375000
H	-1.023414000	-7.509280000	7.458465000
H	-0.020619000	-8.264879000	6.210538000
H	-1.754174000	-8.052100000	5.944254000
C	-0.335691000	-6.366490000	4.233739000
H	-1.229140000	-6.748609000	3.727322000
H	0.478866000	-7.075602000	4.047807000
H	-0.063922000	-5.412923000	3.773100000
C	3.831782000	-5.352902000	-0.826567000
H	4.463581000	-5.088322000	-1.677313000
H	3.759486000	-6.439611000	-0.760335000
H	4.342063000	-4.989398000	0.072041000
C	2.463974000	-4.713599000	-0.931214000
C	1.374629000	-5.544137000	-0.597166000
H	1.654672000	-6.535020000	-0.258610000
C	-0.014347000	-5.354891000	-0.755359000
C	-0.872355000	-6.573273000	-0.489072000
H	-1.302658000	-6.507056000	0.516441000
H	-0.285730000	-7.491827000	-0.544810000
H	-1.707666000	-6.638808000	-1.189218000
C	3.501855000	-2.756411000	-1.845709000
C	3.750987000	-2.809770000	-3.239545000
C	4.814343000	-2.069273000	-3.763822000
H	5.013539000	-2.112634000	-4.831711000
C	5.620929000	-1.282443000	-2.950731000
H	6.439356000	-0.709120000	-3.378123000
C	5.378000000	-1.247992000	-1.583993000
H	6.018392000	-0.647242000	-0.942972000
C	4.336152000	-1.982010000	-1.006593000
C	2.918811000	-3.668235000	-4.181137000
H	2.101220000	-4.102267000	-3.597775000
C	3.743844000	-4.827781000	-4.761311000
H	3.118828000	-5.459921000	-5.402169000

H	4.165262000	-5.461172000	-3.974904000
H	4.576199000	-4.457047000	-5.370331000
C	2.296514000	-2.838294000	-5.310087000
H	1.656625000	-2.044582000	-4.916068000
H	1.686724000	-3.474228000	-5.960417000
H	3.065049000	-2.372770000	-5.935949000
C	4.171570000	-1.947434000	0.504909000
H	3.354484000	-2.628152000	0.766748000
C	3.795803000	-0.549049000	1.011743000
H	4.575263000	0.184313000	0.780358000
H	3.667020000	-0.555908000	2.099654000
H	2.865981000	-0.196204000	0.558889000
C	5.441848000	-2.438207000	1.215201000
H	6.278941000	-1.750604000	1.050017000
H	5.754075000	-3.423581000	0.855023000
H	5.278460000	-2.502621000	2.295032000
C	-1.980455000	-4.168726000	-1.446472000
C	-2.960592000	-3.881585000	-0.468342000
C	-4.295539000	-3.757484000	-0.868576000
H	-5.051685000	-3.531861000	-0.120691000
C	-4.676482000	-3.931028000	-2.192558000
H	-5.720028000	-3.836430000	-2.481101000
C	-3.710310000	-4.240499000	-3.142068000
H	-4.008519000	-4.395008000	-4.175945000
C	-2.360801000	-4.360119000	-2.797846000
C	-2.627664000	-3.742272000	1.008984000
H	-1.555715000	-3.931802000	1.129045000
C	-2.912980000	-2.328910000	1.533009000
H	-2.345380000	-1.576093000	0.980757000
H	-2.647215000	-2.251031000	2.592911000
H	-3.974233000	-2.074613000	1.443008000
C	-3.388538000	-4.777175000	1.851028000
H	-4.468206000	-4.591305000	1.826447000
H	-3.071311000	-4.729099000	2.896972000
H	-3.225008000	-5.796411000	1.487071000
C	-1.354589000	-4.726053000	-3.879297000
H	-0.355969000	-4.661001000	-3.436707000
C	-1.556381000	-6.170658000	-4.363553000
H	-1.478076000	-6.889525000	-3.542488000
H	-0.801353000	-6.433492000	-5.113120000
H	-2.542467000	-6.298997000	-4.824515000
C	-1.403439000	-3.753640000	-5.063364000
H	-2.378788000	-3.773078000	-5.560785000
H	-0.651233000	-4.025484000	-5.811186000
H	-1.207598000	-2.726625000	-4.744827000
Mg	-1.112390000	2.639326000	-5.787831000
O	-1.068546000	3.112605000	-3.736710000
N	-2.838982000	2.930022000	-6.881613000
C	-0.748479000	2.007820000	-3.210816000
Mg	-0.550101000	2.477838000	1.042334000
O	-0.581176000	0.691909000	-5.203863000
N	0.100692000	3.664519000	-7.106351000
C	-0.504320000	0.796571000	-3.946101000
O	0.099037000	-1.100739000	-2.398899000
N	-2.359014000	3.440010000	1.317358000
C	-0.220255000	0.068507000	-2.707456000
O	-0.442942000	1.592643000	-0.727845000

