Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Reduction of highly bulky triphenolamine molybdenum nitrido and chloride complexes

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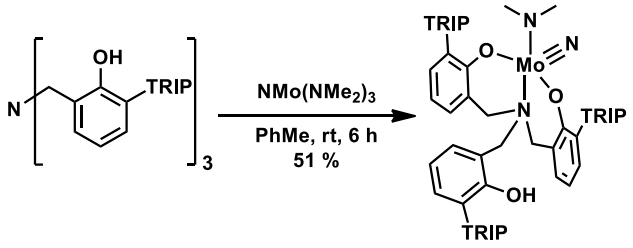
Materials and Methods

All air- and moisture-sensitive manipulations were performed using oven-dried or flame-dried glassware, including basic Schlenk and glovebox techniques under N_2 atmosphere. Air- and moisture-insensitive reactions were carried out under an ambient atmosphere and magnetically stirred. Benzene, benzene-*d*$_6$, diethyl ether, toluene, and THF were distilled from deep purple sodium benzophenone ketyl. Ligand **1**,[1] $NMo(NMe_2)_3$,[2] [LutH]OTf,[3] $MoCl_4(THF)_2$,[4] and KC_8[5] were prepared following the literature procedure. All deuterated solvents were purchased from Aldrich and Cambridge Isotope Laboratories. Unless stated otherwise, all other chemicals were used as received. NMR spectra were recorded on a Bruker DRX 500 spectrometer operating at 500 MHz and 125 MHz for ^{1}H and ^{13}C acquisitions, respectively. ^{1}H chemical shifts were referenced to the residual proton solvent peaks (C_6D_6, δ 7.16) and ^{13}C solvent signals (C_6D_6, δ 128.06). Signals are listed in ppm, and multiplicity identified as s = singlet, br = broad, d = doublet, t = triplet, m = multiplet; coupling constants in Hz; integration. Purified compounds were further dried under high vacuum (~ 10^{-3} Torr). Yields refer to purified and spectroscopically pure compounds. Solution state magnetic susceptibility was measured by Evans' method[6,7] on a Bruker DRX 500 spectrometers in benzene-*d*$_6$ at 297 K. UV-vis spectra were recorded using an Agilent Technologies Cary 6000i UV-Vis-NIR spectrometer. Samples were prepared under N_2 in a sealed 1 cm path length cuvette. Infrared spectra were obtained as thin films formed by evaporation of solutions on KBr windows using a Bruker Alpha system.

Experimental Section

Synthesis of Molybdenum Complexes

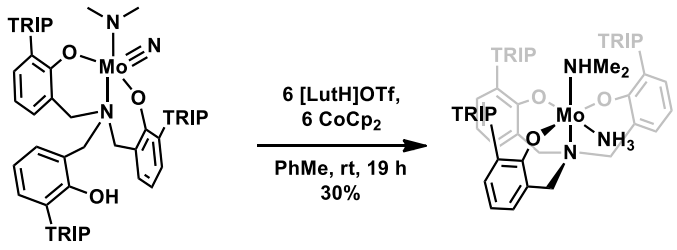
Molybdenum(VI) Nitrido Complex (A)



1 A

$NMo(NMe_2)_3$ (55.3 mg, 0.23 mmol, 1.05 equiv.) and **1** (205.1 mg, 0.218 mmol, 1.0 equiv.) were added to a 20 mL vial. Dry toluene (2.5 mL) was added to the vial. The resulting mixture was stirred at +23 °C for 12 hours. The volatiles were removed *in vacuo*. The solid residue was extracted with ether (3 x 1 mL). The mixture was filtered through a pad of Celite, concentrated *in vacuo*, leading to precipitation of yellow microcrystals, and had stood at –20 °C for several days. The product was rinsed with a small amount of cold ether (3 x 0.5 mL) and dried *in vacuo* at +23 °C to obtain **A** as yellow solid (120.3 mg, 51%). NMR Spectroscopy: ^{1}H NMR (500 MHz, C_6D_6, 23 ºC, δ): 7.35–7.18 (m, 3H), 7.15–6.72 (m, 12H), 5.02 (d, J = 14.9 Hz, 2H), 4.47 (s, 1H), 4.43 (s, 2H), 3.95 (s, 3H), 3.77 (d, J = 15.2 Hz 2H). 3.19 (sept, J = 6.9 Hz, 2H), 2.94 (sept, J = 6.7 Hz, 2H), 2.83 (sept, J = 6.9 Hz, 3H), 2.73 (sept, J = 6.9 Hz, 2H), 2.58 (s, 3H), 1.32 (d, J = 6.9 Hz, 6H), 1.26 (d, J = 6.9 Hz, 6H), 1.25–1.16 (m, 30H), 1.09 (t, J = 7.5 Hz, 12H). ^{13}C NMR (125 MHz, C_6D_6, 23 °C, δ): 159.4, 153.6, 150.3, 148.7, 147.9, 147.6, 147.4, 135.0, 134.2, 131.8, 131.4, 130.7, 129.8, 129.2, 127.2, 122.6, 121.9, 120.1, 120.03, 119.95, 119.3, 118.1, 62.2, 61.0, 46.6, 44.6, 34.9, 34.7, 31.2, 31.1, 31.0, 24.8, 24.7, 24.68, 24.6, 24.4, 24.38, 24.3, 24.27, 24.2, 24.1. IR (KBr, cm^{-1}): 3528 (s, O–H) 2957 (s, C–H), 2865 (s, C–H), 1584 (m), 1438 (m), 1245 (s), 1045 (s, Mo–N), 861 (m), 690 (m). Anal. Calcd. for $C_{69}H_{92}MoN_3O_3$: C, 74.25; H, 8.00; N, 4.01; found: C, 74.83; H, 8.37; N, 4.33.

Molybdenum(III) Amino Complex (B)

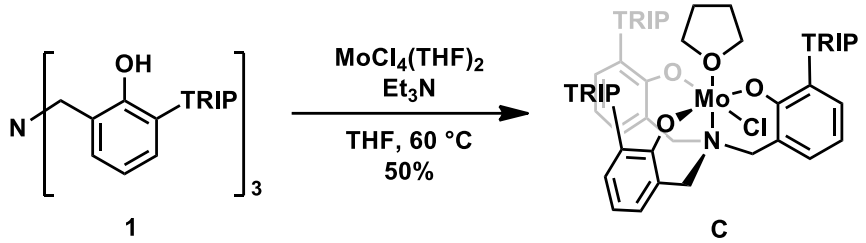


A B

A (100.0 mg, 0.091 mmol, 1.0 equiv.) and [LutH]OTf (141.0 mg, 0.548 mmol, 6.0 equiv.) were added to a 20 mL vial. Dry toluene (4 mL) was added to the vial. The resulting mixture was stirred at +23 °C for 5 minutes followed by the addition of $CoCp_2$ (104.0 mg, 0.548 mmol, 6.0

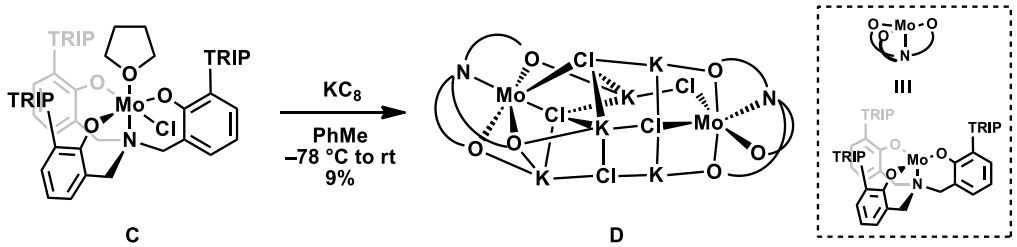
equiv.) to the vial. The mixture was stirred for 19 hours and the volatiles were removed *in vacuo*. The solid residue was extracted with pentane (3 × 1 mL). The solution was filtered through a pad of Celite, concentrated *in vacuo*, leading to precipitation of reddish-yellow microcrystals, and had stood at -40 °C for several days. The product was rinsed with a small amount of cold pentane (3 × 0.5 mL) and dried *in vacuo* at +23 °C to obtain **B** as reddish-yellow solid (30.0 mg, 30%). IR (KBr, cm^{-1}): 3356 (s (w), N–H), 3242 (s (w), N–H), 2954 (s, C–H), 2926 (s, C–H), 2863 (s, C–H), 2737 (s), 1580 (m), 1427 (s), 1262 (s), 754 (m). Anal. Calcd. for $C_{68}H_{94}MoN_3O_3\cdot(H_2O)$: C, 73.22; H, 8.67; N, 3.77; found: C, 72.85; H, 8.37; N, 3.24. Solution magnetic moment (C_6D_6): 3.52 μ_B.

Molybdenum(IV) Chloro THF Complex (C)



Et_3N (49.0 μL, 3.3 equiv.) and **1** (100.0 mg, 1.0 equiv.) were added to a 4 mL vial. Dry THF (10 mL) was added to the vial. The resulting mixture was stirred at +23 °C for 30 minutes. $MoCl_4(THF)_2$ (45.0 mg, 1.1 equiv.) was added to the vial. The mixture was stirred at +60 °C for 24 hours. The solvents were removed *in vacuo*. The solid residue was extracted with pentane (4 × 3 mL). The mixture was filtered through a pad of Celite, concentrated *in vacuo*, leading to precipitation of microcrystals, which were isolated by filtration after the mixture, and had stood at –20 °C for several days. The product was rinsed with a small amount of cold pentane (3 × 1 mL) and dried for 8 h at +23 °C to afford **C** as red solid (60.2 mg, 50 %). IR (KBr, cm^{-1}): 2965 (s, C–H), 2863 (s, C–H), 1581 (m), 1430 (m), 1233 (s), 853 (m), 759 (s). Anal. Calcd. For $C_{70}H_{92}ClMoNO_4\cdot(H_2O)_{0.8}$: C, 72.65; H, 8.15; N, 1.21; found: C, 72.35; H, 7.78; N, 0.97. Solution magnetic moment (C_6D_6): 3.03 μ_B.

Molybdenum(III) KCl Dimer (D)



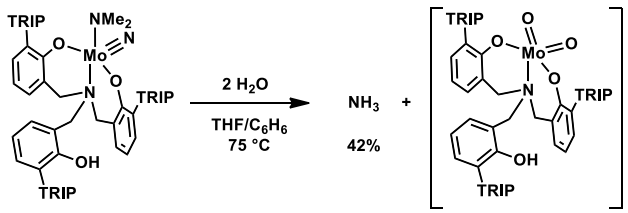
C (50.0 mg, 0.044 mmol, 1.0 equiv.) and KC_8 (6.5 mg, 0.048 mmol, 1.1 equiv.) were added to a 20 mL vial. Dry toluene (5 mL) was added to the vial. The resulting mixture was stirred at –78 °C a coldwell for 12 hours. Then the mixture stirred 5 hours more at +23 °C. The solvents were removed *in vacuo*. The solid residue was extracted with pentane (4 × 3 mL). The mixture was filtered through a pad of Celite, concentrated *in vacuo*, leading to precipitation of microcrystals and had stood at –40 °C for two weeks. The crystalline product was rinsed with

a small amount of cold pentane and dried for 12 h at +23 °C to afford **D** as yellow solid (10.0 mg, 9%). IR (KBr, cm^{-1}): 3030 (s, C–H), 2957 (s, C–H), 2863 (s, C–H), 1591 (m), 1435 (m), 1243 (m), 1071 (m), 754 (m). Anal. Calcd. For $C_{132}H_{168}Cl_5K_5Mo_2N_2O_6(C_7H_8)_4$: C, 68.34; H, 7.17; N, 1.00; found: C, 68.87; H, 7.53; N, 1.31. Solution magnetic moment (C_6D_6): 3.76 μ_B.

