Supporting Information

Synergistic C-H Bond Activation Across Molybdenum-Iridium Multiply Bonded Complexes: a Cascade of Transformations

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General Considerations

Unless otherwise noted, all reactions were performed either using standard Schlenk line techniques or in an MBRAUN glovebox under an atmosphere of purified argon (<1 ppm of O_2/H_2O). Glassware and cannulas were stored in an oven at ~100 °C for at least 16 h prior to use. THF and *n*-pentane were purified by passage through a column of activated alumina, dried over Na/benzophenone, vacuum-transferred to a storage flask, and freeze–pump–thaw degassed prior to use. Deuterated solvents (toluene-d_8, THF-d_8, and C_6D_6) were dried over Na/benzophenone, vacuum-transferred to a storage flask, and freeze–pump–thaw degassed prior to use. The syntheses of Cp^*IrH_4 and $MoCl_4(OEt_2)_2$ were carried out following literature procedures.[1,2] The synthesis of $Mo(NMe_2)_4$ follows a modified literature procedure and is discussed below.[3] All other reagents were acquired from commercial sources and used as received.

IR Spectroscopy
The samples were prepared in a glovebox (either pure crystalline material, or diluted in dry KBr powder), sealed under argon in a Diffuse Reflectance Infrared Fourier Transform (DRIFT) cell fitted with KBr windows, and then analyzed using a Nicolet 670 FT-IR spectrometer.

Elemental Analyses
Elemental analyses were performed under an inert atmosphere at Mikroanalytisches Labor Pascher, Germany.

X-Ray Diffraction - Structural Determinations
Suitable crystals were coated in parabar oil, selected manually under a binocular microscope and mounted on a Rigaku-OD Synergy-S single-crystal diffractometer equipped with an Hypix-100 detector. Intensities were collected at 100K with molybdenum radiation (λ=0.71073 Å) for compounds **1** to **6** and with copper radiation (λ=1.54184 Å) for N,N-dimethyl-N'-*tert*butyl urea by means of the CrysalisPro software.[4] Reflection indexing, unit-cell parameters refinement, Lorentz-polarization correction, peak integration and background determination were carried out with the CrysalisPro software.[4] An analytical absorption correction was applied using the modeled faces of the crystal.[5] The resulting set of *hkl* was used for structure solution and refinement. The structures were solved with the ShelXT structure solution program using the intrinsic phasing solution method and by using Olex2 as the graphical interface.[6,7] The model was refined with version 2018/3 of ShelXL using least-squares minimization.[6]

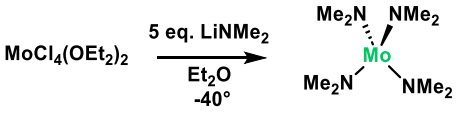
CCDC 2410538-2410544 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Date Centre via www.ccdc.cam.ac.uk/data_request/cif.

NMR Spectroscopy
Solution NMR spectra were recorded on Bruker AV-300 and AV-500 spectrometers. ^1H and ^{13}C chemical shifts were measured relative to residual solvent peaks, which were assigned relative to an external TMS standard set at 0.00 ppm. ^1H and ^{13}C NMR assignments were confirmed by ^1H–^1H COSY, ^1H–^{13}C HSQC, and HMBC experiments. NMR data recorded as follows: chemical shift (δ) [multiplicity, coupling constant(s) *J* (Hz), relative integral], where multiplicity is defined: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet or combinations thereof, and prefixed br = broad.

UV-Visible Spectroscopy
Samples were dissolved in n-pentane or THF and transferred to a quartz cuvette with a J. Young valve inside an argon filled glove box. Solvent backgrounds were subtracted manually from an appropriate solvent blank experiment. Absorption spectra were recorded on a Perkin-Elmer Lambda 1050 UV/Vis/NIR spectrophotometer.

Syntheses

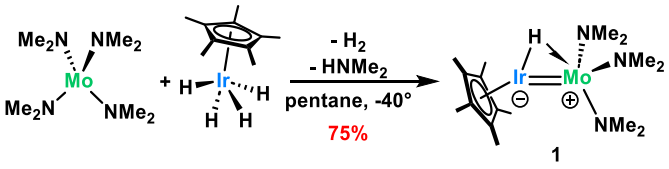
Synthesis of complex $Mo(NMe_2)_4$



In an argon-filled glovebox, a 500 mL Schlenk flask was charged with 3.005 g $MoCl_4(OEt_2)_2$ (7.78 mmol, 1 eq), 250 mL diethylether and a very large, Teflon-coated stir bar. The flask was fitted with a solid addition funnel filled with 1.986 g $LiNMe_2$ ($3.89e^{-2}$ mol, 5 eq). The bright orange suspension of $MoCl_4(OEt_2)_2$ was cooled to -40 °C using an EtOH/liquid nitrogen bath and the $LiNMe_2$ powder was added in one portion with vigourous stirring. The suspension was slowly warmed to room temperature and allowed to stir at room temperature for 4h after which the solvent was removed under reduced pressure. The flask was then fitted with a distillation arm and heated to 60 °C with the rapid evolution of a bright purple material collected in the receiving flask. Yield = 0.712 g, 33%. NMR spectroscopic analysis confirms the formation of $Mo(NMe_2)_4$ and no further characterization was performed.

^{1}H NMR (300 MHz, C_6D_6, 298K) δ 3.27 (s, 24H), matches literature expectation.[3]

Synthesis of complex Cp*Ir(H)Mo$(NMe_2)_3$, **1**



In an argon-filled glovebox, a 50 mL Schlenk flask was charged with 0.150 g of complex $Mo(NMe_2)_4$ (5.56 mmol, 1 eq) and 50 mL pentane was added to yield a deep purple solution. This was brought out to a Schlenk line and cooled to approx. -50°C. A colorless solution of 0.184 g Cp^*IrH_4 (5.56 mmol, 1 eq) in 25 mL pentane was added to the rapidly stirring $Mo(NMe_2)_4$ solution *via* cannula over 2 mins. The solution was slowly warmed to room temperature and left to react for 6 hours. The volatiles were removed *in vacuo* to yield a sticky brown solid, which was extracted and recrystallized from pentane at -35°C to yield brown needles along the edge of the liquid phase in the scintillation vial. The dilute conditions and cold temperature were found to be necessary to avoid over substitution and formation of an excessive amount of complex **2**. Despite these conditions, some complex **2** is always present and complex **1** was only obtained pure through multiple, successive recrystallizations from pentane and manual separation of the crystals, reflected in the lower yield. Isolated mass = 0.231 g, Yield = 75%. Caution: the released dimethylamine is potently odorous.

Characterization data:

^{1}H NMR (500 MHz, C_6D_6, 298 K) δ 3.36 (s, 18H, N**Me$_2$**), 2.28 (s, 15H, Cp*), -6.41, (s, 1H, Ir-H)

^{13}C NMR (125 MHz, C_6D_6, 298K) δ 88.17 (Cp*-**C**), 49.80 (N-**Me**), 11.39 (Cp*-**Me**)

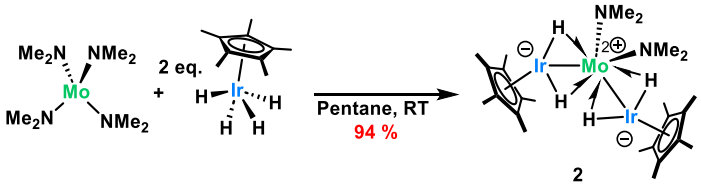
UV-Vis (**Figure S 39**): 495 nm (5500 $M^{-1}cm^{-1}$)

DRIFTS (**Figure S 33**): 2990-2772 cm^{-1} (C-H, s), 1990 (M-H, m)

EA ($C_{16}H_{34}N_3MoIr$) Expected: C 34.52, H 6.16, N 7.55. Found: C 34.97, H 6.35, N 7.43

*Despite several attempts, the carbon analysis for compound **1** is 0.45% higher than the calculated value, slightly exceeding the generally accepted margin of 0.4%.*

Synthesis of complex $(NMe_2)_2Mo(IrH_2Cp^*)_2$, **2**



In an argon-filled glovebox, a 250 mL Schlenk flask was charged with 0.200 g of $Mo(NMe_2)_4$ ($7.35e^{-4}$ mol, 1 eq) and 50 mL pentane was added to it, yielding a deep purple solution. A solution of 0.487 g of complex Cp^*IrH_4 ($1.47e^{-3}$ mol, 2 eq) in 25 mL pentane was added at room temperature to the rapidly stirring Mo solution *via* cannula over 2 minutes, with instant reaction to yield a wine-red solution. The reaction was left to react at room temperature over 18 hours before the volatiles were removed under vacuum to yield a deep red/black solid. This solid was recrystallized from a minimum volume of pentane at -35°C to give X-ray quality, black block shaped crystals of complex **2**. Isolated mass = 0.588 g, Yield = 94%. Caution: the released dimethylamine is potently odorous.

Characterization data:

^{1}H NMR (500 MHz, C_6D_6, 298 K) δ 3.49 (s, 12H, N**Me$_2$**), 2.34 (s, 30H, Cp*), -10.23 (s, 4H, Ir-H).

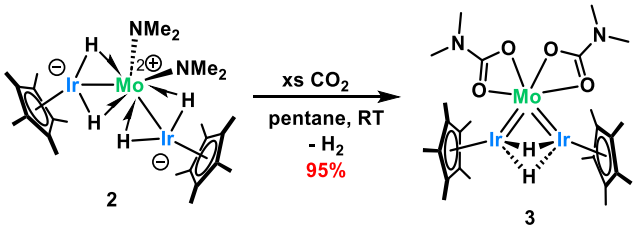
^{13}C NMR (125 MHz, C_6D_6, 298K) δ 90.52 (Cp*-**C**), 55.56 (N-**Me**), 11.80 (Cp*-**Me**)

UV-Vis (**Figure S 40**): 280 nm (11063 $M^{-1}cm^{-1}$), 472 nm (2258 $M^{-1}cm^{-1}$)

DRIFTS (**Figure S 34**): 3002 -2729 cm^{-1} (C-H, s), 2028 cm^{-1} (M-H, m), 1928 cm^{-1} (M-H, m)

EA ($C_{24}H_{46}N_2MoIr_2$) Expected: C 34.19, H 5.50, N 3.32. Found: C 34.12, H 5.54, N 3.25

Reaction of **2** with CO_2 to generate **3**



In an argon-filled glovebox, a 100 mL Teflon screw-capped Schlenk flask was charged with a solution of 0.051 g ($6.05e^{-5}$ mol, 1 eq) of complex **2** dissolved in 20 mL of pentane. The wine-red solution was degassed twice *via* a freeze-pump-thaw procedure and the atmosphere of the flask was replaced with 0.984 bar high-purity CO_2 (N48, $3.2e^{-3}$ mol, 52 eq). The solution was left to stir at room temperature over 18h with a slow colour change to dark green. The solvent was removed under reduced pressure and the solid was recrystallized from pentane at -40°C. Isolated mass = 0.053 g, yield = 95%

Characterization data:

^{1}H NMR (500 MHz, C_6D_6, 298K) δ 2.37 (s, 12H, N**Me$_2$**), 2.32 (s, 30H, Cp*), -6.54 (s; 2H, Ir-**H**).

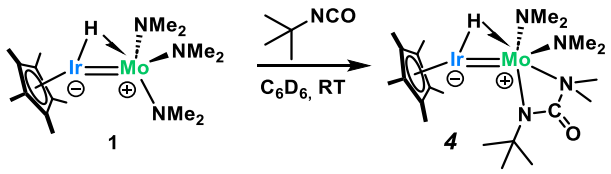
^{13}C NMR (125 MHz, C_6D_6, 298K) δ 168.78 (Me_2N**C**OO), 88.03 (Cp*-**C**), 33.82 (**Me**$_2$NCOO), 10.99 (Cp*-**Me**).

UV-Vis (**Figure S 41**): 290 nm (9420 $M^{-1}cm^{-1}$), 384 nm (2917 $M^{-1}cm^{-1}$), 595 nm (441 $M^{-1}cm^{-1}$)

DRIFTS (**Figure S 35**): 3084 – 2758 cm^{-1} (C-H, s), 2131 (M-H, m), 2019-1849 (M-H, s) 1571 cm^{-1} (C=O, s)

EA ($C_{26}H_{44}N_2MoIr_2$) Expected: C 33.61, H 4.77, N 3.02. Found: C 34.01, H 4.92, N 3.08

Reaction of **1** with 1 equivalent *t*BuNCO and stopping at intermediate product **4**



In an argon-filled glovebox, a 20 mL scintillation vial was charged with 20 mg of complex **1** (3.59e-5 mol, 1 eq) and 2 mL of pentane. 43 µL of a 0.82 mol/L *t*BuNCO (3.59e^{-5} mol, 1 eq) stock solution in pentane was added with a slight darkening of the solution colour. The solution was left to stir for 10 minutes at ambient temperature before the volatiles were removed under reduced pressure to yield a reddish brown powder. This powder was recrystallized from a saturated pentane solution (2.5 mL) at -40 °C to yield 15.3 mg of X-ray quality, dark orange, block shaped crystals in (65% isolated yield, 95% from NMR quantification).

Characterization data:

^{1}H NMR (300 MHz, C_6D_6, 298K) δ 3.49 (br s, 10H, Mo-N**Me$_2$**), 2.86(br s, 6H, (**H**$_3$C)$_2$N$_{urea}$)), 2.02 (s, 15H, Cp*), 1.62 (s, 9 H, (**H**$_3$C)$_3$C-N$_{urea}$) -9.85 (s, 1H, Ir-**H**).

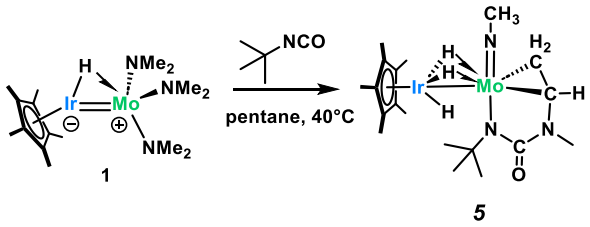
^{1}H NMR (500 MHz, toluene-*d*8, 248K) δ 4.80 (br s, 3H, N**Me**), 3.61 (br s, 3H, N**Me**), 3.35 (br s, 3H, N**Me**), 3.22(br s, 3H, N**Me**), 2.00 (s, 15H, Cp*), 1.60 (s, 9 H, (**H**$_3$C)$_3$C-N$_{urea}$), -9.69 (s, 1H, Ir-**H**).

^{13}C NMR (125 MHz, toluene-*d*8, 248K) δ 164.29 (N$_2$**C**=O), 88.93 (Cp*-**C**), 54.90((H$_3$C)$_3$**C**-N$_{urea}$), 52.65 (N$_{urea}$-**C**H$_3$), 50.91 (N$_{amido}$(**C**H$_3$)$_2$), 4, 30.24 (H$_3$**C**)$_3$C-N$_{urea}$, 10.85 (Cp*-**Me**).

DRIFTS: 3015-2809 cm^{-1} (C-H), 2155 cm^{-1} (M-H)

Owing to the instability of this reaction intermediate, satisfactory elemental analysis results could not be obtained.

Reaction of **1** with 1 equivalent *t*BuNCO and continuing to **5**



In an argon-filled glovebox, a 20 mL Schlenk flask was charged with 25 mg of complex **1** (4.49e^{-5} mol, 1 eq) and 5 mL of pentane. To this solution was added 52.2 µL of a 0.86 mol/L *t*BuNCO solution (4.49e^{-5} mol, 1 eq) in pentane. The solution was stirred at room temperature for 1 hour before removing from the glovebox and heating at 40°C for 1h. The solvent was removed under reduced pressure and the brownish solid was recrystallized from pentane cooled to -40 °C to give orange rhombohedral crystals of X-ray quality. Isolated product mass = 17.8 mg (yield = 59%). Complex **1,** which is generated along **5** in this reaction, can be removed as dark brown needles along the edge of the liquid phase.

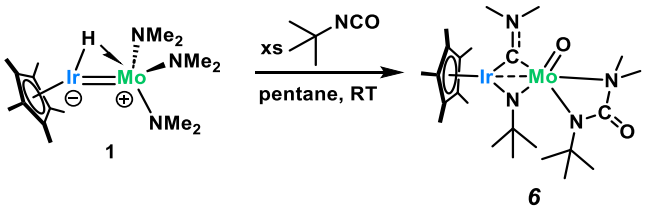
Characterization data:

^{1}H NMR (500 MHz, C_6D_6, 298 K) δ 4.20 (dd, *J* = 9.8, 6.7 Hz, 1H, H$_2$C=C**H**-N), 3.03 (s, 3 H, **H**$_3$C-N=Mo), 2.98 (s, 3 H, **H**$_3$C-N$_{urea}$), 2.69 (t, *J* = 6.2 Hz, 1H **H**$_2$C=CH-N), 2.17 (dd, *J* = 9.7, 5.6 Hz, 1H, **H**$_2$C=CH-N), 1.98 (s, 9 H, (**H**$_3$C)$_3$C-N$_{urea}$), 1.82 (s, 15 H, Cp*), -12.60 (s, 3 H, Ir-**H**).

^{13}C NMR (125 MHz, C_6D_6, 298K) δ 169.77 (N$_2$**C**=O), 92.14 (Cp*-**C**), 73.67 (H$_2$C=**C**H-N), 57.10 ((H$_3$C)$_3$C-N$_{urea}$), 53.19 (N$_{urea}$-**C**H$_3$), 47.22 (H$_2$C=**C**H-N), 37.82 (Mo=N-**C**H$_3$), 31.40 (H$_3$**C**)$_3$C-N$_{urea}$), 10.83 (Cp*-**Me**).

DRIFTS (**Figure S 37**): 3025-2802 cm^{-1} (s, C-H), 1974-1782 cm^{-1} (M-H), 1634 cm^{-1} (C=O)

Reaction of **1** with excess *t*BuNCO to give **6**



In an argon-filled glovebox, a 20 mL scintillation vial was charged with 25 mg of complex **2** (4.49e^{-5} mol, 1 eq) in 4 mL of pentane. To this solution was added 26µL of neat *t*BuNCO (2.24e-4 mol, 5 eq) in one portion. This solution was stirred at room temperature overnight to yield a dark blue/black suspension. The solvent and unreacted *t*BuNCO were removed under reduced pressure and the dark solid was triturated with 2 mL pentane to remove unreacted **1** and N,N-dimethyl-N'-*tert*butylurea. The resulting deep blue powder was recrystallized from 9:1 toluene:pentane to yield 26 mg of X-ray quality crystals of **6** in 82% yield.

Characterization data:

^{1}H NMR (500 MHz, C_6D_6, 298K) δ 3.44 (s, 6H, (**H**$_3$C)$_2$N=C-M), 2.15 (s, 9H, (**H**$_3$C)$_3$C-N$_{imide}$), 1.82 (s, 9H, (**H**$_3$C)$_3$C-N$_{urea}$), 1.68 (s, 21H, Cp* and (**H**$_3$C)$_2$N$_{urea}$).

^{13}C NMR (125 MHz, C_6D_6, 298K) δ 295.43 (**C**=NMe$_2$), 166.07 (N$_2$**C**=O), 93.45(Cp*-**C**), 71.46 (N$_{imide}$-**C**(CH$_3$)$_3$), 55.16 (N$_{urea}$-**C**(CH$_3$)$_3$), 48.33 (C=N**Me**$_2$), 45.46(**Me**$_2$N-C=O), 32.70 (N$_{imide}$-C(**C**H$_3$)$_3$), 30.66(N$_{urea}$-C(**C**H$_3$)$_3$), 11.32 (Cp*-**Me**).

UV-Vis (**Figure S 42**): 302 nm (7285 M^{-1}cm^{-1}), 387 nm (3582 M^{-1}cm^{-1}), 585 nm (2760 M^{-1}cm^{-1})

DRIFTS (**Figure S 38**): 3020-2808 cm^{-1} (s, C-H), 1669 cm^{-1} (C=O)

EA ($C_{24}H_{45}N_4O_2MoIr$) Expected: C 40.61, H 6.39, N 7.89. Found: C 40.74, H 6.45, N 7.82.

NMR Spectra

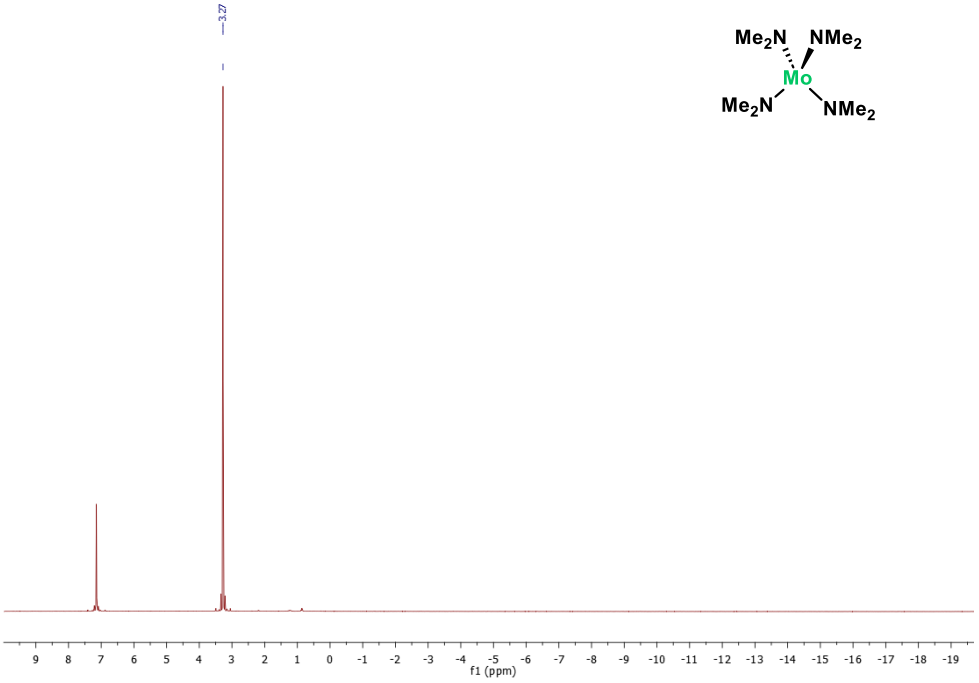


Figure S 1 : ^{1}H NMR spectrum of $Mo(NMe_2)_4$ in C_6D_6 solution, recorded at 300 MHz, 298K. No paramagnetic impurities were observed when expanding the collection window to ±150 ppm.

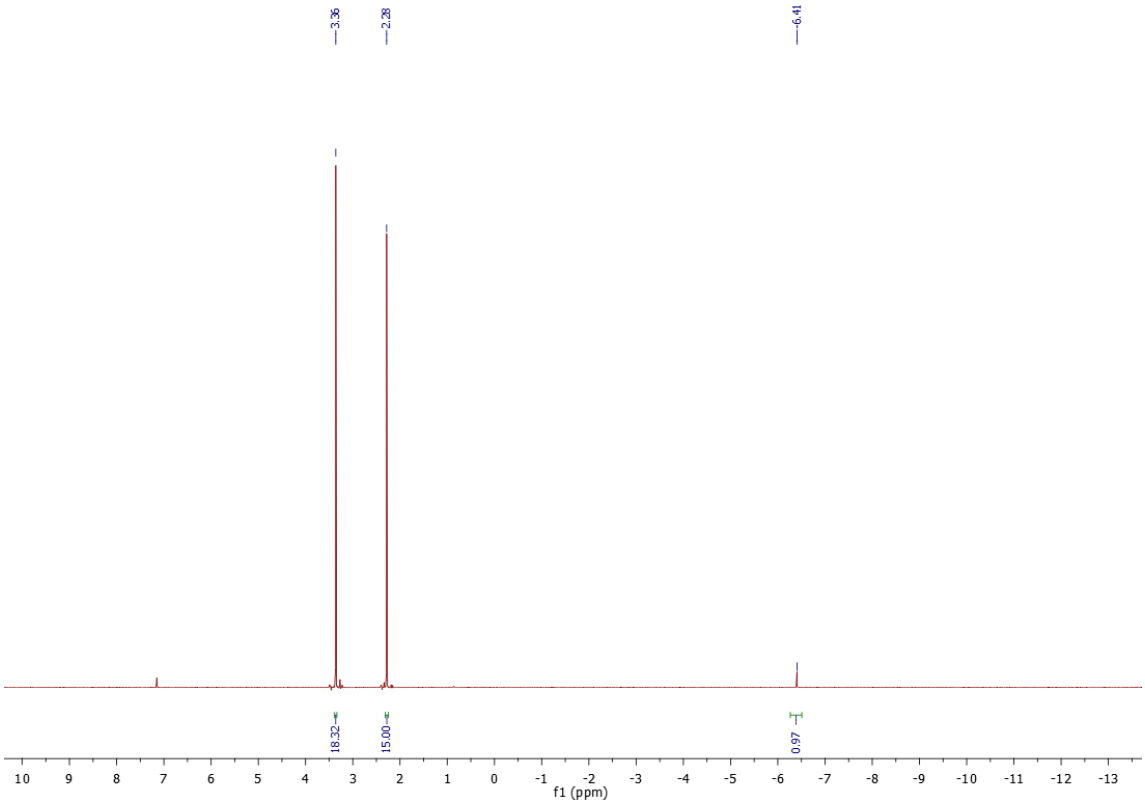


Figure S 2: ^{1}H NMR spectrum of compound 1 in C_6D_6 solution, recorded at 500 MHz, 298K.

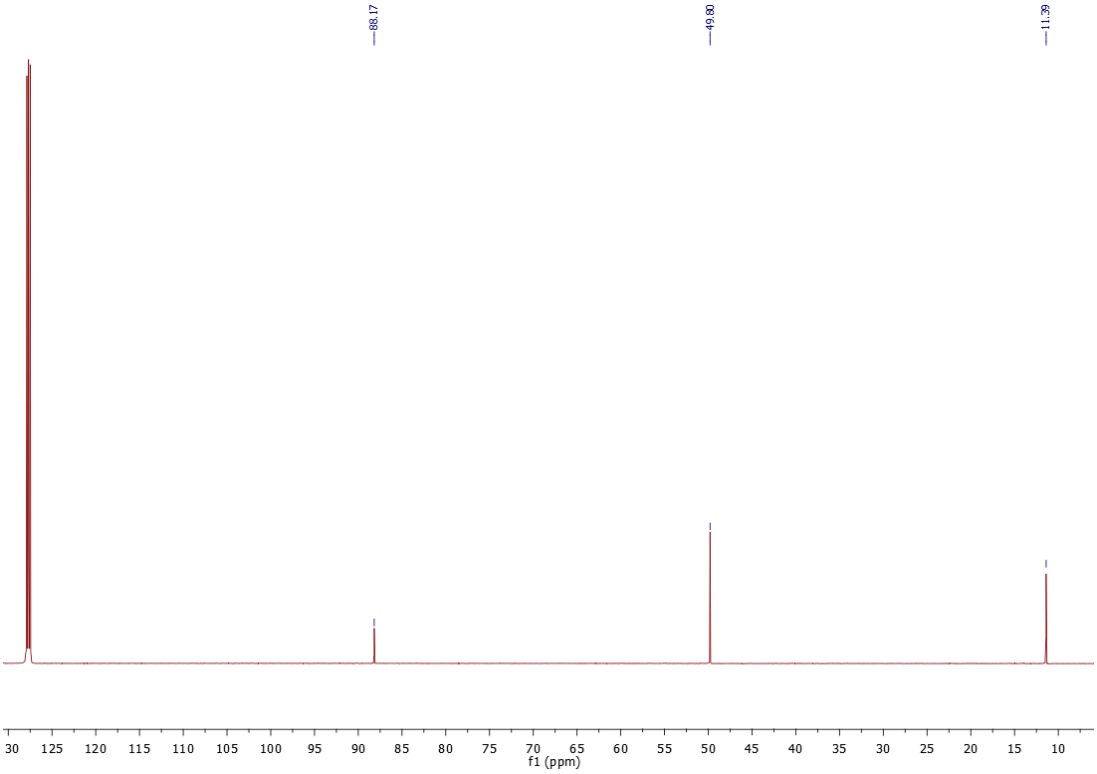


Figure S 3 : ^{13}C NMR spectrum of compound 1 in C_6D_6 solution, recorded at 125 MHz, 298K.

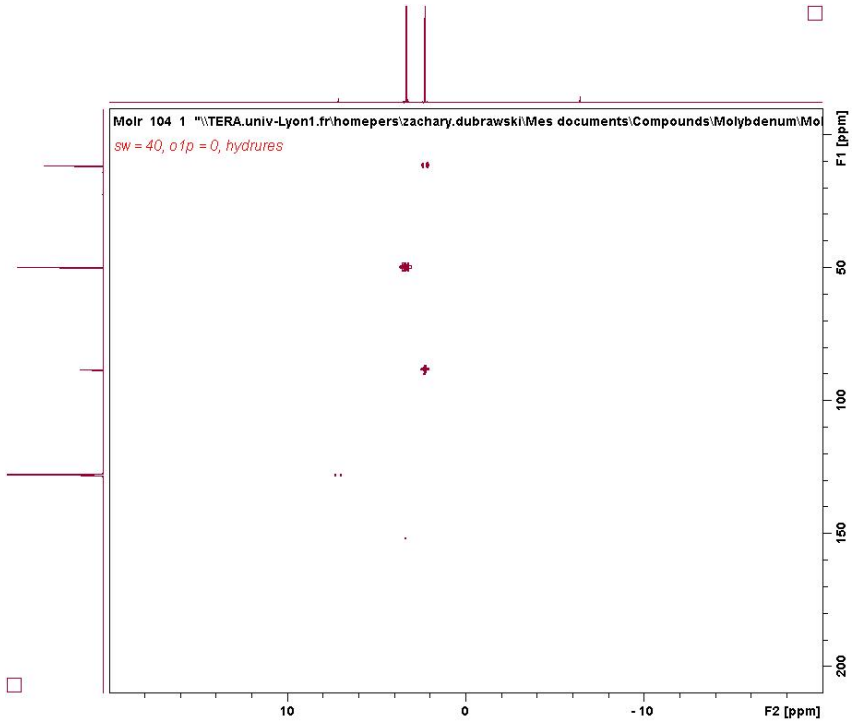


Figure S 4 : ^{1}H-^{13}C HMBC 2D NMR spectrum of compound 1 in C_6D_6 solution, recorded at 500 MHz, 298K. Spectra presented along axes are external projections (for clarity) of ^{1}H and ^{13}C spectra recorded on the same sample.

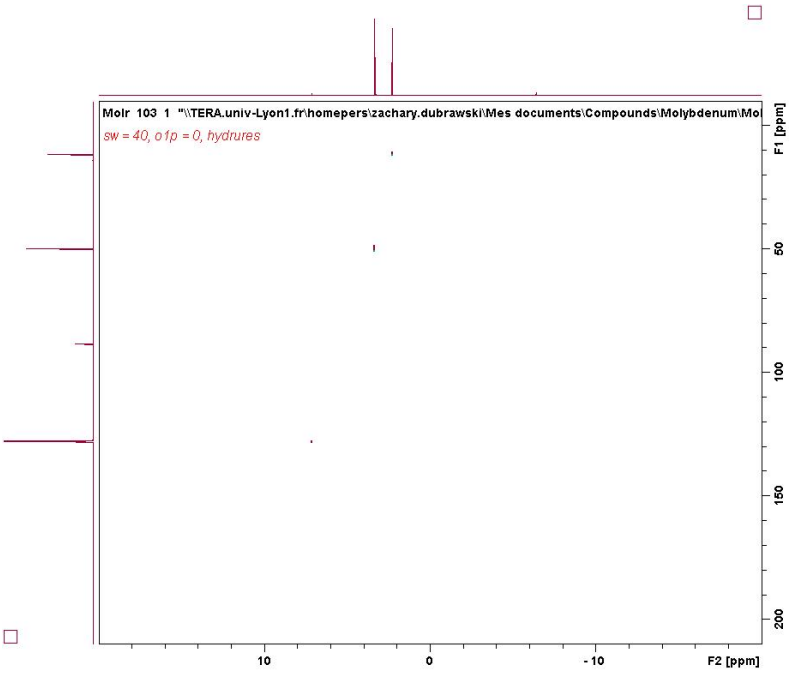


Figure S 5 : ^{1}H-^{13}C HSQC 2D NMR spectrum of compound 1 in C_6D_6 solution, recorded at 500 MHz, 298K. Spectra presented along axes are external projections (for clarity) of ^{1}H and ^{13}C spectra recorded on the same sample.

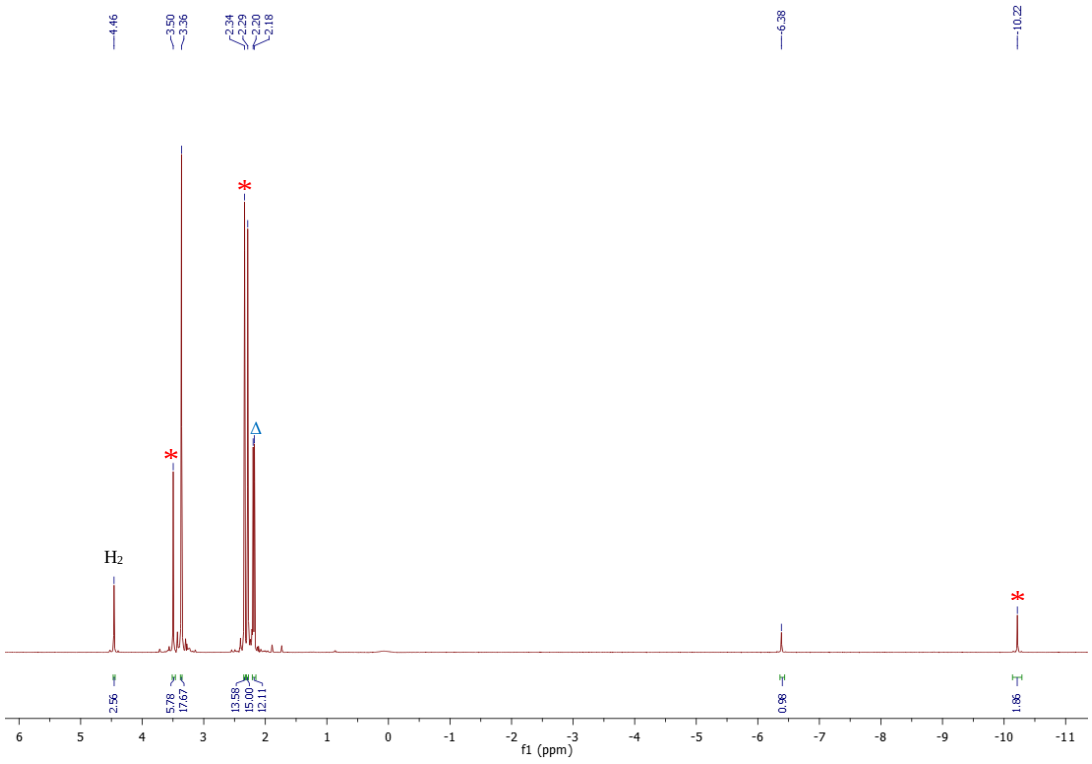


Figure S 6 : ^{1}H NMR spectrum of a synthesis of 1 in a J-Young NMR tube fully filled with C_6D_6 (no headspace). This allows for the detection and titration of dihydrogen produced in this reaction. Due to the speed of the reaction and a lack of good mixing, a full J-Young is challenging to load and mix in a timely manner, significant over substitution of 1 can be observed and a large concentration of 2 (marked with a red asterisk,*) can be observed in this reaction in about a 1:0.5 ratio. 2 equivalents of dimethylamine can also be observed (d, 2.19 ppm, marked with a blue triangle). Dihydrogen (4.46 ppm, chemical shift consistent with literature [8]) can be observed in about 2 equivalent ratio with the product, complex 1.

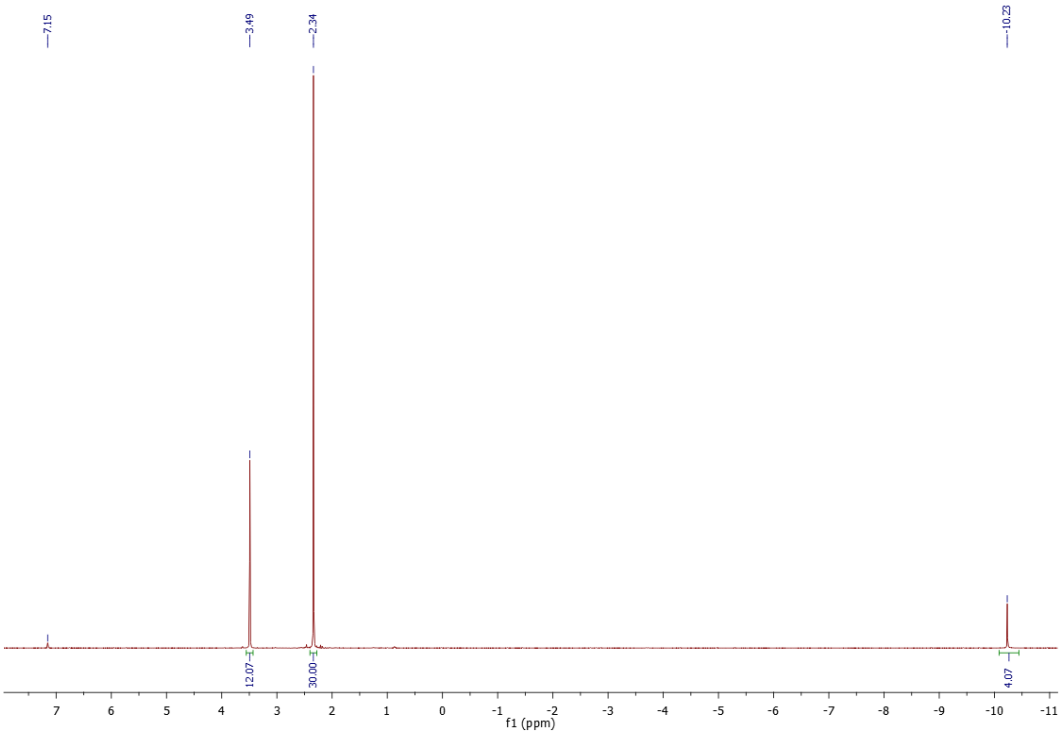


Figure S 7 : ^{1}H NMR spectrum of compound 2 in C_6D_6 solution, recorded at 500 MHz, 298K.

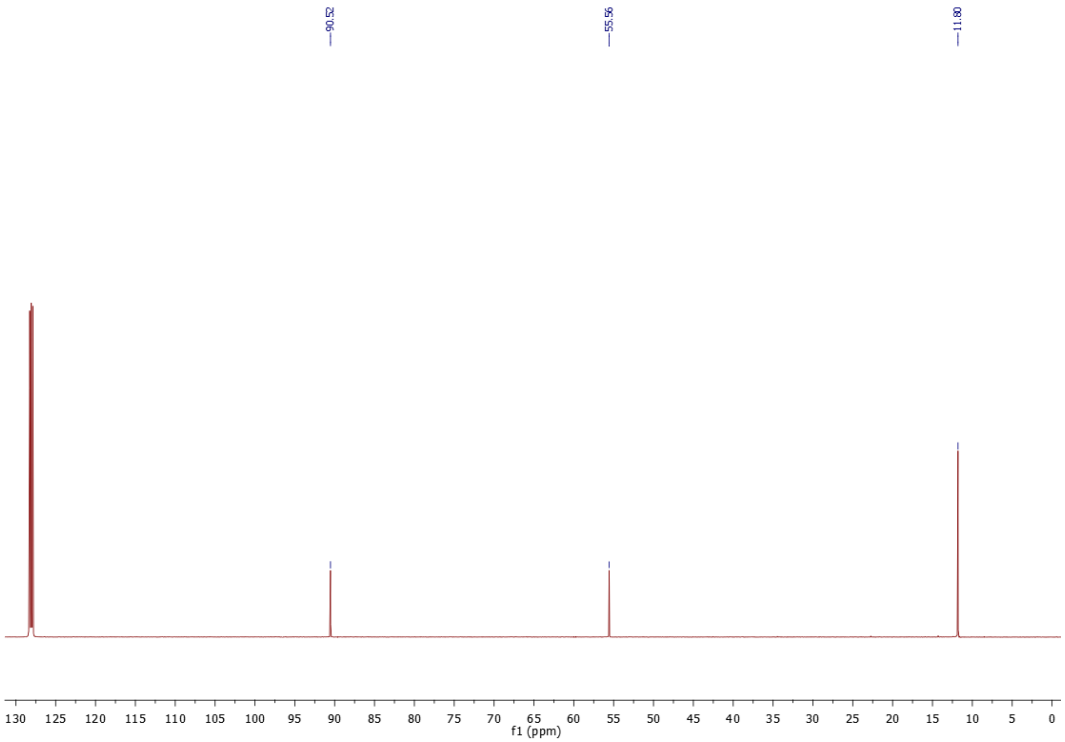


Figure S 8 : ^{13}C NMR spectrum of compound 2 in C_6D_6 solution, recorded at 125 MHz, 298K.

