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Syntheses of Variations of Sterogenic-at-Metal Imido Alkylidene Complexes of Molybdenum

by

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Abstract

In this paper we describe the syntheses of several new stereogenic-at-metal imido alkylidene complexes of molybdenum, Mo(NR)(CHR')(X)(Y), many of which had to be prepared through selective nucleophilic displacement reactions in imido alkylidene complexes. The reported compounds include Mo(NAd)(CHCMe$_2$Ph)(MesPyr)$_2$ (**1a**; MesPyr = 2-mesitylpyrrolide, Ad = 1-adamantyl), Mo(NAd)(CHCMe$_2$Ph)(2-CNPyr)$_2$ (**1b**; 2-CNPyr = 2-cyanopyrrolide), Mo(NAd)(CHCMe$_2$Ph)(MesPyr)(OTPP) (**2a**; OTPP = 2,3,5,6-tetraphenylphenoxide), Mo(NAd)(CHCMe$_2$Ph)(MesPyr)(OBr$_2$Bitet) (**2b**; OBr$_2$Bitet = (*R*)-3,3'-dibromo-2'-(*tert*-butyldimethylsilyloxy)-5,5',6,6',7,7',8,8'-octahydro-1,1'-binaphthyl-2-olate), Mo(NAd)(CHCMe$_2$Ph)(OHIPT)(2-Mespyr) (**2c**; HIPT = 2,6-(2,4,6-i-Pr$_3$C$_6$H$_2$)$_2$C$_6$H$_3$), Mo(NAd)(CHCMe$_2$Ph)(OTf)(OHIPT) (**3)**, Mo(NAd)(CHCMe$_2$Ph)(OTf)(OHIPT)(PMe$_3$) **(3(PMe$_3$))**, Mo(NAd)(CHCMe$_2$Ph)(2-CNPyr)(OHIPT) (**4**), Mo(NAd)(CHCMe$_2$Ph)(OHIPT)(OCMe$_3$) (**5**), Mo(NR)(CHCMe$_2$Ph)(OR$_{F6}$)(OHMT) (OR$_{F6}$ = OCMe(CF$_3$)$_2$; HMT = 2,6-Mes$_2$C$_6$H$_3$); R = Ar (**6a**), 2,6-Me$_2$C$_6$H$_3$ (Ar', **6b**), 2-*i*-PrC$_6$H$_4$ (Ar$^{i\text{Pr}}$, **6c**), or Ad (**6d**)), Mo(NR)(CHCMe$_2$Ph)(OR$_{F6}$)[N(H)HMT] [**7a**, (R = Ar') and **7b** (R = Ar$^{i\text{Pr}}$)], and Mo(NAd)(CHCMe$_2$Ph)(OR$_{F6}$)(HMT) (**8**). X-ray structural studies were carried out on **1b**, **2a**, **2b**, **2c**, **3(PMe$_3$)**, **4**, **5**, **6d**, **7d**, and **8**. Compound **1b** is an octamer in which two η^1-pyrrolides are *trans* to one another at each metal center and cyano groups bind from neighboring Mo centers *trans* to the alkylidene and imido ligands.

INTRODUCTION

Recent advances in olefin metathesis by molybdenum,[1] tungsten,[2] and ruthenium[3] alkylidene complexes have focused on initiators in which the metal is a stereogenic center. For example, the chemistry of high oxidation state molybdenum or tungsten complexes of the type M(NR)(CHR')(OR")(Pyr) where Pyr is a pyrrolide or a substituted pyrrolide (MAP complexes) were first prepared in 2007[4,5] in the process of demonstrating that a $M(NR)(CHR')(Pyr)_2$ complex[6,7] could act as a precursor to a bisalkoxide, a biphenolate, or a binaphtholate imido alkylidene catalyst through addition of the monoalcohol or diol to it. Recent examples of selective metathesis applications by MAP catalysts that contain a sterically demanding HIPTO ligand ($HIPTO^-$ = hexaisopropylterphenoxide = O-2,6-(2,4,6-i-$Pr_3C_6H_2)_2C_6H_3^-$) or HMTO ligand ($HMTO^-$ = hexamethylterphenoxide = O-2,6-$Mesityl_2C_6H_3^-$) include Z-selective metathesis homocoupling of terminal olefins,[8] *Z*-selective ring-opening metathesis polymerization (ROMP) of 2,3-disubstituted norbornenes and norbornadienes,[9] Z-selective ring-opening/cross-metathesis reactions,[10] ethenolysis reactions[11] (including *Z*-selective ethenolysis[12]), and *Z*-selective cross metathesis[1c] or ring-closing metathesis.[2a] Theoretical calculations by Eisenstein and coworkers[13] help explain why olefin metatheses by MAP species are relatively efficient. Isolation of four-coordinate 14-electron methylidene species when the aryloxide is sterically demanding is consistent with the relatively long-lived nature of MAP catalysts under some circumstances.[14]

Syntheses of MAP species via the "protonolysis" route is proposed to involve binding of ROH to the metal through the oxygen atom before a proton migrates to the pyrrolide, probably to the α carbon atom first to yield an intermediate pyrrolenine complex.[15] Therefore, syntheses of MAP species via the protonolysis route strongly depend upon steric factors associated with the size of the pyrrolides (so far usually parent pyrrolide or a 2,5-dimethylpyrrolide), the imido, the alkylidene, and the added ROH. Another persistant synthetic problem is that intermediate MAP species can react with a second equivalent of alcohol to form a bisalkoxide. In short, in our experience, many potentially useful MAP species cannot be made in pure form via "protonolysis" of bispyrrolide species. It should be noted that both bisamido[16] and dialkyl[17]

complexes were explored as precursors to monoalkoxide or bisalkoxide complexes with scant success before bispyrrolides were employed as catalyst precursors to MAP complexes.

Two of the most important features of MAP complexes are that the metal is a stereogenic center and that all ligands are covalently bound to the metal. Therefore, MAP complexes are members of a larger class of stereogenic-at-metal (SAM) complexes. For example, M(D)(CHR')(X)(Y) complexes, in theory, could be prepared where M is Mo or W, D is an imido or oxo ligand,[18] and X and Y are different monoanionic ligands based on, for example, C (e.g., an alkyl),[15] N (e.g., an amide),[14] or O (e.g., an alkoxide). Since MAP species have demonstrated some special reactivities in olefin metathesis reactions (*vide supra*), other SAM complexes besides MAP species might exhibit special properties in metathesis reactions. However, all syntheses of M(D)(CHR')(X)(Y) complexes cannot depend solely upon protonolysis reactions. In this paper we explore some of the problems associated with the synthesis of some new MAP variations and begin to explore possible Mo(NR)(CHR')(X)(Y) variations in which neither X nor Y is a pyrrolide.

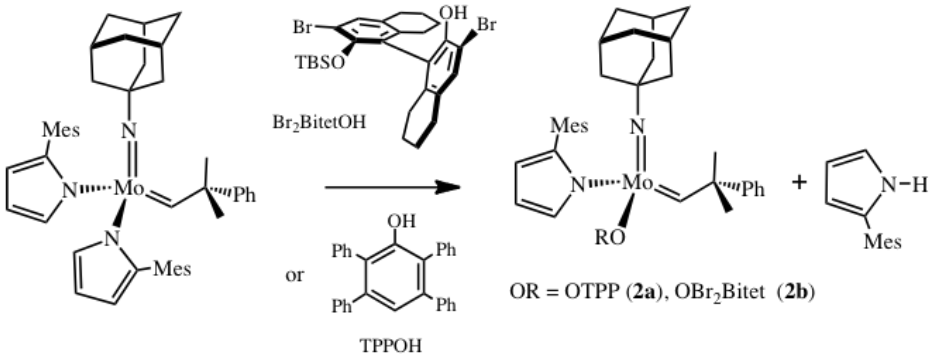
RESULTS AND DISCUSSION

MAP Complexes that contain pyrrolide variations

Potential variations of MAP species include those that contain a sterically demanding pyrrolide, e.g., 2-mesitylpyrrolide. Mo(NAd)(CHCMe$_2$Ph)(MesPyr)$_2$ (**1a**; MesPyr = 2-mesitylpyrrolide, Ad = 1-adamantyl) can be prepared in 75% isolated yield by treating Mo(NAd)(CHCMe$_2$Ph)(OTf)$_2$(DME) with two equivalents of Li(MesPyr) in diethyl ether. Compound **1a** is close relative of Mo(NAd)(CHCMe$_3$)(MesPyr)$_2$, which was prepared in 25% isolated yield in a similar manner.[19] It is also related to structurally characterized Mo(NAr)(CHCMe$_2$Ph)(η^1-MesPyr)$_2$ (Ar = 2,6-diisopropylphenyl),[20] in which for steric reasons the 2-mesitylpyrrolide ligand cannot bind in an η^5 fashion, usually the observed mode of binding one of the two pyrrolides in other imido alkylidene bispyrrolide complexes.[5,21]

Mo(NAd)(CHCMe$_2$Ph)(MesPyr)$_2$ reacts with TPPOH (2,3,5,6-tetraphenylphenol) and

Br_2BitetOH (eq 1) readily to yield Mo(NAd)(CHCMe$_2$Ph)(MesPyr)(OTPP) (**2a**) and Mo(NAd)(CHCMe$_2$Ph)(MesPyr)(OBr$_2$Bitet) (**2b**) in 80% and 53% yields, respectively. These syntheses of **2a** and **2b** are typical protonolysis methods. Compound **2b** is found as two diastereomers with *syn* alkylidene proton shifts of 12.47 ppm (*R*-diastereomer) and 13.14 ppm (*S*-diastereomer). The *S*-diastereomer could be isolated in pure form through crystallization from *n*-pentane. A typical observed ratio of R to S in the crude product mixture is 1:1.



(1)

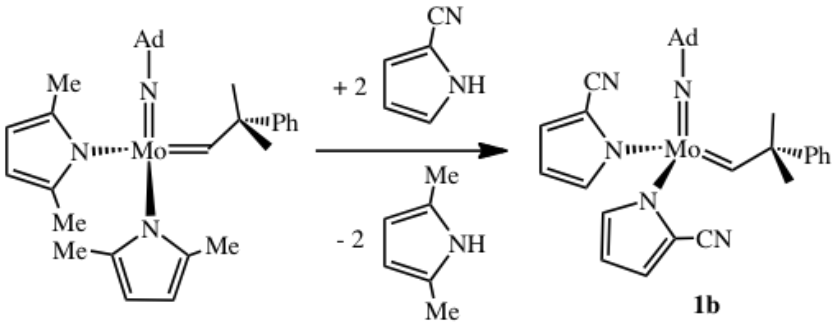
Complexes **2a** and *(S)*-**2b** display distorted tetrahedral geometries typical of MAP species (Figures 1 and 2) with bond lengths and angles similar to those found in other reported MAP complexes. (See a selection of bond lengths and angles in Table 1.) The relatively short Mo–Br distance (3.163 Å) in *(S)*-**2b** is similar to that reported (3.04 Å) for the *R*-diastereomer of Mo(NAr)(CHCMe$_2$Ph)(Me$_2$Pyr)(OBr$_2$Bitet) (Me$_2$Pyr = 2,5-dimethylpyrrolide, Ar = 2,6-i-Pr$_2$C$_6$H$_3$).[22]

While one equivalent of HIPTOH will react with Mo(NAd)(CHCMe$_2$Ph)(Pyr)$_2$ (Pyr = pyrrolide or 2,5-dimethylpyrrolide) to yield Mo(NAd)(CHCMe$_2$Ph)(Pyr)(OHIPT),[9a] attempts to react one equivalent of HIPTOH with **1a** in toluene-d$_8$ led to no reaction, even after heating mixtures (~0.1 M in each) to 80 °C for weeks. This result illustrates the steric limitations in certain protonolysis reactions.

In order to increase the electrophilicity of the metal center, we became interested in the possibility of employing pyrrolides that are less electron-donating than the parent pyrrolide or 2,5-dimethylpyrrolide. Therefore, we explored the synthesis of 2-cyanopyrrolide[23] MAP

complexes.

The reaction of $Mo(NAd)(CHCMe_2Ph)(OTf)_2(DME)$ with two equivalents of Li(2-CNPyr) yielded $Mo(NAd)(CHCMe_2Ph)(2\text{-}CNPyr)_2$ (**1b**) in 55% isolated yield. Alternatively, **1b** can be obtained in 76% yield by treating $Mo(NAd)(CHCMe_2Ph)(Me_2Pyr)_2$ with excess 2-CNPyrH (eq 2). The proton NMR spectrum of **1b** typically contains several alkylidene resonances in the range 14 – 15 ppm, the intensities of which vary from sample to sample. An NMR spectrum of **1b** that had been recrystallized from a mixture of THF and pentane contained only a single alkylidene resonance at 14.47 ppm. An X-ray crystallographic study of this sample showed the product to be an octamer (Figure 3). Therefore we propose that multiple alkylidene resonances arise from other oligomers of $Mo(NAd)(CHCMe_2Ph)(2\text{-}CNPyr)_2$.



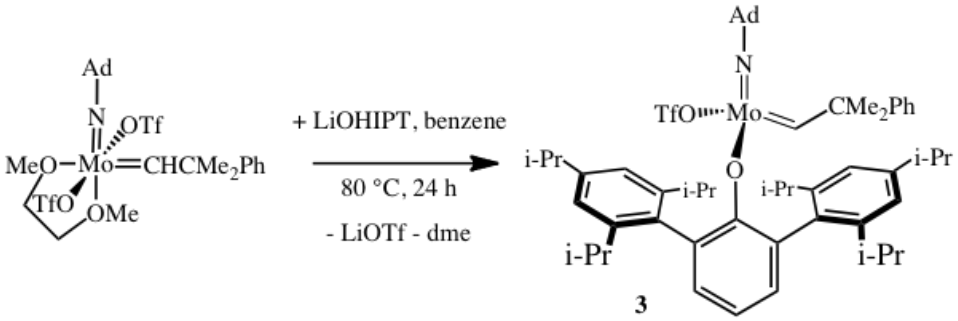
(2)

Each molybdenum center in **1b** (Figure 3) exhibits a pseudo-octahedral geometry. The two η^1-pyrrolides are *trans* to one another and two cyano groups from each of the two adjacent neighboring Mo complexes are coordinated *trans* to the alkylidene and imido ligands. Eight bispyrrolide units of this type are linked through cyano donor interactions to yield the doughnut-like octameric structure. The bond lengths and angles in any one unit in the octamer are not unusual. (See Supporting Information for bond distances and angles.) It should be noted that $Mo(NAr)(CHCMe_2Ph)(NC_4H_4)_2$ was found to be a dimer, $\{Mo(NAr)(\textit{syn}\text{-}CHCMe_2Ph)(\eta^5\text{-}NC_4H_4)(\eta^1\text{-}NC_4H_4)\}\{Mo(NAr)(\textit{syn}\text{-}CHCMe_2Ph)(\eta^1\text{-}NC_4H_4)_2\}$, in which the nitrogen in the η^5-pyrrolide bound to one Mo behaves as a donor to the other Mo.[24]

Compound **1b** reacts with Me_3COH, $(CF_3)_2CHOH$, and $(CF_3)_3COH$ in C_6D_6 at 22 °C to give the known bisalkoxide complexes exclusively, according to NMR studies. However, **1b** does not react with one equivalent of HIPTOH (~0.1 M in **1b** and HIPTOH) even at 100 °C over a period of days. We suspect that the sluggish reaction between **1b** and HIPTOH is a consequence either of an inability of the bulky phenol to compete with the two cyano donors, or the steric demands of the 2-cyanopyrrolides in hypothetical $Mo(NAr)(CHCMe_2Ph)(\eta^1\text{-}2\text{-}CNPyr)_2$.

Formation of a monotriflate monoaryloxide complex and reactions thereof

The reaction between $Mo(NAd)(CHCMe_2Ph)(OTf)_2(DME)$ and LiOHIPT in benzene at 80 °C leads to formation of $Mo(NAd)(CHCMe_2Ph)(OTf)(OHIPT)$ (**3)** in 99% yield (equation 3). Replacement of the triflate in **3** upon reaction of **3** with LiOHIPT to yield hypothetical $Mo(NAd)(CHCMe_2Ph)(OHIPT)_2$ must be slow for steric reasons. Filtration of the reaction



3 (3)

mixture and removal of the benzene *in vacuo* yields **3** as a dark yellow solid that can be employed in subsequent reactions without further purification. Compound **3** shows a single resonance in its ^{19}F NMR spectrum at δ -75.4 ppm, consistent with the formation of a monotriflate species, while a single *syn* alkylidene resonance is found at 12.35 ppm (J_{CH} = 123 Hz) in its ^1H NMR spectrum.

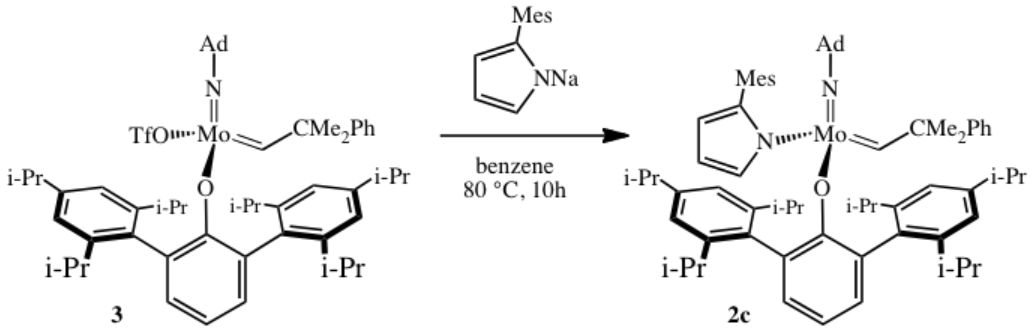
Crystals of **3** suitable for an X-ray study could not be obtained. However, a trimethylphosphine adduct (**3**(PMe_3)**)** could be prepared readily and crystals suitable for an X-ray study obtained. As shown in Figure 4 **3**(PMe_3) is approximately a square pyramid with the

alkylidene in the apical position and PMe_3 coordinated *trans* to the triflate ligand. The bond distances and angles in **3**(PMe_3) are similar to what have been found recently in other PMe_3 adducts of imido alkylidene complexes such as Mo(NAr)($CHCMe_2Ph$)(Me_2Pyr)(OBr_2Bitet)(PMe_3)[25] and Mo(NAr)($CHCMe_2Ph$)(Ph_2Pyr)(OR_{F6})(PMe_3).[6] The structure of a trimethylphosphine adduct has often been viewed as analogous to that of an initial olefin adduct of an imido alkylidene complex before the TBP metallacyclobutane complex is formed. If that were the case, the imido and OHIPT ligands (N(1)-Mo(1)-O(1) = 153.63(5)° in **3**(PMe_3)) would end up in apical positions in a TBP metallacyclobutane intermediate, as found in unsubstituted TBP metallacyclobutane complexes prepared from Mo or W MAP species containing one OHIPT or OBr_2Bitet ligand.[8b,9a,11]

An attempted synthesis of a monotriflate complex in a reaction between Mo(NAr)($CHCMe_2Ph$)($OTf)_2$(DME) (Ar = 2,6-i-$Pr_2C_6H_3$) and LiOHIPT in benzene at 80 °C led only to unidentified products. In contrast, a reaction between Mo(NAr)($CHCMe_2Ph$)($OTf)_2$(DME) and $NaOBr_2Bitet$ led to formation of primarily burgundy red Mo(NAr)($CHCMe_2Ph$)($OBr_2Bitet)_2$ in good yield.[26] Attempts to prepare OHMT analogs of **3** in which NR is NAr, NAr' (N-2,6-$Me_2C_2H_3$), $NAr^{i\text{-}Pr}$ (N-2-i-PrC_2H_4), or NAd were not successful. We propose that in the above circumstances the nucleophile attacks and deprotonates the alkylidene ligand at a rate competitive with nucleophilic attack at the metal center. We have also noted that when Mo(NAr^M)($CHCMe_2Ph$)($OTf)_2$(DME) (Ar^M = 2-mesitylphenyl)[27] and Mo(NAr^T)($CHCMe_3$)($OTf)_2$(DME) (Ar^T = 2-(2',4',6'-triisopropylphenyl)[27] were each treated with one equivalent of LiOHIPT the alkylidene peaks corresponding to the starting materials disappeared over time, no new alkylidene complexes were formed, and HIPTOH is observed as a product of the reaction. Clearly a fine balance of steric and electronic factors allows **3** to form in good yield. There is ample evidence in the literature that alkylidyne ligands can be formed through deprotonation of alkylidene ligands,[28] although other complications could be envisioned.