Standard Reduction Protocol

In a nitrogen atmosphere glovebox, the complex (~10.0 mg, ~9.14 μmol) weighed into a 50 mL Schlenk flask. The 48 equivalents of proton sources and 36 equivalents of electron sources were added in the same flask, containing a magnetic stirring bar. The flask is cooled to 77 K in a cold well using liquid nitrogen. The solvent is added to the flask 4 mL to make the concentration of the solution ~2.3 mM. The reaction system is maintained in the cold well for 5 minutes before transferring to a dry ice/acetone bath outside of the glovebox. The reaction solution was stirred in the cold bath for 5 hours at –78 °C. Then the flask was removed from the bath.

Hydrolysis of molybdenum nitride complex A



A E

In a nitrogen atmosphere glovebox, complex **A** (5.5 mg, 5.03 μmol) weighed into a JY NMR tube and 600 uL of C_6H_6 was added. A stock solution of water in THF (10 μL of water in 10 mL of THF) was prepared outside of the glovebox. 360 μL of the solution was transferred to the tube. The solution was heated at 75 °C for 6 hours. The quantification of the synthesized ammonia was proceeded with below the **Ammonia Quantification** method. The yield of ammonia was 42% by ^{1}H-NMR using 1,3,5-trimethoxybenzene as an internal standard. After vacuum transfer for the ammonia quantification, the residual yellow solid measured for ESI-MS (negative mode) by dissolving C_6H_6/MeCN solution whose m/z value was in accordance with molybdenum dioxo complex **E**.

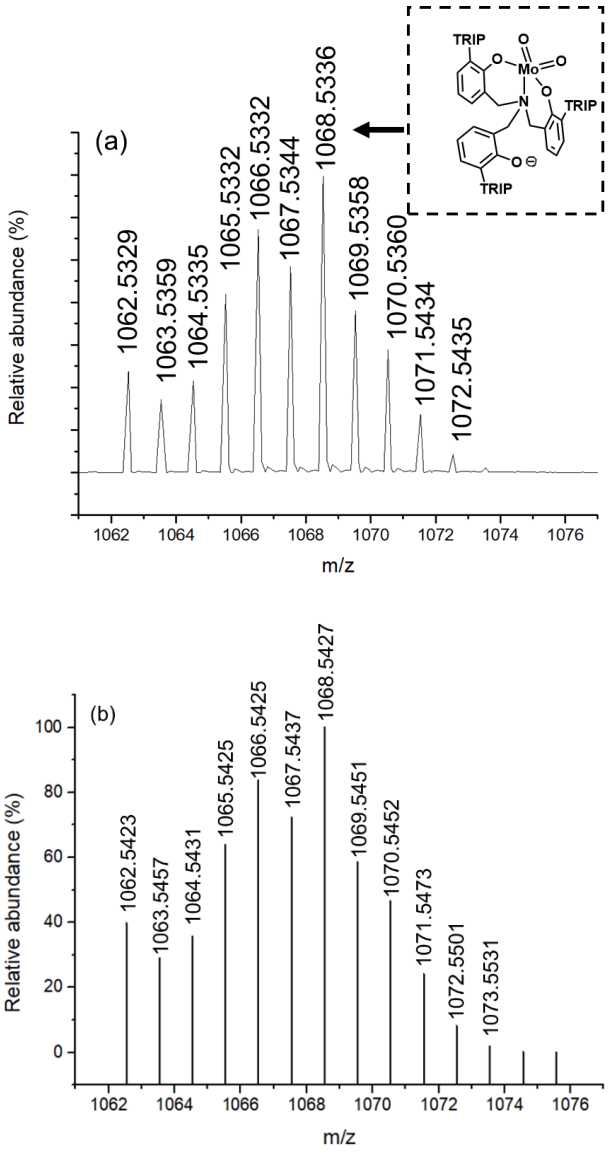


Figure S1. (a) Observed mass spectrum and (b) calculated isotopic pattern of molybdenum dioxo complex **I**

Ammonia Quantification

A Schlenk flask was filled with 3 mL of 2.0 M HCl in diethyl ether to collect NH_3. A glass vacuum transfer apparatus was attached to a high-vacuum (< 10^{-3} Torr) line. The reaction mixture flask and the collection (3 mL of 2.0 M HCl in diethyl ether) flask were connected with the apparatus, and then both of them were placed in liquid nitrogen for 15 minutes. The headspace of the apparatus was evacuated for 15 minutes, by maintaining the line pressure under high-vacuum (< 10^{-3} Torr). The mixture was thawed and the remaining volatiles were vacuum-transferred to the collection flask under static vacuum. After the vacuum-transfer, the reaction flask was taken into the N_2 glovebox. To the solid residue in the reaction flask, 40 mg of potassium *tert*-butoxide in MeOH/THF (4 mL/ 2 mL) was added. The flask was taken out

from the glovebox and attached to the vacuum transfer apparatus. The homogeneous solution was stirred for 15 minutes and the volatiles of the solution were vacuum-transferred to the collection flask. All volatiles of the collection flask were removed under dynamic vacuum at room temperature. The remaining solid including ammonium chloride in the flask was dissolved in 1 mL of H_2O. The amount of ammonia was quantified by the indophenol method using an aliquot of the solution (20 uL). The indophenol absorbance was calibrated using sublimed NH_4Cl within the range of 0.035 to 2.49, and all the sample absorbance data were interpolated in that region. In the case of runs with $PhNH_3OTf$, the anilinium salt in a collection flask could interfere with the indophenol method. The quantification for ammonia was conducted by integrating ^{1}H-NMR peaks. The solid residue of the collection flask was extracted into 1 mL of DMSO-d_6 solvent, which contains 0.67 mmol of 1,3,5-trimethoxybenzene as an internal standard. Ammonium peaks in ^{1}H-NMR were integrated against the two peaks of the internal standard for quantification of ammonium.

entry	Complex	H^+	e^-	Solvent	NH_3/Mo
1	**A**	[LutH]OTf	$CoCp_2$	PhMe	0.95
2	**A**	Ph_2NH_2OTf	$CoCp^*_2$	Diethyl ether	0.64
3[a]	**A**	$PhNH_3OTf$	$CoCp^*_2$	Diethyl ether	0.54
4[a,b]	**A**	$PhNH_3OTf$	$CoCp^*_2$	Diethyl ehter	0.58
5	**A**	ethylene glycol	SmI_2	THF	0.22
6	**A**	$[Cy_3PH][BF_4]$	KC_8	Et_2O	0.28
7[c]	**C**	[LutH]OTf	$CoCp^*_2$	PhMe	0.06
8	**C**	[LutH]OTf	$CoCp_2$	PhMe	0.11

[a]: The synthesized ammonium was quantified by the integration of ^{1}H-NMR peaks of ammonium against the internal standard.

[b]: The reaction was done in Ar atmosphere.

[c]: The reaction was done in rt.

Calibration Curve for Ammonia Quantification

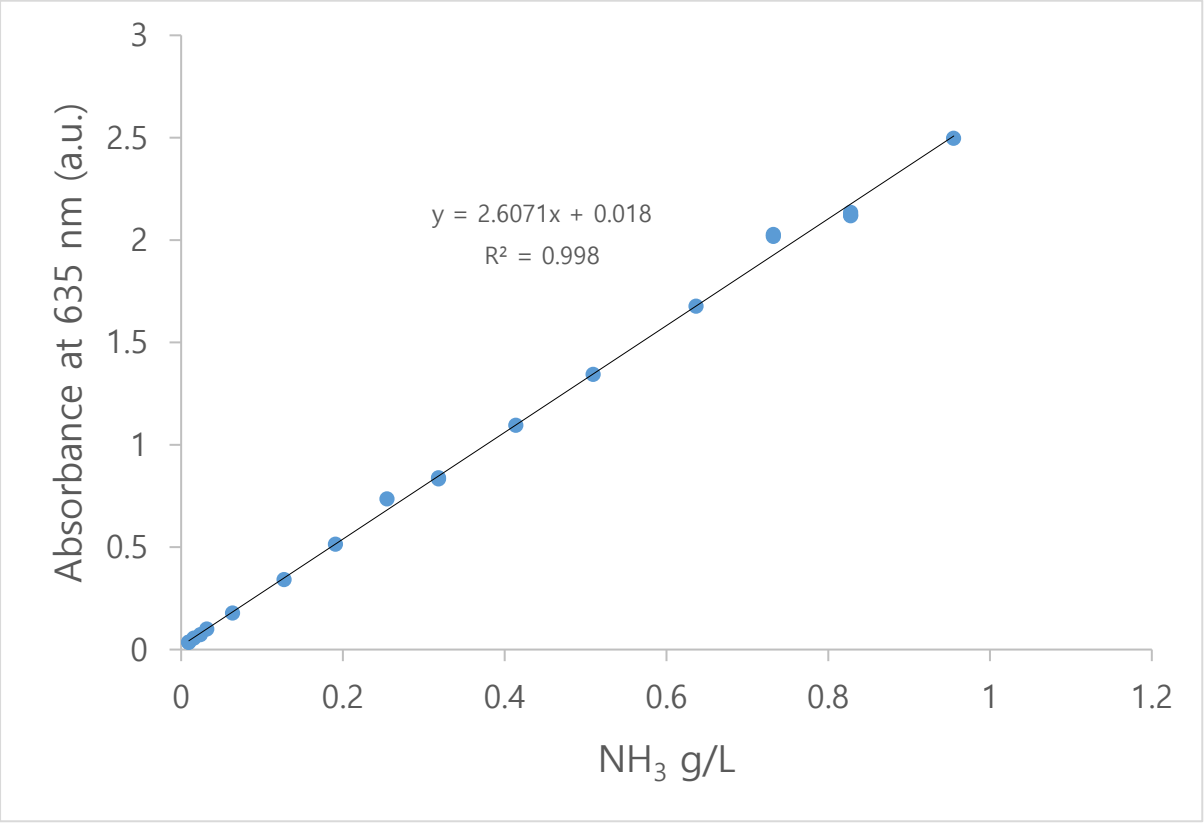


Figure S2. Calibration curve for NH_3 UV-VIS quantification

X-ray Crystallographic Analysis

CCDC 1991108- 1991111 contains the supplementary crystallographic data for **A**, **B**, **C**, and **D**. These data can be obtained free of charge via www.ccdc.cam.ac.uk/cgi-bin/catreq.cgi (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB21EZ, UK; fax (+44) 1223-336-033; or deposit@ccdc.cam.ac.uk).

General information

A suitable crystal was coated with paratone-N oil and the diffraction data measured at 100 K either with synchrotron radiation on a 2D (for **B**), 6D (for **A** and **C**), or 11C (for **D**) beamline at the Pohang Accelerator Laboratory, Korea. Using Olex2 software, the structure was solved by ShelXT using Intrinsic Phasing and refined by ShelXL using Least Squares minimization. All the non-hydrogen atoms were refined anisotropically. All hydrogen atoms were added to their geometrically ideal positions.

