Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information for

A Dinuclear Mo_2H_8 Complex Supported by Bulky $C_5H_2{}^tBu_3$ ligands

Yasuhiro Ohki,* Kodai Ishihara, Moeko Yaoi, Mizuki Tada, W. M. C. Sameera, and Roger E. Cramer

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General Procedures for Experiments

All reactions were carried out under an atmosphere of Ar or N_2 using either Schlenk line or glovebox techniques. Hexane, benzene, THF, and Et_2O were purified by passing over columns of activated alumina and a supported copper catalyst supplied by Hansen & Co. Ltd. Deuterated solvents were dried and vacuum-transferred prior to use. ^1H and ^{13}C NMR spectra were recorded on JEOL JNM ECS600, ECS500, or ECS400 spectrometers. Elemental analyses were carried out on powdered crystalline samples sealed in tin capsules, using an Elementar Analytical vario MICRO cube elemental analyzer. Cyclic voltammograms were measured in a single-compartment cell under an inert atmosphere at room temperature using a BAS ALS-660A electrochemical analyzer. The supporting electrolyte, 0.2 M tetrabutylammonium hexafluorophosphate ($[^nBu_4N][PF_6]$), was recrystallized from THF prior to use. All potentials are referenced to $Ag/AgNO_3$. IR spectra were recorded on an ATR-equipped Bruker Alpha FTIR spectrometer. Electro-spray ionization mass spectra (ESI-MS) were acquired on a Bruker micrOTOF-II spectrometer. Chemicals were purchased from common commercial sources and used without further purification. $C_5H_3{}^tBu_3$[1] and KC_8[2] were synthesized according to the reported procedures. For the synthesis of $(C_5H_2{}^tBu_3)MoCl_4$ in a large scale, we modified the original protocol reported by Poli et al.[3]

References for experiments

(1) E. V. Dehmlow, C. Bollman, *Z. Naturforsch. B* 1993, **48**, 457-460.

(2) D. E. Bergbreiter, J. M. Killough, *J. Am. Chem. Soc.* 1978, **100**, 2126−2134.

(3) M. Baya, J. Houghton, J. –C. Daran, R. Poli, L. Male, A. Albinati, M. Gutman, *Chem. Eur. J.* 2007, **13**, 5347-5359.

Large scale synthesis of $(C_5H_2{}^tBu_3)MoCl_4$. A hexane solution of ^nBuLi (1.54 M, 46.2 mL, 0.0711 mol) was added to a THF (240 mL) solution of $C_5H_3{}^tBu_3$ (16.7 g, 0.0710 mol) at 0 °C. The resultant mixture was stirred overnight at 60 °C, while butane was released through a bubbler to a fume hood. After addition of $Mo(CO)_6$ (18.7 g, 0.0710 mol) at room temperature, the mixture was refluxed for two days. The evolved CO in this process was released to a fume hood. The resulting brown mixture was cooled to room temperature and treated with an excess of MeI (18.8 mL, 0.302 mol), followed by stirring for 3 h. The volatile materials were removed under reduced pressure. The residue was extracted multiple times with hexane (*ca.* 750 mL in total) and filtered through Celite. Evaporation of hexane afforded a dark orange solid (22.0 g). We speculate that this solid contains $(C_5H_2{}^tBu_3)Mo(CO)_3Me$ (***i***)[3] as the major component. On the basis of this speculation, the dark orange solid corresponds to up to 0.0514 mol of ***i***. This solid was dissolved in CH_2Cl_2 (30 mL), and the solution was carefully added to 2 equiv. of PCl_5 (21.4 g, 0.103 mol) in a flask equipped with a reflux condenser and a bubbler. Ice-cooling of the flask is recommended to avoid abrupt CO evolution during addition of the CH_2Cl_2 solution. After refluxing overnight, the mixture was cooled to room temperature, giving a purple suspension. The product was collected by filtration of the suspension followed by washing multiple times with Et_2O (*ca.* 150 mL in total) until the color of filtrate became

light purple (13.9 g). The filtrate was concentrated and cooled to –30 °C to obtain a second crop (1.94 g). The total yield was 47% (15.8 g, 0.0336 mol). Single crystals for X-ray diffraction analysis were grown from a THF solution stored at –35 °C. See Figure S1 for the molecular structure.

$(C_5H_2{}^tBu_3)_2Mo_2H_8$ (1). In a glove box, $(C_5H_2{}^tBu_3)MoCl_4$ (1.00 g, 2.12 mmol) and KC_8 (1.15g, 8.51 mmol) were placed onto frozen THF (15 mL) in a 100 mL round-bottom flask (vacuum-transfer of THF onto a solid mixture of the Mo complex and KC_8 should also work). The flask was closed, taken out from the glove box, evacuated, and then filled with H_2 from a balloon (volume of the balloon: *ca.* 500 mL). The flask was gradually warmed to room temperature, and vigorous stirring was initiated when a part of THF melted. After stirring overnight at room temperature, the solvent was removed under vacuum. The residue was extracted with hexane (20 mL) and the extract was filtered. The resultant dark brown solution was concentrated and stored at –35 °C to grow crystals of **1**·$(hexane)_{0.5}$, which were vacuum-dried to give a dark brown powder of **1** (0.289 g, 0.433 mmol, 41%). ^{1}H NMR (C_6D_6, 600 MHz, r.t.): δ 4.96 (s, 4H, $C_5{}^tBu_3H_2$), 1.37 (s, 36H, $C_5{}^tBu_3H_2$), 1.29 (s, 18H, $C_5{}^tBu_3H_2$), -3.54 (s, 8H, Mo-H). ^{13}C{^{1}H} NMR (C_6D_6, 125 MHz, r.t.): δ 116.0, 115.9, 80.5 ($C_5{}^tBu_3H_2$), 34.7, 32.4, 32.1, 30.3 ($C_5{}^tBu_3H_2$). IR (ATR, cm^{-1}): ν = 2954, 2906, 2867, 1483, 1459, 1389, 1360, 1262, 1243, 1200, 1167, 1095, 1022. Cyclic Voltammogram (THF): a weak feature appeared at $E_{1/2}$ = –1.07 V (vs. Ag/$AgNO_3$). Anal. Calcd for $C_{34}H_{66}Mo_2$: C, 61.24; H, 9.98. Found: C, 60.84; H, 9.99.

$(C_5H_2{}^tBu_3)_2Mo_2H_2(C_6H_6)$ (2). A 30 mL flask was charged with **1** (50.2 mg, 0.0753 mmol) and

benzene (5 mL). The flask was closed and the solution was stirred overnight at 60 °C. The solvent was removed under vacuum, and the residue was extracted with hexane (1 mL), and the solution was stored at –35 °C to furnish black crystals of **2** (48.5 mg, 0.0656 mmol, 87%). ^{1}H NMR (C_6D_6, 600 MHz, r.t.): δ 3.88 (s, 4H, $C_5{}^{t}Bu_3H_2$), 3.82 (s, 6H, C_6H_6), 1.37 (s, 36H, $C_5{}^{t}Bu_3H_2$), 1.31 (s, 18H, $C_5{}^{t}Bu_3H_2$), -7.56 (s, 2H, Mo-H). ^{13}C{^{1}H} NMR (C_6D_6, 125 MHz, r.t.): δ 115.4, 114.6, 83.2 ($C_5{}^{t}Bu_3H_2$), 48.9 (C_6H_6), 34.5, 33.3, 32.6, 30.7 ($C_5{}^{t}Bu_3H_2$). ESI-MS (THF): *m/z* = 737.86 ([**2**]$^{+}$). IR (ATR, cm^{-1}): ν = 3120, 3104, 2954, 2905, 2867, 1483, 1458, 1389, 1358, 1269, 1243, 1199, 1164, 1090, 1023. Cyclic Voltammogram (THF): $E_{1/2}$ = –1.09 V, +0.23 V (vs. Ag/$AgNO_3$). Anal. Calcd for $C_{40}H_{66}Mo_2$: C, 65.02; H, 9.00. Found: C, 64.26-64.33; H, 9.06-9.36. We have been unable to obtain satisfactory elemental analysis values for this compound. Even though we attempted more than 10 times with crystals of diffraction quality or a ground powder, the samples always afforded low carbon values, which may be due to a partial loss of C_6H_6 ligand. This speculation is in accordance with the observed lower C value and higher H value, as a tentative [**2**-C_6H_6] species gives C 61.80% and H 9.15%. Nevertheless, we cannot exclude other possibilities such as incomplete combustion or contamination, while the addition of a combustion accelerator (WO_3 powder) did not improve the results. Regardless, various measurements indicated its sufficient purity, and the chemical formula of **2** was supported by the ESI-MS spectrum (Figure S13).

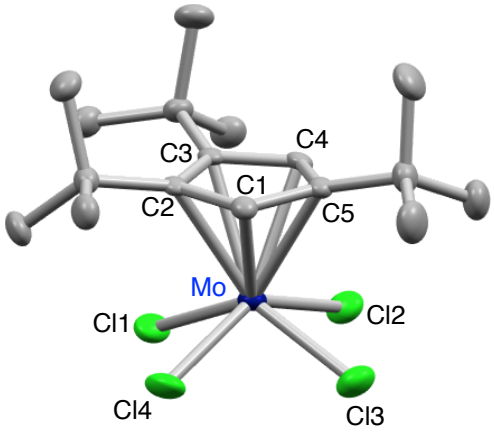

Figure S1. Molecular structure of $(C_5H_2{}^tBu_3)MoCl_4$ with thermal ellipsoids set at the 50% probability level. Only selected atoms are labeled, and hydrogen atoms except hydrides are omitted for clarity. Selected distances (Å): Mo-Cl1, 2.3333(9); Mo-Cl2, 2.3517(7); Mo-Cl3, 2.3430(7); Mo-Cl4, 2.3727(8); Mo-C1, 2.301(2); Mo-C2, 2.388(2); Mo-C3, 2.412(2); Mo-C4, 2.348(3); Mo-C5, 2.396(3).

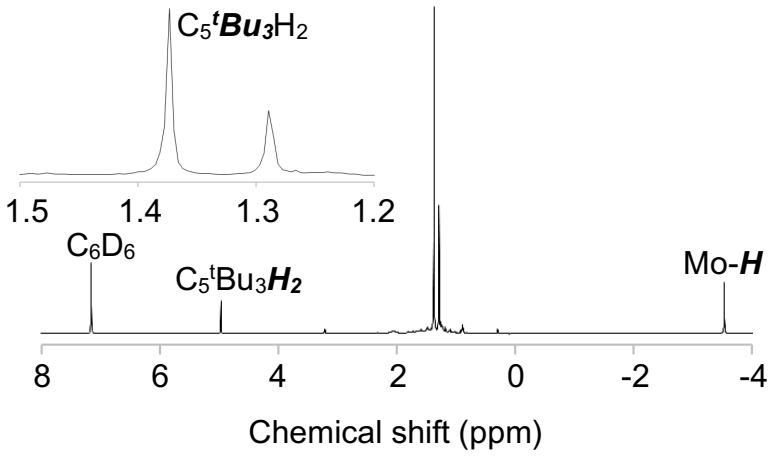

Figure S2. ^1H NMR spectrum of **1** in C_6D_6 at room temperature.

