Experimental Section

General Procedures. All manipulations were carried out under nitrogen using standard Schlenk techniques. Solvents were distilled from Na (hexane and toluene), Na/benzophenone (diethyl ether, tetrahydrofuran and 1, 4-dioxane) and CaH_2 (CH_2Cl_2). CD_2Cl_2, C_6D_6 and acetone-d_6 were dried over molecular sieves (MS-4A) and stored in Young tubes. CD_2Cl_2 was stored in the dark over Na_2CO_3. Elemental analyses were obtained using a Perkin-Elmer 240-B microanalyzer. The IR and NMR spectra were recorded on Perkin-Elmer FT 1720-X (over the range 2200-1600 cm^{-1}), and Bruker AC-200 (or AC-300) spectrometers respectively.

Preparation of $[MoCl(\eta^3\text{-}C_3H_5)(CO)_2(N\text{-}N)]$(1a,b)-.

$[MoCl(\eta^3\text{-}C_3H_5)(CO)_2(bipy)]$(1a). In an adaptation of a literature procedure,[1] a suspension of molybdenum hexacarbonyl (0.10 g, 0.38 mmol) in acetonitrile (20 mL) was refluxed for 3 hours. At this time, the IR of the resulting yellow solution showed that the complex *fac*-$[Mo(CO)_3(NCMe)_3]$ (two bands of similar intensity at 1920 and 1795_{br} cm^{-1}) was formed. Allyl chloride (0.10 mL, 1.23 mmol) was added. Gas evolution was observed, as well as a change in color from golden yellow to orange. The mixture was refluxed for another 30 min and then reduced pressure was applied to remove all volatiles. The resulting solid was redissolved in CH_2Cl_2 (30 mL), and 2, 2'-bipyridine (0.59 g, 0.38 mmol) was added. The color of the solution changed from light orange to red. The solution was concentrated to 10 mL and, by addition of hexane (30 mL), the

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[1] Brisdon, B. J.; Griffin, G. F. *J. Chem. Soc., Dalton Trans.* **1975**, 1999-2002.

chlorocomplex **1a** was obtained as a red microcrystalline solid (0.14 g, 97 %). IR (CH_2Cl_2): 1950, 1865 (ν_{CO}). ^1H RMN (CD_2Cl_2): 8.81, 8.15, 7.97 and 7.49 [m, 2H each, bipy], 3.11 [m, 1H, CH of η^3-C_3H_5], 3.09 [d (6.2), 2H, H_{syn}], 1.35 [d (9.1), 2H, H_{anti}].

[MoCl(η^3-C_3H_5)$(CO)_2$(phen)](1b). A similar procedure using $Mo(CO)_6$ (0.10 g, 0.38 mmol), allyl chloride (0.10 mL, 1.23 mmol) and 1, 10-phenanthroline (0.07 g, 0.38 mmol) gave de chlorocomplex **1b** as a red solid (0.15 g, 96 %). IR (CH_2Cl_2): 1950, 1870 (ν_{CO}). ^1H NMR (CD_2Cl_2): 9.16, 8.26, 7.96 and 7.81 [m, 2H each, phen], 3.16 [d (6.2), 2H, H_{syn}], 2.97 [m, 1H, CH of η^3-C_3H_5], 1.42 [d (9.1), 2H, H_{anti}].

Preparation of $LiCuMe_2$ -.

Following the procedure reported by Templeton,[2] to a suspension of CuI (0.18 g, 0.94 mmol) in THF (10 mL) at 0°C, MeLi (1.30 mL of a 1.6 M solution in hexanes, 2.08 mmol) was added dropwise. First, a yellow solution was formed, and after 5 min of stirring, a colorless solution of $LiCuMe_2$ (0.095 M in THF) was obtained.

Reaction of [MoCl(η^3-C_3H_5)$(CO)_2$(phen)](1b) with $LiCuMe_2$ -.

To a solution of **1b** (0.10 g, 0.24 mmol) in THF (20 mL) at 0°C was added lithium dimethylcuprate (2.50 mL of a 0.095 M solution, 0.24 mmol). The color of the mixture changed from orange to blue, and after 30 min the solvent was evaporated under vacuum.

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[2]Caldarelli, J. L.; Wagner, L. E.; White, P. S; Templeton, J. L. *J. Am. Chem. Soc.* **1994**, *116*, 2878-2888.

The residue was extracted with toluene (4x15 mL) and this solution was filtered through Celite. The solvent was removed under reduced pressure to give the methyl complex **3a** as a blue solid, which was characterized by spectroscopic techniques. Attempted recrystallization from CH_2Cl_2/hexanes at –20°C yielded red crystals of the complex $[MoI(\eta^3\text{-}C_3H_5)(CO)_2(phen)]$ (**4**).

In the preparation of $LiCuMe_2$ lithium iodide is obtained as a byproduct:

$$CuI + 2MeLi \longrightarrow LiCuMe_2 + LiI$$

Lithium iodide is somewhat soluble in toluene and, during the long time required for the crystallization, methyl / iodide exchange takes place.

Reaction of $[MoCl(\eta^3\text{-}C_3H_5)(CO)_2(phen)]$(1b) with MeMgI -.

A solution of methylmagnesium iodide was prepared by dropwise addition of methyl iodide (0.5 mL, 8.03 mmol) to a well stirred suspension of magnesium turnings (0.5 g, 20.58 mmol) in diethyl ether (20 mL). The solution was filtered off from the unreacted magnesium.

To a solution of **1b** (0.10 g, 0.24 mmol) in THF (20 mL), methylmagnesium iodide was added (0.6 mL of the 0.39 M solution in Et_2O prepared as described above, 0.24 mmol). A workup like that described for the reaction with $LiCuMe_2$ afforded, as the main product, the iodocomplex $[MoI(\eta^3\text{-}C_3H_5)(CO)_2(phen)]$ (**4**).

Synthesis of dialkylmagnesium solutions-.

Although published methods[3] for the synthesis of dialkylmagnesium reagents include their isolation as solids, we have found satisfactory the use of the freshly prepared solutions. Although these MgR_2 reagents are extremely moisture and oxygen sensitive, the solutions can be stored in Young tubes under nitrogen atmosphere for several days, and employed assuming nominal concentrations.

(1) Synthesis of $MgMe_2$ -.

In an adaptation of literature procedures,[3] 1,4-dioxane (1.50 mL, 17.60 mmol) was added slowly dropwise (over a period of 15 min) to a stirred, freshly prepared solution of methylmagnesium iodide (20 mL of a 0.39 M solution, 7.80 mmol) in diethyl ether. The resulting cloudy solution was additionally stirred for 20 hours and then allowed to settle. The clear solution of dimethylmagnesium in ether was transferred (by canula under possitive nitrogen pressure) from the white precipitate (the insoluble adduct MgI_2·dioxane) to a Young tube.

(2) Synthesis of $MgEt_2$ -.

Magnesium (turnings, 0.5 g, 20.58 mmol) was suspended in diethyl ether (30 mL) and a drop of MeI was added to start the reaction (indicated by a slight darkening). Then, ethyl bromide (1.00 mL, 13.40 mmol) was added dropwise and the mixture was stirred for 30

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[3] (a) Anderson, R. A.; Wilkinson, G. *J. Chem. Soc., Dalton Trans.* **1977**, 809-811. (b) Anderson, R. A.; Wilkinson, G. *Inorg. Synth.* **1979**, *19*, 262-264. (c) Dryden, N. H.; Legzdins, P.; Rettig, S. J.; Veltheer, J. E. *Organometallics* **1992**, *11*, 2583-2590.

min. The remaining of the procedure is the same as for the $MgMe_2$ solution, and a 0.21 M solution of diethylmagnesium in ether is obtained.

(3) Synthesis of $MgBz_2$ -.

A similar procedure using benzyl chloride (1.00 mL, 8.69 mmol) to prepare a MgBzCl solution,[4] followed by the addition of 1,4-dioxane (0.9 mL, 10.56 mmol) gave the dibenzylmagnesium solution (0.34 M in THF).

Reactions of the $[MoCl(\eta^3\text{-}C_3H_5)(CO)_2(N\text{-}N)]$ complexes with MgR_2 -.

Synthesis of $[Mo(CH_3)(\eta^3\text{-}C_3H_5)(CO)_2(bipy)]$ (2a). To a solution of **1a** (0.10 g, 0.26 mmol) in THF (20 mL) was added an ethereal solution of $MgMe_2$ (0.26 mmol, 0.9 mL of a 0.29 M solution). The color of the solution changed immediatly from orange to green. After stirring for 15 min, the solvent was removed under vacuum. The residue was redissolved in toluene and filtered through Celite. The solvent was then removed under reduced pressure to afford 0.054 g of **2a** (57%) as a green solid. IR (CH_2Cl_2): 1920, 1830 (ν_{CO}). ^1H NMR (CD_2Cl_2): 8.60, 8.19, 7.91 and 7.36 [m, 2H each, bipy], 3.16 [m, 1H, CH of $\eta^3\text{-}C_3H_5$], 2.66 [d (6.3), 2H, H_{syn}], 1.41 [d (9.6), 2H, H_{anti}], -0.32 [s, 3H Mo-CH_3]. Anal. Calcd. for $C_{16}H_{16}MoN_2O_2$: C, 52.76; H, 4.43; N, 7.69. Found: C, 52.44; H, 4.68; N, 7.63.

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[4] Schrauzer, G. N.; Hughes, L. A. *Organometallics* **1983**, 2, 1163.