Crystal data and structure refinements

Crystal data and structure refinement for A

Empirical formula	$C_{72}H_{101}MoN_3O_4$
Formula weight	1168.49
Temperature/K	100
Crystal system	monoclinic
Space group	C2/c
a/Å	39.948(8)
b/Å	9.4800(19)
c/Å	36.213(7)
α/°	90
β/°	99.22(3)
γ/°	90
Volume/Å^3	13537(5)
Z	8
ρcalcg/cm^3	1.147
μ/mm^{-1}	0.188
F(000)	5024.0
Crystal size/mm^3	0.05 × 0.03 × 0.03
Radiation	Synchrotron (λ = 0.660)
2Θ range for data collection/°	2.116 to 66.124
Index ranges	-65 ≤ h ≤ 65, -15 ≤ k ≤ 15, -59 ≤ l ≤ 59
Reflections collected	89521
Independent reflections	27164 [Rint = 0.0968, Rsigma = 0.0708]
Data/restraints/parameters	27164/0/745
Goodness-of-fit on F^2	1.144
Final R indexes [I>=2σ (I)]	R1 = 0.0655, wR2 = 0.1926
Final R indexes [all data]	R1 = 0.0757, wR2 = 0.2003
Largest diff. peak/hole / e Å^{-3}	1.75/-1.16

Crystal data and structure refinement for B

Empirical formula	$C_{68}H_{94}MoN_3O_3$
Formula weight	1097.40
Temperature/K	100
Crystal system	monoclinic
Space group	P21/c
a/Å	21.558(4)
b/Å	16.423(3)
c/Å	18.064(4)
α/°	90
β/°	103.13(3)
γ/°	90
Volume/Å^3	6228(2)
Z	4
ρcalcg/cm^3	1.170
μ/mm^{-1}	0.242
F(000)	2356.0
Crystal size/mm^3	0.2 × 0.1 × 0.06
Radiation	Synchrotron (λ = 0.70000)

2Θ range for data collection/°	4.536 to 48.666
Index ranges	-25 ≤ h ≤ 25, -19 ≤ k ≤ 19, -21 ≤ l ≤ 21
Reflections collected	27742
Independent reflections	10192 [Rint = 0.0283, Rsigma = 0.0258]
Data/restraints/parameters	10192/0/719
Goodness-of-fit on F^2	1.059
Final R indexes [I>=2σ (I)]	R1 = 0.0422, wR2 = 0.1079
Final R indexes [all data]	R1 = 0.0431, wR2 = 0.1086
Largest diff. peak/hole / e $Å^{-3}$	1.28/-0.74

Crystal data and structure refinement for C

Empirical formula	$C_{70}H_{92}ClMoNO_4$
Formula weight	1142.83
Temperature/K	100.0
Crystal system	monoclinic
Space group	P21/c
a/Å	21.259(4)
b/Å	16.589(3)
c/Å	18.108(4)
α/°	90
β/°	102.74(3)
γ/°	90
Volume/$Å^3$	6229(2)
Z	4
ρcalcg/cm^3	1.219
μ/mm^{-1}	0.285
F(000)	2440.0
Crystal size/mm^3	0.05 × 0.05 × 0.03
Radiation	Synchrotron (λ = 0.700)
2Θ range for data collection/°	3.096 to 60.01
Index ranges	-30 ≤ h ≤ 30, -23 ≤ k ≤ 23, -25 ≤ l ≤ 25
Reflections collected	67241
Independent reflections	18922 [Rint = 0.0387, Rsigma = 0.0368]
Data/restraints/parameters	18922/0/733
Goodness-of-fit on F^2	1.071
Final R indexes [I>=2σ (I)]	R1 = 0.0572, wR2 = 0.1691
Final R indexes [all data]	R1 = 0.0738, wR2 = 0.1798
Largest diff. peak/hole / e $Å^{-3}$	1.15/-1.37

Crystal data and structure refinement for D

Empirical formula	$C_{144.5}H_{198}Cl_5K_5Mo_2N_2O_6$
Formula weight	2623.67
Temperature/K	100
Crystal system	triclinic
Space group	P-1
a/Å	18.820(4)
b/Å	21.472(4)
c/Å	23.757(5)
α/°	111.84(3)
β/°	100.76(3)

γ/°	99.58(3)
Volume/Å^3	8457(4)
Z	2
ρcalcg/cm^3	1.030
μ/mm^{-1}	0.314
F(000)	2782.0
Crystal size/mm^3	0.09 × 0.08 × 0.03
Radiation	Synchrotron (λ = 0.660)
2Θ range for data collection/°	2.368 to 54.56
Index ranges	-26 ≤ h ≤ 26, -29 ≤ k ≤ 29, -32 ≤ l ≤ 32
Reflections collected	75919
Independent reflections	41484 [Rint = 0.0479, Rsigma = 0.0718]
Data/restraints/parameters	41484/0/1513
Goodness-of-fit on F^2	0.973
Final R indexes [I>=2σ (I)]	R1 = 0.0770, wR2 = 0.2162
Final R indexes [all data]	R1 = 0.1237, wR2 = 0.2444
Largest diff. peak/hole / e Å^{-3}	1.76/-0.98

IR spectra of metal complexes

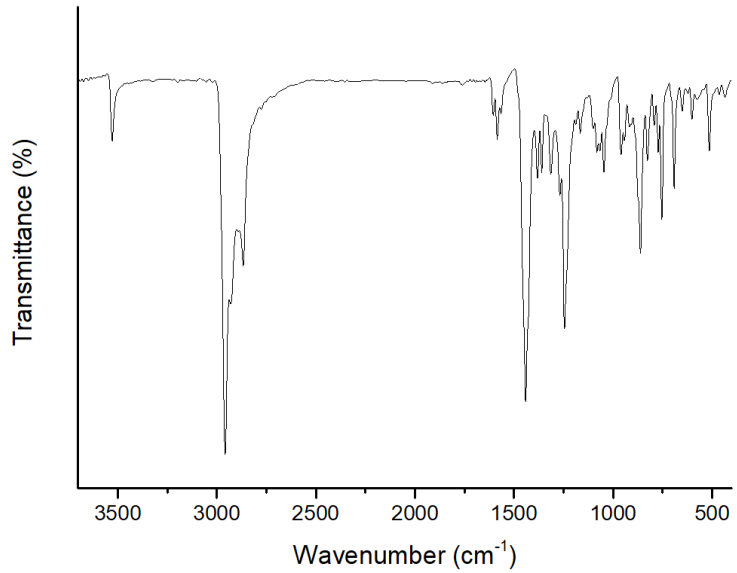


Figure S3. IR spectrum of **A**. IR (KBr, cm^{-1}): 3528 (s, O–H) 2957 (s, C–H), 2865 (s, C–H), 1584 (m), 1438 (m), 1245 (s), 1045 (s, Mo–N), 861 (m), 690 (m).

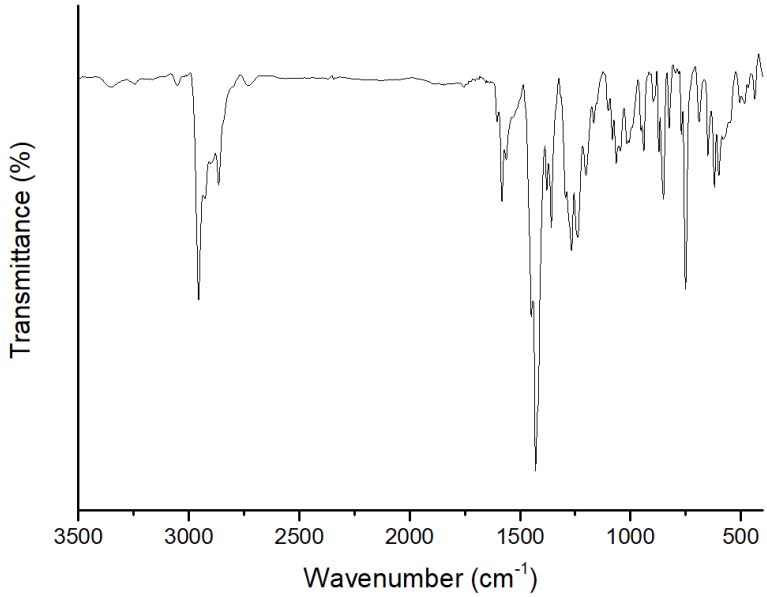


Figure S4. IR spectrum of **B**. IR (KBr, cm^{-1}): 3356 (s (w), N–H), 3242 (s (w), N–H), 2954 (s, C–H), 2926 (s, C–H), 2863 (s, C–H), 2737 (s), 1580 (m), 1427 (s), 1262 (s), 754 (m).

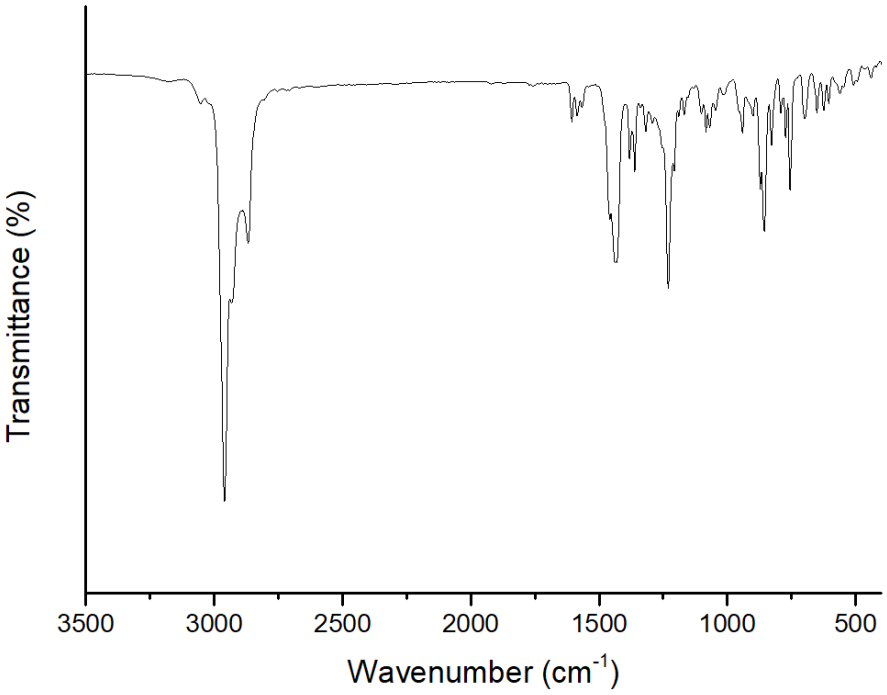


Figure S5. IR spectrum of **C**. IR (KBr, cm^{-1}): 2965 (s, C–H), 2863 (s, C–H), 1581 (m), 1430 (m), 1233 (s), 853 (m), 759 (s).

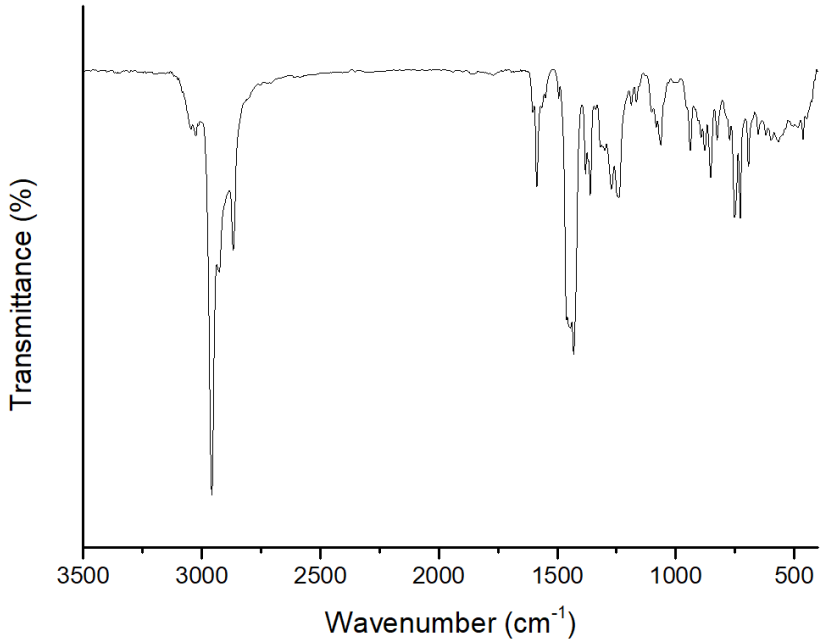


Figure S6. IR spectrum of **D**. IR (KBr, cm^{-1}): 3030 (s, C–H), 2957 (s, C–H), 2863 (s, C–H), 1591 (m), 1435 (m), 1243 (m), 1071 (m), 754 (m).