N	0.589279000	4.202925000	1.105774000
C	-0.473097000	1.320274000	-1.943830000
C	-4.097632000	3.543731000	-8.905928000
H	-4.830509000	4.148944000	-8.364817000
H	-3.925486000	3.994543000	-9.884102000
H	-4.554769000	2.560683000	-9.050168000
C	-2.809554000	3.427634000	-8.121513000
C	-1.652029000	3.884504000	-8.778228000
H	-1.816600000	4.233469000	-9.790313000
C	-0.334976000	4.046691000	-8.310352000
C	0.621311000	4.726863000	-9.264604000
H	1.466386000	4.073951000	-9.500319000
H	0.122835000	5.001476000	-10.195090000
H	1.044384000	5.629315000	-8.814147000
C	-4.113653000	2.610541000	-6.306873000
C	-4.793103000	3.590356000	-5.543638000
C	-6.009233000	3.247754000	-4.944505000
H	-6.541000000	3.994575000	-4.360315000
C	-6.551590000	1.975161000	-5.081294000
H	-7.495785000	1.728008000	-4.603748000
C	-5.879265000	1.024400000	-5.838787000
H	-6.308150000	0.031990000	-5.951985000
C	-4.666100000	1.318210000	-6.469739000
C	-4.255778000	5.004867000	-5.369238000
H	-3.332893000	5.083253000	-5.952782000
C	-5.232588000	6.059573000	-5.911200000
H	-6.169362000	6.069412000	-5.343189000
H	-4.791914000	7.059856000	-5.836282000
H	-5.484996000	5.881886000	-6.961290000
C	-3.905484000	5.302181000	-3.903958000
H	-3.156987000	4.603848000	-3.520165000
H	-3.501971000	6.316386000	-3.806826000
H	-4.793415000	5.236679000	-3.265207000
C	-3.996782000	0.245377000	-7.317396000
H	-3.132552000	0.701986000	-7.811161000
C	-3.478029000	-0.912464000	-6.454729000
H	-4.296522000	-1.397898000	-5.911600000
H	-2.996226000	-1.669413000	-7.083015000
H	-2.740802000	-0.570267000	-5.725165000
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H	-5.340079000	0.508773000	-9.037590000
H	-4.386953000	-0.983624000	-9.066857000
H	-5.776570000	-0.841053000	-7.987626000
C	1.443180000	4.000158000	-6.729577000
C	2.506845000	3.110912000	-7.011893000
C	3.791379000	3.441574000	-6.568177000
H	4.613937000	2.761352000	-6.773947000
C	4.039494000	4.623308000	-5.881381000
H	5.045953000	4.863765000	-5.549933000
C	2.990242000	5.499216000	-5.627636000
H	3.187043000	6.429323000	-5.100337000
C	1.684743000	5.211351000	-6.037587000
C	2.305727000	1.820341000	-7.793875000
H	1.267416000	1.799882000	-8.141284000
C	2.521929000	0.584748000	-6.910314000
H	1.822849000	0.563251000	-6.071487000
H	2.369412000	-0.330605000	-7.492360000