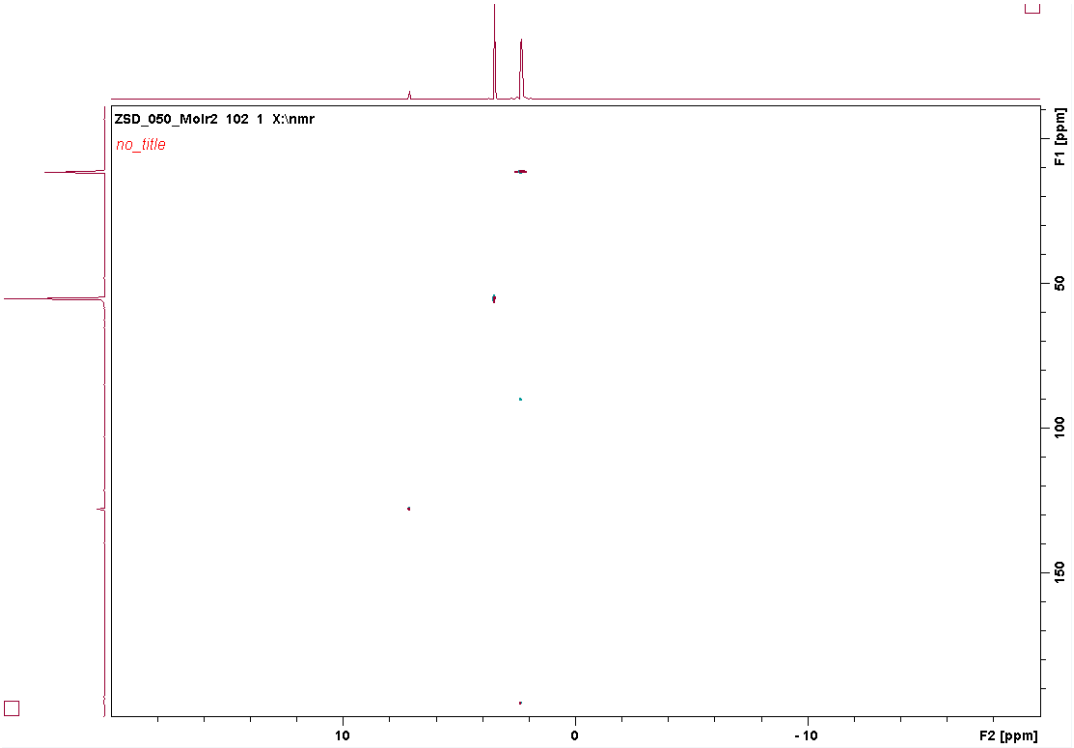


Figure S 9 : ^{1}H-^{13}C HSQC 2D NMR spectrum of compound 2 in C_6D_6 solution, recorded at 500 MHz, 298K. Spectra presented along axes are external projections (for clarity) of ^{1}H and ^{13}C spectra recorded on the same sample.

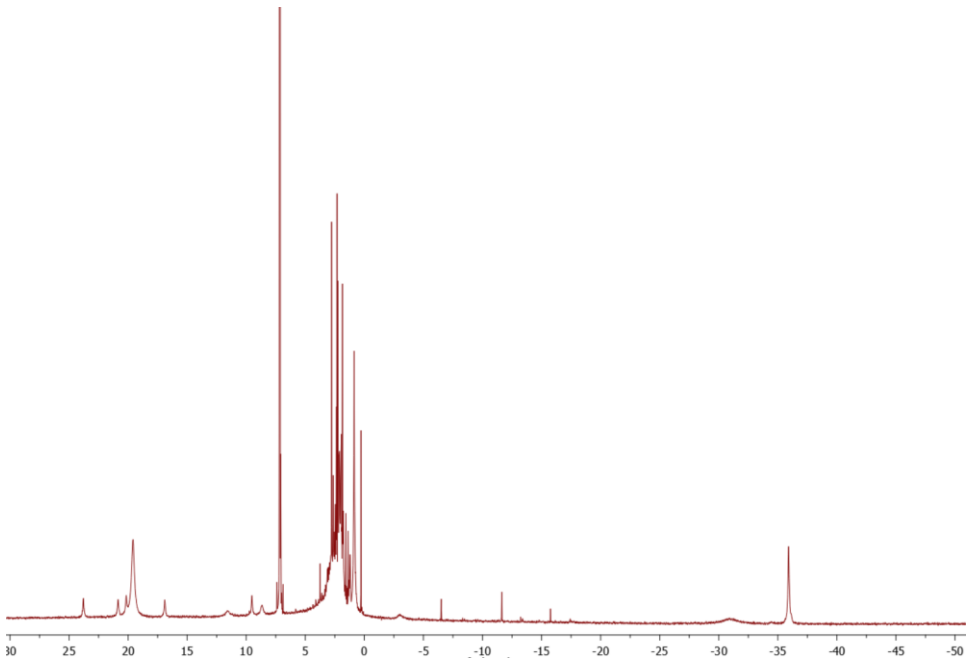


Figure S 10 : The reaction of 1 with CO_2 yields many products, as shown by ^{1}H NMR analysis of the crude reaction mixture. This particular reaction was exposed to an excess of CO_2 in C_6D_6 (300 MHz, 298K) at room temperature but similar results were obtained from reactions performed with stoichiometric amounts of CO_2, reduced temperature or with the exclusion of light.

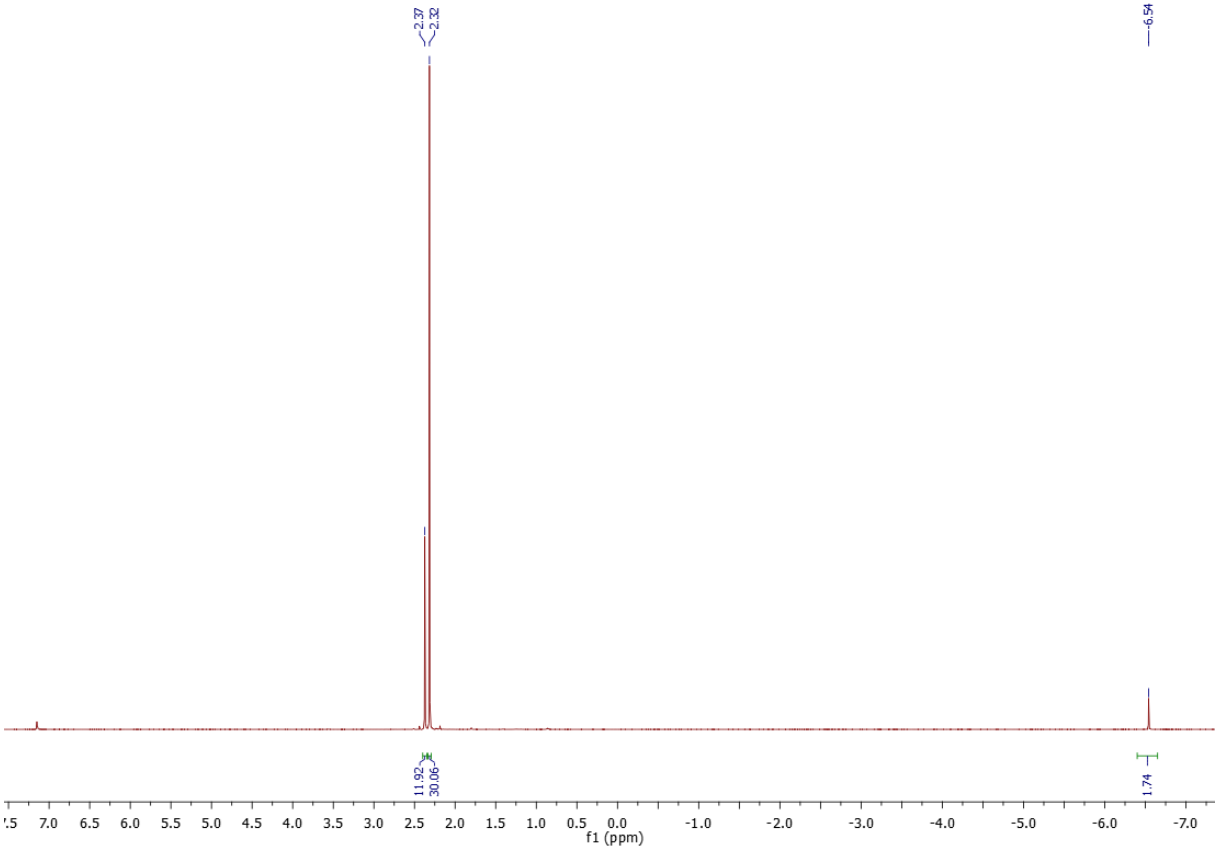


Figure S 11 : ^{1}H NMR spectrum of compound 3 in C_6D_6 solution, recorded at 500 MHz, 298K.

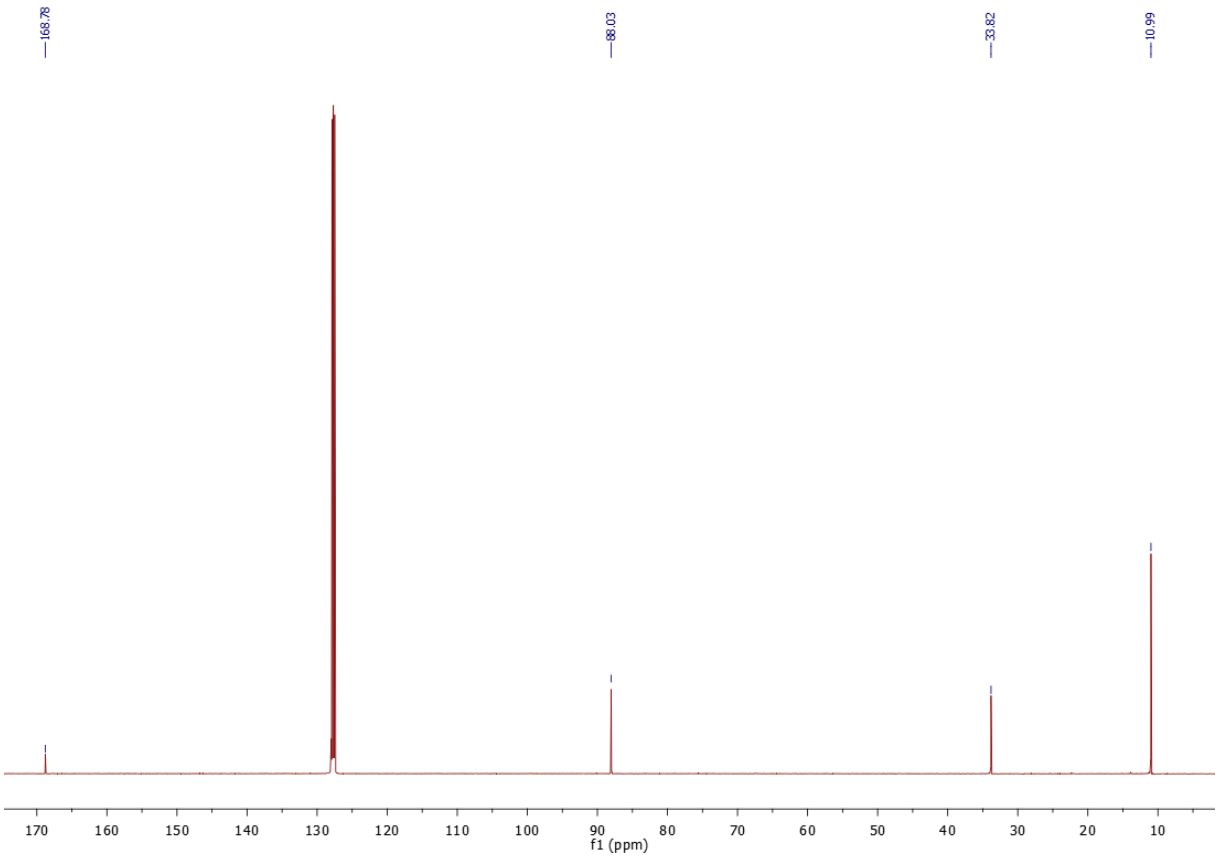


Figure S 12: ^{13}C NMR spectrum of compound 3 in C_6D_6 solution, recorded at 125 MHz, 298K.

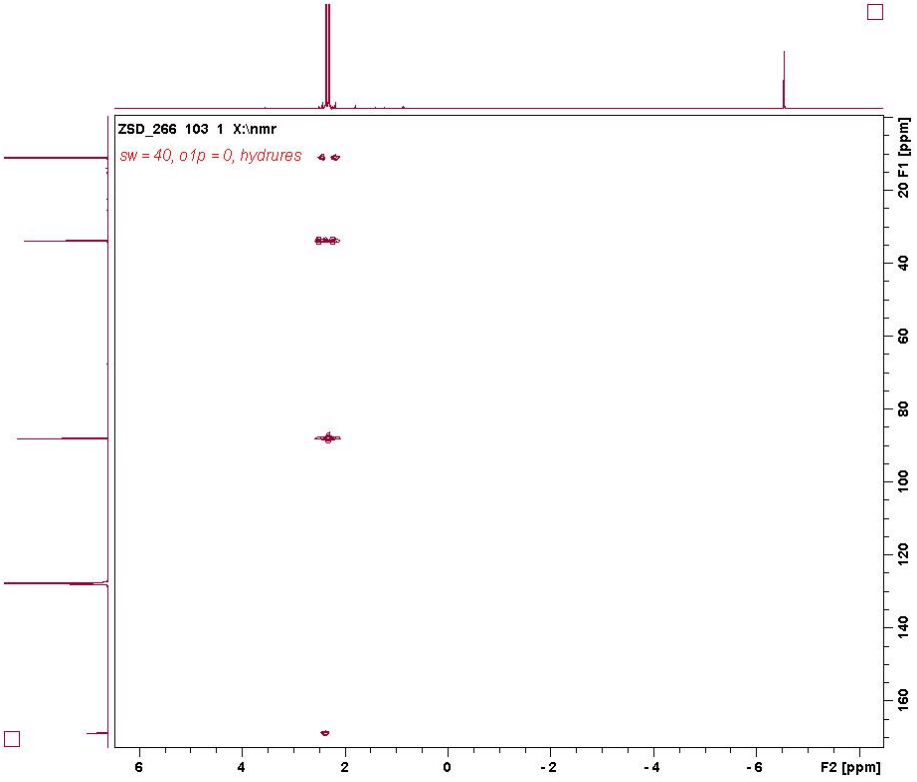


Figure S 13 ^{1}H-^{13}C HMBC 2D NMR spectrum of compound 3 in C_6D_6 solution, recorded at 500 MHz, 298K. Spectra presented along axes are external projections (for clarity) of ^{1}H and ^{13}C spectra recorded on the same sample.

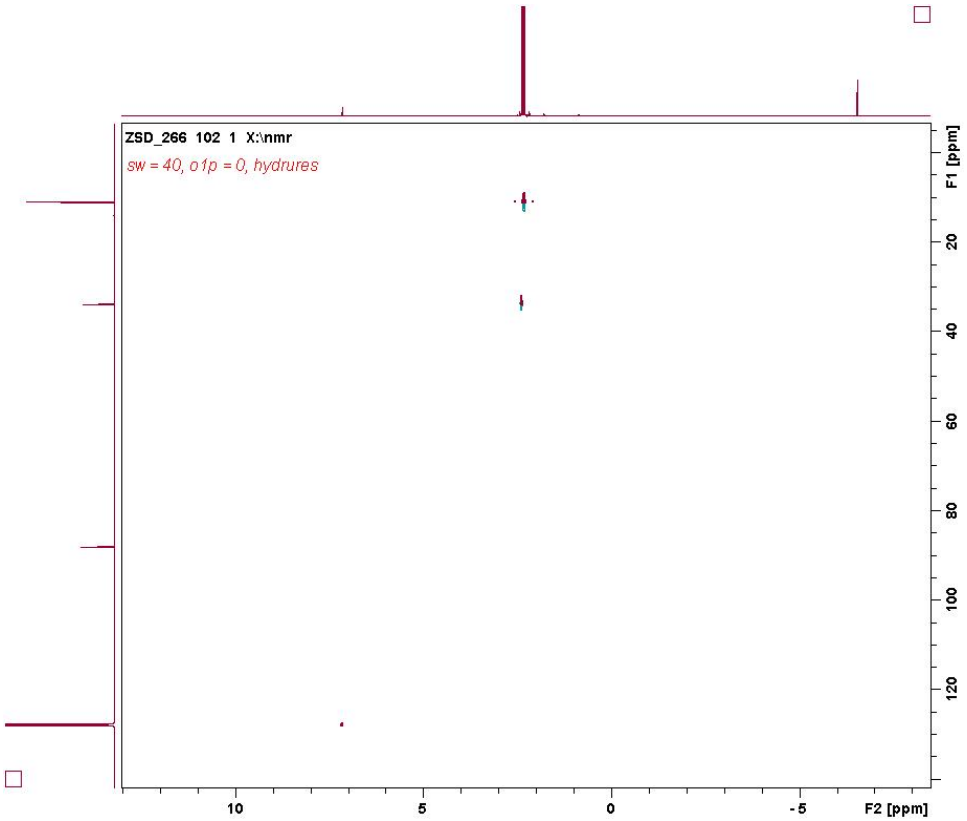


Figure S 14 ^{1}H-^{13}C HSQC 2D NMR spectrum of compound 3 in C_6D_6 solution, recorded at 500 MHz, 298K. Spectra presented along axes are external projections (for clarity) of ^{1}H and ^{13}C spectra recorded on the same sample.

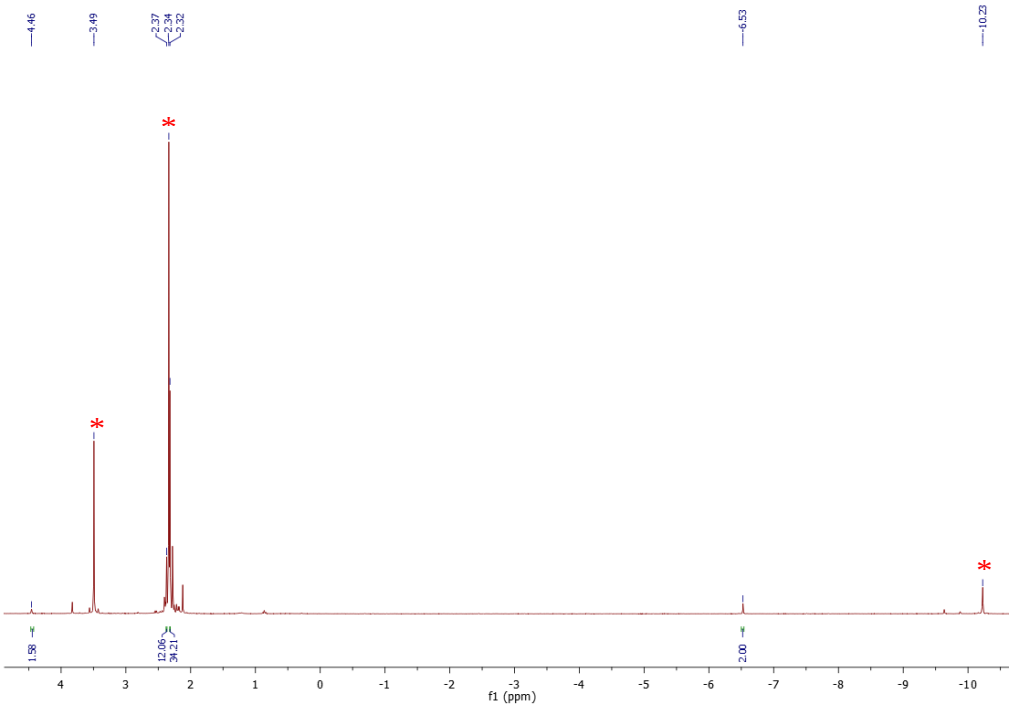


Figure S 15 : ^{1}H NMR spectrum of the crude reaction mixture from the synthesis of 3 in a J-Young NMR tube filled with C_6D_6, recorded at 300 MHz, 298K. This allows for the detection and titration of dihydrogen produced in this reaction. The starting material, complex 2, is marked with red asterisks (*). The necessarily small headspace in the J-Young tube only permits a substoichiometric volume of CO_2 and therefore the reaction cannot go to completion. Dihydrogen (4.46 ppm, chemical shift consistent with literature [8]) can be observed in about 1 equivalent ratio with the product, complex 3.

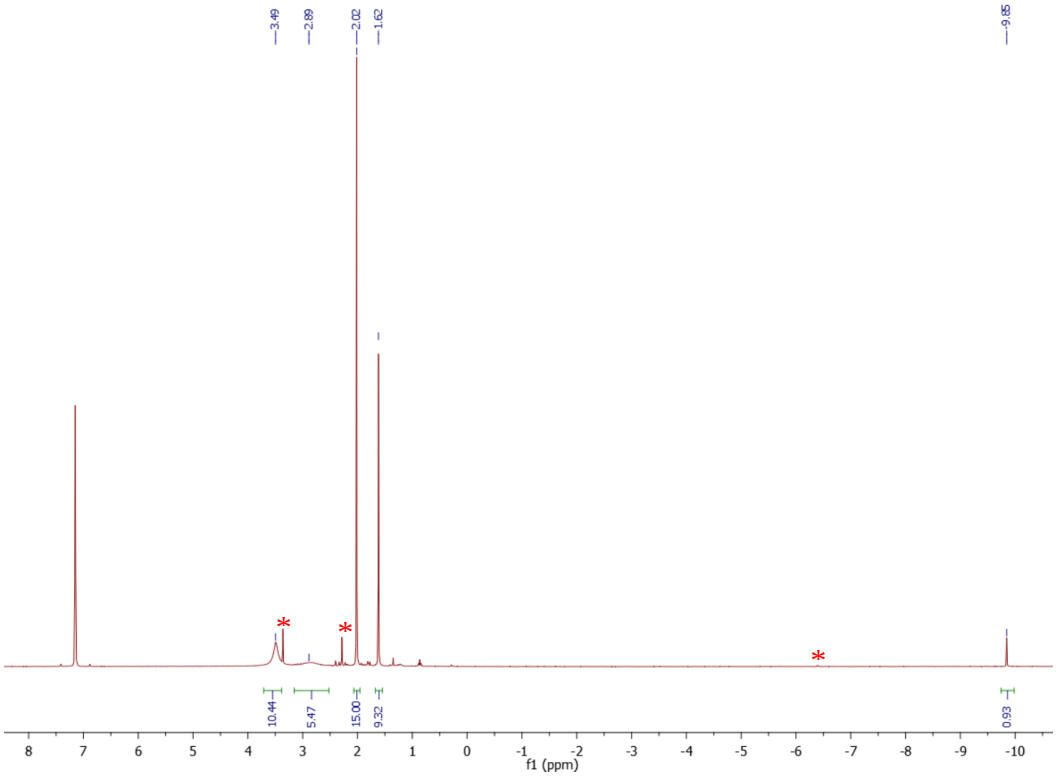


Figure S 16 : ^{1}H NMR spectrum of complex 4 in C_6D_6 solution, recorded at 298K, 300 MHz. The broad signals at 3.49 and 2.89 ppm correspond to the Mo-NMe_2 and the urea NMe_2 moieties, respectively. Some unreacted 1 can be observed and is marked with a red asterisk.

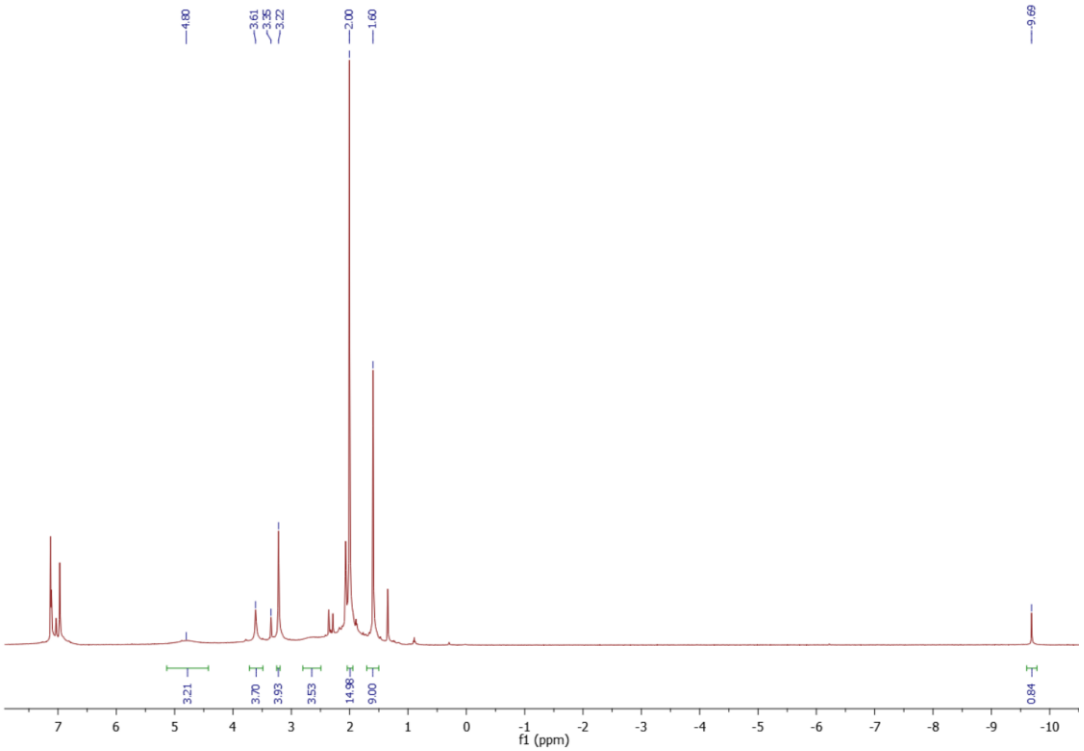


Figure S 17 : ^{1}H NMR spectrum of complex 4 in toluene-*d*8 solution, recorded at 248K, 500 MHz. One can observe some deconvolution of the signals for the NMe_2 signals at this reduced temperature however, the assignment is unclear.

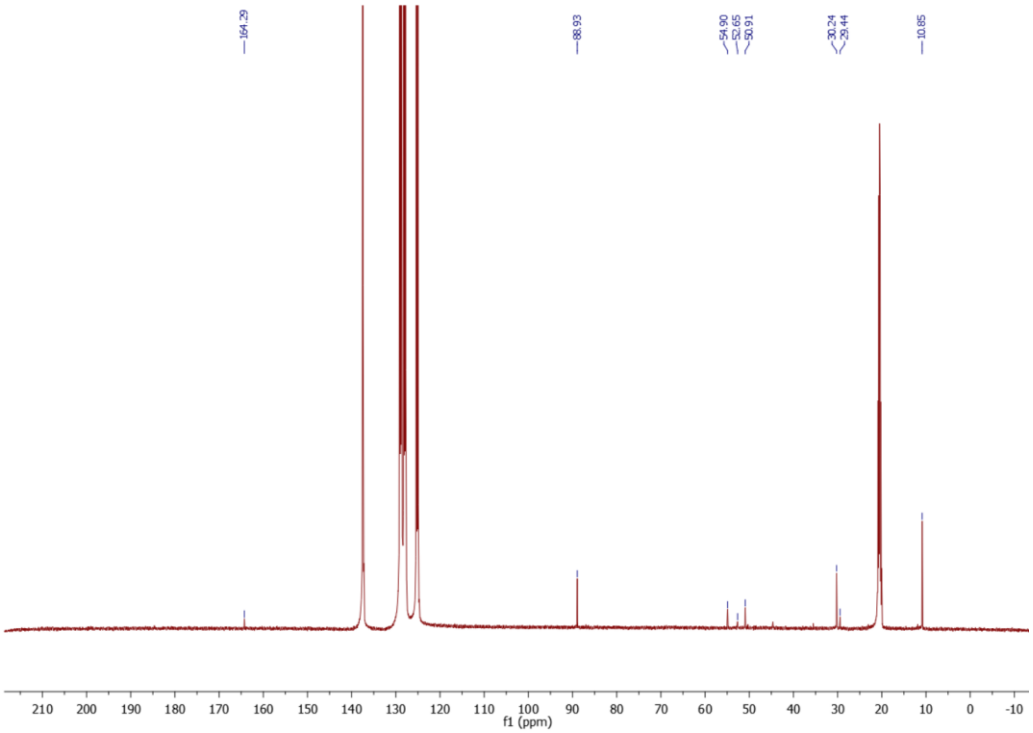


Figure S 18 : ^{13}C NMR spectrum of complex 4 in toluene-*d*8 solution, recorded at 248K to avoid the conversion of the complex to 5 at room temperature.

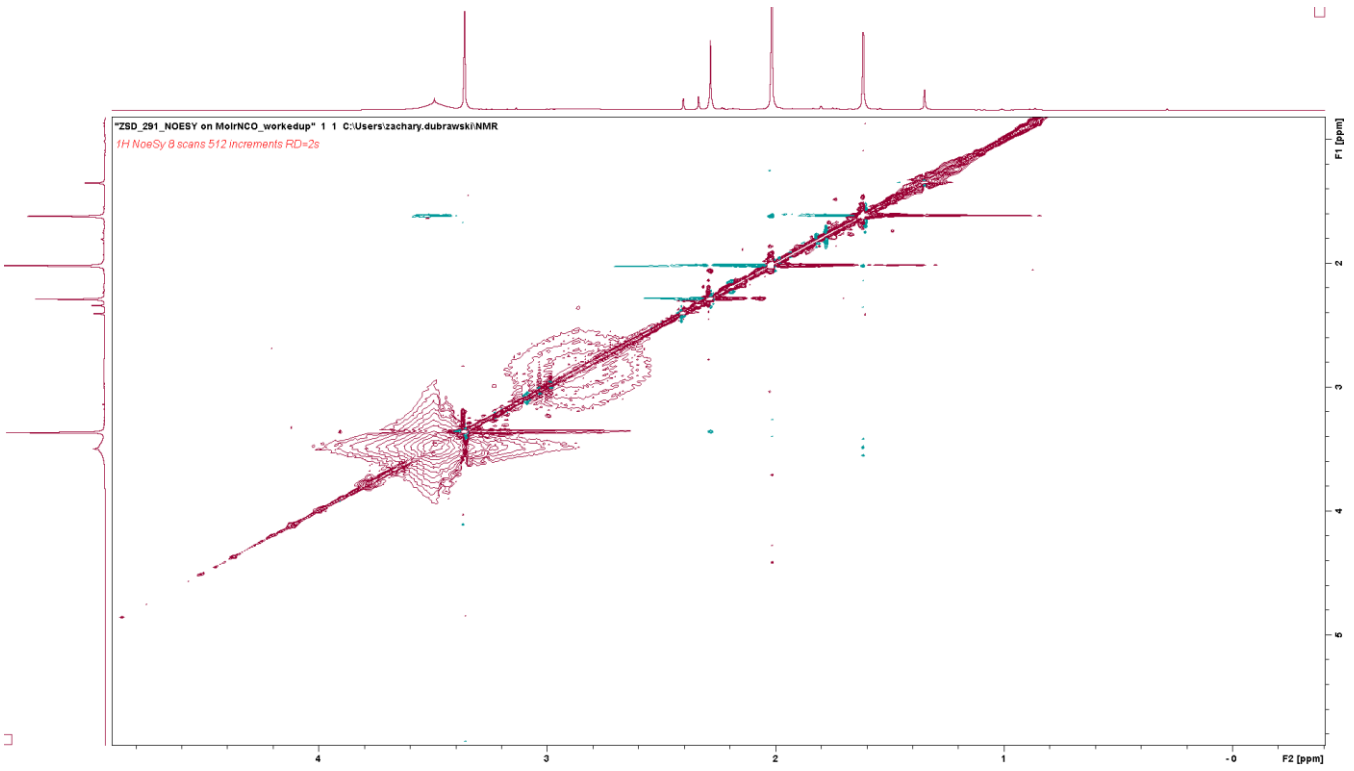


Figure S 19 : The NOESY spectrum (EXSY) of compound 4 in C_6D_6 with a very large broad signal between the NMe_2 groups of compound 4 (3.48ppm) and those of compound 1 (3.36 ppm). The cross peak(s) are in-phase with the diagonal, consistent with chemical exchange. They are however, extremely broad and could be a chemical exchange process with the other NMe_2 groups on complex 4 at (2.86 ppm).

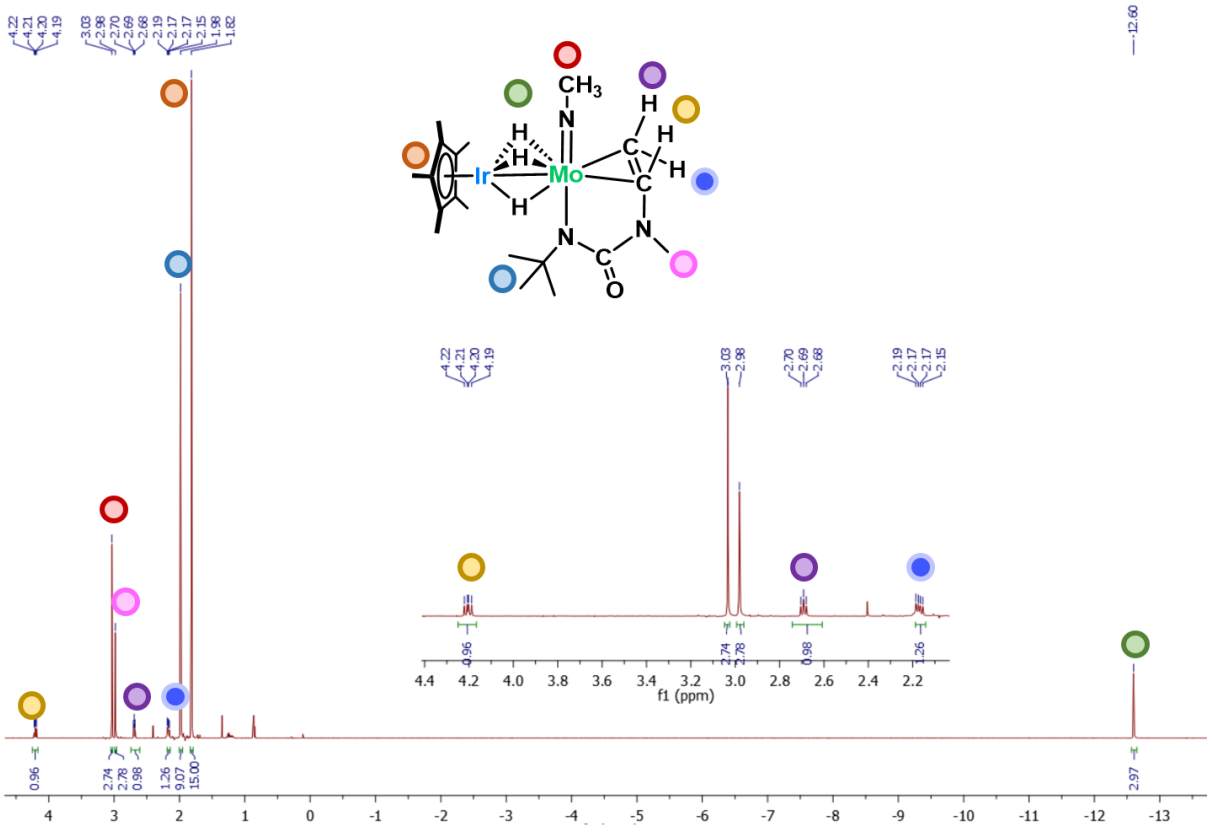


Figure S 20 : ^{1}H NMR spectrum of compound 5 in C_6D_6 solution, recorded at 500 MHz, 298K. The inset is expanding the region between 4.5 – 2.0 ppm, highlighting the diasterotopic protons on the metallacyclopropane moiety.

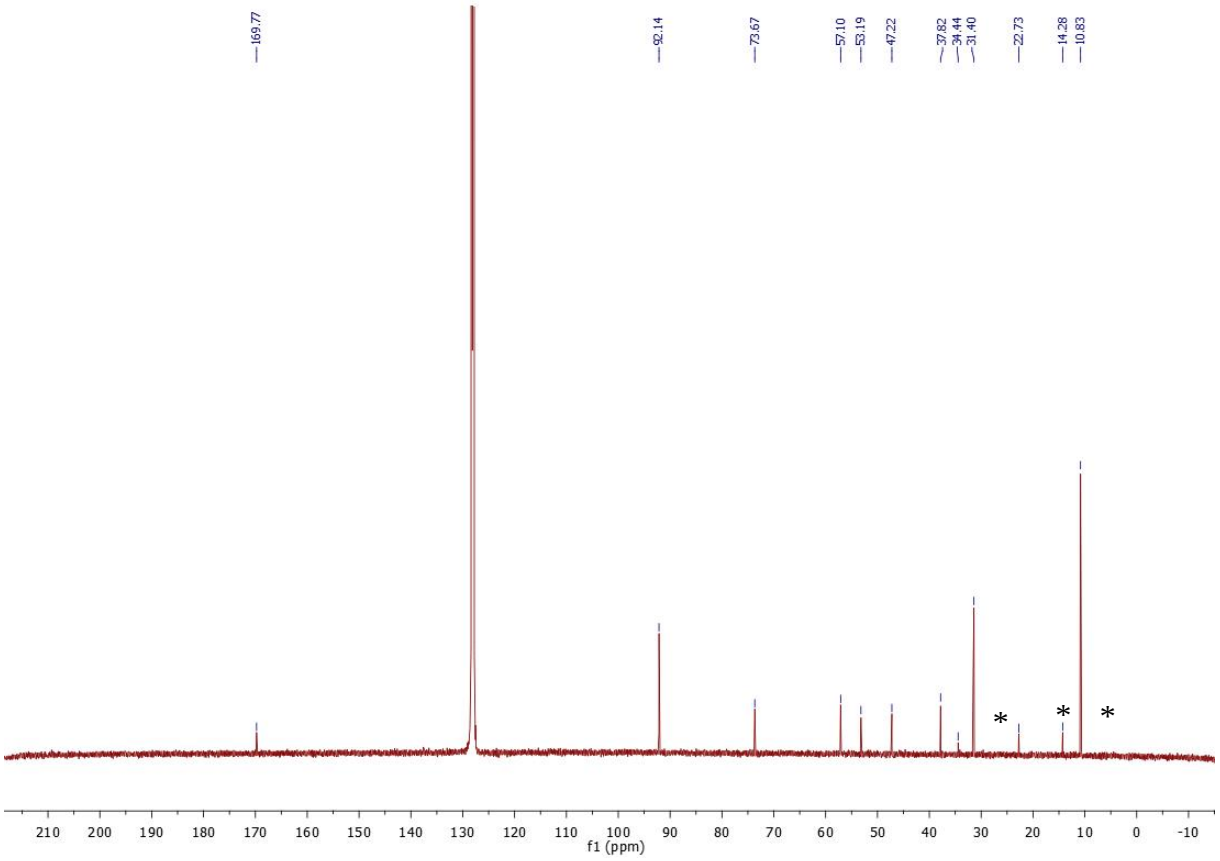


Figure S 21 : ^{13}C NMR spectrum of compound 5 in C_6D_6 solution, recorded at 125 MHz, 298K. Pentane impurity peaks marked with an asterisk (*).

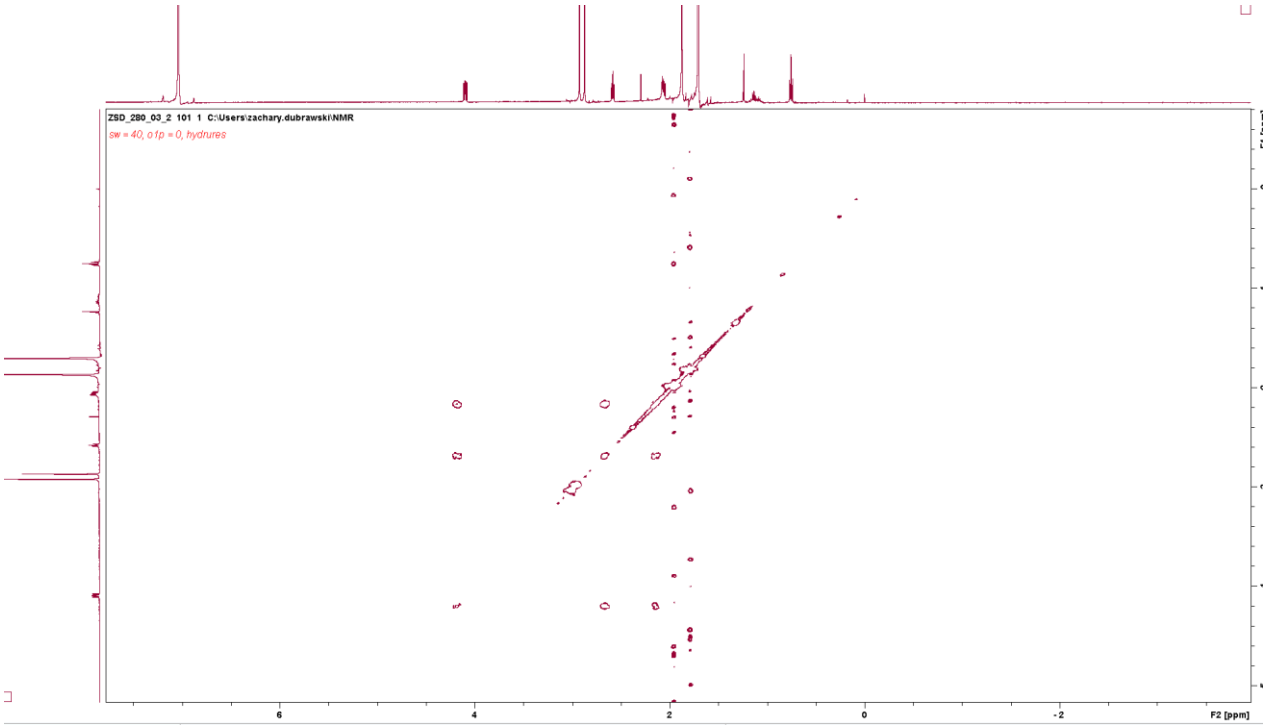


Figure S 22 : ^{1}H-^{1}H COSY 2D NMR spectrum of compound 5 in C_6D_6 solution, recorded at 500 MHz, 298K. Spectra presented along axes are external projections (for clarity) of ^{1}H spectra recorded on the same sample.