A reaction between one equivalent of sodium 2-mesitylpyrrolide and **3** in benzene (80 °C

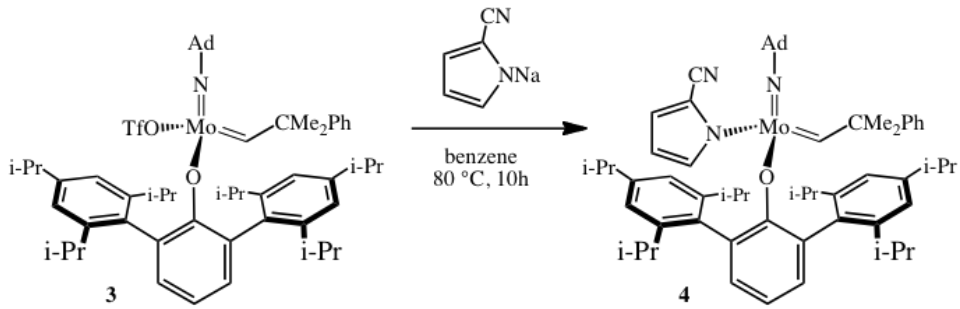
for 10 h) led to the formation of Mo(NAd)(CHCMe$_2$Ph)(OHIPT)(2-Mespyr) (**2c**) in 45% yield (eq 4). A single alkylidene resonance (at 12.25 ppm) with a J_{CH} characteristic of a *syn* species



(4)

(120 Hz) is observed in the ^{1}H NMR spectrum of **2c**. A structural study of **2c** reveals it to have a slightly distorted tetrahedral geometry in which the mesityl group points away from the sterically demanding OHIPT ligand toward the relatively small adamantylimido ligand (Figure 5). Therefore, the imido ligand is bent slightly (Mo(1)-N(1)-C(11) = 163.58(11)°). It is important to note, as stated earlier, that we have not been able to prepare compound **2c** through addition of HIPTOH to Mo(NAd)(CHCMe$_2$Ph)(Mespyr)$_2$, at least not under the conditions we have tried so far. Therefore, **2c** must be assembled through selective nucleophilic displacements. The yield may be limited as a consequence of some competition between deprotonation of the alkylidene ligand and substitution of the triflate ligand.

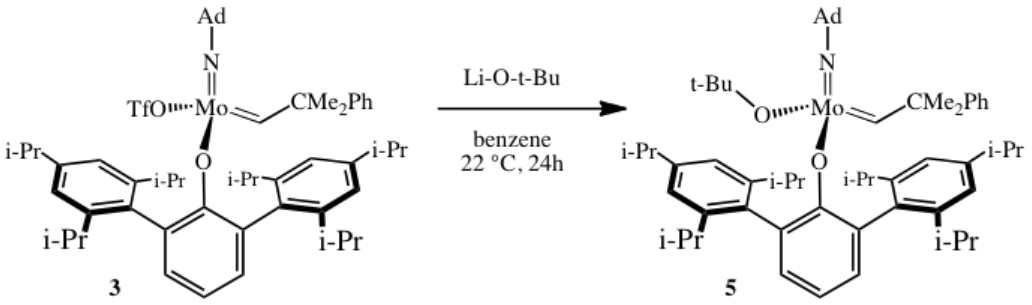
Reaction of **3** with one equivalent of Li(2-CNPyr) in benzene at room temperature gave a complex mixture of products from which Mo(NAd)(CHCMe$_2$Ph)(2-CNPyr)(OHIPT) (**4**) could



(5)

be isolated in 25% yield (equation 5). Formation of free HIPTOH and the relatively low yield we propose is again a consequence of deprotonation of the alkylidene. The ^{1}H NMR spectrum of pure **4** is straightforward; the *syn* alkylidene has a J_{CH} of 121 Hz. An X-ray study of **4** confirmed that it is a monomer (Figure 6). Evidently the steric demands of the HIPTO ligand prevent the cyano group from binding to another Mo center in this circumstance. As noted earlier, we were not able to prepare **4** by heating a mixture of **1b** and HIPTOH, although even the nucleophilic approach to **4** (equation 5) is borderline.

The reaction between one equivalent of LiO-*t*-Bu and **3** in benzene at room temperature for one day led to the formation of Mo(NAd)(CHCMe$_2$Ph)(OHIPT)(OCMe$_3$) (**5**) in 22% isolated yield (eq 6). We propose that the low yield again is a consequence, at least in part, of



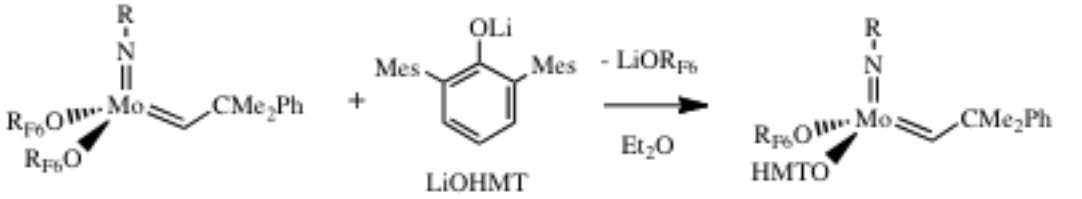
(6)

competitive deprotonation of the alkylidene ligand. A single alkylidene resonance (at 11.16 ppm) with J_{CH} characteristic of a *syn* species (119 Hz) was observed in the ^{1}H NMR spectrum of **5**. A structural study reveals **5** to have the expected tetrahedral geometry (Figure 7). The Mo(1)-O(2)-C(71) angle (143.3(2)°) and the Mo(1)-O(1)-C(21) angle (145.2(2)°) are essentially identical. The extent to which other possible products are formed, e.g., Mo(NAd)(CHCMe$_2$Ph)(OCMe$_3$)$_2$, in the reaction shown in equation 6 is not known. There is no evidence for disproportionation of **5** in solution under mild conditions, perhaps because facile formation of hypothetical Mo(NAd)(CHCMe$_2$Ph)(OHIPT)$_2$ may be unlikely for steric reasons.

Synthesis of SAM complexes from bishexafluoro-t-butoxide complexes

In the previous section we noted that deprotonation of the alkylidene ligand is a likely complication of attempted nucleophilic substitutions at the metal when one or two triflate ligands are present. In past studies we noted that whereas addition of two equivalents of $LiNPh_2$ to $Mo(NAr)(CHCMe_2Ph)(OTf)_2(DME)$ yielded $Mo(NAr)(CHCMe_2Ph)(NPh_2)_2$ in only 35% yield after a difficult isolation,[16] $Mo(NAr)(CHCMe_2Ph)(OR_{F6})_2$ (OR_{F6} = $OCMe(CF_3)_2$) reacts with two equivalents of $LiNPh_2$ to afford $Mo(NAr)(CHCMe_2Ph)(NPh_2)_2$ in 78% isolated yield without formation of any significant side products. We proposed that deprotonation of the alkylidene is significantly reduced in reactions between $Mo(NAr)(CHCMe_2Ph)(OR_{F6})_2$ and amido mucleophiles. Therefore, we evaluated the possibility of employing bishexafluoro-t-butoxide complexes as starting materials for making $Mo(NR)(CHCMe_2Ph)(OR_{F6})(Y)$ complexes.

When $Mo(NR)(CHCMe_2Ph)(OR_{F6})_2$ complexes are treated with one equivalent of LiOHMT, $Mo(NR)(CHCMe_2Ph)(OR_{F6})$(OHMT) complexes are formed where R = Ar (**6a**), Ar' (**6b**), Ar^{iPr} (**6c**), or Ad (**6d**) in moderate to good yields (43-80 %, equation 7). Complexes **6b**-**6d** can be made without formation of any significant byproducts, except in the case of **6a**. The proton NMR spectrum of crude of **6a** shows that a substantial amount of HMTOH forms, consistent



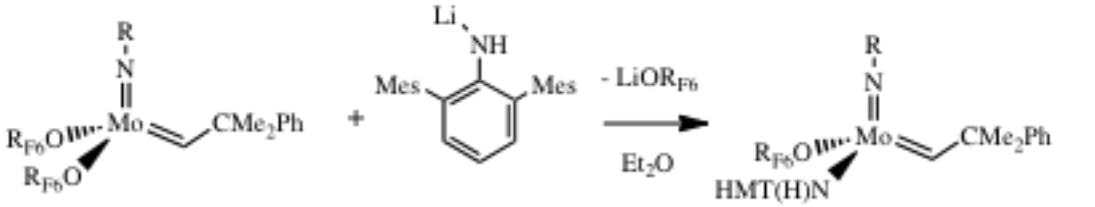
(7)

6a R = Ar (43%); **6b** R = Ar' (80%)
6c R = Ar^{iPr} (71%); **6d** R = Ad (59%)

with deprotonation of the alkylidene ligand. Like **5**, compounds **6** show no tendency to disproportionate to yield bishexafluoro-t-butoxide and bis(OHIPT) complexes.

The structure of complex **6d** is shown in Figure 8. The HMTO ligand is oriented so that one of the mesityl groups points toward the imido group while the other points into the COO face of the tetrahedron. In this case the Mo(1)-O(1)-C(21) bond angle (145.23(12)^{o}) and Mo(1)-O(2)-C(31) bond angle (154.38(10)^{o}) differ in the direction one might expect.

When Mo(NR)(CHCMe$_2$Ph)(OR$_{F6}$)$_2$ is treated with one equivalent of LiN(H)HMT at 22 °C in diethyl ether, **7a** (R = Ar') and **7b** (R = Ar^{iPr}) could be obtained cleanly (equation 8). Proton NMR spectra of **7a and 7b** show only one alkylidene peak (at 11.86 ppm for **7a** and 11.72 ppm for **7b**) and one NH resonance (at 7.82 ppm for **7a** and 7.99 ppm for **7b**).



(8)

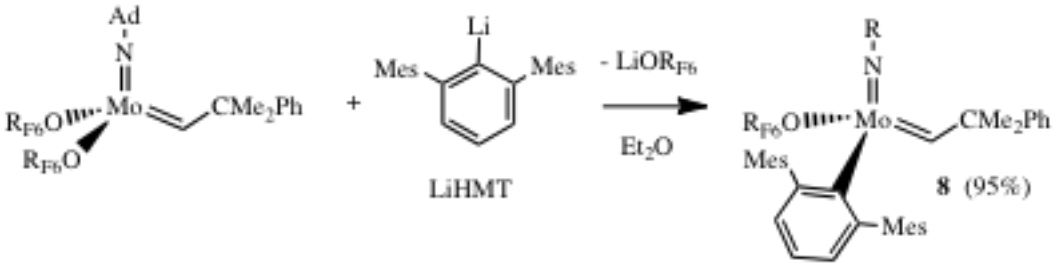
7a R = Ar' (48%); **7b** R = Ar^{iPr} (92%)

The reaction between Mo(NAr)(CHCMe$_2$Ph)(OR$_{F6}$)$_2$ and LiN(H)HMT leads to formation of byproducts, while in the case of the Mo(NAd)(CHCMe$_2$Ph)(OR$_{F6}$)$_2$, substitution appears to be successful, according to proton NMR studies, but the compound could not be isolated in pure form readily. Compounds **7a** and **7b** are believed to be the first examples of imido alkylidene complexes of this general type in which a primary amido ligand is present. Although we have uncovered no evidence that an α proton can mgrate from an amido nitrogen to either an imido nitrogen or an alkylidene carbon atom in the same complex, we would not be surprised if some of the side products formed in reactions of this type were to result from loss of the amido proton from the amido ligand in **7** in the presence of strong nucleophiles.

The structure of **7b** is shown in Figure 9 with relevant bond distances and angles listed either in the figure caption or in Table 1. The Mo(1)-N(2) bond distance (1.9950(13) Å) is similar to Mo-N$_{amido}$ distances in Mo(NAr)(CHCMe$_2$Ph)(NPh$_2$)$_2$ complexess[16] (2.007(3) and 2.009(3) Å),

but the Mo(1)-N(2)-C(31) bond angle (133.32(11)^{o}) is significantly larger than those of the bisamide complex (118.61(19)^{o} and 117.6(3)^{o}), either because of the steric demands of the HMT substituent in the N(H)(HMT) ligand, or an N-H agostic interaction, or both.

When Mo(NAd)(CHCMe$_2$Ph)(OR$_{F6}$)$_2$ was treated with one equivalent of LiHMT Mo(NAd)(CHCMe$_2$Ph)(OR$_{F6}$)(HMT) (**8**) could be obtained as a crystalline yellow solid (equation 9). A proton NMR spectrum of **8** reveals the presence of only one product, as determined by the presence of only one alkylidene peak at 10.99 ppm in its ^{1}H-NMR spectrum and the set of quartets in its ^{19}F-NMR spectrum.



(9)

When the imido ligand is NAr in a reaction analogous to that shown in equation 9 the steric crowding is so significant that even after 5 days of heating the mixture only 18 % of a new alkylidene species is formed. When R = Ar', the reaction reaches 90 % completion after 5 days to yield two alkylidene products with alkylidene resonances at 11.7 ppm (78%) and 11.0 ppm (12%). No product analogous to **8** could be isolated in either of these reactions. When Mo(NAd)(CHCMe$_2$Ph)(OTf)$_2$(DME) is treated with 1 equivalent of LiHMT the alkylidene peak corresponding to the starting material disappears but no new alkylidene peak appears.

The structure of **8** is shown in Figure 10. The hexafluoro-t-butoxide ligand is disordered. A front view of the disordered hexafluoro-t-butoxide ligand is shown in the Supporting Information (Figure S1). The Mo(1)-C(21) bond length (2.188(5) Å) is typical of a Mo-C bond length. However, the HMT ligand is considerably more sterically demanding than an OHMT ligand since no heteroatom is present between the Mo and C(21). No analogous species could be

prepared that contains the NAr group. Compound **8** is a rare example of a SAM Mo complex that contains an carbon-based ligand singly bound to the metal. The only other examples are monoalkoxide mononeopentyl imido alkylidene complexes of Mo and W.[17]

ROMP polymerization of 2,3-dicarbomethoxynorbornadiene has been employed to determine as to whether a given catalyst can produce a polymer with a single structure. For example, DCMNBD (2,3-dicarbomethoxynorbornadiene) was polymerized by Mo(NAd)(CHCMe$_2$Ph)(Pyr)(OHIPT) to give a >99% *cis* and highly tactic poly(DCMNBD) that is proposed to be *syndiotactic* on the basis of formation of what could be proven to be >99% *cis,syndiotactic* polymer employing 2,3-dicarbo*menthoxy*norbornadiene.[9a] Complexes of the type Mo(NR)(CHCMe$_2$Ph)(Pyr)(OHMT) (where R = 2,6-diisopropylphenyl, 2,6-dimethylphenyl, 2-isopropylphenyl, or 1-adamantyl) have also been found to yield >99% *cis,syndiotactic*-poly(DCMNBD).[28] In contrast, with the exception of **6c**, polymerization of DCMNBD with **6a**, **6b**, **6d**, **7a**, **7b**, and **8**, did not produce highly structured poly(DCMNBD). The structures of poly(DCMNBD) samples obtained with initiators **6a** and **7b** were biased toward *cis,isotactic*, behavior that is not readily explicable, but not unusual for bisalkoxide species (Table 2).[29] Finally, it should be noted that polymerization of DCMNBD initiated by **8** was exceedingly slow, requiring days to consume 95% of the 100 equivalents of monomer under the same conditions employed for the other initiators. We attribute the sluggishness of **8** as an initiator to the presence of the extremely high steric demand of the HMT ligand.

CONCLUSIONS

We have found that several stereogenic-at-metal imido alkylidene complexes can be accessed through selective nucleophilic displacement reactions in imido alkylidene complexes of molybdenum. Those that are monopyrrolide complexes could not be made through protonolysis of the required bispyrrolide. A persistant problem that is exacerbated in sterically crowded circumstances is what is proposed to be competitive deprotonation of the alkylidene ligand in competition with substitution of (usually) a triflate ligand; product yield is consequently reduced

and isolation of pure product is compromised by byproduct formation. Several Mo(NR)(CHR')(X)(Y) variations in which neither X nor Y is a pyrrolide could be prepared, including Mo(NR)(CHCMe$_2$Ph)(OR$_{F6}$)(Y) complexes in which Y is OHMT, N(H)HMT, or HMT (HMT = 2,6-dimesitylphenyl). Deprotonation of the alkylidene in Mo(NR)(CHCMe$_2$Ph)(OR$_{F6}$)$_2$ apparently is not facile relative to nucleophilic displacement of the OR$_{F6}$ ligand in the syntheses of Mo(NR)(CHCMe$_2$Ph)(OR$_{F6}$)(Y) complexes.

Acknowledgement. R.R.S. thanks the National Science Foundation (CHE-0841187 and CHE-0946721) for research support. The department of chemistry thanks the NSF (CHE-9808061) for funds to purchase a Varian 500 NMR instrument.

Supporting Information Available. Synthesis and characterization details for all complexes. Crystallographic details, fully labeled thermal ellipsoid diagrams for all crystallographically characterized species and crystallographic information files in CIF format. Supporting Information is available free of charge via the Internet at http://pubs.acs.org. Data for the X-ray structures are also available to the public at http://www.reciprocalnet.org.

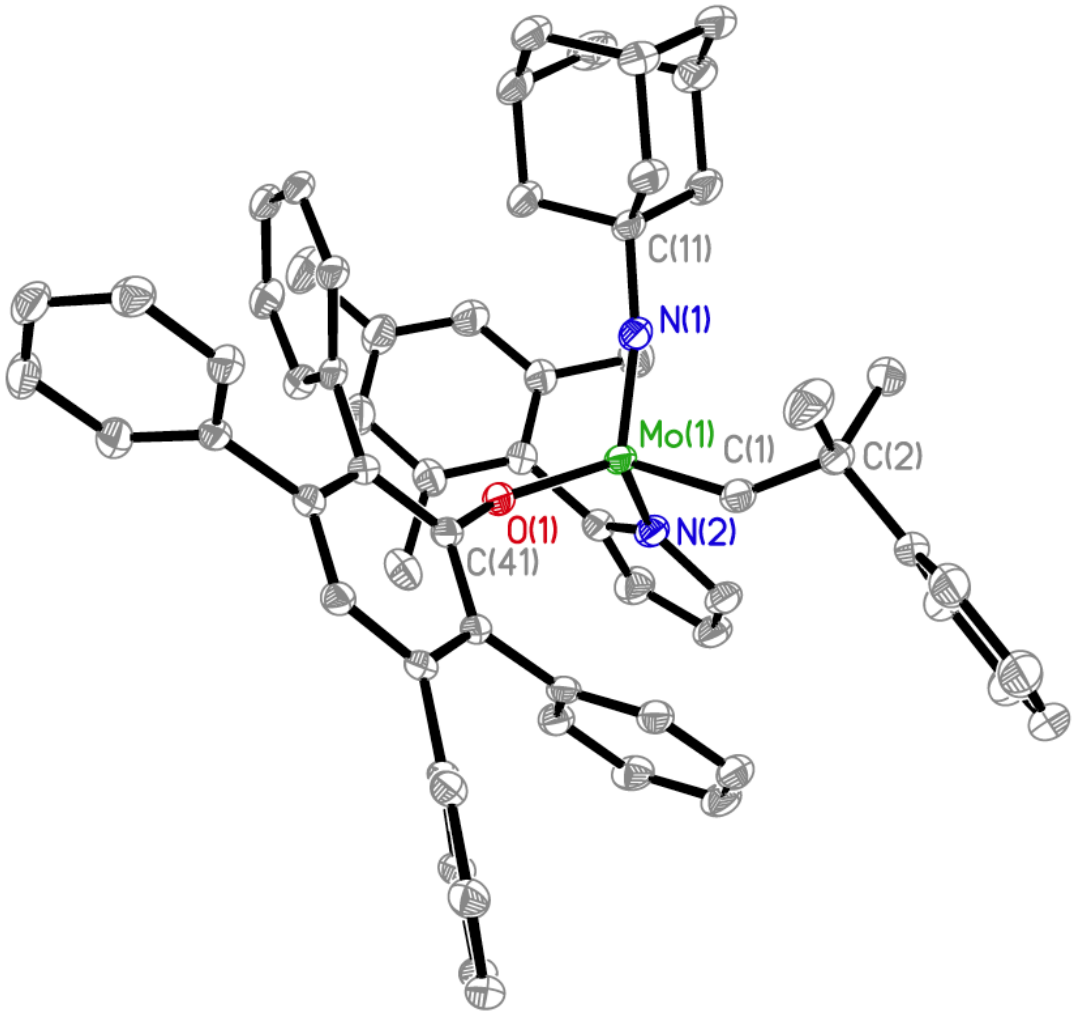


Figure 1. Thermal ellipsoid drawing of Mo(NAd)(CHCMe$_2$Ph)(2-MesPyr)(OTPP) (**2a**) (ellipsoids at 50% probability level). Hydrogen atoms and solvent molecules are omitted for clarity. Selected bond lengths (Å) and angles (°) can be found in Table 1.