Synthesis of $[Mo(CH_2CH_3)(\eta^3\text{-}C_3H_5)(CO)_2(bipy)]$ (2b). A similar procedure using **1a** (0.10 g, 0.26 mmol) and $MgEt_2$ (1.20 mL of a 0.21 M solution, 0.26 mmol in ether) gave the ethyl complex **2b** (0.061 g, 52 %) as a dark green solid. IR (CH_2Cl_2): 1920, 1826 (ν_{CO}). ^1H NMR (CD_2Cl_2): 8.61, 8.18, 7.90 and 7.36 [m, 2H each, bipy], 3.10 [m, 1H, CH of η^3-C_3H_5], 2.63 [d (6.3), 2H, H_{syn}], 1.52 [t (7.8), 3H, Mo-CH_2CH_3], 1.38 [d (9.3), 2H, H_{anti}], -0.29 [q (7.8), 2H, Mo-CH_2CH_3]. Anal. Calcd. for $C_{17}H_{18}MoN_2O_2$: C, 53.99; H, 4.79; N, 7.40. Found: C, 53.77; H, 4.81; N, 7.43.

Synthesis of $[Mo(CH_2C_6H_5)(\eta^3\text{-}C_3H_5)(CO)_2(bipy)]$ (2c). A similar procedure using **1a** (0.10 g, 0.26 mmol) and $MgBz_2$ (0.76 mL of a 0.34 M solution, 0.26 mmol in ether) gave the benzyl complex **2c** (0.091 g, 79 %) as a dark green solid. IR (CH_2Cl_2): 1924, 1836 (ν_{CO}). ^1H NMR (CD_2Cl_2): 8.50, 7.90, 7.81 and 7.31 [m, 2H each, bipy], 6.48 [m, 3H, C_6H_5], 5.84 [m, 2H, C_6H_5], 2.88 [m, 1H, CH of η^3-C_3H_5], 2.65 [d (6.1), 2H, H_{syn}], 1.54 [s, 2H, Mo-$CH_2C_6H_5$], 1.36 [d (9.2), 2H, H_{anti}]. Anal. Calcd. for $C_{22}H_{20}MoN_2O_2$: C, 60.01; H, 4.58; N, 6.36. Found: C, 59.92; H, 4.65; N, 6.39.

Synthesis of $[Mo(CH_3)(\eta^3\text{-}C_3H_5)(CO)_2(phen)]$ (3a). Following the procedure described for **2a**, 0.9 mL of a 0.29 M solution of dimethylmagnesium in diethylether (0.26 mmol of $MgMe_2$) was added to a solution of **1b** (0.10 g, 0.24 mmol) in THF (20 mL). The resulting blue solution was stirred for 15 min. Subsequent workup was as described for **2a**. Yield of complex **3a**: 0.063 g, 66 %. IR (CH_2Cl_2): 1922, 1830 (ν_{CO}). ^1H NMR (CD_2Cl_2): 8.96, 8.42, 7.97 and 7.71 [m, 2H each, phen], 3.05 [m, 1H, CH of η^3-C_3H_5], 2.77 [d (6.4), 2H, H_{syn}], 1.49 [d (9.3), 2H, H_{anti}], -0.69 [s, 3H Mo-CH_3]. $^{13}C\{^1H\}$ NMR (CD_2Cl_2): 235.60 [CO], 151.69, 144.36, 136.02, 130.49, 127.45 and 124.29 [phen], 73.56 [C^2 of η^3-C_3H_5], 51.82 [C^1 and C^3 of η^3-C_3H_5], 12.51 [Mo-CH_3]. Anal. Calcd. for $C_{18}H_{16}MoN_2O_2$: C, 55.69; H, 4.15; N, 7.21. Found: C, 55.58; H, 4.31; N, 7.26.

Synthesis of [Mo(CH_2CH_3)(η^3-C_3H_5)$(CO)_2$(phen)] (3b). Following the procedure described for **2b**, 1.13 mL of a 0.21 M solution of diethylmagnesium in diethyl ether (0.24 mmol of $MgEt_2$) was added to a solution of **1b** (0.10 g, 0.24 mmol) in THF (20 mL). The resulting violet solution was stirred for 15 min. Subsequent workup was as described for **2b**. Yield of complex **3b**: 0.057 g, 58 %. IR (CH_2Cl_2): 1919, 1827 (ν_{CO}). ^{1}H NMR (CD_2Cl_2): 8.96, 8.41, 7.96 and 7.71 [m, 2H each, phen], 3.03 [m, 1H, CH of η^3-C_3H_5], 2.74 [d (6.3), 2H, H_{syn}], 1.52 [t (7.9), 3H, Mo-CH_2CH_3], 1.46 [d (9.3), 2H, H_{anti}], -0.29 [q (7.8), 2H, Mo-CH_2CH_3]. ^{13}C{^{1}H} NMR (CD_2Cl_2): 235.87 [CO], 151.64, 135.87, 130.47, 127.48, 125.23 and 124.27 [phen], 73.68 [C^2 of η^3-C_3H_5], 52.02 [C^1 and C^3 of η^3-C_3H_5], 30.67 [Mo-CH_2CH_3], 19.82 [Mo-CH_2CH_3]. Anal. Calcd. for $C_{19}H_{18}MoN_2O_2$: C, 56.73; H, 4.51; N, 6.96. Found: C, 56.46; H, 4.43; N, 6.91.

Synthesis of [Mo($CH_2C_6H_5$)(η^3-C_3H_5)$(CO)_2$(phen)] (3c). Following the procedure described for **2c**, 0.70 mL of a 0.34 M solution of dibenzylmagnesium in tetrahydrofuran (0.24 mmol of $MgBz_2$) was added to a solution of **1b** (0.10 g, 0.24 mmol) in THF (20 mL). The resulting dark blue solution was stirred for 15 min. Subsequent workup was as described for **2c**. Yield of complex **3c**: 0.095 g, 84 %. IR (CH_2Cl_2): 1925, 1827 (ν_{CO}). ^{1}H NMR (C_6D_6): 8.33, 7.18, 6.91 and 6.52 [m, 2H each, phen], 6.14 [m, 3H, C_6H_5], 5.40 [m, 2H, C_6H_5], 3.00 [s, 2H, Mo-$CH_2C_6H_5$], 2.68 [d (6.4), 2H, H_{syn}], 2.57 [m, 1H, CH of η^3-C_3H_5], 1.73 [d (9.1), 2H, H_{anti}]. ^{13}C{^{1}H} NMR (CD_2Cl_2): 233.44 [CO], 152.07, 151.62, 144.27, 135.59, 130.19, 127.30, 126.26, 124.27, 124.15 and 118.57 [phen and C_6H_5], 72.29 [C^2 of η^3-C_3H_5], 52.91 [C^1 and C^3 of η^3-C_3H_5], 36.65 [Mo-$CH_2C_6H_5$]. Anal. Calcd. for $C_{24}H_{20}MoN_2O_2$: C, 62.08; H, 4.34; N, 6.06. Found: C, 61.78; H, 4.29; N, 6.13.

Synthesis of [MoI(η^3-C_3H_5)(CO)$_2$(phen)] (4) -.

For a comparison with the product obtained by evolution of the solutions of the alkyl complexes prepared using iodide-containing reagents, this iodocomplex was prepared independently by another two different methods:

a) To a solution of **1b** (0.10 g, 0.24 mmol) in CH_2Cl_2 (30 mL), potassium iodide (0.045 g, 0.27 mmol) was added. The mixture was allowed to stir for 3 h at room temperature, and then the solvent was removed under vacuum. The residue was redissolved in CH_2Cl_2 and the combined extracts were filtered through Celite from the KCl white precipitate. The volume was reduced to 5 mL by *in vacuo* evaporation, and hexane (20 mL) was added to precipitate the iodocomplex [MoI(η^3-C_3H_5)(CO)$_2$(phen)] (**4**) as a red solid (0.11 g, 90 %).

b) A suspension of molybdenum hexacarbonyl (0.10 g, 0.38 mmol) in acetonitrile (20 mL) was refluxed under nitrogen for 3 h. At this time, the IR spectrum showed that the complex *fac*-[Mo(CO)$_3$(NCMe)$_3$] was formed, and allyl iodide (0.10 mL, 1.09 mmol) was added. The mixture was refluxed for another 30 min and then reduced presure was applied to remove all volatiles. The resulting solid was redissolved in CH_2Cl_2 (20 mL), and 1,10-phenantroline (0.068 g, 0.38 mmol) was added. The color of the solution changed from light orange to red. The solution was concentrated to 5 mL, and by addition of hexane (20 mL), the iodocomplex **4** was obtained as a red solid (0.17 g, 92 %). IR (CH_2Cl_2): 1951, 1870 (ν_{CO}). ^{1}H NMR (CD_2Cl_2): 9.18, 8.50, 8.00 and 7.84 [m, 2H each, phen], 3.18 [d (6.3), 2H, H_{syn}], 2.86 [m, 1H, CH of η^3-C_3H_5], 1.56 [d (9.1), 2H, H_{anti}]. Anal. Calcd. for $C_{17}H_{13}IMoN_2O_2$: C, 40.83; H, 2.62; N, 5.60. Found: C, 40.91; H, 2.60; N, 5.51.

Preparation of [Mo(OTf)(η^3-C_3H_5)(CO)$_2$(N-N)](5a-b) -.

For the purpose of comparison with the product of the reaction of **3a** and **2c** (see below) with triflic acid, the triflatocomplexes **5a-b** were prepared independently.

[Mo(OTf)(η^3-C_3H_5)(CO)$_2$(bipy)](5a). A mixture of chlorocomplex **1a** (0.18 g, 0.47 mmol), AgOTf (0.12 g, 0.47 mmol) and acetone (1 mL) was stirred in the dark for 2h. The solvent was removed under vacuum, and the residue was extracted in CH_2Cl_2 and filtered through Celite. The solvent was evaporated under reduced pressure, hexane was added and the complex **5a** was obtained as a red precipitate (0.19 g, 82 %). IR (CH_2Cl_2): 1951, 1865 (ν_{CO}). ^{1}H NMR (CD_2Cl_2): 9.18, 8.19, 8.11 and 7.69 [m, 2H each, bipy], 4.04 [m, 1H, CH of η^3-C_3H_5], 3.76 [d (6.6), 2H, H_{syn}], 1.59 [d (9.6), 2H, H_{anti}]. ^{19}F NMR (CD_2Cl_2): -79.27. Anal. Calcd. for $C_{16}H_{13}F_3MoN_2O_5S$: C, 38.57; H, 2.63; N, 5.62. Found: C, 38.19; H, 2.56; N, 5.55.