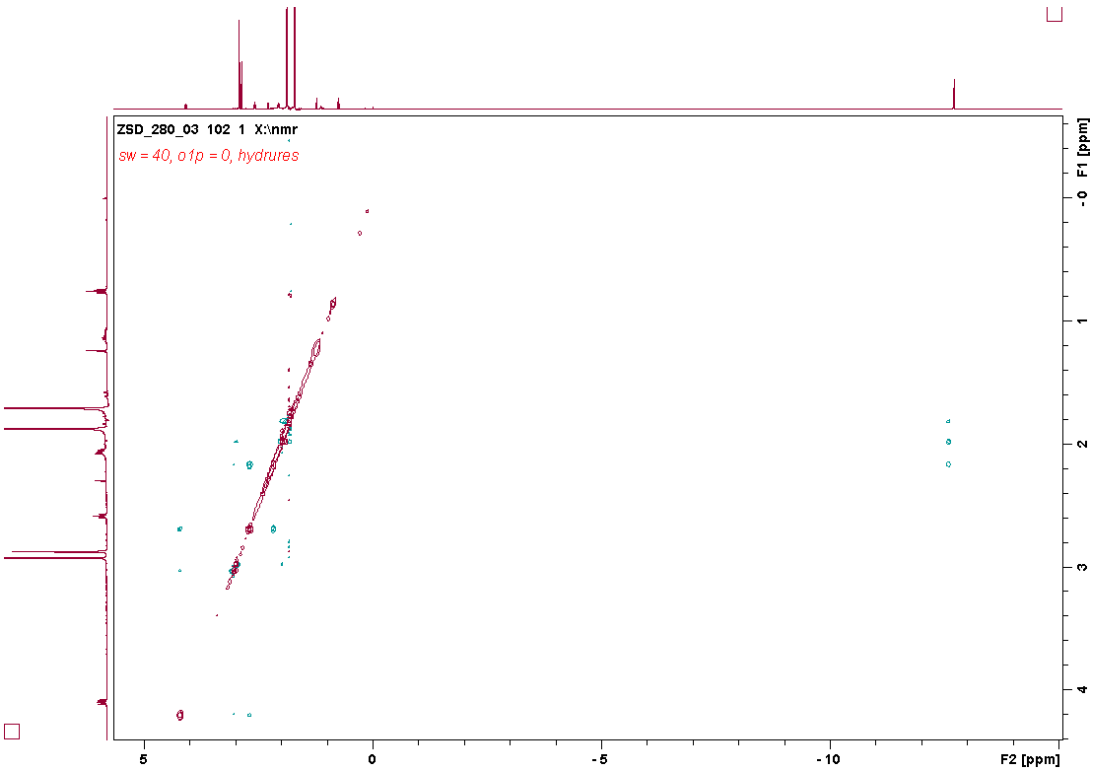


Figure S 23 : 2D ^{1}H-^{1}H NOESY NMR spectrum of compound 5 in C_6D_6 solution, recorded at 500 MHz, 298K. Spectra presented along axes are external projections (for clarity) of ^{1}H spectra recorded on the same sample.

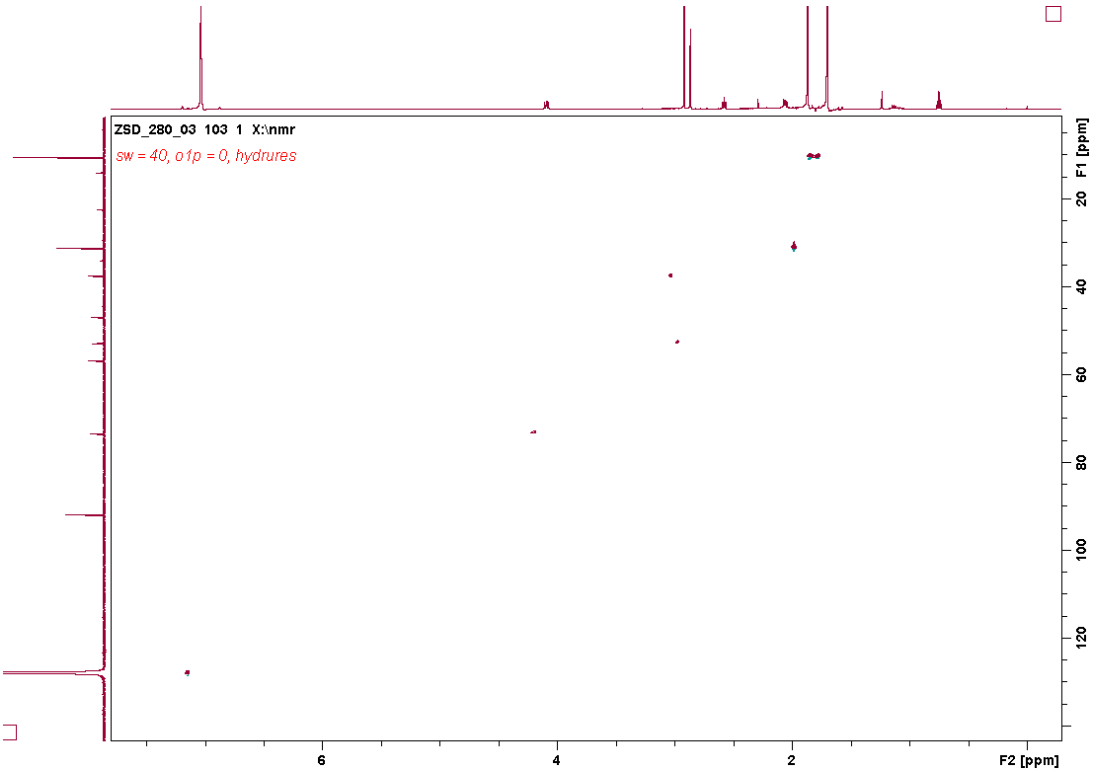


Figure S 24 : ^{1}H-^{13}C HSQC 2D NMR spectrum of compound 5 in C_6D_6 solution, recorded at 500 MHz, 298K. Spectra presented along axes are external projections (for clarity) of ^{1}H and ^{13}C spectra recorded on the same sample.

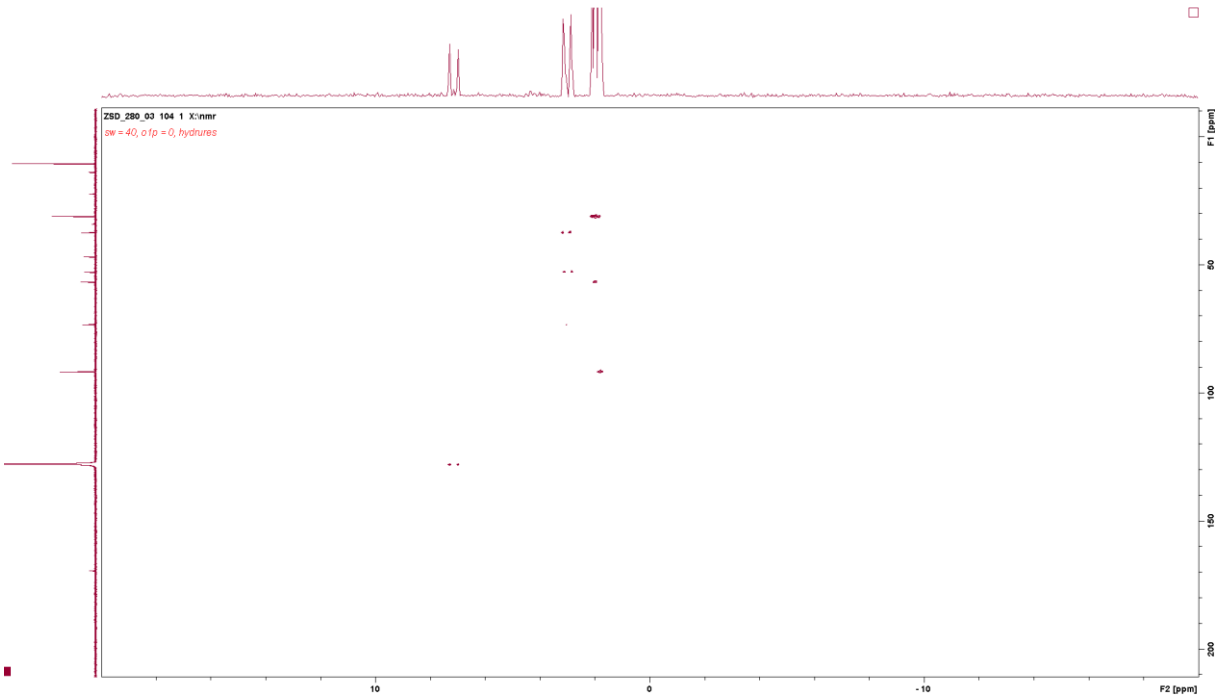


Figure S 25 : ^{1}H-^{13}C HMBC 2D NMR spectrum of compound 5 in C_6D_6 solution, recorded at 500 MHz, 298K. Spectra presented along axes are external projections (for clarity) of ^{1}H and ^{13}C spectra recorded on the same sample.

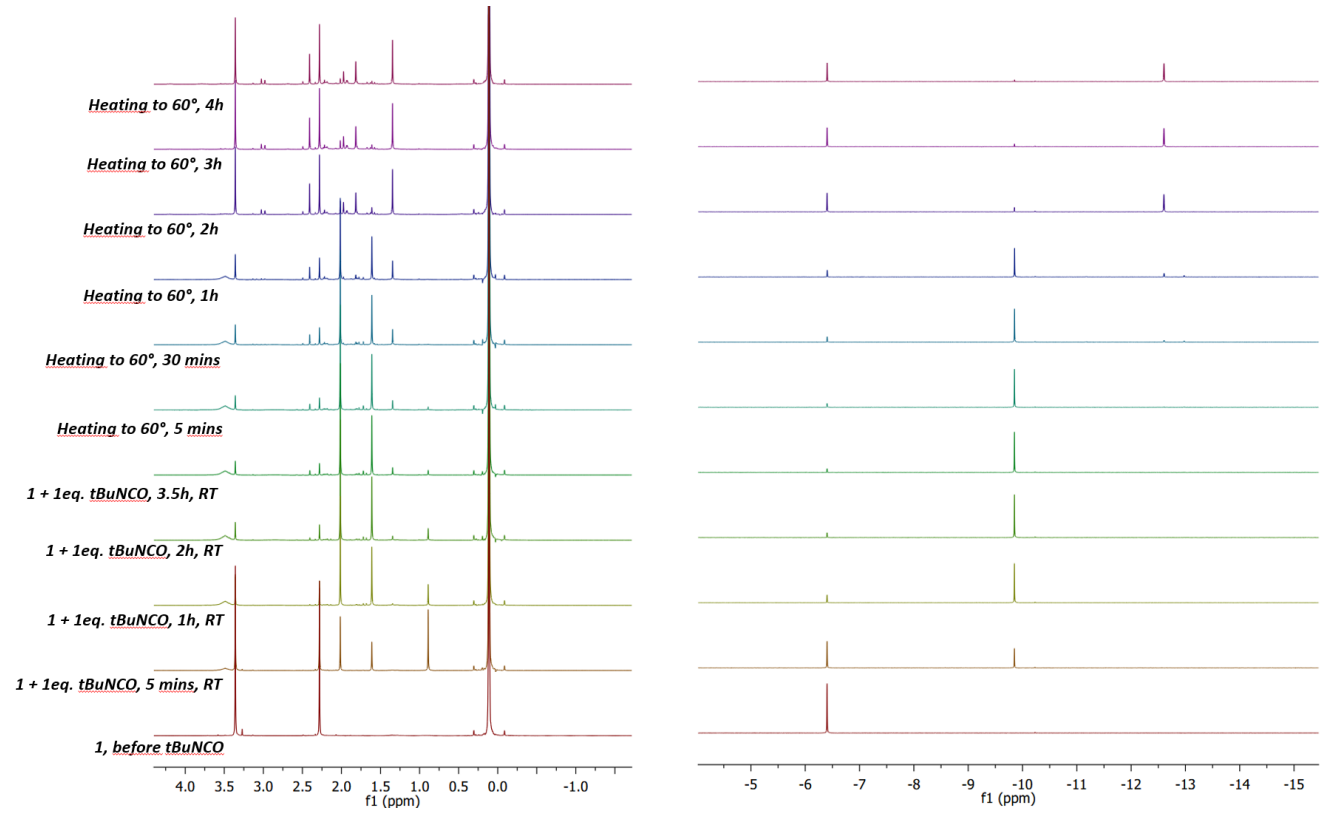


Figure S 26 : ^{1}H NMR spectra recorded (300 MHz, 298K, d1 = 20s) in C_6D_6 (with 0.184 M HMDSO as internal standard, 0.01 ppm) during the reaction of 1 with one equivalent of tBuNCO, passing through complex 4 to yield complex 5. The consumption and subsequent regeneration of 1 can be most easily observed from the hydride signal at -6.4 ppm. Complex 4 converts to 5 at room temperature (as observed in the signal at 1.8 ppm, attributed to the Cp*- Me moiety) however, heating was used to ensure conversion and a timely experiment duration.

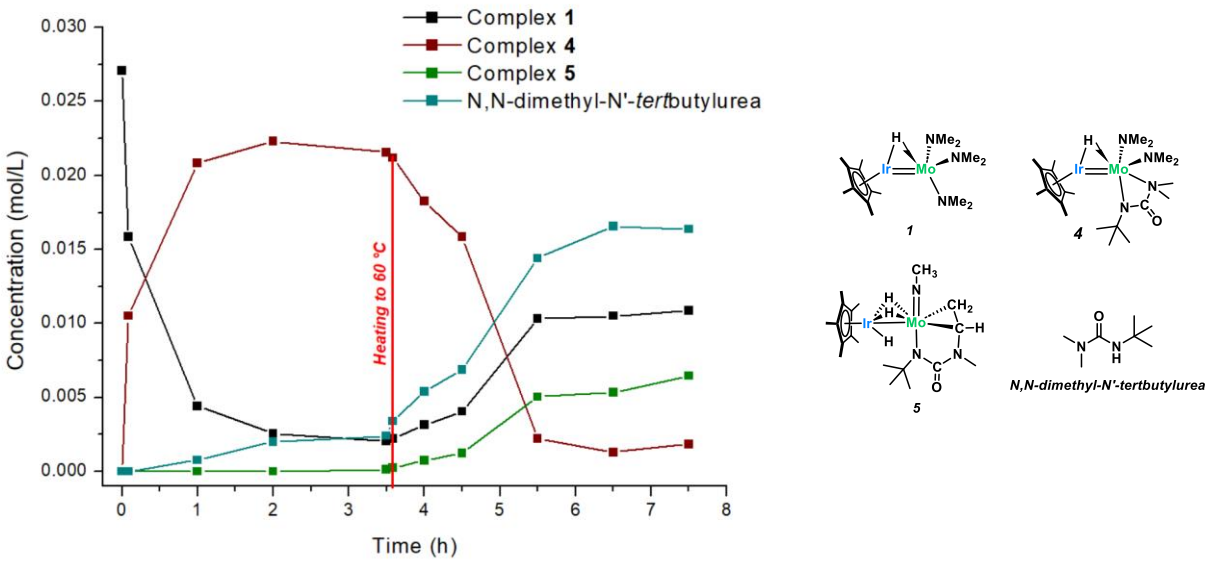


Figure S 27: Concentrations of species from Figure S 26 as determined from NMR integration against the HMDSO internal standard compared to the Cp* groups of 1, 4 and 5 and the *t*Bu group of the N,N-dimethyl-N'-tert-butyl-urea. The concentration of the urea equals 95% of the sum of the final concentrations of 1 and 4 Note that the yield of 5 from this reaction (24%) is quite low

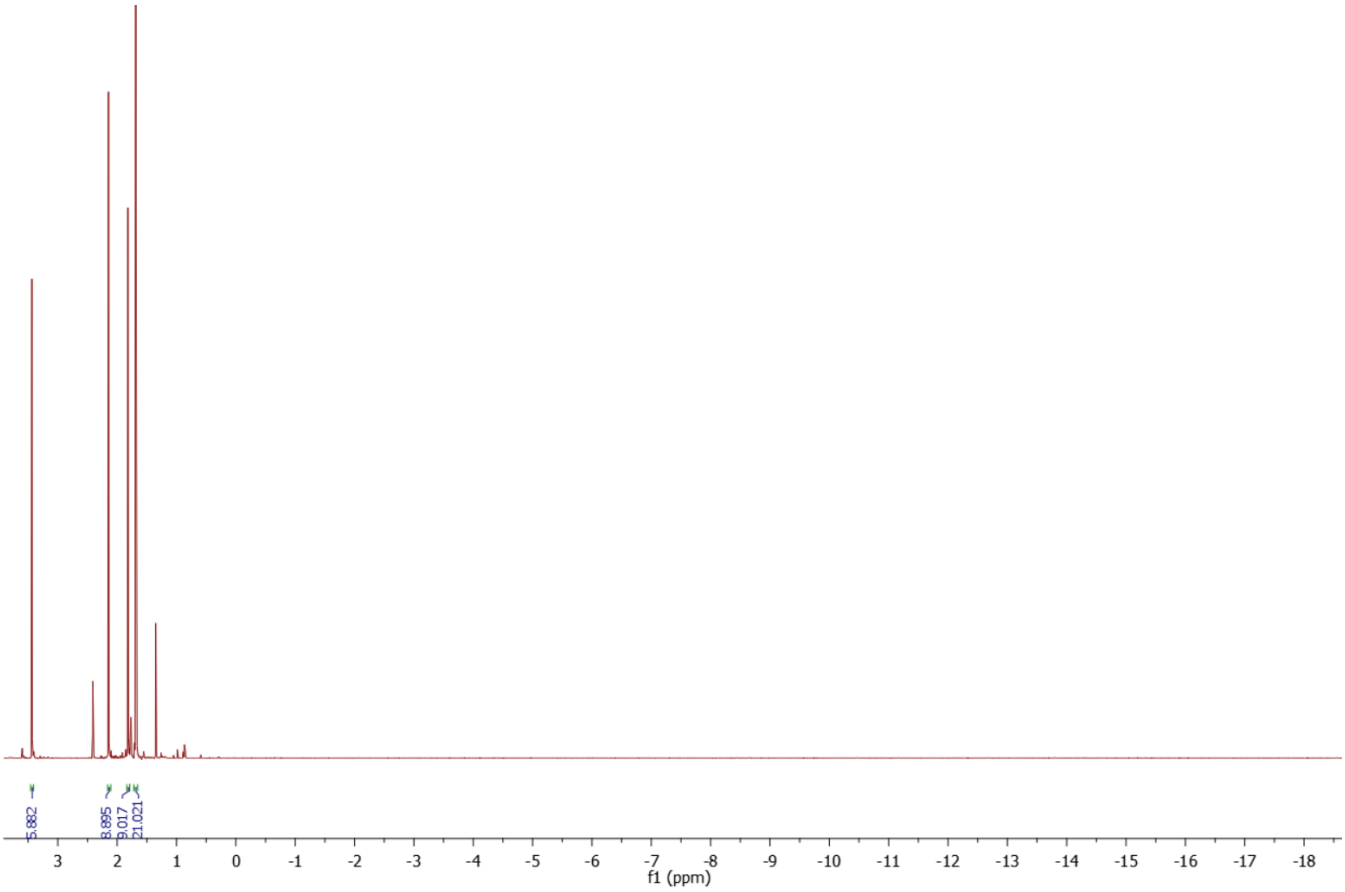


Figure S 28 : ^{1}H NMR spectrum of compound 6 in C_6D_6 solution, recorded at 500 MHz, 298K.

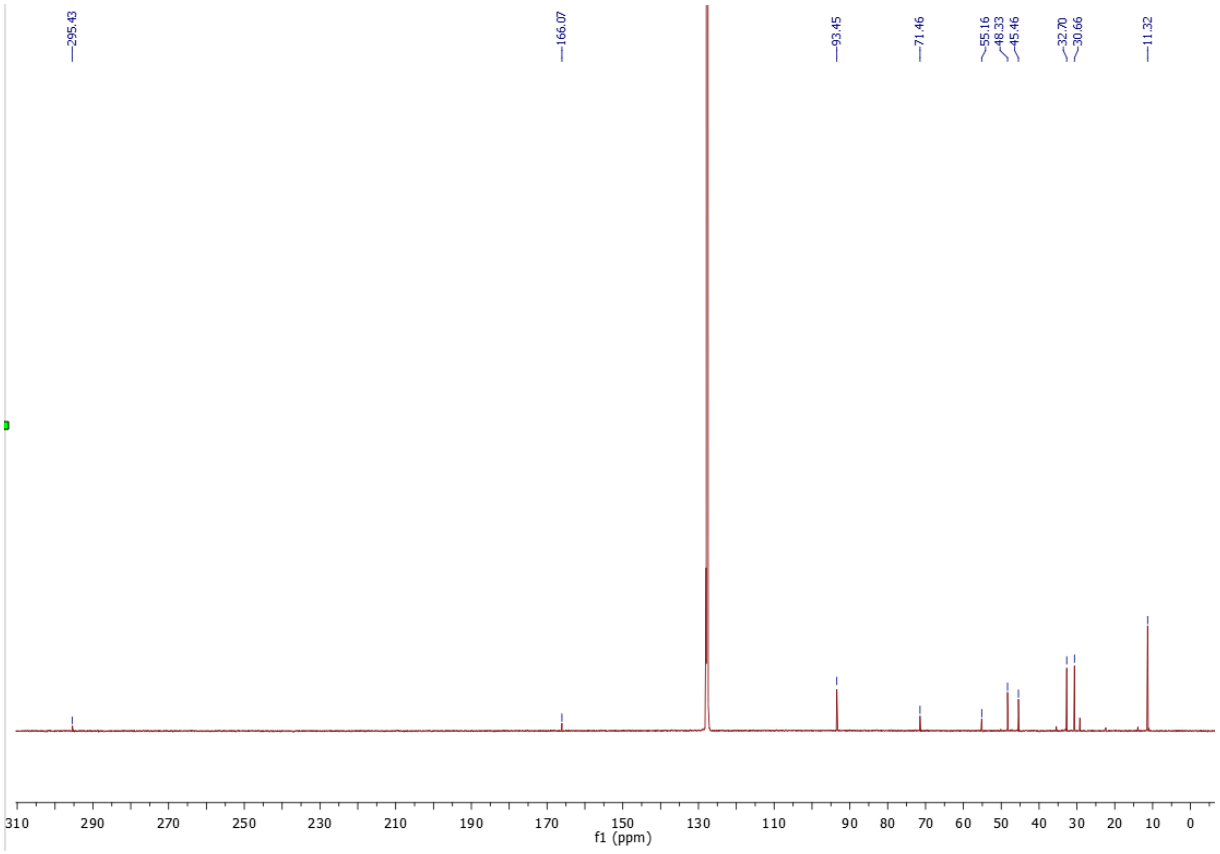


Figure S 29 : ^{13}C NMR spectrum of compound 6 in C_6D_6 solution, recorded at 125 MHz, 298K.

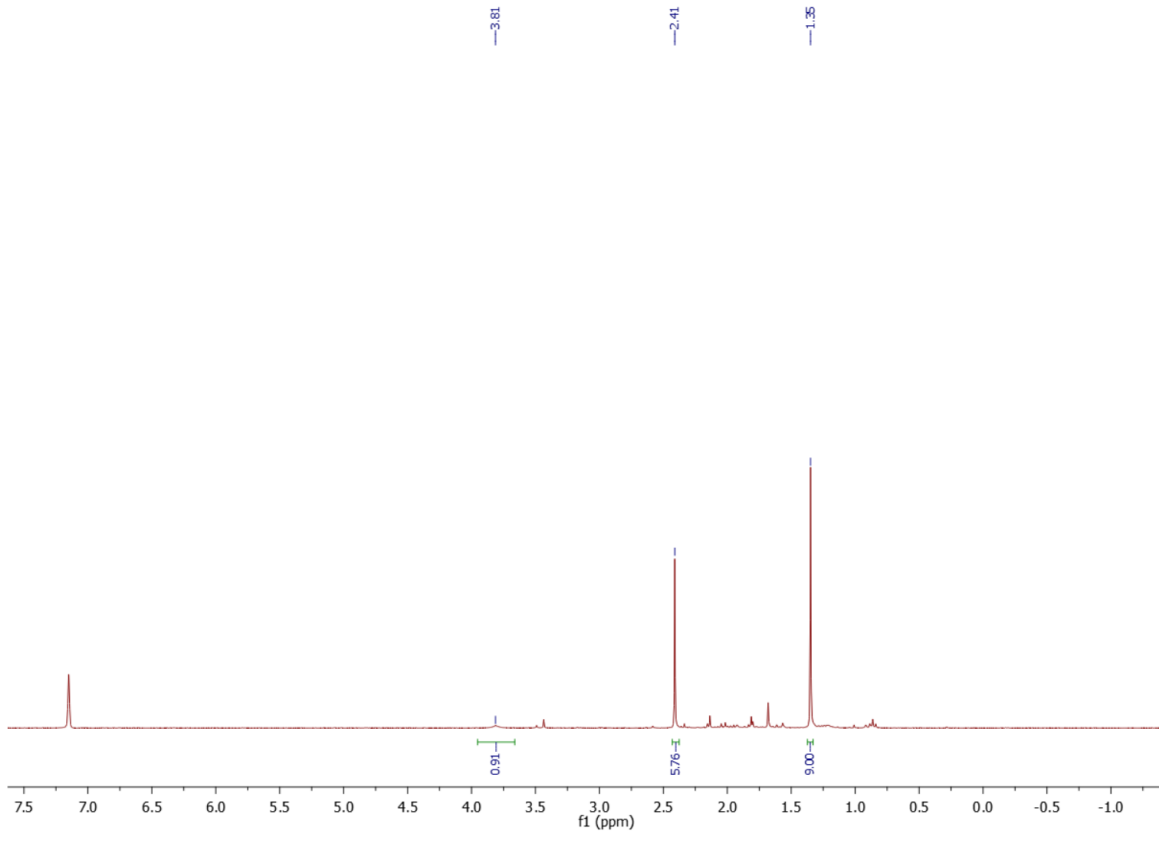


Figure S 30 : ^{1}H NMR spectrum of N,N-dimethyl-N'-*tert*butylurea isolated from the reaction mixture, recorded in C_6D_6 solution, at 300 MHz, 298K.

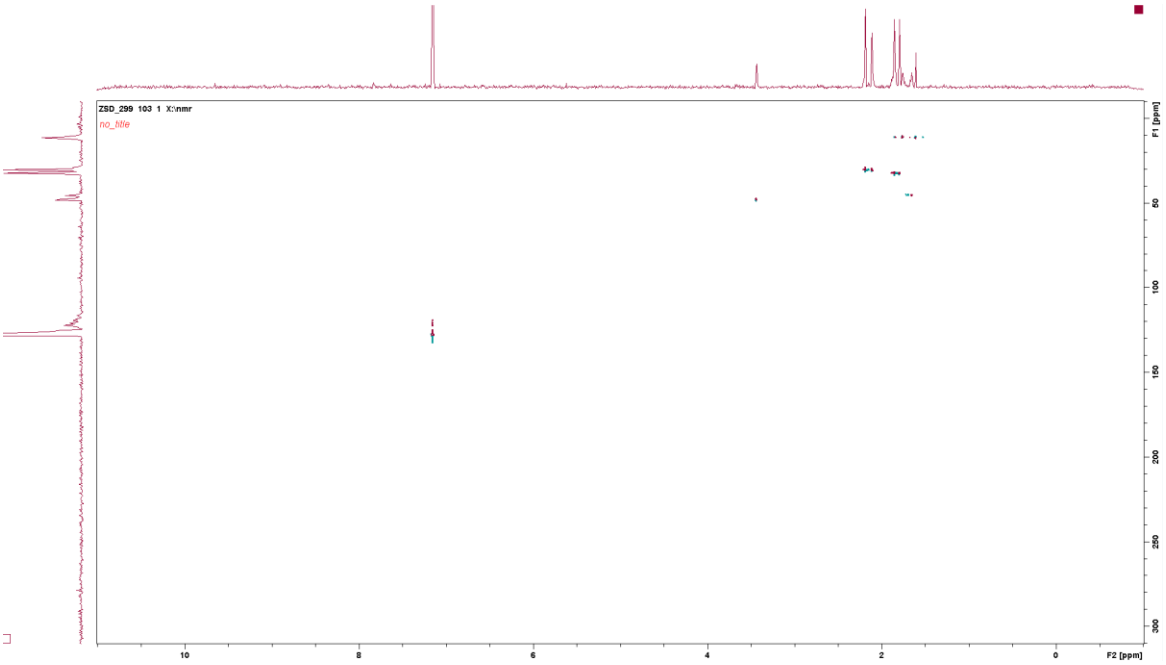


Figure S 31 : ^{1}H-^{13}C HSQC 2D NMR spectrum of compound 6 in C_6D_6 solution, recorded at 500 MHz, 298K.

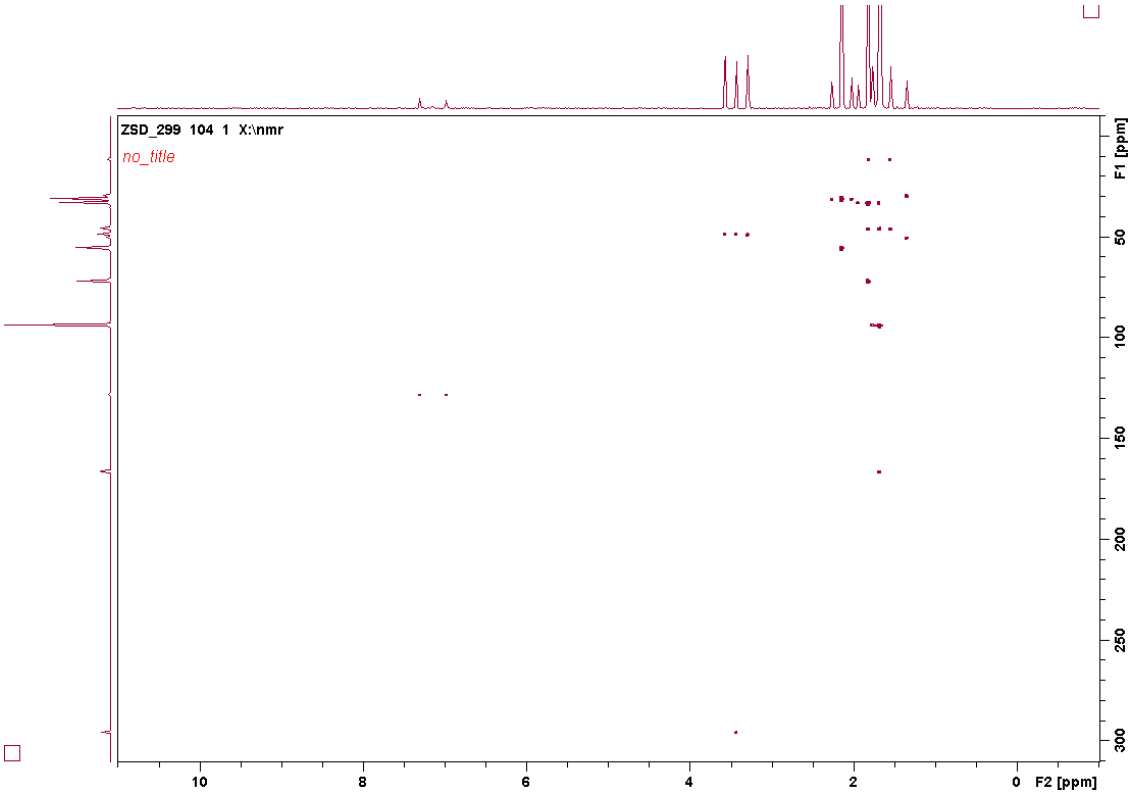


Figure S 32: ^{1}H-^{13}C HMBC 2D NMR spectrum of compound 6 in C_6D_6 solution, recorded at 500 MHz, 298K.

Diffuse Reflectance Infrared Fourier Transform (DRIFT) Spectra

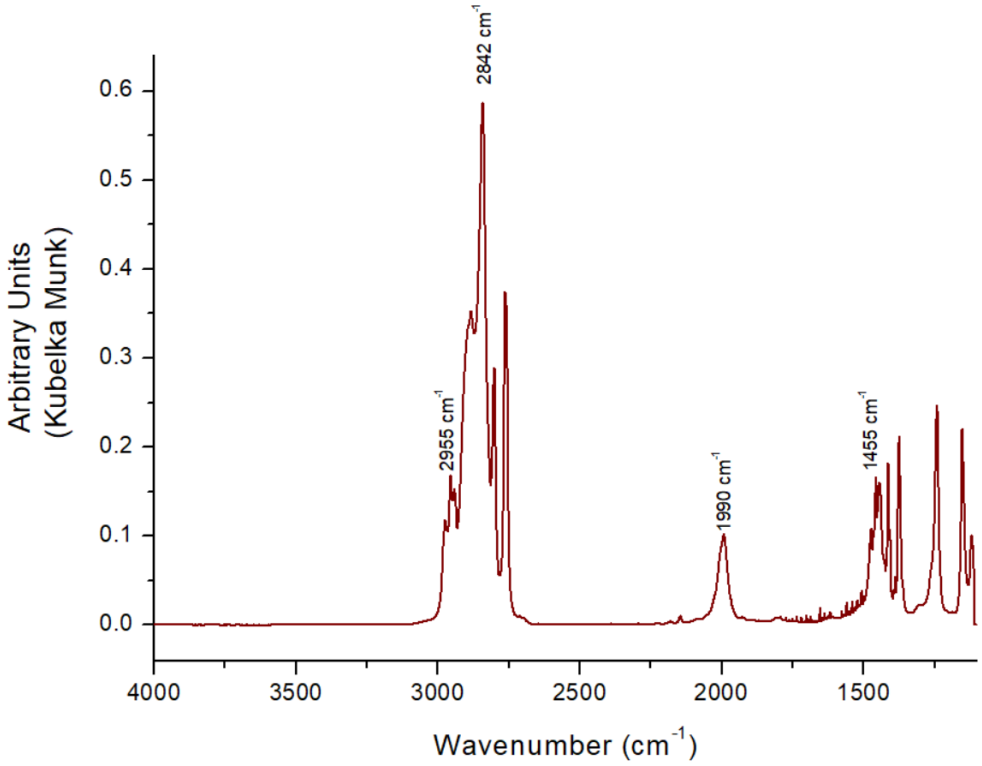


Figure S 33 : DRIFT spectrum of compound 1, diluted in KBr.

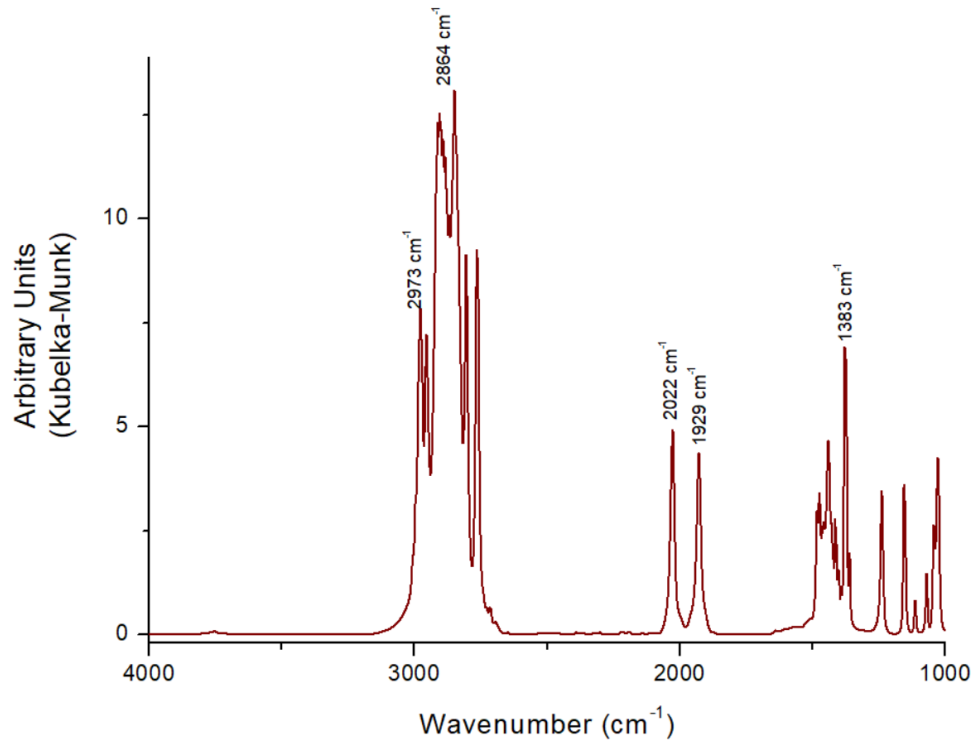


Figure S 34 : DRIFT spectrum of compound 2, pure crystalline material.

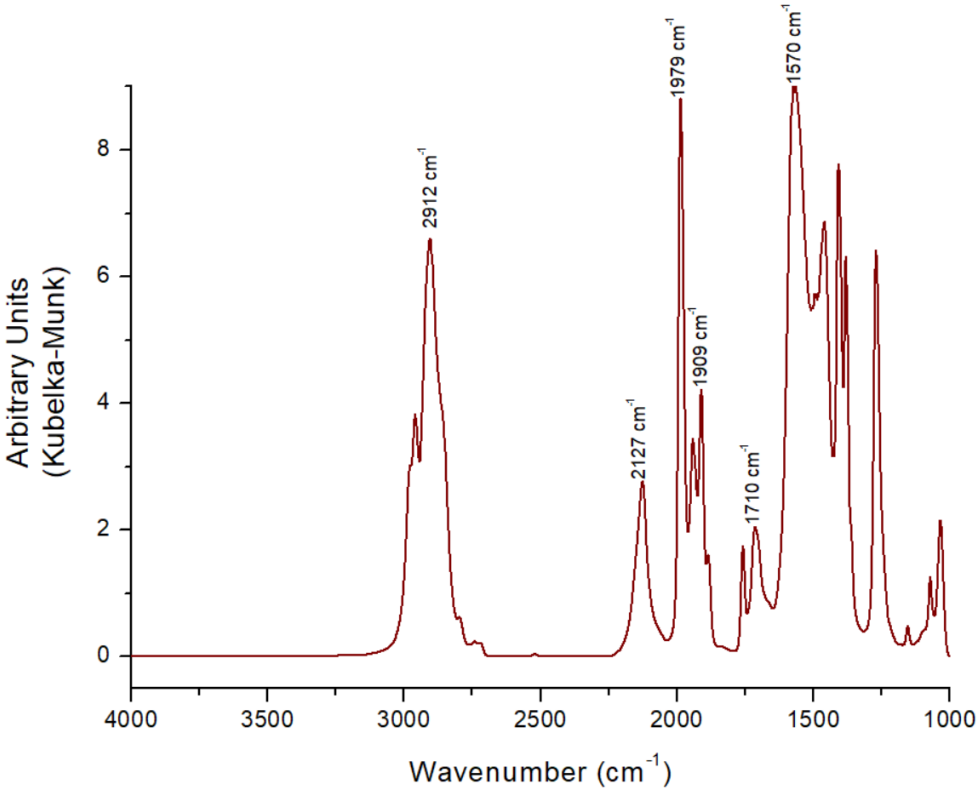


Figure S 35 : DRIFT spectrum of compound 3, pure crystalline material.

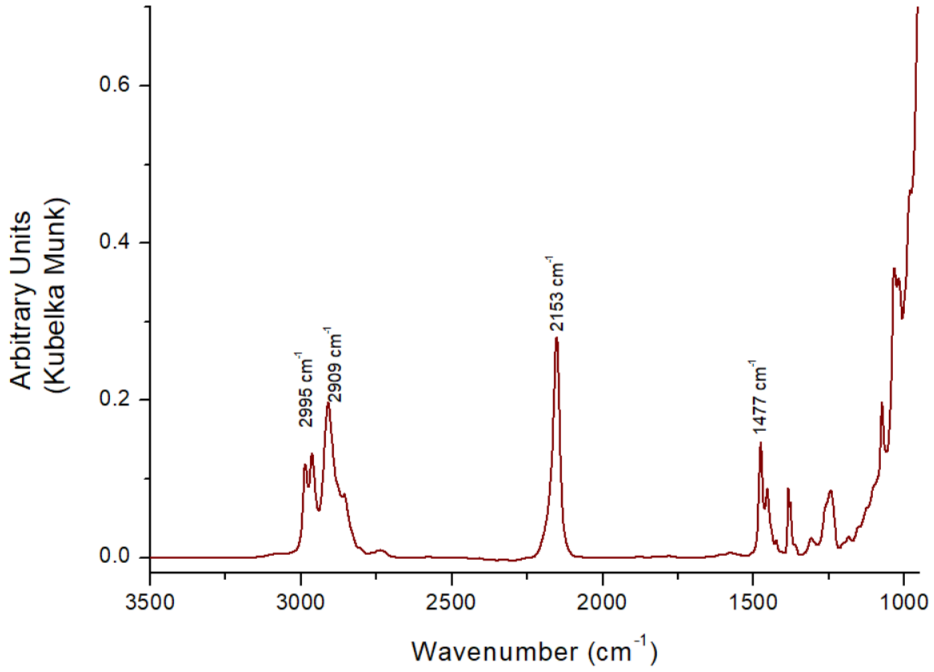


Figure S 36 : DRIFT spectrum of compound 4, diluted in KBr.

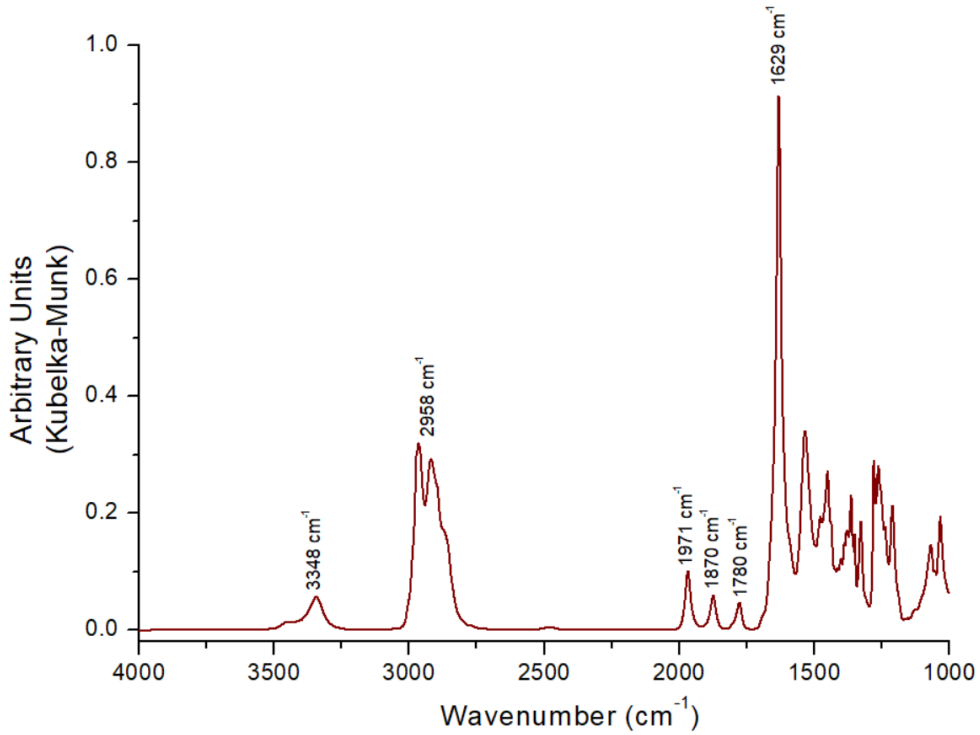


Figure S 37 : DRIFT spectrum of compound 5, diluted in KBr.