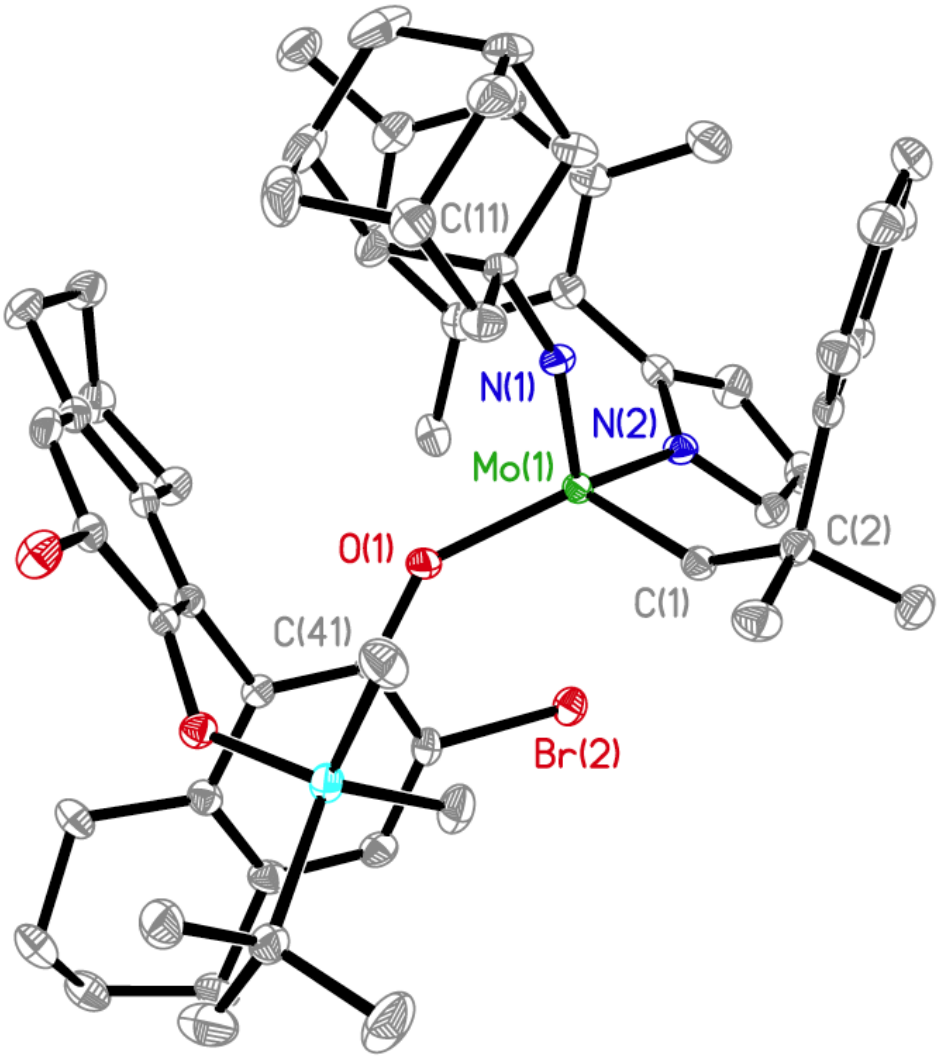


Figure 2. Thermal ellipsoid drawing of (*S*)-Mo(NAd)(CHCMe$_2$Ph)(2-MesPyr)(OBr$_2$Bitet) ((*S*)-**2b**) (ellipsoids at 50% probability level). Hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (°) can be found in Table 1.

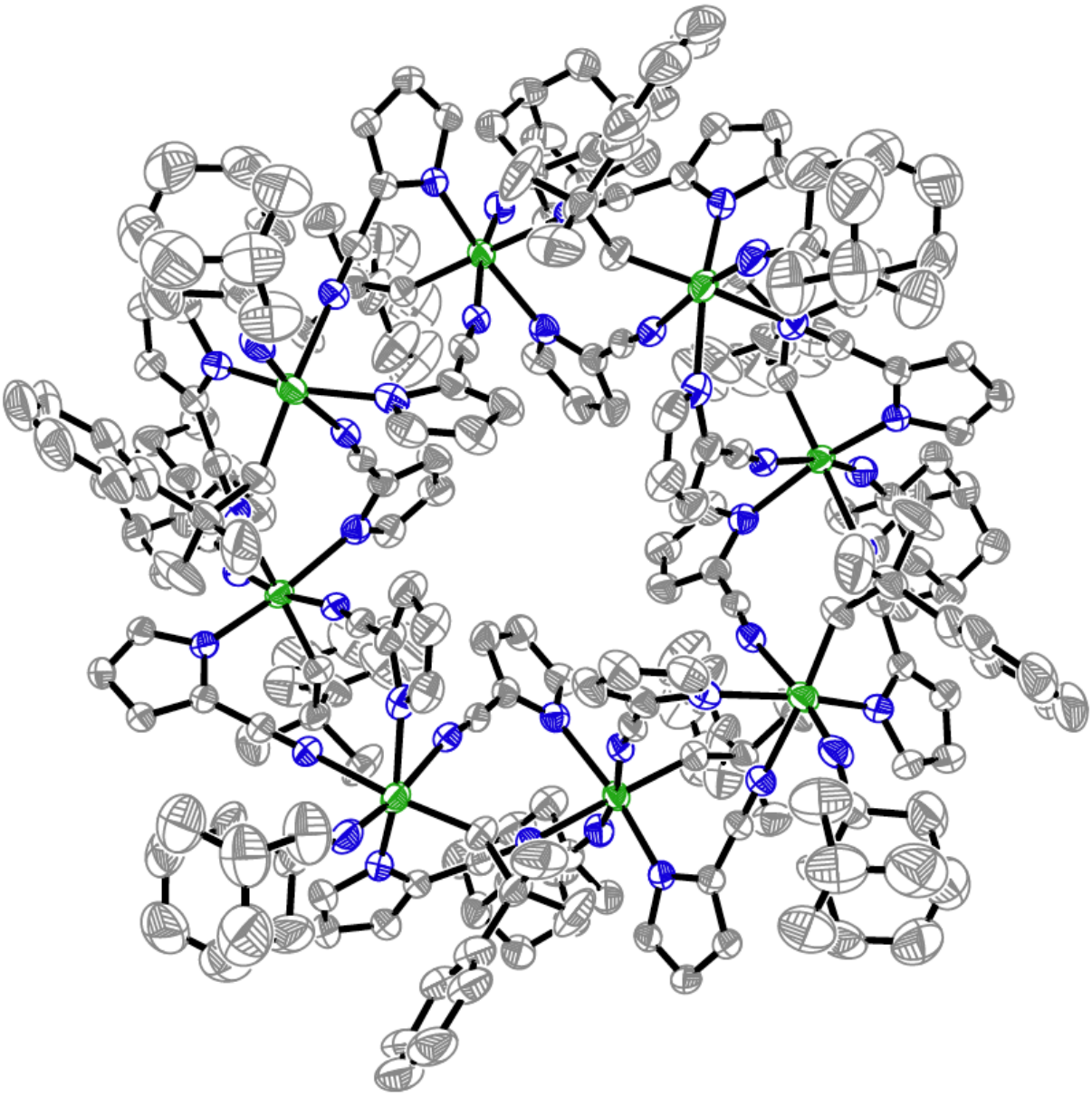


Figure 3. Thermal ellipsoid drawing of Mo(NAd)(CHCMe$_2$Ph)(2-CNPyr)$_2$ (**1b**) (ellipsoids at 30% probability level). Hydrogen atoms, minor components of disorders, and solvent molecules are omitted for clarity. Atom colors: Mo (green); N (blue); C (gray).

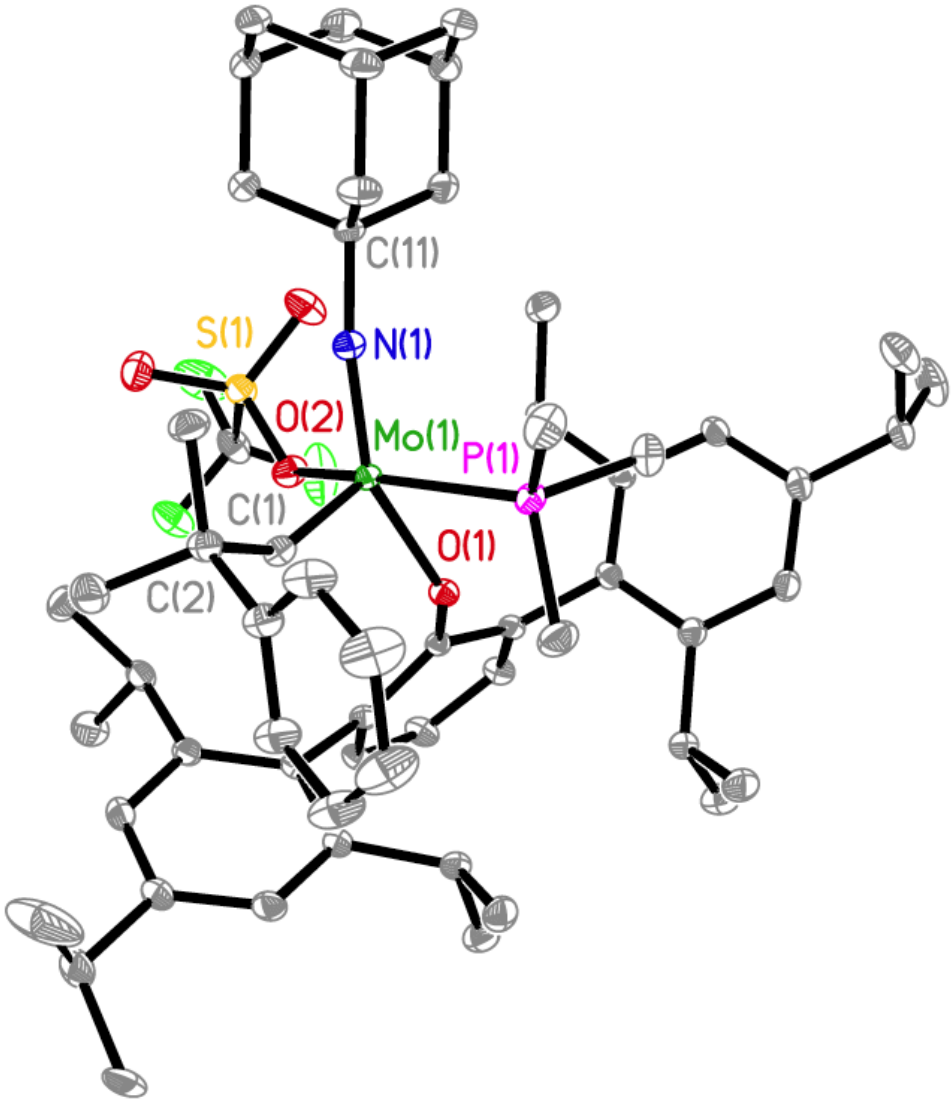


Figure 4. Thermal ellipsoid drawing of **3**(PMe_3) (ellipsoids at 50% probability level). Hydrogen atoms and the minor component of the disorder are omitted for clarity. Selected bond lengths (Å) and angles (°) can be found in Table 1.

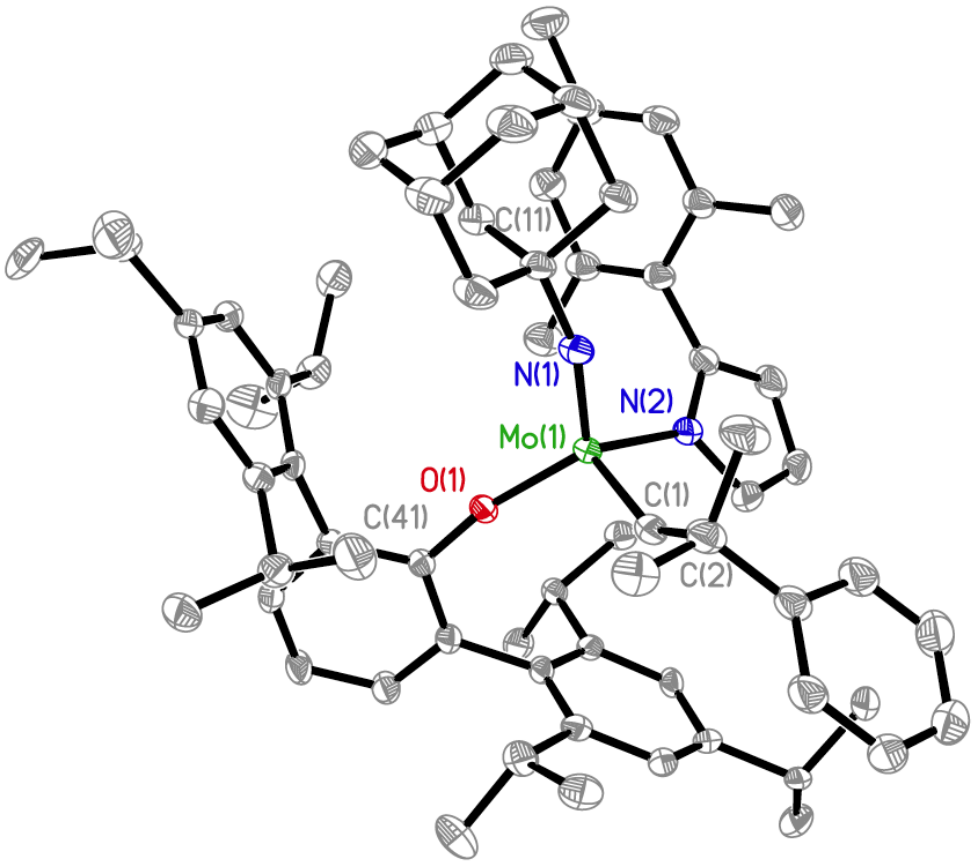


Figure 5. Thermal ellipsoid drawing of **2c** (ellipsoids at 50% probability level). Hydrogen atoms, minor components of disorders, and the solvent molecule are omitted for clarity. Selected bond lengths (Å) and angles (°) can be found in Table 1.

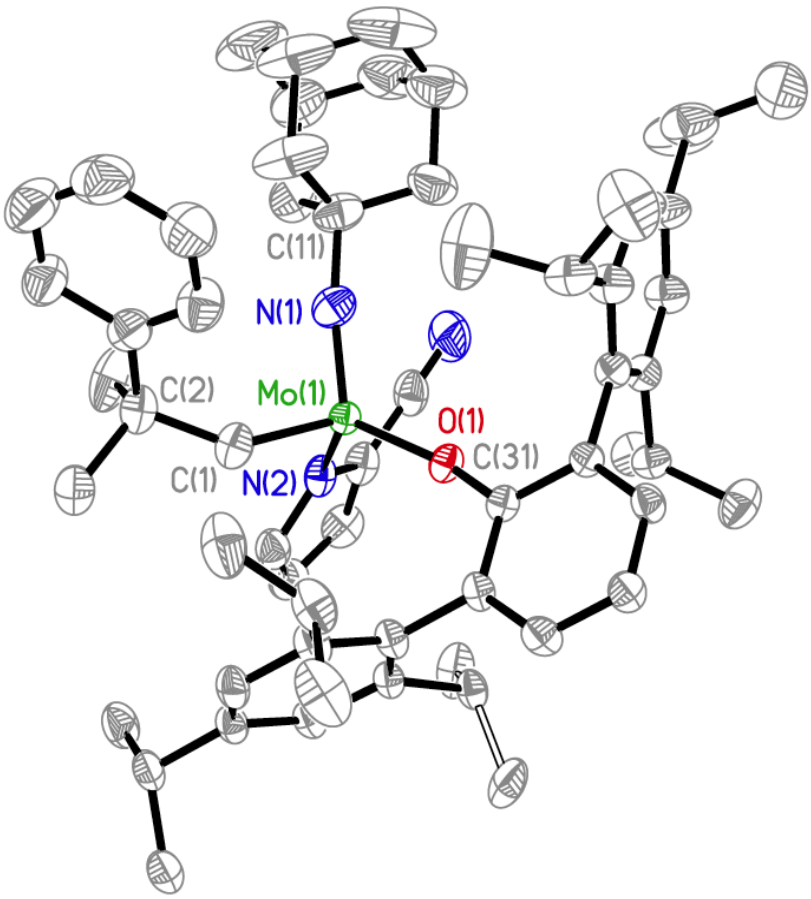


Figure 6. Thermal ellipsoid drawing of Mo(NAd)($CHCMe_2Ph$)(2-CNPyr)(OHIPT) (**4**). (ellipsoids at 50% probability level). Hydrogen atoms and minor components of disorders are omitted for clarity. Selected bond lengths (Å) and angles (°) can be found in Table 1.

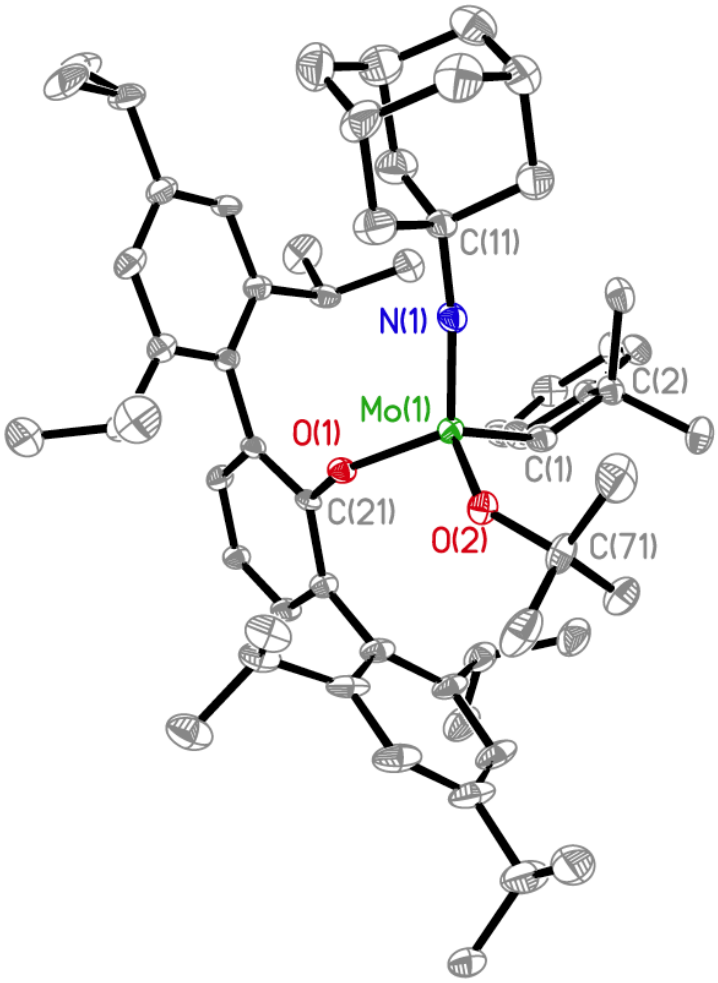


Figure 7. Thermal ellipsoid drawing of **5** (ellipsoids at 50% probability level). Hydrogen atoms are omitted for clarity; only one independent molecule is shown. Selected bond lengths (Å) and angles (°) can be found in Table 1.

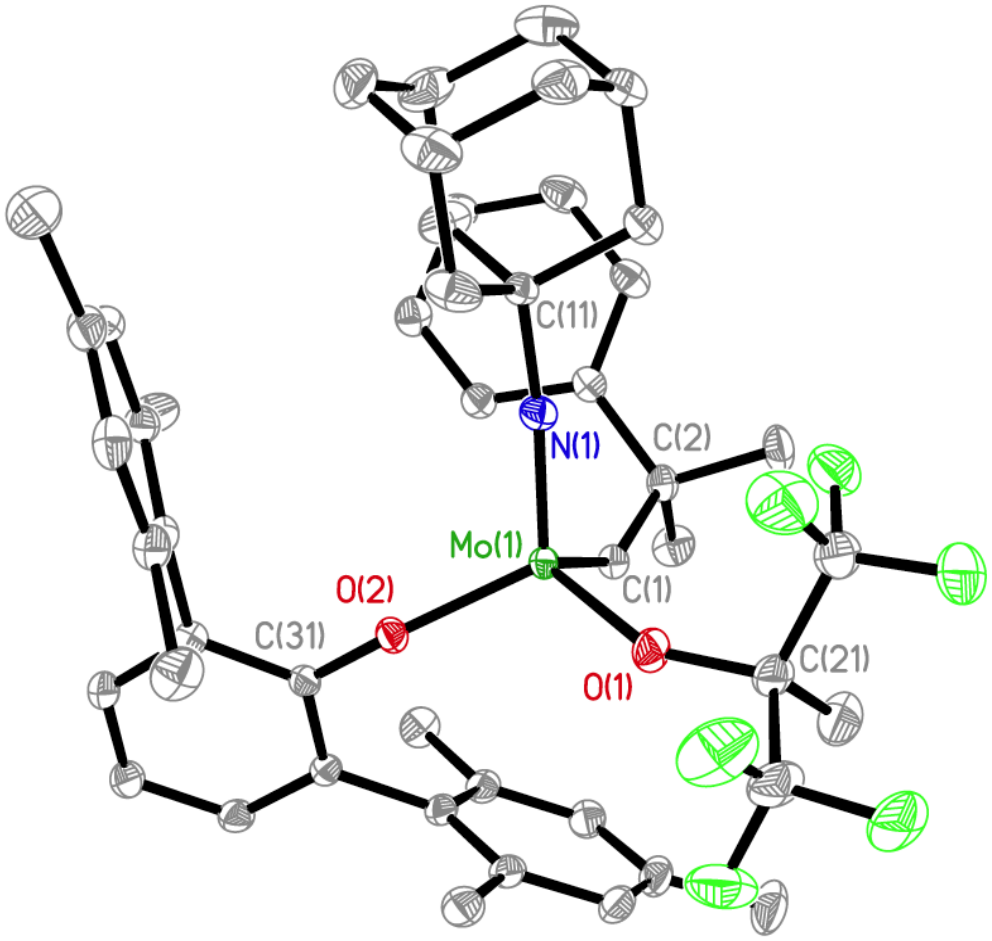


Figure 8. The solid state structure of **6d** (50% probability ellipsoids). Hydrogen atoms are omitted for clarity. Selected bond lengths (Å) and angles (°) can be found in Table 1.