[Mo(OTf)(η^3-C_3H_5)(CO)$_2$(phen)](5b). A similar procedure using **1b** (0.10 g, 0.24 mmol) and AgOTf (0.063 g, 0.24 mmol) gave **5b** as a red solid (0.11 g, 86 %). IR (CH_2Cl_2): 1948, 1864 (ν_{CO}). ^{1}H NMR (CD_2Cl_2): 9.54, 8.62, 8.04 and 8.00 [m, 2H each, phen], 4.24 [m, 1H, CH of η^3-C_3H_5], 3.90 [d (6.4), 2H, H_{syn}], 1.70 [d (9.7), 2H, H_{anti}]. ^{13}C{^{1}H} NMR (CD_2Cl_2): 225.72 [CO], 152.96, 144.90, 139.29, 130.34, 127.74 and 125.59 [phen], 73.81 [C^2 of η^3-C_3H_5], 55.92 [C^1 and C^3 of η^3-C_3H_5]. Anal. Calcd. for $C_{16}H_{13}F_3MoN_2O_5S$: C, 41.39; H, 2.51; N, 5.36. Found: C, 41.13; H, 2.49; N, 5.29.

Reaction of [Mo(CH_3)(η^3-C_3H_5)(CO)$_2$(phen)](3a) with HOTf -.

Complex **3a** (15 mg, 0.04 mmol) was charged in a 5 mm NMR tube, which was then capped with a rubber septum. The tube was evacuated using a needle attached to the vacuum line, and 0.5 mL of CD_2Cl_2 was injected. The sample was shaken and HOTf (3 μL, 0.037 mmol) was injected, causing an inmediate color change from dark blue to bright

red. The ^{1}H NMR spectrum of this sample showed a singlet at 0.19 ppm, indicating the formation of methane, as well as the signals of the complex [Mo(OTf)(η^3-C_3H_5)$(CO)_2$(phen)] (**5b**).

Reaction of [Mo($CH_2C_6H_5$)(η^3-C_3H_5)$(CO)_2$(bipy)](2c) with HOTf -.

The procedure is the same as for the reaction of **3a** with HOTf. The ^{1}H NMR using complex **2c** (0.01 g, 0.02 mmol) and HOTf (2.5 μL, 0.02 mmol), in acetone-d_6, showed a multiplet centered at 7.24 ppm and a singlet at 2.31 ppm, indicating the formation of toluene, as well as the signals of the complex [Mo(OTf)(η^3-C_3H_5)$(CO)_2$(bipy)] (**5a**).

Reaction of [Mo(CH_3)(η^3-C_3H_5)$(CO)_2$(phen)](3a) with benzenethiol -.

Complex **3a** (15 mg, 0.04 mmol) was charged in a 5 mm NMR tube, which was capped with a rubber septum. The tube was evacuated using a needle attached to the vacuum line, and 0.5 mL of CD_2Cl_2 was injected. The sample was shaken and HSPh (4 μL, 0.04 mmol) was injected. After 8 hours, the color changed from dark blue to red. The ^{1}H NMR spectrum of this sample showed a singlet at 0.19 ppm, indicating the formation of methane, as well as the signals of the complex [Mo(SPh)(η^3-C_3H_5)$(CO)_2$(phen)]. ^{1}H NMR (CD_2Cl_2): 9.15, 8.28, 7.74 and 7.67 [m, 2H each, phen], 6.06 [m, 3H, Ph], 5.86 [m, 2H, Ph], 3.15 [d (6.0), 2H, H_{syn}], 2.87 [m, 1H, CH of η^3-C_3H_5], 1.52 [d (9.7), 2H, H_{anti}].

X-Ray Structure determination of 2a and 3a. Data were measured using the ω-2θ scan technique with a scan angle of 1.5° and a variable scan rate with a maximum scan time of 60 s per reflection. Mo Kα radiation was used with a graphite-crystal

monochromator on a Nonius CAD4 single-crystal diffractometer. On all reflections, profile analysis was performed.[5] Multiple measured reflections were averaged and Lorentz and polarization corrections were applied.

The structures were solved by Patterson methods using DIRDIF99.[6] Isotropic least-squares refinement on F^2 using SHELXL97.[7] During the final stages of the refinements, all positional parameters and the anisotropic temperature factors of all the non-H atoms were refined. The H-atoms were refined isotropically as a mixture of independent and constrained refinement. A statistical disordered model accounting for the partial substitution of (Cl/CH_3) was refined for structures **2a** and **3a** with occupation factors ca. 44:56 for **2a** and ca. 75:25 for **3a**. Atomic scattering factors were taken from International tables for X-ray Crystallography.[8] Plots were made with the EUCLID package.[9] Geometrical calculations were made with PARST.[10] All calculations were made on the Scientific Computer Centre at the University of Oviedo.

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Table 1. Crystal Data and Structure Refinement for 2a.

empirical formula	$C_{15}H_{13}MoN_2O_2$
Fw	384.66
temperature	293 (2) K
wavelength	0.71073 Å
space group, crystal system	$P2_1/c$, monoclinic
unit cell dimensions	a= 8.379 (4) Å, α= 90°
	b= 13.572 (6) Å, β= 102.78 (4)°
	c= 13.958 (5) Å, γ= 90°
volume	1548.0 (11) $Å^3$
Z, calcd density	4, 1.651 $Mg\,m^{-3}$
abs coeff	1.024 mm^{-1}
F(000)	768
cryst size	0.23 x 0.13 x 0.07 mm^3
θ range for data collection	0.98 to 25.97°
limiting indices	$-10 \le h \le 10$, $0 \le k \le 16$, $0 \le l \le 17$
no of rflns collected/unique	3161/3030 (R_{int}=0.0616)
completeness to θ=25.99°	94.1 %
refinement method	full-matrix least-squares on F^2
no of data/restraints/params	3030/ 0/ 225
goodness-of-fit on F^2	1.038
final R indices [I>2 sigma(I)]	R1=0.0415, wR2=0.1008
R indices (all data)	R1=0.1063, wR2=0.1234
largest diff peak and hole	0.489 and -0.614 e $Å^{-3}$

Table 2. Crystal Data and Structure Refinement for 3a.

empirical formula	$C_{18}H_{16}ClMoN_2O_2$
fw	423.72
temperature	293 (2) K
wavelength	0.71073 Å
space group, crystal system	$P2_1/c$, monoclinic
unit cell dimensions	a= 9.32 (6) Å, α= 90°
	b= 12.351 (10) Å, β=100.8 (5)°
	c= 14.38 (6) Å, γ= 90°
volume	1626.0 (12) $Å^3$
Z, calcd density	4, 1.731 Mg m^{-3}
abs coeff	0.984 mm^{-1}
F(000)	852
cryst size	0.23 x 0.20 x 0.17 mm
θ range for data collection	0.83 to 26.11°
limiting indices	$-11 \leq h \leq 11$, $0 \leq k \leq 15$, $0 \leq l \leq 17$
no of rflns collected/unique	3200/3200
completeness to θ=25.99°	96.0 %
refinement method	full-matrix least-squares on F^2
no of data/restraints/params	3200/ 0/ 230
goodness-of-fit on F^2	1.064
final R indices [I>2 sigma(I)]	R1=0.0471, wR2=0.1215
R indices (all data)	R1=0.0980, wR2=0.1440
largest diff peak and hole	0.737 and –0.946 e $Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 2A. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mo(1)	6383(1)	3147(1)	2436(1)	33(1)
C(1)	5080(8)	4065(5)	1513(5)	51(2)
O(1)	4287(6)	4586(5)	938(4)	84(2)
C(2)	5003(8)	2221(5)	1554(5)	48(2)
O(2)	4186(7)	1694(4)	1001(4)	74(2)
Cl(1)	8244(8)	3128(6)	1141(4)	59(2)
C(3)	8070(3)	3120(2)	1480(16)	59(2)
C(4)	4742(9)	2307(6)	3320(6)	60(2)
C(5)	5363(8)	3181(7)	3783(5)	52(2)
C(6)	4809(10)	4064(6)	3282(6)	63(2)
N(1)	8327(6)	2166(4)	3284(3)	36(1)
C(11)	9754(7)	2595(5)	3765(4)	37(1)
C(12)	11068(7)	2024(5)	4254(5)	52(2)
C(13)	10934(9)	1015(6)	4238(5)	58(2)
C(14)	9496(9)	601(7)	3744(5)	54(2)
C(15)	8227(8)	1180(5)	3286(5)	45(2)
N(2)	8392(6)	4116(4)	3245(3)	38(1)
C(21)	9797(7)	3670(5)	3721(4)	37(1)
C(22)	11179(8)	4231(6)	4129(4)	49(2)
C(23)	11125(9)	5235(6)	4049(5)	59(2)
C(24)	9705(10)	5674(7)	3579(5)	59(2)
C(25)	8370(9)	5097(5)	3182(5)	48(2)

Table S3. Bond lengths [Å] and angles [deg] for 2A.