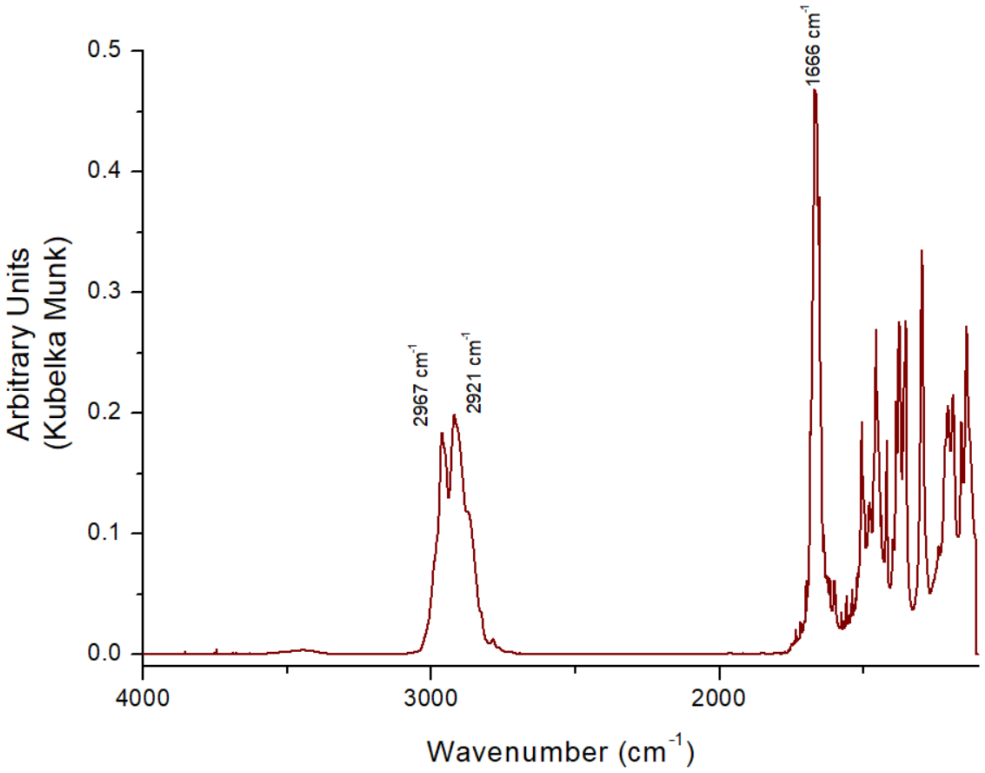


Figure S 38 : DRIFT spectrum of compound 6, diluted in KBr.

UV-Vis Spectra

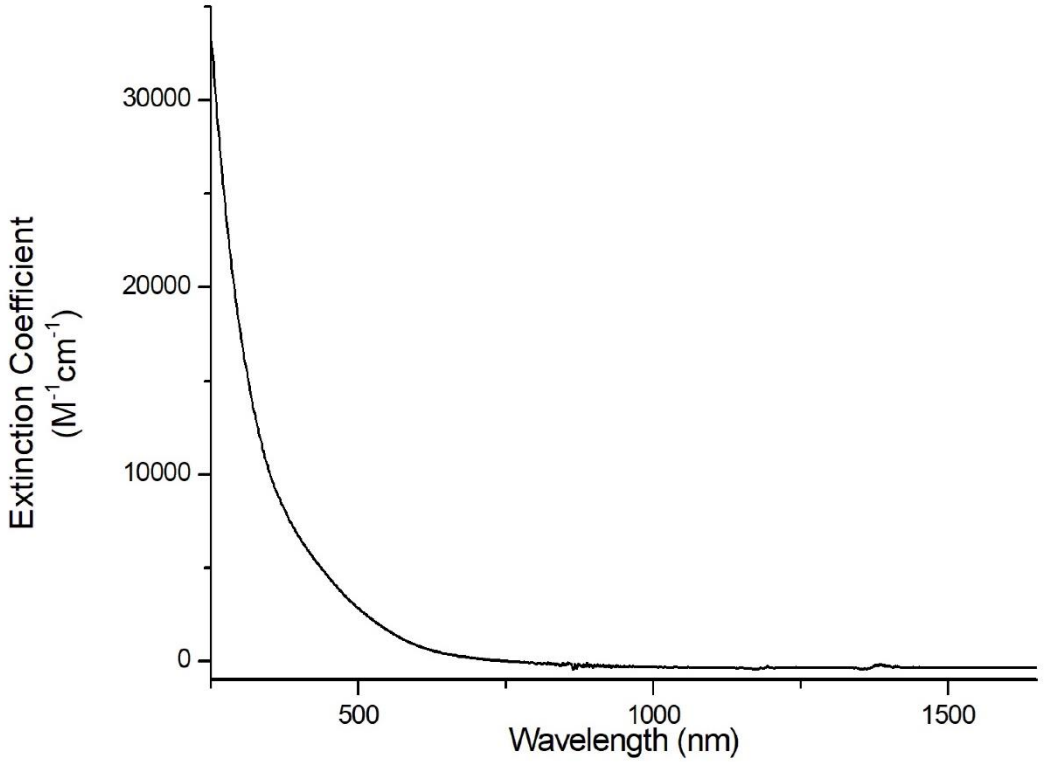


Figure S 39 : UV-Vis spectrum of 1, recorded in THF solution (0.061 mM). Signal noise at 850, 1200 and 1350 nm are artifacts from the instrument.

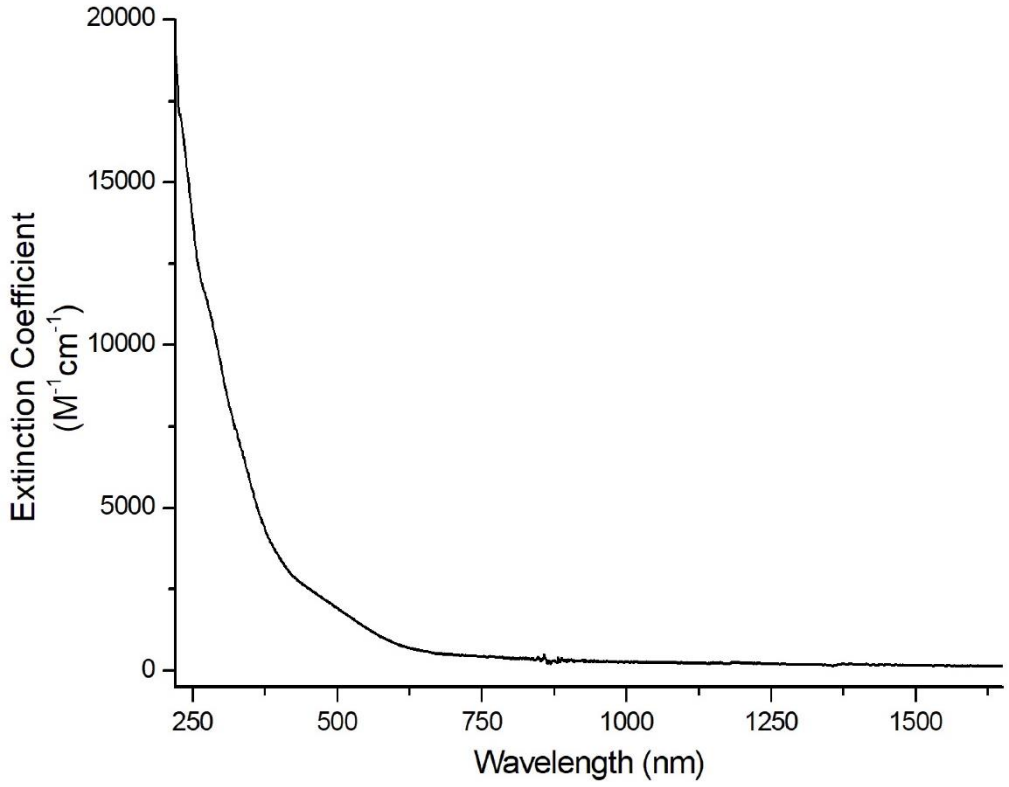


Figure S 40: UV-Vis spectrum of complex 2, recorded in THF solution (0.091 mM). Signal noise at 850, 1200 and 1350 nm are artifacts from the instrument

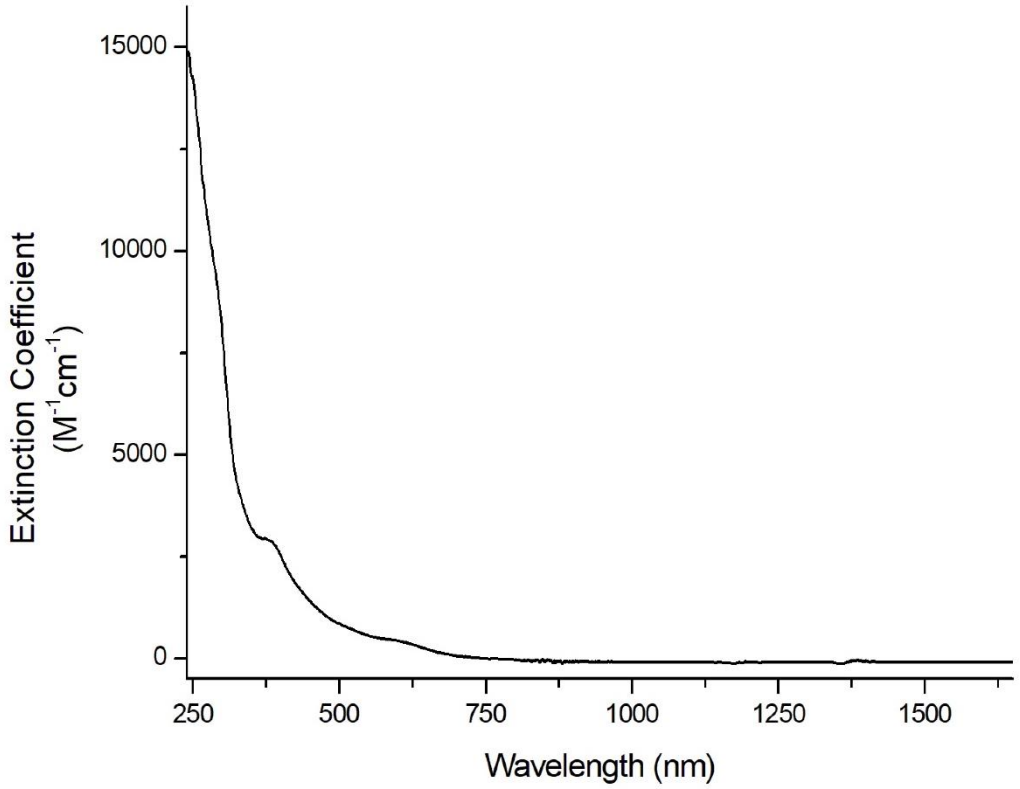


Figure S 41: UV Vis spectrum of complex 3, recorded in THF solution (0.16 mM). Signal noise at 850, 1200 and 1350 nm are artifacts from the instrument.

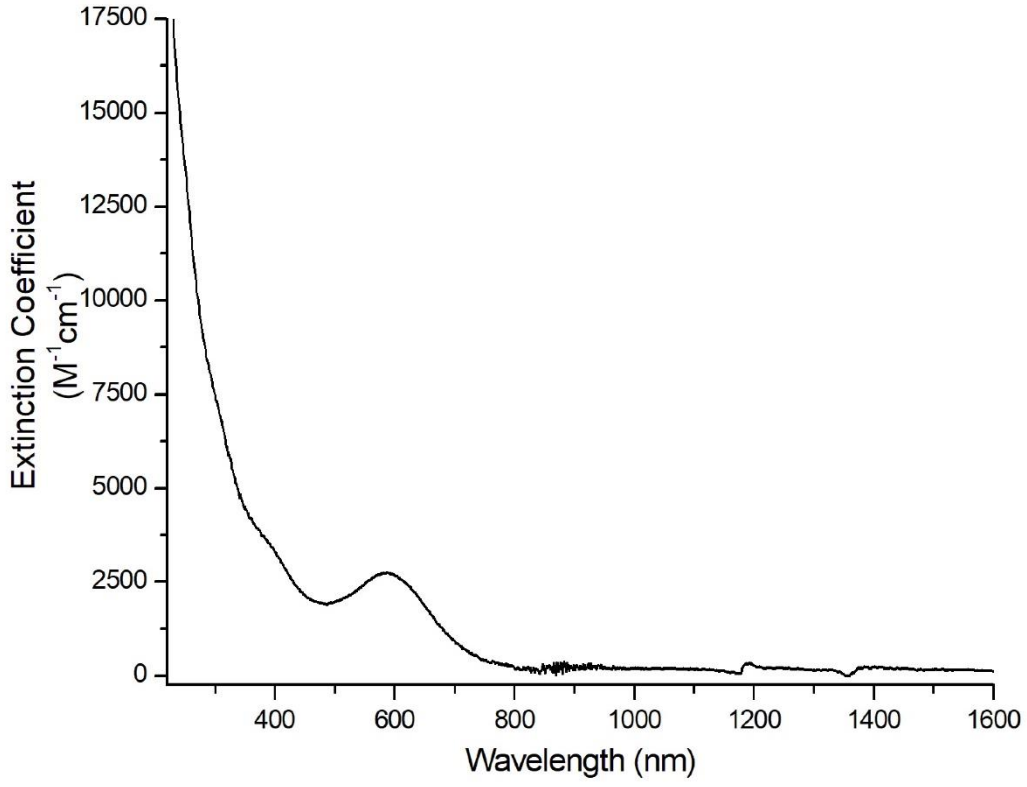
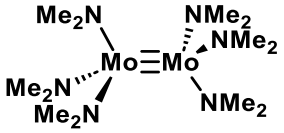
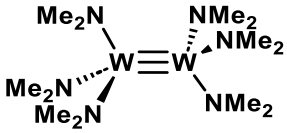
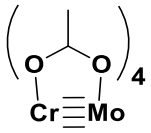
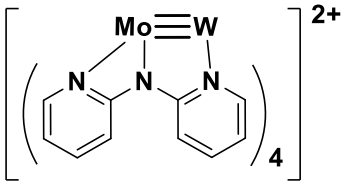
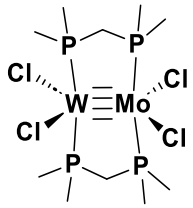
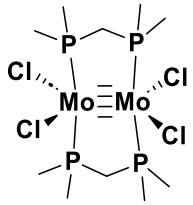
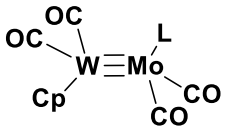
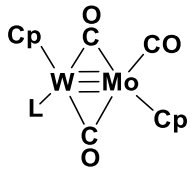
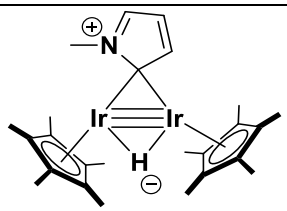
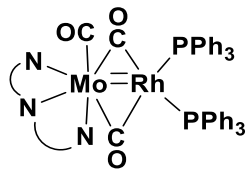
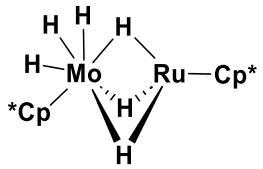
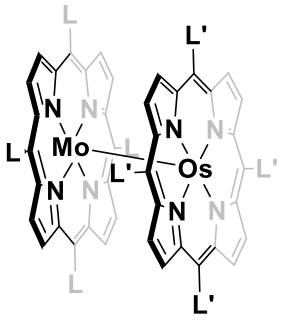
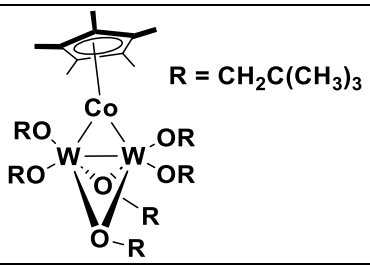
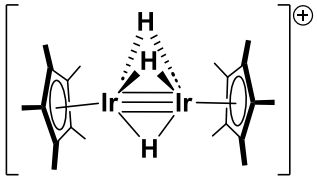
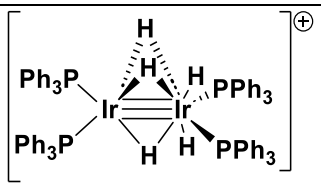
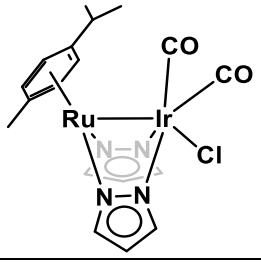


Figure S 42 : UV Vis spectrum of compounds 6, recorded in THF solution (0.043 mM). Signal noise at 850, 1200 and 1350 nm are artifacts from the instrument

X-ray Crystallography Data

Table S1: Literature bond lengths and FSR analysis of homo- and heterobimetallic complexes involving molybdenum and iridium, found in the CCDC database. The structures are drawn as they appear in their respective articles.

	Structure	M-M' Bond Length	Formal Shortness ratio	Reference
1		2.211(2)	0.856	[9]
2		2.294(1)	0.883	[10]
3		2.050(1)	0.832	[11]
4		2.736(4)	1.056	[12]
5		2.193(2)	0.846	[13]
6		2.1271(8)	0.823	[13]
7		2.562(1)	0.988	[14]
8		2.526(1)	0.975	[15]
9		2.462(2)	0.977	[16]

10		2.6066(5)	1.027	[17]
11		2.5255(7)	0.997	[18]
12		2.238(3)	0.880	[19]
13		Co – W = 2.279(5) – 2.340(5) W – W = 2.504(3)	Co – W = 0.928 W – W =0.96	[20]
14		2.465(3)	0.978	[21]
15		2.518	0.999	[22]
16		2.6962	1.078	[23]

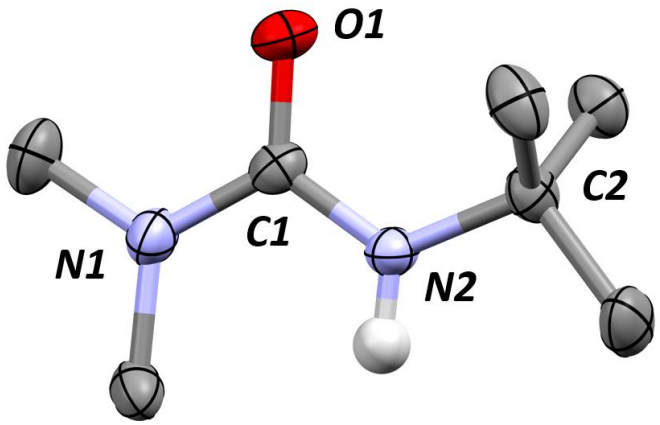


Figure S 43: X-ray crystal structure of N,N-dimethyl-N'-*tert*butyl urea. Displacement ellipsoids represented at 50% with most hydrogens removed for clarity. Relevant bond distances (Å): N1 – C1 = 1.369(2), C1 – O1 = 1.239(2), C1 – N2 = 1.358(2), N2 – C2 = 1.478(2)

Table S2: Crystallographic data collections and refinements details

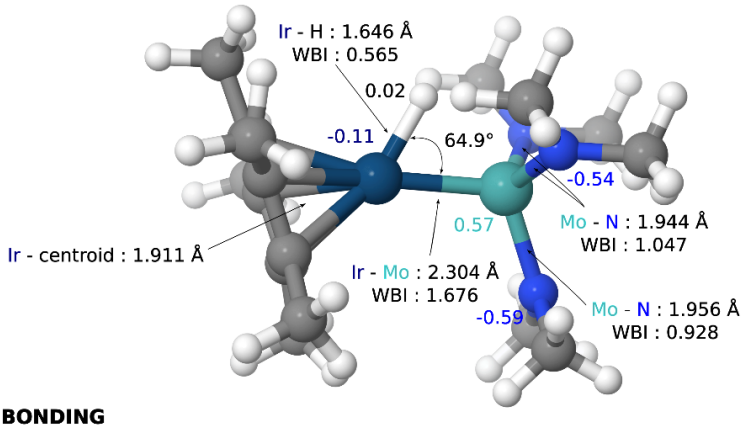
Compound	**1**	**2**	**3**	**4**
Formula	$C_{16}H_{33}IrMoN_3$	$C_{24}H_{42}N_2MoIr_2$	$C_{26}H_{42}N_2O_4MoIr_2$	$C_{21}H_{42}IrMoN_4O$
$D_{calc.}$/ g cm^{-3}	1.827	2.079	2.100	1.713
μ/mm^{-1}	7.201	10.378	9.507	5.749
Formula Weight	555.59	838.93	926.95	654.72
Colour	black	black	black	dark red
Shape	plate-shaped	block-shaped	plate-shaped	block-shaped
Size/mm^3	0.35×0.28×0.05	0.33×0.26×0.15	0.27×0.20×0.07	0.44×0.30×0.22
T/K	100.0(2)	100.1(4)	150.01(10)	100.0(3)
Crystal System	monoclinic	triclinic	monoclinic	triclinic
Space Group	$P2_1/c$	P-1	$P2/n$	P-1
a/Å	18.3443(4)	10.3728(2)	10.9967(2)	10.5680(2)
b/Å	8.22852(16)	11.1282(2)	10.9728(2)	14.3581(2)
c/Å	13.3820(3)	11.9391(2)	12.1515(2)	17.6451(2)
α/°	90	86.4790(10)	90	100.1480(10)
β/°	90.251(2)	80.4780(10)	90.354(2)	101.6170(10)
γ/°	90	80.6460(10)	90	98.0710(10)
V/Å^3	2019.94(7)	1340.23(4)	1466.23(4)	2538.22(7)
Z	4	2	2	4
Z'	1	1	0.5	2
Wavelength/Å	0.71073	0.71073	0.71073	0.71073
Radiation type	Mo K$_\alpha$	Mo K$_\alpha$	Mo K$_\alpha$	Mo K$_\alpha$
Θ_{min}/°	2.713	2.440	2.490	2.411
Θ_{max}/°	30.334	30.615	30.307	30.731
Measured Refl's.	46772	36487	33776	112854
Indep't Refl's	5431	6919	3901	13733
Refl's I≥2 σ(I)	4428	6208	3310	12780
R_{int}	0.0822	0.0840	0.0461	0.0459
Parameters	298	276	263	800
Restraints	919	0	623	2607
Largest Peak	2.741	3.306	2.020	1.769
Deepest Hole	-4.443	-3.973	-2.134	-1.801
GooF	1.060	1.029	1.028	1.029
wR_2 (all data)	0.1181	0.1113	0.0668	0.0635
wR_2	0.1114	0.1095	0.0638	0.0626
R_1 (all data)	0.0646	0.0445	0.0448	0.0293
R_1	0.0495	0.0409	0.0352	0.0265

Compound	**5**	**6**	**N,N-dimethyl-N'-tertbutylurea**
Formula	$C_{19}H_{33}IrMoN_3O$	$C_{24}H_{45}IrMoN_4O_2$	$C_7H_{16}N_2O$
$D_{calc.}$/ g cm^{-3}	1.766	1.712	1.086
μ/mm^{-1}	6.376	5.309	0.585
Formula Weight	607.62	709.78	144.22
Colour	black	black	black
Shape	block-shaped	block-shaped	block-shaped
Size/mm^3	0.51×0.23×0.13	0.21×0.15×0.09	0.20×0.10×0.10
T/K	100.02(16)	100.0(4)	100.0(3)
Crystal System	monoclinic	monoclinic	orthorhombic
Space Group	$P2_1/n$	$P2_1/c$	$Pbca$
a/Å	10.4733(2)	10.3416(2)	9.9756(3)
b/Å	14.1270(3)	18.4312(4)	11.6881(3)
c/Å	15.9700(3)	14.9177(3)	15.1321(4)
α/°	90	90	90
β/°	104.700(2)	104.443(2)	90
γ/°	90	90	90
V/Å^3	2285.52(8)	2753.56(11)	1764.34(8)
Z	4	4	8
Z'	1	1	1
Wavelength/Å	0.71073	0.71073	1.54184
Radiation type	Mo Kα	Mo Kα	Cu Kα
Θ_{min}/°	2.474	2.314	5.848
Θ_{max}/°	30.508	29.940	74.130
Measured Refl's.	49581	119373	8064
Indep't Refl's	6080	7504	1722
Refl's I≥2 σ(I)	5164	6502	1454
R_{int}	0.0610	0.0767	0.0308
Parameters	236	304	96
Restraints	0	0	0
Largest Peak	3.224	1.447	0.292
Deepest Hole	-1.926	-2.891	-0.310
GooF	1.038	1.253	1.081
wR_2 (all data)	0.0880	0.1010	0.1086
wR_2	0.0828	0.0988	0.1030
R_1 (all data)	0.0442	0.0617	0.0522
R_1	0.0337	0.0520	0.0418

Computational Data

All DFT calculations were carried out with the Gaussian 09 suite of programs.[24] Geometries were fully optimized in gas phase without symmetry constraints, employing the B3PW91 functional.[25,26] The nature of the extrema was verified by analytical frequency calculations. The calculation of electronic energies and enthalpies of the extrema of the potential energy surface (minima and transition states) were performed at the same level of theory as the geometry optimizations. IRC calculations were performed to confirm the connections of the optimized transition states. Iridium and Molybdenum atoms were treated with a small-core effective core potential (60 MWB), associated with its adapted basis set[27–29] augmented with a polarization function (ζ_f = 0.938 and 1.0434 respectively for Ir and Mo).[30] For the other elements (H, C, N and O), Pople's triple-ζ basis set 6-311G(d,p) was used.[31–33] The electronic charges (at the DFT level) were computed using the natural population analysis (NPA) technique.[34]

Figure S 44: Computational data for complex 1.



BONDING

(1.75512) BD (1)Ir 6 -Mo 7

(49.13%) 0.7009*Ir 6 s(38.03%) p 0.16(6.06%) d 1.47(55.89%) f 0.00(0.03%

(50.87%) 0.7132*Mo 7 s(32.26%) p 0.54(17.53%) d 1.55(50.13%) f 0.00(0.07

(1.87579) BD (2)Ir 6 -Mo 7

(55.25%) 0.7433*Ir 6 s(0.01%) p 1.00(1.58%) d 62.40(98.40%) f 0.01(0.01%

(44.75%) 0.6689*Mo 7 s(0.00%) p 1.00(18.08%) d 4.53(81.85%) f 0.00(0.07%

(1.65990) BD (1)Ir 6 - H 55

(47.66%) 0.6904*Ir 6 s(42.97%)p 0.26(11.31%)d 1.06(45.68%) f 0.00(0.03%)

(52.34%) 0.7234* H 55 s(99.88%)p 0.00(0.12%)

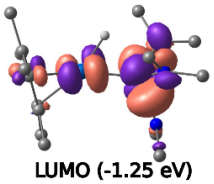
Second Order Perturbation Theory Analysis

LP Ir 6 -> LP* Mo 7 180.49

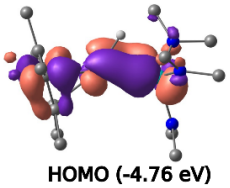
LP Ir 6 -> BD*(1)Ir 6 -Mo 7 153.08

BD Ir 6 - H 55 -> LP*(1)Mo 7 1848.15

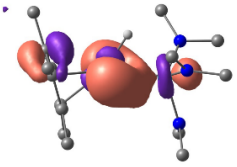
BD Ir 6 - H 55 -> BD*(1)Ir 6 -Mo 7 1721.62



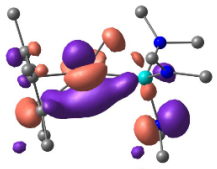
LUMO (-1.25 eV)



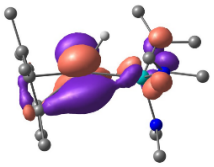
HOMO (-4.76 eV)



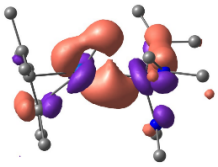
HOMO-1 (-4.97 eV)



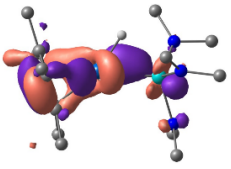
HOMO-2 (-5.46 eV)



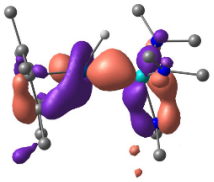
HOMO-4 (-5.78 eV)



HOMO-7 (-7.15 eV)

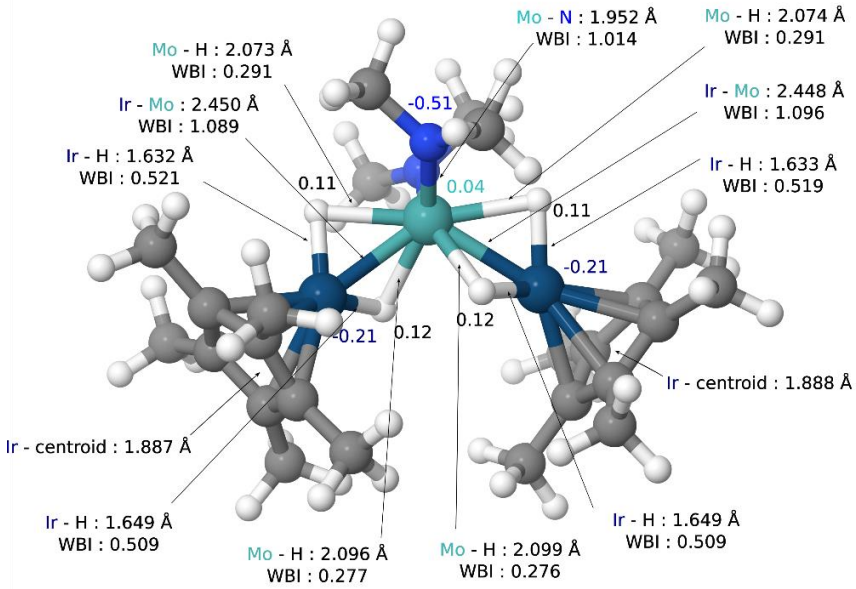


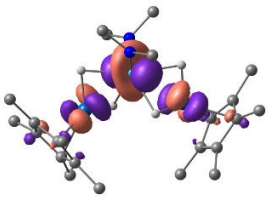
HOMO-8 (-7.49 eV)



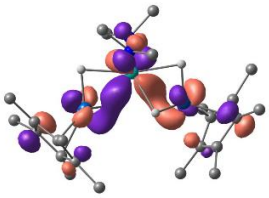
HOMO-9 (-7.50 eV)

Figure S 45: Computational data for complex 2.

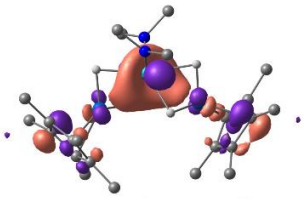




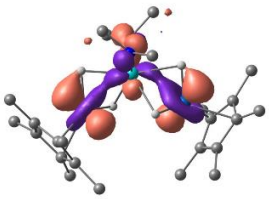
LUMO (-1.33 eV)



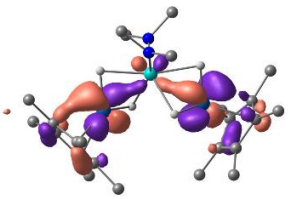
HOMO (-4.70 eV)



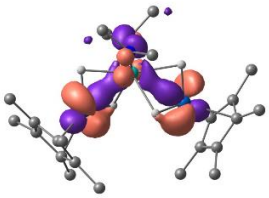
HOMO-2 (-5.05 eV)



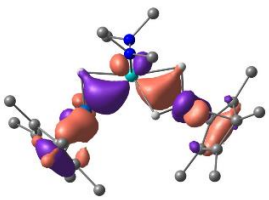
HOMO-9 (-6.80 eV)



HOMO-10 (-7.01 eV)



HOMO-11 (-7.12 eV)



HOMO-12 (-7.57 eV)

BONDING

(1.92397) BD (1)Ir 6 -Mo 7

(44.95%) 0.6704*Ir 6 s(15.18%)p 0.24(3.68%)d 5.34(81.13%)f 0.00(0.01%)

(55.05%) 0.7420*Mo 7 s(1.46%)p 2.87(4.20%)d64.53(94.32%) f 0.01(0.02%)

(1.61124) BD (1)Ir 6 - H 73

(53.77%) 0.7333*Ir 6 s(31.02%)p 0.37(11.55%)d 1.85(57.40%)f 0.00(0.03%)

(46.23%) 0.6800* H 73 s(99.85%)p 0.00(0.15%)

(1.62558) BD (1)Ir 6 - H 75

(53.54%) 0.7317*Ir 6 s(30.96%)p 0.37(11.60%)d 1.85(57.41%) f 0.00(0.03%)

(46.46%) 0.6816* H 75 s(99.85%)p 0.00(0.15%)

(1.50586) BD (1)Ir 15 - H 72

(45.95%) 0.6779*Ir 15 s(37.63%)p 0.73(27.40%)d 0.93(34.85%) f 0.00(0.12%)

(54.05%) 0.7352* H 72 s(99.85%)p 0.00(0.15%)

(1.53706) BD (1)Ir 15 - H 74

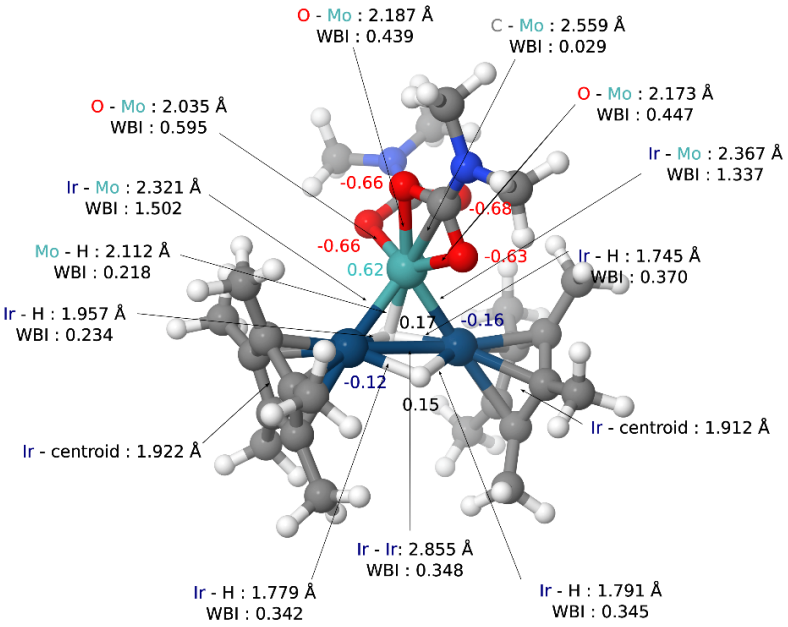
(46.74%) 0.6837*Ir 15 s(28.44%)p 1.18(33.58%)d 1.33(37.85%) f 0.00(0.13%)

(54.26%) 0.7298* H 74 s(99.86%)p 0.00(0.14%)

Second Order Perturbation Theory Analysis

LP Mo 7	-> LP* Ir 6	109.6
LP Ir 6	-> LP* Mo 7	47.7
LP (1)Ir 6	-> BD* Ir 6 -Mo 7	15.6
BD Ir 6 -Mo 7	-> LP* Ir 6	226.9
BD Ir 6 -Mo 7	-> LP* Mo 7	648.4
BD Ir 6 -Mo 7	-> BD* Ir 6 -Mo 7	214.2
BD Ir 6 -Mo 7	-> BD* Ir 6 - H 73	283.7
BD Ir 6 -Mo 7	-> BD* Ir 6 - H 75	281.5
BD Ir 6 - H 73	-> LP* Mo 7	1980.8
BD Ir 6 - H 73	-> BD* Ir 6 -Mo 7	4620.9
BD Ir 6 - H 75	-> LP* Mo 7	2054.7
BD Ir 6 - H 75	-> BD* Ir 6 -Mo 7	4673.4
LP Mo 7	-> LP* Ir 15	590.8
LP Mo 7	-> BD* Ir 15 - H 72	386.6
LP Mo 7	-> BD* Ir 15 - H 74	392.7
LP Ir 15	-> LP* Mo 7	13.5
BD Ir 15 - H 72	-> LP* Mo 7	3812.9
BD Ir 15 - H 72	-> BD* Ir 6 -Mo 7	1.02
BD Ir 15 - H 74	-> LP* Mo 7	34627.7
BD Ir 15 - H 74	-> BD* Ir 6 -Mo 7	50.1

Figure S 46: Computational data for complex 3.



BONDING

(1.94225) BD (1)Ir 6 -Mo 7

(62.51%) 0.7907*Ir 6 s(5.29%)p 0.34(1.81%)d17.57(92.88%) f 0.00(0.01%)

(37.49%) 0.6123*Mo 7 s(9.77%)p 0.45(4.42%)d 8.78(85.75%) f 0.01(0.05%)

(1.82095) BD (2)Ir 6 -Mo 7

(61.81%) 0.7862*Ir 6 s(0.05%)p29.55(1.55%)d99.99(98.39%) f 0.20(0.01%)

(38.19%) 0.6180*Mo 7 s(0.36%)p 4.68(1.70%)d99.99(97.89%) f 0.13(0.05%)

(1.94394) BD (1)Mo 7 -Ir 16

(39.74%) 0.6304*Mo 7 s(6.97%)p 0.59(4.11%)d12.75(88.87%) f 0.01(0.05%)

(60.26%) 0.7763*Ir 16 s(4.05%)p 0.34(1.39%)d23.36(94.55%) f 0.00(0.01%)

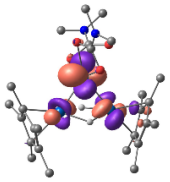
(1.74197) BD (2)Mo 7 -Ir 16

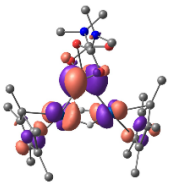
(34.24%) 0.5852*Mo 7 s(0.76%)p 2.69(2.05%)d99.99(97.15%) f 0.06(0.05%)

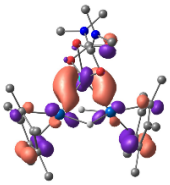
(65.76%) 0.8109*Ir 16 s(0.17%)p10.44(1.76%)d99.99(98.07%) f 0.03(0.01%)

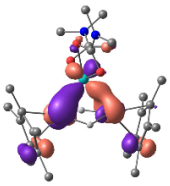
Second Order Perturbation Theory Analysis

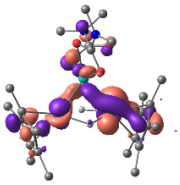
LP Ir 6	-> LP* Mo 7	242.3
LP Ir 6	-> BD* Ir 6 -Mo 7	94.5
LP Ir 6	-> BD* Mo 7 -Ir 16	18.9
LP Ir 16	-> BD* Ir 6 -Mo 7	10.2
LP Ir 16	-> LP* Mo 7	115.9
LP Ir 16	-> BD* Mo 7 -Ir 16	62.0
LP Ir 6	-> LP* Ir 16	114.1
LP Ir 16	-> LP* Ir 6	17.7
BD Ir 6 -Mo 7	-> LP* Ir 16	197.6
BD Ir 6 -Mo 7	-> BD* Mo 7 -Ir 16	112.5
BD Mo 7 -Ir 16	-> LP* Ir 6	171.9

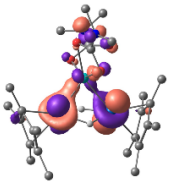

LUMO (-1.22 eV)

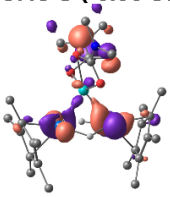

HOMO (-4.07 eV)


HOMO-1 (-5.02 eV)


HOMO-2 (-5.29 eV)


HOMO-3 (-5.68 eV)


HOMO-5 (-6.06 eV)


HOMO-6 (-6.28 eV)

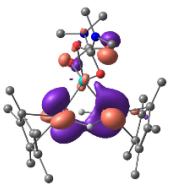
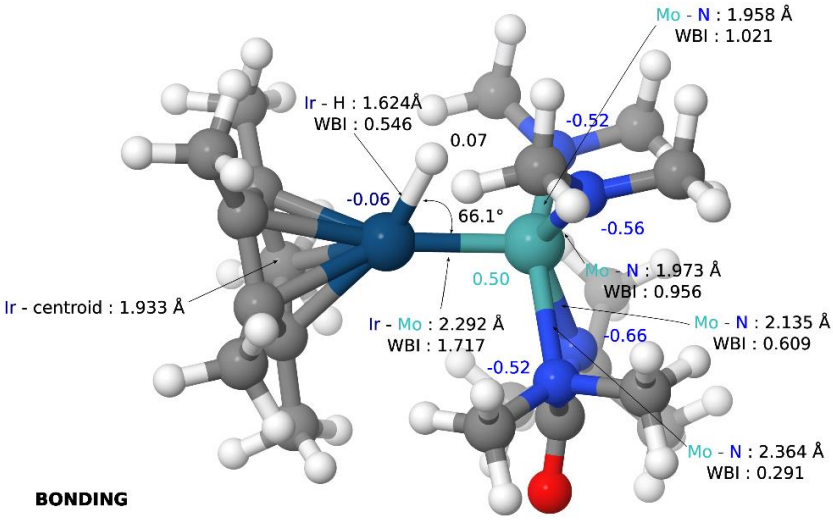

HOMO-8 (-6.55 eV)

Figure S 47: Computational data for complex 4.