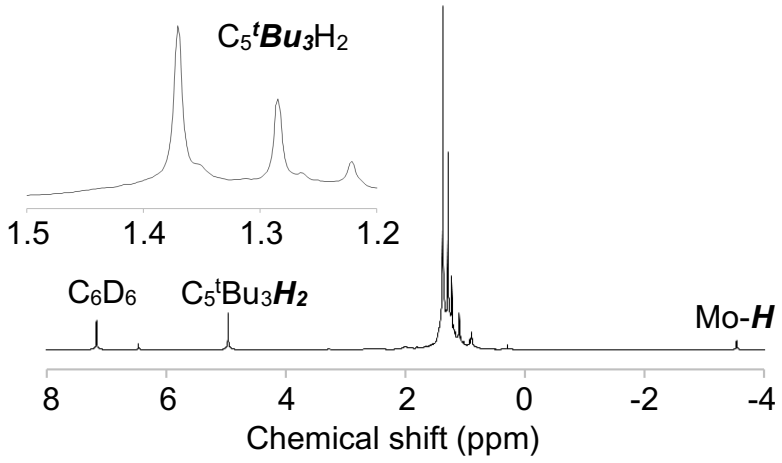

Figure S3. ^{1}H NMR spectrum of **1**-d_8 (obtained by using $(C_5H_2{}^tBu_3)MoCl_4$, KC_8, and D_2) in C_6D_6 at room temperature. Complete disappearance of the hydride signal was not achieved.

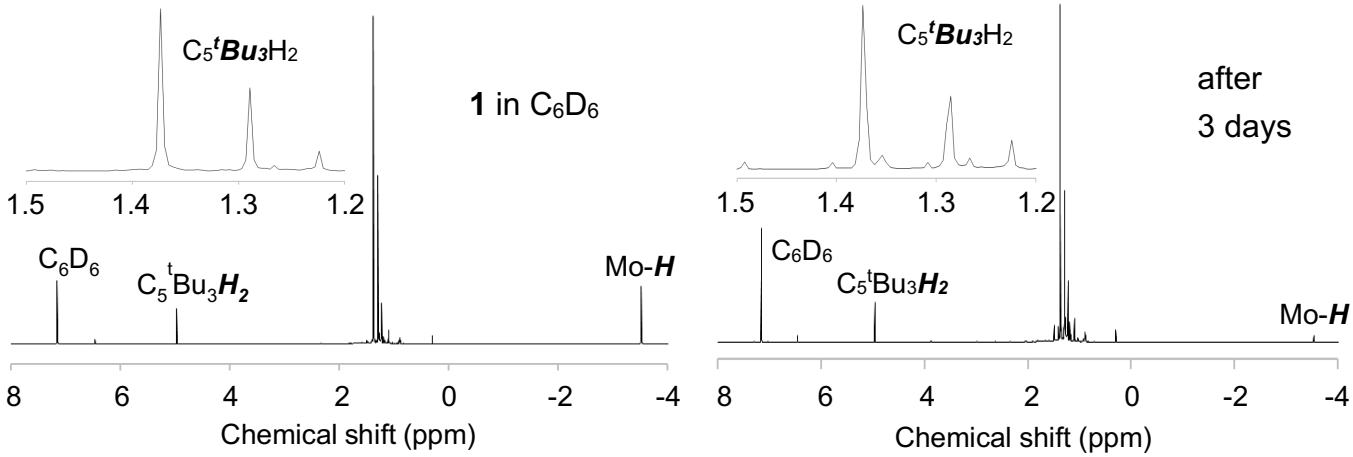

Figure S4. ^{1}H NMR of a C_6D_6 solution of **1** (left) and after three days (right) at room temperature, causing the H/D exchange between hydrides in **1** and C_6D_6. Partial degradation of **1** also underwent to give some minor signals after three days.

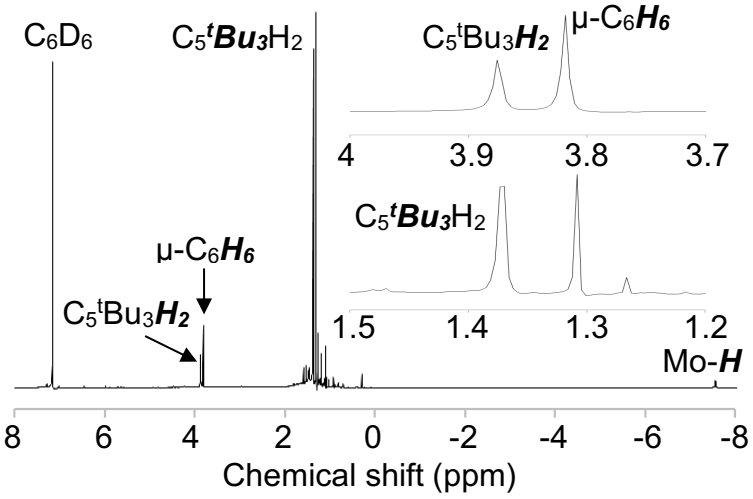

Figure S5. ^{1}H NMR spectrum of **2** in C_6D_6 at room temperature.

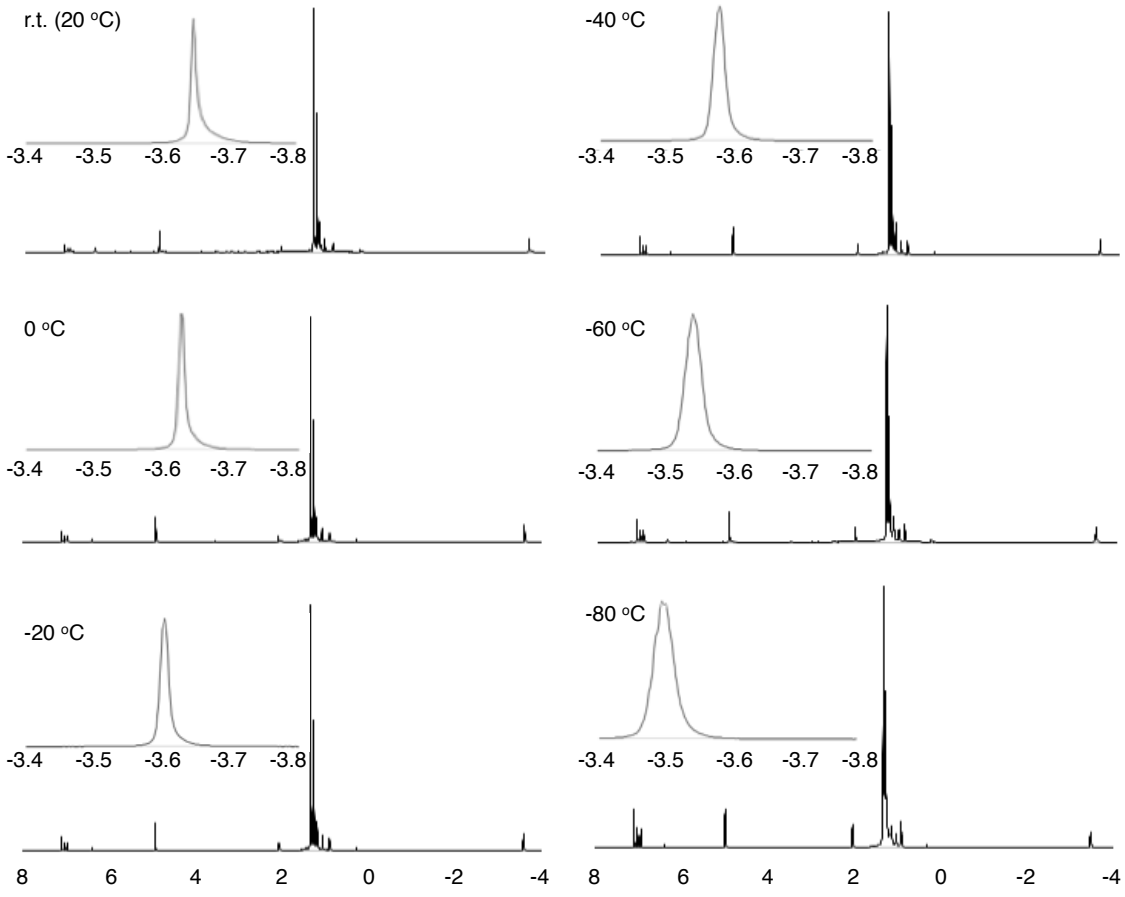

Figure S6. Variable-temperature ^{1}H NMR spectra of **1** in toluene-d_8. The hydride signal became broad upon lowering the measurement temperatures but remained a single signal even at -80 °C.

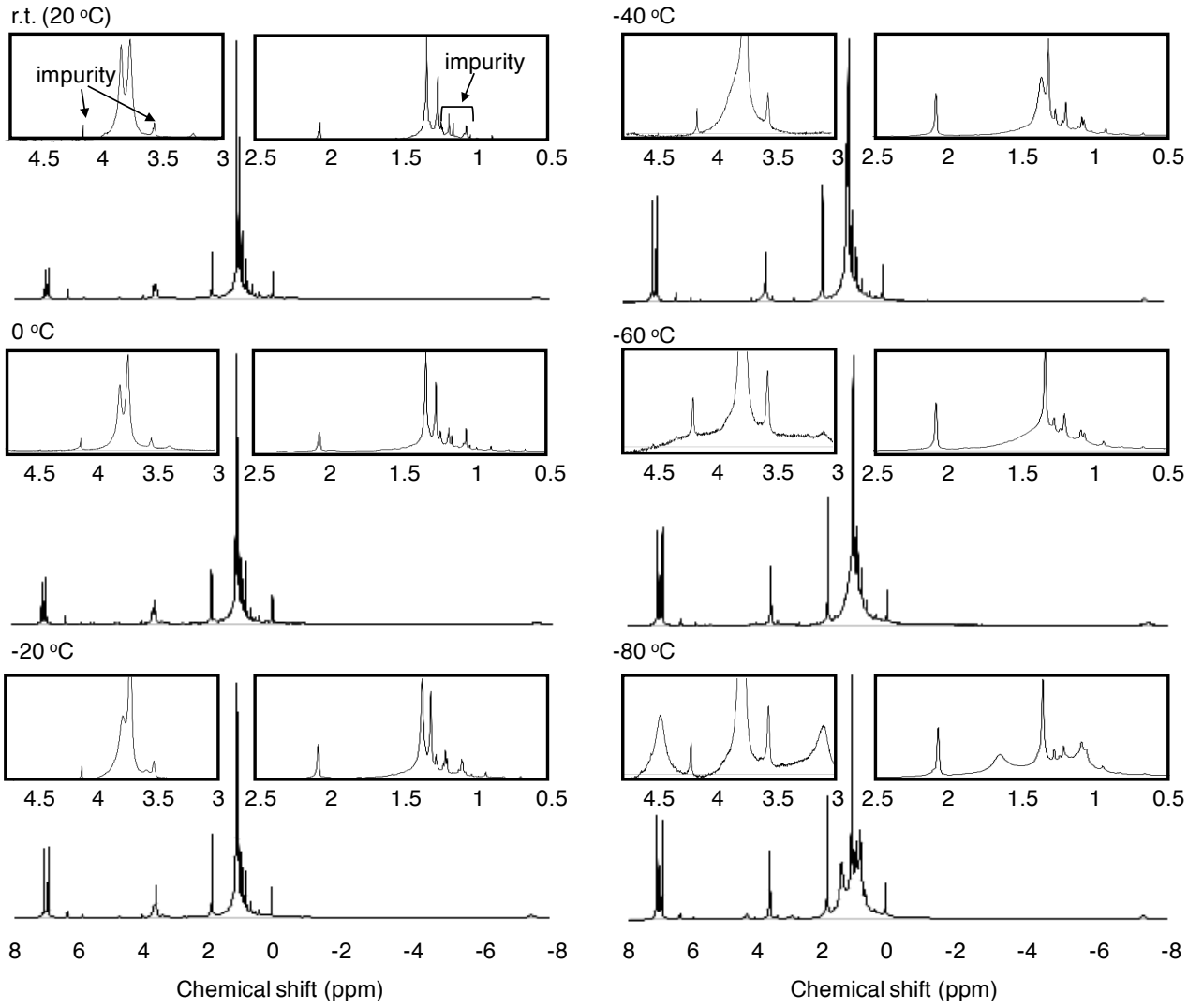

Figure S7. Variable-temperature ^{1}H NMR spectra of **2** in toluene-d_8. At –80 °C, the benzene ligand exhibited two broad signals in a 4:2 intensity ratio at 4.5 and 3.1 ppm (left inset in each chart). Upon lowering the measurement temperature, one of the $C_5H_2{}^{t}\underline{Bu}_3$ signals also broadened and split into two (right inset in each chart), indicating hindered rotation of $C_5H_2{}^{t}Bu_3$ ligands in **2**.