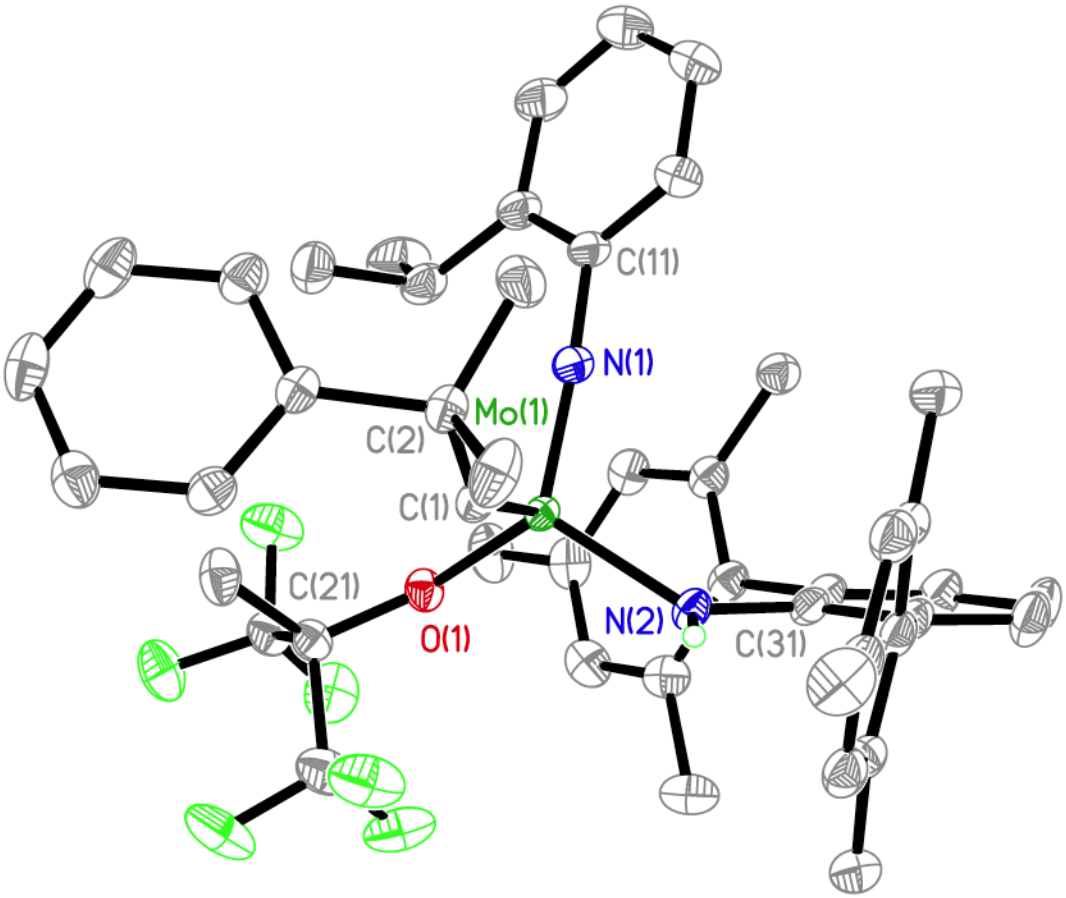


Figure 9. The solid state structure of **7b** (50% probability ellipsoids). Hydrogen atoms are omitted for clarity, except for the hydrogen on N(2). Selected bond lengths (Å) and angles (°) can be found in Table 1.

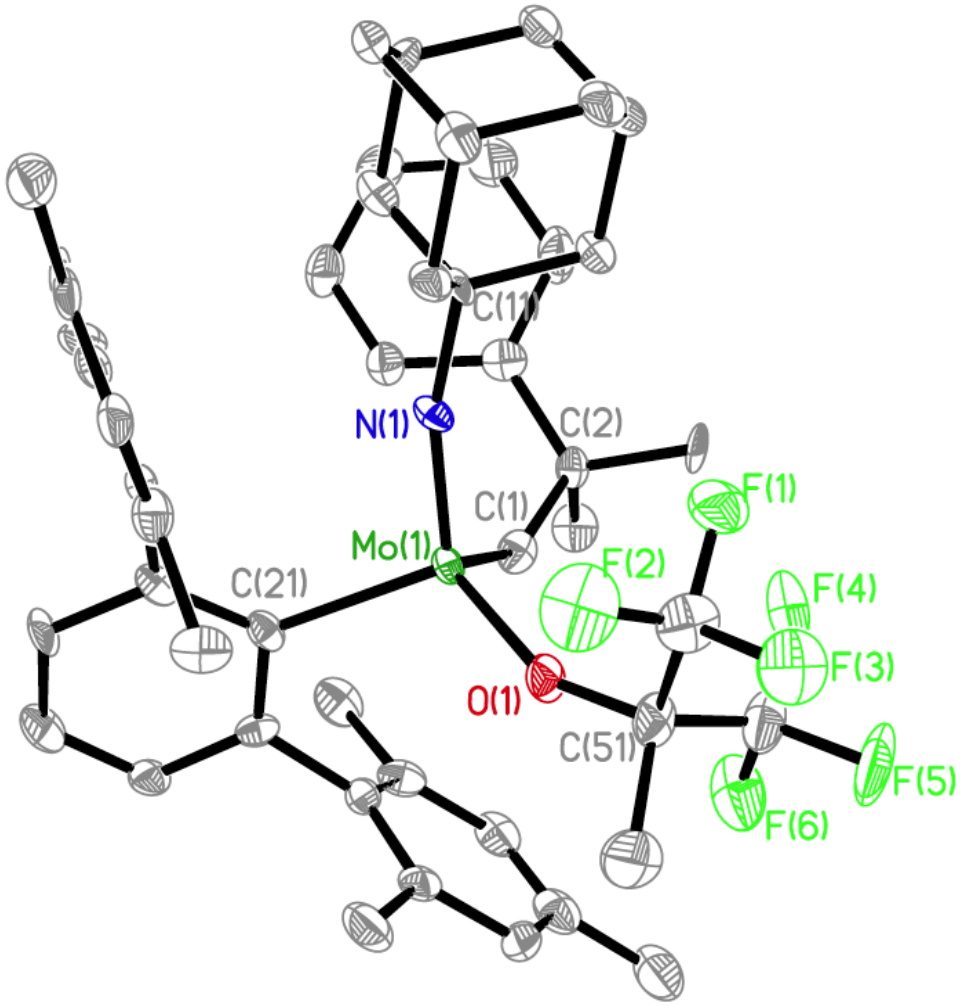


Figure 10. The solid state structure of **8** (50% probability ellipsoids). Hydrogen atoms and minor disorder components are omitted for clarity; only one independent molecule is shown. Selected bond lengths (Å) and angles (°) can be found in Table 1.

Table 1. Selected bond lengths (Å) and bond angles (°) in Mo(NR)(CHR')(OR'')(X) complexes.

	2a	**2b**	**2c**	**3(PMe$_3$)**	**4**	**5**	**6d**	**7b**	**8**
Mo=C	1.886(2)	1.888(2)	1.8811(16)	1.8951(16)	1.883(4)	1.880(3)	1.8821(16)	1.8833(16)	1.895(5)
Mo–X	2.0527(19)	2.0608(18)	2.0551(13)	1.7413(13)	2.053(3)	1.879(2)	1.9444(12)	1.9950(13)	2.188(5)
Mo=N	1.7099(17)	1.7074(18)	1.7127(13)	2.0180(11)	1.714(3)	1.713(3)	1.7028(14)	1.7261(13)	1.703(4)
Mo–O	1.9334(14)	1.9654(15)	1.909(5)	2.1721(11)	1.906(2)	1.941(2)	1.9230(11)	1.9518(11)	1.943(5)
Mo=N–C	167.81(15)	159.50(15)	163.58(11)	168.35(11)	171.6(3)	168.73(3)	169.14(12)	173.09(12)	162.1(4)
Mo–O–C	150.88(13)	142.25(14)	169.3(10)	139.66(9)	163.00(19)	145.2(2)	154.38(10)	140.93(10)	156.2(8)
Mo-C-C	145.64(15)	144.77(16)	144.53(12)	147.17(12)	142.4(3)	145.6(3)	141.90(12)	144.78(12)	144.7(4)

Table 2. ROMP of 2,3-dicarbomethoxynorbornadiene (DCMNBD).[a]

Catalyst	**[Cat] (mM)**	**Eq DCMNBD**	**Structure**
6a Mo(NAr)(CHR')(OR_{F6})(OHMT)	4.6	50	> 98% *cis*,78% iso
6b Mo(NAr')(CHR')(OR_{F6})(OHMT)	4.9	50	95% *cis*,73% syndio
6c Mo(NAr^{iPr})(CHR')(OR_{F6})(OHMT)	4.8	50	98% *cis*,95% syndio
6d Mo(NAd)(CHR')(OR_{F6})(OHMT)	4.7	50	90% *cis*,76% syndio
7a Mo(NAr')(CHR')(OR_{F6})[N(H)HMT]	4.9	50	95% *cis*,71% syndio
7b Mo(NAr^{iPr})(CHR')(OR_{F6})[N(H)HMT]	4.8	50	90% *cis*,54% iso
8 Mo(NAd)(CHR')(OR_{F6})(HMT)	4.8	100	83% *cis*,91% syndio[b]

[a] R' = CMe_2Ph. [b] Five days were required to reach full conversion.

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Supporting Information for

Synthesis of Monoaryloxide Monotriflate Alkylidene Complexes of Molybdenum

by

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EXPERIMENTAL SECTION

General. All manipulations of air and moisture sensitive materials were conducted under a nitrogen atmosphere in a Vacuum Atmospheres glovebox or on a dual-manifold Schlenk line. All glassware, including NMR tubes, was dried in an oven prior to use. Ether, pentane, toluene, dichloromethane, toluene, and benzene were degassed with dinitrogen, passed through activated alumina columns, and stored over 4 Å Linde-type molecular sieves. Dimethoxyethane was distilled *in vacuo* from a dark purple solution of sodium benzophenone ketyl and degassed three times by a freeze-pump-thaw procedure. Deuterated solvents were dried over 4 Å Linde-type molecular sieves prior to use. Proton and carbon NMR spectra were acquired using 500 MHz Varian and 400 MHz Bruker spectrometers at room temperature, are reported as parts per million relative to tetramethylsilane, and are referenced to the residual $^{1}H/^{13}C$ resonances of the deuterated solvent (^{1}H: $CDCl_3$, δ 7.26; C_6D_6, δ 7.16. ^{13}C: $CDCl_3$, δ 77.23; C_6D_6, δ 128.39). Compounds 2-CNPyrH,[1b] 2-MesPyrH,[1] HMTOH,[3] $HMTNH_2$,[4] HMTLi,[5] DCMNBD,[6] $Mo(NAd)(CHCMe_2Ph)(OTf)_2(DME)$[2a], and $Mo(NR)(CHCMe_2Ph)(OR_{F6})_2$[2] were synthesized according to literature procedures. Li(2-CNPyr), Li(2-MesPyr), LiOHMT, and LiN(H)HMT were obtained by treating 2-CNPyrH, 2-MesPyrH, HMTOH, and $HMTNH_2$ each with one equivalent of *n*-BuLi at -35 ^{o}C in diethyl ether. Elemental analyses were performed by Midwest Microlab, Indianapolis, Indiana.

Synthesis of $Mo(NAd)(CHCMe_2Ph)(2\text{-}MesPyr)_2$ (1a).

$Mo(NAd)(CHCMe_2Ph)(OTf)_2(DME)$ (0.962 g, 1.26 mmol) was dissolved in ether (15 mL) and the solution was cooled to – 30 °C. Li(MesPyr) (0.505 g, 2.64 mmol, 2.1 equivalents) was added in portions to the ethereal suspension. The reaction mixture was allowed to warm to room temperature and was stirred for 2 h. A large amount of yellow precipitate of the product formed during the reaction. The yellow solid was filtered off and washed with cold ether. The filtrate was concentrated and recrystallized to yield another crop of product; total yield 0.70 g (75%):

^{1}H NMR (500 MHz, C_6D_6) δ 10.24 (s, 1H, *syn* Mo=C*H*, J_{CH} = 117.5 Hz), 7.30 (d, 2H, *Ar*, *J* = 7.5 Hz), 7.08–7.12 (overlapping resonances, 4H, *Ar & pyr*), 6.99 (t, 1H, *Ar*, *J* = 7.5 Hz), 6.89 (s, 2H, *Ar*), 6.84 (s, 2H, *Ar*), 6.54 (m, 2H, *Pyr*), 6.23 (m, 2H, *Pyr*), 2.18 (s, 6H, *Pyr*), 2.10 (s, 12H, *Pyr*), 1.74 (br s, 3H, *Ad*), 1.44 (br s, 6H, *Ad*), 1.35 (s, 6H, C*Me*$_2$Ph), 1.32 (br s, 6H, *Ad*); ^{13}C{^{1}H} NMR (125 MHz, C_6D_6) δ 281.8 (Mo=*C*), 149.9, 140.2, 139.8, 138.7, 137.6, 135.1, 133.1, 128.8, 128.6, 128.4, 128.3, 127.5, 126.3, 111.5, 110.0, 78.5, 53.3, 43.5, 35.6, 31.3, 29.9, 21.3, 21.2, 21.1. Anal. Calcd for $C_{46}H_{55}N_3Mo$: C, 74.07; H, 7.43; N, 5.64. Found: C, 74.09; H, 7.30; N, 5.93.

Synthesis of Mo(NAd)(CHCMe$_2$Ph)(2-CNPyr)$_2$ (1b).

Method 1. Mo(NAd)(CHCMe$_2$Ph)(OTf)$_2$(DME) (1.000 g, 1.31 mmol) was suspended in ether (20 mL) and the solution was cooled to – 30 ^{o}C. Li(2-CNPyr) (0.282, 2.87 mmol, 2.2 equivalents) was added in portions to the ethereal suspension. The reaction was warmed to room temperature and stirred for 4 h. The volatiles were then removed *in vacuo*. Toluene was added to the residue and the mixture was filtered through Celite in order to remove LiOTf. The filtrate was taken to dryness to yield a yellow microcrystalline solid. The crude product was recrystallized from a mixture of THF and *n*-pentane at – 30 ^{o}C to give yellow blocks; yield 0.40 g (55%).

Method 2. Mo(NAd)(CHCMe$_2$Ph)(Me$_2$Pyr)$_2$ (1.001 g, 1.77 mmol) was suspended in ether (20 mL) and the solution was cooled to – 30 ^{o}C. 2-CNPyrH (0.360 g, 3.91 mmol, 2.2 equivalents) was added dropwise to the ethereal suspension. The reaction was warmed to room temperature and stirred for 4 h. The volatiles were then removed *in vacuo* to yield a yellow microcrystalline solid. The crude product was recrystallized from a mixture of THF and *n*-pentane at – 30 °C to give yellow blocks; yield 0.75 g (76%): ^{1}H NMR (500 MHz, C_6D_6) δ 14.47 (s, 1H, Mo=C*H*), 7.49 (s, 1H, *Ar*), 7.44 (s, 1H, *Ar*), 7.12–7.17 (overlapping resonances, 3H, *Ar & Pyr*), 6.99–7.04 (overlapping resonances, 3H, *Ar & Pyr*), 6.58 (m, 1H, *Pyr*), 6.45 (m, 1H, *Pyr*), 6.27 (m, 1H, *Pyr*), 1.98 (m, 6H, *Ad*), 1.79 (br s, 3H, *Ad*), 1.54 (s, 3H, C*Me*$_2$Ph), 1.35 (m, 6H, *Ad*), 1.08 (s, 6H, C*Me*$_2$Ph). Anal. Calcd for $C_{30}H_{33}N_5Mo$: C, 64.39; H, 5.94; N, 12.52. Found: C, 64.05; H, 5.95; N, 12.39.

Synthesis of Mo(NAd)(CHCMe$_2$Ph)(2-MesPyr)(OTPP) (2a). A solution of Mo(NAd)(CHCMe$_2$Ph)(2-MesPyr)$_2$ (0.200 g, 0.270 mmol) and HOTPP (0.107 g, 0.270 mmol) in benzene (10 mL) was heated at 60 ^{o}C in a Schlenk flask for two days. The solvents were removed from the reaction mixture *in vacuo*. An amount of pentane sufficient to dissolve the yellow residue was added and the soluytion was stored at – 30 ^{o}C overnight. Yellow crystals were filtered off and washed with cold pentane. Analytically pure product can be recrystallized from a mixture of toluene and pentane; yield 0.205 g (80%): ^{1}H NMR (500 MHz, C_6D_6) δ 11.17 (s, 1H, *syn* Mo=C*H*, J_{CH} = 119.5 Hz), 7.32 (br m, 4H, *Ar*), 7.24 (s, 2H, *Pyr*), 7.19 (overlapping resonances, 4H, *Ar*), 6.95–7.08 (overlapping resonances, 17H, *Ar*), 6.84 (s, 1H, *Ar*), 6.52 (m, 1H, *Pyr*), 6.50 (m, 1H, *Pyr*), 6.25 (m, 1H, *Pyr*), 2.65 (s, 3H, *Pyr*), 2.26 (s, 3H, *Pyr*), 2.24 (s, 3H, *Pyr*), 1.65 (br s, 3H, *Ad*), 1.44 (s, 3H, C*Me*$_2$Ph), 1.29 (br s, 6H, *Ad*), 1.14 (s, 3H, C*Me*$_2$Ph), 1.06 (m, 6H, *Ad*); ^{13}C NMR (125 MHz, C_6D_6) δ 285.7 (Mo=*C*), 159.3, 149.7, 142.4, 142.3, 140.3, 139.6, 138.9, 138.0, 137.9, 137.0, 135.3, 132.6, 132.2 (br), 130.7, 130.1, 129.3, 128.9, 128.7, 128.5, 128.1, 127.0, 126.9, 126.4, 126.0, 110.1, 109.5, 109.4, 77.0, 52.6, 42.9, 35.7, 35.6, 35.5, 32.8, 29.9, 29.8, 29.5, 21.9, 21.4. Anal. Calcd for $C_{63}H_{62}N_2OMo$: C, 78.89; H, 6.52; N, 2.92. Found: C, 79.09; H, 6.89; N, 2.86.

Synthesis of Mo(NAd)(CHCMe$_2$Ph)(2-MesPyr)(OBitetBr$_2$) (2b).

Mo(NAd)(CHCMe$_2$Ph)(2-MesPyr)$_2$ (0.192 g, 0.250 mmol) was suspended in ether (10 mL) and cooled to – 30 ^{o}C for 2 h. Br$_2$BitetOH (0.156 g, 0.280 mmol, 1.10 equivalents) was then added to the ethereal suspension. The reaction was warmed to room temperature and stirred for two days. An amount of pentane sufficient to dissolve the yellow residue was added and the solution was stored at – 30 ^{o}C overnight. The yellow crystals were collected via filtration and washed with cold pentane. Analytically pure product (a mixture of diastereomers in ~ 1:1 ratio) can be obtained through recrystallization from pentane; yield 0.153 g (53%): ^{1}H NMR (500 MHz, C_6D_6, selected resonances for *R*-diastereomer) δ 12.47 (s, 1H, *syn* Mo=C*H*, J_{CH} = 120.5 Hz), 1.00 (s, 9H, OSi^t*Bu*), 0.32 (s, 3H, OSi*Me*$_2$), – 0.18 (s, 3H, OSi*Me*$_2$): ^{1}H NMR (500 MHz, C_6D_6; selected resonances for *S*-diastereomer) δ 13.14 (s, 1H, Mo=C*H*, J_{CH} = 120.0 Hz), 1.01 (s, 9H,

OSi^t*Bu*), 0.32 (s, 3H, OSi*Me*$_2$), –0.50 (s, 3H, OSi*Me*$_2$); ^{13}C NMR of both diastereomers (125 MHz, C_6D_6) δ 290.3, 288.5 (Mo=*C*), 158.5, 157.8, 149.6, 149.3, 147.9, 147.5, 140.2, 140.0, 139.7, 139.4, 139.2, 138.7, 137.1, 136.9, 136.8, 136.6, 136.5, 136.2, 136.1, 133.7, 132.0, 131.7, 131.5, 131.2, 130.8, 130.6, 128.9, 127.5, 127.3, 126.3, 126.2, 114.0, 113.7, 112.6, 112.0, 111.2, 109.5, 109.0, 77.9, 77.5, 53.5, 52.9, 43.2, 35.7, 32.4, 32.1, 31.3, 30.9, 30.7, 30.1, 30.0, 29.6, 29.4, 27.5, 26.6, 25.9, 23.4, 23.2, 23.0, 22.7, 22.1, 21.9, 21.6, 21.4, 21.3, 19.1, 18.9, –2.5, –2.8, –3.15. Anal. Calcd for $C_{59}H_4N_2Br_2O_2SiMo$: C, 62.87; H, 6.62; N, 2.49. Found: C, 62.59; H, 6.52; N, 2.43.