BONDING

(1.80264) BD (1)Ir 1 -Mo 2

(48.23%) 0.6945*Ir 1 s(26.02%)p 0.18(4.68%)d 2.66(69.27%) f 0.00(0.03%)

(51.77%) 0.7195*Mo 2 s(32.87%)p 0.23(7.42%)d 1.81(59.58%) f 0.00(0.13%)

(1.89080) BD (2)Ir 1 -Mo 2

(55.55%) 0.7453*Ir 1 s(1.34%)p 0.79(1.06%)d72.96(97.59%) f 0.01(0.02%)

(44.45%) 0.6667*Mo 2 s(1.09%)p12.38(13.48%)d78.28(85.21%) f 0.21(0.23%)

(1.67948) BD (3)Ir 1 -Mo 2

(81.61%) 0.9034*Ir 1 s(9.82%)p 0.33(3.22%)d 8.85(86.95%) f 0.00(0.02%)

(18.39%) 0.4288*Mo 2 s(1.63%)p20.73(33.73%)d39.56(64.37%) f 0.17(0.27%)

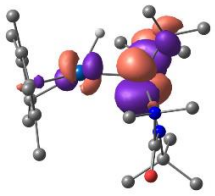
(1.73869) BD (1)Ir 1 - H 71

(57.81%) 0.7603*Ir 1 s(43.75%)p 0.21(9.31%)d 1.07(46.91%) f 0.00(0.03%)

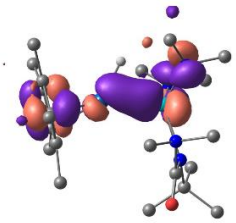
(42.19%) 0.6496* H 71 s(99.82%)p 0.00(0.18%)

Second Order Perturbation Theory Analysis

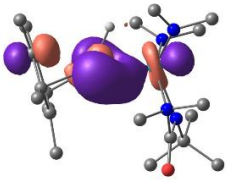
LP Ir 1	-> LP* Mo 2	179.2
LP Ir 1	-> BD* Ir 1 -Mo 2	283.2
BD Ir 1 - H 71	-> LP* Mo 2	2734.67
BD Ir 1 - H 71	-> BD* Ir 1 -Mo 2	2964.53



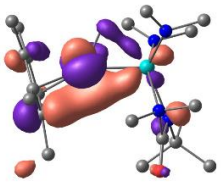
LUMO (-1.29 eV)



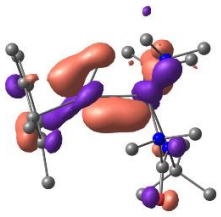
HOMO (-4.97 eV)



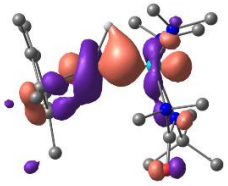
HOMO-1 (-5.16 eV)



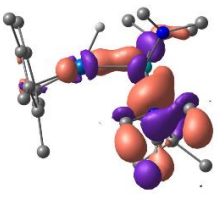
HOMO-3 (-5.72 eV)



HOMO-8 (-7.36 eV)

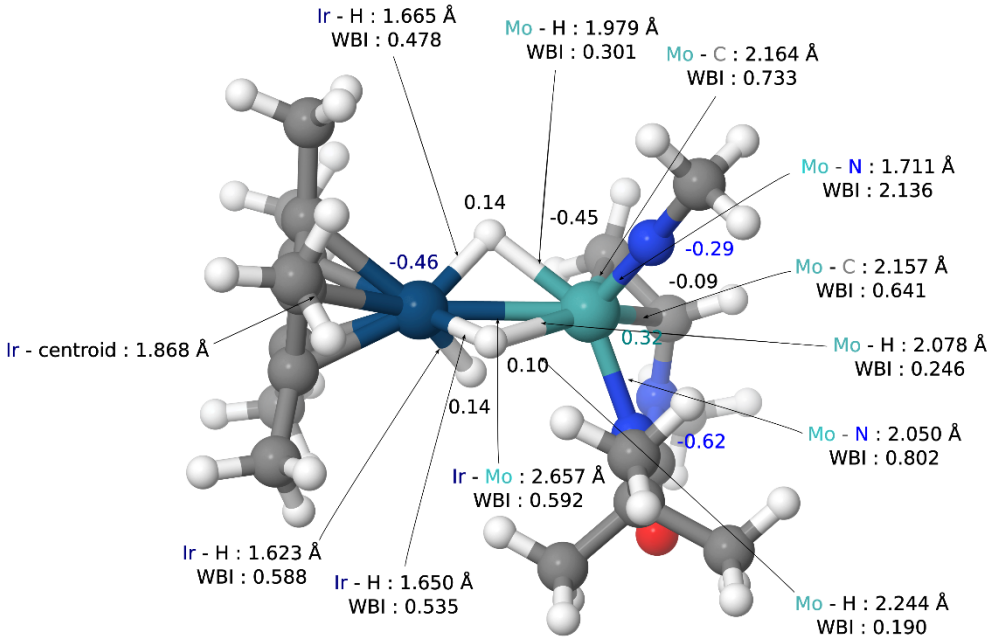


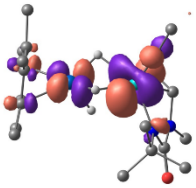
HOMO-9 (-7.51 eV)



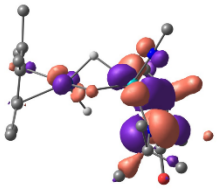
HOMO-11 (-7.76 eV)

Figure S 48: Computational data for complex 5.

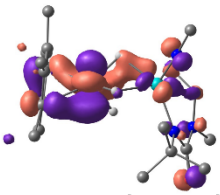




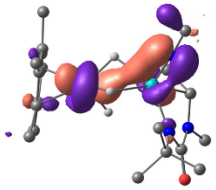
LUMO (-1.54 eV)



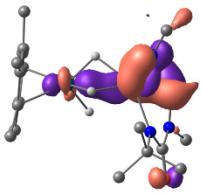
HOMO (-5.27 eV)



HOMO-3 (-6.32 eV)



HOMO-6 (-7.32 eV)



HOMO-11 (-8.10 eV)

BONDING

(1.75512) BD (1)Ir 6 -Mo 7

(49.13%) 0.7009*Ir 6 s(38.03%) p 0.16(6.06%) d 1.47(55.89%) f 0.00(0.03%)

(50.87%) 0.7132*Mo 7 s(32.26%) p 0.54(17.53%) d 1.55(50.13%) f 0.00(0.07%)

(1.87579) BD (2)Ir 6 -Mo 7

(55.25%) 0.7433*Ir 6 s(0.01%) p 1.00(1.58%) d 62.40(98.40%) f 0.01(0.01%)

(44.75%) 0.6689*Mo 7 s(0.00%) p 1.00(18.08%) d 4.53(81.85%) f 0.00(0.07%)

(1.65990) BD (1)Ir 6 - H 55

(47.66%) 0.6904*Ir 6 s(42.97%)p 0.26(11.31%)d 1.06(45.68%) f 0.00(0.03%)

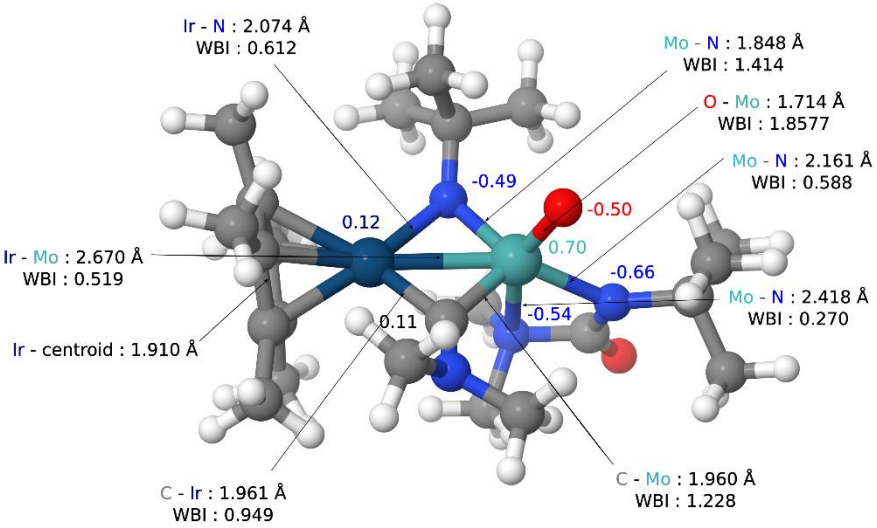
(52.34%) 0.7234* H 55 s(99.88%)p 0.00(0.12%)

Second Order Perturbation Theory Analysis

LP Ir 1	-> LP* Mo 2	8.11
LP H 59	-> LP* Ir 1	145.9

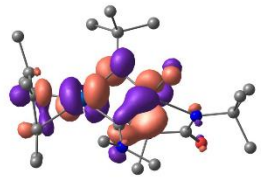
BD Ir 1 - H 60	-> LP*(1)Mo 2	1909.8
BD Ir 1 - H 61	-> LP*(1)Mo 2	2674.6
BD Ir 1 - H 61	-> BD* Ir 1 - H 60	822.11
BD Ir 1 - H 60	-> BD* Ir 1 - H 61	744.01

Figure S 49: Computational data for complex 6.

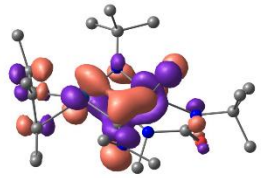


Second Order Perturbation Theory Analysis

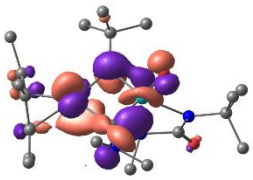
BD Ir 1 - N 7	-> LP* Mo 2	828.3
BD Ir 1 - C 44	-> LP*)Mo 2	1080.8
BD Mo 2 - O 3	-> LP*(5)Ir 1	45.0
BD Mo 2 - N 6	-> LP*(5)Ir 1	12.9
BD Mo 2 - N 7	-> LP*(5)Ir 1	68.3
BD Mo 2 - C 44	-> LP*(5)Ir 1	133.7
BD Mo 2 - C 44	-> LP*(6)Ir 1	4.7
LP Ir 1	-> LP* Mo 2	793.8



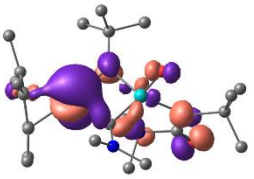
LUMO (-1.77 eV)



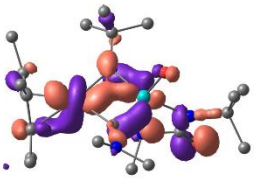
HOMO (-4.55 eV)



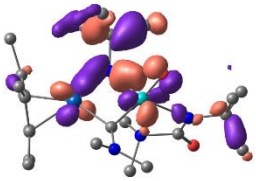
HOMO-1 (-5.55 eV)



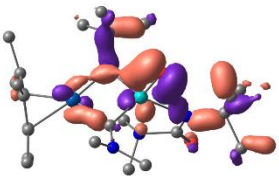
HOMO-2 (-6.10 eV)



HOMO-7 (-7.30 eV)



HOMO-12 (-8.32 eV)



HOMO-13 (-8.55 eV)

	Int 1	Compd 4	Int 2	Int 3	Int 3’	Int 3’’	Int 4	Int 5
Distances in Å and Angles in °								
d(Ir - Mo)	2,299	2,285	2,292	2,285	2,244	2,313	2,242	2,210
d(Ir - H)	1,644	1,621	1,624	1,613	-	-	-	-
d(Mo - H)	2,214	2,212	2,200	2,285	-	-	-	-
d(Ir - Cp)	1,917	1,936	1,933	1,928	1,931	1,956	1,954	1,951
Cp-Ir-Mo	161,3	166,1	166,1	168,1	179,4	166,3	173,9	169,4
Wiberg Bond Indices								
Ir - Mo	1,688	1,735	1,719	1,678	2,112	1,721	2,107	2,413
Ir - H	0,571	0,548	0,543	0,542	-	-	-	-
Mo - H	0,296	0,319	0,321	0,310	-	-	-	-
Natural Charges								
Ir	-0,12	-0,05	-0,06	-0,01	-0,02	-0,01	-0,03	-0,02
Mo	0,58	0,51	0,50	0,59	0,22	0,44	0,26	0,49
H	0,02	0,08	0,07	0,09	-	-	-	-
QTAIM – Ir – Mo Bond								
Density of all electrons	0.13817868	0.14178894	0.13983436	0.14149116	0.15117225	0.13505756	0.15170664	0.16198112
Laplacian of electron density	0.22839847	0.25005742	0.24508059	0.26087553	0.34241592	0.23979208	0.34196980	0.32173476
Lagrangian kinetic energy G(r)	0.12375363	0.13179036	0.12895682	0.13410578	0.16223080	0.12354756	0.16248950	0.16685695
Potential energy density V(r)	-0.1915681	-0.2023856	-0.19790791	-0.20434828	-0.24065786	-0.18842817	-0.24132236	-0.25522421
Energy density E(r) or H(r)	-0.06781438	-0.07059529	-0.06895109	-0.07024250	-0.07842706	-0.06488061	-0.07883286	-0.08836726
Ellipticity of electron density	0.216291	0.217052	0.226151	0.218064	0.017855	0.275401	0.015123	0.051861
Type	(3,-1)	(3,-1)	(3,-1)	(3,-1)	(3,-1)	(3,-1)	(3,-1)	(3,-1)

Table S3 – Bond distances, angles, Wiberg Bond Indices, Natural Charges and QTAIM results for the Ir – Mo bond of intermediates and complexes of Scheme 5.

	Int 5	Int 6	Int 7	Int 8	Int 8’	Int 9	Int 9’	Int 9’’	Compd 5	Compd 5’
Distances in Å and Angles in °										
d(Ir - Mo)	2,210	2,315	2,434	2,628	2,502	2,592	2,590	2,456	2,639	2,657
d(Ir - H)	-	1,670	1,650 / 1,636	1,689 / 1,633 / 1,626	1,640 / 1,653	1,689 / 1,676 / 1,628	1,670 / 1,754 / 1,605	1,635 / 1,679	1,650 / 1,657 / 1,625	1,650 / 1,665 / 1,623
d(Mo - H)	-	2,051	2,061 / 2,238	1,897 / 2,135 / 2,232	2,139 / 2,013	1,917 / 1,955 / 2,263	2,060 / 1,790 / 2,393	2,230 / 1,988	2,029 / 2,016 / 2,239	2,078 / 1,979 / 2,244
d(Ir - Cp)	1,951	1,897	1,891	1,874	1,870	1,872	1,875	1,880	1,870	1,868
Cp-Ir-Mo	169,4	164,8	159,4	170,9	165,7	169,1	164,4	158,5	174,3	174,4
Wiberg Bond Indices										
Ir - Mo	2,413	1,625	1,143	0,618	0,984	0,688	0,713	1,070	0,618	0,592
Ir - H	-	0,509	0,520 / 0,588	0,445 / 0,542 / 0,601	0,529 / 0,490	0,471 / 0,480 / 0,609	0,541 / 0,385 / 0,610	0,482 / 0,577	0,510 / 0,594 / 0,506	0,534 / 0,478 / 0,588
Mo - H	-	0,375	0,289 / 0,214	0,344 / 0,542 / 0,179	0,283 / 0,302	0,323 / 0,324 / 0,172	0,249 / 0,442 / 0,156	0,332 / 0,236	0,274 / 0,184 / 0,269	0,246 / 0,301 / 0,190
Natural Charges										
Ir	-0,02	-0,07	-0,30	-0,48	-0,20	-0,46	-0,44	-0,25	-0,47	-0,46
Mo	0,49	0,36	0,34	0,13	0,12	0,25	0,36	0,35	0,30	0,32
H	-	0,02	0,10 / 0,07	0,11 / 0,15 / 0,17	0,08 / 0,08	0,14 / 0,12 / 0,13	0,10 / 0,16 / 0,11	0,08 / 0,07	0,13 / 0,12 / 0,14	0,10 / 0,14 / 0,14
QTAIM – Ir – Mo Bond										
Density of all electrons	0.16198112	0.13186215	0.10647817	0.07112934	0.09156807	0.07588834	0.07913922	0.10365319	0.06708042	0.06552125
Laplacian of electron density	0.32173476	0.23577310	0.13870597	0.13642017	0.13599296	0.14145584	0.13029446	0.12323384	0.14540137	0.14231628
Lagrangian kinetic energy G(r)	0.16685695	0.12065617	0.07776420	0.05362804	0.06738457	0.05802710	0.05692818	0.05692818	0.05345017	0.05174926
Potential energy density V(r)	-0.2552242	-0.1833743	-0.1213637	-0.0732660	-0.1010581	-0.0808309	-0.0814581	-0.1136806	-0.0706443	-0.0680068
Energy density E(r) or H(r)	-0.0883672	-0.0627181	-0.0435995	-0.0196380	-0.0336735	-0.0228038	-0.0245299	-0.0416519	-0.0171941	-0.0162576
Ellipticity of electron density	0.051861	0.199350	0.025125	0.987941	0.046144	0.416995	0.906974	0.022598	0.537625	1.000349
Type	(3,-1)	(3,-1)	(3,-1)	(3,-1)	(3,-1)	(3,-1)	(3,-1)	(3,-1)	(3,-1)	(3,-1)

Table S4 – Bond distances, angles, Wiberg Bond Indices, Natural Charges and QTAIM results for the Ir – Mo bond of intermediates and complexes of Scheme 6.

	Int 5	**Int 10**	**Int 11**	**Int 12**	**Int 13**	**Int 13'**	**Complex 6**
Distances in Å and Angles in °							
d(Ir - Mo)	2,210	2,210	2,235	2,219	2,312	2,374	2,670
d(Ir - Cp)	1,951	1,955	1,934	1,938	1,933	1,995	1,910
Cp-Ir-Mo	169,4	168,2	178,4	175,6	164,7	154,0	174,0
Wiberg Bond Indices							
Ir - Mo	2,413	2,423	2,182	2,274	1,579	1,444	0,519
Natural Charges							
Ir	-0,02	-0,02	-0,1	0,04	0,12	-0,02	0,12
Mo	0,49	0,50	0,27	0,45	0,39	0,77	0,70
QTAIM – Ir – Mo Bond							
Density of all electrons	0.16198112	0.16230043	0.15376372	0.15869890	0.13267179	0.12172361	0.06086824
Laplacian of electron density	0.32173476	0.32074537	0.35299537	0.35155026	0.21439951	0.16626852	0.16445957
Lagrangian kinetic energy G(r)	0.16685695	0.16688538	0.16702128	0.17118673	0.11612116	0.09600807	0.051748673
Potential energy density V(r)	-0.25522421	-0.25553658	-0.24771216	-0.25649923	-0.17953340	-0.15105300	-0.06246698
Energy density E(r) or H(r)	-0.08836726	-0.08865120	-0.08069088	-0.08531249	-0.06341224	-0.0550449	-0.01071831
Ellipticity of electron density	0.051861	0.051158	0.014444	0.027835	0.233211	0.276613	-2.208075
Type	(3,-1)	(3,-1)	(3,-1)	(3,-1)	(3,-1)	(3,-1)	(3,+1)

Table S5 – Bond distances, angles, Wiberg Bond Indices, Natural Charges and QTAIM results for the Ir – Mo bond of intermediates and complexes of Scheme 7.

NBO Analysis of the Ir – Mo Bond for all the intermediates and final complexes.

- **Int 1 :**

Bond Orbitals
(1.75459) BD (1)Ir 6 -Mo 7
(49.35%) 0.7025*Ir 6 s(38.02%)p 0.16(6.00%)d 1.47(55.96%)f 0.00(0.03%)
(50.65%) 0.7117*Mo 7 s(32.39%)p 0.54(17.39%)d 1.55(50.15%)f 0.00(0.07%)
(1.87474) BD (2)Ir 6 -Mo 7
(55.57%) 0.7455*Ir 6 s(0.00%)p 1.00(1.55%)d63.30(98.43%)f 0.01(0.01%)
(44.43%) 0.6666*Mo 7 s(0.00%)p 1.00(18.40%)d 4.43(81.53%)f 0.00(0.07%)

Second Order Perturbation Analysis :
LP Ir → LP*Mo 185.12 kcal/mol

- **Complex 4 :**

Bond Orbitals
(1.79588) BD (1)Ir 6 -Mo 7
(47.71%) 0.6908*Ir 6 s(27.64%)p 0.17(4.76%)d 2.44(67.57%)f 0.00(0.03%)
(52.29%) 0.7231*Mo 7 s(34.82%)p 0.22(7.56%)d 1.65(57.49%)f 0.00(0.12%)
(1.89319) BD (2)Ir 6 -Mo 7
57.56%) 0.7587*Ir 6 s(0.04%)p25.83(0.91%)d99.99(99.04%)f 0.41(0.01%)
(42.44%) 0.6514*Mo 7 s(0.12%)p99.99(13.54%)d99.99(86.13%)f 1.66(0.20%)
(1.69979) BD (3)Ir 6 -Mo 7
(79.78%) 0.8932*Ir 6 s(9.30%)p 0.33(3.05%)d 9.42(87.63%)f 0.00(0.02%)
(20.22%) 0.4496*Mo 7 s(2.61%)p10.92(28.50%)d26.30(68.66%)f 0.09(0.23%)

Second Order Perturbation Analysis :
LP (1)Ir → LP*(1)Mo 97.88 kcal/mol
LP (2)Ir → LP*(1)Mo 78.55 kcal/mol

- **Int 2 :**

Bond Orbitals
(1.80415) BD (1)Ir 6 -Mo 7
(48.48%) 0.6963*Ir 6 s(25.87%)p 0.18(4.63%)d 2.69(69.47%)
(51.52%) 0.7178*Mo 7 s(32.62%)p 0.23(7.59%)d 1.83(59.66%)f 0.00(0.13%)
(1.89089) BD (2)Ir 6 -Mo 7
(55.76%) 0.7467*Ir 6 s(1.24%)p 0.84(1.04%)d78.54(97.70%)f 0.01(0.02%)
(44.24%) 0.6652*Mo 7 s(1.02%)p13.27(13.52%)d83.68(85.23%)f 0.23(0.24%)
(1.67489) BD (3)Ir 6 -Mo 7
(81.59%) 0.9033*Ir 6 s(10.07%)p 0.32(3.24%)d 8.61(86.68%)f 0.00(0.02%)
(18.41%) 0.4290*Mo 7 s(1.61%)p21.07(33.95%)d39.81(64.16%)f 0.17(0.28%)

Second Order Perturbation Analysis :
LP (1)Ir → LP*(1)Mo 121.52 kcal/mol
LP (2)Ir → LP*(1)Mo 56.57 kcal/mol

- **Int 3 :**

Bond Orbitals
(1.80549) BD (1)Ir 6 -Mo 7
(51.93%) 0.7206*Ir 6 s(18.99%)p 0.22(4.26%)d 4.04(76.72%)f 0.00(0.03%)
(48.07%) 0.6933*Mo 7 s(31.66%)p 0.33(10.42%)d 1.83(57.86%)f 0.00(0.07%)
(1.64428) BD (2)Ir 6 -Mo 7
(76.65%) 0.8755*Ir 6 s(17.11%)p 0.26(4.44%)d 4.58(78.43%)f 0.00(0.02%)
(23.35%) 0.4832*Mo 7 s(7.19%)p 3.49(25.09%)d 9.37(67.44%)f 0.04(0.27%)
(1.85080) BD (3)Ir 6 -Mo 7
(55.04%) 0.7419*Ir 6 s(1.74%)p 0.37(0.64%)d56.16(97.61%)f 0.01(0.02%)
(44.96%) 0.6705*Mo 7 s(3.45%)p 4.85(16.75%)d23.08(79.74%)f 0.02(0.06%)

Second Order Perturbation Analysis :
LP Ir → LP*Mo 133.30 kcal/mol

- **Int 3' :**

Bond Orbitals
(1.84220) BD (1)Ir 6 -Mo 7
(51.22%) 0.7157*Ir 6 s(10.74%)p 0.13(1.44%)d 8.18(87.80%)f 0.00(0.02%)
(48.78%) 0.6985*Mo 7 s(8.93%)p 1.93(17.27%)d 8.27(73.77%)f 0.00(0.03%)
(1.82259) BD (2)Ir 6 -Mo 7
(55.03%) 0.7418*Ir 6 s(9.18%)p 0.17(1.56%)d 9.73(89.25%)f 0.00(0.02%)
(44.97%) 0.6706*Mo 7 s(7.31%)p 2.69(19.62%)d 9.99(73.01%)f 0.01(0.06%)
(1.74481) BD (3)Ir 6 -Mo 7
(39.68%) 0.6299*Ir 6 s(61.61%)p 0.11(6.61%)d 0.52(31.74%)f 0.00(0.04%)
(60.32%) 0.7767*Mo 7 s(43.47%)p 0.33(14.47%)d 0.97(42.02%)f 0.00(0.04%)
Second Order Perturbation Analysis :
LP (1)Ir → LP* Mo 15.75 kcal/mol
LP (2)Ir → LP* Mo 326.78 kcal/mol

- **Int 3" :**

Bond Orbitals
(1.88795) BD (1)Ir 6 -Mo 7
(30.97%) 0.5566*Ir 6 s(57.70%)p 0.07(4.10%)d 0.66(38.14%)f 0.00(0.06%)
(69.03%) 0.8308*Mo 7 s(17.93%)p 0.41(7.43%)d 4.16(74.62%)f 0.00(0.02%)
(1.93331) BD (2)Ir 6 -Mo 7
(48.39%) 0.6956*Ir 6 s(2.34%)p 0.25(0.59%)d41.52(97.05%)f 0.01(0.02%)
(51.61%) 0.7184*Mo 7 s(0.13%)p24.22(3.26%)d99.99(96.58%)f 0.19(0.03%)

Second Order Perturbation Analysis :
LP (1)Ir → LP*Mo ~285 kcal/mol
LP (2)Ir → LP*Mo ~300 kcal/mol
LP (3)Ir → LP*Mo ~94 kcal/mol

- **Int 4 :**

Bond Orbitals
(1.82401) BD (1)Ir 6 -Mo 7
(50.81%) 0.7128*Ir 6 s(15.28%)p 0.13(1.92%)d 5.42(82.78%)f 0.00(0.02%)
(49.19%) 0.7013*Mo 7 s(14.28%)p 1.11(15.82%)d 4.89(69.84%)f 0.00(0.06%)
(1.85703) BD (2)Ir 6 -Mo 7
(58.34%) 0.7638*Ir 6 s(3.33%)p 0.12(0.39%)d28.93(96.27%)f 0.00(0.01%)
(41.66%) 0.6454*Mo 7 s(1.84%)p12.14(22.33%)d41.17(75.76%)f 0.03(0.06%)
(1.71393) BD (3)Ir 6 -Mo 7
(39.02%) 0.6247*Ir 6 s(63.51%)p 0.10(6.16%)d 0.48(30.30%)f 0.00(0.03%)
(60.98%) 0.7809*Mo 7 s(45.56%)p 0.29(13.11%)d 0.91(41.31%)f 0.00(0.02%)

Second Order Perturbation Analysis :

LP (1)Ir	→	LP* Mo	2.85	kcal/mol
LP (2)Ir	→	LP* Mo	359.24	kcal/mol
LP (3)Ir	→	LP* Mo	203.78	kcal/mol

- **Int 5 :**

Bond Orbitals
(1.74612) BD (1)Ir 6 -Mo 7
(47.73%) 0.6908*Ir 6 s(44.01%)p 0.14(6.23%)d 1.13(49.60%)f 0.00(0.17%)
(52.27%) 0.7230*Mo 7 s(39.78%)p 0.21(8.20%)d 1.30(51.89%)f 0.00(0.13%)
(1.66405) BD (2)Ir 6 -Mo 7
(36.02%) 0.6001*Ir 6 s(3.22%)p11.37(36.65%)d18.45(59.47%)f 0.20(0.66%)
(63.98%) 0.7999*Mo 7 s(7.35%)p 0.48(3.52%)d12.12(89.09%)f 0.01(0.04%)
(1.86680) BD (3)Ir 6 -Mo 7
(41.78%) 0.6464*Ir 6 s(30.63%)p 0.38(11.64%)d 1.88(57.63%)f 0.00(0.09%)
(58.22%) 0.7630*Mo 7 s(15.90%)p 0.25(3.99%)d 5.04(80.08%)f 0.00(0.03%)

Second Order Perturbation Analysis :

LP (2)Ir	→	LP* Mo	~335	kcal/mol
LP (3)Ir	→	LP* Mo	~840	kcal/mol

- **Int 6 :**

Bond Orbitals
(1.86461) BD (1)Ir 6 -Mo 7
(54.46%) 0.7379*Ir 6 s(10.48%)p 0.20(2.07%)d 8.34(87.42%)f 0.00(0.02%)
(45.54%) 0.6749*Mo 7 s(2.02%)p 2.84(5.74%)d45.63(92.21%)f 0.02(0.03%)
(1.93175) BD (2)Ir 6 -Mo 7
(50.69%) 0.7120*Ir 6 s(1.43%)p 1.40(2.01%)d67.48(96.55%)f 0.01(0.01%)
(49.31%) 0.7022*Mo 7 s(0.04%)p45.81(1.77%)d99.99(98.17%)f 0.62(0.02%)

Second Order Perturbation Analysis :

LP (1)Ir	→	LP* Mo	~356	kcal/mol
LP (2)Ir	→	LP* Mo	~27	kcal/mol
LP (3)Ir	→	LP* Mo	~36	kcal/mol

- **Int 7 :**

Bond Orbitals
(1.83668) BD (1)Ir 6 -Mo 7
(51.90%) 0.7204*Ir 6 s(17.39%)p 0.37(6.39%)d 4.38(76.21%)f 0.00(0.01%)
(48.10%) 0.6935*Mo 7 s(22.86%)p 0.26(6.01%)d 3.11(71.05%)f 0.00(0.08%)

Second Order Perturbation Analysis :
LP (1)Ir → LP* Mo ~26 kcal/mol
LP (2)Ir → LP* Mo ~34 kcal/mol

- **Int 8 :**

Bond Orbitals
-
Second Order Perturbation Analysis :
LP Ir → LP* Mo <10 kcal/mol

- **Int 8' :**

Bond Orbitals
(1.83600) BD (1)Ir 6 -Mo 7
(50.53%) 0.7108*Ir 6 s(11.54%)p 0.24(2.73%)d 7.43(85.72%)f 0.00(0.01%)
(49.47%) 0.7034*Mo 7 s(7.74%)p 0.97(7.53%)d10.95(84.71%)f 0.00(0.02%)

Second Order Perturbation Analysis :
LP (1)Ir → LP* Mo 7 ~20 kcal/mol
LP (2)Ir → LP* Mo 7 ~8 kcal/mol
LP (3)Ir → LP* Mo 7 ~15 kcal/mol

- **Int 9 :**

Bond Orbitals
-
Second Order Perturbation Analysis :
LP Ir → LP* Mo <5 kcal/mol
LP Mo → LP*Ir 8.99 kcal/mol

- **Int 9' :**

Bond Orbitals
-
Second Order Perturbation Analysis :
LP (1)Ir → LP* Mo ~15 kcal/mol
LP (2)Ir → LP* Mo <5 kcal/mol
LP Mo → LP* Ir ~50 kcal/mol

- **Int 9" :**

Bond Orbitals
(1.84514) BD (1)Ir 6 -Mo 7
(45.08%) 0.6714*Ir 6 s(17.58%)p 0.56(9.76%)d 4.13(72.61%)f 0.00(0.05%)
(54.92%) 0.7411*Mo 7 s(8.03%)p 0.71(5.70%)d10.73(86.23%)f 0.00(0.03%)

Second Order Perturbation Analysis :
LP (1)Ir → LP*(1)Mo 7 ~45 kcal/mol

- **Complex 5 :**

Bond Orbitals

-

Second Order Perturbation Analysis :

LP Ir → LP* Mo <5 kcal/mol

- **Complex 5':**

Bond Orbitals

-

Second Order Perturbation Analysis :

LP Ir → LP* Mo <5 kcal/mol

- **Int 10 :**

Bond Orbitals

(1.91393) BD (1)Ir 6 -Mo 7

(49.08%) 0.7005*Ir 6 s(34.27%)p 0.13(4.51%)d 1.79(61.19%)f 0.00(0.03%)

(50.92%) 0.7136*Mo 7 s(26.39%)p 0.22(5.93%)d 2.56(67.63%)f 0.00(0.05%)

(1.89287) BD (2)Ir 6 -Mo 7

(51.27%) 0.7160*Ir 6 s(11.50%)p 0.16(1.86%)d 7.53(86.61%)f 0.00(0.03%)

(48.73%) 0.6981*Mo 7 s(13.03%)p 0.35(4.54%)d 6.32(82.38%)f 0.00(0.04%)

(1.89518) BD (3)Ir 6 -Mo 7

(42.83%) 0.6545*Ir 6 s(33.61%)p 0.16(5.40%)d 1.81(60.97%)f 0.00(0.03%)

(57.17%) 0.7561*Mo 7 s(16.22%)p 0.14(2.19%)d 5.03(81.55%)f 0.00(0.03%)

Second Order Perturbation Analysis :

LP (1)Ir → LP* Mo 7 ~285 kcal/mol

LP (2)Ir → LP* Mo 7 ~18 kcal/mol

LP (3)Ir → LP* Mo 7 ~1071 kcal/mol

- **Int 11 :**

Bond Orbitals

(1.90388) BD (1)Ir 6 -Mo 7

(54.05%) 0.7352*Ir 6 s(0.06%)p11.90(0.67%)d99.99(99.26%)f 0.30(0.02%)

(45.95%) 0.6778*Mo 7 s(0.39%)p44.56(17.45%)d99.99(82.12%)f 0.10(0.04%)

(1.65437) BD (2)Ir 6 -Mo 7

(36.94%) 0.6078*Ir 6 s(78.27%)p 0.10(7.62%)d 0.18(14.05%)f 0.00(0.05%)

(63.06%) 0.7941*Mo 7 s(64.16%)p 0.13(8.23%)d 0.43(27.59%)f 0.00(0.02%)

(1.84243) BD (3)Ir 6 -Mo 7

(57.65%) 0.7593*Ir 6 s(3.40%)p 0.30(1.01%)d28.07(95.56%)f 0.01(0.02%)

(42.35%) 0.6508*Mo 7 s(1.48%)p15.64(23.22%)d50.67(75.21%)f 0.06(0.08%)

Second Order Perturbation Analysis :

LP (1)Ir → LP* Mo 7 84.25 kcal/mol

LP (2)Ir → LP* Mo 7 304.92 kcal/mol

LP (3)Ir → LP* Mo 7 213.79 kcal/mol

- **Int 12 :**

Bond Orbitals
(1.93529) BD (1)Ir 6 -Mo 7
(49.80%) 0.7057*Ir 6 s(10.51%)p 0.15(1.56%)d 8.37(87.91%)f 0.00(0.02%)
(50.20%) 0.7085*Mo 7 s(11.00%)p 0.33(3.61%)d 7.76(85.34%)f 0.00(0.05%)
(1.83196) BD (2)Ir 6 -Mo 7
(55.77%) 0.7468*Ir 6 s(5.78%)p 0.20(1.16%)d16.11(93.04%)f 0.00(0.02%)
(44.23%) 0.6651*Mo 7 s(4.88%)p 3.88(18.96%)d15.59(76.14%)f 0.00(0.02%)
1.74617) BD (3)Ir 6 -Mo 7
(38.08%) 0.6171*Ir 6 s(63.94%)p 0.12(7.44%)d 0.45(28.58%)f 0.00(0.04%)
(61.92%) 0.7869*Mo 7 s(46.73%)p 0.23(10.84%)d 0.91(42.41%)f 0.00(0.01%)

Second Order Perturbation Analysis :
LP (1)Ir → LP* Mo ~290 kcal/mol
LP (3)Ir → LP* Mo ~400 kcal/mol

- **Int 13 :**

Bond Orbitals
(1.53554) BD (1)Ir 6 -Mo 7
(33.48%) 0.5786*Ir 6 s(32.88%)p 0.70(23.17%)d 1.33(43.63%)f 0.01(0.32%)
(66.52%) 0.8156*Mo 7 s(15.50%)p 0.59(9.12%)d 4.86(75.35%)f 0.00(0.03%)
(1.89715) BD (2)Ir 6 -Mo 7
(53.69%) 0.7327*Ir 6 s(1.04%)p 1.39(1.45%)d93.81(97.50%)f 0.01(0.01%)
(46.31%) 0.6805*Mo 7 s(2.47%)p 1.82(4.50%)d37.67(93.00%)f 0.01(0.03%)

Second Order Perturbation Analysis :
LP (1)Ir → LP* Mo ~450 kcal/mol
LP (2)Ir → LP* Mo <5 kcal/mol
LP (3)Ir → LP* Mo 7 ~80 kcal/mol

- **Int 13' :**

Bond Orbitals
(1.80257) BD (1)Ir 6 -Mo 7
(54.34%) 0.7371*Ir 6 s(32.98%)p 0.16(5.28%)d 1.87(61.72%)f 0.00(0.02%)
(45.66%) 0.6757*Mo 7 s(5.00%)p 3.00(15.00%)d16.00(79.96%)f 0.01(0.04%)
(1.92385) BD (2)Ir 6 -Mo 7
(38.54%) 0.6208*Ir 6 s(14.99%)p 0.19(2.80%)d 5.48(82.18%)f 0.00(0.02%)
(61.46%) 0.7840*Mo 7 s(3.09%)p 0.71(2.21%)d30.68(94.69%)f 0.00(0.01%)

Second Order Perturbation Analysis :
LP (1)Ir → LP* Mo ~301 kcal/mol
LP (2)Ir → LP* Mo ~10 kcal/mol
LP (3)Ir → LP* Mo ~73 kcal/mol

- **Complex 6 :**

Bond Orbitals
-
Second Order Perturbation Analysis :
LP (1)Ir → LP* Mo 129.02 kcal/mol
LP (3)Ir → LP* Mo 103.57 kcal/mol
LP (4)Ir → LP* Mo 537.45 kcal/mol

Cartesian coordinates of all optimized structures:

3
CO2
C 0.09117 0.00000 1.21200
O 0.16203 0.00000 2.37702
O 0.02083 0.00000 0.04695
2
H2
H 0.00000 0.00000 0.02728
H 0.00000 0.00000 0.77272
10
HNMe2
N 0.00115 0.00195 -0.07128
H -0.05152 -0.08872 0.93667
C 1.39253 -0.00723 -0.48369
C -0.70259 1.20205 -0.48419
H 1.44877 -0.04174 -1.57687
H 1.97257 0.87343 -0.15118
H 1.88578 -0.90547 -0.10291
H -0.76292 1.23202 -1.57731
H -1.72638 1.18112 -0.10138
H -0.22872 2.14478 -0.15384
16
tBuNCO
N -0.04039 -0.13462 0.18583
C 0.20987 0.28473 1.28213
O 0.51353 0.79362 2.29300
C -0.72073 -1.27259 -0.42929
C -0.62859 -1.08466 -1.94450
C -0.01485 -2.56516 -0.00826
C -2.18550 -1.28333 0.01895
H -1.12294 -1.91158 -2.46111
H -1.10863 -0.14999 -2.24412
H 0.41594 -1.04972 -2.26303
H -2.72291 -2.10566 -0.46200
H -2.26057 -1.41319 1.10228
H -2.67690 -0.34554 -0.25129
H -0.48386 -3.42737 -0.49081
H 1.03861 -2.53871 -0.29735
H -0.07241 -2.70589 1.07471
26
tBuNHCONMe2
C 1.35409 -0.05752 -0.57653
N 0.04353 0.13849 -0.19965
C -0.73812 1.33397 -0.56804
H -0.25981 -0.31330 0.64747
O 1.95508 0.70261 -1.32513
N 1.93952 -1.20403 -0.07323

C -0.89323 1.40480 -2.09069
C -2.11412 1.14770 0.07653
C -0.08103 2.61343 -0.03262
H -2.75979 1.99650 -0.16030
H -2.59738 0.23706 -0.29001
H -2.03567 1.08611 1.16830
H -1.52221 2.25777 -2.36252
H 0.08016 1.51639 -2.56772
H -1.36572 0.49289 -2.46685
H -0.68238 3.48983 -0.29337
H 0.00646 2.57365 1.05804
H 0.91531 2.73042 -0.46000
C 3.36179 -1.39275 -0.26279
C 1.24084 -2.16905 0.74336
H 1.75754 -3.12933 0.67693
H 1.19849 -1.88979 1.80771
H 0.22274 -2.32422 0.37681
H 3.90231 -1.35263 0.69191
H 3.56408 -2.36044 -0.73611
H 3.72436 -0.59789 -0.91138
55
Complex 1
C 7.76677 5.26046 5.98147
C 7.14648 5.66028 7.20689
C 6.46219 4.51501 7.75631
C 6.63842 3.42206 6.84257
C 7.44563 3.88978 5.74196
Ir 5.45073 5.01005 5.84251
Mo 3.19942 5.23090 5.40732
N 2.80705 7.13249 5.30496
C 3.69260 8.27723 5.19186
C 7.29357 6.98731 7.87730
C 5.82979 4.44729 9.10994
C 6.21236 2.00671 7.06579
C 7.95072 3.04865 4.61468
C 8.61199 6.12961 5.10664
N 2.07804 4.46367 6.81470
C 1.78601 3.04651 6.91190
N 2.84056 4.24402 3.77119
C 1.45797 4.15684 3.32191
C 1.71959 5.18244 8.02243
C 3.75014 3.71312 2.77202
C 1.41932 7.52255 5.09624
H 2.24684 4.78640 8.90338
H 0.63911 5.09927 8.21875
H 1.97018 6.24079 7.92785
H 2.05264 2.53414 5.98547
H 0.71327 2.88287 7.09981
H 2.34192 2.57140 7.73490

H 3.61268 4.21673 1.80226
H 3.56277 2.64037 2.61559
H 4.77771 3.84512 3.10554
H 1.18489 3.11213 3.11212
H 1.29460 4.73396 2.39987
H 0.77308 4.52898 4.08824
H 1.26607 7.95426 4.09614
H 1.11583 8.27931 5.83455
H 0.74918 6.66621 5.20876
H 4.72550 7.95560 5.30732
H 3.46222 9.01666 5.97309
H 3.57246 8.77755 4.21816
H 7.43359 7.78969 7.15022
H 8.16208 6.99187 8.54874
H 6.41189 7.23144 8.47309
H 5.36439 5.39716 9.38137
H 6.57736 4.21054 9.87808
H 5.05660 3.67808 9.15072
H 5.32727 1.95484 7.70202
H 7.01022 1.43279 7.55438
H 5.97124 1.50865 6.12432
H 7.24374 2.25715 4.35687
H 8.90239 2.56949 4.87864
H 8.12087 3.64464 3.71552
H 8.55080 5.82341 4.06024
H 9.66627 6.08144 5.40591
H 8.30035 7.17489 5.16094
H 5.08256 5.79094 4.44057
55
Complex 1 - triplet
C 7.88467 4.96546 5.83812
C 7.14730 5.95333 6.60442
C 6.38523 5.26426 7.59490
C 6.58959 3.84376 7.39466
C 7.55557 3.68183 6.33033
Ir 5.57148 4.67611 5.61039
Mo 3.21713 5.07762 5.24629
N 2.61927 6.78417 5.97718
C 3.41051 7.99584 5.86648
C 7.34120 7.43218 6.49469
C 5.63578 5.88277 8.73097
C 6.11206 2.75653 8.30092
C 8.11542 2.37508 5.86851
C 8.85630 5.28592 4.74966
N 2.24318 3.73800 6.28007
C 2.06981 2.38660 5.78036
N 2.71322 4.97330 3.36828
C 1.32661 4.88793 2.95541
C 1.92620 3.83905 7.68940