Detection of H_2 evolved in the reaction of 1 with benzene.

All the following procedures were carried out using the same setup. The GC condition is summarized in Table S1, and the calibration curve is shown in Figure S8. For the preparation of the calibration curve, a Schlenk tube was charged with a stirring bar and benzene (3 mL) under an Ar atmosphere, before closing with a rubber septum. H_2 (0.5, 1.0, 1.5, 2.0, 2.5 mL) was injected with a gas-tight syringe, and the benzene solution was left stirring for 30 min. 0.5 mL of the gas phase was taken with a gas-tight syringe and subjected to GC analysis. Retention times were 2.14 min for H_2 and 6.92 min for Ar.

Table S1. Conditions for the GC analysis.

Instrument	Shimadzu GC-8A
Column	Molecular Sieve 13X-S 60/80 SUS 4m x 4.0mm I.D.
Col. Temp.	40 ºC
Carrier Gas	N_2, 60 mL/min
Detector	TCD, 100 mA
Sample Volume	0.5 mL

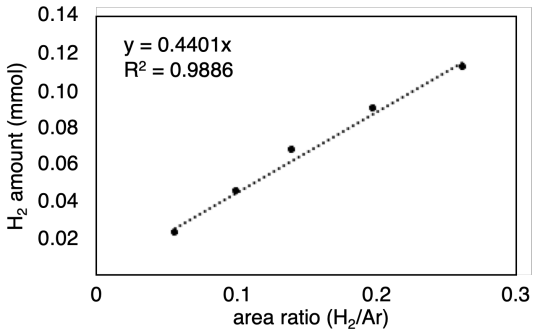

Figure S8 Calibration curve for H_2 quantification.

For the H_2 detection experiment, the same Schlenk tube used for the preparation of the calibration curve was charged with benzene (3 mL) and **1** (7.8 mg, 0.0117 mmol) under an Ar atmosphere. The solution was stirred overnight at 60 °C, before 0.5 mL of the gas phase was taken with a gas-tight syringe and subjected to GC analysis. The yield of H_2 per **1** was 1.75 equiv, which is lower than the ideal amount of 3 equiv (according to **1** + C_6H_6 → **2** + $3H_2$). The low yield is probably be due to gradual loss of H_2 through a septum during overnight stirring, while we cannot exclude the possibility of benzene hydrogenation.

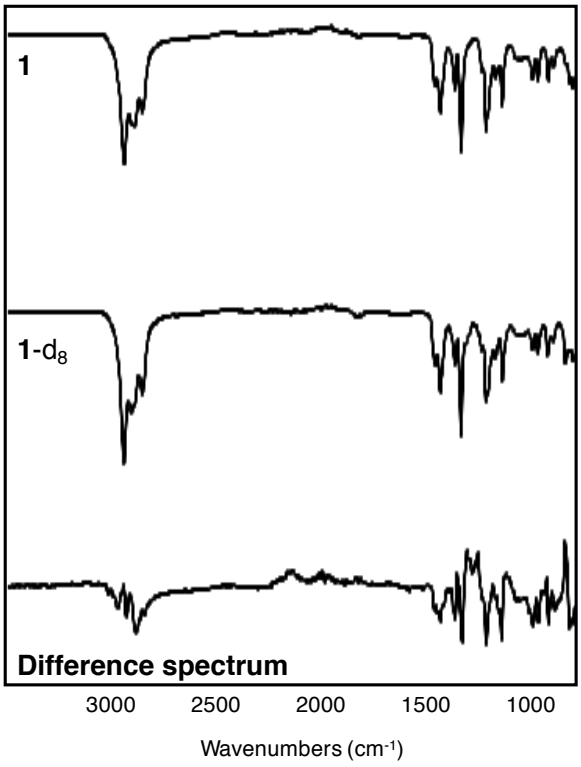

Figure S9. IR spectra of solid state samples of **1** and deuterated derivative **1** (obtained by using $(C_5H_2{}^tBu_3)MoCl_4$, KC_8, and D_2, see Figure S3), alongside the corresponding difference spectrum. Unfortunately, we have been unable to assign Mo-H/Mo-D bands from the difference spectrum.

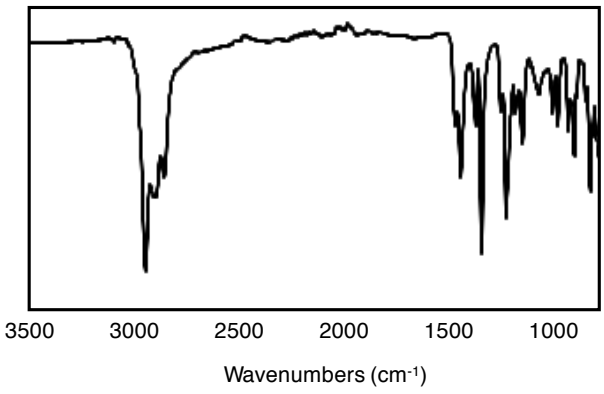

Figure S10. IR spectrum of complex **2** in the solid state.

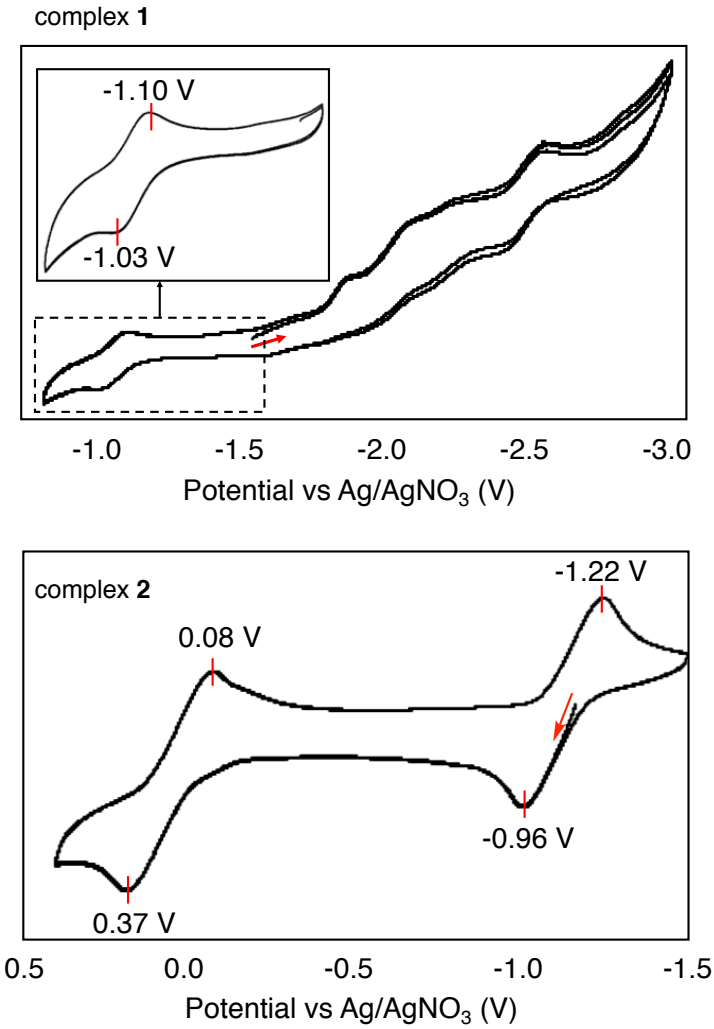

Figure S11. Cyclic voltammograms of **1** (top, 5.0 mM in THF) and **2** (bottom, 2.0 mM in THF). Supporting electrolyte: 0.1 M [^{n}Bu$_4$N][PF$_6$]; working electrode: glassy carbon; scan rate: 20 mV/s (**1**) or 100 mV/s (**2**). For the measurement of **1**, we first applied the same condition as for **2**, but the voltammogram was nearly featureless. Therefore, a higher concentration (5.0 mM) and slower scan rate (20 mV/s) were applied to find electrochemical features. Various weak features appeared by scanning toward negative region, and we have been unable to assign these features. Partial degradation of **1** is possible. What we can conclude from the voltammogram of **1** is its difficulty in electronic oxidation/reduction, that was supported by the appearance of only degraded species in the ESI-MS spectrum (Figure S12).

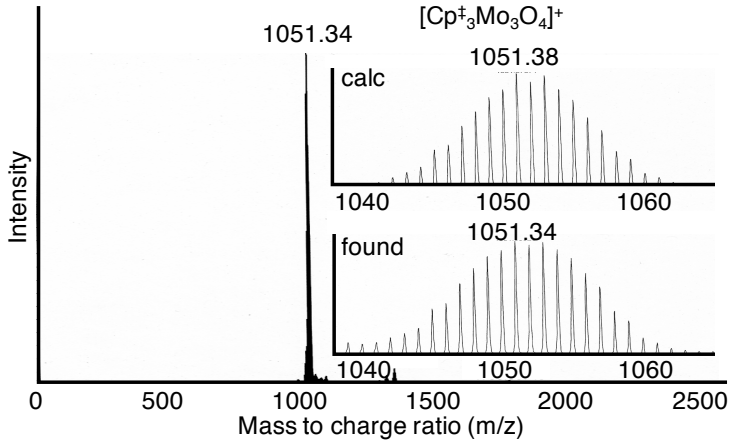

Figure S12. ESI-MS spectrum (positive mode) of **1** in THF. The most intense signal is assignable as the cationic trinuclear molybdenum-oxide without hydride, $[(C_5H_2{}^tBu_3)_3Mo_3O_4]^+$. As a short-time air-exposure is inevitable for the ESI-MS measurement of this air-sensitive compound **1**, partial air-decomposition of **1** probably generated the cationic species $[(C_5H_2{}^tBu_3)_3Mo_3O_4]^+$, which was readily detected in the mass spectrometer. Detection of the signal of **1** requires 1e-oxidation (or 1e-reduction) in the spectrometer, but 1e-oxidation of **1** is difficult as observed by the cyclic voltammogram (Figure S11 top), where *ca.* 0.5 V difference is found between the rest potential (–1.54 V) and a weak oxidation process at $E_{1/2} = -1.07$ V. The formal oxidation state of **1** is high and Mo(V)-Mo(V), which would also explain why 1e-oxidation of **1** in the spectrometer is difficult. It should be also noted that the signal for **1** was not detected either in the negative ESI-MS mode, indicating that 1e-reduction of **1** in the spectrometer is also difficult.