UV-Vis spectra of metal complexes

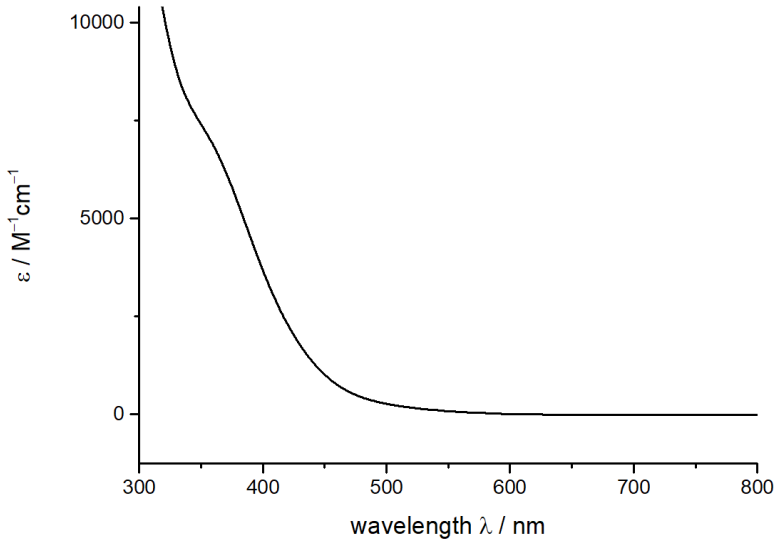


Figure S7. Electronic adsorption spectrum of **A**, recorded in benzene. UV/Vis (Benzene, 0.1 mM, 25 °C, nm ($\varepsilon = M^{-1}cm^{-1}$)): λ (ε) = ca. 361 (ca. 6769, shoulder).

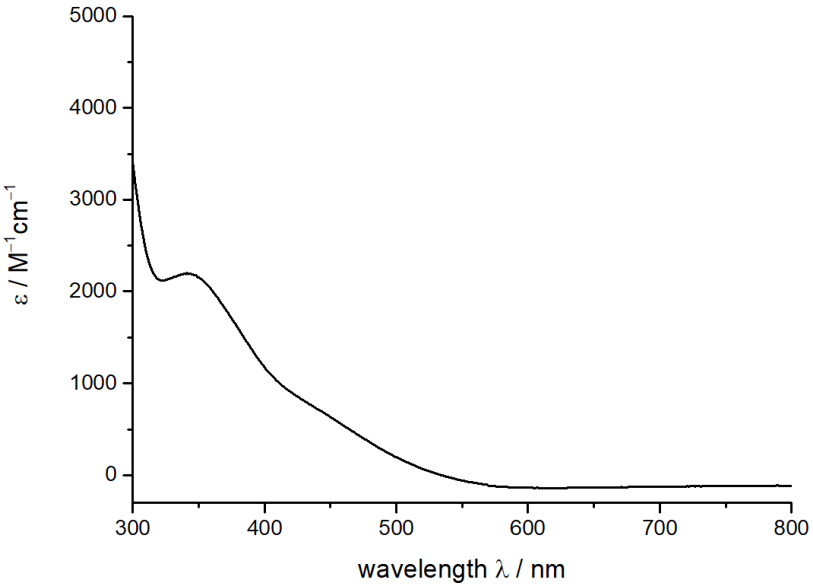


Figure S8. Electronic adsorption spectrum of **B**, recorded in benzene. UV/Vis (Benzene, 0.1 mM, 25 °C, nm ($\varepsilon = M^{-1}cm^{-1}$)): λ (ε) = 342 (2190).

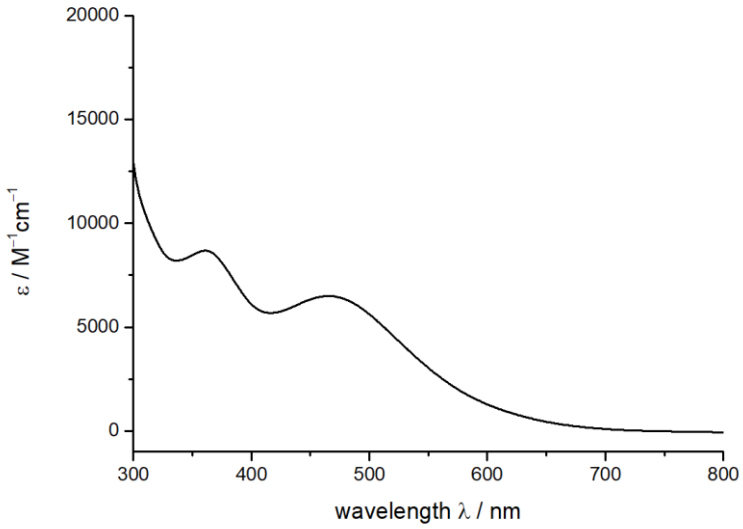


Figure S9. Electronic adsorption spectrum of **C**, recorded in benzene. UV/Vis (Benzene, 0.1 mM, 25 °C, nm ($\varepsilon = M^{-1}cm^{-1}$)): λ (ε) = 362 (8687), 465 (6490).

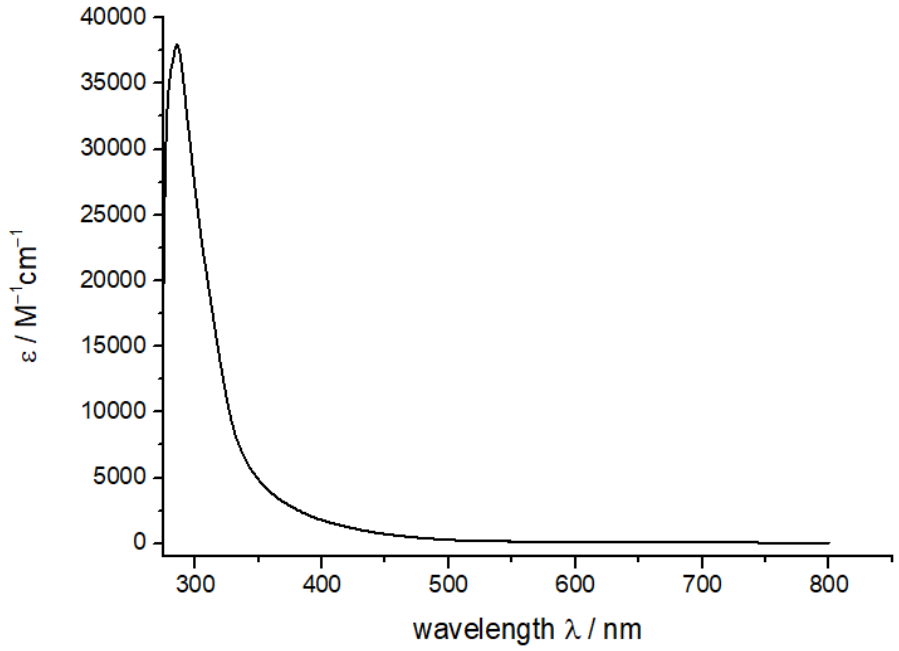


Figure S10. Electronic adsorption spectrum of **D**, recorded in benzene. UV/Vis (Benzene, 0.1 mM, 25 °C, nm ($\varepsilon = M^{-1}cm^{-1}$)): λ (ε) = 285 (37892), ca. 639 (ca. 112, shoulder).

DFT

Density functional theory (DFT) calculations were performed using Gaussian09[8] at the clusters at Pohang University of Science and Technology (POSTECH). Geometry optimizations were carried out using the atomic coordinates from crystal structures (for **A**, **B**, and **C**). The nature of all stationary points calculated from full optimizations was confirmed via frequency analysis, which revealed zero imaginary frequency for the ground state. All geometries were optimized using the B3PW91[9,10] under standard convergence criteria with the following basis sets, which include SDD quasirelativistic pseudopotentials on Mo (28) with associated basis set (8s7p6d1f)/[6s5p3d1f])[11] augmented by polarization functions (Mo: f, 1.043),[12] and 6-31G(d,p)[13] on H, C, N and O.

Intramolecular Proton Transfer from **A** Generating Molybdenum Nitride **A'**

Figure S11 illustrates a thermodynamically demanding energy in the activation of molybdenum nitride complex (**A**) by the deprotonation from the dative amide ligand. Computational result insists that this process is endergonic with requiring ~ 7 kcal/mol. The reason for this unfavorable transformation is coming from the geometric change from square pyramidal to trigonal bipyramidal structure. The resulting shift in relative position of nitride and axial amine ligand caused by the deprotonation makes both ligands to be located in the axial position of trigonal bipyramidal symmetry. In that case (**A'**), the strong trans-influence from the nitride ligand weakens orbital interaction between the metal center and the axial amine ligand, originating the destabilization of the whole structure.

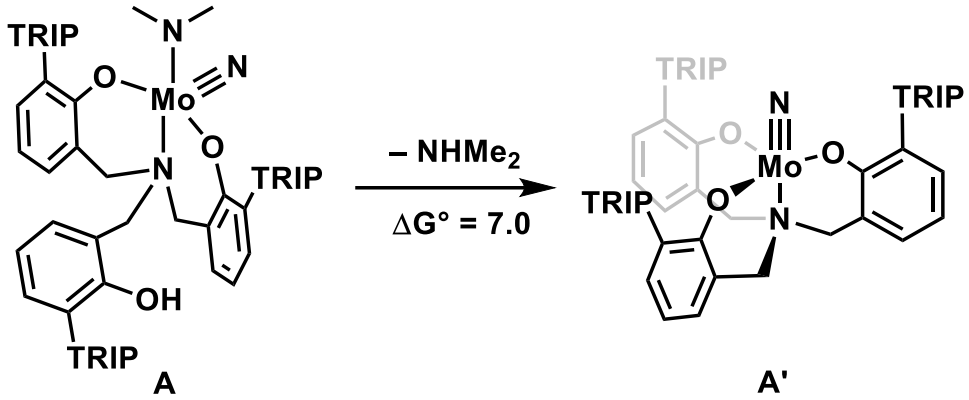


Figure S11. Transformation of **A** to **A'** with the liberation of $NHMe_2$. The energy represents the Gibbs free energy change in kcal/mol.