Mo(NAd)(CHCMe$_2$Ph)(2-MesPyr)(OHIPT) (2c). Solid sodium 2-Mespyrrolide (80.4 mg, 0.388 mmol, 1 equiv) was added to a solution of Mo(NAd)(CHCMe$_2$Ph)(OTf)(OHIPT) (398 mg, 0.388 mmol, 1 equiv) in benzene (20 mL). The reaction mixture was heated at 80 °C for 10 hours, cooled to 22 °C, and filtered through Celite. The volatiles were removed under vacuum. The yellow product was recrystallized from a mxiture of pentane and tetramethylsilane; yield 183 mg (45%): ^{1}H NMR (500 MHz, C_6D_6) δ 12.25 (s, 1H, *syn*-Mo=C*H*, J_{CH} = 120.0 Hz), 7.23 (s, 2H, *Ar*), 7.20 (s, 2H, *Ar*), 7.18-7.10 (m, 4H, *Ar*), 7.06 (d, 1H, *Ar*, *J* = 7.5 Hz), 7.03 (d, 2H, *Ar*, *J* = 7.5 Hz), 6.83 (s, 1H, *Ar*), 6.80 (t, 1H, *Ar*, *J* = 7.5 Hz), 6.76 (s, 1H, *Ar*), 6.36 (t, 1H, NC$_4$*H*$_3$, *J* = 2.5 Hz), 6.15 (dd, 1H, NC$_4$*H*$_3$, *J* = 2.5 Hz, 1.2Hz), 5.99 (dd, 1H, NC$_4$*H*$_3$, *J* = 2.5 Hz, 1.2Hz), 3.05 (sept, 2H, MeC*H*Me, *J* = 7.0 Hz), 2.97 (sept, 4H, MeC*H*Me, *J* = 7.0 Hz), 2.33 (s, 3H, *Me*), 2.16 (s, 3H, *Me*), 2.15 (s, 3H, *Me*), 1.73 (br, 3H), 1.53 (s, 3H, *Me*), 1.48 (s, 3H, *Me*), 1.36 (app q, 12H, *Me*CH*Me*), 1.33 (br, 9H), 1.27 (d, 6H, *Me*CH*Me*, *J* = 7.0 Hz), 1.23 (d, 6H, *Me*CH*Me*, *J* = 7.0 Hz), 1.15 (t, 12H, *Me*CH*Me*, *J* = 7.0 Hz), 1.11 (br, 3H); ^{13}C NMR (125 MHz, C_6D_6) δ 288.0, 160.2, 150.6, 148.2, 147.7, 147.6, 140.0, 139.6, 139.3, 136.9, 136.7, 135.8, 135.2 (br), 133.3, 131.3, 129.1 (br), 128.9 (br), 127.5, 126.4, 122.1, 121.6, 120.8, 111.5, 111.4, 111.2, 111.1, 100.5, 77.1, 53.2, 43.7, 35.9, 35.1, 35.0, 34.6, 31.8, 31.6, 30.2, 30.1, 26.4, 26.1, 24.7, 24.7, 24.6. Anal. Calcd for $C_{69}H_{90}MoN_2O$: C, 78.22; H, 8.56; N, 2.64. Found: C, 77.91; H, 8.60; N, 2.65.

Mo(NAd)(CHCMe$_2$Ph)(OTf)(OHIPT) (3). Solid LiOHIPT (371mg, 0.735 mmol) was added to a suspension of Mo(NAd)(CHCMe$_2$Ph)(OTf)$_2$(dme) (563 mg, 0.735 mmol) in benzene

(20 mL). The reaction mixture was heated at 80 °C for 24 hours, cooled to 22 °C, and filtered through Celite. The solvents were removed *in vacuo* to yield a yellow-brown solid; yield 750 mg (99%): ^{1}H NMR (500 MHz, C_6D_6) δ 12.35 (s, 1H, *syn*-Mo=C*H*, J_{CH} = 123.0 Hz), 7.33 (s, 4H, *Ar*), 7.25-7.00 (m, 7H, *Ar*), 6.84 (t, 1H, *Ar*, *J* = 7.5 Hz), 2.98 (sept, 4H, MeC*H*Me, *J* = 7.0 Hz), 2.92 (sept, 2H, MeC*H*Me, *J* = 7.0 Hz), 1.78 (br, 6H), 1.74 (br, 6H), 1.58 (s, 3H, *Me*), 1.37 (d, 6H, *Me*CH*Me*, *J* = 7.0 Hz), 1.35 (br, 6H), 1.33 (t, 12H, *Me*CH*Me*, *J* = 7.0 Hz), 1.17 (d, 6H, *Me*CH*Me*, *J* = 7.0 Hz), 1.11 (t, 12H, *Me*CH*Me*, *J* = 7.0 Hz); ^{13}C NMR (125 MHz, C_6D_6) δ 301.5, 159.8, 152.0, 149.7, 149.5, 149.2, 148.5, 147.8, 147.2, 134.1, 132.3, 131.8, 128.9, 128.7, 127.3, 126.9, 123.3, 122.2, 122.0, 121.7, 81.5, 54.0, 44.0, 35.9, 34.8, 34.5, 31.6 (br), 30.2 (br), 25.4 (br), 24.7 (br); ^{19}F NMR (282 MHz, C_6D_6) δ -75.4. Anal. Calcd for $C_{57}H_{76}F_3MoNO_4S$: C, 66.84; H, 7.48; N, 1.37. Found: 66.75; H, 7.50; N, 1.44.

Mo(NAd)(CHCMe$_2$Ph)(OTf)(OHIPT)(PMe$_3$) (3(PMe$_3$)). Trimethylphosphine (57 mL, 0.552 mmol, 1.50 equiv) was added to a solution of Mo(NAd)(CHCMe$_2$Ph)(OTf)(OHIPT) (378 mg, 0.368 mmol) in benzene (20 mL). The reaction mixture was stirred at room temperature for 15 minutes and the volatiles were removed *in vacuo*. Pentane was added and the off-white solid was collected on a medium porosity frit; yield 303 mg (75%): ^{1}H NMR (500 MHz, C_6D_6) δ 12.74 (d, 1H, *syn*-Mo=C*H*, J_{CH} = 122.2 Hz, J_{PH} = 4.6 Hz), 7.48 (s, 1H, *Ar*), 7.32 (d, 2H, *Ar*, *J* = 11.6 Hz), 7.25-7.19 (m, 3H, *Ar*), 7.10 (t, 2H, *Ar*, *J* = 7.5 Hz), 7.04 (s, 1H, *Ar*), 6.99 (t, 1H, *Ar*, *J* = 7.5 Hz), 6.87 (d, 2H, *Ar*, *J* = 7.5 Hz), 6.80 (t, 1H, *Ar*, *J* = 7.5 Hz), 3.73 (sept, 1H, MeC*H*Me, *J* = 6.5 Hz), 3.58 (sept, 1H, MeC*H*Me, *J* = 6.5 Hz), 3.08 (sept, 1H, MeC*H*Me, *J* = 6.5 Hz), 2.95 (sept, 1H, MeC*H*Me, *J* = 6.5 Hz), 2.83 (sept, 1H, MeC*H*Me, *J* = 6.5 Hz), 2.76 (sept, 1H, MeC*H*Me, *J* = 6.5 Hz), 2.20 (br, 6H), 2.03 (s, 3H, *Me*), 1.93 (br, 3H), 1.80 (d, 3H, *Me*CH*Me*, *J* = 6.5 Hz), 1.73 (d, 3H, *Me*CH*Me*, *J* = 6.5 Hz), 1.58-1.14 (m, 33H), 1.05 (d, 3H, *Me*CH*Me*, *J* = 6.5 Hz), 1.02 (d, 3H, *Me*CH*Me*, *J* = 6.5 Hz), 0.39 (d, 9H, P*Me$_3$*, J_{PH} = 10.2 Hz); ^{13}C NMR (125 MHz, C_6D_6:CD_2Cl_2 = 1:1) δd 314.5 (d, J_{CP} = 19.9 Hz), 161.5, 149.2 (br), 148.1, 147.9 (br), 138.4 (br), 137.5 (br), 134.2 (br), 133.3 (br), 130.1, 129.0 (br), 127.1 (br), 126.6, 126.5, 122.9 (br), 121.5 (br), 120.8 (br), 117.9 (br), 75.2, 52.0, 44.8, 36.3, 34.9 (br), 31.1 (br), 30.3 (br), 25.0 (br),

16.1 (t, J_{CP} = 31.0 Hz); ^{19}F NMR (282 MHz, C_6D_6:CD_2Cl_2 = 1:1) δ -75.2; ^{31}P NMR (121 MHz, C_6D_6:CD_2Cl_2 = 1:1) δ 8.6. Anal. Calcd for $C_{60}H_{85}F_3MoNO_4PS$: C, 65.49; H, 7.79; N, 1.27. Found: 65.56; H, 7.78; N, 1.13.

Synthesis of Mo(NAd)(CHCMe$_2$Ph)(2-CNPyr)(OHIPT) (4).

Mo(NAd)(CHCMe$_2$Ph)(OTf)(OHIPT) (0.300 g, 0.29 mmol) was dissolved in benzene (15 mL) and Li(2-CNPyr) (0.029 g, 0.30 mmol, 1.1 equivalents) was added in portions to the solution. The reaction mixture was stirred at room temperature for 18 h. The white LiOTf salt was removed by filtration through Celite, and the solvents were removed from the filtrate *in vacuo*. Tetramethylsilane was added to the orange residue to produce some dark orange solids. The orange solids were washed with *n*-pentane and the washings were combined and taken to dryness *in vacuo*. Upon addition of fresh *n*-pentane, a yellow microcrystalline solid was obtained. The yellow solid was recrystallized from a concentrated solution of *n*-pentane; yield 70 mg (25%): ^{1}H NMR (500 MHz, C_6D_6) δ 12.69 (s, 1H, *syn* Mo=C*H*, J_{CH} = 121.0 Hz), 7.11–7.24 (overlapping resonances, 8H, *Ar*), 7.01–7.04 (m, 3H, *Ar*), 6.84 (t, 1H, *Ar*, *J* = 7.5 Hz), 6.78 (m, 1H, *Pyr*), 6.21 (m, 1H, *Pr*), 6.09 (m, 1H, *Pyr*), 3.00 (overlapping sept, 4H, ^{i}*Pr*), 2.93 (sept, 2H, C*H*Me$_2$, *J* = 7.0 Hz), 1.80 (m, 6H, *Ad*), 1.66 (m, 3H, *Ad*), 1.59 (s, 3H, C*Me*$_2$Ph), 1.51 (s, 3H, C*Me*$_2$Ph), 1.45 (m, 3H, *Ad*), 1.31–1.37 (overlapping resonances, 15H, *Ad* & CH*Me*$_2$), 1.25 (d, 9H, CH*Me*$_2$, *J* = 7.0 Hz), 1.13–1.19 (overlapping resonances, 15H, CH*Me*$_2$); ^{13}C NMR (125 MHz, C_6D_6) δ 296.2 (Mo=*C*), 159.5, 149.8, 148.1, 147.4, 147.0, 142.2, 134.5, 131.8, 131.6, 127.4, 126.3, 122.1, 121.9, 121.6, 118.4, 113.2, 111.1, 78.7, 53.9, 43.4, 35.7, 34.6, 34.2, 32.8, 32.0, 31.5, 30.8, 30.0, 29.9, 25.1, 24.9, 24.8, 24.3, 24.2. Anal. Calcd for $C_{61}H_{79}N_3OMo$: C, 75.82; H, 8.24; N, 4.35. Found: C, 75.90; H, 8.16; N, 4.32.

Mo(NAd)(CHCMe$_2$Ph)(OCMe$_3$)(OHIPT) (5). LiOCMe$_3$ (80.0 mg, 0.360 mmol, 1 equiv) was added to a solution of Mo(NAd)(CHCMe$_2$Ph)(OTf)(OHIPT) (368.4 mg, 0.360 mmol, 1 equiv) in benzene (20 mL). The reaction mixture was stirred at room temperature for 24 hours and the reaction mixture was filtered through Celite. The volatiles were removed from the filtrate *in vacuo*. The residue was recrystallized from a mixture of pentane and tetramethylsilane

to yield a yellow solid; yield 75 mg (22%): ^{1}H NMR (500 MHz, C_6D_6) δ 11.16 (s, 1H, *syn*-Mo=C*H*, J_{CH} = 119.0 Hz), 7.26 (s, 4H, *Ar*), 7.21 (d, 2H, *Ar*, *J* = 1.5 Hz), 7.11 (d, 2H, *Ar*, *J* = 7.5 Hz), 7.08 (d, 2H, *Ar*, *J* = 7.5 Hz), 7.02 (t, 1H, *Ar*, *J* = 7.5 Hz), 6.82 (t, 1H, *Ar*, *J* = 7.5 Hz), 3.16 (sept, 4H, MeC*H*Me, *J* = 6.5 Hz), 2.95 (sept, 2H, MeC*H*Me, *J* = 6.5 Hz), 1.90 (br, 6H), 1.71 (app q, 6H, *J* = 11.8 Hz), 1.55 (s, 3H, *Me*), 1.45 (br, 6H), 1.41 (d, 6H, *Me*CH*Me*, *J* = 6.5 Hz), 1.35 (t, 12H, *Me*CH*Me*, *J* = 6.5 Hz), 1.28 (d, 6H, *Me*CH*Me*, *J* = 6.5 Hz), 1.23 (t, 12H, *Me*CH*Me*, *J* = 6.5 Hz), 1.01 (s, 9H, OC*Me$_3$*); ^{13}C NMR (125 MHz, C_6D_6) δ 263.1, 161.8, 150.9, 148.2, 148.1, 147.7, 135.8, 132.7, 131.6, 128.9, 128.7, 128.3, 127.1, 126.3, 121.6, 121.5, 120.2, 77.9, 74.1, 49.7, 45.0, 36.5, 34.8, 34.7, 32.0, 31.5, 30.5, 30.2, 26.5, 26.3, 26.1, 25.9, 25.4, 25.2, 25.1, 24.9, 24.8, 24.7, 24.4. Anal. Calcd for $C_{60}H_{85}MoNO_2$: C, 75.99; H, 9.03; N, 1.48. Found: C, 75.64; H, 8.80; N, 1.55.

Mo(NAr)(CHCMe$_2$Ph)(OR$_{F6}$) (OHMT) (6a). Mo(NAr)(CHCMe$_2$Ph)(OR$_{F6}$)$_2$ (0.3118 g, 0.41 mmol) was dissolved in Et_2O and LiOHMT (0.1370 g, 0.41 mmol) was added in one portion. The reaction mixture was left stirring at RT overnight. The volatiles were removed and the crude was dissolved in minimal pentane and placed at – 35 ^{o}C overnight to yield orange crystalline solid (0.1600 g, 43%): ^{1}H NMR (400 MHz, C_6D_6) δ 11.59 (s, 1H, Mo=C*H*CMe$_2$Ph, J_{CH} = 124.2 Hz), 7.25-6.85 (overlapping peaks, 15H, aromatics), 3.45 (sept, 2H, C*H*Me$_2$), 2.30 (s, 12H, HMTO), 2.20 (s, 6H, HMTO), 1.79 (s, 3H, C*H$_3$*), 1.31 (d, 6H, CH*Me$_2$*), 1.25 (s, 3H, C*H$_3$*), 1.18 (d, 6H, CH*Me$_2$*), 0.78 (s, 3H, C*H$_3$*); ^{13}C NMR (100 MHz, C_6D_6) δ 281.3 (Mo=*C*HCMe$_2$Ph), 158.4, 153.4, 148.7, 143.0, 136.6, 132.3, 130.0, 129.2, 128.4, 128.4, 126.4, 125.6, 123.3, 123.1, 122.9, 54.3, 31.6, 29.8, 28.3, 24.3, 23.8, 20.9, 20.8, 19.2; ^{19}F NMR (376 MHz, C_6D_6) δ – 77.2 (q, 3F, C*F$_3$*), - 77.7 (q, 3F, C*F$_3$*). Anal. Calcd for $C_{50}H_{57}F_6MoNO_2$: C, 65.71; H, 6.29, N, 1.53. Found: C, 65.65; H, 6.11; N, 1.34.

Mo(NAr')(CHCMe$_2$Ph)(OR$_{F6}$)(OHMT) (6b). The procedure is the same as that of **6a**, employing Mo(NAr')(CHCMe$_2$Ph)(OR$_{F6}$)$_2$ (0.3065 g, 0.43 mmol) and LiOHMT (0.1453 g, 0.43 mmol) to yield yellow solid (0.2977 g, 80%): ^{1}H NMR (400 MHz, C_6D_6) δ 11.40 (s, 1H, Mo=C*H*CMe$_2$Ph, J_{CH} = 123.8 Hz), 7.05-6.55 (overlapping peaks, 15H, aromatics), 2.19 (s, 6H,

HMTO), 2.15 (s, 6H, HMTO), 2.06 (s, 6H, Ar' C*H*$_3$), 2.03 (s, 6H, HMTO), 1.45 (s, 3H, C*H*$_3$), 1.22 (s, 3H, C*H*$_3$), 0.80 (s, 3H, C*H*$_3$); ^{13}C NMR (100 MHz, C_6D_6) δ 281.7 (Mo=*C*HCMe$_2$Ph), 158.0, 156.0, 148.6, 136.6, 136.4, 136.2, 135.7, 135.3, 132.0, 129.6, 129.1, 128.4, 128.1, 128.0, 126.9, 126.5, 126.2, 126.0, 125.9, 122.6, 53.6, 40.3, 31.1, 29.6, 29.1, 20.8, 20.6, 19.5, 19.2; ^{19}F NMR (376 MHz, C_6D_6) δ – 77.4 (q, 3F, C*F*$_3$), - 77.6 (q, 3F, C*F*$_3$). Anal. Calcd for $C_{46}H_{44}F_6MoNO_2$: C, 64.41; H, 5.76, N, 1.63. Found: C, 64.81; H, 5.82; N, 1.38.

Mo(NAr^{iPr})(CHCMe$_2$Ph)(OR$_{F6}$)(OHMT) (6c). The procedure is the same as that of **6a**, employing Mo(NAr^{iPr})(CHCMe$_2$Ph)(OR$_{F6}$)$_2$ (0.3602 g, 0.50 mmol) and LiOHMT (0.1675 g, 0.50 mmol) to yield orange crystalline solid (0.3672 g, 71%): ^{1}H NMR (400 MHz, C_6D_6) δ 11.20 (s, 1H, Mo=C*H*CMe$_2$Ph, J_{CH} = 124.5 Hz), 7.14 (dd, 2H, aromatic), 7.08 (td, 2H, Ar^{iPr}), 7.02-6.78 (overlapping peaks, 8H, aromatics), 6.76 (s, 2H, HMTO), 6.67 (s, 2H, HMTO), 3.31 (sept, 1H, C*H*Me$_2$), 2.14 (s, 6H, HMTO), 2.08 (s, 6H, HMTO), 2.04 (s, 6H, HMTO), 1.49 (s, 3H, C*H*$_3$), 1.43 (s, 3H, C*H*$_3$), 1.15 (d, 3H, CH(Me)C*H*$_3$), 1.13 (d, 3H, CH(C*H*$_3$)Me), 0.94 (s, 3H, C*H*$_3$); ^{13}C NMR (100 MHz, C_6D_6) δ 281.7 (Mo=*C*HCMe$_2$Ph), 157.9, 155.3, 149.0, 146.7, 136.5, 136.4, 136.0, 135.4, 132.1, 129.7, 128.7, 128.4, 127.9, 127.9, 126.2, 125.5, 122.9, 54.3, 32.4, 30.5, 28.2, 23.6, 21.1, 20.9, 20.5, 18.6; ^{19}F NMR (375 MHz, C_6D_6) δ – 77.7 (q, 3F, C*F*$_3$), - 78.1 (1, 3F, C*F*$_3$). Anal. Calcd for $C_{47}H_{51}F_6MoNO_2$: C, 64.75; H, 5.90, N, 1.61. Found: C, 64.60; H, 6.01; N, 1.41.

Mo(NAd)(CHCMe$_2$Ph)(OR$_{F6}$)(OHMT) (6d). The procedure is the same as that of **6a**, employing Mo(NAd)(CHCMe$_2$Ph)(OR$_{F6}$)$_2$ (0.1900 g, 0.26 mmol) and LiOHMT (0.0864 g, 0.26 mmol) to yield yellow crystalline solid (0.1353 g, 59%): ^{1}H NMR (400 MHz, C_6D_6) δ 10.64 (s, 1H, Mo=C*H*CMe$_2$Ph, J_{CH} = 122.7 Hz), 7.25-7.08 (overlapping peaks, 4H, aromatics), 7.05-6.93 (overlapping peaks 3H, aromatics), 6.92-6.53 (overlapping peaks 3H, aromatics), 6.72 (s, 2H, HMTO), 2.26 (s, 6H, HMTO), 2.20 (s, 6H, HMTO), 1.97 (s, 6H, HMTO), 1.80 (s, 3H, Ad), 1.70-1.50 (overlapping peaks, 9H, MoCHC*Me$_2$*Ph + Ad), 1.47-1.30 (overlapping peaks, 9H, MoCHC*Me$_2$*Ph + Ad), 1.16 (s, 3H, C*H*$_3$); ^{13}C NMR (100 MHz, C_6D_6) δ 276.0 (Mo=*C*HCMe$_2$Ph), 158.7, 150.3, 137.5, 136.6, 136.4, 136.3, 131.9, 130.5, 129.2, 128.7, 126.7,

126.1, 122.2, 76.9, 50.5, 43.7, 35.6, 33.2, 31.0, 29.9, 21.1, 20.7, 20.6; ^{19}F NMR (376 MHz, C_6D_6) δ – 77.4 (q, 3F, C*F*$_3$), - 78.1 (q, 3F, C*F*$_3$). Anal. Calcd for $C_{48}H_{55}F_6MoNO_2$: C, 64.93; H, 6.24, N, 1.58. Found: C, 64.95; H, 6.12; N, 1.56.