C 3.62258 5.09839 2.24462
C 1.26518 7.06118 6.41662
H 2.54981 3.16229 8.29421
H 0.87534 3.56613 7.87626
H 2.08286 4.85765 8.04809
H 2.29864 2.33939 4.71378
H 1.03317 2.04577 5.92604
H 2.73396 1.67842 6.29908
H 3.42600 6.01622 1.66935
H 3.51278 4.24427 1.55853
H 4.65703 5.11890 2.59268
H 1.16196 4.01920 2.29934
H 1.01328 5.78614 2.40148
H 0.67242 4.78044 3.82450
H 0.74986 7.74687 5.72595
H 1.26007 7.53519 7.41076
H 0.68219 6.14012 6.47630
H 4.41448 7.75604 5.51122
H 3.50344 8.49491 6.84371
H 2.95162 8.71719 5.17156
H 7.44433 7.74668 5.45328
H 8.24858 7.74789 7.02575
H 6.50082 7.98033 6.92409
H 5.29390 6.88897 8.48310
H 6.27402 5.95594 9.62101
H 4.75647 5.29391 8.99853
H 5.16754 3.02289 8.77795
H 6.84474 2.56506 9.09636
H 5.95948 1.82127 7.75890
H 7.37614 1.57570 5.94922
H 8.98512 2.08607 6.47180
H 8.43569 2.42101 4.82587
H 9.03204 4.42588 4.10083
H 9.82511 5.58998 5.16678
H 8.49819 6.10627 4.12291
H 4.97258 3.53346 4.61251
71
Int 1
C -0.53215 1.26416 -3.48327
C -0.37005 2.51747 -2.81656
C -1.07556 2.44873 -1.55910
C -1.64894 1.13795 -1.44932
C -1.29778 0.40217 -2.64069
Ir 0.56766 0.95694 -1.43771
Mo 2.03162 0.50495 0.27689
N -2.79872 -2.67881 3.62771
C -3.34086 -1.61340 3.52926
O -3.75507 -0.51834 3.46715
C 0.29657 3.73345 -3.37243

C	-1.30190	3.59853	-0.62947
C	-2.59189	0.66603	-0.38929
C	-1.77197	-0.97253	-2.98331
C	0.00629	0.91658	-4.83407
N	1.32406	1.04545	2.01481
C	0.38047	0.24002	2.76816
N	3.63936	1.54753	-0.05719
C	4.70543	1.47803	0.93189
N	2.29871	-1.42167	0.31985
C	1.96226	-2.44513	-0.65278
C	1.38074	2.41531	2.48838
C	4.06865	2.26557	-1.24310
C	3.14022	-1.95999	1.37944
C	-3.10143	-4.09883	3.46234
C	-4.02782	-4.54074	4.59941
C	-3.76858	-4.32107	2.10179
C	-1.77182	-4.85231	3.53382
H	1.36101	-2.01181	-1.44978
H	1.38858	-3.25162	-0.17180
H	2.86908	-2.89793	-1.08391
H	4.36696	0.96538	1.83619
H	5.02794	2.48810	1.22484
H	5.58724	0.94819	0.54214
H	4.08954	-2.35177	0.98502
H	2.63001	-2.78585	1.89702
H	3.36589	-1.19427	2.12623
H	4.95574	1.79492	-1.69557
H	4.33970	3.29998	-0.98449
H	3.25972	2.28619	-1.97087
H	-1.09827	-4.51117	2.74407
H	-1.93639	-5.92627	3.41311
H	-1.28478	-4.68072	4.49681
H	-3.56564	-4.34358	5.56964
H	-4.23313	-5.61246	4.52553
H	-4.98024	-4.00537	4.55539
H	0.35409	-0.78062	2.38198
H	-0.63845	0.64967	2.71185
H	0.66656	0.20143	3.83042
H	-4.71589	-3.77815	2.03984
H	-3.97368	-5.38453	1.95016
H	-3.11855	-3.97723	1.29356
H	0.40344	2.91366	2.40492
H	2.10346	2.99220	1.90776
H	1.68261	2.44746	3.54668
H	-2.48243	-0.40486	-0.20655
H	-3.63238	0.84992	-0.68595
H	-2.42374	1.17715	0.55962
H	-1.07027	-1.48572	-3.64432
H	-2.74326	-0.93686	-3.49379

H -1.89095 -1.58646 -2.08810
H -1.54362 3.25539 0.37788
H -2.13606 4.22135 -0.97745
H -0.41795 4.23604 -0.55802
H 0.72038 4.35225 -2.57887
H -0.41824 4.35190 -3.93082
H 1.10712 3.46916 -4.05486
H 0.93535 1.45054 -5.04456
H -0.71159 1.17671 -5.62170
H 0.21663 -0.15167 -4.91836
H 1.98200 0.27522 -1.92447
71
TS Int - complex 4
C 0.43293 1.80409 6.35347
C 0.68448 2.99473 7.10904
C -0.24495 3.03007 8.20796
C -1.04361 1.84045 8.13940
C -0.62371 1.08440 6.98814
Ir 1.09469 1.25316 8.51077
Mo 2.36910 0.66392 10.34399
N 0.39197 -0.36759 11.56130
C -0.10289 0.70304 11.94842
O -0.83424 1.54770 12.31071
C 1.63174 4.08823 6.73707
C -0.46539 4.18246 9.13507
C -2.24835 1.55409 8.97607
C -1.25842 -0.17399 6.49236
C 1.14042 1.39891 5.10019
N 1.92523 1.65543 12.07649
C 2.24160 1.15538 13.40122
N 3.96768 1.72372 9.96453
C 4.98298 1.88547 10.99310
N 3.08412 -1.15650 10.21521
C 3.04458 -2.14542 9.15704
C 1.85597 3.10497 12.05980
C 4.43777 2.29895 8.72042
C 4.07468 -1.50594 11.21362
C -0.35365 -1.66281 11.61425
C -1.60231 -1.55673 12.49253
C -0.73998 -2.05560 10.18932
C 0.60792 -2.69388 12.20588
H 2.26840 -1.90596 8.43324
H 2.84215 -3.14529 9.57259
H 4.00822 -2.20371 8.62570
H 4.65141 1.48870 11.95430
H 5.22340 2.94945 11.13893
H 5.91975 1.37690 10.71816
H 5.08207 -1.58715 10.77644
H 3.83880 -2.47204 11.68607

H 4.11526 -0.76115 12.01403
H 5.38884 1.83626 8.40938
H 4.62485 3.37850 8.83368
H 3.69410 2.14821 7.94065
H 1.51466 -2.74803 11.60285
H 0.13707 -3.68117 12.22907
H 0.88577 -2.42239 13.22809
H -1.34377 -1.26961 13.51599
H -2.10514 -2.52717 12.53236
H -2.31263 -0.82517 12.09943
H 2.19716 0.06448 13.42075
H 1.52824 1.53931 14.14672
H 3.24645 1.46757 13.72910
H -1.46953 -1.35315 9.78267
H -1.18167 -3.05727 10.18262
H 0.13331 -2.04356 9.53653
H 1.02747 3.45010 12.69613
H 1.68157 3.46476 11.04582
H 2.78546 3.56124 12.43269
H -2.44928 0.48303 9.03855
H -3.13516 2.02620 8.53369
H -2.13962 1.93562 9.99208
H -0.56010 -0.76628 5.89731
H -2.12762 0.04660 5.85940
H -1.59982 -0.80208 7.31753
H -0.80814 3.84947 10.11643
H -1.22317 4.86523 8.72961
H 0.44953 4.76101 9.27978
H 2.03894 4.58247 7.62120
H 1.12456 4.85036 6.13171
H 2.47243 3.71028 6.15214
H 2.16883 1.76527 5.08301
H 0.63022 1.79987 4.21579
H 1.17872 0.31264 4.99660
H 2.21522 0.12366 8.17479
71
Complex4
C -2.45256 0.72685 -1.62442
C -1.75479 0.55325 -2.85580
C -0.64957 1.45144 -2.87803
C -0.68790 2.23144 -1.66369
C -1.80814 1.78572 -0.88788
Ir -0.29992 0.10989 -0.99992
Mo 0.98694 -0.85693 0.59727
N 2.61836 0.15350 0.34957
C 2.99056 1.17268 -0.61296
C -2.11662 -0.42045 -3.93108
C 0.30155 1.65295 -4.01221
C 0.13892 3.44532 -1.38253

C	-2.34841	2.43489	0.34812
C	-3.73037	0.06002	-1.23138
N	1.71116	-2.58320	-0.06716
C	2.77925	-2.68792	-1.04173
N	0.42389	0.15668	2.47363
C	0.82144	1.30387	3.30931
C	1.96012	0.84225	4.21863
C	-0.75068	-0.34932	2.65782
O	-1.84173	-0.24170	3.11313
N	-0.54078	-1.75501	1.93325
C	-0.06150	-2.58795	3.03963
C	0.81712	-3.72178	-0.20805
C	-1.84479	-2.19740	1.47438
C	3.73655	-0.18715	1.21310
C	1.27884	2.43027	2.39014
C	-0.33314	1.80904	4.17768
H	0.02562	-3.70100	0.54063
H	1.37549	-4.66190	-0.08729
H	0.33557	-3.74524	-1.20035
H	3.45745	-0.96189	1.93152
H	4.10357	0.69029	1.76388
H	4.57448	-0.57525	0.61691
H	2.39580	-2.63143	-2.07387
H	3.29157	-3.65566	-0.93116
H	3.51307	-1.89355	-0.91585
H	3.84666	0.82904	-1.21283
H	3.29778	2.10414	-0.11387
H	2.14886	1.36719	-1.27365
H	1.61944	0.03952	4.87823
H	2.30942	1.67125	4.84189
H	2.80573	0.47207	3.63745
H	2.07907	2.09722	1.73173
H	1.63796	3.28108	2.97748
H	0.44800	2.76728	1.76555
H	-2.14721	-1.59406	0.61931
H	-2.59006	-2.10586	2.27410
H	-1.79598	-3.24704	1.16211
H	-1.18181	2.13471	3.57561
H	0.01942	2.66410	4.76232
H	-0.68680	1.04768	4.87441
H	-0.78886	-2.61897	3.86402
H	0.88545	-2.20410	3.42477
H	0.10282	-3.61806	2.70351
H	-3.78965	-0.96042	-1.61586
H	-4.59209	0.61272	-1.62691
H	-3.84038	0.01565	-0.14628
H	-1.23597	-0.76018	-4.47984
H	-2.80272	0.03625	-4.65484
H	-2.61022	-1.30394	-3.52099

H -2.77974 1.70582 1.03626
H -3.13037 3.16119 0.09114
H -1.56881 2.97383 0.88951
H 0.27236 3.60660 -0.31166
H -0.34617 4.33874 -1.79563
H 1.13015 3.37644 -1.83445
H 1.28525 1.97145 -3.66133
H -0.06826 2.42166 -4.70284
H 0.44107 0.73402 -4.58496
H 0.07659 -1.31314 -1.63642
71
Complex4- triplet
Ir 1.24870 1.36111 8.37031
Mo 2.07312 0.56396 10.47161
N 4.00971 0.67788 10.81555
N 2.11202 -1.29602 9.68527
O -0.38694 2.52054 12.65070
N 0.79765 0.56703 12.11430
N 1.77343 2.56004 11.70173
C 0.93411 -2.08630 9.39704
H 0.03796 -1.61792 9.80327
H 1.02296 -3.10247 9.81479
H 0.79271 -2.19241 8.31129
C 0.56446 1.89696 12.22769
C -0.75532 1.07383 7.38929
C 4.69070 -0.33107 11.59929
H 3.99418 -1.11253 11.91403
H 5.14100 0.10580 12.50515
H 5.50605 -0.81474 11.03601
C 3.27320 -1.89307 9.05365
H 3.11696 -1.99289 7.96888
H 3.46060 -2.90269 9.45182
H 4.15743 -1.27929 9.20979
C 4.90860 1.71035 10.35039
H 5.65117 1.31097 9.64029
H 5.47147 2.15710 11.18647
H 4.35579 2.49973 9.83975
C 0.69168 -1.73798 12.90042
H 0.86873 -2.11246 11.89353
H 0.09519 -2.47601 13.44456
H 1.65978 -1.64765 13.40187
C 0.23737 0.98937 6.33734
C -0.02874 -0.38929 12.89279
C -0.15023 0.08232 14.35122
H 0.84193 0.21824 14.79256
H -0.67655 -0.67803 14.93577
H -0.69936 1.02047 14.42591
C 2.73930 2.72531 12.80763
H 2.93182 1.76075 13.27458

H 2.34555 3.42433 13.55616
H 3.67504 3.11822 12.40950
C -0.69172 2.38698 7.94470
C -1.42718 -0.51590 12.27639
H -1.92976 0.45312 12.28831
H -2.03286 -1.22986 12.84363
H -1.36903 -0.86515 11.24261
C 1.49238 3.86361 11.09504
H 2.42867 4.28370 10.72335
H 1.04200 4.54619 11.82406
H 0.82396 3.71630 10.25091
C -1.79581 0.04172 7.68383
H -1.40229 -0.97227 7.58741
H -2.63940 0.13474 6.98770
H -2.18982 0.15100 8.69554
C 0.89500 2.24527 6.24001
C 0.35745 3.10927 7.24959
C 0.45946 -0.19200 5.45148
H 1.49414 -0.24609 5.10715
H -0.18480 -0.14048 4.56410
H 0.23163 -1.12684 5.96742
C -1.66400 2.97261 8.91724
H -1.99834 2.23248 9.64468
H -2.54774 3.35312 8.38932
H -1.23556 3.80489 9.47729
C 0.67478 4.56135 7.39654
H 0.43171 4.93318 8.39291
H 0.09822 5.15632 6.67650
H 1.73381 4.75864 7.21672
C 1.95550 2.61473 5.25340
H 2.67124 3.32030 5.68033
H 1.51617 3.08389 4.36441
H 2.51695 1.73933 4.92108
H 2.87090 1.43135 8.44203
71
TS Complex 4 - Int 3''
C -1.77430 1.56781 -1.69309
C -1.88165 0.21097 -2.21159
C -0.82946 -0.01646 -3.11369
C -0.10585 1.29134 -3.35214
C -0.65167 2.17909 -2.24933
Ir 0.09692 0.29492 -1.04794
Mo 1.15809 -0.65633 0.69565
N -0.31708 -0.91444 2.38530
C 0.02039 -1.92973 3.39644
C -3.00255 -0.72954 -1.91062
C -0.64005 -1.19727 -4.00580
C -0.22959 1.89986 -4.75956
C -0.21165 3.59413 -2.08160

C	-2.74598	2.19741	-0.75030
N	3.07895	-0.42035	0.46881
C	3.80575	-0.15505	-0.75502
N	0.95571	-2.58179	0.26842
C	1.73372	-3.54769	1.01839
N	0.94847	0.92664	2.20258
C	1.38933	2.32786	2.39558
C	0.20568	3.26419	2.11208
C	3.96161	-0.63817	1.59527
C	0.14667	-3.24910	-0.72522
C	-0.04444	0.45760	2.94149
O	-0.70703	0.88368	3.87069
C	-1.73532	-1.04975	2.00727
C	1.90341	2.52955	3.82815
C	2.50800	2.64404	1.40453
H	-0.41485	-2.50870	-1.29205
H	-0.55356	-3.96816	-0.26445
H	0.77658	-3.82044	-1.42722
H	3.39552	-0.75661	2.52384
H	4.64467	0.21430	1.73507
H	4.58201	-1.53647	1.45220
H	2.42778	-4.08788	0.35441
H	1.10080	-4.30780	1.50681
H	2.33480	-3.06662	1.79518
H	4.48167	-0.99031	-0.99726
H	4.41890	0.75417	-0.65353
H	3.10890	-0.01376	-1.58042
H	3.40247	2.05270	1.61091
H	2.77537	3.70260	1.48211
H	2.18382	2.42834	0.38351
H	-0.15993	3.07217	1.09937
H	0.52007	4.31042	2.18289
H	-0.60524	3.09317	2.82204
H	-1.98190	-0.28353	1.27305
H	-2.36813	-0.93475	2.89330
H	-1.88741	-2.03212	1.55748
H	1.11514	2.33106	4.55556
H	2.25110	3.55925	3.95992
H	2.74515	1.85985	4.02969
H	-0.16667	-2.92371	2.98995
H	-0.58776	-1.77301	4.29325
H	1.07441	-1.84412	3.66821
H	-3.34421	-0.63811	-0.87844
H	-2.70606	-1.76714	-2.07309
H	-3.85973	-0.52345	-2.56384
H	0.42195	-1.38301	-4.18504
H	-1.12218	-1.03792	-4.97997
H	-1.06679	-2.10420	-3.57417
H	-3.57545	2.64999	-1.30778

H -2.27502 2.98399 -0.15954
H -3.17470 1.47174 -0.05671
H 0.87568 3.67847 -2.15535
H -0.50955 3.99689 -1.11255
H -0.64835 4.23978 -2.85589
H 0.32927 2.83674 -4.81781
H -1.27648 2.10227 -5.00207
H 0.17652 1.21838 -5.51147
H 0.98159 1.12556 -3.17048
71
Int 3''
C -2.10092 1.52400 -1.73415
C -2.19624 0.16375 -2.21182
C -0.94982 -0.16453 -2.84056
C -0.25142 1.15412 -3.16951
C -0.82217 2.03425 -2.05891
Ir -0.52070 0.19996 -0.75391
Mo 0.76762 -0.84045 0.86061
N -0.47746 -1.21775 2.66254
C -0.01171 -2.23059 3.62335
C -3.40481 -0.70874 -2.10552
C -0.68180 -1.39596 -3.64442
C -0.59678 1.68488 -4.57649
C -0.34199 3.43156 -1.84554
C -3.15984 2.22210 -0.94508
N 2.67428 -0.64503 0.57041
C 3.26826 -0.84547 -0.73897
N 0.55511 -2.72826 0.31602
C 1.40394 -3.74193 0.92025
N 0.57345 0.73936 2.38365
C 0.90444 2.17505 2.54884
C -0.38140 3.00204 2.41061
C 3.65979 -0.50353 1.61838
C -0.44970 -3.35315 -0.51625
C -0.26260 0.16644 3.23171
O -0.84185 0.50353 4.24769
C -1.90969 -1.41613 2.36133
C 1.55043 2.41560 3.92115
C 1.88168 2.59000 1.45026
H -1.10910 -2.58640 -0.92216
H -1.04906 -4.08605 0.05118
H 0.01514 -3.90177 -1.35097
H 3.17594 -0.31482 2.57832
H 4.34077 0.33533 1.40890
H 4.27854 -1.41032 1.70956
H 1.91977 -4.32389 0.14099
H 0.83206 -4.46282 1.52760
H 2.16792 -3.28923 1.55709
H 3.91981 -1.73331 -0.74583

H 3.87693 0.02580 -1.02137
H 2.49066 -0.97218 -1.49316
H 2.83896 2.07556 1.55440
H 2.06690 3.66681 1.51355
H 1.47232 2.35225 0.46578
H -0.83479 2.80547 1.43461
H -0.15690 4.07090 2.48407
H -1.09685 2.74179 3.19286
H -2.20821 -0.70245 1.58843
H -2.50144 -1.25882 3.26817
H -2.05760 -2.42809 1.98247
H 0.86746 2.14707 4.72794
H 1.81989 3.47131 4.02585
H 2.46496 1.82307 4.02272
H -0.18815 -3.22754 3.21954
H -0.54982 -2.11143 4.56880
H 1.05676 -2.09968 3.80642
H -3.93800 -0.54939 -1.16521
H -3.13923 -1.76644 -2.16120
H -4.10804 -0.50361 -2.92335
H 0.38947 -1.60848 -3.68688
H -1.03844 -1.27217 -4.67587
H -1.18015 -2.27278 -3.22852
H -3.92145 2.64670 -1.61103
H -2.74347 3.04058 -0.35501
H -3.66474 1.53830 -0.25873
H 0.74613 3.45798 -1.74612
H -0.76737 3.87629 -0.94436
H -0.61364 4.07706 -2.69246
H -0.13874 2.66453 -4.74019
H -1.67849 1.78325 -4.70184
H -0.21776 1.00837 -5.34810
H 0.83618 1.05639 -3.08536
71
TS Complex 4 - Int 3'
C -1.16617 2.37598 7.76840
C -0.85023 1.21932 6.98402
C 0.42014 1.44072 6.36228
C 0.88313 2.74407 6.74706
C -0.09882 3.32441 7.61362
Ir 0.73566 1.46195 8.62289
Mo 1.82331 0.68543 10.44193
N 0.83199 1.61444 12.33639
C 0.88833 0.76651 13.54119
C 1.07526 0.53730 5.36797
C 2.10974 3.41976 6.22573
C -1.72887 0.02978 6.76968
C -0.08629 4.71772 8.15440
C -2.44852 2.61994 8.49577

N	3.30376	-0.29829	9.68249
C	3.68878	-0.62433	8.32375
N	0.47214	-0.97874	10.56783
C	0.99498	-2.33228	10.67238
N	2.78283	2.29612	11.40638
C	3.91565	3.20522	11.09368
C	4.87332	3.27656	12.29087
C	4.24695	-0.86121	10.64235
C	-0.93338	-0.90017	10.91650
C	1.94909	2.61156	12.39851
O	1.95382	3.48662	13.24184
C	-0.45663	2.33048	12.28499
C	4.66322	2.66651	9.87567
C	3.36700	4.59815	10.75469
H	-1.32983	0.06021	10.58025
H	-1.10361	-0.99957	11.99729
H	-1.50147	-1.70190	10.42146
H	3.99093	-0.56846	11.66504
H	5.26909	-0.51267	10.43849
H	4.25627	-1.95956	10.59253
H	0.28251	-3.05292	10.24585
H	1.17982	-2.63076	11.71477
H	1.93368	-2.41460	10.12381
H	3.76861	-1.71442	8.19069
H	4.67340	-0.19271	8.09050
H	2.94605	-0.22435	7.63707
H	5.13431	1.70509	10.09091
H	5.44911	3.37161	9.58909
H	3.98068	2.53341	9.03222
H	2.66896	4.52139	9.91680
H	4.18527	5.26559	10.46739
H	2.84702	5.03330	11.60902
H	-0.50408	2.90160	11.35830
H	-0.55197	2.99713	13.14852
H	-1.26977	1.60433	12.29120
H	4.36699	3.67574	13.17037
H	5.72250	3.92458	12.05196
H	5.26274	2.28198	12.52902
H	0.10214	0.01229	13.49415
H	0.75781	1.37542	14.44242
H	1.85643	0.26362	13.59253
H	2.16171	0.65011	5.37503
H	0.73014	0.76201	4.35039
H	0.84798	-0.51241	5.56723
H	2.49057	4.16241	6.92934
H	1.89810	3.93713	5.28107
H	2.91120	2.70261	6.03640
H	-1.14288	-0.88511	6.65536
H	-2.33757	0.14927	5.86419

H -2.41316 -0.11963 7.60723
H -2.88749 1.68827 8.85897
H -3.18608 3.09762 7.83799
H -2.30364 3.27644 9.35648
H -0.57438 4.77612 9.12957
H -0.61374 5.40303 7.47840
H 0.93113 5.09432 8.27512
H 0.49298 -0.32544 9.40516
71
Int 3'
C -2.38648 0.95185 -1.73688
C -1.99855 -0.19369 -2.51103
C -0.73675 0.09918 -3.12711
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61
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N 1.44959 -1.18820 0.06285

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N	-0.83376	-0.09104	1.55341
C	-0.65992	-1.33895	2.32250
C	-0.99887	-6.11836	0.14306
N	-1.04866	-7.14596	-0.46911
C	-1.85688	-8.35748	-0.58373
C	-1.80380	-9.11668	0.74544
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O	-1.76552	1.43872	3.07225
C	-2.10111	-0.15455	0.81705
C	4.00614	0.81792	1.47620
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C	2.33949	2.89748	3.31668
H	0.35316	-1.25691	-1.72138
H	0.41977	-2.79554	-0.82718
H	1.83812	-2.23548	-1.73240
H	3.54352	0.22629	2.26921
H	4.58897	1.61430	1.96077
H	4.71515	0.17403	0.93457
H	2.52087	-1.57526	1.84387
H	3.15806	-2.38572	0.40348
H	1.67317	-2.97453	1.17397
H	4.47333	1.74438	-0.90871
H	4.11699	3.11953	0.15234
H	2.93324	2.62870	-1.09076
H	2.93525	2.03537	3.62294
H	2.57395	3.72385	3.99398
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H	0.29748	4.14491	2.00637
H	0.35005	4.68130	3.69721
H	-1.00844	3.69087	3.12557
H	-2.24148	0.77925	0.27832
H	-2.94011	-0.32226	1.50174
H	-2.04163	-0.96984	0.09418
H	-0.53234	1.97698	4.97969
H	0.84174	2.94865	5.53673
H	1.08505	1.25085	5.09830
H	-0.60322	-2.18184	1.63432
H	-1.50738	-1.48305	3.00368
H	0.25872	-1.29022	2.90762
H	-2.00083	4.10516	0.52936
H	-3.09609	2.86940	-0.06889

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87
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C	-0.27634	-4.39016	-3.04803
C	1.96087	-2.36398	1.97041
C	-0.86624	1.25677	2.59168
O	-1.84376	1.88850	2.93502
C	-2.25267	-0.48655	1.58716
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H	4.24623	0.92498	-0.91885
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H	2.61373	4.09798	3.31587
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H	-2.26098	-1.55118	1.36163
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H	0.94344	2.22992	5.06272
H	-0.84117	-2.01274	3.18949
H	-1.63368	-0.71665	4.12804
H	0.13414	-0.71019	3.93624
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H	-2.89885	2.77101	0.24798
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H	0.10834	4.73500	-0.83261
H	0.10386	5.02186	-2.57293
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H	4.23814	1.05812	1.95963
H	4.33685	-0.63460	1.45524
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H	2.70473	-2.28252	2.31053
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H	3.72438	1.97063	-0.21297
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H	-3.19280	2.30249	0.16163
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H	-3.25346	-0.84723	-2.03671
H	-4.09430	0.54936	-2.72063
H	-3.85520	0.42757	-0.97816
H	-0.11826	4.36897	-0.73913
H	-0.02692	4.63726	-2.47922
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H	1.95718	2.33368	-3.31323
H	0.90833	2.29947	-4.73044
H	1.55433	0.79239	-4.07416
H	-1.55061	-0.24044	-4.90409
H	-1.57880	-1.36752	-3.54210
H	-0.03923	-0.82977	-4.20169
H	0.32797	-0.88207	-1.04813
H	-2.96462	-4.70112	-1.81248
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H	-1.44047	-6.63667	-1.07388

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87
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87
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Ir	-0.08233	0.73381	-0.91976
Mo	0.97756	-0.19624	0.82378
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C	1.28036	1.27667	-3.98605
C	0.81322	3.79769	-2.08797
C	-2.08066	3.50713	-0.77384
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C	-0.00920	-3.35202	0.26075
N	-1.13412	-2.87453	-0.28730
C	-2.33866	-3.71850	-0.49377
C	-2.87052	-4.26995	0.83562
N	0.66619	1.17129	2.40490
C	1.09205	2.54628	2.77247
C	-0.15040	3.43249	2.94503
C	3.81494	-0.02972	1.44550
C	2.27542	-3.02521	0.93016
C	1.58418	-2.46203	-1.30391
C	-0.16219	0.51572	3.21336
O	-0.59491	0.74099	4.32844
C	-2.02908	-0.52969	2.13073
O	0.12325	-4.43337	0.79967
C	1.90826	2.51614	4.07277
C	1.94632	3.12007	1.64564
C	-3.40531	-2.83255	-1.13104
C	-1.99407	-4.87436	-1.44188
H	0.82476	-1.96969	-1.90628
H	1.75570	-3.49686	-1.62771
H	2.50570	-1.88959	-1.39467
H	3.35232	-0.45142	2.34171
H	4.31321	0.90659	1.73323
H	4.59931	-0.72001	1.10056
H	3.15935	-2.41623	0.75941
H	2.46884	-4.05878	0.63531
H	2.02143	-3.01624	1.98914
H	4.26516	0.17114	-1.13839
H	3.90812	1.78281	-0.49683
H	2.70609	0.96333	-1.53358
H	2.90224	2.59887	1.56550
H	2.15325	4.17611	1.84340
H	1.42623	3.02388	0.68977
H	-0.73115	3.44208	2.01952

H 0.15157 4.45902 3.17508
H -0.78309 3.06845 3.75548
H -2.13187 0.36177 1.51256
H -2.61828 -0.43718 3.05043
H -2.36643 -1.39094 1.55644
H 1.30951 2.13111 4.89898
H 2.24536 3.52683 4.32441
H 2.79330 1.88373 3.95494
H -0.73645 -2.79240 2.77905
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H -3.56361 -0.17305 -2.12908
H -4.09112 1.46122 -2.52296
H -3.70660 1.03627 -0.85348
H -0.37854 -1.08655 -4.06527
H -1.70057 -0.22342 -4.85256
H -2.01821 -1.21533 -3.43059
H -2.76029 3.03312 -0.06171
H -2.67092 4.20770 -1.37904
H -1.36129 4.09474 -0.20014
H 0.67756 4.31158 -1.13447
H 0.61248 4.52565 -2.88457
H 1.86477 3.51189 -2.16085
H 2.17222 1.80272 -3.63899
H 1.05202 1.65510 -4.99098
H 1.53596 0.21851 -4.08318
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H -3.64831 -1.97830 -0.49442
H -3.07655 -2.45855 -2.10320
H -3.76411 -4.87123 0.64458
H -2.12728 -4.89781 1.32542
H -3.15365 -3.46104 1.51413
H -2.88350 -5.48304 -1.62747
H -1.63586 -4.49095 -2.40136
H -1.22552 -5.51610 -1.00809
77
Int 5
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C 0.04287 1.53640 -3.03310
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Mo 1.06551 0.25486 0.80705
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C -1.31374 -0.69565 -3.11860

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C	-2.13311	4.03567	-1.24094
N	2.92068	0.17335	0.27081
C	3.56859	0.48373	-0.99103
N	0.67145	1.25785	2.57016
C	0.95354	2.61380	3.10123
C	-0.26032	3.51710	2.85549
C	3.87620	-0.36318	1.23216
C	-0.31543	0.51552	3.08525
O	-1.08548	0.67670	4.00816
C	-1.80874	-0.97460	1.83229
C	1.27879	2.52864	4.59848
C	2.16584	3.16607	2.35245
H	3.39896	-0.55508	2.19755
H	4.69436	0.35205	1.40011
H	4.31946	-1.30353	0.87472
H	4.02223	-0.41667	-1.43234
H	4.37311	1.21696	-0.83222
H	2.83677	0.89735	-1.67961
H	3.04605	2.53742	2.51786
H	2.39424	4.17437	2.71012
H	1.97149	3.20687	1.27755
H	-0.49177	3.53813	1.78651
H	-0.04784	4.53730	3.18996
H	-1.13319	3.14894	3.39815
H	-2.20758	-0.10079	1.32005
H	-2.40795	-1.19403	2.72198
H	-1.83141	-1.82324	1.14595
H	0.42881	2.14667	5.16449
H	1.53385	3.52287	4.97756
H	2.13741	1.87110	4.76646
H	0.14204	-2.74780	2.26990
H	-0.47427	-2.10183	3.81718
H	1.16002	-1.67642	3.25703
H	-3.40907	0.06414	-1.23490
H	-4.13638	1.26675	-2.30186
H	-3.71870	1.69564	-0.64088
H	-0.37318	-1.24535	-3.19369
H	-1.79424	-0.71331	-4.10541
H	-1.95850	-1.24073	-2.42601
H	-2.82185	3.73405	-0.44898
H	-2.70491	4.62143	-1.97178
H	-1.39204	4.70325	-0.79495
H	0.57334	4.76064	-1.90686
H	0.41867	4.57379	-3.65537
H	1.72700	3.76310	-2.78558
H	2.04271	1.74695	-3.79686
H	0.84386	1.26927	-4.99961

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87

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C -2.35679 0.09368 -1.89598
C -2.54327 1.47849 -1.64294
Ir -1.02555 0.57129 -0.06156
Mo 0.92082 0.21145 1.07416
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N 0.92528 -1.22651 2.39187
C 1.89912 -1.29162 3.46602
C -3.84104 0.01635 1.58351
C -2.86585 -2.11594 -0.60441
C -1.91734 -0.51740 -3.18680
C -2.27411 2.58769 -2.60697
C -3.41374 2.92681 0.34036
C 1.37909 2.30899 1.07217
N 2.70939 2.49430 0.75781
C 3.36194 3.77710 0.94549
N 2.62623 0.34535 -0.09946
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O 4.50330 1.68536 -0.41306
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C 2.05782 -1.83430 -1.00406
C 3.20328 -0.16127 -2.45691
C 4.44780 -1.28753 -0.56718
H 1.08302 1.77205 2.12590
H 1.40914 -1.24434 4.45006
H 2.60708 -0.46079 3.39812
H 2.47569 -2.22744 3.42377
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H 4.74253 -2.11671 -1.21897
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H -3.16114 2.80255 -3.21593
H -1.45853 2.33681 -3.28854
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H -2.77796 3.74744 0.00035
H 1.99980 -2.29487 -0.01115
H 2.32828 -2.62032 -1.71549
H 1.06698 -1.45061 -1.27441
H 2.77140 4.58233 0.49553
H 4.33120 3.72401 0.45179
H 3.50949 3.99325 2.00846
H -3.45463 -0.90787 2.01674

H -4.92418 -0.10151 1.44849
H -3.67960 0.81156 2.31357
H -2.77365 -0.68125 -3.85334
H -1.43445 -1.48376 -3.02910
H -1.20670 0.12336 -3.71314
H 2.23358 0.23067 -2.77707
H 3.50021 -0.95528 -3.14966
H 3.94348 0.63779 -2.50913
H -2.84277 -2.44999 0.43429
H -2.06581 -2.63042 -1.14072
H -3.82086 -2.44342 -1.03450
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H 0.48072 1.83536 0.19984
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H -0.55786 -2.33566 3.40498
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61
Int 6
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C -3.01234 -0.00860 0.31788
C -2.99522 -1.04733 -0.68108
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Ir -0.93065 -0.20718 -0.33982
Mo 1.09939 -0.25737 0.77242
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C 2.56874 -2.34196 2.23335
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C -3.43353 -2.46084 -0.47693
C -2.50889 -1.16952 -3.23994
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C 2.99303 1.59291 1.02949
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C 4.36520 1.16511 -1.59792
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H 4.69039 1.43753 -2.60674

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H 4.05974 0.78561 3.25174
H 2.56082 0.35741 4.12009
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H -3.24742 -2.79335 0.54628
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H 3.21536 3.57320 -0.83053
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H -4.59524 -0.03369 1.76513
H -3.06027 0.59321 2.37947
H 0.40991 2.11239 1.85535
H 0.28741 -1.23558 -0.83678
H 1.15632 -3.99632 0.74948
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61
TS Int 6 - Int 7
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C -2.80760 0.41385 0.51613
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C -2.88605 -0.43863 -1.64414
Ir -0.97073 -0.42951 -0.40396
Mo 1.08757 -0.92925 0.60993
C 1.08109 -3.85582 -0.37219
N 1.63176 -2.76259 0.41368
C 2.89735 -3.12910 1.04018
C -1.83237 2.78353 0.00064
C -3.07478 0.58442 1.97711
C -3.89262 -1.94896 0.23089
C -3.17734 -1.32480 -2.81183
C -1.93944 1.60584 -2.95552
C 1.38870 -0.19155 2.45895
N 1.54290 1.14820 2.42397

C	1.34550	2.02331	3.56746
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C	2.10324	1.69969	1.20017
O	2.36302	2.88985	1.16111
C	2.88742	1.15103	-1.04499
C	3.04624	-0.12366	-1.87832
C	1.98596	2.13433	-1.79833
C	4.28081	1.74952	-0.80759
H	1.41809	-0.65189	3.44898
H	2.75007	-3.95550	1.74885
H	3.31361	-2.28051	1.59038
H	3.63206	-3.45053	0.28935
H	4.21995	2.67487	-0.23608
H	4.75880	1.96157	-1.76926
H	4.91151	1.03975	-0.26320
H	-2.44761	-1.18562	-3.61191
H	-4.17026	-1.10842	-3.22491
H	-3.15997	-2.37890	-2.52778
H	-1.14463	2.33143	-2.77411
H	-2.80553	2.15464	-3.34724
H	-1.59627	0.92664	-3.73853
H	3.67277	-0.85502	-1.35620
H	3.52626	0.10832	-2.83355
H	2.07227	-0.57439	-2.09477
H	0.29048	2.05172	3.85303
H	1.67177	3.02221	3.28175
H	1.93777	1.67494	4.41954
H	-1.50846	2.83713	1.04119
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H	-1.00065	3.12745	-0.61633
H	-3.63991	-2.83044	-0.36147
H	-4.98140	-1.81585	0.18659
H	-3.62563	-2.16231	1.26768
H	0.99682	1.68597	-1.92785
H	2.40372	2.35624	-2.78587
H	1.88930	3.06805	-1.24245
H	-2.95485	-0.35732	2.51699
H	-4.09950	0.93822	2.14634
H	-2.39627	1.31280	2.42519
H	0.04377	-0.68192	2.00958
H	-0.00138	-1.45524	-1.24103
H	1.78179	-4.16428	-1.16132
H	0.90311	-4.72538	0.27508
H	0.13826	-3.55520	-0.82261

61

Int 7

C	-2.18797	1.07173	-1.47057
C	-2.20872	1.50577	-0.09667
C	-2.88486	0.50467	0.67930

C	-3.29486	-0.54374	-0.22556
C	-2.87824	-0.19091	-1.54245
Ir	-1.02936	-0.37716	-0.22009
Mo	1.22032	-0.73335	0.63948
C	1.18241	-3.72624	0.00372
N	1.83057	-2.54159	0.54061
C	3.20389	-2.79766	0.95709
C	-1.72920	2.82964	0.40277
C	-3.25457	0.60283	2.12484
C	-4.09721	-1.74818	0.14840
C	-3.16817	-0.95437	-2.79421
C	-1.72872	1.88067	-2.64057
C	1.56233	-0.06552	2.42284
N	1.54125	1.29535	2.24128
C	1.10619	2.22180	3.27481
N	2.39604	0.83330	0.13557
C	2.08254	1.83579	1.02153
O	2.18173	3.04334	0.87767
C	3.10661	1.18272	-1.11978
C	3.40259	-0.12865	-1.84990
C	2.23240	2.06916	-2.01401
C	4.43446	1.87846	-0.79106
H	1.65400	-0.41118	3.45424
H	3.22748	-3.55025	1.75655
H	3.66280	-1.88133	1.33763
H	3.80608	-3.16939	0.11726
H	4.26132	2.82625	-0.28140
H	4.99058	2.07358	-1.71327
H	5.05029	1.24088	-0.14945
H	-2.38066	-0.81660	-3.53726
H	-4.11119	-0.61744	-3.24231
H	-3.25657	-2.02498	-2.60049
H	-0.93730	2.57670	-2.35988
H	-2.55864	2.46909	-3.05176
H	-1.34423	1.24608	-3.44164
H	4.02602	-0.78592	-1.23653
H	3.93921	0.07604	-2.78084
H	2.47763	-0.65648	-2.10093
H	0.05615	2.04936	3.52249
H	1.23946	3.23573	2.90048
H	1.71110	2.08215	4.17677
H	-1.48108	2.78678	1.46397
H	-2.50882	3.59056	0.27215
H	-0.83741	3.16625	-0.12737
H	-3.89037	-2.58946	-0.51569
H	-5.17052	-1.53001	0.08706
H	-3.88224	-2.07030	1.16880
H	1.28058	1.56787	-2.20905
H	2.73309	2.25217	-2.97029

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H -3.28513 -0.38012 2.59902
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H -2.53834 1.21148 2.67941
H -0.64744 -1.58159 0.84185
H 0.06126 -1.02569 -1.25251
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61
TS Int 7 - Int 8'
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Ir 2.00585 7.95081 4.28614
Mo 4.29077 8.41585 5.11881
C 3.28921 9.40504 7.19470
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C 4.67189 7.24182 8.03862
C 0.35179 5.11238 4.96073
C 0.37134 6.12799 1.94167
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C -0.35767 10.22508 5.00196
C -0.16426 7.64341 6.84994
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C 5.63096 11.75270 2.94171
N 5.67149 8.13984 3.55117
C 5.84516 9.25574 2.81630
O 6.28890 9.41710 1.69204
C 6.23025 6.86954 3.01169
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H 5.04006 11.17232 5.44714
H 5.38844 6.42543 7.90797
H 3.71572 6.82124 8.37484
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H 7.89335 7.76835 1.91627
H 8.14196 6.07369 2.37397
H 8.26723 7.34645 3.60021
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H 0.30925 6.77709 7.31546
H -1.23853 7.59232 7.06906
H 0.22578 8.54111 7.33461

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H 5.04680 5.57807 4.31612
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H 4.69395 12.08824 2.48824
H 0.99719 4.52646 4.30366
H -0.64496 4.65490 4.94444
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H 5.82935 5.47166 1.39719
H 5.58054 7.17481 0.96224
H 0.80979 6.66104 1.09601
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H 3.25847 6.85286 4.34148
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H 2.61944 8.78388 7.77832
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61
Int 8'
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C -2.89825 -0.00709 -1.13962
C -3.10208 0.57515 0.15804
Ir -1.05645 -0.26744 0.11461
Mo 1.21144 0.41179 0.92302
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C -3.47128 1.99183 0.45503
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N 2.86410 2.49624 -0.37033
C 3.48043 3.75111 -0.79052
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O 3.50267 1.61174 -2.39783
C 2.92786 -1.04468 -1.49766
C 2.63891 -2.25181 -0.60209
C 2.07991 -1.13639 -2.77106