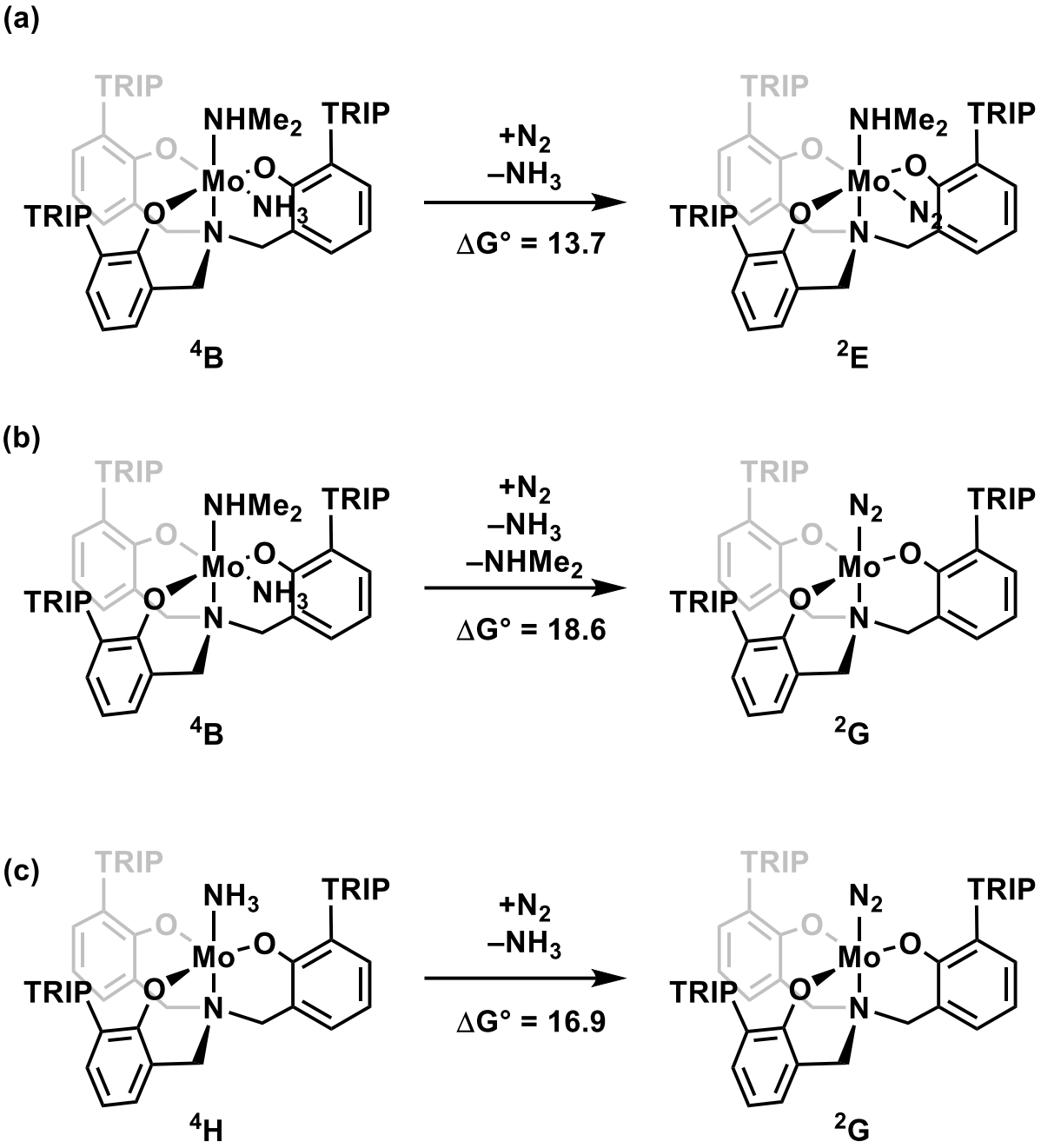


Figure S12. The reaction energy for the NH_3/N_2 exchange. Superscripts indicate spin multiplicities. The energy represents the Gibbs free energy change in kcal/mol.

Coordinates of optimized structures

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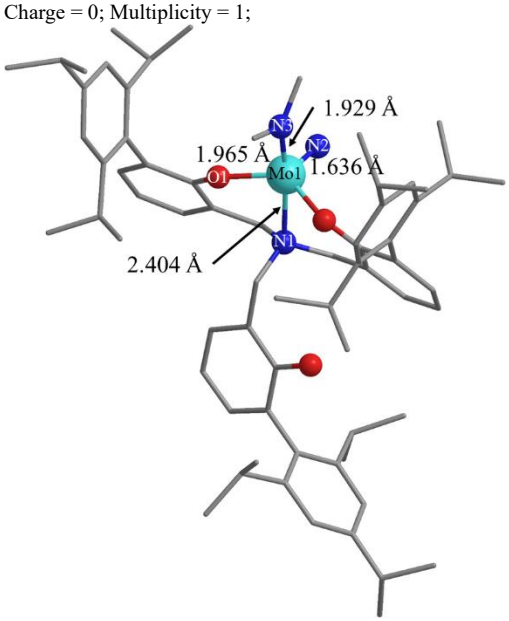

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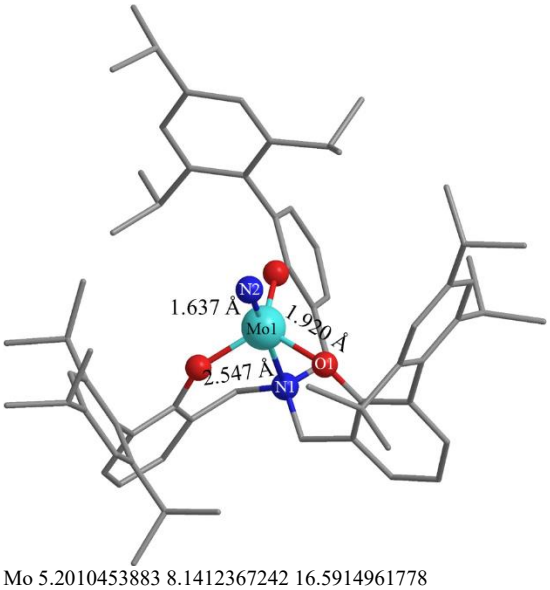

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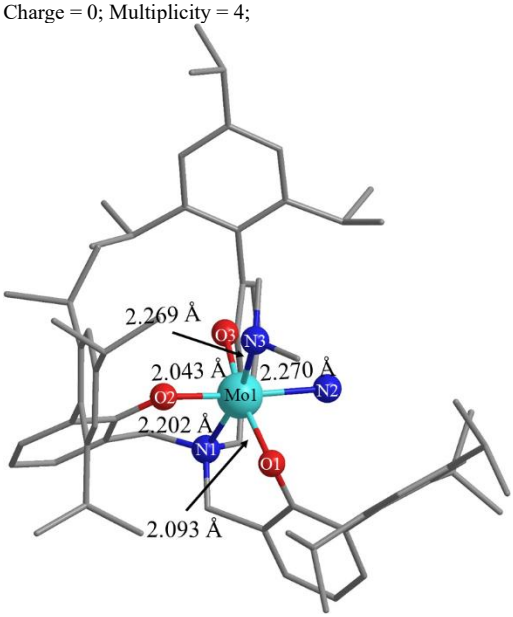

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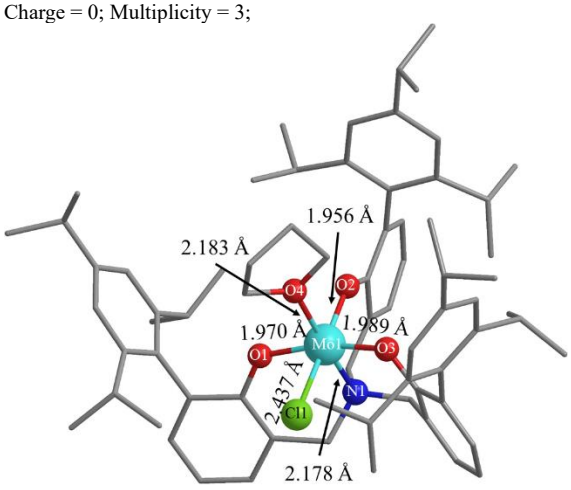

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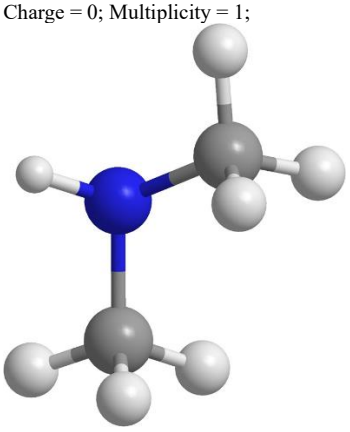
H -5.5031740694 1.5912690979 0.4560708761
H -3.8838558725 1.1143367789 0.9976262894

NHMe$_2$
E° = –135.1241566; G° = –135.056727
Charge = 0; Multiplicity = 1;



N -0.3297430941 0.1769425216 -0.4832298972
C 0.733921066 0.9539061339 0.1249087302
C -0.503966971 -1.1219265358 0.1391417381
H -1.1999254713 0.6961314732 -0.4254172287
H 1.6945298974 0.4550258188 -0.0498937295
H 0.7873308602 1.9413853163 -0.3437513431
H 0.6330726376 1.0957983873 1.2178029289
H 0.3900230445 -1.7322131172 -0.0355726649
H -0.6696545539 -1.0896175901 1.2328385269
H -1.3507214154 -1.6424514081 -0.3187880608

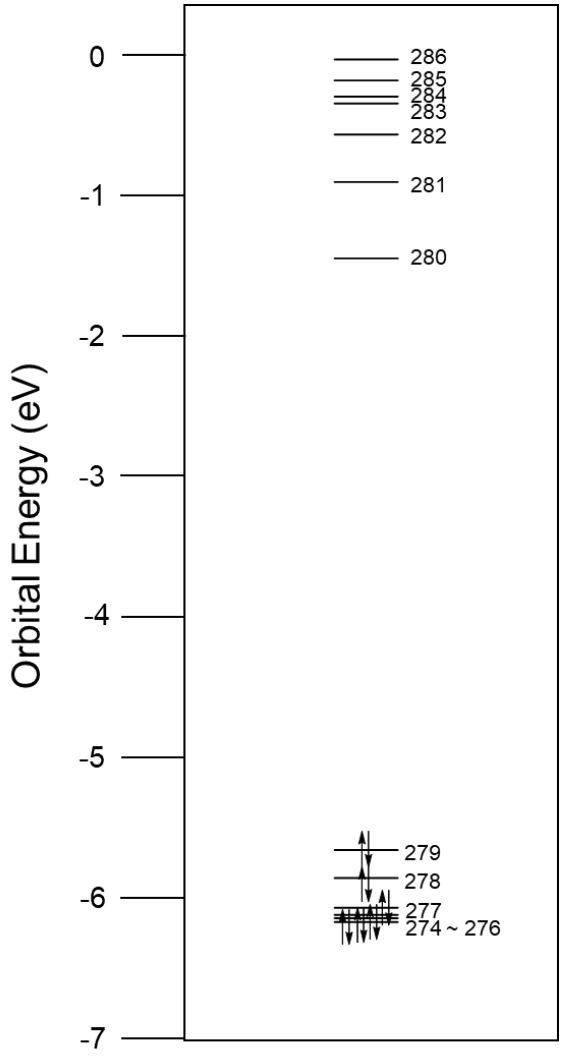
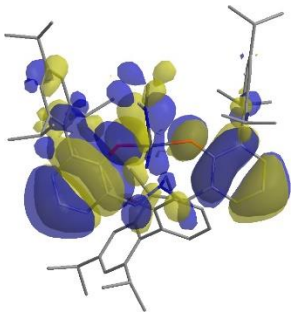


Figure S13. Computed orbital energies for **A**



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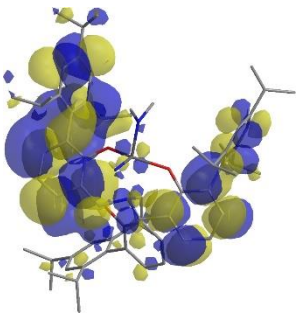

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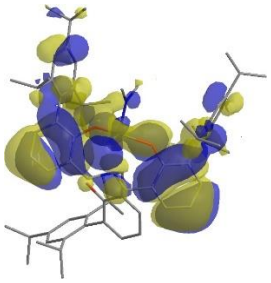

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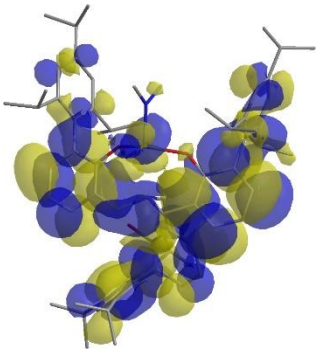

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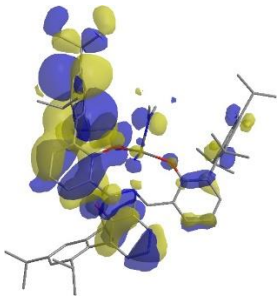

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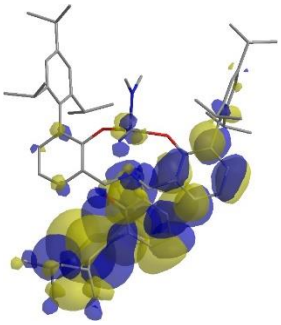

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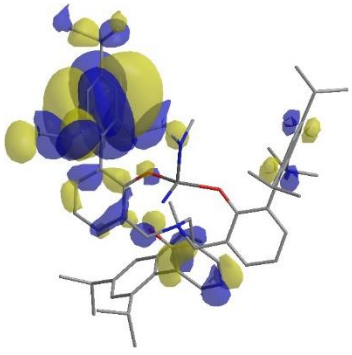