Mo(1)-C(1)	1.946(7)
Mo(1)-C(2)	1.949(7)
Mo(1)-C(3)	2.15(2)
Mo(1)-N(1)	2.230(5)
Mo(1)-C(5)	2.231(6)
Mo(1)-N(2)	2.236(5)
Mo(1)-C(6)	2.317(7)
Mo(1)-C(4)	2.337(7)
Mo(1)-Cl(1)	2.636(6)
C(1)-O(1)	1.161(7)
C(2)-O(2)	1.158(8)
C(3)-H(31)	0.9600
C(3)-H(32)	0.9600
C(3)-H(33)	0.9600
C(4)-C(5)	1.395(11)
C(4)-H(41)	0.9700
C(4)-H(42)	0.9700
C(5)-C(6)	1.413(11)
C(5)-H(5)	0.73(6)

C(6)-H(61)	0.9700
C(6)-H(62)	0.9700
N(1)-C(15)	1.340(8)
N(1)-C(11)	1.366(8)
C(11)-C(12)	1.395(8)
C(11)-C(21)	1.461(8)
C(12)-C(13)	1.373(10)
C(12)-H(12)	0.9300
C(13)-C(14)	1.370(10)
C(13)-H(13)	1.07(6)
C(14)-C(15)	1.363(10)
C(14)-H(14)	0.76(6)
C(15)-H(15)	1.00(6)
N(2)-C(25)	1.333(8)
N(2)-C(21)	1.359(7)
C(21)-C(22)	1.397(8)
C(22)-C(23)	1.368(11)
C(22)-H(22)	0.84(7)
C(23)-C(24)	1.363(11)
C(23)-H(23)	0.94(7)
C(24)-C(25)	1.378(10)
C(24)-H(24)	0.87(7)
C(25)-H(25)	1.09(7)

C(1)-Mo(1)-C(2)	80.0(3)
C(1)-Mo(1)-C(3)	87.2(8)
C(2)-Mo(1)-C(3)	88.6(8)
C(1)-Mo(1)-N(1)	166.2(2)
C(2)-Mo(1)-N(1)	102.2(2)
C(3)-Mo(1)-N(1)	79.3(7)
C(1)-Mo(1)-C(5)	106.3(3)
C(2)-Mo(1)-C(5)	105.2(3)
C(3)-Mo(1)-C(5)	162.0(7)
N(1)-Mo(1)-C(5)	86.4(2)
C(1)-Mo(1)-N(2)	101.9(2)
C(2)-Mo(1)-N(2)	166.7(2)
C(3)-Mo(1)-N(2)	78.4(7)
N(1)-Mo(1)-N(2)	72.76(17)
C(5)-Mo(1)-N(2)	87.0(2)
C(1)-Mo(1)-C(6)	72.2(3)
C(2)-Mo(1)-C(6)	110.1(3)
C(3)-Mo(1)-C(6)	148.5(9)
N(1)-Mo(1)-C(6)	118.8(2)
C(5)-Mo(1)-C(6)	36.1(3)
N(2)-Mo(1)-C(6)	82.9(3)
C(1)-Mo(1)-C(4)	110.6(3)
C(2)-Mo(1)-C(4)	71.6(3)
C(3)-Mo(1)-C(4)	149.8(9)
N(1)-Mo(1)-C(4)	82.8(2)
C(5)-Mo(1)-C(4)	35.5(3)
N(2)-Mo(1)-C(4)	119.0(2)
C(6)-Mo(1)-C(4)	61.7(3)
C(1)-Mo(1)-Cl(1)	83.2(3)
C(2)-Mo(1)-Cl(1)	85.3(3)
C(3)-Mo(1)-Cl(1)	4.7(8)
N(1)-Mo(1)-Cl(1)	83.39(19)
C(5)-Mo(1)-Cl(1)	166.7(2)
N(2)-Mo(1)-Cl(1)	81.86(19)

C(6)-Mo(1)-Cl(1)	147.6(3)
C(4)-Mo(1)-Cl(1)	149.8(3)
O(1)-C(1)-Mo(1)	177.5(6)
O(2)-C(2)-Mo(1)	177.5(6)
Mo(1)-C(3)-H(31)	109.5
Mo(1)-C(3)-H(32)	109.5
H(31)-C(3)-H(32)	109.5
Mo(1)-C(3)-H(33)	109.5
H(31)-C(3)-H(33)	109.5
H(32)-C(3)-H(33)	109.5
C(5)-C(4)-Mo(1)	68.1(4)
C(5)-C(4)-H(41)	116.9
Mo(1)-C(4)-H(41)	116.9
C(5)-C(4)-H(42)	116.9
Mo(1)-C(4)-H(42)	116.9
H(41)-C(4)-H(42)	113.9
C(4)-C(5)-C(6)	116.3(7)
C(4)-C(5)-Mo(1)	76.4(4)
C(6)-C(5)-Mo(1)	75.3(4)
C(4)-C(5)-H(5)	127(6)
C(6)-C(5)-H(5)	117(6)
Mo(1)-C(5)-H(5)	120(5)
C(5)-C(6)-Mo(1)	68.6(4)
C(5)-C(6)-H(61)	116.8
Mo(1)-C(6)-H(61)	116.8
C(5)-C(6)-H(62)	116.8
Mo(1)-C(6)-H(62)	116.8
H(61)-C(6)-H(62)	113.8
C(15)-N(1)-C(11)	118.2(5)
C(15)-N(1)-Mo(1)	123.9(4)
C(11)-N(1)-Mo(1)	117.6(4)
N(1)-C(11)-C(12)	120.9(6)
N(1)-C(11)-C(21)	115.6(5)
C(12)-C(11)-C(21)	123.5(6)
C(13)-C(12)-C(11)	119.5(6)
C(13)-C(12)-H(12)	120.2
C(11)-C(12)-H(12)	120.2
C(14)-C(13)-C(12)	118.5(7)
C(14)-C(13)-H(13)	115(3)
C(12)-C(13)-H(13)	127(3)
C(15)-C(14)-C(13)	120.5(8)
C(15)-C(14)-H(14)	116(6)
C(13)-C(14)-H(14)	124(6)
N(1)-C(15)-C(14)	122.3(7)
N(1)-C(15)-H(15)	121(4)
C(14)-C(15)-H(15)	117(4)
C(25)-N(2)-C(21)	118.4(6)
C(25)-N(2)-Mo(1)	123.8(5)
C(21)-N(2)-Mo(1)	117.2(4)
N(2)-C(21)-C(22)	120.4(6)
N(2)-C(21)-C(11)	116.1(5)
C(22)-C(21)-C(11)	123.5(6)
C(23)-C(22)-C(21)	120.0(7)
C(23)-C(22)-H(22)	126(5)
C(21)-C(22)-H(22)	114(5)
C(24)-C(23)-C(22)	119.0(7)
C(24)-C(23)-H(23)	115(4)
C(22)-C(23)-H(23)	126(4)

C(23)-C(24)-C(25)	119.3(8)
C(23)-C(24)-H(24)	124(5)
C(25)-C(24)-H(24)	117(5)
N(2)-C(25)-C(24)	122.9(7)
N(2)-C(25)-H(25)	116(4)
C(24)-C(25)-H(25)	121(4)

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for 2A. The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Mo(1)	21(1)	37(1)	38(1)	0(1)	-1(1)	-1(1)
C(1)	32(3)	47(4)	66(4)	4(3)	-5(3)	2(3)
O(1)	65(3)	85(4)	88(4)	23(3)	-16(3)	26(3)
C(2)	41(4)	54(4)	44(4)	6(3)	-4(3)	-7(3)
O(2)	74(3)	70(4)	63(3)	-6(3)	-19(3)	-33(3)
Cl(1)	54(3)	49(2)	68(4)	-1(4)	3(3)	-1(2)
C(3)	54(3)	49(2)	68(4)	-1(4)	3(3)	-1(2)
C(4)	37(4)	74(5)	70(5)	14(4)	16(4)	-2(4)
C(5)	34(3)	77(5)	46(4)	-2(5)	10(3)	-4(4)
C(6)	48(4)	64(5)	85(5)	-8(4)	28(4)	3(4)
N(1)	31(3)	36(3)	38(3)	3(2)	2(2)	1(2)
C(11)	27(3)	51(4)	32(3)	8(3)	7(2)	8(3)
C(12)	30(3)	68(6)	52(4)	6(3)	-2(3)	5(3)
C(13)	42(4)	72(6)	56(4)	13(4)	2(3)	22(4)
C(14)	62(5)	41(4)	60(4)	15(4)	20(4)	10(4)
C(15)	49(4)	37(4)	44(4)	10(3)	3(3)	0(3)
N(2)	28(2)	42(3)	39(3)	-5(2)	0(2)	-5(2)
C(21)	29(3)	47(4)	32(3)	-5(3)	3(2)	-5(3)
C(22)	33(3)	71(6)	38(3)	-8(3)	1(3)	-13(3)
C(23)	49(4)	70(6)	57(4)	-18(4)	13(4)	-27(4)
C(24)	65(5)	50(4)	66(4)	-10(4)	25(4)	-21(4)
C(25)	46(4)	47(4)	52(4)	-8(3)	9(3)	-5(3)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for 2A.

	x	y	z	U(eq)
H(31)	8970	2689	1749	120(4)
H(32)	8479	3772	1419	120(4)
H(33)	7524	2882	844	120(4)
H(41)	3576	2288	3034	54(14)
H(42)	5174	1697	3636	54(14)
H(5)	5900(8)	3230(5)	4270(4)	40(2)
H(61)	5283	4673	3580	50(2)
H(62)	3648	4109	2989	51(18)

H(12)	12028	2324	4589	47(9)
H(13)	11810(7)	500(5)	4630(4)	47(9)
H(14)	9330(9)	50(5)	3730(5)	47(9)
H(15)	7260(7)	840(4)	2870(4)	47(9)
H(22)	11980(9)	3900(5)	4430(5)	60(10)
H(23)	12000(8)	5670(6)	4280(5)	60(10)
H(24)	9610(9)	6300(5)	3450(5)	60(10)
H(25)	7230(8)	5420(5)	2780(4)	60(10)

Table S6. Torsion angles [deg] for 2A.