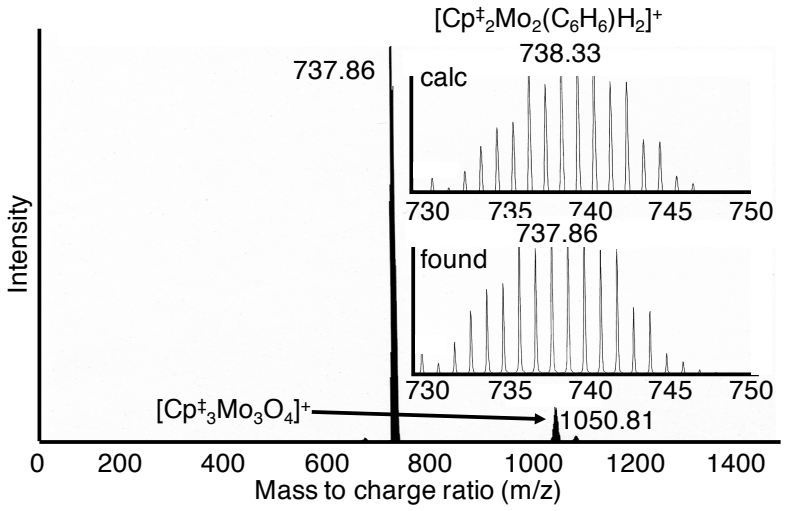

Figure S13. ESI-MS spectrum (positive mode) of **2** in THF. The most intense signal is assignable as the 1e-oxidized form $[\mathbf{2}]^+$. Facile 1e-oxidation of **2** is supported by the cyclic voltammogram (Figure S11 bottom). Appearance of a relatively weak signal of $[(C_5H_2{}^tBu_3)_3Mo_3O_4]^+$ indicates partial air-decomposition of **2** in the spectrometer.

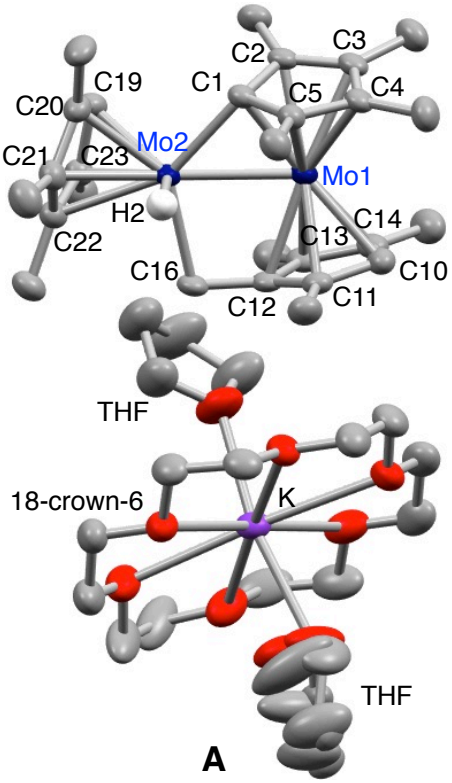

Figure S14. Structure of **A** with thermal ellipsoids set at the 50% probability level. Only selected atoms are labeled, and hydrogen atoms except the hydride are omitted for clarity. There is no hydrogen on C1, as far as the crystallographic analysis is concerned. We tried to locate a hydrogen atom on C1, but the possible hydrogen atom did not refine to any chemically reasonable position and the R value increased. There may be more hydrides in this molecule, but we have been unable to reasonably locate more hydrides around molybdenum atoms. Selected distances (Å): Mo1-Mo2, 2.6719(6); Mo1-C1, 2.149(5); Mo1-C2, 2.289(5); Mo1-C3, 2.353(4); Mo1-C4, 2.317(4); Mo1-C5, 2.240(4); Mo1-C10, 2.274(5); Mo1-C11, 2.242(5); Mo1-C12, 2.265(4); Mo1-C13, 2.322(5); Mo1-C14, 2.330(5); Mo2-C1, 2.207(4); Mo2-C16, 2.277(5); Mo2-C19, 2.184(5), Mo2-C20, 2.255(5); Mo2-C21, 2.393(4); Mo2-C22, 2.382(4); Mo2-C23, 2.229(4).

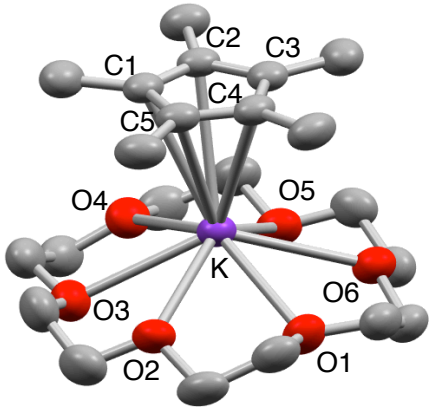

Figure S15. Structure of Cp*K(18-crown-6) with thermal ellipsoids set at the 50% probability level. Only selected atoms are labeled, and the crystal solvent (THF) and hydrogen atoms are omitted for clarity. Selected distances (Å):K-O1, 3.0058(15); K-O2, 2.8472(14); K-O3, 2.9563(15); K-O4, 2.9636(16); K-O5, 2.9415(15); K-O6, 3.0356(16); K-C1, 3.0812(19); K-C2, 3.1034(19); K-C3, 3.0844(19); K-C4, 3.0574(19); K-C5, 3.0576(19).

X-ray Crystal Structure Determination

The crystallographic data and refinement parameters for **1**, **2**, $(C_5H_2{}^tBu_3)MoCl_4$, Cp*K(18-crown-6), and **A** are summarized in Table S2. Single crystals were coated with oil (immersion Oil, type B: Code 1248, Cargille laboratories, Inc.) and mounted on loops. Diffraction data were collected at –100 ºC under a cold nitrogen stream on a Rigaku RA-Micro7 equipped with a PILATUS 200K detector, using graphite-monochromated MoKα radiation (λ = 0.710690 Å). Eighteen preliminary data frames were measured at 0.5° increments of ω in order to assess the crystal quality and preliminary unit cell parameters. The intensity images were also measured at 0.5° intervals of ω. The frame data were integrated using the CrystalClear program package, and the data sets were corrected for absorption using a REQAB program. The calculations were performed with the CrystalStructure program package. All structures were solved by direct methods, and refined by full-matrix least squares. Anisotropic refinement was applied to all non-hydrogen atoms, while the position of hydrogen atoms except hydrides was calculated. Isotropic refinement was applied to hydrides. The atomic coordinates for **1**, **2**, $(C_5H_2{}^tBu_3)MoCl_4$, Cp*K(18-crown-6), and **A** have been deposited with the Cambridge Crystallographic Data Centre under reference nos. 1990372-1990376.

Table S2. Crystallographic data for complexes **1**, **2**, $(C_5H_2{}^tBu_3)MoCl_4$, Cp*K(18-crown-6), and **A**

	1·(hexane)$_{0.5}$	**2**	$(C_5H_2{}^tBu_3)MoCl_4$
Formula	$C_{37}H_{73}Mo_2$	$C_{40}H_{64}Mo_2$	$C_{17}H_{29}Cl_4Mo$
Fw (g mol^{-1})	709.86	736.79	471.17
Crystal system	triclinic	monoclinic	monoclinic
Space group	*P-1* (#2)	*Cc* (#9)	*P2$_1$/c* (#14)
a (Å)	9.4411(6)	21.340(4)	8.443(2)
b (Å)	9.8160(7)	19.875(3)	26.099(6)
c (Å)	22.4360(14)	19.984(3)	9.924(3)
α(deg)	97.004(2)	90	90
β(deg)	91.791(2)	119.218(3)	113.425(5)
γ(deg)	113.348(3)	90	90
V (Å^3)	1887.5(2)	7398(2)	2006.6(9)
Z	2	8	4
D_{calc} (g cm^{-3})	1.249	1.323	1.560
μ (Mo Kα) (cm^{-1})	0.685	0.703	1.179
$2\theta_{max}$ (deg)	55.0	55.0	55.0
No. of measured reflections	Total: 62357	Total: 124897	Total: 64672
No. of Observation	8570	17091	4572
No. of Variables	400	794	199
*R*1[a]	0.0184	0.0504	0.0267
*wR*2[b]	0.0527	0.1321	0.0569
GOF[c]	1.064	1.040	1.010

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$ ($I > 2\sigma(I)$). [b] $wR_2 = [(\Sigma(w(|F_o|-|F_c|)^2/\Sigma wF_o^2))^{1/2}$ (all reflections).

[c] GOF = $[\Sigma w(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$ (where N_o = number of observations, N_v = number of variables).

Table S2. Crystallographic data (continued)

	Cp*K(18-crown-6) ·1/2(THF)	**A**
Formula	$C_{24}H_{43}KO_{6.5}$	$C_{35}H_{50}FeMoP_2$
Fw (g mol^{-1})	474.68	684.51
Crystal system	monoclinic	Triclinic
Space group	$P2_1/n$ (#14)	P-1 (#2)
a (Å)	9.704(2)	10.038(2)
b (Å)	15.687(3)	13.927(3)
c (Å)	17.654(5)	18.546(4)
α(deg)	90	99.992(4)
β(deg)	97.336(5)	105.254(4)
γ(deg)	90	94.410(4)
V (Å^3)	2665.4(11)	2442.9(9)
Z	4	2
D_{calc} (g cm^{-3})	1.183	1.362
μ (Mo Kα) (cm^{-1})	0.235	0.647
$2\theta_{max}$ (deg)	55.0	55.0
No. of measured reflections	Total: 86209	Total: 77076
No. of Observation	6201	11268
No. of Variables	278	581
$R1$[a]	0.0448	0.0572
$wR2$[b]	0.1269	0.1620
GOF[c]	0.883	1.089

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$ ($I > 2\sigma(I)$). [b] $wR_2 = [(\Sigma(w(|F_o|-|F_c|)^2/\Sigma wF_o^2))^{1/2}$ (all reflections).

[c] GOF = $[\Sigma w(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$ (where N_o = number of observations, N_v = number of variables).

Computational Studies

Structure optimizations were performed using density functional theory as implemented in the ADF program (version 2019.103).[1] The revPBE functional,[2] including the Grimme D3 corrections and the Becke–Johnson damping,[3] was employed. The TZP[4] basis sets were applied for all electrons in the system, and the relativistic Scalar ZORA[5] approach was used Mo. The COSMO[6] implicit solvation model was used with the benzene solvent. The numerical quality was set to "normal". Vibrational frequency calculations, at 298.15 K and 1 atm, were performed to confirm the local minima (*i.e.* no imaginary frequency). The Mayer bond order[7] analysis and QTAIM[8] analysis were performed using the methods mentioned above.

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[8] R. Bader, *Chem. Rev.* 1991, **91**, 893-928.

Table S3. Selected bond distances (Å) of the X-ray structure and computed structures of **1**, computed relative energies, $<S^2>$ values, and spin densities.