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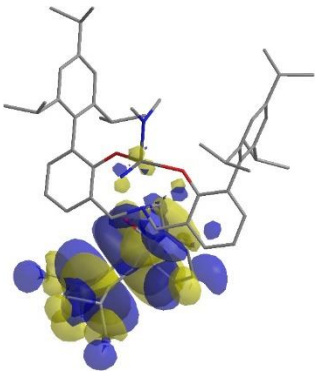

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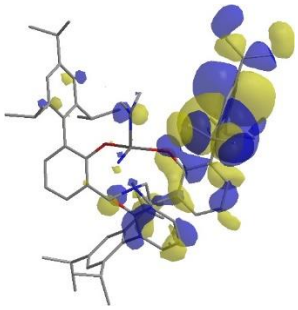

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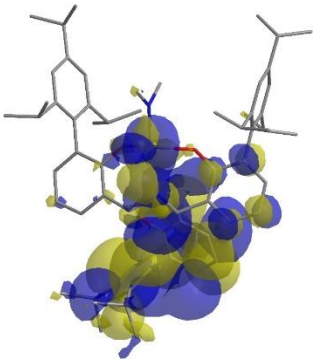

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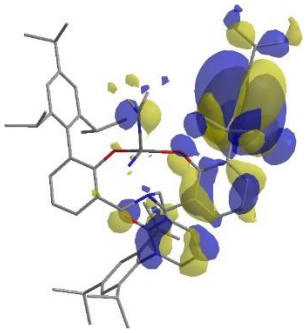

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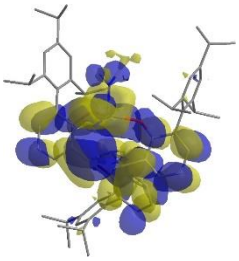

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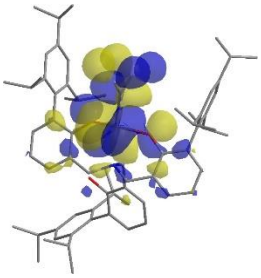


280

Figure S14. Computed frontier molecular orbitals of **A**

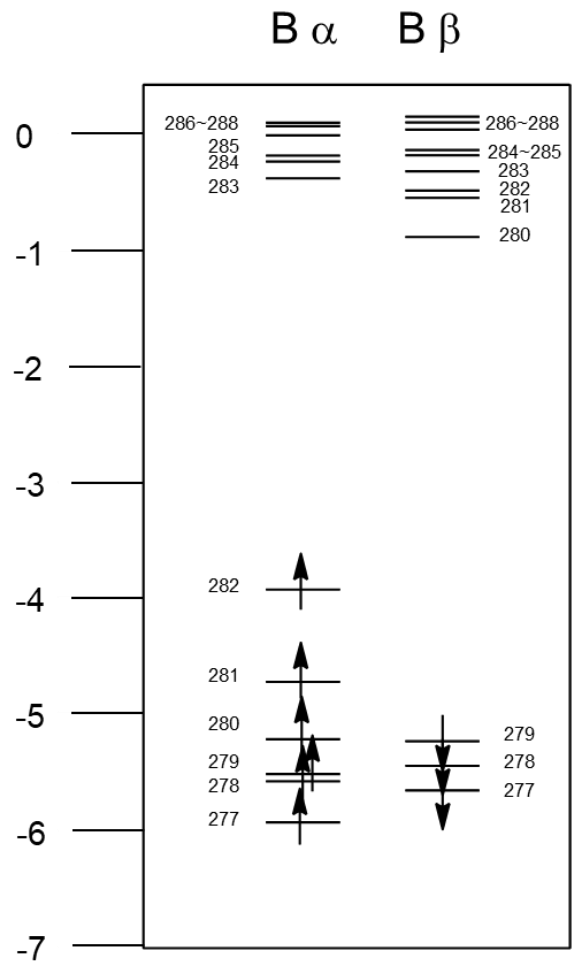
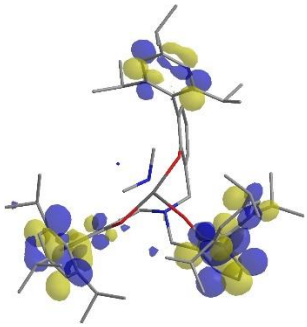
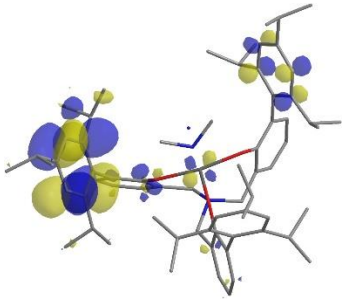


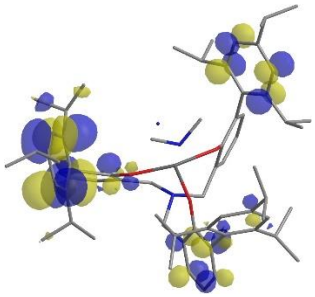
Figure S15. Computed orbital energies for **B**



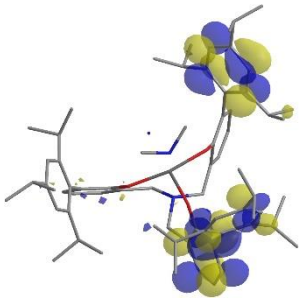
288 α



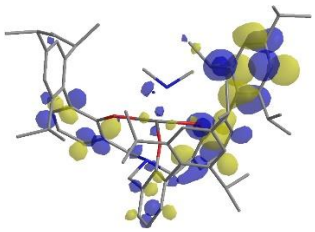
288 β



287 α



287 β



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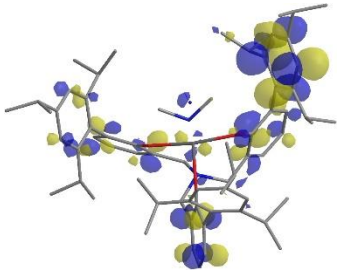
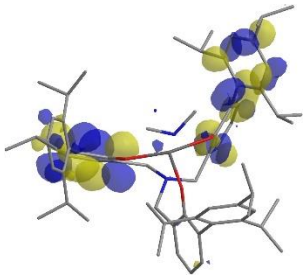


286 β



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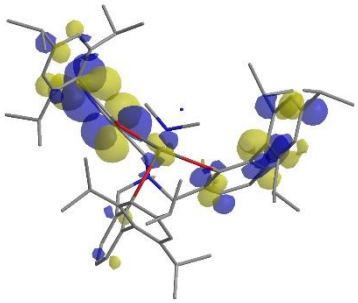

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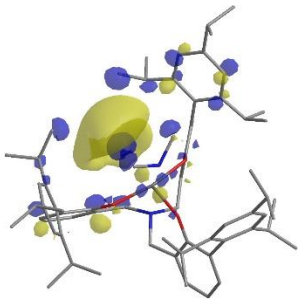
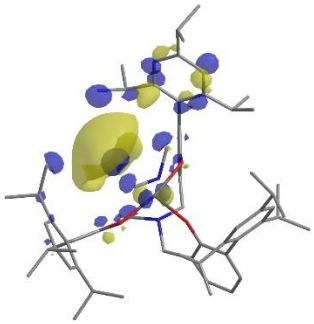
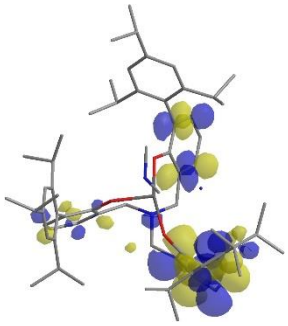


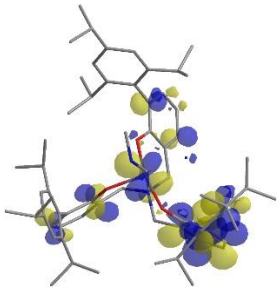
284 α



284 β



283 α



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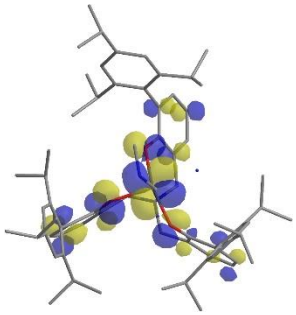

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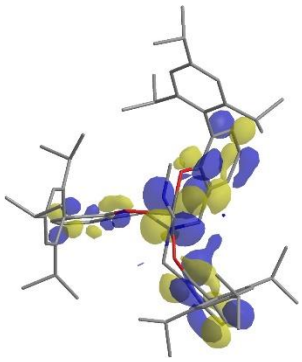

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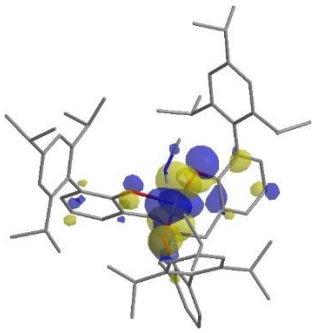

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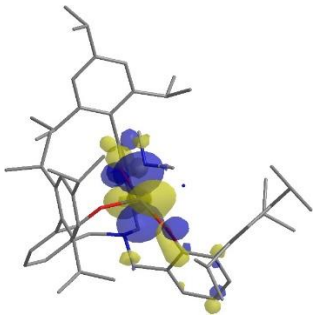

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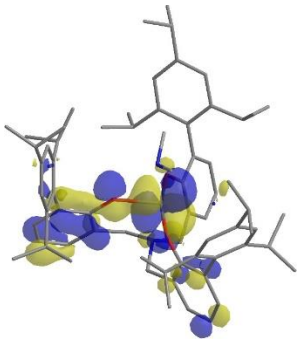

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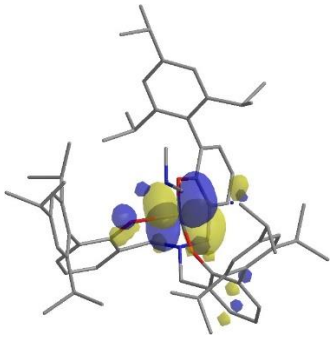

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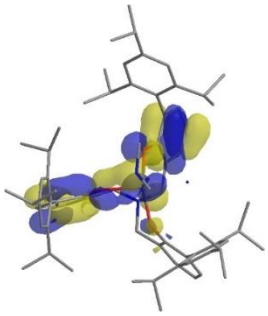

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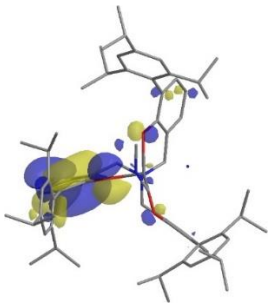

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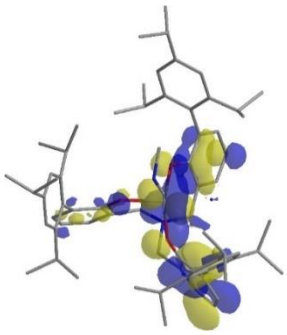
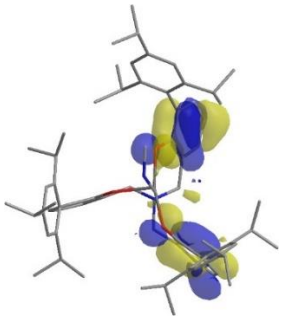
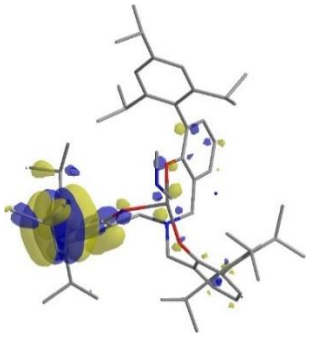