C(2)-Mo(1)-C(1)-O(1)	-19(14)
C(3)-Mo(1)-C(1)-O(1)	70(14)
N(1)-Mo(1)-C(1)-O(1)	82(14)
C(5)-Mo(1)-C(1)-O(1)	-122(14)
N(2)-Mo(1)-C(1)-O(1)	148(14)
C(6)-Mo(1)-C(1)-O(1)	-134(14)
C(4)-Mo(1)-C(1)-O(1)	-85(14)
Cl(1)-Mo(1)-C(1)-O(1)	67(14)
C(1)-Mo(1)-C(2)-O(2)	36(14)
C(3)-Mo(1)-C(2)-O(2)	-51(14)
N(1)-Mo(1)-C(2)-O(2)	-130(14)
C(5)-Mo(1)-C(2)-O(2)	141(14)
N(2)-Mo(1)-C(2)-O(2)	-63(15)
C(6)-Mo(1)-C(2)-O(2)	103(14)
C(4)-Mo(1)-C(2)-O(2)	152(15)
Cl(1)-Mo(1)-C(2)-O(2)	-48(14)
C(1)-Mo(1)-C(4)-C(5)	-89.4(5)
C(2)-Mo(1)-C(4)-C(5)	-160.7(5)
C(3)-Mo(1)-C(4)-C(5)	147.9(14)
N(1)-Mo(1)-C(4)-C(5)	93.8(4)
N(2)-Mo(1)-C(4)-C(5)	28.1(5)
C(6)-Mo(1)-C(4)-C(5)	-34.5(4)
Cl(1)-Mo(1)-C(4)-C(5)	157.3(5)
Mo(1)-C(4)-C(5)-C(6)	65.7(5)
C(1)-Mo(1)-C(5)-C(4)	102.8(5)
C(2)-Mo(1)-C(5)-C(4)	19.0(5)
C(3)-Mo(1)-C(5)-C(4)	-120(3)
N(1)-Mo(1)-C(5)-C(4)	-82.7(4)
N(2)-Mo(1)-C(5)-C(4)	-155.6(5)
C(6)-Mo(1)-C(5)-C(4)	122.4(6)
Cl(1)-Mo(1)-C(5)-C(4)	-122.3(12)
C(1)-Mo(1)-C(5)-C(6)	-19.6(5)
C(2)-Mo(1)-C(5)-C(6)	-103.4(5)
C(3)-Mo(1)-C(5)-C(6)	118(3)
N(1)-Mo(1)-C(5)-C(6)	154.9(5)
N(2)-Mo(1)-C(5)-C(6)	82.0(5)
C(4)-Mo(1)-C(5)-C(6)	-122.4(6)
Cl(1)-Mo(1)-C(5)-C(6)	115.3(12)
C(4)-C(5)-C(6)-Mo(1)	-66.4(5)
C(1)-Mo(1)-C(6)-C(5)	160.3(5)
C(2)-Mo(1)-C(6)-C(5)	88.4(5)
C(3)-Mo(1)-C(6)-C(5)	-148.4(13)
N(1)-Mo(1)-C(6)-C(5)	-28.9(5)
N(2)-Mo(1)-C(6)-C(5)	-94.7(5)

C(4)-Mo(1)-C(6)-C(5)	33.8(4)
Cl(1)-Mo(1)-C(6)-C(5)	-157.2(4)
C(1)-Mo(1)-N(1)-C(15)	-111.6(10)
C(2)-Mo(1)-N(1)-C(15)	-13.4(5)
C(3)-Mo(1)-N(1)-C(15)	-99.7(9)
C(5)-Mo(1)-N(1)-C(15)	91.3(5)
N(2)-Mo(1)-N(1)-C(15)	179.3(5)
C(6)-Mo(1)-N(1)-C(15)	107.9(5)
C(4)-Mo(1)-N(1)-C(15)	55.8(5)
Cl(1)-Mo(1)-N(1)-C(15)	-97.2(5)
C(1)-Mo(1)-N(1)-C(11)	63.0(11)
C(2)-Mo(1)-N(1)-C(11)	161.2(4)
C(3)-Mo(1)-N(1)-C(11)	74.9(9)
C(5)-Mo(1)-N(1)-C(11)	-94.1(4)
N(2)-Mo(1)-N(1)-C(11)	-6.1(4)
C(6)-Mo(1)-N(1)-C(11)	-77.5(5)
C(4)-Mo(1)-N(1)-C(11)	-129.5(4)
Cl(1)-Mo(1)-N(1)-C(11)	77.4(4)
C(15)-N(1)-C(11)-C(12)	-0.6(8)
Mo(1)-N(1)-C(11)-C(12)	-175.5(4)
C(15)-N(1)-C(11)-C(21)	178.9(5)
Mo(1)-N(1)-C(11)-C(21)	4.0(6)
N(1)-C(11)-C(12)-C(13)	1.1(9)
C(21)-C(11)-C(12)-C(13)	-178.4(6)
C(11)-C(12)-C(13)-C(14)	-0.6(10)
C(12)-C(13)-C(14)-C(15)	-0.4(10)
C(11)-N(1)-C(15)-C(14)	-0.4(9)
Mo(1)-N(1)-C(15)-C(14)	174.2(5)
C(13)-C(14)-C(15)-N(1)	1.0(10)
C(1)-Mo(1)-N(2)-C(25)	11.9(5)
C(2)-Mo(1)-N(2)-C(25)	109.0(11)
C(3)-Mo(1)-N(2)-C(25)	96.4(9)
N(1)-Mo(1)-N(2)-C(25)	178.7(6)
C(5)-Mo(1)-N(2)-C(25)	-94.2(6)
C(6)-Mo(1)-N(2)-C(25)	-58.1(5)
C(4)-Mo(1)-N(2)-C(25)	-110.1(5)
Cl(1)-Mo(1)-N(2)-C(25)	93.1(5)
C(1)-Mo(1)-N(2)-C(21)	-159.2(4)
C(2)-Mo(1)-N(2)-C(21)	-62.0(11)
C(3)-Mo(1)-N(2)-C(21)	-74.7(9)
N(1)-Mo(1)-N(2)-C(21)	7.6(4)
C(5)-Mo(1)-N(2)-C(21)	94.7(4)
C(6)-Mo(1)-N(2)-C(21)	130.8(4)
C(4)-Mo(1)-N(2)-C(21)	78.8(5)
Cl(1)-Mo(1)-N(2)-C(21)	-78.0(4)
C(25)-N(2)-C(21)-C(22)	-0.2(8)
Mo(1)-N(2)-C(21)-C(22)	171.4(4)
C(25)-N(2)-C(21)-C(11)	-179.8(5)
Mo(1)-N(2)-C(21)-C(11)	-8.2(7)
N(1)-C(11)-C(21)-N(2)	2.8(8)
C(12)-C(11)-C(21)-N(2)	-177.7(5)
N(1)-C(11)-C(21)-C(22)	-176.8(5)
C(12)-C(11)-C(21)-C(22)	2.7(10)
N(2)-C(21)-C(22)-C(23)	-0.1(9)
C(11)-C(21)-C(22)-C(23)	179.5(6)
C(21)-C(22)-C(23)-C(24)	0.7(10)
C(22)-C(23)-C(24)-C(25)	-1.0(10)
C(21)-N(2)-C(25)-C(24)	-0.1(9)

Mo(1)-N(2)-C(25)-C(24)	-171.1(5)
C(23)-C(24)-C(25)-N(2)	0.7(10)

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 3A. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mo(1)	1247(1)	2630(1)	3421(1)	30(1)
Cl(1)	2716(3)	1594(2)	2376(2)	63(1)
C(100)	2562(3)	1760(2)	2772(2)	63(1)
C(1)	417(3)	3415(2)	2266(2)	39(2)
O(1)	-70(3)	3833(2)	1569(2)	60(2)
C(2)	-422(3)	1702(2)	2922(2)	42(2)
O(2)	-1424(3)	1188(2)	2606(2)	61(2)
C(3)	381(3)	4299(2)	3821(2)	46(2)
C(4)	529(8)	3569(6)	4570(5)	44(2)
C(5)	-404(9)	2684(7)	4432(6)	51(2)
C(6)	6715(7)	2713(7)	5628(6)	52(2)
C(7)	6236(7)	1842(8)	6025(5)	55(2)
N(1)	3424(5)	3435(4)	3872(4)	34(1)
C(11)	4360(6)	2918(5)	4571(4)	33(1)
C(12)	5800(6)	3283(5)	4884(5)	39(2)
C(13)	6245(8)	4199(6)	4440(6)	50(2)
C(14)	5303(8)	4713(6)	3742(6)	51(2)
C(15)	3884(7)	4297(5)	3478(5)	43(2)
N(2)	2496(5)	1612(4)	4585(4)	32(1)
C(21)	3884(6)	1963(5)	4964(4)	32(1)
C(22)	4803(7)	1415(6)	5685(5)	43(2)
C(23)	4284(8)	454(6)	6023(5)	52(2)
C(24)	2914(9)	94(6)	5632(6)	55(2)
C(25)	2072(8)	697(5)	4929(5)	44(2)

Table S9. Selected bond lengths [Å] and angles [deg] for 3A.