	X-ray	Optimized structures	
		***S* = 0**	***S* =1**
Mo1-Mo2	2.55911(19)	2.54	2.86
Mo1-H1	1.57(2)	1.69	1.71
Mo1-H2	1.59(2)	1.68	1.69
Mo1-H5	1.766(19)	1.84	1.91
Mo1-H6	1.76(2)	1.88	1.90
Mo1-H7	1.664(16)	1.74	1.91
Mo1-H8	2.25(2)	2.24	1.94
Mo2-H3	1.611(18)	1.67	1.70
Mo2-H4	1.58(2)	1.68	1.68
Mo2-H5	1.78(2)	1.87	1.81
Mo2-H6	1.860(16)	1.84	1.83
Mo2-H7	2.02(2)	2.17	1.81
Mo2-H8	1.59(2)	1.73	1.77
Relative potential energy (kcal/mol)	-	0.0	24.3
$<S^2>$	-	-	2.01
Spin densities			
ρ(Mo1)	-	-	0.32
ρ(Mo2)	-	-	2.00

Table S4. A quantum theory of atoms in molecules (QTAIM) analysis of the Mo-Mo bond of **1** and **2**.

Bond	$\boldsymbol{\rho(r)}$	$\boldsymbol{\varepsilon(r)}$	$\boldsymbol{\nabla^2\rho(r)}$	$\boldsymbol{G_b}$	$\boldsymbol{V_b}$	$\boldsymbol{H_b}$	$\boldsymbol{\lvert V_b\rvert / G_b}$
1, Mo-Mo bond	0.0816	0.0904	0.0901	0.0591	-0.0956	-0.0365	1.6175
2, Mo-Mo bond	0.0790	0.0630	0.1191	0.0616	-0.0934	-0.0318	1.5162

$\rho(r)$: Electron density of the bond critical point (BCP).

$\varepsilon(r)$: Elepticity of the BCP.

$\nabla^2\rho(r)$: Laplacian of the BCP.

G_b : Kinetic energy.

V_b : Local Potential energy.

H_b : Total energy density.

In both complexes,

- (3, -1) BCP between the two Mo atoms was found.
- computed $\nabla^2\rho(r)$ of the BCP is positive, indicating closed-shell or ionic interactions.
- H_b is negative, but nearly zero, suggesting ionic interactions.
- $1 < \lvert V_b\rvert / G_b < 2$, indicating fairly ionic with modest covalent bonding combination.

Table S5. Selected bond distances (Å) of the X-ray structure and computed structures of **2** and **2'**, computed relative energies, $<S^2>$ values, and spin densities. Compound **2'** is a computed analogue of **2** without bridging hydrides. The computed Mo-Mo distance of **2'** became 2.38 Å, which is significantly shorter than that in the X-ray structure of **2**. Therefore, two bridging hydrides are important, and they must be present in **2**.

	X-ray	**Optimized structures of 2**		**Optimized structures of 2'**	
		***S* = 0**	***S* = 1**	***S* = 0**	***S* = 1**
Mo1-Mo2	2.5906(13)	2.57	2.71	2.38	2.53
Mo1-C3	2.534(12)	2.51	2.57	2.16	2.16
Mo1-C4	2.197(13)	2.22	2.23	2.16	2.16
Mo1-C5	2.194(13)	2.25	2.25	2.51	2.52
Mo2-C1	2.191(12)	2.22	2.23	2.16	2.16
Mo1-C2	2.212(12)	2.23	2.25	2.53	2.52
Mo2-C6	2.579(14)	2.52	2.58	2.16	2.16
C1-C2	1.43(2)	1.44	1.43	1.45	1.46
C1-C6	1.38(2)	1.43	1.43	1.45	1.45
C2-C3	1.434(19)	1.46	1.45	1.45	1.46
C3-C4	1.37(2)	1.43	1.43	1.45	1.45
C4-C5	1.45(2)	1.44	1.43	1.45	1.46
C5-C6	1.43(2)	1.46	1.45	1.45	1.46
Mo1-H	-	1.82, 1.86	1.84, 1.86	-	-
Mo2-H	-	1.86, 1.82	1.86, 1.84	-	-
Relative potential energy (kcal/mol)	-	0.0	15.0	0.0	8.9
$<S^2>$	-	-	2.02	-	2.01
Spin densities					
ρ(Mo1)	-	-	1.09	-	1.07
ρ(Mo2)	-	-	1.18	-	1.08

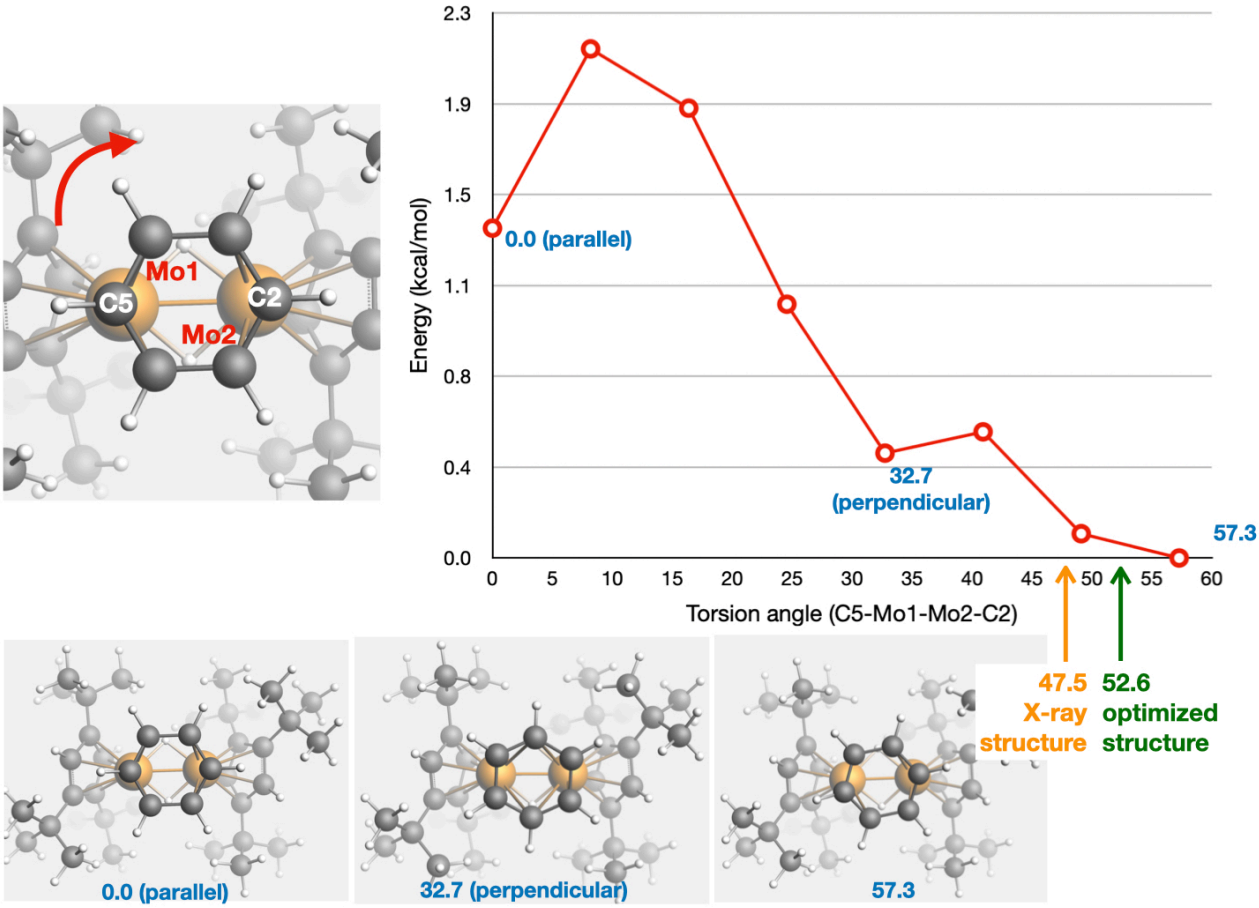

Figure S16. Relaxed potential energy surface for the rotation of the C_6H_6 ligand of **2**. For this purpose, we have selected the C5-Mo1-Mo2-C2 torsion angle as the reaction coordinate. The lowest energy structure, in which the C_6H_6 ligand is close to the μ-η^2:η^2-coordination mode, was found at the torsion angle of 57.3°. This is consistent with the torsion angle of the ground state optimized structure (52.6°) or the X-ray structure (47.5°).

At 32.7°, an isomeric μ-η^2:η^2-coordination mode of C_6H_6 (denoted as "perpendicular") is present, which is only 0.5 kcal/mol higher in energy. Approximate barrier for converting the lowest energy structure to the "perpendicular" mode is only 0.6 kcal/mol, and the reverse process is almost barrierless. Therefore, the interconversion of **2** and its isomeric "perpendicular" form should be possible even at low temperautres. Starting from the μ-η^2:η^2-coordination mode at 32.7°, structure optimization without constraints gave a local minimum. In this optimized structure, the torsion angle

is 35.4°, and the compound is only 0.5 kcal/mol above the fully optimized ground state of **2**.

At 0.0°, the μ-η^3:η^3-coordination mode (denoted as "parallel") of C_6H_6 is present. Approximate barrier for going from the lowest energy structure to the μ-η^3:η^3-coordination (parallel) mode of C_6H_6 is about 2.1 kcal/mol. This barrier may be difficult to achieve at low-temperatures. Starting from the μ-η^3:η^3-coordination (parallel) mode of C_6H_6 at 0.0°, we have optimized the structure without any constraint. Despite a number of attempts, we were unable to locate a local minimum for the μ-η^3:η^3-coordination mode. All attempts ultimately converged to the μ-η^2:η^2-coordination mode. Therefore, we concluded that the μ-η^3:η^3-coordination (parallel) mode is not a local minimum.