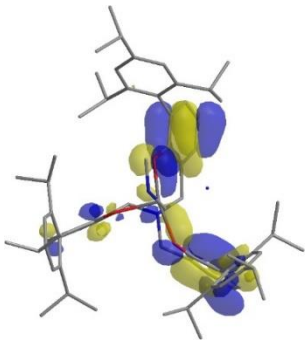
278 α



278 β



277 α



277 β

Figure S16. Computed frontier molecular orbitals of **B**

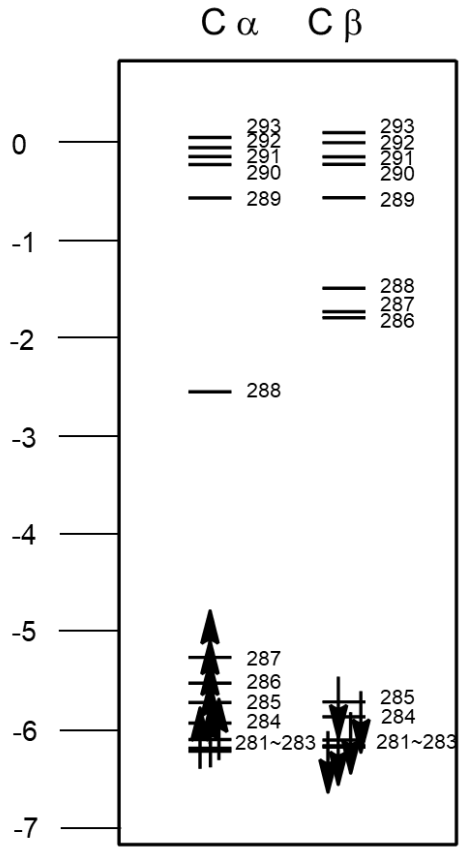
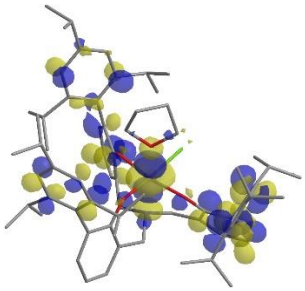
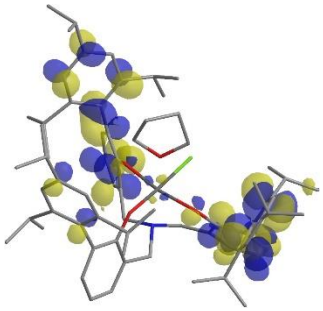


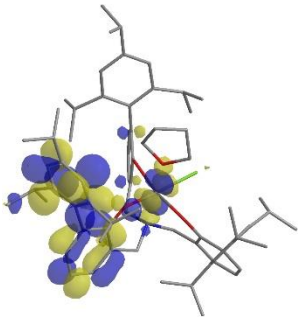
Figure S17. Computed orbital energies for **C**



293 α



293 β



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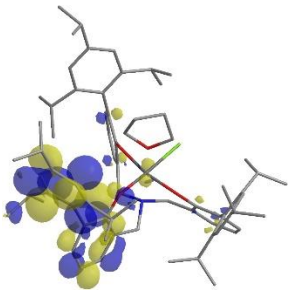

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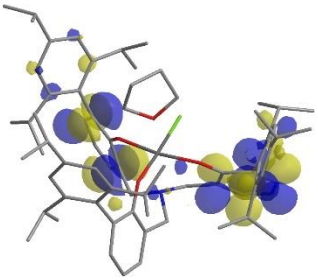

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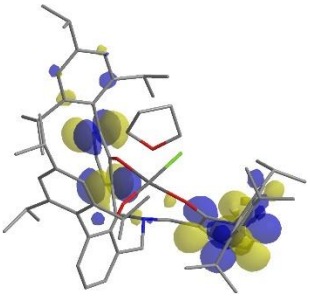

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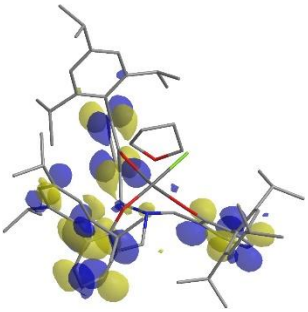
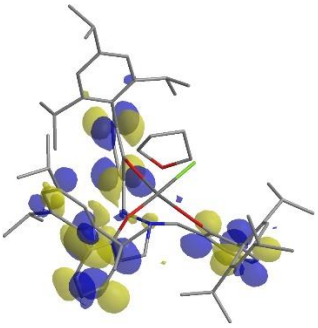
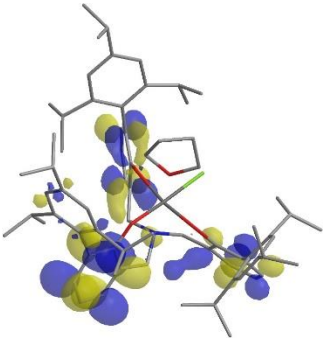


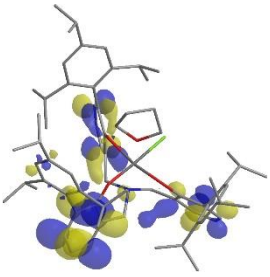
290 α



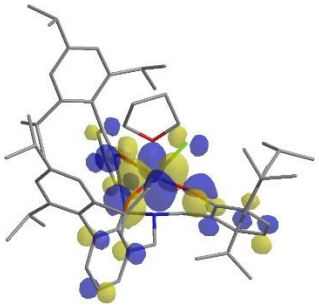
290 β



289 α



289 β



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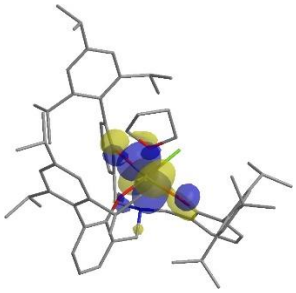

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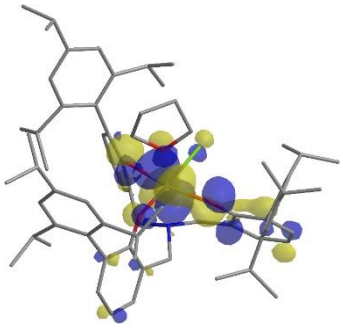

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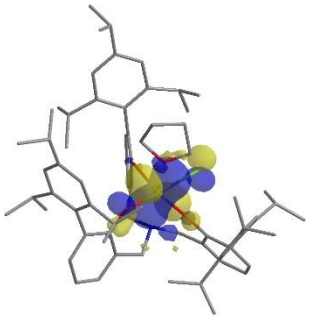

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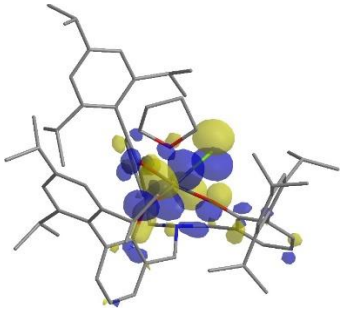

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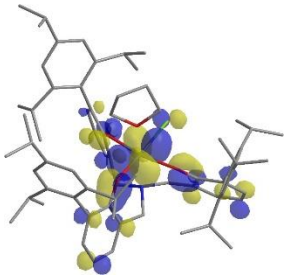
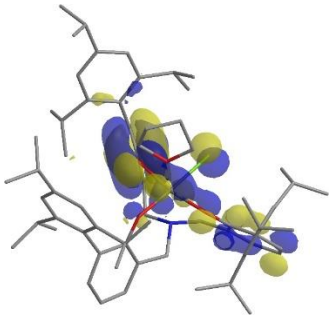
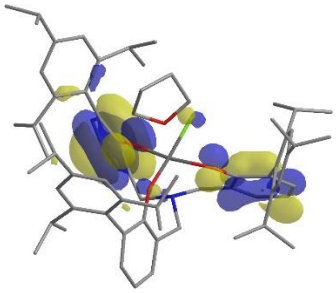


286 β



285 α



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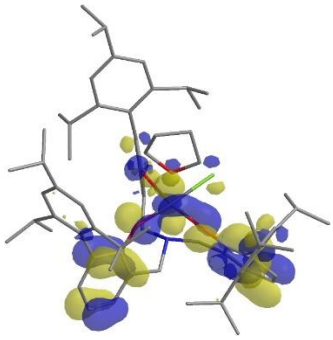

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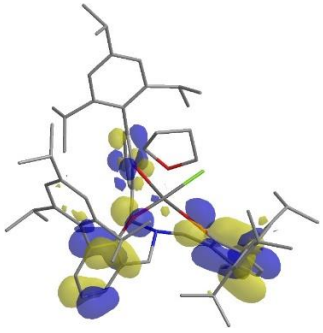

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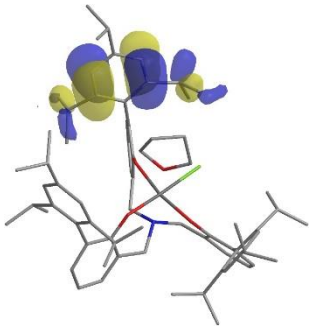
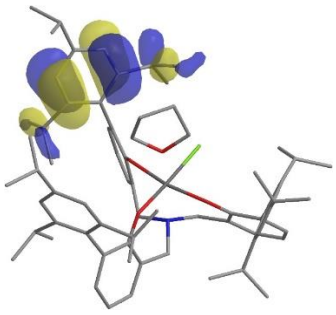


283 α



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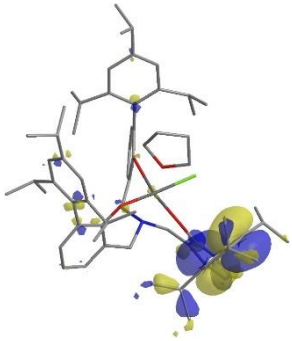
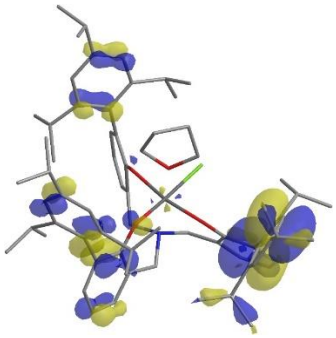
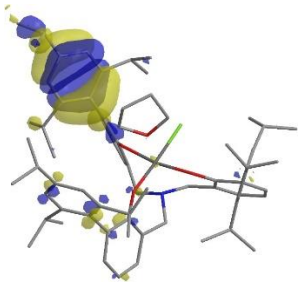


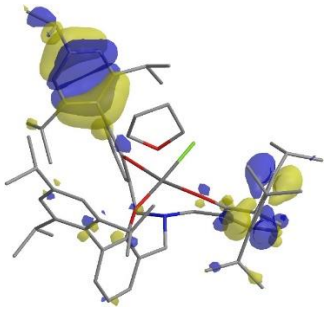
282 α



282 β



281 α



281 β

Figure S3. Computed frontier molecular orbitals of **C**

Electron Paramagnetic Resonance (EPR) Data

EPR spectrum of **B** was recorded on a Bruker X-band A200 spectrometer at room temperature.