Mo(NAr')(CHCMe$_2$Ph)(OR$_{F6}$)(N(H)HMT) (7a). The procedure is the same as that of **6a**, employing Mo(NAr')(CHCMe$_2$Ph)(OR$_{F6}$)$_2$ (0.2094 g, 0.30 mmol) and LiN(H)HMT (0.0990 g, 0.30 mmol) to yield yellow solid (0.1205 g, 48%): ^{1}H NMR (400 MHz, C_6D_6) δ 11.86 (s, 1H, Mo=C*H*CMe$_2$Ph, J_{CH} = 121.2 Hz), 7.82 (s, 1H, MoN(*H*)HMT), 7.25-7.10 (overlapping peaks, 3H, aromatics), 7.00-6.55 (overlapping peaks, 11H, aromatics), 6.40 (s br, 1H, aromatic), 2.38 (s, 3H, C*H*$_3$), 2.23 (s, 6H, C*H*$_3$), 2.19 (s, 3H, C*H*$_3$), 2.10 (s, 3H, C*H*$_3$), 2.03 (s, 6H, C*H*$_3$), 1.67 (s, 3H, C*H*$_3$), 1.19 (s, 3H, C*H*$_3$), 1.16 (s, 3H, C*H*$_3$), 1.00 (s, 3H, C*H*$_3$); ^{13}C NMR (100 MHz, C_6D_6) δ 287.3 (Mo=*C*HCMe$_2$Ph), 156.1, 149.5, 148.2, 135.6, 131.3, 130.7, 130.2, 129.2, 129.2, 128.9, 128.6, 127.1, 126.1, 125.8, 121.1, 54.5, 30.5, 28.8, 21.2, 20.6, 20.5, 20.3, 20.0, 19.4, 19.3; ^{19}F NMR (376 MHz, C_6D_6) δ – 76.7 (q, 3F, C*F*$_3$), - 77.2 (q, 3F, C*H*$_3$). Anal. Calcd for $C_{46}H_{50}F_6MoN_2O$: C, 64.48; H, 5.88, N, 3.27. Found: C, 64.20; H, 6.01; N, 3.22.

Mo(NAr$^{i\mathrm{Pr}}$)(CHCMe$_2$Ph)(OR$_{F6}$)(N(H)HMT) (7b). The procedure is the same as that of **6a**, employing Mo(NAr$^{i\mathrm{Pr}}$)(CHCMe$_2$Ph)(OR$_{F6}$)$_2$ (0.2959 g, 0.41 mmol) and LiN(H)HMT (0.1372 g, 0.41 mmol) to yield orange crystalline solid (0.3260 g, 92%): ^{1}H NMR (400 MHz, C_6D_6) δ; 11.72 (s, 1H, Mo=C*H*CMe$_2$Ph, J_{CH} = 117.9 Hz), 7.99 (s, 1H, MoN(*H*)HMT), 7.23 (dd, 1H, aromatic), 7.08 (dd, 1H, aromatic), 7.05-6.70 (overlapping peaks, 12H, aromatics), 6.72 (s br, 2H, aromatic), 3.22 (sept, 1H, C*H*Me$_2$), 2.31 (s, 6H, C*H*$_3$), 2.24 (s, 6H, C*H*$_3$), 1.94 (s br, 6H, C*H*$_3$), 1.53 (s, 3H, C*H*$_3$), 1.25 (d, 3H, CH(Me)C*H*$_3$), 1.19 (s, 3H, C*H*$_3$), 1.12 (d, 3H, CH(C*H*$_3$)Me), 0.82 (s, 3H, C*H*$_3$); ^{13}C NMR (100 MHz, C_6D_6) δ 286.5 (Mo=*C*HCMe$_2$Ph), 155.5, 149.4, 148.0, 146.1, 137.9, 137.4, 137.4, 135.5, 130.3, 129.0, 128.5, 128.2, 126.3, 125.7, 125.6, 125.5, 121.5, 55.6, 30.4, 30.1, 27.8, 24.4, 22.6, 21.2, 20.5, 19.4; ^{19}F NMR (376 MHz, C_6D_6) δ – 77.1 (q, 3F, C*F*$_3$), - 77.7 (q, 3F, C*H*$_3$). Anal. Calcd for $C_{47}H_{52}F_6MoN_2O$: C, 64.82; H, 6.02, N, 3.22. Found: C, 64.43; H, 5.89; N, 3.15.

Mo(NAd)(CHCMe$_2$Ph)(OR$_{F6}$)(HMT) (8). Mo(NAd)(CHCMe$_2$Ph)(OR$_{F6}$)$_2$(DME) (0.300 g, 0.360 mmoles) and LiHMT (0.1159 g, 0.36 mmoles) were added to 3 mL of toluene at RT and the mixture was stirred for 12 h. The solution was placed at -35 ^{o}C overnight and then passed through celite. The celite was washed with cold toluene until the color was gone. At this point the solvent was removed from the filtrate under reduced pressure and the product was washed with pentane 3 times and twice with TMS to induce precipitation of the product, which was collected by filtration (0.3080 g, 95%). Orange-yellow crystals were grown by dissolving **8** in pentane and placing the solution at – 35 °C a few days: ^{1}H NMR (400 MHz, C_6D_6) δ 10.99 (s, 1H, MoC*H*, J_{CH} = 120.2 Hz), 7.40 (d, 2H, HMT), 7.20-7.10 (m, 3H, Ph), 7.03 (t, 1H, HMT), 6.90 (s, 2H, Mes), 6.84 (m, 2H, Ph), 6.79 (s, 2H, Mes), 2.23 (s, 6H, *o*-Mes), 2.21 (s, 6H, *o*-Mes), 2.16 (s, 6H, *p*-Mes), 1.71 (s, 3H, Ad), 1.44 (s, 6H, C*Me$_2$*Ph), 1.36 (s, 6H, C*Me$_2$*Ph *syn*), 1.33 (s, 6H, Ad), 1.13 (s, 3H, (CF$_3$)$_2$C*H$_3$*C); ^{13}C NMR (100 MHz, C_6D_6) δ 279.4 (Mo*CH*, J_{CH} = 120.23 Hz), 173.7 (*C*F$_3$), 150.9, 150.5, 145.6, 136.7, 136.2, 136.0, 135.7, 129.7, 129.5, 129.3, 128.1, 125.9, 77.6, 53.5, 42.5, 35.6, 35.2, 30.4, 30.0, 22.1, 21.8, 21.1; ^{19}F NMR (375 MHz, C_6D_6) δ -77.2 (q, 1F), -77.9 (q, 1F). Anal. Calcd for $C_{48}H_{55}F_6MoNO$: C, 66.12; H, 6.36, N, 1.61. Found: C, 66.37; H, 6.30; N, 1.74.

X-Ray Structure Determination

Low-temperature diffraction data (ϕ-and ω-scans) were collected on a Siemens Platform three-circle diffractometer coupled to a Bruker-AXS Smart Apex CCD detector with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) for **2b** and **3**(PMe_3), on a Bruker D8 three-circle diffractometer coupled to a Bruker-AXS Smart Apex CCD detector with graphite-monochromated Cu Kα radiation (λ = 1.54178 Å) for **1b**, and on a Bruker-AXS X8 Kappa Duo diffractometer coupled to a Smart Apex2 CCD detector with Mo K_α radiation (λ = 0.71073 Å) from an *IμS* micro-source for the structure of compounds **2a**, **2c**, **4**, **5, 6d**, **7b**, and **8**. All structures were solved by direct methods using SHELXS[7] and refined against F^2 on all data by full-matrix least squares with SHELXL-97[8] using established refinement techniques.[9] All non-hydrogen atoms were refined anisotropically. Unless otherwise noted below all hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). All disordered atoms were refined with the help of similarity restraints on the 1,2- and 1,3- distances and displacement parameters as well as rigid bond restraints for anisotropic displacement parameters.

Compound 1b

Compound **1b** crystallizes in the tetragonal space group *P*4/*nnc* with four octameric molecules of **3d** (monomeric subunit corresponds to $Mo(NAd)(CHCMe_2Ph)(2\text{-}CNPyr)_2$) in the unit cell, corresponding to two Mo centers per asymmetric unit. In addition the asymmetric unit contains highly disordered solvent, which was modeled to be a mixture of thf and pentane. This solvent disorder is uncommonly complex and all solvent molecules are found near crystallographic fourfold axes. The first solvent site consists of eight-fold disordered thf (two independent) components, the second site of eight-fold disordered pentane (two independent positions) and the third site of twelve-fold disordered solvent (crystallographically independent are one thf position and two pentane positions). The main molecule also shows disorder, namely

one of the two independent adamantly ligands as well as both $CHCMe_2Ph$ ligands were modeled as disordered over two positions. The eight-fold disordered pentane (described above as the second site) interferes with one orientation of each of the disordered $CHCMe_2Ph$ ligands and the occupancies of the disorder components were linked accordingly. In addition to the similarity restraints mentioned above, all disordered solvent atoms were restrained to behave approximately isotropically within 0.1 Å (0.2 Å for terminal atoms). Even though all attempts to resolve more disorders failed, larger than average thermal parameter for all atoms suggest high molecular motion and probably more disorders. It also seems likely that the solvent disorder model, although fairly complex, is still not reflecting all aspects of the actual solvent situation and a bulk solvent correction based on Babinet's principle was applied.[10] The circumstance that the structure contains only fractions of solvent molecules per octamer leads to non-integer values in the empirical formula for the elements C, H and O.

Compound 2a

Compound **2a** crystallizes in the triclinic space group *P*-1 with one molecule of **2a** and half a molecule of pentane in the asymmetric unit. The pentane molecule is located close to a crystallographic inversion center and disordered over four positions, two of which are crystallographically independent. In addition to the similarity restraints mentioned above, the disordered solvent atoms were restrained to behave approximately isotropically within 0.1 Å (0.2 Å for terminal atoms). Coordinates for the hydrogen atom on C1, the carbon binding directly to Mo, were taken from the difference Fourier synthesis. This hydrogen atom was subsequently refined semi-freely with the help of a distance restraint while constraining its U_{iso} to 1.2 times the U_{eq} value of C1. The circumstance that the structure contains only half a pentane per molecule of **2a** leads to a non-integer value in the empirical formula for the element C.

Compound 2b

Compound **2b** crystallizes in the monoclinic space group $P2_1$ with one molecule of **2b** in the asymmetric unit. Coordinates for the hydrogen atom on C1, the carbon binding directly to Mo, were taken from the difference Fourier synthesis. This hydrogen atom was subsequently refined semi-freely with the help of a distance restraint while constraining its U_{iso} to 1.2 times the U_{eq} value of C1. The Flack x parameter refined to -0.006(3).[11]

Compound 2c

Compound **2c** crystallizes in the monoclinic space group $C2/c$ with one molecule of **2c** and half a molecule of tetramethylsilane (tms) in the asymmetric unit. The tms molecule is located close to but not on a crystallographic two-fold axis and disordered accordingly over two positions. The alkoxide ligand was modeled as a two part disorder. The ratio was refined freely and converged at 0.710(3). In addition to the similarity restraints mentioned above some almost overlapping atoms were pair-wise constrained to have identical anisotropic displacement parameters (O1/O1A, C41/C41A, C42/C42A, and C46/C46A). Coordinates for the hydrogen atom on C1, the carbon binding directly to Mo, were taken from the difference Fourier synthesis. This hydrogen atom was subsequently refined semi-freely with the help of a distance restraint while constraining its U_{iso} to 1.2 times the U_{eq} value of C1. The circumstance that the structure contains only half a tms per molecule of **2c** leads to a non-integer value in the empirical formula for the element Si.

Compound 3(PMe_3)

Compound **3(PMe_3)** crystallizes in the monoclinic space group $P2_1/n$ with one molecule of **3(PMe_3)** in the asymmetric unit. Coordinates for the hydrogen atom on C1, the carbon binding directly to Mo, were taken from the difference Fourier synthesis. This hydrogen atom was subsequently refined semi-freely with the help of a distance restraint while constraining its

U_{iso} to 1.2 times the U_{eq} value of C1. One of the ^{i}Pr groups was treated as disordered over two positions.

Compound 4

Compound **4** crystallizes in the monoclinic space group $P2_1/c$ with one molecule of **4** in the asymmetric unit. Coordinates for the hydrogen atom on C1, the carbon binding directly to Mo, were taken from the difference Fourier synthesis. This hydrogen atom was subsequently refined semi-freely with the help of a distance restraint while constraining its U_{iso} to 1.2 times the U_{eq} value of C1. Two of the ^{i}Pr groups were treated as disordered over two positions. The highest residual electron density maximum in the difference Fourier map was significantly higher than all other maxima (7.0 electrons per Å^3, compared to 1.1 electrons for second highest peak). This maximum was located 0.82 Å away from the Mo position and the deepest electron density hole (-2.7 electrons per Å^3) was located 0.58 Å from Mo1, suggesting a second position for the metal atom. Upon very careful examination of the difference Fourier synthesis, alternative positions for the ligand atoms could also be distinguished (interestingly with the alkylidene and imido places switched), however a refinement of the whole-molecule disorder was not stable. Therefore the final model contains only the second Mo position; the ratio between first and second component of this incomplete whole-molecule disorder was refined freely and converged at 0.849 (6). Introduction of the second Mo site improved the model significantly: the $R1$ dropped by over three points and the highest residual electron density maximum is down to 0.75 electrons.

Compound 5

Compound **5** crystallizes in the triclinic space group P-1 with two molecules of **5** in the asymmetric unit. One of these two molecules shows extensive disorder, which was treated as described above. The other molecule shows no disorder and the discussion of the structure of **5** in the main text is limited to the well-behaved molecule. Coordinates for the hydrogen atoms on

C1 and C101, the carbon atoms binding directly to the two Mo centers, were taken from the difference Fourier synthesis. These hydrogen atoms were subsequently refined semi-freely with the help of a distance restraints while constraining their U_{iso} to 1.2 times the U_{eq} value of C1 or C101, respectively. The crystal was non-merohedrally twinned. Two independent orientation matrices for the unit cell were found using the program CELL_NOW,[12] and data reduction taking into account the twinning was performed with SAINT.[13] The program TWINABS[14] was used to perform absorption correction and to set up the HKLF5 format file for structure refinement. The twin ratio was refined freely and converged at a value of 0.4642(6).

Compound 6d

Compound **6d** crystallizes in the triclinic space group *P*-1 with one molecule of **6d** in the asymmetric unit. Coordinates for the hydrogen atom on C1, the carbon binding directly to Mo, were taken from the difference Fourier synthesis. This hydrogen atom was subsequently refined semi-freely with the help of a distance restraint while constraining its U_{iso} to 1.2 times the U_{eq} value of C1. The crystal was non-merohedrally twinned which was addressed as described for the structure of compound **5**. The twin ratio was refined freely and converged at a value of 0.0916(4).

Compound 7b

Compound **7b** crystallizes in the monoclinic space group $P2_1/c$ with one molecule of **7b** in the asymmetric unit. Coordinates for the hydrogen atoms on C1, the carbon atom binding directly to Mo, and N2were taken from the difference Fourier synthesis. These hydrogen atoms were subsequently refined semi-freely with the help of a distance restraints while constraining their U_{iso} to 1.2 times the U_{eq} value of C1 or N2, respectively.

Compound 8

Compound **8** crystallizes in the triclinic space group *P*-1 with two molecules of **8** in the asymmetric unit. In both independent molecules, there is a three part disorder for the alkoxide ligand, approximately corresponding to a rotation of the $C(CF_3)_2(CH_3)$ group about the Mo-O bond. The anisotropic displacement parameters of the F and C atoms in the CF_3 groups were pairwise constrained to be identical. The crystal was non-merohedrally twinned which was addressed as described for the structure of compound **5**. The twin ratio was refined freely and converged at a value of 0.3032(17).

Table S1A. Crystal data and structure refinement for **1b**.

Identification code	d10066	
Empirical formula	C253.45 H301.80 Mo8 N40 O1.55	
Formula weight	4700.87	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Tetragonal	
Space group	P4/ncc	
Unit cell dimensions	a = 28.5841(4) Å	α= 90°
	b = 28.5841(4) Å	β= 90°
	c = 31.1532(7) Å	γ = 90°
Volume	25453.7(8) $Å^3$	
Z	4	
Density (calculated)	1.227 Mg/m^3	
Absorption coefficient	3.570 mm^{-1}	
F(000)	9804	
Crystal size	0.40 x 0.15 x 0.10 mm^3	
Theta range for data collection	2.19 to 61.16°	
Index ranges	-32<=h<=31, -32<=k<=32, -35<=l<=35	
Reflections collected	385460	
Independent reflections	9789 [R(int) = 0.1364]	
Completeness to theta = 61.16°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7166 and 0.3293	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9789 / 2725 / 1149	
Goodness-of-fit on F^2	1.070	
Final R indices [I>2sigma(I)]	R1 = 0.0724, wR2 = 0.1999	
R indices (all data)	R1 = 0.1151, wR2 = 0.2503	
Largest diff. peak and hole	0.740 and -0.499 $e.Å^{-3}$	

Table S1B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	400(1)	2802(1)	-718(1)	71(1)
N(1)	995(3)	2392(2)	-952(2)	72(1)
C(1)	1212(4)	2460(3)	-1336(3)	88(2)
C(2)	1599(4)	2190(3)	-1378(3)	99(3)
C(3)	1647(4)	1926(3)	-1000(3)	96(3)
C(4)	1270(3)	2051(3)	-748(3)	75(2)
C(5)	1163(3)	1829(3)	-354(3)	66(2)
N(2)	1098(2)	1619(2)	-51(2)	63(1)
N(3)	-141(2)	3054(2)	-293(3)	76(2)
C(6)	-577(3)	2879(3)	-278(4)	95(2)
C(7)	-836(3)	3082(4)	40(4)	103(3)
C(8)	-559(3)	3415(3)	239(4)	88(2)
C(9)	-132(3)	3386(3)	29(3)	71(2)
C(10)	279(3)	3653(3)	123(3)	64(2)
N(4)	609(2)	3856(2)	211(2)	65(2)
N(5)	42(3)	2677(2)	-1141(2)	87(2)
C(11)	-243(4)	2463(3)	-1465(3)	112(3)
C(12)	-654(4)	2765(4)	-1563(4)	161(4)
C(13)	-974(4)	2526(5)	-1930(4)	175(4)
C(14)	-1113(4)	2071(4)	-1742(5)	174(4)
C(15)	-718(4)	1745(4)	-1682(4)	150(4)
C(16)	-384(4)	1978(3)	-1327(4)	137(3)
C(17)	37(5)	2404(5)	-1872(3)	162(4)
C(18)	-269(5)	2161(5)	-2243(4)	172(4)
C(19)	-666(5)	2491(5)	-2309(4)	196(5)
C(20)	-412(5)	1700(4)	-2067(4)	176(4)
C(23)	596(8)	4290(4)	-931(7)	138(7)
C(24)	833(6)	3783(8)	-1547(5)	132(6)
C(23A)	28(6)	3997(7)	-1045(7)	119(6)
C(24A)	868(7)	4220(5)	-1074(6)	107(6)
C(21)	616(3)	3425(2)	-861(3)	76(2)

C(22)	512(3)	3833(3)	-1162(3)	91(2)
C(25)	10(5)	3874(3)	-1346(5)	99(4)
C(26)	-100(7)	3937(6)	-1763(5)	109(4)
C(27)	-550(7)	3976(8)	-1947(7)	130(5)
C(28)	-912(8)	3962(8)	-1638(7)	137(6)
C(29)	-835(6)	3923(8)	-1190(7)	128(5)
C(30)	-364(6)	3848(7)	-1072(6)	107(4)
C(25A)	546(6)	3719(4)	-1630(5)	111(4)
C(26A)	192(8)	3778(7)	-1910(6)	126(5)
C(27A)	232(10)	3674(9)	-2352(6)	142(6)
C(28A)	672(9)	3499(9)	-2474(8)	151(7)
C(29A)	1064(9)	3437(9)	-2206(7)	146(6)
C(30A)	962(8)	3547(8)	-1774(6)	129(5)
Mo(2)	821(1)	1244(1)	556(1)	64(1)
N(6)	232(2)	1048(2)	165(2)	67(1)
C(31)	12(3)	622(3)	186(3)	74(2)
C(32)	-362(3)	597(3)	-88(3)	82(2)
C(33)	-389(3)	1024(3)	-300(3)	80(2)
C(34)	-23(3)	1295(3)	-144(3)	72(2)
C(35)	99(3)	1750(3)	-275(3)	69(2)
N(7)	199(2)	2116(2)	-386(2)	72(2)
N(8)	1540(2)	1387(2)	762(2)	67(1)
C(36)	1650(3)	1598(3)	1144(3)	77(2)
C(37)	2117(4)	1678(3)	1175(3)	90(2)
C(38)	2327(3)	1515(4)	804(3)	91(2)
C(39)	1965(3)	1323(3)	562(3)	70(2)
C(40)	2041(3)	1092(3)	176(3)	63(2)
N(9)	2141(2)	882(2)	-125(2)	66(2)
N(10)	699(2)	894(2)	991(2)	77(2)
C(41)	719(2)	542(3)	1313(2)	83(2)
C(42)	245(4)	449(5)	1499(5)	95(3)
C(43)	290(5)	62(5)	1864(4)	100(3)
C(44)	493(5)	-362(4)	1652(5)	101(3)
C(45)	980(5)	-284(4)	1495(4)	97(3)
C(46)	961(5)	111(4)	1142(4)	87(3)
C(47)	1057(5)	713(5)	1672(4)	96(3)