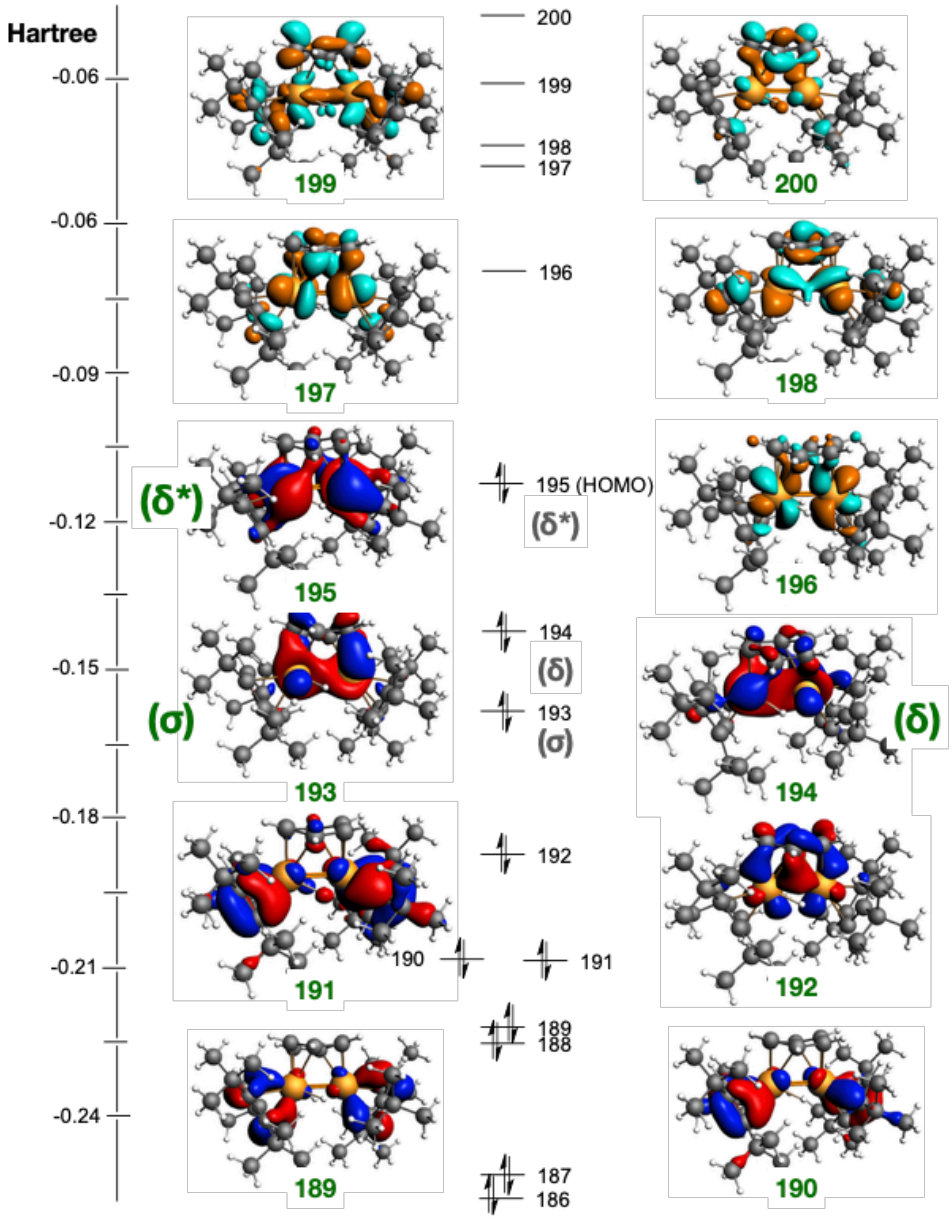

Figure S17. Kohn-Sham frontier molecular orbitals of the optimized ground state structure of **2**. The HOMO (195) and HOMO-1 (194) orbitals show δ^* and δ characters, respectively. The HOMO-2 (193) orbital shows σ character. The HOMO-3 (192) represents the Mo-H-Mo bonding orbital. Therefore, the $\sigma^2\delta^2\delta^{*2}$ configuration of **2** suggests a Mo-Mo single bond.

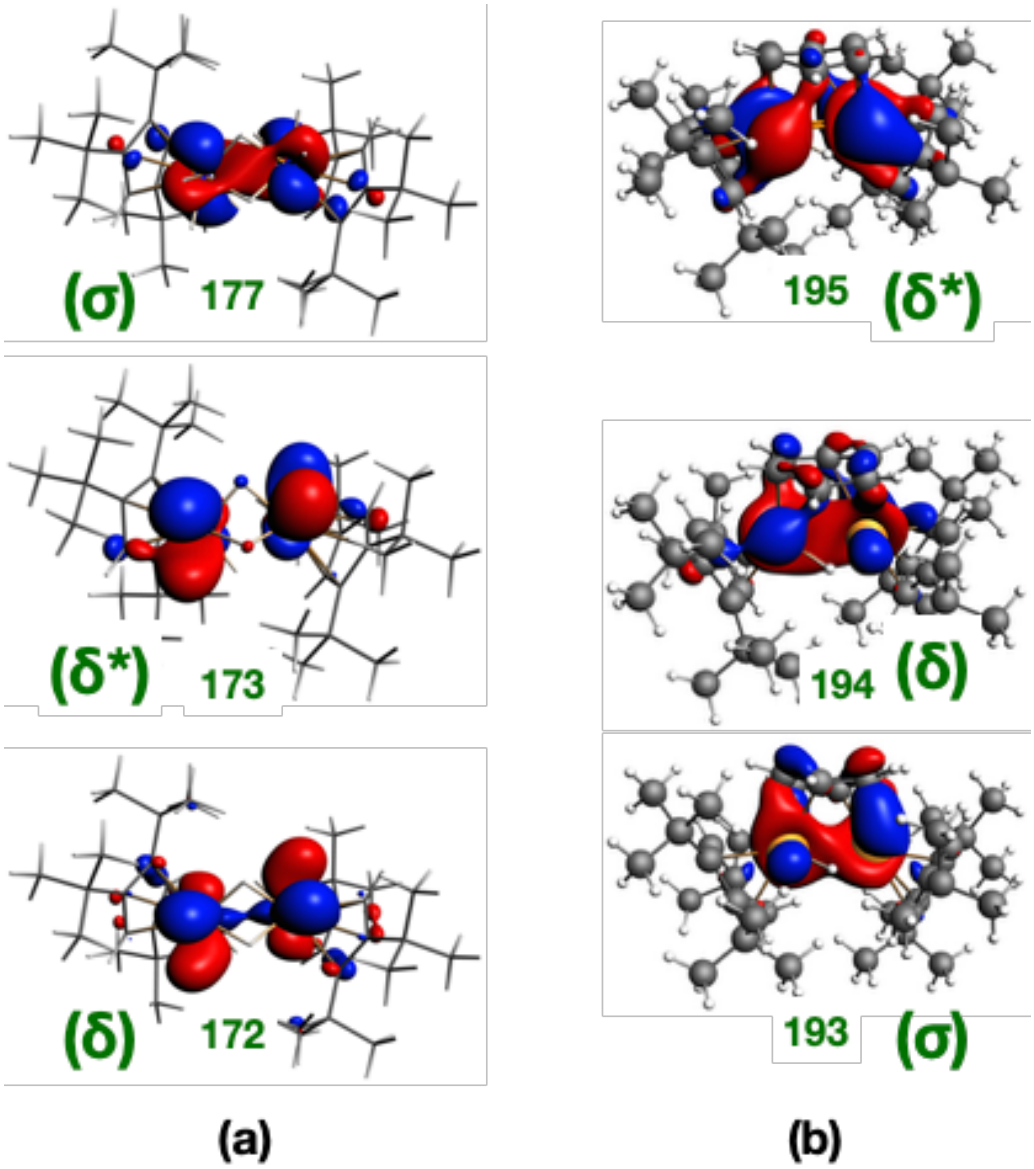

Figure S18. Expanded molecular orbital drawings highlighting Mo-Mo interactions. (a) Mo_2H_8 complex **1**. (b) $Mo_2(C_6H_6)$ complex **2**.

Cartesian coordinates (Å) of the optimized structures

1

S=0

Mo	2.827709	-1.483598	17.874304
Mo	1.750491	-1.907402	15.609488
C	2.128325	-1.931325	20.066584
C	1.406529	-0.803553	19.565822
C	2.292576	0.312619	19.320691
C	3.627110	-0.135977	19.701101
C	3.484960	-1.505466	20.137307
C	1.555862	-3.229636	20.618815
C	1.278366	-2.993795	22.126679
H	0.564141	-2.169032	22.266054
H	2.206568	-2.737936	22.658048
H	0.855091	-3.901877	22.582331
C	2.558328	-4.390049	20.455474
H	3.497342	-4.193792	20.992212
H	2.793805	-4.542980	19.394155
H	2.125400	-5.315065	20.863940
C	0.239202	-3.602479	19.911230
H	-0.529381	-2.829330	20.046822
H	-0.154051	-4.542736	20.324742
H	0.410979	-3.731134	18.835505
C	1.720395	1.673629	18.859380
C	2.227364	2.127802	17.468631
H	1.910486	3.166668	17.288553
H	1.793821	1.490534	16.688750
H	3.313216	2.074243	17.373104
C	2.021585	2.752806	19.929014
H	3.085887	3.001797	19.982189
H	1.696009	2.415329	20.923755
H	1.474880	3.674709	19.680946
C	0.177741	1.586072	18.739372
H	-0.122074	0.835101	17.995709
H	-0.204403	2.560064	18.402113
H	-0.298526	1.351091	19.702015
C	4.977771	0.575604	19.901267
C	5.306218	1.649418	18.848102

H	5.291198	1.208489	17.841872
H	6.314695	2.044074	19.039288
H	4.613446	2.495193	18.872740
C	6.142389	-0.446937	19.864278
H	6.131163	-1.018588	18.927289
H	6.106171	-1.149481	20.707359
H	7.095132	0.096565	19.935089
C	4.960242	1.205492	21.321163
H	4.173107	1.960503	21.426116
H	5.929862	1.683327	21.527972
H	4.790202	0.428343	22.080255
C	-0.403573	-2.628249	15.044503
C	0.367140	-3.748175	15.489204
C	1.459031	-4.018875	14.580154
C	1.354800	-3.030337	13.512929
C	0.219704	-2.199540	13.839104
C	-1.736992	-2.142617	15.596338
C	-2.843119	-2.960900	14.879673
H	-3.837612	-2.654744	15.238330
H	-2.718886	-4.036048	15.075436
H	-2.801293	-2.802324	13.792237
C	-1.940004	-0.641222	15.309398
H	-2.900972	-0.309629	15.729257
H	-1.956923	-0.433626	14.230011
H	-1.130128	-0.053498	15.760991
C	-1.831441	-2.381993	17.114674
H	-1.744203	-3.448305	17.364519
H	-2.802611	-2.027635	17.489983
H	-1.030396	-1.841643	17.634102
C	2.369701	-5.247574	14.801980
C	3.857583	-4.890591	15.035769
H	4.455940	-5.814531	15.039119
H	3.973080	-4.396496	16.008219
H	4.259403	-4.220363	14.273806
C	2.220983	-6.223919	13.608316
H	2.651242	-5.824192	12.684998
H	1.160942	-6.451022	13.423564
H	2.740554	-7.165887	13.839054
C	1.914315	-6.021292	16.064877
H	2.579538	-6.884772	16.207261

H	0.886710	-6.399291	15.966221
H	1.983471	-5.393885	16.964125
C	2.025665	-2.863194	12.136792
C	3.527135	-3.199365	12.097149
H	3.733106	-4.251927	12.310381
H	4.074156	-2.578473	12.819547
H	3.916272	-2.985755	11.090950
C	1.889826	-1.400534	11.640025
H	2.436998	-1.294285	10.692575
H	2.310998	-0.699182	12.372108
H	0.845738	-1.122687	11.444021
C	1.250470	-3.765805	11.137493
H	1.325987	-4.827302	11.400034
H	1.654933	-3.629622	10.123216
H	0.185191	-3.493155	11.123233
H	0.341423	-0.794789	19.373171
H	4.303160	-2.122032	20.485422
H	0.170089	-4.306141	16.395573
H	-0.122591	-1.369239	13.235721
H	3.419263	-2.283074	16.290643
H	2.057875	-2.995216	17.539038
H	0.932318	-1.069505	16.894074
H	2.728133	-0.487486	16.328483
H	4.422406	-1.043154	17.545580
H	3.955629	-2.708122	18.107707
H	2.812088	-1.284270	14.454394
H	1.298495	-0.404793	15.006991