Mo(1)-C(1)	1.954(8)
Mo(1)-C(2)	1.956(9)
Mo(1)-C(100)	1.989(8)
Mo(1)-C(4)	2.222(10)
Mo(1)-N(2)	2.239(10)
Mo(1)-N(1)	2.244(12)
Mo(1)-C(5)	2.308(14)
Mo(1)-C(3)	2.325(4)
Mo(1)-Cl(1)	2.557(10)
C(1)-O(1)	1.1422
C(2)-O(2)	1.1494

C(3)-C(4)	1.391(8)
C(4)-C(5)	1.387(11)
C(6)-C(7)	1.333(12)
C(6)-C(12)	1.423(12)
C(7)-C(22)	1.433(13)
N(1)-C(15)	1.314(9)
N(1)-C(11)	1.361(10)
C(11)-C(12)	1.407(11)
C(11)-C(21)	1.415(9)
C(12)-C(13)	1.400(11)
C(13)-C(14)	1.360(13)
C(14)-C(15)	1.402(12)
N(2)-C(25)	1.323(8)
N(2)-C(21)	1.376(11)
C(21)-C(22)	1.391(10)
C(22)-C(23)	1.403(11)
C(23)-C(24)	1.369(13)
C(24)-C(25)	1.376(11)

C(1)-Mo(1)-C(2)	79.5(4)
C(1)-Mo(1)-C(100)	92.9(3)
C(2)-Mo(1)-C(100)	91.7(4)
C(1)-Mo(1)-C(4)	104.3(3)
C(2)-Mo(1)-C(4)	104.4(4)
C(100)-Mo(1)-C(4)	158.2(2)
C(1)-Mo(1)-N(2)	169.29(17)
C(2)-Mo(1)-N(2)	102.2(4)
C(100)-Mo(1)-N(2)	76.6(3)
C(4)-Mo(1)-N(2)	85.6(3)
C(1)-Mo(1)-N(1)	102.6(4)
C(2)-Mo(1)-N(1)	168.30(16)
C(100)-Mo(1)-N(1)	76.8(4)
C(4)-Mo(1)-N(1)	86.3(4)
N(2)-Mo(1)-N(1)	73.6(4)
C(1)-Mo(1)-C(5)	108.5(4)
C(2)-Mo(1)-C(5)	70.8(4)
C(100)-Mo(1)-C(5)	148.6(3)
C(4)-Mo(1)-C(5)	35.6(3)
N(2)-Mo(1)-C(5)	81.9(4)
N(1)-Mo(1)-C(5)	118.6(4)
C(1)-Mo(1)-C(3)	70.7(2)
C(2)-Mo(1)-C(3)	108.8(3)
C(100)-Mo(1)-C(3)	150.21(15)
C(4)-Mo(1)-C(3)	35.5(2)
N(2)-Mo(1)-C(3)	118.0(2)
N(1)-Mo(1)-C(3)	82.7(3)
C(5)-Mo(1)-C(3)	61.0(3)
C(1)-Mo(1)-Cl(1)	85.4(3)
C(2)-Mo(1)-Cl(1)	88.2(4)
C(100)-Mo(1)-Cl(1)	7.81(11)
C(4)-Mo(1)-Cl(1)	165.2(2)
N(2)-Mo(1)-Cl(1)	84.1(3)
N(1)-Mo(1)-Cl(1)	80.6(4)
C(5)-Mo(1)-Cl(1)	151.5(3)
C(3)-Mo(1)-Cl(1)	146.89(11)
O(1)-C(1)-Mo(1)	177.04(8)
O(2)-C(2)-Mo(1)	177.36(9)
C(4)-C(3)-Mo(1)	68.2(4)

C(5)-C(4)-C(3)	115.6(7)
C(5)-C(4)-Mo(1)	75.6(5)
C(3)-C(4)-Mo(1)	76.3(4)
C(4)-C(5)-Mo(1)	68.8(5)
C(7)-C(6)-C(12)	121.3(7)
C(6)-C(7)-C(22)	121.1(7)
C(15)-N(1)-C(11)	118.9(6)
C(15)-N(1)-Mo(1)	125.8(5)
C(11)-N(1)-Mo(1)	115.1(5)
N(1)-C(11)-C(12)	121.8(7)
N(1)-C(11)-C(21)	118.8(6)
C(12)-C(11)-C(21)	119.4(6)
C(13)-C(12)-C(11)	117.3(6)
C(13)-C(12)-C(6)	123.8(7)
C(11)-C(12)-C(6)	118.9(7)
C(14)-C(13)-C(12)	120.5(7)
C(13)-C(14)-C(15)	118.3(8)
N(1)-C(15)-C(14)	123.2(7)
C(25)-N(2)-C(21)	116.5(6)
C(25)-N(2)-Mo(1)	127.6(5)
C(21)-N(2)-Mo(1)	115.9(5)
N(2)-C(21)-C(22)	122.9(7)
N(2)-C(21)-C(11)	116.5(5)
C(22)-C(21)-C(11)	120.5(6)
C(21)-C(22)-C(23)	117.7(7)
C(21)-C(22)-C(7)	118.6(8)
C(23)-C(22)-C(7)	123.6(7)
C(24)-C(23)-C(22)	119.2(7)
C(23)-C(24)-C(25)	119.1(8)
N(2)-C(25)-C(24)	124.6(7)

Table S10. Bond lengths [Å] and angles [deg] for 3A.

Mo(1)-C(1)	1.954(8)
Mo(1)-C(2)	1.956(9)
Mo(1)-C(100)	1.989(8)
Mo(1)-C(4)	2.222(10)
Mo(1)-N(2)	2.239(10)
Mo(1)-N(1)	2.244(12)
Mo(1)-C(5)	2.308(14)
Mo(1)-C(3)	2.325(4)
Mo(1)-Cl(1)	2.557(10)
C(1)-O(1)	1.1422
C(2)-O(2)	1.1494
C(3)-C(4)	1.391(8)
C(4)-C(5)	1.387(11)
C(6)-C(7)	1.333(12)
C(6)-C(12)	1.423(12)
C(7)-C(22)	1.433(13)
N(1)-C(15)	1.314(9)
N(1)-C(11)	1.361(10)
C(11)-C(12)	1.407(11)
C(11)-C(21)	1.415(9)
C(12)-C(13)	1.400(11)
C(13)-C(14)	1.360(13)

C(14)-C(15)	1.402(12)
N(2)-C(25)	1.323(8)
N(2)-C(21)	1.376(11)
C(21)-C(22)	1.391(10)
C(22)-C(23)	1.403(11)
C(23)-C(24)	1.369(13)
C(24)-C(25)	1.376(11)

C(1)-Mo(1)-C(2)	79.5(4)
C(1)-Mo(1)-C(100)	92.9(3)
C(2)-Mo(1)-C(100)	91.7(4)
C(1)-Mo(1)-C(4)	104.3(3)
C(2)-Mo(1)-C(4)	104.4(4)
C(100)-Mo(1)-C(4)	158.2(2)
C(1)-Mo(1)-N(2)	169.29(17)
C(2)-Mo(1)-N(2)	102.2(4)
C(100)-Mo(1)-N(2)	76.6(3)
C(4)-Mo(1)-N(2)	85.6(3)
C(1)-Mo(1)-N(1)	102.6(4)
C(2)-Mo(1)-N(1)	168.30(16)
C(100)-Mo(1)-N(1)	76.8(4)
C(4)-Mo(1)-N(1)	86.3(4)
N(2)-Mo(1)-N(1)	73.6(4)
C(1)-Mo(1)-C(5)	108.5(4)
C(2)-Mo(1)-C(5)	70.8(4)
C(100)-Mo(1)-C(5)	148.6(3)
C(4)-Mo(1)-C(5)	35.6(3)
N(2)-Mo(1)-C(5)	81.9(4)
N(1)-Mo(1)-C(5)	118.6(4)
C(1)-Mo(1)-C(3)	70.7(2)
C(2)-Mo(1)-C(3)	108.8(3)
C(100)-Mo(1)-C(3)	150.21(15)
C(4)-Mo(1)-C(3)	35.5(2)
N(2)-Mo(1)-C(3)	118.0(2)
N(1)-Mo(1)-C(3)	82.7(3)
C(5)-Mo(1)-C(3)	61.0(3)
C(1)-Mo(1)-Cl(1)	85.4(3)
C(2)-Mo(1)-Cl(1)	88.2(4)
C(100)-Mo(1)-Cl(1)	7.81(11)
C(4)-Mo(1)-Cl(1)	165.2(2)
N(2)-Mo(1)-Cl(1)	84.1(3)
N(1)-Mo(1)-Cl(1)	80.6(4)
C(5)-Mo(1)-Cl(1)	151.5(3)
C(3)-Mo(1)-Cl(1)	146.89(11)
O(1)-C(1)-Mo(1)	177.04(8)
O(2)-C(2)-Mo(1)	177.36(9)
C(4)-C(3)-Mo(1)	68.2(4)
C(5)-C(4)-C(3)	115.6(7)
C(5)-C(4)-Mo(1)	75.6(5)
C(3)-C(4)-Mo(1)	76.3(4)
C(4)-C(5)-Mo(1)	68.8(5)
C(7)-C(6)-C(12)	121.3(7)
C(6)-C(7)-C(22)	121.1(7)
C(15)-N(1)-C(11)	118.9(6)
C(15)-N(1)-Mo(1)	125.8(5)
C(11)-N(1)-Mo(1)	115.1(5)
N(1)-C(11)-C(12)	121.8(7)
N(1)-C(11)-C(21)	118.8(6)

C(12)-C(11)-C(21)	119.4(6)
C(13)-C(12)-C(11)	117.3(6)
C(13)-C(12)-C(6)	123.8(7)
C(11)-C(12)-C(6)	118.9(7)
C(14)-C(13)-C(12)	120.5(7)
C(13)-C(14)-C(15)	118.3(8)
N(1)-C(15)-C(14)	123.2(7)
C(25)-N(2)-C(21)	116.5(6)
C(25)-N(2)-Mo(1)	127.6(5)
C(21)-N(2)-Mo(1)	115.9(5)
N(2)-C(21)-C(22)	122.9(7)
N(2)-C(21)-C(11)	116.5(5)
C(22)-C(21)-C(11)	120.5(6)
C(21)-C(22)-C(23)	117.7(7)
C(21)-C(22)-C(7)	118.6(8)
C(23)-C(22)-C(7)	123.6(7)
C(24)-C(23)-C(22)	119.2(7)
C(23)-C(24)-C(25)	119.1(8)
N(2)-C(25)-C(24)	124.6(7)