H	3.540415000	0.560615000	-6.506984000
C	3.213235000	1.747144000	-9.031918000
H	4.269902000	1.675884000	-8.751779000
H	2.971792000	0.858949000	-9.625815000
H	3.104455000	2.624184000	-9.677790000
C	0.578351000	6.215827000	-5.742615000
H	-0.344650000	5.832865000	-6.189589000
C	0.863276000	7.585084000	-6.378375000
H	1.023414000	7.509280000	-7.458465000
H	0.020619000	8.264879000	-6.210538000
H	1.754174000	8.052100000	-5.944254000
C	0.335691000	6.366490000	-4.233739000
H	1.229140000	6.748609000	-3.727322000
H	-0.478866000	7.075602000	-4.047807000
H	0.063922000	5.412923000	-3.773100000
C	-3.831782000	5.352902000	0.826567000
H	-4.463581000	5.088322000	1.677313000
H	-3.759486000	6.439611000	0.760335000
H	-4.342063000	4.989398000	-0.072041000
C	-2.463974000	4.713599000	0.931214000
C	-1.374629000	5.544137000	0.597166000
H	-1.654672000	6.535020000	0.258610000
C	0.014347000	5.354891000	0.755359000
C	0.872355000	6.573273000	0.489072000
H	1.302658000	6.507056000	-0.516441000
H	0.285730000	7.491827000	0.544810000
H	1.707666000	6.638808000	1.189218000
C	-3.501855000	2.756411000	1.845709000
C	-3.750987000	2.809770000	3.239545000
C	-4.814343000	2.069273000	3.763822000
H	-5.013539000	2.112634000	4.831711000
C	-5.620929000	1.282443000	2.950731000
H	-6.439356000	0.709120000	3.378123000
C	-5.378000000	1.247992000	1.583993000
H	-6.018392000	0.647242000	0.942972000
C	-4.336152000	1.982010000	1.006593000
C	-2.918811000	3.668235000	4.181137000
H	-2.101220000	4.102267000	3.597775000
C	-3.743844000	4.827781000	4.761311000
H	-3.118828000	5.459921000	5.402169000
H	-4.165262000	5.461172000	3.974904000
H	-4.576199000	4.457047000	5.370331000
C	-2.296514000	2.838294000	5.310087000
H	-1.656625000	2.044582000	4.916068000
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H	-3.065049000	2.372770000	5.935949000
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H	-2.865981000	0.196204000	-0.558889000
C	-5.441848000	2.438207000	-1.215201000
H	-6.278941000	1.750604000	-1.050017000
H	-5.754075000	3.423581000	-0.855023000
H	-5.278460000	2.502621000	-2.295032000
C	1.980455000	4.168726000	1.446472000

C	2.960592000	3.881585000	0.468342000
C	4.295539000	3.757484000	0.868576000
H	5.051685000	3.531861000	0.120691000
C	4.676482000	3.931028000	2.192558000
H	5.720028000	3.836430000	2.481101000
C	3.710310000	4.240499000	3.142068000
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C	2.360801000	4.360119000	2.797846000
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C	2.912980000	2.328910000	-1.533009000
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H	2.647215000	2.251031000	-2.592911000
H	3.974233000	2.074613000	-1.443008000
C	3.388538000	4.777175000	-1.851028000
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H	3.225008000	5.796411000	-1.487071000
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C	1.556381000	6.170658000	4.363553000
H	1.478076000	6.889525000	3.542488000
H	0.801353000	6.433492000	5.113120000
H	2.542467000	6.298997000	4.824515000
C	1.403439000	3.753640000	5.063364000
H	2.378788000	3.773078000	5.560785000
H	0.651233000	4.025484000	5.811186000
H	1.207598000	2.726625000	4.744827000

6

Mo	2.686687000	4.386119000	-0.146633000
Mg	-2.826156000	0.199938000	-0.046233000
O	-0.848900000	0.573055000	0.009370000
N	-2.700445000	-2.754645000	1.263112000
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N	-3.297891000	-3.015125000	-0.767942000
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N	-3.779339000	1.224710000	-1.595242000
C	1.253977000	2.526263000	-0.084616000
O	-0.992594000	3.599866000	-0.074865000
N	-3.795609000	1.306425000	1.459553000
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C	2.561004000	4.504682000	1.887806000
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C	1.227650000	5.800506000	-0.278219000
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C	4.013033000	5.868276000	-0.200093000

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