C 4.42918 -1.08700 -1.83292
H 2.30406 3.11235 1.45895
H 2.87532 -1.54877 3.66176
H 1.24146 -2.16308 3.31853
H 1.45297 -0.74219 4.36268
H 4.71777 -0.28458 -2.50949
H 4.66621 -2.04385 -2.30755
H 5.02218 -1.00943 -0.91609
H -3.00706 2.33556 1.38242
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H -3.14758 2.66274 -0.34275
H -2.84709 -1.14737 3.17409
H -4.36689 -0.32735 2.79239
H -2.87880 0.60548 2.97900
H 3.16517 -2.16318 0.35234
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H 1.57252 -2.36297 -0.40425
H 4.55102 3.60336 -0.93701
H 3.29728 4.50385 -0.02468
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H -3.62270 -3.57251 1.00663
H -2.33217 -3.02759 2.08512
H -2.68990 1.75814 -2.34869
H -4.01399 0.68995 -2.82905
H -2.34028 0.25596 -3.19902
H 1.01820 -1.10048 -2.51233
H 2.27966 -2.07853 -3.29230
H 2.31052 -0.31109 -3.44683
H -2.03385 -1.97073 -2.94921
H -3.47408 -2.82087 -2.37657
H -1.87872 -3.25296 -1.75179
H 0.17969 -1.27546 0.54948
H -0.06693 0.69814 -0.76750
H -0.78822 1.46837 2.61295
H -0.38802 2.69822 1.40437
H 0.69762 2.41540 2.78473
61
TS Int 8' - Int 9''
C -2.89884 0.52521 0.40622
C -2.87508 -0.74926 1.08490
C -2.77094 -1.77914 0.09498
C -2.74550 -1.14437 -1.20430
C -2.83028 0.26763 -1.00834
Ir -0.94977 -0.48025 0.01502
Mo 1.39199 -0.33452 0.87213
C 0.55251 1.02039 2.57211
N 1.89471 -1.81495 1.59167
C 1.91133 -3.19171 1.95049

C	-3.04582	-0.94679	2.55600
C	-2.83282	-3.25334	0.34048
C	-2.73741	-1.85138	-2.52039
C	-2.90747	1.29778	-2.08872
C	-3.13097	1.85275	1.05339
C	2.44304	1.11268	1.87643
N	2.77466	2.14788	1.09212
C	3.25356	3.42688	1.58866
N	2.62634	0.54729	-0.59508
C	2.91158	1.84641	-0.32746
O	3.29127	2.72941	-1.07465
C	2.94401	0.04240	-1.96337
C	2.72962	-1.47331	-1.97122
C	2.03182	0.69117	-3.01196
C	4.42323	0.30207	-2.29021
H	2.91754	1.07913	2.85545
H	1.76825	-3.30325	3.03185
H	2.86832	-3.65424	1.68122
H	1.10403	-3.73147	1.44160
H	4.64239	1.36787	-2.33190
H	4.66621	-0.14271	-3.26024
H	5.06365	-0.16220	-1.53380
H	-2.48561	2.25038	-1.76384
H	-3.95011	1.47517	-2.37930
H	-2.36146	0.98320	-2.97986
H	-2.68607	1.89547	2.05051
H	-4.20412	2.05299	1.16456
H	-2.70246	2.66645	0.46466
H	3.33051	-1.95406	-1.19322
H	3.03687	-1.88046	-2.93904
H	1.67995	-1.73041	-1.81478
H	3.58827	4.01029	0.73205
H	4.08858	3.28032	2.28171
H	2.45084	3.96424	2.10099
H	-2.63194	-1.90266	2.88160
H	-4.10896	-0.93142	2.82718
H	-2.54854	-0.15732	3.12428
H	-2.25670	-1.25005	-3.29428
H	-3.76063	-2.06790	-2.85267
H	-2.20195	-2.80093	-2.46128
H	0.98388	0.49379	-2.77054
H	2.24278	0.27631	-4.00322
H	2.19226	1.76962	-3.04520
H	-2.25728	-3.80584	-0.40476
H	-3.86831	-3.61270	0.29481
H	-2.43350	-3.51212	1.32282
H	0.20132	-1.62905	-0.24246
H	0.06172	0.70982	-0.45807
H	0.14617	0.17272	3.13041

H -0.22340 1.58323 2.06371
H 1.03427 1.67160 3.30667
61
Int 9''
C -3.24484 0.59590 -0.85475
C -3.65690 0.18968 0.44604
C -3.19078 -1.16415 0.67060
C -2.48194 -1.58043 -0.49932
C -2.48319 -0.47649 -1.43804
Ir -1.38227 0.12016 0.37956
Mo 0.94779 0.03542 1.15175
N 2.58906 0.79105 0.16183
C 3.57479 0.32636 -0.83724
C 3.40895 1.12356 -2.13889
C -4.50185 0.98001 1.39141
C -3.52563 -2.01231 1.85600
C -1.93596 -2.94420 -0.77070
C -1.96783 -0.52301 -2.84110
C -3.57257 1.89354 -1.52016
N 1.36745 -1.55966 1.66185
C 1.66805 -2.83150 2.21656
C 0.74359 1.68233 3.98853
C 1.51600 1.24925 2.77050
N 1.57826 2.17284 1.64861
C 0.89315 3.46281 1.70515
C 2.62037 2.06141 0.63041
O 3.26333 3.03143 0.28481
C 4.99565 0.49244 -0.28092
C 3.30710 -1.15273 -1.11082
H 2.51659 0.88613 3.02431
H 2.26937 -3.42153 1.51316
H 0.74980 -3.39448 2.42650
H 2.23641 -2.73743 3.15036
H 5.21576 1.54288 -0.08507
H 5.72746 0.11309 -1.00040
H 5.10743 -0.07177 0.64967
H -2.77847 -2.79242 2.01072
H -4.49909 -2.50092 1.72463
H -3.57365 -1.41848 2.77098
H -1.02022 -2.89573 -1.36249
H -2.66599 -3.54491 -1.32787
H -1.70381 -3.47344 0.15452
H 3.43262 -1.74712 -0.20321
H 4.00490 -1.52142 -1.86811
H 2.28899 -1.30622 -1.48170
H 1.38028 4.13398 2.41897
H -0.14964 3.31559 1.98253
H 0.93654 3.91943 0.71816
H -1.66276 0.46661 -3.18621

H -2.73937 -0.89387 -3.52769
H -1.10207 -1.18218 -2.92720
H -4.26540 0.74320 2.43054
H -5.56617 0.76377 1.23557
H -4.35699 2.05338 1.25545
H 2.39658 0.99767 -2.53355
H 4.11829 0.76514 -2.89154
H 3.58747 2.18545 -1.96642
H -3.73024 2.68990 -0.79046
H -4.48866 1.80133 -2.11635
H -2.77180 2.21276 -2.18954
H -0.38916 1.33960 -0.06597
H -0.84684 0.32585 1.95727
H 0.74184 0.85557 4.70271
H 1.20123 2.54846 4.48295
H -0.29683 1.91875 3.75942
61
TS Int 7 - Int 8
C 0.18679 8.92879 4.29642
C 0.07337 8.07131 5.43168
C 0.06152 6.70059 4.96415
C 0.14953 6.72720 3.53099
C 0.24337 8.09626 3.11201
Ir 2.00434 7.62786 4.38748
Mo 4.43596 7.78640 5.11113
C 3.86994 6.78137 7.06916
N 4.77514 6.19984 6.18285
C 4.72013 4.78890 5.87790
C -0.12432 8.50582 6.84799
C -0.18640 5.49241 5.80956
C 0.06950 5.54069 2.62548
C 0.25239 8.58922 1.70166
C 0.13659 10.42322 4.30539
C 4.96730 9.28994 6.23277
N 5.58692 10.34178 5.63420
C 5.80930 11.63031 6.25929
N 5.74080 8.83901 3.89349
C 6.04581 10.10943 4.30848
O 6.62152 10.99140 3.69042
C 6.21500 8.42092 2.54565
C 5.86583 6.94031 2.37364
C 5.51599 9.23233 1.44709
C 7.74155 8.56263 2.44085
H 4.77825 9.43749 7.29956
H 5.22652 4.20890 6.65919
H 5.22709 4.59477 4.93030
H 3.68056 4.43953 5.79946
H 8.04658 9.60533 2.51376
H 8.08402 8.16166 1.48130

H 8.22926 7.99645 3.24038
H 0.80842 9.52393 1.61051
H -0.77008 8.77247 1.34853
H 0.71330 7.86493 1.02793
H 0.52354 10.83129 5.24060
H -0.89518 10.77590 4.18660
H 0.72858 10.84738 3.49246
H 6.34119 6.33583 3.15502
H 6.23194 6.58017 1.40744
H 4.78461 6.77656 2.40248
H 6.34353 11.51012 7.20683
H 4.86116 12.14514 6.44547
H 6.41175 12.22934 5.57741
H 0.31363 7.79622 7.55307
H -1.19414 8.58165 7.07885
H 0.32581 9.48220 7.03466
H 0.61459 5.71170 1.69574
H -0.97451 5.32552 2.36793
H 0.48799 4.64945 3.09578
H 4.43189 9.10300 1.51629
H 5.84032 8.89055 0.45850
H 5.75427 10.29192 1.54460
H 0.25653 4.59766 5.36855
H -1.26260 5.30984 5.92249
H 0.23257 5.61027 6.81103
H 3.08199 6.49025 3.91100
H 3.11848 8.74401 3.91007
H 3.00923 6.16058 7.34334
H 4.28691 7.31957 7.92286
H 3.02935 7.60816 6.28113
61
Int 8
C -2.85342 0.98048 -0.57943
C -3.07765 0.47139 0.73367
C -3.17062 -0.97201 0.64922
C -3.01507 -1.33646 -0.72877
C -2.80370 -0.14030 -1.49724
Ir -1.13092 -0.35260 -0.04800
Mo 1.40091 -0.39097 0.65506
C 1.77904 -1.69399 2.35916
N 2.10454 -2.12624 1.08834
C 1.82414 -3.44724 0.57241
C -3.29396 1.28111 1.97146
C -3.53495 -1.89150 1.77058
C -3.14773 -2.71759 -1.28646
C -2.73098 -0.04671 -2.98776
C -2.79315 2.42231 -0.97027
C 1.93905 0.93524 1.99513
N 2.33710 2.14180 1.51076

C 2.49644 3.33957 2.31439
N 2.56992 0.90966 -0.40502
C 2.74710 2.14968 0.15330
O 3.18147 3.16420 -0.37035
C 3.05683 0.69135 -1.79549
C 2.80841 -0.77666 -2.15363
C 2.30062 1.58168 -2.79078
C 4.56765 0.95657 -1.86667
H 1.91786 0.89095 3.08466
H 2.62322 -4.13589 0.87148
H 1.77561 -3.43059 -0.51873
H 0.87277 -3.83168 0.96487
H 4.79089 1.99751 -1.63471
H 4.93693 0.73383 -2.87285
H 5.09815 0.31459 -1.15724
H -2.10760 0.79111 -3.30504
H -3.72970 0.09789 -3.41818
H -2.30856 -0.95332 -3.42441
H -2.42512 3.04386 -0.15277
H -3.79076 2.78487 -1.24578
H -2.13416 2.57810 -1.82585
H 3.31770 -1.44259 -1.44984
H 3.19959 -0.98201 -3.15462
H 1.73910 -1.01353 -2.16353
H 3.16350 3.14843 3.16063
H 1.52912 3.68310 2.69152
H 2.92961 4.11087 1.67846
H -2.94049 0.75484 2.85992
H -4.36156 1.49014 2.11042
H -2.77042 2.23713 1.92229
H -2.55026 -2.84229 -2.19071
H -4.19355 -2.92339 -1.54331
H -2.82561 -3.47241 -0.56754
H 1.22653 1.38067 -2.73665
H 2.63662 1.37116 -3.81142
H 2.47503 2.63549 -2.57464
H -3.14502 -2.89716 1.60447
H -4.62491 -1.96832 1.87100
H -3.13864 -1.53810 2.72421
H -0.13760 -1.57814 -0.44346
H 0.05542 0.56023 -0.70189
H 0.91032 -2.15581 2.84381
H 2.58757 -1.41532 3.03091
H -0.31506 -0.09828 1.40887
61
TS Int 8 - Int 9'
C 0.17445 9.05600 3.49905
C -0.33401 8.62609 4.78665
C -0.53918 7.21112 4.72151

C	-0.14260	6.74842	3.41693
C	0.28345	7.90648	2.66028
Ir	1.63714	7.61711	4.41640
Mo	4.07080	7.67750	5.35118
N	4.32755	6.49029	6.87812
C	4.11955	5.17172	7.40997
C	-0.71689	9.52781	5.91583
C	-1.14295	6.36225	5.79406
C	-0.32600	5.36665	2.87587
C	0.66211	7.90205	1.21435
C	0.42007	10.47443	3.09446
C	5.10702	8.85024	6.59701
N	5.13822	10.15531	6.17041
C	5.72021	11.23740	6.94718
C	3.94536	7.68367	7.54609
N	5.23281	8.91923	4.18430
C	5.30470	10.18796	4.74153
O	5.52549	11.23623	4.17051
C	5.65541	8.75542	2.76586
C	5.69562	7.25294	2.47165
C	4.65847	9.43766	1.82079
C	7.07176	9.31124	2.55419
H	2.87552	7.88240	7.69493
H	4.49021	7.94973	8.45543
H	5.96410	8.56031	7.21697
H	4.41559	4.43661	6.65800
H	3.06489	4.98844	7.66857
H	4.72520	4.99973	8.31131
H	7.10453	10.38854	2.70999
H	7.40055	9.09573	1.53259
H	7.77331	8.83207	3.24400
H	1.32431	8.73357	0.96934
H	-0.23332	7.99199	0.58766
H	1.17145	6.97774	0.93665
H	0.77161	11.07518	3.93483
H	-0.50478	10.93080	2.72070
H	1.17004	10.54481	2.30522
H	6.38814	6.74276	3.14840
H	6.03568	7.08365	1.44538
H	4.70801	6.79466	2.57543
H	6.71654	10.97176	7.32538
H	5.07297	11.48295	7.79216
H	5.80680	12.10831	6.29792
H	-0.68353	9.00575	6.87379
H	-1.73640	9.90926	5.77932
H	-0.04787	10.38755	5.98492
H	0.41190	5.14082	2.10409
H	-1.32209	5.25021	2.43076
H	-0.22033	4.61400	3.65912

H 3.65664 9.03285 1.98830
H 4.93923 9.25895 0.77751
H 4.64050 10.51349 1.99963
H -0.75482 5.34302 5.76166
H -2.23111 6.31134 5.66969
H -0.93891 6.76487 6.78737
H 2.18425 6.58975 5.55363
H 2.61164 8.79735 5.19828
H 2.94333 6.97122 3.65918
61
Int 9'
C -2.70727 0.84278 -0.90184
C -2.96780 0.17230 0.36037
C -3.03196 -1.22627 0.10909
C -2.80995 -1.44152 -1.31129
C -2.65698 -0.15424 -1.92626
Ir -0.98520 -0.51442 -0.46654
Mo 1.41003 -0.41732 0.51520
N 1.00463 -0.80332 2.38378
C -0.02035 -1.55392 3.06663
C -3.23439 0.86115 1.65961
C -3.39527 -2.29411 1.08934
C -2.93186 -2.75151 -2.02150
C -2.51165 0.10278 -3.39169
C -2.67418 2.32342 -1.10668
C 2.60125 0.60699 1.96432
N 2.85783 1.94778 1.56424
C 3.48036 2.91925 2.43601
C 1.69409 0.24266 3.11133
N 2.63825 0.86569 -0.44062
C 3.01208 2.06267 0.20040
O 3.42570 3.06833 -0.35514
C 3.08138 0.66952 -1.85417
C 2.91265 -0.81585 -2.20662
C 2.25243 1.54006 -2.80591
C 4.57855 0.98906 -2.00062
H 1.00471 1.05777 3.37424
H 2.17484 -0.11234 4.03988
H 3.53050 -0.00078 2.00287
H -0.45801 -2.29903 2.40435
H -0.81668 -0.89024 3.43442
H 0.41524 -2.06775 3.93516
H 4.77989 2.04481 -1.83215
H 4.90287 0.72040 -3.01118
H 5.16437 0.39867 -1.28923
H -1.94046 1.01212 -3.58462
H -3.49852 0.22317 -3.85388
H -2.00537 -0.72208 -3.89557
H -2.24154 2.83673 -0.24623

H -3.68759 2.71592 -1.25611
H -2.07973 2.59327 -1.98093
H 3.53918 -1.44353 -1.56401
H 3.22434 -0.98276 -3.24231
H 1.87634 -1.16000 -2.13078
H 4.45654 2.56879 2.80019
H 2.84069 3.12681 3.29859
H 3.62719 3.83840 1.86836
H -3.03244 0.20675 2.50881
H -4.28408 1.17336 1.71958
H -2.61631 1.75340 1.77344
H -2.34677 -2.76090 -2.94267
H -3.97702 -2.95512 -2.28567
H -2.57852 -3.57626 -1.40011
H 1.19057 1.29297 -2.72216
H 2.56616 1.37607 -3.84218
H 2.39177 2.59288 -2.55811
H -2.85352 -3.22106 0.89219
H -4.46729 -2.51705 1.02781
H -3.17866 -1.99081 2.11457
H -0.03679 -1.79885 0.02420
H -0.02797 0.64613 0.43605
H 0.19816 -0.44160 -1.54766
61
TS Int 9' - Complex 5'
C -0.64720 8.46237 4.98743
C -0.47860 7.10764 4.51966
C 0.18922 7.17243 3.24010
C 0.44389 8.54074 2.92061
C -0.05359 9.33719 4.02105
Ir 1.51983 7.98880 4.85416
Mo 3.98846 8.21623 5.65686
N 4.08761 8.56263 7.46014
C 3.89335 8.55372 8.87401
C -1.06339 5.87989 5.14151
C 0.45683 5.99788 2.35610
C 1.00823 9.07171 1.64233
C -0.06699 10.83156 4.06578
C -1.40233 8.87867 6.20866
C 5.60075 9.56238 5.74307
N 5.69880 10.14478 4.45957
C 6.56253 11.28875 4.22552
C 4.81727 10.01175 6.90985
N 5.17610 7.92414 3.97492
C 5.67308 9.13741 3.47763
O 6.03690 9.35264 2.33359
C 5.37772 6.72136 3.11405
C 5.02195 5.47074 3.92482
C 4.48497 6.79002 1.86883

C 6.85728 6.58738 2.71270
H 4.09236 10.80858 6.75677
H 5.42097 10.18551 7.80400
H 6.51804 9.04073 6.06012
H 3.50861 7.57033 9.15489
H 3.15826 9.30755 9.18639
H 4.82847 8.73369 9.42496
H 7.18294 7.42214 2.09496
H 6.99896 5.65895 2.15035
H 7.48696 6.53915 3.60686
H -0.09294 11.20114 5.09206
H -0.95217 11.21927 3.54739
H 0.81436 11.25386 3.58022
H -1.32896 8.12771 6.99696
H -2.46463 9.01646 5.97362
H -1.02495 9.81972 6.61227
H 5.60992 5.42400 4.84680
H 5.24741 4.57861 3.33222
H 3.96425 5.43964 4.19168
H 7.58845 11.10576 4.57742
H 6.16538 12.16706 4.73988
H 6.59153 11.47972 3.15315
H -0.46911 4.99440 4.90958
H -2.08252 5.70455 4.77496
H -1.10996 5.96701 6.22842
H 0.20581 9.30277 0.93048
H 1.67712 8.35215 1.16803
H 1.58146 9.98603 1.80559
H 3.44186 6.89773 2.17752
H 4.58308 5.87294 1.27817
H 4.76225 7.64323 1.24954
H 1.27808 6.19086 1.66541
H -0.43448 5.76844 1.76020
H 0.70811 5.10834 2.93603
H 1.74778 7.70389 6.41490
H 2.66813 9.28311 4.99139
H 2.73756 6.85731 4.81008
61
Complex 5'
Ir 1.68954 7.81049 4.44465
Mo 4.20504 7.65225 5.28416
O 6.24239 10.96027 3.95720
N 5.59357 10.08505 5.96747
N 5.42970 8.77434 4.08214
N 4.83811 6.10681 5.65538
C 4.14117 8.53640 7.25830
H 3.36356 9.29588 7.27693
H 4.11036 7.83237 8.08325
C -0.31068 6.80901 4.68308

C	0.06538	6.74917	3.31208
C	-0.11430	8.99405	3.90332
C	0.20395	8.10663	2.81858
C	5.81057	10.01079	4.59578
C	5.38695	8.84659	6.63604
H	6.28994	8.34352	6.98981
C	5.81758	8.48349	2.67176
C	-0.41117	8.20646	5.06493
C	5.28968	4.77455	5.84607
H	6.07178	4.51709	5.12190
H	4.46400	4.06126	5.74089
H	5.70833	4.66671	6.85372
C	7.32593	8.71097	2.46806
H	7.59481	9.75436	2.62140
H	7.60649	8.42052	1.45051
H	7.89774	8.09209	3.16694
C	0.44146	8.49914	1.39596
H	0.89872	9.48716	1.32534
H	-0.50342	8.52687	0.83916
H	1.10370	7.79410	0.89044
C	-0.19817	10.48400	3.81205
H	0.00390	10.95605	4.77449
H	-1.20265	10.78566	3.49304
H	0.51734	10.88155	3.09108
C	5.54875	7.00615	2.36641
H	6.07791	6.35873	3.07101
H	5.90862	6.77777	1.35879
H	4.48453	6.76161	2.39886
C	6.09807	11.22133	6.70565
H	7.06588	11.00000	7.17808
H	5.38906	11.50980	7.48717
H	6.23138	12.04712	6.00690
C	-0.90634	8.71800	6.37957
H	-0.60988	8.06207	7.20022
H	-2.00135	8.78399	6.38420
H	-0.51125	9.71230	6.59406
C	0.19748	5.51352	2.48116
H	0.96026	5.63085	1.70963
H	-0.75156	5.28858	1.98000
H	0.46835	4.64823	3.08807
C	5.00250	9.35182	1.70261
H	3.93344	9.17111	1.84844
H	5.25657	9.10701	0.66548
H	5.21042	10.40741	1.87719
C	-0.64924	5.64842	5.56240
H	-0.12907	4.74208	5.24891
H	-1.72642	5.44555	5.52863
H	-0.38046	5.84276	6.60209
H	2.35360	7.27823	5.87546

H 2.64882 9.11157 4.58950
H 2.98032 7.10561 3.69725
61
TS Int 8 - Int 9
C -3.01208 0.63798 -1.61504
C -3.52335 1.05393 -0.32841
C -3.58846 -0.11492 0.50932
C -3.08874 -1.22882 -0.23538
C -2.74278 -0.76507 -1.56582
Ir -1.44963 0.27206 -0.06280
Mo 1.06509 0.85802 0.31810
N 2.55475 -0.51345 -0.02348
C 3.33002 -0.35781 -1.13732
O 4.19885 -1.08727 -1.59366
C -4.05719 2.40964 0.00872
C -4.15365 -0.16590 1.89234
C -3.06573 -2.65412 0.21595
C -2.31778 -1.63169 -2.70766
C -2.88783 1.51423 -2.81990
N 1.73259 2.03926 1.66462
C 2.43021 2.59189 0.58131
C 2.03335 1.59773 -1.26475
N 3.02070 0.86067 -1.80747
C 3.84980 1.25554 -2.93278
C 1.22897 2.81088 2.77677
C 2.83499 -1.71834 0.81845
C 1.95421 -1.66986 2.06951
C 2.51869 -3.00156 0.03780
C 4.30069 -1.70890 1.28367
H 1.83140 2.51227 -1.83026
H 2.04861 3.08884 3.45025
H 0.50614 2.21621 3.33873
H 0.73650 3.73269 2.43710
H 4.98451 -1.78121 0.43938
H 4.48084 -2.55454 1.95504
H 4.51280 -0.78764 1.83528
H -3.69110 -0.95627 2.48557
H -5.23223 -0.36059 1.85573
H -4.00362 0.77681 2.42117
H -2.23966 -3.20310 -0.23916
H -3.99767 -3.16016 -0.06388
H -2.95664 -2.73026 1.29900
H 2.13596 -0.75681 2.64455
H 2.19554 -2.52576 2.70792
H 0.89077 -1.72108 1.82442
H 3.35026 2.06311 -3.46995
H 3.99275 0.40068 -3.59377
H 4.83580 1.59497 -2.60042
H -1.74422 -1.06744 -3.44475

H -3.19072 -2.05850 -3.21706
H -1.69208 -2.45908 -2.36901
H -3.95981 2.62185 1.07495
H -5.11998 2.48842 -0.25219
H -3.52349 3.19408 -0.53087
H 1.47259 -2.99636 -0.28342
H 2.67656 -3.87947 0.67286
H 3.15771 -3.08671 -0.84124
H -2.64306 2.54115 -2.54337
H -3.83349 1.53391 -3.37474
H -2.11005 1.15666 -3.49641
H -0.88080 0.78136 1.38032
H -0.16918 -0.76425 0.05724
H 2.13255 3.59649 0.26524
H 3.50888 2.41553 0.55604
H -0.41043 1.47141 -0.68918
61
Int 9
C -3.26363 0.89299 -0.64514
C -3.28408 0.16516 0.57884
C -2.98443 -1.22549 0.28125
C -2.80621 -1.33888 -1.13496
C -2.94387 -0.03133 -1.71694
Ir -1.23409 0.01846 -0.30752
Mo 1.19319 0.73200 0.20500
N 2.48541 -0.70276 0.82811
C 3.39460 -1.19831 -0.10320
O 4.14910 -2.15423 0.04352
C -3.66004 0.69783 1.92406
C -3.02667 -2.35290 1.26203
C -2.57331 -2.60783 -1.88952
C -2.95006 0.28658 -3.17780
C -3.60500 2.33784 -0.82130
N 2.07503 2.34292 0.57738
C 3.00884 1.96371 -0.52972
C 2.51241 0.64605 -1.33499
N 3.37832 -0.46841 -1.28216
C 4.29271 -0.78583 -2.35226
C 2.18860 3.66026 1.13037
C 2.56061 -1.30686 2.19515
C 1.62801 -0.54523 3.14113
C 2.12357 -2.77855 2.15871
C 3.98369 -1.17488 2.76829
H 2.28193 0.92011 -2.36607
H 3.16879 3.80720 1.60380
H 1.41557 3.80194 1.88833
H 2.06433 4.43269 0.35796
H 4.70370 -1.72865 2.16902
H 4.00662 -1.55968 3.79298

H 4.28073 -0.12124 2.79807
H -2.39266 -3.18228 0.94513
H -4.04958 -2.73404 1.36899
H -2.68498 -2.03681 2.24924
H -1.99893 -2.43101 -2.79999
H -3.53110 -3.05702 -2.17720
H -2.02749 -3.33686 -1.28915
H 1.86926 0.52257 3.16327
H 1.75085 -0.93951 4.15505
H 0.57844 -0.65827 2.86171
H 5.10019 -0.04591 -2.43564
H 3.76252 -0.83106 -3.31002
H 4.73381 -1.75851 -2.13610
H -2.62507 1.31168 -3.36446
H -3.95791 0.17401 -3.59588
H -2.28271 -0.37539 -3.73215
H -3.11571 0.18955 2.72171
H -4.73165 0.55252 2.10648
H -3.44893 1.76514 2.00638
H 1.11047 -2.85578 1.75222
H 2.12038 -3.19924 3.17031
H 2.79967 -3.36327 1.53568
H -3.38017 2.91442 0.07717
H -4.67392 2.45347 -1.03705
H -3.04855 2.78199 -1.64815
H -0.32575 -0.09261 1.09949
H 0.02987 -0.84009 -0.87656
H 3.01183 2.77832 -1.25942
H 4.01307 1.76959 -0.13736
H -0.32062 1.27777 -0.92906
61
TS Int 9 - Complex 5
C -3.37945 1.06068 -1.03333
C -3.44540 0.46973 0.26158
C -3.18754 -0.95319 0.11430
C -2.99420 -1.22258 -1.27806
C -3.07931 0.02094 -1.99733
Ir -1.38697 0.15603 -0.56779
Mo 1.04810 0.89900 -0.07853
N 2.35577 -0.57311 0.45911
C 3.36262 -0.92730 -0.43718
O 4.13836 -1.86981 -0.32742
C -3.82739 1.15393 1.53487
C -3.27379 -1.96858 1.20797
C -2.79761 -2.57158 -1.89090
C -3.06065 0.18126 -3.48389
C -3.66337 2.49019 -1.36548
N 1.71054 2.44941 0.53155
C 2.62301 2.24565 -1.11791

C 2.42742 0.91217 -1.67367
N 3.44674 -0.06448 -1.51969
C 4.34449 -0.35021 -2.61227
C 2.09460 3.69526 1.10318
C 2.39529 -1.30100 1.77019
C 1.36537 -0.71208 2.73838
C 2.06542 -2.78869 1.57118
C 3.77209 -1.13012 2.43985
H 1.91145 0.88544 -2.63564
H 3.16597 3.72295 1.34166
H 1.53593 3.82386 2.03504
H 1.85755 4.54173 0.44536
H 4.56535 -1.56990 1.83881
H 3.76706 -1.61328 3.42229
H 3.98551 -0.06642 2.58906
H -2.65061 -2.83859 0.99526
H -4.30679 -2.31572 1.33151
H -2.94580 -1.55454 2.16302
H -2.17122 -2.51824 -2.78252
H -3.76409 -2.99890 -2.18302
H -2.32298 -3.26225 -1.19266
H 1.50522 0.36538 2.86677
H 1.49290 -1.19087 3.71472
H 0.34050 -0.89021 2.40909
H 4.98076 0.51389 -2.83669
H 3.79621 -0.62196 -3.52521
H 4.97090 -1.19057 -2.31346
H -2.70069 1.16988 -3.77444
H -4.06687 0.05612 -3.90268
H -2.40938 -0.55689 -3.95524
H -3.31686 0.71396 2.39322
H -4.90702 1.06885 1.70881
H -3.57559 2.21536 1.50990
H 1.08728 -2.89071 1.09108
H 2.02738 -3.30045 2.53919
H 2.81687 -3.26941 0.94667
H -3.42195 3.15077 -0.53144
H -4.72613 2.62063 -1.60191
H -3.08669 2.82158 -2.23048
H -0.49308 0.08052 0.84378
H -0.14965 -0.74108 -1.12274
H 2.19899 3.08473 -1.66039
H 3.60258 2.42005 -0.67891
H -0.43498 1.39136 -1.22248
61
Complex 5
C -3.26324 1.05655 -0.70995
C -3.29417 0.50414 0.60248
C -3.07899 -0.92817 0.48873

C	-2.93527	-1.23976	-0.90133
C	-3.02332	-0.01507	-1.65414
Ir	-1.26920	0.10952	-0.29556
Mo	1.29095	0.66516	0.02641
N	2.66025	-0.76561	0.65745
C	3.87696	-0.83726	-0.01300
O	4.86538	-1.47272	0.33013
C	-3.60769	1.23552	1.86794
C	-3.16158	-1.91005	1.61276
C	-2.80205	-2.61077	-1.48212
C	-3.06357	0.10417	-3.14410
C	-3.52136	2.48354	-1.07207
N	1.81799	1.95345	1.02681
C	2.05841	1.56090	-1.82595
C	2.59589	0.26082	-1.63735
N	3.88971	-0.05304	-1.16682
C	4.95182	-0.26612	-2.12958
C	2.35471	2.94988	1.87985
C	2.61756	-1.48374	1.96899
C	1.24670	-1.30590	2.62335
C	2.82178	-2.99281	1.74808
C	3.67176	-0.92852	2.94233
H	2.10448	-0.54403	-2.20241
H	3.22502	2.56535	2.42503
H	1.60762	3.29480	2.60447
H	2.67798	3.81420	1.28622
H	4.67787	-1.06951	2.55098
H	3.59387	-1.43895	3.90814
H	3.50075	0.13907	3.11165
H	-2.60125	-2.81984	1.39195
H	-4.20429	-2.19577	1.79744
H	-2.76251	-1.49333	2.53911
H	-2.22935	-2.59880	-2.41053
H	-3.79307	-3.02364	-1.70394
H	-2.30198	-3.29136	-0.79182
H	1.03743	-0.25799	2.85813
H	1.23135	-1.86434	3.56430
H	0.44556	-1.68666	1.98620
H	5.14455	0.65898	-2.67842
H	4.70161	-1.05808	-2.85121
H	5.84701	-0.56557	-1.58536
H	-2.68252	1.07071	-3.47866
H	-4.09144	0.00500	-3.51444
H	-2.46140	-0.66985	-3.62301
H	-3.09301	0.79293	2.72236
H	-4.68436	1.20337	2.07390
H	-3.30978	2.28352	1.80904
H	2.05673	-3.37576	1.06551
H	2.72627	-3.52464	2.70083

H 3.80467 -3.19747 1.32794
H -3.24243 3.15980 -0.26288
H -4.58681 2.63276 -1.28326
H -2.96133 2.77869 -1.96076
H -0.38111 0.22957 1.09028
H -0.09109 -0.84862 -0.87493
H 1.31982 1.71657 -2.60556
H 2.66216 2.42867 -1.58002
H -0.36968 1.37828 -0.86710
75

Int 10
C -3.23742 -0.40109 -1.91489
C -1.94509 -0.19286 -2.48811
C -1.60658 1.20307 -2.33329
C -2.71176 1.84548 -1.65853
C -3.70046 0.84657 -1.40285
Ir -1.63289 0.34559 -0.31444
Mo -0.13253 0.07965 1.28607
N 0.42974 1.85119 1.82171
C 0.15152 3.15584 1.24819
C -1.14711 -1.20039 -3.25106
C -0.44356 1.89582 -2.96674
C -2.87359 3.31617 -1.44730
C -5.01230 1.07728 -0.72433
C -3.99268 -1.69097 -1.89980
N -0.95801 -1.12995 2.74540
C -2.08789 -1.01938 3.69884
C -2.33541 0.46573 3.96242
N 0.55015 -2.06108 1.32103
C 1.89965 -2.24103 1.89540
C -0.49281 -2.33007 2.37538
O -0.77645 -3.46547 2.69437
C 0.37251 -2.95938 0.16455
C 1.36624 1.95816 2.93316
C -3.34113 -1.64993 3.08150
C -1.72194 -1.71031 5.01966
N 6.18034 -1.12510 -1.89616
C 7.20032 -0.21804 -2.41734
C 6.60461 0.58620 -3.57661
C 5.09123 -1.12035 -1.40218
O 4.03016 -1.24471 -0.91309
C 7.66076 0.71092 -1.29011
C 8.36357 -1.08210 -2.90722
H 1.55449 0.98057 3.38619
H 0.96331 2.61837 3.71502
H 2.33008 2.37440 2.60587
H 1.07210 3.62074 0.86286
H -0.26261 3.82621 2.01589

H -0.57008 3.04926 0.44185
H -1.44529 0.94003 4.38704
H -3.15780 0.58340 4.67435
H -2.59398 0.98721 3.03769
H -3.55809 -1.16858 2.12337
H -4.20035 -1.51641 3.74629
H -3.19331 -2.71840 2.91357
H -0.62178 -2.80227 -0.25019
H 0.49336 -4.00246 0.47439
H 1.11802 -2.70283 -0.58969
H -1.54400 -2.77563 4.87030
H -2.53889 -1.58894 5.73754
H -0.82242 -1.26017 5.45124
H 2.64763 -1.95495 1.15430
H 2.04814 -3.28753 2.18538
H 2.00961 -1.61193 2.78069
H -0.07549 -1.01074 -3.16273
H -1.40502 -1.17552 -4.31770
H -1.33365 -2.21487 -2.89212
H -0.14585 2.77826 -2.39658
H -0.69018 2.22175 -3.98580
H 0.42411 1.23566 -3.02766
H -3.31942 -2.55074 -1.88873
H -4.63136 -1.78466 -2.78764
H -4.63805 -1.77110 -1.02227
H -5.33601 0.19644 -0.16514
H -5.79736 1.30995 -1.45506
H -4.95913 1.91229 -0.02226
H -3.44878 3.53439 -0.54478
H -3.40054 3.77501 -2.29417
H -1.90840 3.81840 -1.35450
H 7.36327 1.24603 -4.00679
H 6.24271 -0.08097 -4.36253
H 5.76912 1.20319 -3.23447
H 9.16028 -0.45153 -3.31016
H 8.77194 -1.67684 -2.08674
H 8.03053 -1.76543 -3.69197
H 8.45188 1.37558 -1.64819
H 6.83237 1.32760 -0.93080
H 8.05163 0.13185 -0.45001
77
TS Int 10 - Int 11
O 0.94071 -3.72969 0.84913
Mo 0.82448 0.03593 1.46013
N 2.75319 -0.00540 1.33245
C 3.50169 -0.39190 2.52185
Ir 0.10341 0.89952 -0.44435
C 0.40172 0.59334 -2.61557
C 0.61954 1.99807 -2.37800

C	-0.62823	2.56962	-1.96967
C	-1.61308	1.54269	-1.93951
C	-0.98333	0.31455	-2.32630
C	1.87514	2.75715	-2.66459
C	-0.85463	4.01089	-1.64592
C	-3.06219	1.72113	-1.62000
C	-1.67035	-0.99372	-2.55316
C	1.36648	-0.35437	-3.25032
N	-0.00068	1.17721	2.97408
C	-1.07768	0.44634	3.28599
O	-2.07026	0.66987	3.94681
N	-0.90630	-0.87265	2.57417
C	-2.15988	-1.27537	1.90979
C	1.00659	-4.26293	-0.19622
N	1.01119	-4.70754	-1.30673
C	1.45018	-5.88526	-2.05400
C	0.95687	-5.71875	-3.49213
C	0.10274	2.59173	3.40609
C	-1.02629	3.40481	2.76292
C	0.03554	2.67338	4.93678
C	1.45354	3.12551	2.93049
C	2.97971	-5.95191	-2.01618
C	0.83524	-7.13615	-1.41920
C	-0.49782	-1.90977	3.54462
C	3.63984	0.18617	0.19906
H	2.84005	-0.50253	3.38583
H	4.25059	0.37441	2.76990
H	4.03047	-1.34394	2.37136
H	4.22101	-0.72680	-0.00283
H	4.35464	0.99581	0.40812
H	3.05182	0.44520	-0.67827
H	2.27643	2.55827	3.37626
H	1.56289	4.17369	3.22416
H	1.53435	3.05183	1.84280
H	-0.98201	3.28981	1.67580
H	-0.92014	4.46532	3.01190
H	-2.00056	3.06021	3.11473
H	-2.43830	-0.50975	1.18749
H	-2.95569	-1.40385	2.65066
H	-1.98452	-2.21380	1.38119
H	-0.91977	2.30157	5.30834
H	0.15503	3.71320	5.25625
H	0.84149	2.08566	5.38725
H	-0.28071	-2.83529	3.00959
H	-1.29754	-2.07935	4.27463
H	0.40003	-1.58582	4.07404
H	-0.99484	-1.83377	-2.37929
H	-2.03967	-1.06731	-3.58443
H	-2.52686	-1.11615	-1.88676

H 2.40086 -0.07079 -3.04616
H 1.23715 -0.36725 -4.34065
H 1.22284 -1.37223 -2.88325
H -3.63318 1.99293 -2.51729
H -3.21904 2.50829 -0.87937
H -3.50039 0.80445 -1.21945
H -1.67114 4.13966 -0.93224
H -1.11353 4.57933 -2.54835
H 0.03726 4.47016 -1.21345
H 2.75844 2.12105 -2.57865
H 2.00418 3.59009 -1.97003
H 1.86295 3.17023 -3.68169
H 3.33359 -6.80600 -2.60032
H 3.41573 -5.04243 -2.43600
H 3.33933 -6.06655 -0.98992
H 1.25988 -6.57762 -4.09651
H -0.13267 -5.64240 -3.51848
H 1.37431 -4.81399 -3.93994
H 1.12242 -8.02606 -1.98613
H 1.18059 -7.26110 -0.38916
H -0.25536 -7.06892 -1.41389
77
Int 11
C -2.56384 1.78963 -0.43165
C -1.81912 1.74995 -1.65426
C -1.98147 0.44468 -2.22832
C -2.83938 -0.31451 -1.36568
C -3.19339 0.51502 -0.25714
Ir -0.90195 0.22974 -0.24714
Mo 0.91797 -0.52587 0.80687
O 2.50154 -0.12376 -0.73106
C 2.60134 0.76109 -1.52825
N 2.75476 1.54581 -2.39002
C 3.33328 2.76289 -2.94684
C 2.95495 3.93784 -2.04200
C -1.45352 0.00604 -3.55632
C -1.12659 2.91006 -2.29115
C -3.35698 -1.69253 -1.62275
C -4.15465 0.16257 0.83116
C -2.77443 2.99143 0.43145
N 1.24922 -2.68038 0.08502
C 2.64282 -3.15562 0.13166
N 0.21214 -2.09096 2.01460
C -0.64417 -2.21566 3.21848
C -0.85460 -0.82298 3.81019
N 1.37129 0.93950 1.98602
C 0.80429 2.25807 2.18756
C 0.59361 -3.16597 -1.14279
C 0.51248 -3.17313 1.29739

O	0.29795	-4.36068	1.44977
C	2.52245	0.72851	2.85528
C	-2.00397	-2.80250	2.81837
C	0.04729	-3.11100	4.25611
C	4.85303	2.57725	-3.00036
C	2.76297	2.94997	-4.35343
H	2.93486	-0.27623	2.72336
H	2.24096	0.84053	3.91238
H	3.31857	1.45799	2.64468
H	1.56252	3.03936	2.01912
H	0.44576	2.36708	3.22227
H	-0.02674	2.39401	1.49796
H	0.09124	-0.39207	4.14998
H	-1.52855	-0.88695	4.66984
H	-1.28832	-0.15291	3.06300
H	-2.46148	-2.16857	2.05513
H	-2.66883	-2.84304	3.68705
H	-1.88865	-3.81165	2.41979
H	-0.43709	-2.81468	-1.15026
H	0.62864	-4.26035	-1.18684
H	1.10968	-2.74029	-2.00564
H	0.19954	-4.11657	3.86223
H	-0.56760	-3.17756	5.15929
H	1.01841	-2.69135	4.53649
H	3.19261	-2.74655	-0.71788
H	2.67341	-4.25005	0.09811
H	3.11689	-2.81725	1.05580
H	-4.19544	-0.91528	0.99971
H	-5.16994	0.49348	0.57529
H	-3.88408	0.63425	1.77850
H	-2.69271	-2.25315	-2.28378
H	-4.34386	-1.66025	-2.10262
H	-3.45709	-2.26369	-0.69693
H	-2.92813	2.71233	1.47623
H	-3.65740	3.55879	0.10830
H	-1.91893	3.67040	0.39375
H	-0.70636	3.58193	-1.53867
H	-1.82035	3.49509	-2.91010
H	-0.31053	2.57592	-2.93563
H	-1.32008	-1.07706	-3.59564
H	-0.48332	0.46231	-3.76648
H	-2.13888	0.28487	-4.36776
H	3.36474	4.86357	-2.45458
H	1.87054	4.03754	-1.97120
H	3.35786	3.80021	-1.03568
H	3.19015	3.84719	-4.80789
H	3.00366	2.09261	-4.98614
H	1.67765	3.06270	-4.32027
H	5.31676	3.46802	-3.43192