Table S11. Anisotropic displacement parameters (A^2 x 10^3) for 3A.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Mo(1)	20(1)	32(1)	32(1)	-1(1)	-9(1)	1(1)
Cl(1)	53(2)	62(2)	66(2)	-14(1)	-7(1)	17(1)
C(100)	53(2)	62(2)	66(2)	-14(1)	-7(1)	17(1)
C(1)	23(3)	45(4)	44(4)	-5(3)	-6(3)	-5(3)
O(1)	56(3)	65(3)	47(3)	14(3)	-18(3)	-1(3)
C(2)	38(4)	35(4)	46(4)	2(3)	-10(3)	5(3)
O(2)	42(3)	60(3)	70(4)	0(3)	-18(3)	-24(3)
C(3)	35(4)	41(4)	58(4)	-11(3)	-3(3)	6(3)
C(4)	39(4)	44(4)	45(4)	-7(3)	-2(3)	7(3)
C(5)	42(4)	60(5)	53(5)	12(4)	11(4)	11(4)
C(6)	21(3)	73(5)	54(4)	-18(4)	-14(3)	4(3)
C(7)	31(4)	86(6)	38(4)	0(4)	-17(3)	14(4)
N(1)	26(3)	34(3)	36(3)	-2(2)	-7(2)	-1(2)
C(11)	19(3)	40(3)	34(3)	-8(3)	-5(2)	4(2)
C(12)	23(3)	49(4)	39(4)	-17(3)	-8(3)	4(3)
C(13)	24(3)	53(5)	74(6)	-26(4)	6(4)	-10(3)
C(14)	40(4)	49(4)	65(5)	-6(4)	11(4)	-16(3)
C(15)	33(4)	39(4)	56(4)	0(3)	4(3)	-3(3)
N(2)	20(2)	35(3)	36(3)	-3(2)	-4(2)	-3(2)
C(21)	23(3)	40(3)	29(3)	-7(3)	-4(2)	6(3)
C(22)	36(4)	50(4)	38(4)	-3(3)	-6(3)	16(3)
C(23)	54(5)	62(5)	39(4)	16(3)	4(3)	22(4)
C(24)	66(5)	39(4)	58(5)	12(3)	7(4)	7(4)
C(25)	39(4)	35(4)	53(4)	3(3)	-1(3)	-1(3)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for 3A.

	x	y	z	U(eq)
H(101)	1986	1318	2294	150(14)
H(102)	3169	1306	3226	150(14)
H(103)	3165	2237	2484	150(14)
H(31)	1063	4900	3887	240(8)
H(32)	-606	4492	3520	80(3)
H(4)	1180	3708	5176	90(3)
H(51)	-1270(7)	2780(5)	4020(4)	32(18)
H(52)	-290(8)	2260(6)	4850(5)	40(2)
H(6)	7550(7)	2970(5)	5890(4)	29(16)
H(7)	7000(7)	1400(5)	6480(5)	40(18)
H(13)	7040(9)	4510(7)	4530(6)	70(3)
H(14)	5650(7)	5350(6)	3440(5)	43(19)
H(15)	3260(8)	4730(6)	2960(5)	60(2)
H(23)	4863	66	6507	36(10)
H(24)	2557	-548	5838	36(10)
H(25)	1140	443	4679	36(10)

Table S13. Selected torsion angles [deg] for 3A.

C(2)-Mo(1)-C(1)-O(1)	-50.0(17)
C(100)-Mo(1)-C(1)-O(1)	41.1(17)
C(4)-Mo(1)-C(1)-O(1)	-152.4(16)
N(2)-Mo(1)-C(1)-O(1)	50(2)
N(1)-Mo(1)-C(1)-O(1)	118.2(16)
C(5)-Mo(1)-C(1)-O(1)	-115.5(16)
C(3)-Mo(1)-C(1)-O(1)	-164.3(16)
Cl(1)-Mo(1)-C(1)-O(1)	38.9(16)
C(1)-Mo(1)-C(2)-O(2)	-14.7(18)
C(100)-Mo(1)-C(2)-O(2)	-107.3(17)
C(4)-Mo(1)-C(2)-O(2)	87.5(18)
N(2)-Mo(1)-C(2)-O(2)	176(100)
N(1)-Mo(1)-C(2)-O(2)	-116.3(18)
C(5)-Mo(1)-C(2)-O(2)	99.3(18)
C(3)-Mo(1)-C(2)-O(2)	50.6(18)
Cl(1)-Mo(1)-C(2)-O(2)	-100.3(18)
C(1)-Mo(1)-C(3)-C(4)	159.9(3)
C(2)-Mo(1)-C(3)-C(4)	88.7(5)
C(100)-Mo(1)-C(3)-C(4)	-140.4(5)
N(2)-Mo(1)-C(3)-C(4)	-26.9(4)
N(1)-Mo(1)-C(3)-C(4)	-93.9(6)
C(5)-Mo(1)-C(3)-C(4)	34.6(5)
Cl(1)-Mo(1)-C(3)-C(4)	-154.0(4)
Mo(1)-C(3)-C(4)-C(5)	-66.3(6)
C(1)-Mo(1)-C(4)-C(5)	101.9(6)
C(2)-Mo(1)-C(4)-C(5)	19.3(5)
C(100)-Mo(1)-C(4)-C(5)	-117.2(7)
N(2)-Mo(1)-C(4)-C(5)	-82.2(6)
N(1)-Mo(1)-C(4)-C(5)	-156.0(5)

C(3)-Mo(1)-C(4)-C(5)	121.5(6)
Cl(1)-Mo(1)-C(4)-C(5)	-128.4(8)
C(1)-Mo(1)-C(4)-C(3)	-19.5(3)
C(2)-Mo(1)-C(4)-C(3)	-102.2(4)
C(100)-Mo(1)-C(4)-C(3)	121.4(5)
N(2)-Mo(1)-C(4)-C(3)	156.3(3)
N(1)-Mo(1)-C(4)-C(3)	82.5(4)
C(5)-Mo(1)-C(4)-C(3)	-121.5(6)
Cl(1)-Mo(1)-C(4)-C(3)	110.1(7)
C(3)-C(4)-C(5)-Mo(1)	66.7(6)
C(1)-Mo(1)-C(5)-C(4)	-88.8(5)
C(2)-Mo(1)-C(5)-C(4)	-160.2(5)
C(100)-Mo(1)-C(5)-C(4)	140.7(5)
N(2)-Mo(1)-C(5)-C(4)	93.8(5)
N(1)-Mo(1)-C(5)-C(4)	27.5(5)
C(3)-Mo(1)-C(5)-C(4)	-34.5(4)
Cl(1)-Mo(1)-C(5)-C(4)	155.3(4)
C(12)-C(6)-C(7)-C(22)	3.0(12)
C(1)-Mo(1)-N(1)-C(15)	6.5(6)
C(2)-Mo(1)-N(1)-C(15)	105.8(9)
C(100)-Mo(1)-N(1)-C(15)	96.5(6)
C(4)-Mo(1)-N(1)-C(15)	-97.3(6)
N(2)-Mo(1)-N(1)-C(15)	176.2(6)
C(5)-Mo(1)-N(1)-C(15)	-112.9(6)
C(3)-Mo(1)-N(1)-C(15)	-61.8(6)
Cl(1)-Mo(1)-N(1)-C(15)	89.6(6)
C(1)-Mo(1)-N(1)-C(11)	-168.5(4)
C(2)-Mo(1)-N(1)-C(11)	-69.2(10)
C(100)-Mo(1)-N(1)-C(11)	-78.5(5)
C(4)-Mo(1)-N(1)-C(11)	87.7(5)
N(2)-Mo(1)-N(1)-C(11)	1.2(4)
C(5)-Mo(1)-N(1)-C(11)	72.1(5)
C(3)-Mo(1)-N(1)-C(11)	123.3(5)
Cl(1)-Mo(1)-N(1)-C(11)	-85.4(5)
C(15)-N(1)-C(11)-C(12)	0.3(9)
Mo(1)-N(1)-C(11)-C(12)	175.6(5)
C(15)-N(1)-C(11)-C(21)	-177.2(6)
Mo(1)-N(1)-C(11)-C(21)	-1.9(7)
N(1)-C(11)-C(12)-C(13)	-0.7(9)
C(21)-C(11)-C(12)-C(13)	176.8(6)
N(1)-C(11)-C(12)-C(6)	179.0(6)
C(21)-C(11)-C(12)-C(6)	-3.5(9)
C(7)-C(6)-C(12)-C(13)	-179.8(7)
C(7)-C(6)-C(12)-C(11)	0.5(11)
C(11)-C(12)-C(13)-C(14)	0.7(10)
C(6)-C(12)-C(13)-C(14)	-179.0(7)
C(12)-C(13)-C(14)-C(15)	-0.3(11)
C(11)-N(1)-C(15)-C(14)	0.2(10)
Mo(1)-N(1)-C(15)-C(14)	-174.6(6)
C(13)-C(14)-C(15)-N(1)	-0.1(12)
C(1)-Mo(1)-N(2)-C(25)	-107.6(9)
C(2)-Mo(1)-N(2)-C(25)	-9.4(6)
C(100)-Mo(1)-N(2)-C(25)	-98.1(6)
C(4)-Mo(1)-N(2)-C(25)	94.5(7)
N(1)-Mo(1)-N(2)-C(25)	-178.1(6)
C(5)-Mo(1)-N(2)-C(25)	58.8(6)
C(3)-Mo(1)-N(2)-C(25)	109.8(6)
Cl(1)-Mo(1)-N(2)-C(25)	-96.2(6)