C(48)	1091(5)	328(5)	2039(4)	106(3)
C(49)	603(5)	260(6)	2201(4)	113(4)
C(50)	1294(5)	-104(5)	1842(5)	112(3)
C(42A)	1210(5)	450(7)	1447(6)	90(3)
C(43A)	1217(5)	53(6)	1807(5)	101(3)
C(44A)	903(6)	210(7)	2157(5)	101(4)
C(45A)	399(6)	236(6)	2026(4)	94(4)
C(46A)	365(6)	626(6)	1666(5)	85(4)
C(47A)	509(7)	85(4)	1124(5)	91(3)
C(48A)	550(6)	-335(5)	1452(5)	94(3)
C(49A)	1049(6)	-375(6)	1582(7)	104(4)
C(50A)	239(6)	-213(6)	1822(6)	96(4)
C(53)	158(8)	2569(4)	946(6)	122(7)
C(54)	-270(5)	1813(7)	948(6)	110(5)
C(53A)	480(6)	2170(9)	1426(5)	129(6)
C(54A)	-24(8)	2482(6)	846(7)	126(8)
C(51)	535(3)	1839(3)	708(3)	72(2)
C(52)	192(2)	2042(3)	1036(3)	85(2)
C(55)	345(4)	2008(4)	1496(5)	117(4)
C(56)	733(6)	2240(8)	1637(5)	153(6)
C(57)	916(8)	2228(11)	2060(6)	178(7)
C(58)	647(9)	1956(11)	2348(7)	189(8)
C(59)	233(9)	1713(11)	2235(5)	174(7)
C(60)	108(7)	1757(8)	1796(4)	142(5)
C(55A)	-205(5)	1732(4)	1174(3)	105(4)
C(56A)	-463(5)	1480(6)	887(6)	116(5)
C(57A)	-865(6)	1211(8)	985(7)	139(6)
C(58A)	-961(8)	1174(9)	1430(7)	143(7)
C(59A)	-711(7)	1419(9)	1752(6)	139(6)
C(60A)	-336(7)	1692(8)	1593(5)	124(5)
O(1S)	2580(20)	2095(13)	9904(17)	99(10)
C(1S)	2231(17)	2412(17)	10127(19)	102(12)
C(2S)	2160(20)	2760(30)	9900(30)	103(12)
C(3S)	2680(30)	2846(17)	9717(19)	102(12)
C(4S)	2773(17)	2448(17)	9589(16)	100(11)
O(1SA)	3480(30)	1830(30)	10100(30)	116(14)

C(1SA)	3060(40)	1990(40)	10350(30)	112(13)
C(2SA)	2800(30)	2220(50)	10120(50)	109(12)
C(3SA)	3190(50)	2490(30)	9830(40)	110(12)
C(4SA)	3430(40)	2160(40)	9720(30)	115(13)
C(1X)	1420(30)	2880(30)	2370(30)	120(20)
C(2X)	1930(30)	2510(30)	2440(30)	122(15)
C(3X)	1910(20)	2034(19)	2400(30)	122(15)
C(4X)	2270(30)	1700(20)	2400(40)	121(15)
C(5X)	2160(30)	1090(20)	2320(30)	120(20)
C(1Y)	1800(40)	2990(30)	2370(30)	121(18)
C(2Y)	2290(20)	2590(30)	2410(30)	123(15)
C(3Y)	2230(30)	2110(20)	2410(40)	123(15)
C(4Y)	2550(30)	1750(30)	2340(30)	123(16)
C(5Y)	2420(40)	1150(30)	2450(30)	125(18)
C(1T)	8800(70)	2210(70)	6480(60)	119(5)
C(2T)	8430(70)	2630(80)	6210(50)	119(5)
C(3T)	8500(40)	2760(70)	5780(50)	119(5)
C(4T)	8220(50)	3010(70)	5510(50)	119(5)
C(5T)	7590(40)	3050(70)	5570(60)	119(5)
C(1U)	8540(80)	2510(80)	6410(60)	119(5)
C(2U)	8250(60)	2930(60)	6070(50)	119(5)
C(3U)	8240(40)	2890(80)	5620(50)	119(5)
C(4U)	7880(60)	2890(70)	5330(50)	119(5)
C(5U)	7310(50)	3140(80)	5450(70)	119(5)
O(1V)	8320(20)	2580(20)	6754(16)	128(8)
C(1V)	8720(30)	2280(30)	6590(20)	122(8)
C(2V)	8630(30)	2160(30)	6220(20)	121(7)
C(3V)	8400(30)	2640(30)	6037(19)	121(7)
C(4V)	8120(20)	2720(30)	6320(20)	123(7)

Table S1C. Bond lengths [Å] and angles [°] for **1b**.

Mo(1)-N(5)	1.705(7)
Mo(1)-C(21)	1.938(7)
Mo(1)-N(3)	2.159(8)
Mo(1)-N(1)	2.189(7)
Mo(1)-N(7)	2.290(7)
Mo(1)-N(9)#1	2.309(7)
N(1)-C(1)	1.363(11)
N(1)-C(4)	1.404(11)
C(1)-C(2)	1.357(14)
C(1)-H(1)	0.9500
C(2)-C(3)	1.406(13)
C(2)-H(2)	0.9500
C(3)-C(4)	1.381(13)
C(3)-H(3)	0.9500
C(4)-C(5)	1.416(12)
C(5)-N(2)	1.135(9)
N(2)-Mo(2)	2.312(7)
N(3)-C(6)	1.344(11)
N(3)-C(9)	1.379(11)
C(6)-C(7)	1.367(15)
C(6)-H(6)	0.9500
C(7)-C(8)	1.386(13)
C(7)-H(7)	0.9500
C(8)-C(9)	1.387(12)
C(8)-H(8)	0.9500
C(9)-C(10)	1.434(11)
C(10)-N(4)	1.139(9)
N(4)-Mo(2)#1	2.305(7)
N(5)-C(11)	1.436(10)
C(11)-C(12)	1.489(11)
C(11)-C(16)	1.508(10)
C(11)-C(17)	1.510(11)
C(12)-C(13)	1.617(11)
C(12)-H(12A)	0.9900

C(12)-H(12B)	0.9900
C(13)-C(19)	1.478(11)
C(13)-C(14)	1.479(11)
C(13)-H(13)	1.0000
C(14)-C(15)	1.476(11)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(20)	1.491(11)
C(15)-C(16)	1.605(11)
C(15)-H(15)	1.0000
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.608(12)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(20)	1.485(11)
C(18)-C(19)	1.489(11)
C(18)-H(18)	1.0000
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(23)-C(22)	1.511(12)
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-C(22)	1.516(13)
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(23A)-C(22)	1.506(12)
C(23A)-H(23D)	0.9800
C(23A)-H(23E)	0.9800
C(23A)-H(23F)	0.9800
C(24A)-C(22)	1.527(12)
C(24A)-H(24D)	0.9800

C(24A)-H(24E)	0.9800
C(24A)-H(24F)	0.9800
C(21)-C(22)	1.526(10)
C(21)-H(21A)	0.9900
C(21)-H(21B)	0.9900
C(22)-C(25A)	1.495(17)
C(22)-C(25)	1.550(16)
C(25)-C(26)	1.350(14)
C(25)-C(30)	1.370(15)
C(26)-C(27)	1.411(16)
C(26)-H(26)	0.9500
C(27)-C(28)	1.413(17)
C(27)-H(27)	0.9500
C(28)-C(29)	1.419(17)
C(28)-H(28)	0.9500
C(29)-C(30)	1.412(16)
C(29)-H(29)	0.9500
C(30)-H(30)	0.9500
C(25A)-C(26A)	1.348(15)
C(25A)-C(30A)	1.362(16)
C(26A)-C(27A)	1.412(16)
C(26A)-H(26A)	0.9500
C(27A)-C(28A)	1.406(17)
C(27A)-H(27A)	0.9500
C(28A)-C(29A)	1.408(17)
C(28A)-H(28A)	0.9500
C(29A)-C(30A)	1.415(16)
C(29A)-H(29A)	0.9500
C(30A)-H(30A)	0.9500
Mo(2)-N(10)	1.720(6)
Mo(2)-C(51)	1.945(7)
Mo(2)-N(6)	2.153(7)
Mo(2)-N(8)	2.193(7)
Mo(2)-N(4)#2	2.305(7)
N(6)-C(31)	1.373(10)
N(6)-C(34)	1.398(10)

C(31)-C(32)	1.371(12)
C(31)-H(31)	0.9500
C(32)-C(33)	1.389(12)
C(32)-H(32)	0.9500
C(33)-C(34)	1.389(11)
C(33)-H(33)	0.9500
C(34)-C(35)	1.406(11)
C(35)-N(7)	1.138(9)
N(8)-C(36)	1.371(10)
N(8)-C(39)	1.377(11)
C(36)-C(37)	1.357(13)
C(36)-H(36)	0.9500
C(37)-C(38)	1.383(13)
C(37)-H(37)	0.9500
C(38)-C(39)	1.393(12)
C(38)-H(38)	0.9500
C(39)-C(40)	1.389(12)
C(39)-O(1SA)#3	1.59(11)
C(39)-C(1SA)#3	1.88(13)
C(40)-N(9)	1.151(10)
C(40)-O(1SA)#3	1.38(10)
C(40)-C(4SA)#3	1.99(12)
N(9)-Mo(1)#2	2.309(7)
N(10)-C(41)	1.423(9)
C(41)-C(42A)	1.487(12)
C(41)-C(42)	1.498(11)
C(41)-C(46)	1.510(11)
C(41)-C(46A)	1.513(12)
C(41)-C(47A)	1.553(12)
C(41)-C(47)	1.557(11)
C(42)-C(43)	1.591(12)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-C(49)	1.491(11)
C(43)-C(44)	1.498(11)
C(43)-H(43)	1.0000

C(44)-C(45)	1.494(11)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(45)-C(50)	1.495(12)
C(45)-C(46)	1.579(12)
C(45)-H(45)	1.0000
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-C(48)	1.591(12)
C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900
C(48)-C(49)	1.495(11)
C(48)-C(50)	1.495(12)
C(48)-H(48)	1.0000
C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(42A)-C(43A)	1.595(13)
C(42A)-H(42C)	0.9900
C(42A)-H(42D)	0.9900
C(43A)-C(44A)	1.483(12)
C(43A)-C(49A)	1.492(12)
C(43A)-H(43A)	1.0000
C(44A)-C(45A)	1.498(12)
C(44A)-H(44C)	0.9900
C(44A)-H(44D)	0.9900
C(45A)-C(50A)	1.503(12)
C(45A)-C(46A)	1.585(13)
C(45A)-H(45A)	1.0000
C(46A)-H(46C)	0.9900
C(46A)-H(46D)	0.9900
C(47A)-C(48A)	1.580(13)
C(47A)-H(47C)	0.9900
C(47A)-H(47D)	0.9900
C(48A)-C(49A)	1.488(12)

C(48A)-C(50A)	1.498(12)
C(48A)-H(48A)	1.0000
C(49A)-H(49C)	0.9900
C(49A)-H(49D)	0.9900
C(50A)-H(50C)	0.9900
C(50A)-H(50D)	0.9900
C(53)-C(52)	1.536(12)
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800
C(54)-C(52)	1.497(12)
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(53A)-C(52)	1.515(12)
C(53A)-H(53D)	0.9800
C(53A)-H(53E)	0.9800
C(53A)-H(53F)	0.9800
C(54A)-C(52)	1.520(12)
C(54A)-H(54D)	0.9800
C(54A)-H(54E)	0.9800
C(54A)-H(54F)	0.9800
C(51)-C(52)	1.530(10)
C(51)-H(51A)	0.9900
C(51)-H(51B)	0.9900
C(52)-C(55A)	1.502(15)
C(52)-C(55)	1.503(15)
C(55)-C(60)	1.361(12)
C(55)-C(56)	1.366(12)
C(56)-C(57)	1.417(12)
C(56)-H(56)	0.9500
C(57)-C(58)	1.415(13)
C(57)-H(57)	0.9500
C(58)-C(59)	1.416(13)
C(58)-H(58)	0.9500
C(59)-C(60)	1.417(12)

C(59)-H(59)	0.9500
C(60)-H(60)	0.9500
C(55A)-C(56A)	1.364(12)
C(55A)-C(60A)	1.364(12)
C(56A)-C(57A)	1.416(12)
C(56A)-H(56A)	0.9500
C(57A)-C(58A)	1.416(13)
C(57A)-H(57A)	0.9500
C(58A)-C(59A)	1.416(13)
C(58A)-H(58A)	0.9500
C(59A)-C(60A)	1.416(12)
C(59A)-H(59A)	0.9500
C(60A)-H(60A)	0.9500
O(1S)-C(1S)	1.51(4)
O(1S)-C(4S)	1.51(4)
C(1S)-C(2S)	1.23(6)
C(1S)-H(1S1)	0.9900
C(1S)-H(1S2)	0.9900
C(2S)-C(3S)	1.63(10)
C(2S)-H(2S1)	0.9900
C(2S)-H(2S2)	0.9900
C(3S)-C(4S)	1.23(6)
C(3S)-H(3S1)	0.9900
C(3S)-H(3S2)	0.9900
C(4S)-H(4S1)	0.9900
C(4S)-H(4S2)	0.9900
O(1SA)-C(40)#4	1.38(10)
O(1SA)-C(1SA)	1.51(4)
O(1SA)-C(4SA)	1.51(4)
O(1SA)-C(39)#4	1.59(11)
C(1SA)-C(2SA)	1.23(6)
C(1SA)-C(39)#4	1.88(13)
C(1SA)-H(1S3)	0.9900
C(1SA)-H(1S4)	0.9900
C(2SA)-C(3SA)	1.63(10)
C(2SA)-H(2S3)	0.9900

C(2SA)-H(2S4)	0.9900
C(3SA)-C(4SA)	1.23(6)
C(3SA)-H(3S3)	0.9900
C(3SA)-H(3S4)	0.9900
C(4SA)-C(40)#4	1.99(12)
C(4SA)-H(4S3)	0.9900
C(4SA)-H(4S4)	0.9900
C(1X)-C(2X)	1.80(6)
C(1X)-H(1X1)	0.9800
C(1X)-H(1X2)	0.9800
C(1X)-H(1X3)	0.9800
C(2X)-C(3X)	1.38(6)
C(2X)-H(2X1)	0.9900
C(2X)-H(2X2)	0.9900
C(3X)-C(4X)	1.38(6)
C(3X)-H(3X1)	0.9900
C(3X)-H(3X2)	0.9900
C(4X)-C(5X)	1.80(6)
C(4X)-H(4X1)	0.9900
C(4X)-H(4X2)	0.9900
C(5X)-H(5X1)	0.9800
C(5X)-H(5X2)	0.9800
C(5X)-H(5X3)	0.9800
C(1Y)-C(2Y)	1.80(6)
C(1Y)-H(1Y1)	0.9800
C(1Y)-H(1Y2)	0.9800
C(1Y)-H(1Y3)	0.9800
C(2Y)-C(3Y)	1.38(6)
C(2Y)-H(2Y1)	0.9900
C(2Y)-H(2Y2)	0.9900
C(3Y)-C(4Y)	1.38(6)
C(3Y)-H(3Y1)	0.9900
C(3Y)-H(3Y2)	0.9900
C(4Y)-C(5Y)	1.80(6)
C(4Y)-H(4Y1)	0.9900
C(4Y)-H(4Y2)	0.9900

C(5Y)-H(5Y1)	0.9800
C(5Y)-H(5Y2)	0.9800
C(5Y)-H(5Y3)	0.9800
C(1T)-C(2T)	1.80(6)
C(1T)-H(1T1)	0.9800
C(1T)-H(1T2)	0.9800
C(1T)-H(1T3)	0.9800
C(2T)-C(3T)	1.38(6)
C(2T)-H(2T1)	0.9900
C(2T)-H(2T2)	0.9900
C(3T)-C(4T)	1.38(6)
C(3T)-H(3T1)	0.9900
C(3T)-H(3T2)	0.9900
C(4T)-C(5T)	1.80(6)
C(4T)-H(4T1)	0.9900
C(4T)-H(4T2)	0.9900
C(5T)-H(5T1)	0.9800
C(5T)-H(5T2)	0.9800
C(5T)-H(5T3)	0.9800
C(1U)-C(2U)	1.80(6)
C(1U)-H(1U1)	0.9800
C(1U)-H(1U2)	0.9800
C(1U)-H(1U3)	0.9800
C(2U)-C(3U)	1.38(6)
C(2U)-H(2U1)	0.9900
C(2U)-H(2U2)	0.9900
C(3U)-C(4U)	1.38(6)
C(3U)-H(3U1)	0.9900
C(3U)-H(3U2)	0.9900
C(4U)-C(5U)	1.80(6)
C(4U)-H(4U1)	0.9900
C(4U)-H(4U2)	0.9900
C(5U)-H(5U1)	0.9800
C(5U)-H(5U2)	0.9800
C(5U)-H(5U3)	0.9800
O(1V)-C(4V)	1.51(4)

O(1V)-C(1V)	1.52(4)
C(1V)-C(2V)	1.23(6)
C(1V)-H(1V1)	0.9900
C(1V)-H(1V2)	0.9900
C(2V)-C(3V)	1.63(10)
C(2V)-H(2V1)	0.9900
C(2V)-H(2V2)	0.9900
C(3V)-C(4V)	1.23(6)
C(3V)-H(3V1)	0.9900
C(3V)-H(3V2)	0.9900
C(4V)-H(4V1)	0.9900
C(4V)-H(4V2)	0.9900

N(5)-Mo(1)-C(21)	101.8(3)
N(5)-Mo(1)-N(3)	96.5(3)
C(21)-Mo(1)-N(3)	93.6(3)
N(5)-Mo(1)-N(1)	95.6(3)
C(21)-Mo(1)-N(1)	99.6(3)
N(3)-Mo(1)-N(1)	159.9(3)
N(5)-Mo(1)-N(7)	91.1(3)
C(21)-Mo(1)-N(7)	166.3(3)
N(3)-Mo(1)-N(7)	80.2(2)
N(1)-Mo(1)-N(7)	83.5(2)
N(5)-Mo(1)-N(9)#1	171.9(3)
C(21)-Mo(1)-N(9)#1	85.9(3)
N(3)-Mo(1)-N(9)#1	85.1(3)
N(1)-Mo(1)-N(9)#1	80.8(2)
N(7)-Mo(1)-N(9)#1	81.4(2)
C(1)-N(1)-C(4)	104.0(8)
C(1)-N(1)-Mo(1)	124.7(6)
C(4)-N(1)-Mo(1)	131.0(6)
C(2)-C(1)-N(1)	112.0(9)
C(2)-C(1)-H(1)	124.0
N(1)-C(1)-H(1)	124.0
C(1)-C(2)-C(3)	107.7(9)
C(1)-C(2)-H(2)	126.1

C(3)-C(2)-H(2)	126.1
C(4)-C(3)-C(2)	105.2(9)
C(4)-C(3)-H(3)	127.4
C(2)-C(3)-H(3)	127.4
C(3)-C(4)-N(1)	111.1(8)
C(3)-C(4)-C(5)	123.1(8)
N(1)-C(4)-C(5)	125.5(8)
N(2)-C(5)-C(4)	173.9(9)
C(5)-N(2)-Mo(2)	168.9(6)
C(6)-N(3)-C(9)	104.3(8)
C(6)-N(3)-Mo(1)	124.1(7)
C(9)-N(3)-Mo(1)	131.5(5)
N(3)-C(6)-C(7)	111.7(9)
N(3)-C(6)-H(6)	124.2
C(7)-C(6)-H(6)	124.2
C(6)-C(7)-C(8)	107.8(9)
C(6)-C(7)-H(7)	126.1
C(8)-C(7)-H(7)	126.1
C(7)-C(8)-C(9)	104.5(9)
C(7)-C(8)-H(8)	127.8
C(9)-C(8)-H(8)	127.8
N(3)-C(9)-C(8)	111.7(8)
N(3)-C(9)-C(10)	122.0(8)
C(8)-C(9)-C(10)	126.3(9)
N(4)-C(10)-C(9)	177.6(9)
C(10)-N(4)-Mo(2)#1	165.3(7)
C(11)-N(5)-Mo(1)	166.7(6)
N(5)-C(11)-C(12)	110.2(7)
N(5)-C(11)-C(16)	110.1(7)
C(12)-C(11)-C(16)	112.4(10)
N(5)-C(11)-C(17)	109.7(8)
C(12)-C(11)-C(17)	108.0(10)
C(16)-C(11)-C(17)	106.3(10)
C(11)-C(12)-C(13)	110.3(8)
C(11)-C(12)-H(12A)	109.6
C(13)-C(12)-H(12A)	109.6