S=1

Mo	2.868487	-1.569252	18.000989
Mo	1.797773	-1.875741	15.364524
C	2.173764	-1.959184	20.214195
C	1.402406	-0.889125	19.672921
C	2.243210	0.245790	19.364792
C	3.607302	-0.141199	19.730768
C	3.520856	-1.488829	20.240315
C	1.630222	-3.237591	20.838250
C	1.241581	-2.886067	22.298859
H	0.475910	-2.096942	22.319439
H	2.117949	-2.530698	22.860076

H	0.840170	-3.774687	22.808637
C	2.694752	-4.352199	20.850167
H	3.576644	-4.062503	21.438887
H	3.021450	-4.583243	19.827502
H	2.274507	-5.262106	21.303152
C	0.380506	-3.733482	20.082654
H	-0.428423	-2.989774	20.103029
H	0.001736	-4.653479	20.551448
H	0.629028	-3.942378	19.034049
C	1.615793	1.577562	18.894770
C	2.111995	2.072164	17.514626
H	1.761305	3.102736	17.351532
H	1.703914	1.434792	16.720721
H	3.198234	2.054843	17.419413
C	1.862504	2.654288	19.982553
H	2.917762	2.934944	20.057072
H	1.532685	2.292411	20.967243
H	1.290011	3.560940	19.736764
C	0.080543	1.420066	18.761006
H	-0.176851	0.642072	18.029534
H	-0.341400	2.369226	18.401365
H	-0.396869	1.181027	19.721960
C	4.939842	0.618236	19.886309
C	5.193069	1.730427	18.853842
H	5.166631	1.316405	17.836750
H	6.191857	2.156301	19.028096
H	4.471855	2.549689	18.923024
C	6.137227	-0.359684	19.772000
H	6.108555	-0.894389	18.814272
H	6.157363	-1.095195	20.586837
H	7.072068	0.215434	19.830860
C	4.952612	1.214625	21.320802
H	4.134535	1.928628	21.474019
H	5.905682	1.735101	21.499398
H	4.850918	0.414462	22.068175
C	-0.428311	-2.591956	14.889550
C	0.294176	-3.724427	15.357402
C	1.391355	-4.021917	14.466517
C	1.326201	-3.047430	13.373891
C	0.207033	-2.189655	13.676361

C	-1.690101	-1.990302	15.492994
C	-2.899872	-2.598805	14.737410
H	-3.841147	-2.192503	15.138597
H	-2.917345	-3.692673	14.848773
H	-2.848274	-2.362279	13.664797
C	-1.693568	-0.456205	15.320361
H	-2.599915	-0.030001	15.775073
H	-1.678932	-0.169695	14.259743
H	-0.812761	-0.009271	15.802552
C	-1.798276	-2.331235	16.993136
H	-1.874733	-3.415243	17.157478
H	-2.698421	-1.863584	17.417788
H	-0.919423	-1.963832	17.539806
C	2.293858	-5.248193	14.724319
C	3.786299	-4.892203	14.935595
H	4.378083	-5.819840	14.960581
H	3.914337	-4.374563	15.894375
H	4.187949	-4.247373	14.152506
C	2.127055	-6.258856	13.561955
H	2.537484	-5.883391	12.619749
H	1.064503	-6.494447	13.404056
H	2.654583	-7.191693	13.810707
C	1.844905	-5.973163	16.017486
H	2.506648	-6.834885	16.184922
H	0.814352	-6.348660	15.941773
H	1.926400	-5.312269	16.891791
C	2.005101	-2.925369	11.995619
C	3.493343	-3.317374	11.953953
H	3.664080	-4.373041	12.182772
H	4.066727	-2.702379	12.660542
H	3.881339	-3.134327	10.941336
C	1.931339	-1.460079	11.492117
H	2.478142	-1.382003	10.541789
H	2.388156	-0.779197	12.221835
H	0.900280	-1.135044	11.300220
C	1.197254	-3.808179	11.005911
H	1.234560	-4.869278	11.280977
H	1.606156	-3.699108	9.990039
H	0.142392	-3.497811	10.988496
H	0.332871	-0.925216	19.510608

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H	0.078714	-4.259028	16.273734
H	-0.120689	-1.367393	13.053455
H	3.304881	-2.359654	16.427989
H	2.626558	-3.231269	18.163119
H	1.364539	-2.118125	17.235437
H	2.485223	-0.546602	16.529040
H	4.236852	-0.802686	17.341681
H	4.279471	-2.479954	18.127886
H	3.192830	-1.377730	14.512369
H	1.618133	-0.369067	14.612581

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Mo	3.543293	0.695450	12.199240
C	3.899600	-0.945500	10.548864
H	3.427955	-1.920325	10.610367
C	5.224866	-0.656382	11.029008
C	6.157373	-1.778770	11.532858
C	5.439974	0.766873	10.804586
C	6.650300	1.714044	10.926895
C	4.247268	1.258221	10.149185
H	4.101542	2.285327	9.838465
C	3.263688	0.216416	9.993148
C	6.538969	-1.654958	13.028910
H	7.372592	-2.337994	13.254720
H	5.696147	-1.940395	13.669116
H	6.834420	-0.640784	13.302580
C	5.474747	-3.158097	11.358528
H	5.239411	-3.363260	10.304381
H	4.547794	-3.238478	11.942619
H	6.158401	-3.942255	11.715078
C	7.440341	-1.822889	10.664378
H	8.018040	-2.727461	10.907508
H	8.088978	-0.959111	10.837415
H	7.183729	-1.853207	9.595707
C	7.533647	1.473603	12.165228
H	6.921776	1.512418	13.076458
H	8.296805	2.263337	12.226932
H	8.057125	0.513493	12.134794

C	6.168363	3.187482	11.012356
H	5.449673	3.315506	11.829911
H	5.699892	3.524560	10.078729
H	7.034380	3.838676	11.197850
C	7.491717	1.590678	9.627991
H	8.329195	2.305024	9.656493
H	6.869266	1.824253	8.751981
H	7.902036	0.583950	9.492942
C	2.049225	0.243541	9.074189
C	1.542369	1.685608	8.884788
H	1.289646	2.129783	9.855754
H	0.642995	1.689493	8.251327
H	2.297196	2.320276	8.399361
C	2.491247	-0.331176	7.703780
H	3.326939	0.253908	7.292371
H	1.657944	-0.303259	6.984137
H	2.824194	-1.373990	7.810161
C	0.897920	-0.608714	9.641551
H	1.216035	-1.642763	9.837950
H	0.064958	-0.643436	8.922903
H	0.536054	-0.171396	10.580665
Mo	2.626824	2.488277	13.794869
C	3.522514	4.229178	14.953061
C	4.833677	4.404359	15.707941
C	3.255962	4.627193	13.593778
H	4.022788	4.851879	12.862770
C	1.835328	4.655037	13.319212
C	1.363611	5.195476	11.954704
C	1.171657	4.309151	14.568467
C	-0.313048	4.325295	14.991191
C	2.216515	4.037101	15.519824
H	2.041767	3.713908	16.540254
C	6.030561	4.333566	14.741257
H	6.973542	4.414812	15.302144
H	6.006326	5.149493	14.004842
H	6.023720	3.379234	14.200152
C	4.798999	5.799577	16.383176
H	3.971292	5.860443	17.105254
H	4.653516	6.588449	15.630595
H	5.742195	5.996506	16.916805

C	5.010955	3.317405	16.785883
H	5.110417	2.332467	16.312055
H	4.156429	3.287353	17.477104
H	5.916638	3.517939	17.378357
C	2.436270	4.913733	10.868324
H	2.687003	3.847162	10.836616
H	3.358267	5.484836	11.038302
H	2.041202	5.212842	9.887181
C	1.229778	6.737961	12.068664
H	0.967176	7.164142	11.088141
H	2.185402	7.176868	12.390300
H	0.460636	7.034949	12.790250
C	0.049833	4.579998	11.438504
H	0.131932	3.484973	11.414470
H	-0.142456	4.935559	10.415653
H	-0.815929	4.854313	12.048508
C	-0.438021	4.081938	16.516024
H	0.087152	4.855101	17.094807
H	-0.045454	3.099911	16.813301
H	-1.501679	4.110866	16.793671
C	-1.180787	3.247416	14.295357
H	-2.246396	3.465645	14.466727
H	-0.976526	2.254804	14.712978
H	-1.003673	3.197153	13.220060
C	-0.909921	5.732045	14.731851
H	-1.903219	5.803593	15.200508
H	-1.031541	5.941332	13.664959
H	-0.266433	6.511036	15.165188
C	1.467125	0.993156	14.951343
H	0.724431	1.453989	15.594723
C	2.844087	0.879474	15.364800
H	3.148181	1.195775	16.359656
C	3.694964	-0.028088	14.602798
H	4.718566	-0.183428	14.942033
C	3.141948	-0.932437	13.649966
H	3.654247	-1.853593	13.390977
C	1.882977	-0.583436	13.039975
H	1.393564	-1.270998	12.354893
C	1.111362	0.482690	13.669021
H	0.125888	0.713875	13.266049

H	4.298765	2.050219	13.234442
H	2.312392	2.016976	12.015993

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Mo	3.468217	0.561889	12.199189
C	3.904159	-0.983267	10.513380
H	3.493201	-1.985788	10.562060
C	5.200851	-0.605436	11.021261
C	6.199364	-1.668889	11.530067
C	5.339184	0.827203	10.753575
C	6.506497	1.830767	10.856928
C	4.135010	1.242432	10.088817
H	3.942605	2.248197	9.738173
C	3.227837	0.141332	9.941637
C	6.613764	-1.489085	13.010826
H	7.454375	-2.161846	13.242025
H	5.783629	-1.750278	13.676647
H	6.914565	-0.467030	13.243640
C	5.574753	-3.081874	11.417849
H	5.341551	-3.340933	10.375209
H	4.656412	-3.173523	12.013260
H	6.294759	-3.820343	11.799606
C	7.456628	-1.682185	10.623224
H	8.087251	-2.546875	10.879782
H	8.065381	-0.780712	10.741130
H	7.168098	-1.766257	9.565634
C	7.439047	1.629484	12.065598
H	6.857663	1.630181	12.996461
H	8.157101	2.461440	12.109377
H	8.015704	0.702000	12.009722
C	5.958730	3.276046	10.969660
H	5.268375	3.357146	11.816279
H	5.434620	3.594664	10.060437
H	6.797422	3.969874	11.124571
C	7.319934	1.747044	9.536805
H	8.138119	2.483864	9.555241
H	6.671273	1.971680	8.677854
H	7.754452	0.752896	9.382202
C	1.965976	0.123401	9.088136
C	1.378643	1.542676	8.961623