C(1)-Mo(1)-N(2)-C(21)	70.1(10)
C(2)-Mo(1)-N(2)-C(21)	168.3(4)
C(100)-Mo(1)-N(2)-C(21)	79.5(5)
C(4)-Mo(1)-N(2)-C(21)	-87.9(6)
N(1)-Mo(1)-N(2)-C(21)	-0.4(4)
C(5)-Mo(1)-N(2)-C(21)	-123.5(5)
C(3)-Mo(1)-N(2)-C(21)	-72.5(5)
Cl(1)-Mo(1)-N(2)-C(21)	81.5(5)
C(25)-N(2)-C(21)-C(22)	-1.5(9)
Mo(1)-N(2)-C(21)-C(22)	-179.4(5)
C(25)-N(2)-C(21)-C(11)	177.6(6)
Mo(1)-N(2)-C(21)-C(11)	-0.4(7)
N(1)-C(11)-C(21)-N(2)	1.5(8)
C(12)-C(11)-C(21)-N(2)	-176.0(6)
N(1)-C(11)-C(21)-C(22)	-179.4(6)
C(12)-C(11)-C(21)-C(22)	3.0(9)
N(2)-C(21)-C(22)-C(23)	1.1(10)
C(11)-C(21)-C(22)-C(23)	-177.9(6)
N(2)-C(21)-C(22)-C(7)	179.4(6)
C(11)-C(21)-C(22)-C(7)	0.4(10)
C(6)-C(7)-C(22)-C(21)	-3.5(11)
C(6)-C(7)-C(22)-C(23)	174.7(8)
C(21)-C(22)-C(23)-C(24)	0.3(10)
C(7)-C(22)-C(23)-C(24)	-177.9(7)
C(22)-C(23)-C(24)-C(25)	-1.3(11)
C(21)-N(2)-C(25)-C(24)	0.5(10)
Mo(1)-N(2)-C(25)-C(24)	178.1(6)
C(23)-C(24)-C(25)-N(2)	0.9(12)

Table S14. Torsion angles [deg] for 3A.

C(2)-Mo(1)-C(1)-O(1)	-50.0(17)
C(100)-Mo(1)-C(1)-O(1)	41.1(17)
C(4)-Mo(1)-C(1)-O(1)	-152.4(16)
N(2)-Mo(1)-C(1)-O(1)	50(2)
N(1)-Mo(1)-C(1)-O(1)	118.2(16)
C(5)-Mo(1)-C(1)-O(1)	-115.5(16)
C(3)-Mo(1)-C(1)-O(1)	-164.3(16)
Cl(1)-Mo(1)-C(1)-O(1)	38.9(16)
C(1)-Mo(1)-C(2)-O(2)	-14.7(18)
C(100)-Mo(1)-C(2)-O(2)	-107.3(17)
C(4)-Mo(1)-C(2)-O(2)	87.5(18)
N(2)-Mo(1)-C(2)-O(2)	176(100)
N(1)-Mo(1)-C(2)-O(2)	-116.3(18)
C(5)-Mo(1)-C(2)-O(2)	99.3(18)
C(3)-Mo(1)-C(2)-O(2)	50.6(18)
Cl(1)-Mo(1)-C(2)-O(2)	-100.3(18)
C(1)-Mo(1)-C(3)-C(4)	159.9(3)
C(2)-Mo(1)-C(3)-C(4)	88.7(5)
C(100)-Mo(1)-C(3)-C(4)	-140.4(5)
N(2)-Mo(1)-C(3)-C(4)	-26.9(4)
N(1)-Mo(1)-C(3)-C(4)	-93.9(6)
C(5)-Mo(1)-C(3)-C(4)	34.6(5)
Cl(1)-Mo(1)-C(3)-C(4)	-154.0(4)
Mo(1)-C(3)-C(4)-C(5)	-66.3(6)

C(1)-Mo(1)-C(4)-C(5)	101.9(6)
C(2)-Mo(1)-C(4)-C(5)	19.3(5)
C(100)-Mo(1)-C(4)-C(5)	-117.2(7)
N(2)-Mo(1)-C(4)-C(5)	-82.2(6)
N(1)-Mo(1)-C(4)-C(5)	-156.0(5)
C(3)-Mo(1)-C(4)-C(5)	121.5(6)
Cl(1)-Mo(1)-C(4)-C(5)	-128.4(8)
C(1)-Mo(1)-C(4)-C(3)	-19.5(3)
C(2)-Mo(1)-C(4)-C(3)	-102.2(4)
C(100)-Mo(1)-C(4)-C(3)	121.4(5)
N(2)-Mo(1)-C(4)-C(3)	156.3(3)
N(1)-Mo(1)-C(4)-C(3)	82.5(4)
C(5)-Mo(1)-C(4)-C(3)	-121.5(6)
Cl(1)-Mo(1)-C(4)-C(3)	110.1(7)
C(3)-C(4)-C(5)-Mo(1)	66.7(6)
C(1)-Mo(1)-C(5)-C(4)	-88.8(5)
C(2)-Mo(1)-C(5)-C(4)	-160.2(5)
C(100)-Mo(1)-C(5)-C(4)	140.7(5)
N(2)-Mo(1)-C(5)-C(4)	93.8(5)
N(1)-Mo(1)-C(5)-C(4)	27.5(5)
C(3)-Mo(1)-C(5)-C(4)	-34.5(4)
Cl(1)-Mo(1)-C(5)-C(4)	155.3(4)
C(12)-C(6)-C(7)-C(22)	3.0(12)
C(1)-Mo(1)-N(1)-C(15)	6.5(6)
C(2)-Mo(1)-N(1)-C(15)	105.8(9)
C(100)-Mo(1)-N(1)-C(15)	96.5(6)
C(4)-Mo(1)-N(1)-C(15)	-97.3(6)
N(2)-Mo(1)-N(1)-C(15)	176.2(6)
C(5)-Mo(1)-N(1)-C(15)	-112.9(6)
C(3)-Mo(1)-N(1)-C(15)	-61.8(6)
Cl(1)-Mo(1)-N(1)-C(15)	89.6(6)
C(1)-Mo(1)-N(1)-C(11)	-168.5(4)
C(2)-Mo(1)-N(1)-C(11)	-69.2(10)
C(100)-Mo(1)-N(1)-C(11)	-78.5(5)
C(4)-Mo(1)-N(1)-C(11)	87.7(5)
N(2)-Mo(1)-N(1)-C(11)	1.2(4)
C(5)-Mo(1)-N(1)-C(11)	72.1(5)
C(3)-Mo(1)-N(1)-C(11)	123.3(5)
Cl(1)-Mo(1)-N(1)-C(11)	-85.4(5)
C(15)-N(1)-C(11)-C(12)	0.3(9)
Mo(1)-N(1)-C(11)-C(12)	175.6(5)
C(15)-N(1)-C(11)-C(21)	-177.2(6)
Mo(1)-N(1)-C(11)-C(21)	-1.9(7)
N(1)-C(11)-C(12)-C(13)	-0.7(9)
C(21)-C(11)-C(12)-C(13)	176.8(6)
N(1)-C(11)-C(12)-C(6)	179.0(6)
C(21)-C(11)-C(12)-C(6)	-3.5(9)
C(7)-C(6)-C(12)-C(13)	-179.8(7)
C(7)-C(6)-C(12)-C(11)	0.5(11)
C(11)-C(12)-C(13)-C(14)	0.7(10)
C(6)-C(12)-C(13)-C(14)	-179.0(7)
C(12)-C(13)-C(14)-C(15)	-0.3(11)
C(11)-N(1)-C(15)-C(14)	0.2(10)
Mo(1)-N(1)-C(15)-C(14)	-174.6(6)
C(13)-C(14)-C(15)-N(1)	-0.1(12)
C(1)-Mo(1)-N(2)-C(25)	-107.6(9)
C(2)-Mo(1)-N(2)-C(25)	-9.4(6)
C(100)-Mo(1)-N(2)-C(25)	-98.1(6)

C(4)-Mo(1)-N(2)-C(25)	94.5(7)
N(1)-Mo(1)-N(2)-C(25)	-178.1(6)
C(5)-Mo(1)-N(2)-C(25)	58.8(6)
C(3)-Mo(1)-N(2)-C(25)	109.8(6)
Cl(1)-Mo(1)-N(2)-C(25)	-96.2(6)
C(1)-Mo(1)-N(2)-C(21)	70.1(10)
C(2)-Mo(1)-N(2)-C(21)	168.3(4)
C(100)-Mo(1)-N(2)-C(21)	79.5(5)
C(4)-Mo(1)-N(2)-C(21)	-87.9(6)
N(1)-Mo(1)-N(2)-C(21)	-0.4(4)
C(5)-Mo(1)-N(2)-C(21)	-123.5(5)
C(3)-Mo(1)-N(2)-C(21)	-72.5(5)
Cl(1)-Mo(1)-N(2)-C(21)	81.5(5)
C(25)-N(2)-C(21)-C(22)	-1.5(9)
Mo(1)-N(2)-C(21)-C(22)	-179.4(5)
C(25)-N(2)-C(21)-C(11)	177.6(6)
Mo(1)-N(2)-C(21)-C(11)	-0.4(7)
N(1)-C(11)-C(21)-N(2)	1.5(8)
C(12)-C(11)-C(21)-N(2)	-176.0(6)
N(1)-C(11)-C(21)-C(22)	-179.4(6)
C(12)-C(11)-C(21)-C(22)	3.0(9)
N(2)-C(21)-C(22)-C(23)	1.1(10)
C(11)-C(21)-C(22)-C(23)	-177.9(6)
N(2)-C(21)-C(22)-C(7)	179.4(6)
C(11)-C(21)-C(22)-C(7)	0.4(10)
C(6)-C(7)-C(22)-C(21)	-3.5(11)
C(6)-C(7)-C(22)-C(23)	174.7(8)
C(21)-C(22)-C(23)-C(24)	0.3(10)
C(7)-C(22)-C(23)-C(24)	-177.9(7)
C(22)-C(23)-C(24)-C(25)	-1.3(11)
C(21)-N(2)-C(25)-C(24)	0.5(10)
Mo(1)-N(2)-C(25)-C(24)	178.1(6)
C(23)-C(24)-C(25)-N(2)	0.9(12)