H 5.26384 2.42740 -1.99870
H 5.11832 1.71691 -3.61927
77
TS Int 11 - Int 12
C 1.75672 1.20541 6.56547
C 2.66172 2.28173 6.84821
C 1.90576 3.35970 7.41973
C 0.53838 2.94970 7.49895
C 0.44781 1.61763 6.97789
Ir 1.80976 1.54422 8.80667
Mo 2.25111 0.71858 10.83309
N 4.06719 -0.13817 10.59050
C 4.72589 -0.64495 11.79576
C 4.10565 2.34360 6.46857
C 2.43977 4.71560 7.74584
C -0.60568 3.80173 7.94392
C -0.80658 0.82316 6.81175
C 2.09348 -0.06477 5.85454
N 1.87699 2.27123 12.17026
C 0.60720 2.06079 12.51631
O -0.19679 2.69602 13.16595
O 1.75595 -1.37804 10.61557
C 2.80304 -1.75567 10.08330
N 3.51263 -2.55894 9.51666
C 3.17037 -3.91988 9.04205
C 1.88511 -3.87334 8.21303
N 0.24666 0.73863 11.90030
C -1.02838 0.82679 11.16646
C 2.57401 3.53213 12.49303
C 2.63085 3.71991 14.01400
C 3.99222 3.41010 11.93434
C 1.85044 4.70567 11.82442
C 4.34124 -4.40074 8.18697
C 2.99537 -4.82477 10.26525
C 0.14354 -0.28137 12.96304
C 5.00735 -0.05015 9.48495
H 4.01350 -0.73909 12.62037
H 5.52041 0.04291 12.11088
H 5.17801 -1.62765 11.60744
H 5.47283 -1.02710 9.30008
H 5.79273 0.67625 9.72958
H 4.47573 0.28650 8.59693
H 4.53112 2.58846 12.41780
H 4.55344 4.33200 12.11117
H 3.96136 3.22498 10.85477
H 1.77388 4.51700 10.75083
H 2.40315 5.63670 11.98484
H 0.84571 4.82064 12.23511
H -0.94513 1.60648 10.41141

H -1.84754 1.05151 11.85791
H -1.20806 -0.12627 10.66650
H 1.62649 3.79696 14.43269
H 3.18183 4.63404 14.25651
H 3.14433 2.87652 14.48571
H -0.04164 -1.25494 12.50831
H -0.67159 -0.02736 13.64866
H 1.07933 -0.32406 13.52420
H 3.10851 -0.39583 6.08413
H 2.02134 0.06230 4.76637
H 1.41243 -0.86960 6.13884
H 4.68642 2.91615 7.19542
H 4.22969 2.82498 5.48995
H 4.54764 1.34725 6.40011
H -0.61805 -0.24678 6.92325
H -1.24479 0.98448 5.81846
H -1.55748 1.10313 7.55323
H -1.44187 3.19696 8.30089
H -0.97902 4.41804 7.11587
H -0.31819 4.47498 8.75441
H 1.82821 5.21861 8.49691
H 2.45404 5.35267 6.85190
H 3.46060 4.66322 8.13040
H 1.64068 -4.87377 7.84376
H 1.04351 -3.51223 8.80941
H 2.00766 -3.20957 7.35412
H 2.79813 -5.85319 9.94846
H 3.90009 -4.82299 10.87866
H 2.15711 -4.49146 10.88314
H 4.15174 -5.41062 7.81249
H 4.48865 -3.73593 7.33248
H 5.26388 -4.41457 8.77249
77
Int 12
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C 0.64764 1.40955 -2.80104
C -0.12798 2.46865 -2.20554
C -1.49084 2.04663 -2.17023
C -1.56134 0.73742 -2.75177
Ir -0.18928 0.60951 -0.88688
Mo 0.37945 -0.21609 1.09266
N 2.20765 -1.39015 0.65608
C 2.99945 -1.61600 1.88728
C 2.09018 1.50509 -3.17934
C 0.38684 3.82336 -1.84505
C -2.65133 2.86615 -1.70673
C -2.80621 -0.06564 -2.94935
C 0.10299 -0.89157 -3.91893
N -0.12517 1.24893 2.49377

C	-1.38458	0.92418	2.78066
O	-2.27766	1.46551	3.39434
O	0.14841	-2.28316	0.88940
C	1.32972	-2.57616	0.41600
N	1.82742	-3.59200	-0.13624
C	1.02833	-4.79535	-0.41478
C	-0.13677	-4.46749	-1.35824
N	-1.56905	-0.42275	2.13740
C	-2.82565	-0.50133	1.37437
C	0.45495	2.55272	2.86740
C	0.43795	2.71071	4.39211
C	1.89953	2.54730	2.36385
C	-0.32960	3.68123	2.19117
C	1.97394	-5.78877	-1.09710
C	0.50305	-5.40768	0.89119
C	-1.54164	-1.47090	3.18033
C	3.10645	-1.08379	-0.47039
H	2.33611	-1.88794	2.71016
H	3.53610	-0.70132	2.14802
H	3.71412	-2.42832	1.71899
H	3.82612	-1.89661	-0.60229
H	3.62454	-0.14621	-0.25843
H	2.50611	-0.95835	-1.36723
H	2.47635	1.75447	2.85269
H	2.38856	3.50154	2.57951
H	1.92362	2.38974	1.27886
H	-0.35734	3.50432	1.11309
H	0.14573	4.64814	2.38380
H	-1.35349	3.71367	2.56806
H	-2.82596	0.28868	0.62445
H	-3.68111	-0.38990	2.04815
H	-2.86150	-1.46825	0.87070
H	-0.58561	2.69980	4.76932
H	0.90459	3.65962	4.67428
H	0.99657	1.89971	4.86920
H	-1.55370	-2.44844	2.70009
H	-2.40712	-1.35696	3.84054
H	-0.62865	-1.37435	3.77107
H	1.12506	-1.21460	-3.71069
H	0.02059	-0.72559	-5.00098
H	-0.55920	-1.71977	-3.65941
H	2.66618	2.05981	-2.43532
H	2.20160	2.02399	-4.13994
H	2.54491	0.51850	-3.28744
H	-2.60795	-1.13651	-2.86741
H	-3.23587	0.11831	-3.94205
H	-3.56956	0.18745	-2.21059
H	-3.47700	2.23838	-1.36477
H	-3.03511	3.49565	-2.51973

H -2.37621 3.52355 -0.87970
H -0.22518 4.29541 -1.07457
H 0.38012 4.48436 -2.72151
H 1.41307 3.77937 -1.47424
H -0.70147 -5.37500 -1.59440
H -0.81313 -3.74009 -0.90549
H 0.24222 -4.04918 -2.29472
H -0.01932 -6.34795 0.68863
H 1.33244 -5.62105 1.57238
H -0.18988 -4.72645 1.38892
H 1.45372 -6.71965 -1.34327
H 2.37440 -5.35956 -2.01955
H 2.81748 -6.02369 -0.44204
77
TS Int 12 - Int 13'
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C 0.01081 1.54278 -2.61713
C -1.09582 1.98058 -1.81287
C -2.02407 0.89083 -1.74674
Ir -0.14507 0.27220 -0.75144
Mo 0.66735 -0.16741 1.31619
N 2.69385 -0.15128 0.45631
C 3.79589 -0.67790 1.28620
C 0.60584 -0.53081 -4.05345
C 1.14746 2.40202 -3.07031
C -1.31031 3.36247 -1.28850
C -3.38927 0.94118 -1.13969
C -2.28675 -1.43040 -2.89392
N -0.18520 1.02891 2.80100
C -1.22115 0.30247 3.23446
O -2.11954 0.52021 4.01735
C 1.93383 -1.25205 -0.23412
N 2.54775 -2.01074 -1.04032
C 2.13557 -3.35504 -1.43634
C 0.61878 -3.50007 -1.58973
N -1.08457 -0.99587 2.51013
C -2.34528 -1.39231 1.86393
C 0.06361 2.40804 3.25890
C 0.32237 2.41362 4.77012
C 1.30884 2.88956 2.51171
C -1.13076 3.30279 2.91137
C 2.82687 -3.66541 -2.76884
C 2.64355 -4.34271 -0.37099
C -0.65033 -2.04965 3.45082
C 3.21188 0.83744 -0.49339
O 1.24779 -1.90145 1.15573
H 3.40990 -1.43919 1.96144
H 4.23463 0.14252 1.85886

H 4.55463 -1.12713 0.63783
H 4.00836 0.38523 -1.09420
H 3.60438 1.69591 0.05661
H 2.39382 1.15672 -1.13697
H 2.17901 2.27654 2.77267
H 1.54087 3.92668 2.76918
H 1.14855 2.83501 1.42799
H -1.31378 3.27720 1.83446
H -0.92876 4.33730 3.20544
H -2.02868 2.96150 3.42891
H -2.64823 -0.61257 1.16847
H -3.12484 -1.54756 2.61738
H -2.17487 -2.31469 1.30700
H -0.55279 2.04908 5.31058
H 0.54388 3.42945 5.11166
H 1.17662 1.77598 5.01644
H -0.39882 -2.94557 2.88296
H -1.44704 -2.26341 4.17078
H 0.23910 -1.71803 3.98950
H -1.66234 -2.17517 -3.38835
H -3.13478 -1.21683 -3.55651
H -2.68554 -1.88900 -1.98613
H 1.55936 -0.77015 -3.57088
H 0.82158 0.04905 -4.95766
H 0.14989 -1.47013 -4.37028
H -3.74401 -0.05442 -0.86531
H -4.11082 1.35813 -1.85380
H -3.41202 1.56535 -0.24388
H -1.98567 3.36247 -0.43156
H -1.75625 4.00318 -2.06040
H -0.37315 3.82739 -0.97467
H 1.44847 3.11693 -2.30101
H 0.85822 2.97913 -3.95787
H 2.02230 1.80696 -3.34129
H 0.36574 -4.51045 -1.92792
H 0.11682 -3.30581 -0.64019
H 0.24100 -2.78433 -2.32053
H 2.40539 -5.37191 -0.66082
H 3.72854 -4.25788 -0.26290
H 2.17871 -4.13157 0.59348
H 2.62499 -4.69506 -3.08052
H 2.47559 -2.99285 -3.55563
H 3.90817 -3.53625 -2.67164
77
Int 13'
C -1.61566 -0.58240 -2.90672
C -0.41922 0.02872 -3.29783
C -0.26699 1.25561 -2.54172
C -1.45903 1.44170 -1.74449

C	-2.24724	0.26585	-1.90850
Ir	-0.28845	-0.23397	-0.85709
Mo	0.32776	-0.19970	1.43505
N	2.32353	-0.09964	0.39085
C	3.46749	-0.69753	1.10071
C	0.53823	-0.42666	-4.34972
C	0.72249	2.32584	-2.87393
C	-1.86475	2.71052	-1.06484
C	-3.65391	0.05745	-1.44542
C	-2.23551	-1.82865	-3.44945
N	-0.28566	1.27689	2.79166
C	-1.41043	0.77068	3.32046
O	-2.15144	1.14950	4.20122
C	1.61476	-1.05199	-0.58571
N	2.34889	-2.02071	-0.91272
C	2.01213	-3.26065	-1.60164
C	0.52974	-3.48469	-1.89535
N	-1.64023	-0.50248	2.58373
C	-2.94769	-0.46649	1.91172
C	0.29165	2.52812	3.33776
C	0.68508	2.31860	4.80594
C	1.53655	2.86083	2.52026
C	-0.71852	3.67595	3.20927
C	2.82903	-3.29533	-2.90032
C	2.51043	-4.37944	-0.67062
C	-1.60719	-1.64049	3.52761
C	2.76832	1.12316	-0.29160
O	0.85547	-1.70591	1.99968
H	3.15730	-1.63780	1.55023
H	3.79054	-0.00265	1.88115
H	4.29157	-0.88721	0.40769
H	3.51951	0.86842	-1.04932
H	3.21480	1.80846	0.43111
H	1.91726	1.59950	-0.76983
H	2.27942	2.06098	2.59566
H	1.99465	3.78244	2.88960
H	1.28408	3.00901	1.46587
H	-1.00262	3.81948	2.16284
H	-0.27326	4.60721	3.57262
H	-1.61707	3.46932	3.79106
H	-2.99262	0.40330	1.26024
H	-3.75388	-0.40924	2.65139
H	-3.05588	-1.36617	1.30597
H	-0.19183	2.08521	5.41158
H	1.15060	3.22509	5.20482
H	1.40267	1.49757	4.89489
H	-1.69978	-2.56714	2.96077
H	-2.42689	-1.55162	4.24711
H	-0.65260	-1.65655	4.05185

H -1.55181 -2.37378 -4.10196
H -3.12882 -1.58911 -4.03991
H -2.54566 -2.51134 -2.65349
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H -1.00730 3.22927 -0.63147
H 0.83152 3.04835 -2.06218
H 0.38908 2.88261 -3.75936
H 1.70978 1.91708 -3.09967
H 0.38811 -4.46305 -2.36673
H -0.05627 -3.45316 -0.97353
H 0.13921 -2.71777 -2.56212
H 2.35376 -5.36058 -1.13061
H 3.57591 -4.25435 -0.46249
H 1.97033 -4.34842 0.27898
H 2.71617 -4.26351 -3.39792
H 2.50078 -2.51440 -3.59028
H 3.88866 -3.13622 -2.68436
77
TS Int 12 - Int 13
C -1.51818 2.53118 -1.75494
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C -2.45424 0.60770 -2.66293
C -1.29805 0.95049 -3.43614
C -0.70687 2.11191 -2.88027
Ir -0.80199 0.58223 -1.08811
Mo -0.32945 -0.23648 1.05098
C 1.62552 -0.55574 0.56711
O 1.48408 -1.36352 1.55939
C -3.84889 1.80387 -0.80257
C -3.45156 -0.45382 -2.99646
C -0.82634 0.21511 -4.64932
C 0.47159 2.86009 -3.41432
C -1.38036 3.84236 -1.04972
N 0.48869 -0.99617 -0.59605
C 0.79140 -2.24434 -1.34087
C -0.54181 -2.81197 -1.84008
C 1.68517 -1.90098 -2.54008
C 1.48531 -3.31622 -0.49251
N -1.53527 -0.39568 2.90446
C -2.99820 -0.30297 2.76462
N 2.84170 -0.12016 0.12869
C 4.03225 -0.44070 0.88637

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C	-0.96150	0.86916	3.47043
O	-1.34400	1.30299	4.53782
C	-1.15487	-1.55293	3.73712
C	2.96392	0.86430	-0.92126
C	0.71418	2.49111	2.81847
C	1.63509	2.74158	1.63186
C	-0.22533	3.69412	2.98953
C	1.56069	2.29447	4.08498
H	3.81093	-1.25134	1.57873
H	4.39153	0.42407	1.46185
H	4.83319	-0.75372	0.20686
H	3.66799	0.51732	-1.68691
H	3.33042	1.82030	-0.52765
H	1.98507	1.02493	-1.37574
H	2.37254	1.94285	1.54594
H	2.16362	3.69012	1.76812
H	1.06425	2.77638	0.70140
H	-0.82225	3.83871	2.08546
H	0.36163	4.60225	3.15851
H	-0.89561	3.55124	3.83765
H	-3.24721	0.53797	2.11582
H	-3.46345	-0.15519	3.74403
H	-3.37257	-1.22205	2.30930
H	0.92652	2.15042	4.96108
H	2.19089	3.17329	4.25400
H	2.21169	1.42262	3.97399
H	-1.50987	-2.46948	3.26047
H	-1.59606	-1.46157	4.73464
H	-0.06791	-1.59490	3.81663
H	-2.99422	-1.28879	-3.53147
H	-4.24503	-0.05075	-3.63959
H	-3.92669	-0.85576	-2.09910
H	0.23316	0.39204	-4.84576
H	-1.38067	0.54459	-5.53677
H	-0.97241	-0.86397	-4.55941
H	-4.28105	0.84516	-0.50823
H	-4.61603	2.35688	-1.36018
H	-3.63144	2.36737	0.10671
H	-1.90284	3.84247	-0.09227
H	-1.80681	4.64858	-1.66045
H	-0.33519	4.09209	-0.85688
H	1.02609	3.35806	-2.61573
H	0.15667	3.63613	-4.12419
H	1.16794	2.20270	-3.94024
H	1.61892	-4.20915	-1.11178
H	2.46878	-2.99353	-0.14859
H	0.89285	-3.58235	0.38363
H	1.82516	-2.77957	-3.17741

H 1.23017 -1.10607 -3.13455
H 2.66911 -1.56658 -2.20530
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77
Int 13
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C -2.28312 0.35795 -2.44089
C -1.21893 0.35379 -3.39675
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Ir -0.42698 0.16282 -1.07702
Mo 0.49715 -0.51392 0.93183
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O 2.61516 -1.21206 1.98460
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C -1.09229 -0.58536 -4.55300
C 0.90233 1.78819 -3.84398
C -0.32123 3.40876 -1.40284
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C -0.50653 -3.47253 -1.75327
C 1.74942 -2.54112 -2.37678
C 1.47990 -3.88212 -0.26804
N -0.99060 -1.06632 2.50144
C -2.42006 -1.01909 2.14228
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C 5.00772 -0.21181 0.95132
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O -1.17304 0.26711 4.44181
C -0.68359 -2.31636 3.22502
C 3.57713 1.10689 -0.58822
C 0.82772 2.04416 3.24842
C 1.79441 2.66183 2.24022
C -0.30775 3.04488 3.51540
C 1.57860 1.72874 4.54996
H 4.90923 -0.94448 1.75125
H 5.54431 0.66632 1.32760
H 5.58701 -0.64570 0.12880
H 4.11771 0.73810 -1.46764
H 4.00142 2.07710 -0.30297
H 2.52075 1.22137 -0.84037
H 2.67809 2.03562 2.10738
H 2.12200 3.64398 2.59451
H 1.31179 2.78237 1.26704
H -0.82946 3.28418 2.58376

H 0.10280 3.97383 3.92319
H -1.02761 2.64095 4.22788
H -2.62787 -0.07762 1.63535
H -3.03473 -1.10085 3.04526
H -2.64472 -1.84107 1.46045
H 0.89811 1.32508 5.30130
H 2.03948 2.63756 4.95011
H 2.36773 0.99585 4.36063
H -0.94177 -3.16697 2.59142
H -1.25801 -2.36045 4.15574
H 0.38315 -2.35011 3.45232
H -3.26302 -1.50855 -2.87662
H -4.28098 -0.08289 -3.09251
H -3.90256 -0.66602 -1.46833
H -0.04926 -0.75545 -4.82913
H -1.59961 -0.17909 -5.43662
H -1.54342 -1.55772 -4.34351
H -3.71975 1.20714 -0.17927
H -3.72731 2.74192 -1.05064
H -2.59637 2.48373 0.28583
H -0.64069 3.58438 -0.37441
H -0.69778 4.23662 -2.01743
H 0.76978 3.45071 -1.42151
H 1.66442 2.22118 -3.19270
H 0.65616 2.54000 -4.60498
H 1.35114 0.93597 -4.35884
H 1.74350 -4.79958 -0.80310
H 2.38726 -3.45369 0.16221
H 0.80836 -4.14587 0.55311
H 1.96988 -3.43767 -2.96409
H 1.29251 -1.79175 -3.02595
H 2.68874 -2.13638 -1.99282
H -0.30886 -4.38644 -2.32174
H -1.18114 -3.71752 -0.92882
H -1.00723 -2.75058 -2.40057
77
Int 13 - Complex 6
C 6.38857 13.78399 9.25212
C 6.19397 15.13434 8.79777
C 7.18228 15.39705 7.78299
C 7.97433 14.22266 7.60511
C 7.47538 13.21337 8.51255
Ir 5.80273 13.68097 7.11417
C 5.65291 11.84789 6.11985
N 6.35701 10.69598 6.28195
C 7.71420 10.69996 5.74572
C 5.28413 16.13095 9.44206
C 7.49329 16.72545 7.17359
C 9.20869 14.14899 6.76597

C	8.11276	11.89892	8.83800
C	5.70249	13.14482	10.41487
N	4.26064	14.37582	5.93583
Mo	3.89848	12.58136	5.79718
N	2.30900	12.12322	7.40315
C	1.54712	13.28763	7.89326
C	4.01996	15.56521	5.11820
C	5.24234	15.82438	4.23077
C	2.79154	15.32156	4.23131
C	3.74135	16.76309	6.03005
O	5.06561	11.92666	4.48258
N	2.08925	11.59297	5.23314
C	1.48944	11.36588	6.40517
O	0.52976	10.70558	6.74670
C	1.56170	10.97718	3.98985
C	0.08914	11.36574	3.79577
C	2.37820	11.50101	2.80831
C	1.70392	9.45173	4.07754
C	2.67418	11.25636	8.53467
C	5.65833	9.45336	5.96802
H	2.19611	13.89771	8.52265
H	0.67352	12.95665	8.46664
H	1.21310	13.88706	7.04593
H	3.27425	10.41912	8.17610
H	1.77322	10.86943	9.02195
H	3.26869	11.83333	9.24265
H	2.21978	12.57524	2.67411
H	2.05640	11.00166	1.88957
H	3.44718	11.32745	2.95378
H	2.75681	9.17498	4.17944
H	1.31614	8.98329	3.16765
H	1.14724	9.06028	4.93121
H	-0.53294	10.97889	4.60352
H	-0.27653	10.96194	2.84668
H	-0.01533	12.45448	3.76159
H	2.97616	14.50471	3.52921
H	2.55974	16.21917	3.65006
H	1.91362	15.07308	4.83430
H	2.86721	16.57394	6.65870
H	3.55254	17.66139	5.43406
H	4.59502	16.95554	6.67941
H	6.13010	15.98463	4.84462
H	5.08448	16.70602	3.60062
H	5.42861	14.95915	3.58987
H	8.31432	9.92452	6.23163
H	8.16371	11.67458	5.91736
H	7.70059	10.51748	4.66249
H	5.52848	9.32826	4.88623
H	4.67546	9.45433	6.44085

H 6.23430 8.61119 6.36279
H 9.54340 13.12107 6.62139
H 10.03232 14.69046 7.24843
H 9.05480 14.58905 5.77840
H 7.38471 11.08552 8.83609
H 8.57969 11.94378 9.82883
H 8.89398 11.64036 8.12337
H 4.67839 13.50629 10.52766
H 6.23678 13.37746 11.34543
H 5.67239 12.05847 10.31462
H 5.08260 16.98206 8.79092
H 5.73339 16.52346 10.36321
H 4.32228 15.68692 9.70807
H 7.91966 16.62456 6.17372
H 8.23022 17.25339 7.79221
H 6.61515 17.36800 7.09949
77
Complex6
Ir 5.89821 13.78601 6.92534
Mo 4.08917 12.71530 5.27963
O 4.43545 12.79267 3.60322
O 0.61696 11.13017 6.56469
N 2.67118 12.11708 7.14459
N 2.31585 11.51345 4.99649
N 4.21237 14.44623 5.91412
N 6.52742 10.93519 5.91748
C 2.04112 13.20027 7.90863
H 2.80630 13.68244 8.51901
H 1.23566 12.81319 8.54267
H 1.63172 13.94141 7.22261
C 3.15438 11.08043 8.06973
H 3.56250 10.24144 7.50471
H 2.33677 10.71557 8.70347
H 3.94824 11.50157 8.68670
C 1.71139 11.51353 6.19365
C 1.59762 10.88865 3.84863
C 2.48435 10.89144 2.60520
H 2.73450 11.90199 2.28468
H 1.95548 10.38164 1.79398
H 3.42420 10.36454 2.78745
C 1.25714 9.42793 4.18877
H 2.17282 8.86358 4.39229
H 0.75748 8.95929 3.33541
H 0.60070 9.36180 5.05601
C 0.31506 11.67919 3.55044
H -0.35723 11.67083 4.40945
H -0.20651 11.23776 2.69538
H 0.55923 12.71544 3.29911
C 3.86341 15.73624 5.29471

C 2.58233 15.53773 4.46917
H 2.74661 14.81354 3.66793
H 2.28293 16.48704 4.01426
H 1.75785 15.18821 5.09689
C 3.59516 16.78767 6.36998
H 2.80430 16.45791 7.04875
H 3.28213 17.72875 5.90759
H 4.49301 16.97783 6.95488
C 4.99496 16.17951 4.36122
H 5.92437 16.29635 4.92037
H 4.74834 17.13261 3.88185
H 5.15356 15.42634 3.58580
C 5.73878 12.02375 6.08011
C 7.93532 11.07614 5.58340
H 8.54028 10.31877 6.09282
H 8.26900 12.06928 5.86564
H 8.07823 10.96196 4.49987
C 5.93643 9.71995 5.37065
H 5.98045 9.71299 4.27312
H 4.89357 9.64865 5.67594
H 6.47683 8.84556 5.74779
C 7.98730 14.46348 7.45775
C 7.56542 13.40601 8.34393
C 6.43638 13.88513 9.08842
C 6.17973 15.23846 8.68734
C 7.13726 15.59806 7.68237
C 9.22587 14.50146 6.62123
H 9.65058 13.50930 6.46464
H 9.99415 15.10646 7.11830
H 9.03712 14.94333 5.64081
C 8.27628 12.12260 8.64385
H 7.62611 11.25407 8.51410
H 8.63096 12.12916 9.68027
H 9.14879 11.98398 8.00548
C 5.78607 13.17654 10.23054
H 4.73936 13.46457 10.34356
H 6.29801 13.42068 11.17064
H 5.82838 12.09328 10.10498
C 5.22260 16.14273 9.39780
H 5.16715 17.12725 8.93428
H 5.55405 16.28901 10.43264
H 4.21076 15.73334 9.43093
C 7.39930 16.96523 7.13776
H 7.78213 16.92889 6.11591
H 8.15242 17.47581 7.75166
H 6.50635 17.59128 7.13251
77
Complex 6 - triplet
Ir 5.89315 13.87484 6.80015

Mo	3.98424	12.77949	5.20026
O	4.27548	12.81590	3.50473
O	0.63955	11.08967	6.63414
N	2.67195	12.18425	7.09835
N	2.29997	11.41759	5.01018
N	4.28022	14.56731	5.82245
N	6.51594	11.10589	5.52177
C	2.00414	13.23404	7.87620
H	2.76121	13.78923	8.43139
H	1.26682	12.80214	8.56159
H	1.49435	13.92250	7.20157
C	3.29348	11.20564	8.00559
H	3.71849	10.38956	7.41948
H	2.55156	10.79876	8.70398
H	4.09786	11.69616	8.55394
C	1.71400	11.47849	6.21316
C	1.59662	10.68473	3.92129
C	2.47166	10.63853	2.66986
H	2.68841	11.63554	2.28835
H	1.95315	10.06422	1.89591
H	3.42858	10.15078	2.87233
C	1.31622	9.23991	4.36748
H	2.25382	8.72697	4.60578
H	0.83151	8.69040	3.55467
H	0.66746	9.21139	5.24279
C	0.28086	11.40217	3.58420
H	-0.37782	11.43543	4.45316
H	-0.23642	10.87818	2.77426
H	0.48301	12.42426	3.25093
C	3.87103	15.87066	5.29106
C	2.51316	15.70721	4.59095
H	2.58495	14.98798	3.77080
H	2.18639	16.66485	4.17392
H	1.74617	15.36875	5.29379
C	3.73056	16.90780	6.40413
H	3.00335	16.57953	7.15132
H	3.39674	17.86643	5.99463
H	4.68800	17.06436	6.89875
C	4.91337	16.32810	4.25962
H	5.89092	16.43811	4.73502
H	4.62768	17.28757	3.81489
H	5.00237	15.58299	3.46546
C	5.71778	12.11867	5.84364
C	7.96445	11.19273	5.48889
H	8.42386	10.40960	6.10079
H	8.25946	12.17421	5.84249
H	8.30995	11.07034	4.45550
C	5.97836	9.93238	4.84204
H	6.16310	9.99337	3.76375

H 4.90510 9.87398 5.01362
H 6.46010 9.03045 5.23367
C 7.97630 14.33617 7.55433
C 7.41751 13.32314 8.41395
C 6.35110 13.91010 9.16934
C 6.20667 15.25992 8.74601
C 7.19867 15.52976 7.74420
C 9.29030 14.30845 6.83606
H 9.70804 13.30230 6.77497
H 10.02447 14.92134 7.37360
H 9.21289 14.70224 5.81971
C 8.00718 11.98195 8.73135
H 7.27334 11.17609 8.65123
H 8.39017 11.97932 9.75807
H 8.84355 11.73801 8.07733
C 5.61907 13.27128 10.30262
H 4.57221 13.58188 10.34424
H 6.07606 13.55014 11.26179
H 5.64521 12.18164 10.24090
C 5.30356 16.24654 9.41499
H 5.34421 17.22849 8.94447
H 5.60954 16.37350 10.46012
H 4.26077 15.91988 9.41835
C 7.57295 16.86737 7.18925
H 7.95671 16.78611 6.17029
H 8.36084 17.32479 7.80168
H 6.73232 17.56248 7.17044
61
Complex 2
C 4.31800 9.66262 5.62896
C 5.32044 10.68846 5.64183
C 5.11916 11.47723 6.83108
C 3.99865 10.94223 7.54341
C 3.49977 9.80876 6.79588
Ir 5.58916 9.38815 7.48438
Mo 6.55660 7.99940 9.25586
N 6.63037 9.01405 10.92175
C 7.43003 10.22269 11.01132
C 5.88539 12.70924 7.19425
C 6.31765 10.96336 4.56372
C 3.35310 11.53300 8.75541
C 2.25921 9.03986 7.11343
C 4.11317 8.66908 4.53049
Ir 5.26494 5.94640 9.58438
C 4.26808 4.15105 10.55557
C 3.36957 4.69004 9.58206
C 3.99770 4.62244 8.29357
C 5.30029 4.02354 8.47241
C 5.46762 3.73785 9.86536

C	3.36516	4.94041	6.97789
C	1.98298	5.17772	9.85517
C	6.23300	3.63948	7.36948
C	6.62110	3.01639	10.48666
C	3.97924	3.95145	12.00795
N	8.40832	7.56215	8.82144
C	9.13161	7.81521	7.58917
C	9.23062	6.82653	9.76536
C	5.91267	8.77361	12.15971
H	7.54052	3.16957	9.91913
H	6.42706	1.93747	10.52598
H	6.80339	3.35855	11.50731
H	6.20019	4.36039	6.55083
H	5.96221	2.65628	6.96351
H	7.26463	3.58313	7.71993
H	1.90393	5.61780	10.85103
H	1.26461	4.35114	9.79610
H	1.67784	5.93685	9.13325
H	8.70667	6.68352	10.71052
H	10.16607	7.37000	9.97016
H	9.50116	5.83545	9.36990
H	2.56049	5.66895	7.09019
H	2.93393	4.03868	6.52433
H	4.09183	5.35343	6.27567
H	5.25336	9.62241	12.39902
H	6.61341	8.65587	13.00166
H	5.30682	7.87309	12.07939
H	9.44002	6.86973	7.11653
H	10.04622	8.39710	7.78548
H	8.50811	8.36791	6.88890
H	4.88995	4.01030	12.60728
H	3.52572	2.96831	12.18801
H	3.28879	4.70918	12.38396
H	8.00965	10.37553	10.10083
H	8.13119	10.16204	11.85815
H	6.79587	11.10910	11.16694
H	7.22315	11.42115	4.96695
H	5.90618	11.64804	3.81076
H	6.61467	10.04642	4.05053
H	5.88103	12.87846	8.27226
H	5.44711	13.59239	6.71384
H	6.92729	12.63917	6.87565
H	5.06129	8.37878	4.07365
H	3.47817	9.09263	3.74296
H	3.62925	7.76217	4.89593
H	2.28989	8.04191	6.67394
H	1.37181	9.55180	6.71950
H	2.12843	8.92293	8.19076
H	2.90077	10.76207	9.38148

H 2.56266 12.23759 8.46608
H 4.07386 12.07550 9.36930
H 4.57798 7.44223 9.68093
H 6.06263 7.82981 7.22640
H 6.45847 6.41886 10.59454
H 7.02164 9.71683 8.19244
75
Complex 2 - triplet
C 3.91989 9.37042 5.85929
C 5.08400 10.19727 5.93249
C 5.12119 10.79288 7.25073
C 3.98620 10.31401 7.98327
C 3.25002 9.42585 7.12018
Ir 5.40000 8.57371 7.47904
Mo 6.94109 8.10810 9.52563
N 7.02750 9.53509 10.85897
C 8.00461 10.60576 10.78655
C 6.06220 11.87088 7.68597
C 5.99417 10.53514 4.79353
C 3.52421 10.78713 9.32340
C 1.91990 8.82225 7.43357
C 3.43400 8.65805 4.63734
Ir 4.84908 6.55270 9.20798
C 4.22083 4.56821 10.10874
C 3.31129 4.83169 9.03755
C 4.05704 4.89056 7.81890
C 5.44253 4.61852 8.12820
C 5.54453 4.42475 9.54053
C 3.48609 5.00101 6.44289
C 1.82442 4.93781 9.16206
C 6.52108 4.39729 7.11784
C 6.76337 3.98169 10.28530
C 3.85130 4.30029 11.53362
N 8.72488 7.32747 9.33355
C 9.39712 7.01373 8.08718
C 9.50975 6.92269 10.48667
C 6.16044 9.67078 12.01403
H 7.67298 4.32647 9.79113
H 6.80560 2.88711 10.34951
H 6.77446 4.37426 11.30425
H 6.45750 5.11965 6.30123
H 6.44597 3.39209 6.68356
H 7.51146 4.49288 7.56558
H 1.53058 5.32709 10.13861
H 1.35680 3.95263 9.04228
H 1.40327 5.59845 8.40239
H 8.99250 7.17537 11.41542
H 10.48719 7.42895 10.49477
H 9.69911 5.83790 10.48772

H 2.54260 5.55007 6.44629
H 3.28708 4.00606 6.02387
H 4.16987 5.51943 5.76916
H 5.63486 10.63846 12.00881
H 6.73731 9.61739 12.95056
H 5.40976 8.87914 12.02850
H 9.63507 5.94052 8.01856
H 10.34689 7.56413 8.00320
H 8.77134 7.27819 7.23382
H 4.65920 4.57696 12.21373
H 3.63733 3.23500 11.68848
H 2.96458 4.86347 11.83121
H 8.63538 10.49233 9.90197
H 8.65849 10.60443 11.67245
H 7.52232 11.59471 10.73755
H 6.99163 10.80391 5.14641
H 5.60468 11.38555 4.21949
H 6.10518 9.69355 4.10681
H 6.17933 11.88030 8.77025
H 5.69226 12.85707 7.37828
H 7.05374 11.73773 7.24837
H 4.26238 8.34289 4.00001
H 2.78759 9.31429 4.04138
H 2.85546 7.76875 4.89235
H 1.73093 7.93542 6.82562
H 1.11439 9.53992 7.23074
H 1.85274 8.52648 8.48164
H 3.09407 9.97052 9.90773
H 2.75667 11.56496 9.21918
H 4.34792 11.20754 9.90220
H 3.80334 7.70646 9.48366
H 5.70315 7.19076 6.77878
H 5.34832 7.24160 10.57445
H 6.98743 8.51638 7.35289
79
Complex 3
C 10.75119 10.24724 10.91029
C 11.16299 8.89211 11.18751
C 10.28167 8.35553 12.19880
C 9.28792 9.36969 12.48260
C 9.61179 10.53458 11.70322
Ir 9.12245 8.58275 10.39811
Mo 8.29935 6.70750 9.30507
C 9.36097 5.08039 7.43150
N 10.23640 4.34971 6.68676
C 11.66387 4.38218 6.91043
C 12.40379 8.23661 10.67123
C 10.48133 7.08284 12.95970
C 8.24839 9.29466 13.55442

C	8.86624	11.82981	11.74267
C	11.44209	11.18060	9.96992
Ir	7.42404	8.54896	8.10336
C	6.19232	10.40904	7.25091
C	5.37737	9.25570	7.53768
C	5.83104	8.17090	6.69799
C	6.97522	8.65003	5.95718
C	7.16791	10.04455	6.29127
C	4.16098	9.23564	8.40696
C	5.16493	6.84359	6.52858
C	7.68742	7.90548	4.87331
C	8.20037	10.93676	5.68247
C	6.01622	11.76122	7.86331
O	8.01095	4.75659	10.25124
C	6.81166	5.05677	10.57465
N	6.00543	4.17684	11.20159
C	4.64732	4.53147	11.55219
O	6.41224	6.23198	10.27262
O	8.13312	5.05585	7.24248
O	9.88170	5.82339	8.38019
C	6.44953	2.82780	11.47820
C	9.74584	3.46565	5.65544
H	7.48162	2.72126	11.15146
H	5.82707	2.10031	10.94404
H	6.38624	2.61664	12.55173
H	4.48346	5.58115	11.31847
H	4.47666	4.36927	12.62244
H	3.92907	3.92199	10.99073
H	4.00723	8.24840	8.84548
H	3.26341	9.49535	7.83114
H	4.24709	9.94974	9.22855
H	5.89437	6.06559	6.29901
H	4.42635	6.88571	5.71781
H	4.64896	6.54675	7.44320
H	7.67889	6.83177	5.06545
H	8.72991	8.22120	4.79362
H	7.20810	8.08598	3.90242
H	8.43764	11.78179	6.33182
H	7.85007	11.34401	4.72564
H	9.12955	10.39651	5.48915
H	5.68513	11.69145	8.90149
H	5.26343	12.34149	7.31564
H	6.94621	12.33284	7.84939
H	8.66016	3.53032	5.62820
H	10.03952	2.42887	5.86209
H	10.14967	3.74778	4.67512
H	11.88639	5.09752	7.69797
H	12.18942	4.68053	5.99476
H	12.03362	3.39308	7.20973

H 13.27167 8.51173 11.28398
H 12.61230 8.53473 9.64188
H 12.31146 7.14967 10.68419
H 9.53106 6.66979 13.30139
H 11.11088 7.25867 13.84146
H 10.96669 6.32265 12.34537
H 7.90565 8.26955 13.70401
H 7.37419 9.89997 13.30646
H 8.64713 9.65917 14.51006
H 7.79943 11.67398 11.91704
H 8.97235 12.38426 10.80817
H 9.24134 12.47055 12.55023
H 11.88965 10.64277 9.13155
H 12.24637 11.72766 10.47814
H 10.75326 11.91984 9.55600
H 9.13233 8.44790 8.44591
H 7.53740 9.12269 9.79657
79
Complex 3 - triplet
C 10.67534 10.35770 11.02169
C 11.13695 8.98563 10.81887
C 10.41638 8.12200 11.71909
C 9.38094 8.92626 12.31133
C 9.60220 10.31760 11.91581
Ir 9.07071 8.79639 10.15406
Mo 8.14674 6.67137 9.17965
C 9.30369 4.94257 7.60528
N 10.09614 4.11788 6.88040
C 11.53897 4.19024 6.94883
C 12.34385 8.60210 10.02274
C 10.75283 6.70276 12.04490
C 8.43833 8.48501 13.38593
C 8.79155 11.47100 12.40926
C 11.26079 11.56166 10.35881
Ir 7.47756 8.82487 8.06612
C 6.11438 10.51957 7.04530
C 5.45628 9.25734 7.37290
C 6.03409 8.21511 6.56254
C 7.17324 8.79550 5.90440
C 7.16726 10.23455 6.17035
C 4.20991 9.13272 8.19011
C 5.48478 6.83785 6.37135
C 8.03534 8.11407 4.89000
C 8.13838 11.20262 5.57831
C 5.71459 11.85518 7.58181
O 8.07043 4.96697 10.86471
C 6.82641 5.14977 10.83026
N 5.96375 4.44243 11.59688
C 4.53451 4.65439 11.53245

O	6.35298	6.05440	10.02630
O	8.04865	4.87742	7.57366
O	9.86302	5.83807	8.36336
C	6.44874	3.39184	12.46391
C	9.51423	3.06808	6.07419
H	7.53309	3.34696	12.38855
H	6.02732	2.42299	12.16980
H	6.16589	3.58989	13.50447
H	4.32710	5.48347	10.86047
H	4.13792	4.88879	12.52724
H	4.02570	3.75628	11.16134
H	4.10783	8.12653	8.59863
H	3.32316	9.34557	7.57951
H	4.21286	9.83141	9.02939
H	6.27252	6.11121	6.16988
H	4.77285	6.82403	5.53595
H	4.96327	6.49771	7.26755
H	8.09250	7.04267	5.08724
H	9.05367	8.50848	4.89983
H	7.63168	8.25284	3.87860
H	8.19635	12.12465	6.15964
H	7.84417	11.46979	4.55578
H	9.14293	10.77672	5.52746
H	5.43019	11.79575	8.63503
H	4.85286	12.25549	7.03293
H	6.52453	12.58256	7.49861
H	8.43032	3.14388	6.12831
H	9.82433	2.08148	6.43978
H	9.83251	3.16471	5.02964
H	11.82463	5.04021	7.56352
H	11.96190	4.31328	5.94506
H	11.95408	3.27472	7.38823
H	13.25612	8.71456	10.62228
H	12.44879	9.22918	9.13494
H	12.27992	7.56577	9.68888
H	9.86007	6.11084	12.24907
H	11.41393	6.65828	12.91995
H	11.26370	6.22188	11.20927
H	8.22701	7.41774	13.30682
H	7.48642	9.01743	13.32835
H	8.86670	8.67280	14.37912
H	7.73535	11.20589	12.49466
H	8.86606	12.33308	11.74382
H	9.13089	11.78663	13.40364
H	11.51936	11.35936	9.31680
H	12.17914	11.88091	10.86726
H	10.56729	12.40479	10.36948
H	9.16813	9.18352	8.42664
H	7.45949	9.38963	9.74381

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