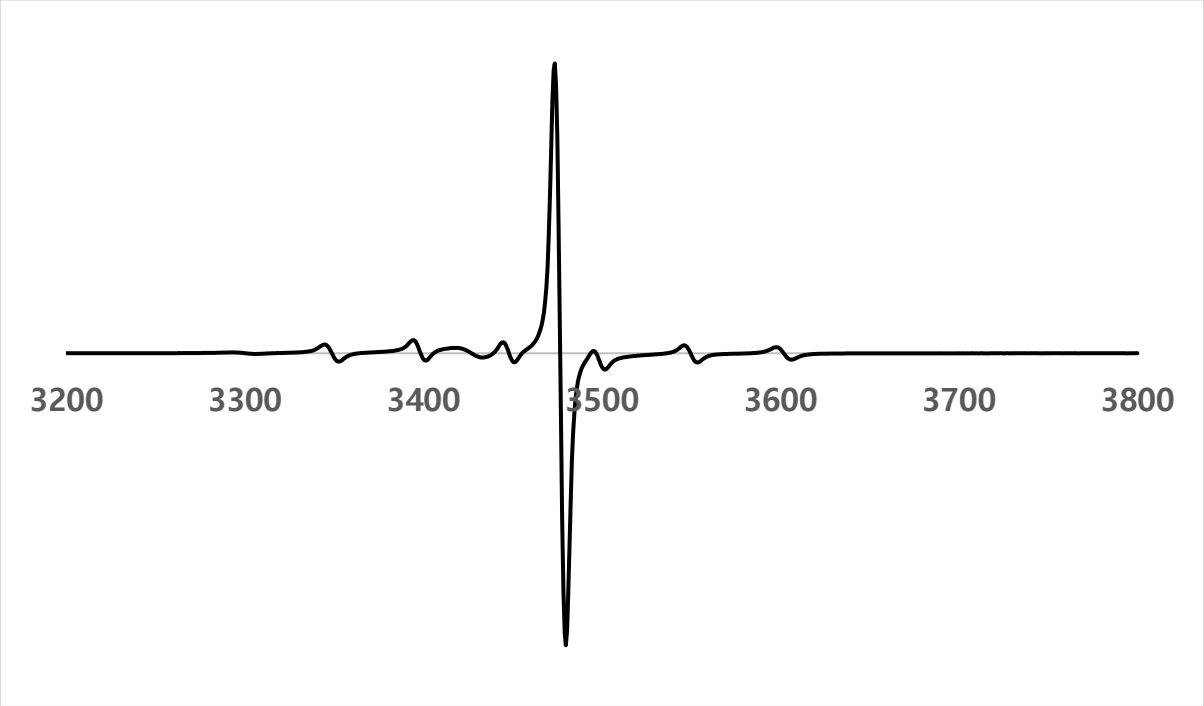


Figure S4. X-band of electron paramagnetic resonance of **B** in pentane.

NMR Data

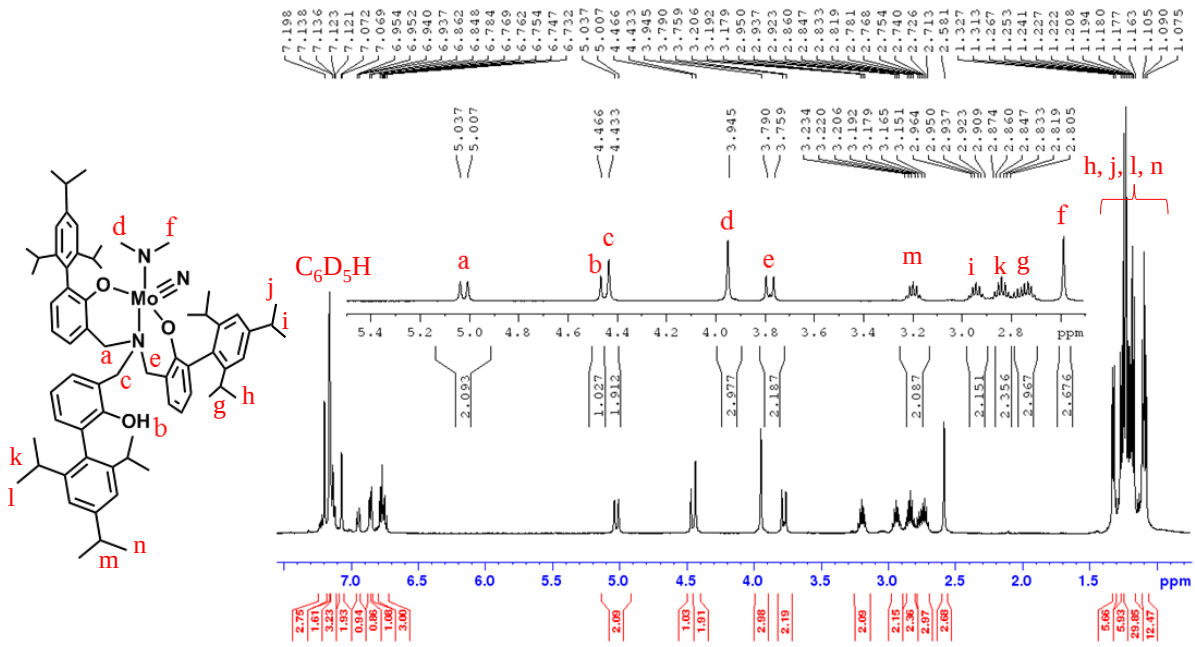


Figure S20. NMR Spectra of **A**. ^{1}H-NMR in C_6D_6.

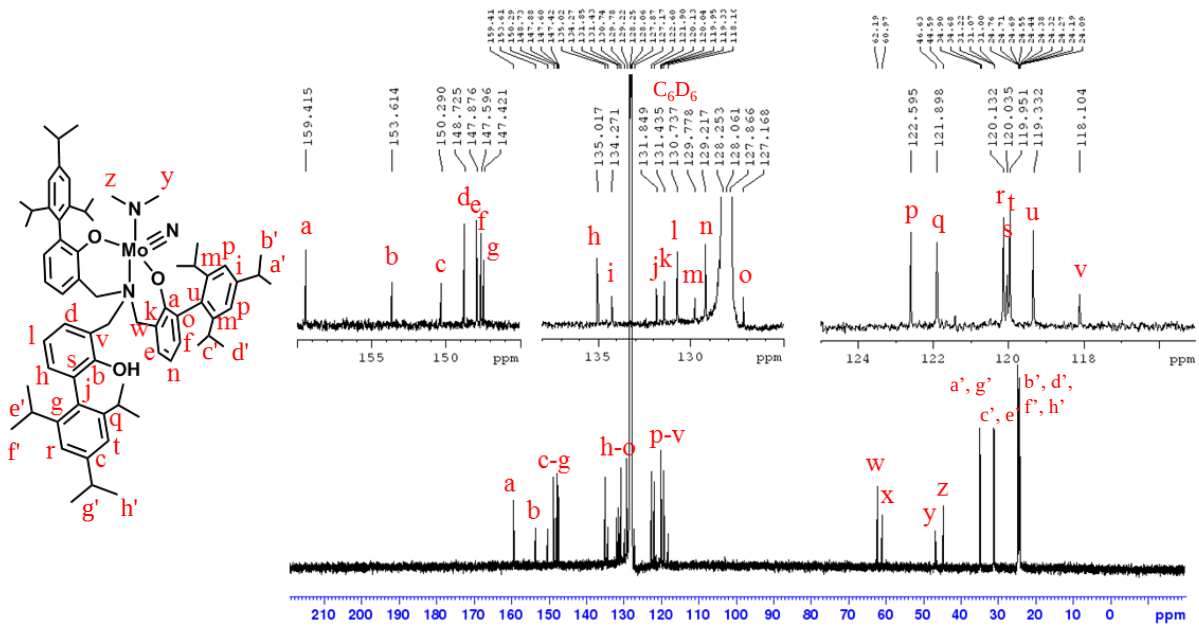


Figure S21. NMR Spectra of **A**. ^{13}C-NMR in C_6D_6.

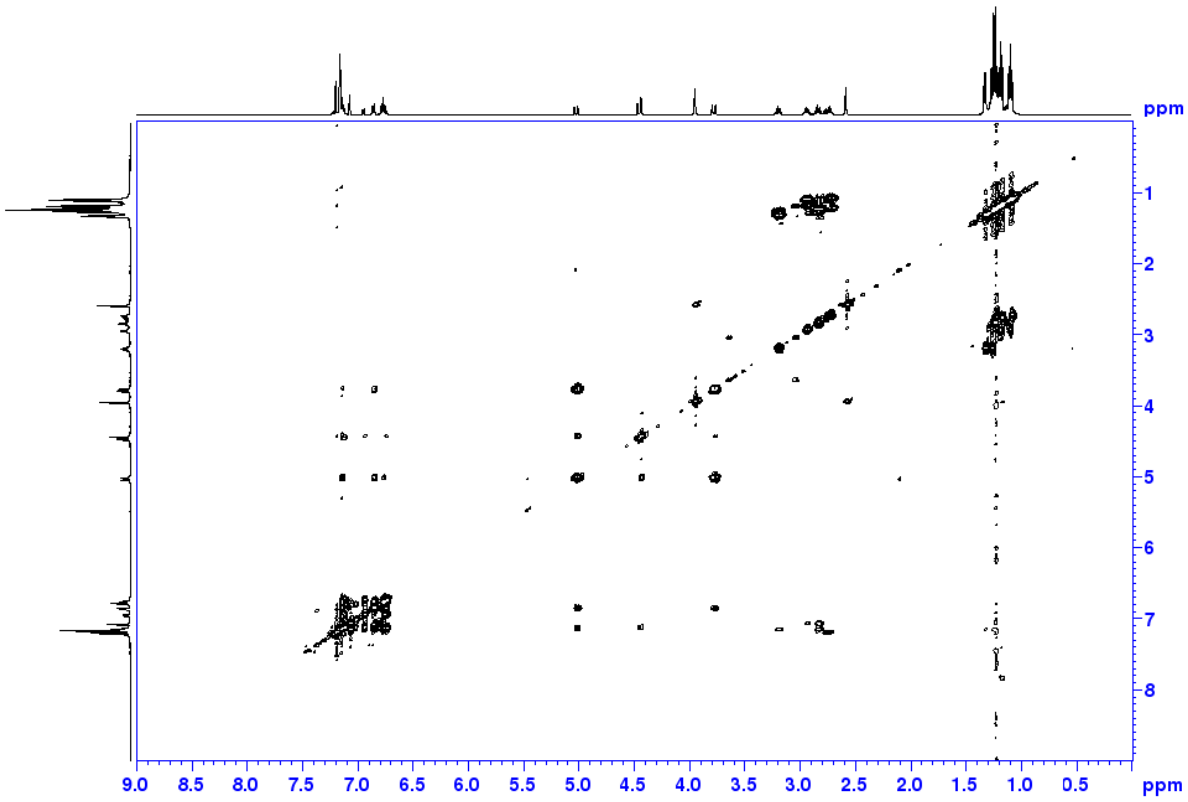


Figure S22. NMR Spectra of **A**. ^{1}H–^{1}H COSY NMR in C_6D_6.

References

1. D. Y. Bae, G. S. Park, N. Ko, K. S. Son and E. Lee, *Dalton Trans.*, 2019, **48**, 9617-9624.
2. M. J. A. Johnson, P. M. Lee, A. L. Odom, W. M. Davis and C. C. Cummins, *Angew. Chem., Int. Ed. Engl.*, 1997, **36**, 87-91.
3. A. M. Thomas, B.-L. Lin, E. C. Wasinger and T. D. P. Stack, *J. Am. Chem. Soc.*, 2013, **135**, 18912-18919.
4. F. Stoffelbach, D. Saurenz and R. Poli, *Eur. J. Inorg. Chem.*, 2001, **2001**, 2699-2703.
5. D. E. Bergbreiter and J. M. Killough, *J. Am. Chem. Soc.*, 1978, **100**, 2126-2134.
6. D. F. Evans, *J. Chem. Soc.*, 1959, DOI: 10.1039/JR9590002003, 2003-2005.
7. G. A. Bain and J. F. Berry, *J. Chem. Educ.*, 2008, **85**, 532.
8. M. J. Frisch *et al*., *Gaussian 09, Revision A.02*, Gaussian, Inc., Wallingford CT, 2009.
9. A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648-5652.
10. J. P. Perdew and Y. Wang, *Phys. Rev. B*, 1992, **45**, 13244-13249.
11. M. Dolg, U. Wedig, H. Stoll and H. Preuss, *J. Chem. Phys.*, 1987, **86**, 866-872.
12. A. W. Ehlers, M. Bohme, S. Dapprich, A. Gobbi, A. Hollwarth, V. Jonas, K. F. Kohler, R. Stegmann, A. Veldkamp and G. Frenking, *Chem. Phys. Lett.*, 1993, **208**, 111-114.
13. P. C. Hariharan and J. A. Pople, *Theor. Chim. Acta.*, 1973, **28**, 213-222.