H	1.170857	1.956544	9.956868
H	0.441038	1.513113	8.387259
H	2.068599	2.222518	8.442432
C	2.364804	-0.397874	7.683481
H	3.143747	0.240509	7.241499
H	1.492984	-0.400928	7.010952
H	2.758733	-1.422818	7.748107
C	0.890952	-0.801340	9.692392
H	1.274348	-1.818260	9.855869
H	0.028618	-0.870378	9.012137
H	0.546663	-0.400997	10.654505
Mo	2.601747	2.456546	13.924973
C	3.542395	4.256038	15.030759
C	4.843897	4.331093	15.819804
C	3.358092	4.628068	13.658121
H	4.161248	4.860195	12.970350
C	1.960884	4.662568	13.322881
C	1.549754	5.201428	11.936705
C	1.225610	4.322377	14.543164
C	-0.276092	4.374759	14.900575
C	2.223116	4.079941	15.556085
H	2.004745	3.798409	16.580496
C	6.056549	4.198571	14.878550
H	6.988550	4.198883	15.462574
H	6.107795	5.031761	14.163514
H	5.996014	3.260940	14.311756
C	4.881973	5.714246	16.519395
H	4.038855	5.819009	17.217956
H	4.814709	6.524256	15.778205
H	5.819560	5.834701	17.084367
C	4.922096	3.217641	16.883115
H	4.960983	2.233998	16.397592
H	4.054046	3.238369	17.556886
H	5.827982	3.344319	17.495190
C	2.639365	4.861566	10.888418
H	2.830942	3.783047	10.873093
H	3.584930	5.381069	11.087656
H	2.294944	5.177027	9.893056
C	1.469830	6.748834	12.036113
H	1.230953	7.175256	11.049579

H	2.436684	7.157048	12.364073
H	0.704305	7.077614	12.748263
C	0.228737	4.637947	11.381632
H	0.264049	3.540691	11.362419
H	0.087830	4.994649	10.350892
H	-0.644601	4.953783	11.959030
C	-0.472110	4.106281	16.413553
H	0.030466	4.865388	17.029482
H	-0.097407	3.116052	16.706198
H	-1.546980	4.138518	16.643789
C	-1.143937	3.331759	14.154312
H	-2.209680	3.562255	14.308039
H	-0.960895	2.325537	14.547252
H	-0.946726	3.307385	13.082101
C	-0.820114	5.803102	14.642178
H	-1.831521	5.897413	15.066087
H	-0.885012	6.036463	13.575095
H	-0.173644	6.553147	15.119945
C	1.343876	0.910897	14.925715
H	0.531960	1.338926	15.507840
C	2.672058	0.800345	15.451121
H	2.910118	1.124667	16.462606
C	3.613937	-0.011101	14.700884
H	4.642320	-0.062775	15.060505
C	3.169424	-1.000873	13.765989
H	3.740507	-1.906487	13.576108
C	1.906023	-0.761982	13.132720
H	1.462405	-1.490933	12.457237
C	1.125806	0.358133	13.619788
H	0.187930	0.585268	13.111245
H	4.207023	1.965054	13.122843
H	2.388531	2.074696	12.141610

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Mo	3.393936	0.593071	12.384916
C	3.923776	-0.936771	10.493360
H	3.531951	-1.947154	10.507980
C	5.177726	-0.543770	11.059538
C	6.191140	-1.590301	11.564521

C	5.275159	0.910488	10.890122
C	6.464392	1.894652	10.898623
C	4.054877	1.320140	10.239648
H	3.849689	2.325699	9.898911
C	3.214254	0.192639	10.000122
C	6.659787	-1.351103	13.024281
H	7.617269	-1.864968	13.201192
H	5.931046	-1.759046	13.734188
H	6.785473	-0.293065	13.257288
C	5.567765	-3.007618	11.525173
H	5.334061	-3.321466	10.497658
H	4.649593	-3.064486	12.125187
H	6.289179	-3.725612	11.941889
C	7.411876	-1.634480	10.607476
H	8.056960	-2.486879	10.870222
H	8.020795	-0.727253	10.662347
H	7.077798	-1.760509	9.567618
C	7.512831	1.689368	12.008679
H	7.046670	1.764092	12.998605
H	8.269847	2.484085	11.932718
H	8.035208	0.731593	11.937049
C	5.937546	3.337323	11.063559
H	5.284043	3.383823	11.940892
H	5.370577	3.674114	10.187829
H	6.780577	4.030525	11.197648
C	7.153695	1.800296	9.510079
H	7.977178	2.529262	9.449650
H	6.431304	2.026025	8.712550
H	7.563363	0.801217	9.321940
C	1.921024	0.190454	9.194416
C	1.113544	1.476448	9.457777
H	0.905309	1.574960	10.532194
H	0.162950	1.449692	8.904596
H	1.663347	2.371569	9.139848
C	2.308548	0.126885	7.694082
H	2.928297	0.991974	7.416899
H	1.405001	0.130311	7.065120
H	2.880267	-0.787726	7.478186
C	1.043644	-1.027368	9.544298
H	1.569992	-1.974767	9.360774

H	0.135536	-1.023450	8.923702
H	0.740657	-0.996025	10.599074
Mo	2.611508	2.288118	13.857676
C	3.567018	4.213349	14.985509
C	4.874633	4.221358	15.767227
C	3.408085	4.483334	13.593430
H	4.216783	4.699176	12.908257
C	2.007219	4.533928	13.248002
C	1.592552	5.135866	11.891457
C	1.271708	4.294761	14.493582
C	-0.234932	4.328644	14.814109
C	2.251682	4.121788	15.519583
H	2.026872	3.872280	16.550040
C	6.022078	3.646567	14.914661
H	6.952566	3.613239	15.500485
H	6.208177	4.256497	14.020768
H	5.767462	2.630451	14.582104
C	5.187882	5.696111	16.129951
H	4.384178	6.122233	16.748019
H	5.280901	6.306934	15.220333
H	6.132301	5.760469	16.692280
C	4.759926	3.393017	17.063324
H	4.563078	2.337812	16.832931
H	3.955948	3.763620	17.714426
H	5.702122	3.452591	17.627887
C	2.643902	4.768727	10.821343
H	2.800964	3.684644	10.827107
H	3.607057	5.261544	11.001577
H	2.291994	5.081593	9.827519
C	1.594833	6.680988	12.044169
H	1.350122	7.155062	11.080747
H	2.590541	7.026903	12.357339
H	0.868836	7.022403	12.791047
C	0.232054	4.663193	11.345762
H	0.230465	3.575317	11.209359
H	0.060412	5.128113	10.363219
H	-0.607854	4.932878	11.990483
C	-0.470717	3.997873	16.309194
H	-0.011181	4.747579	16.968940
H	-0.073483	3.009285	16.576195

H	-1.552728	3.992325	16.505681
C	-1.068100	3.308891	13.972126
H	-1.984961	3.773071	13.581047
H	-1.376925	2.456048	14.590424
H	-0.494974	2.911867	13.130411
C	-0.775768	5.769210	14.611171
H	-1.807566	5.834440	14.989481
H	-0.788740	6.064438	13.557752
H	-0.157847	6.492153	15.163128
C	1.205486	0.924846	14.771676
H	0.309516	1.338533	15.221531
C	2.463015	0.880628	15.488719
H	2.552922	1.261014	16.503426
C	3.554254	0.161270	14.849780
H	4.529095	0.171773	15.339119
C	3.277714	-0.923064	13.924994
H	3.934342	-1.783986	13.851069
C	2.027281	-0.868744	13.199451
H	1.708393	-1.684913	12.555151
C	1.158929	0.263964	13.478349
H	0.241681	0.357682	12.895476

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Mo	3.493965	0.541275	12.388899
C	3.966468	-0.944455	10.518699
H	3.575147	-1.954127	10.551527
C	5.238678	-0.547512	11.041510
C	6.259576	-1.595403	11.531018
C	5.322885	0.908057	10.865526
C	6.497459	1.909009	10.852938
C	4.084821	1.309469	10.241821
H	3.860020	2.315667	9.915531
C	3.237355	0.181508	10.038882
C	6.774132	-1.354978	12.970683
H	7.588519	-2.062625	13.191002
H	5.972880	-1.523049	13.697725
H	7.149880	-0.343837	13.124554
C	5.617892	-3.005342	11.527414
H	5.339548	-3.323406	10.512513
H	4.723794	-3.044508	12.164198

H	6.345679	-3.730219	11.920018
C	7.455206	-1.655110	10.544986
H	8.109943	-2.500752	10.805814
H	8.061006	-0.743890	10.571222
H	7.096868	-1.799020	9.515592
C	7.570125	1.716795	11.941119
H	7.118623	1.743137	12.940781
H	8.294659	2.542031	11.875833
H	8.130184	0.784249	11.826280
C	5.950766	3.343870	11.029861
H	5.303447	3.379191	11.912652
H	5.371004	3.675452	10.160586
H	6.784778	4.048755	11.157660
C	7.163499	1.822985	9.453124
H	7.975083	2.563659	9.376620
H	6.424642	2.034974	8.667060
H	7.584936	0.828911	9.262038
C	1.921349	0.174772	9.271982
C	1.105745	1.444259	9.589760
H	0.946235	1.531009	10.673895
H	0.131009	1.409482	9.080456
H	1.627086	2.350625	9.256402
C	2.262417	0.149062	7.759545
H	2.859235	1.029737	7.481392
H	1.339827	0.150109	7.158896
H	2.841298	-0.751419	7.506749
C	1.075705	-1.066101	9.619371
H	1.609302	-1.998387	9.386118
H	0.144653	-1.057540	9.034012
H	0.813536	-1.072745	10.685060
Mo	2.482085	2.301269	13.896316
C	3.504343	4.164736	14.982808
C	4.809259	4.141461	15.768410
C	3.361940	4.460684	13.595435
H	4.182353	4.647721	12.916224
C	1.965826	4.550534	13.237724
C	1.602064	5.171855	11.872719
C	1.210342	4.320606	14.476171
C	-0.293612	4.410082	14.806412
C	2.180219	4.100512	15.505505

H	1.943226	3.844566	16.531206
C	5.935888	3.504936	14.929352
H	6.859631	3.434820	15.522854
H	6.156633	4.099584	14.033235
H	5.639948	2.499154	14.598472
C	5.176783	5.611827	16.096749
H	4.389161	6.081493	16.703860
H	5.293172	6.197851	15.173509
H	6.122479	5.654730	16.658980
C	4.661124	3.353950	17.085795
H	4.415435	2.303095	16.887174
H	3.877010	3.779951	17.727204
H	5.606926	3.386989	17.646284
C	2.669022	4.770800	10.828465
H	2.809261	3.684606	10.852124
H	3.636114	5.249858	11.022638
H	2.344799	5.077479	9.823569
C	1.653647	6.715528	12.032619
H	1.459036	7.200323	11.063046
H	2.648682	7.026332	12.382173
H	0.912258	7.078295	12.754383
C	0.239869	4.760754	11.283812
H	0.170340	3.669721	11.191023
H	0.140746	5.192844	10.276842
H	-0.605171	5.122945	11.875799
C	-0.529991	4.073793	16.299432
H	-0.031749	4.793691	16.963778
H	-0.174098	3.063966	16.546150
H	-1.608901	4.112965	16.508161
C	-1.182650	3.435692	13.996231
H	-2.243034	3.661682	14.188664
H	-0.996445	2.400937	14.302432
H	-1.009824	3.496489	12.921914
C	-0.782161	5.867280	14.599359
H	-1.805734	5.976276	14.989449
H	-0.796589	6.152488	13.542568
H	-0.129771	6.571036	15.135857
C	1.155647	0.825590	14.760403
H	0.204666	1.113062	15.199487
C	2.394232	0.864133	15.509201

H	2.441286	1.200550	16.542422
C	3.534340	0.223984	14.863094
H	4.507775	0.334391	15.346605
C	3.362557	-0.922999	13.975381
H	4.032696	-1.777114	14.008644
C	2.138354	-0.933214	13.202510
H	1.835893	-1.787495	12.601104
C	1.235075	0.184619	13.450204
H	0.358896	0.269252	12.803168