C(11)-C(12)-H(12B)	109.6
C(13)-C(12)-H(12B)	109.6
H(12A)-C(12)-H(12B)	108.1
C(19)-C(13)-C(14)	114.7(12)
C(19)-C(13)-C(12)	104.8(9)
C(14)-C(13)-C(12)	104.1(8)
C(19)-C(13)-H(13)	111.0
C(14)-C(13)-H(13)	111.0
C(12)-C(13)-H(13)	111.0
C(15)-C(14)-C(13)	113.7(10)
C(15)-C(14)-H(14A)	108.8
C(13)-C(14)-H(14A)	108.8
C(15)-C(14)-H(14B)	108.8
C(13)-C(14)-H(14B)	108.8
H(14A)-C(14)-H(14B)	107.7
C(14)-C(15)-C(20)	113.6(11)
C(14)-C(15)-C(16)	106.3(8)
C(20)-C(15)-C(16)	103.9(8)
C(14)-C(15)-H(15)	110.9
C(20)-C(15)-H(15)	110.9
C(16)-C(15)-H(15)	110.9
C(11)-C(16)-C(15)	110.1(8)
C(11)-C(16)-H(16A)	109.6
C(15)-C(16)-H(16A)	109.6
C(11)-C(16)-H(16B)	109.6
C(15)-C(16)-H(16B)	109.6
H(16A)-C(16)-H(16B)	108.2
C(11)-C(17)-C(18)	111.2(9)
C(11)-C(17)-H(17A)	109.4
C(18)-C(17)-H(17A)	109.4
C(11)-C(17)-H(17B)	109.4
C(18)-C(17)-H(17B)	109.4
H(17A)-C(17)-H(17B)	108.0
C(20)-C(18)-C(19)	113.9(12)
C(20)-C(18)-C(17)	105.5(9)
C(19)-C(18)-C(17)	103.9(8)

C(20)-C(18)-H(18)	111.0
C(19)-C(18)-H(18)	111.0
C(17)-C(18)-H(18)	111.0
C(13)-C(19)-C(18)	112.7(11)
C(13)-C(19)-H(19A)	109.1
C(18)-C(19)-H(19A)	109.1
C(13)-C(19)-H(19B)	109.1
C(18)-C(19)-H(19B)	109.1
H(19A)-C(19)-H(19B)	107.8
C(18)-C(20)-C(15)	112.5(10)
C(18)-C(20)-H(20A)	109.1
C(15)-C(20)-H(20A)	109.1
C(18)-C(20)-H(20B)	109.1
C(15)-C(20)-H(20B)	109.1
H(20A)-C(20)-H(20B)	107.8
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(22)-C(23A)-H(23D)	109.5
C(22)-C(23A)-H(23E)	109.5
H(23D)-C(23A)-H(23E)	109.5
C(22)-C(23A)-H(23F)	109.5
H(23D)-C(23A)-H(23F)	109.5
H(23E)-C(23A)-H(23F)	109.5
C(22)-C(24A)-H(24D)	109.5
C(22)-C(24A)-H(24E)	109.5
H(24D)-C(24A)-H(24E)	109.5

C(22)-C(24A)-H(24F)	109.5
H(24D)-C(24A)-H(24F)	109.5
H(24E)-C(24A)-H(24F)	109.5
C(22)-C(21)-Mo(1)	141.5(6)
C(22)-C(21)-H(21A)	101.6
Mo(1)-C(21)-H(21A)	101.6
C(22)-C(21)-H(21B)	101.6
Mo(1)-C(21)-H(21B)	101.6
H(21A)-C(21)-H(21B)	104.6
C(25A)-C(22)-C(23A)	111.2(10)
C(25A)-C(22)-C(23)	130.0(10)
C(23A)-C(22)-C(23)	76.2(11)
C(25A)-C(22)-C(24)	33.9(10)
C(23A)-C(22)-C(24)	141.0(12)
C(23)-C(22)-C(24)	111.3(12)
C(25A)-C(22)-C(21)	114.8(7)
C(23A)-C(22)-C(21)	105.5(8)
C(23)-C(22)-C(21)	109.8(9)
C(24)-C(22)-C(21)	107.2(8)
C(25A)-C(22)-C(24A)	106.9(8)
C(23A)-C(22)-C(24A)	110.2(11)
C(23)-C(22)-C(24A)	35.3(13)
C(24)-C(22)-C(24A)	79.0(12)
C(21)-C(22)-C(24A)	108.2(8)
C(25A)-C(22)-C(25)	73.5(8)
C(23A)-C(22)-C(25)	38.2(10)
C(23)-C(22)-C(25)	104.9(8)
C(24)-C(22)-C(25)	106.0(9)
C(21)-C(22)-C(25)	117.6(7)
C(24A)-C(22)-C(25)	129.1(9)
C(26)-C(25)-C(30)	115.2(16)
C(26)-C(25)-C(22)	125.5(13)
C(30)-C(25)-C(22)	119.3(12)
C(25)-C(26)-C(27)	127.8(17)
C(25)-C(26)-H(26)	116.1
C(27)-C(26)-H(26)	116.1

C(26)-C(27)-C(28)	113.0(16)
C(26)-C(27)-H(27)	123.5
C(28)-C(27)-H(27)	123.5
C(27)-C(28)-C(29)	123.9(18)
C(27)-C(28)-H(28)	118.1
C(29)-C(28)-H(28)	118.1
C(30)-C(29)-C(28)	114.6(16)
C(30)-C(29)-H(29)	122.7
C(28)-C(29)-H(29)	122.7
C(25)-C(30)-C(29)	125.0(16)
C(25)-C(30)-H(30)	117.5
C(29)-C(30)-H(30)	117.5
C(26A)-C(25A)-C(30A)	119.2(17)
C(26A)-C(25A)-C(22)	123.7(14)
C(30A)-C(25A)-C(22)	117.1(14)
C(25A)-C(26A)-C(27A)	122.9(17)
C(25A)-C(26A)-H(26A)	118.5
C(27A)-C(26A)-H(26A)	118.5
C(28A)-C(27A)-C(26A)	114.3(18)
C(28A)-C(27A)-H(27A)	122.9
C(26A)-C(27A)-H(27A)	122.9
C(27A)-C(28A)-C(29A)	127(2)
C(27A)-C(28A)-H(28A)	116.6
C(29A)-C(28A)-H(28A)	116.6
C(28A)-C(29A)-C(30A)	111.7(18)
C(28A)-C(29A)-H(29A)	124.1
C(30A)-C(29A)-H(29A)	124.1
C(25A)-C(30A)-C(29A)	125.1(17)
C(25A)-C(30A)-H(30A)	117.5
C(29A)-C(30A)-H(30A)	117.5
N(10)-Mo(2)-C(51)	103.5(3)
N(10)-Mo(2)-N(6)	97.7(3)
C(51)-Mo(2)-N(6)	92.1(3)
N(10)-Mo(2)-N(8)	93.9(3)
C(51)-Mo(2)-N(8)	99.2(3)
N(6)-Mo(2)-N(8)	161.4(2)

N(10)-Mo(2)-N(4)#2	89.4(3)
C(51)-Mo(2)-N(4)#2	166.2(3)
N(6)-Mo(2)-N(4)#2	81.0(2)
N(8)-Mo(2)-N(4)#2	84.7(2)
N(10)-Mo(2)-N(2)	169.3(3)
C(51)-Mo(2)-N(2)	86.5(3)
N(6)-Mo(2)-N(2)	85.8(2)
N(8)-Mo(2)-N(2)	80.3(2)
N(4)#2-Mo(2)-N(2)	81.1(2)
C(31)-N(6)-C(34)	104.1(7)
C(31)-N(6)-Mo(2)	124.2(6)
C(34)-N(6)-Mo(2)	131.7(5)
C(32)-C(31)-N(6)	111.8(7)
C(32)-C(31)-H(31)	124.1
N(6)-C(31)-H(31)	124.1
C(31)-C(32)-C(33)	107.1(7)
C(31)-C(32)-H(32)	126.4
C(33)-C(32)-H(32)	126.4
C(32)-C(33)-C(34)	106.4(8)
C(32)-C(33)-H(33)	126.8
C(34)-C(33)-H(33)	126.8
C(33)-C(34)-N(6)	110.6(7)
C(33)-C(34)-C(35)	126.9(8)
N(6)-C(34)-C(35)	122.5(8)
N(7)-C(35)-C(34)	179.1(11)
C(35)-N(7)-Mo(1)	170.8(7)
C(36)-N(8)-C(39)	104.4(7)
C(36)-N(8)-Mo(2)	123.5(6)
C(39)-N(8)-Mo(2)	132.0(5)
C(37)-C(36)-N(8)	111.2(9)
C(37)-C(36)-H(36)	124.4
N(8)-C(36)-H(36)	124.4
C(36)-C(37)-C(38)	108.1(9)
C(36)-C(37)-H(37)	125.9
C(38)-C(37)-H(37)	125.9
C(37)-C(38)-C(39)	105.2(9)

C(37)-C(38)-H(38)	127.4
C(39)-C(38)-H(38)	127.4
N(8)-C(39)-C(40)	126.3(7)
N(8)-C(39)-C(38)	111.0(8)
C(40)-C(39)-C(38)	122.7(8)
N(8)-C(39)-O(1SA)#3	98(3)
C(40)-C(39)-O(1SA)#3	55(3)
C(38)-C(39)-O(1SA)#3	122(3)
N(8)-C(39)-C(1SA)#3	94(3)
C(40)-C(39)-C(1SA)#3	98(3)
C(38)-C(39)-C(1SA)#3	78(3)
O(1SA)#3-C(39)-C(1SA)#3	51(3)
N(9)-C(40)-O(1SA)#3	115(4)
N(9)-C(40)-C(39)	173.4(8)
O(1SA)#3-C(40)-C(39)	70(4)
N(9)-C(40)-C(4SA)#3	74(3)
O(1SA)#3-C(40)-C(4SA)#3	49(4)
C(39)-C(40)-C(4SA)#3	108(3)
C(40)-N(9)-Mo(1)#2	168.7(6)
C(41)-N(10)-Mo(2)	163.6(5)
N(10)-C(41)-C(42A)	111.2(7)
N(10)-C(41)-C(42)	111.2(7)
C(42A)-C(41)-C(42)	135.5(9)
N(10)-C(41)-C(46)	110.2(6)
C(42A)-C(41)-C(46)	61.5(11)
C(42)-C(41)-C(46)	114.1(9)
N(10)-C(41)-C(46A)	111.9(7)
C(42A)-C(41)-C(46A)	117.0(12)
C(42)-C(41)-C(46A)	30.9(9)
C(46)-C(41)-C(46A)	133.9(9)
N(10)-C(41)-C(47A)	108.1(7)
C(42A)-C(41)-C(47A)	108.8(12)
C(42)-C(41)-C(47A)	69.4(10)
C(46)-C(41)-C(47A)	50.1(9)
C(46A)-C(41)-C(47A)	98.7(12)
N(10)-C(41)-C(47)	108.1(6)

C(42A)-C(41)-C(47)	42.9(10)
C(42)-C(41)-C(47)	109.8(10)
C(46)-C(41)-C(47)	102.9(10)
C(46A)-C(41)-C(47)	81.0(10)
C(47A)-C(41)-C(47)	140.8(9)
C(41)-C(42)-C(43)	109.1(8)
C(41)-C(42)-H(42A)	109.9
C(43)-C(42)-H(42A)	109.9
C(41)-C(42)-H(42B)	109.9
C(43)-C(42)-H(42B)	109.9
H(42A)-C(42)-H(42B)	108.3
C(49)-C(43)-C(44)	112.6(11)
C(49)-C(43)-C(42)	106.7(9)
C(44)-C(43)-C(42)	106.3(9)
C(49)-C(43)-H(43)	110.4
C(44)-C(43)-H(43)	110.4
C(42)-C(43)-H(43)	110.4
C(45)-C(44)-C(43)	112.7(10)
C(45)-C(44)-H(44A)	109.1
C(43)-C(44)-H(44A)	109.1
C(45)-C(44)-H(44B)	109.1
C(43)-C(44)-H(44B)	109.1
H(44A)-C(44)-H(44B)	107.8
C(44)-C(45)-C(50)	111.8(12)
C(44)-C(45)-C(46)	107.7(9)
C(50)-C(45)-C(46)	106.1(9)
C(44)-C(45)-H(45)	110.4
C(50)-C(45)-H(45)	110.4
C(46)-C(45)-H(45)	110.4
C(41)-C(46)-C(45)	110.7(9)
C(41)-C(46)-H(46A)	109.5
C(45)-C(46)-H(46A)	109.5
C(41)-C(46)-H(46B)	109.5
C(45)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	108.1
C(41)-C(47)-C(48)	109.8(9)

C(41)-C(47)-H(47A)	109.7
C(48)-C(47)-H(47A)	109.7
C(41)-C(47)-H(47B)	109.7
C(48)-C(47)-H(47B)	109.7
H(47A)-C(47)-H(47B)	108.2
C(49)-C(48)-C(50)	113.2(12)
C(49)-C(48)-C(47)	105.9(9)
C(50)-C(48)-C(47)	107.4(9)
C(49)-C(48)-H(48)	110.1
C(50)-C(48)-H(48)	110.1
C(47)-C(48)-H(48)	110.1
C(43)-C(49)-C(48)	111.9(10)
C(43)-C(49)-H(49A)	109.2
C(48)-C(49)-H(49A)	109.2
C(43)-C(49)-H(49B)	109.2
C(48)-C(49)-H(49B)	109.2
H(49A)-C(49)-H(49B)	107.9
C(45)-C(50)-C(48)	110.5(10)
C(45)-C(50)-H(50A)	109.5
C(48)-C(50)-H(50A)	109.5
C(45)-C(50)-H(50B)	109.5
C(48)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	108.1
C(41)-C(42A)-C(43A)	109.6(10)
C(41)-C(42A)-H(42C)	109.8
C(43A)-C(42A)-H(42C)	109.8
C(41)-C(42A)-H(42D)	109.8
C(43A)-C(42A)-H(42D)	109.8
H(42C)-C(42A)-H(42D)	108.2
C(44A)-C(43A)-C(49A)	113.5(13)
C(44A)-C(43A)-C(42A)	107.1(10)
C(49A)-C(43A)-C(42A)	104.5(10)
C(44A)-C(43A)-H(43A)	110.5
C(49A)-C(43A)-H(43A)	110.5
C(42A)-C(43A)-H(43A)	110.5
C(43A)-C(44A)-C(45A)	113.4(11)

C(43A)-C(44A)-H(44C)	108.9
C(45A)-C(44A)-H(44C)	108.9
C(43A)-C(44A)-H(44D)	108.9
C(45A)-C(44A)-H(44D)	108.9
H(44C)-C(44A)-H(44D)	107.7
C(44A)-C(45A)-C(50A)	111.5(12)
C(44A)-C(45A)-C(46A)	106.6(9)
C(50A)-C(45A)-C(46A)	106.4(10)
C(44A)-C(45A)-H(45A)	110.7
C(50A)-C(45A)-H(45A)	110.7
C(46A)-C(45A)-H(45A)	110.7
C(41)-C(46A)-C(45A)	111.2(10)
C(41)-C(46A)-H(46C)	109.4
C(45A)-C(46A)-H(46C)	109.4
C(41)-C(46A)-H(46D)	109.4
C(45A)-C(46A)-H(46D)	109.4
H(46C)-C(46A)-H(46D)	108.0
C(41)-C(47A)-C(48A)	111.5(10)
C(41)-C(47A)-H(47C)	109.3
C(48A)-C(47A)-H(47C)	109.3
C(41)-C(47A)-H(47D)	109.3
C(48A)-C(47A)-H(47D)	109.3
H(47C)-C(47A)-H(47D)	108.0
C(49A)-C(48A)-C(50A)	112.2(13)
C(49A)-C(48A)-C(47A)	107.8(10)
C(50A)-C(48A)-C(47A)	106.0(10)
C(49A)-C(48A)-H(48A)	110.2
C(50A)-C(48A)-H(48A)	110.2
C(47A)-C(48A)-H(48A)	110.2
C(48A)-C(49A)-C(43A)	111.9(11)
C(48A)-C(49A)-H(49C)	109.2
C(43A)-C(49A)-H(49C)	109.2
C(48A)-C(49A)-H(49D)	109.2
C(43A)-C(49A)-H(49D)	109.2
H(49C)-C(49A)-H(49D)	107.9
C(48A)-C(50A)-C(45A)	110.1(11)

C(48A)-C(50A)-H(50C)	109.6
C(45A)-C(50A)-H(50C)	109.6
C(48A)-C(50A)-H(50D)	109.6
C(45A)-C(50A)-H(50D)	109.6
H(50C)-C(50A)-H(50D)	108.1
C(52)-C(53)-H(53A)	109.5
C(52)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
C(52)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
C(52)-C(54)-H(54A)	109.5
C(52)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(52)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(52)-C(53A)-H(53D)	109.5
C(52)-C(53A)-H(53E)	109.5
H(53D)-C(53A)-H(53E)	109.5
C(52)-C(53A)-H(53F)	109.5
H(53D)-C(53A)-H(53F)	109.5
H(53E)-C(53A)-H(53F)	109.5
C(52)-C(54A)-H(54D)	109.5
C(52)-C(54A)-H(54E)	109.5
H(54D)-C(54A)-H(54E)	109.5
C(52)-C(54A)-H(54F)	109.5
H(54D)-C(54A)-H(54F)	109.5
H(54E)-C(54A)-H(54F)	109.5
C(52)-C(51)-Mo(2)	139.7(6)
C(52)-C(51)-H(51A)	102.1
Mo(2)-C(51)-H(51A)	102.1
C(52)-C(51)-H(51B)	102.1
Mo(2)-C(51)-H(51B)	102.1
H(51A)-C(51)-H(51B)	104.8
C(54)-C(52)-C(55A)	29.6(9)

C(54)-C(52)-C(55)	113.8(9)
C(55A)-C(52)-C(55)	84.7(6)
C(54)-C(52)-C(53A)	137.1(12)
C(55A)-C(52)-C(53A)	108.8(9)
C(55)-C(52)-C(53A)	24.6(9)
C(54)-C(52)-C(54A)	86.2(12)
C(55A)-C(52)-C(54A)	107.1(9)
C(55)-C(52)-C(54A)	122.8(12)
C(53A)-C(52)-C(54A)	109.4(12)
C(54)-C(52)-C(51)	106.1(7)
C(55A)-C(52)-C(51)	116.9(5)
C(55)-C(52)-C(51)	115.2(5)
C(53A)-C(52)-C(51)	106.2(8)
C(54A)-C(52)-C(51)	108.3(9)
C(54)-C(52)-C(53)	109.9(11)
C(55A)-C(52)-C(53)	125.8(10)
C(55)-C(52)-C(53)	104.8(8)
C(53A)-C(52)-C(53)	86.6(13)
C(54A)-C(52)-C(53)	24.8(16)
C(51)-C(52)-C(53)	106.9(8)
C(60)-C(55)-C(56)	116.1(14)
C(60)-C(55)-C(52)	123.1(8)
C(56)-C(55)-C(52)	120.8(8)
C(55)-C(56)-C(57)	125.9(12)
C(55)-C(56)-H(56)	117.0
C(57)-C(56)-H(56)	117.0
C(58)-C(57)-C(56)	113.8(13)
C(58)-C(57)-H(57)	123.1
C(56)-C(57)-H(57)	123.1
C(57)-C(58)-C(59)	124.3(17)
C(57)-C(58)-H(58)	117.8
C(59)-C(58)-H(58)	117.8
C(58)-C(59)-C(60)	114.1(13)
C(58)-C(59)-H(59)	122.9
C(60)-C(59)-H(59)	122.9
C(55)-C(60)-C(59)	125.7(12)

C(55)-C(60)-H(60)	117.2
C(59)-C(60)-H(60)	117.2
C(56A)-C(55A)-C(60A)	115.7(14)
C(56A)-C(55A)-C(52)	122.1(8)
C(60A)-C(55A)-C(52)	122.2(8)
C(55A)-C(56A)-C(57A)	125.8(12)
C(55A)-C(56A)-H(56A)	117.1
C(57A)-C(56A)-H(56A)	117.1
C(58A)-C(57A)-C(56A)	114.0(13)
C(58A)-C(57A)-H(57A)	123.0
C(56A)-C(57A)-H(57A)	123.0
C(57A)-C(58A)-C(59A)	124.1(17)
C(57A)-C(58A)-H(58A)	118.0
C(59A)-C(58A)-H(58A)	118.0
C(58A)-C(59A)-C(60A)	113.9(13)
C(58A)-C(59A)-H(59A)	123.1
C(60A)-C(59A)-H(59A)	123.1
C(55A)-C(60A)-C(59A)	126.1(12)
C(55A)-C(60A)-H(60A)	116.9
C(59A)-C(60A)-H(60A)	116.9
C(1S)-O(1S)-C(4S)	98(4)
C(2S)-C(1S)-O(1S)	109(4)
C(2S)-C(1S)-H(1S1)	109.8
O(1S)-C(1S)-H(1S1)	109.8
C(2S)-C(1S)-H(1S2)	109.8
O(1S)-C(1S)-H(1S2)	109.8
H(1S1)-C(1S)-H(1S2)	108.2
C(1S)-C(2S)-C(3S)	100(3)
C(1S)-C(2S)-H(2S1)	111.9
C(3S)-C(2S)-H(2S1)	111.9
C(1S)-C(2S)-H(2S2)	111.9
C(3S)-C(2S)-H(2S2)	111.9
H(2S1)-C(2S)-H(2S2)	109.6
C(4S)-C(3S)-C(2S)	99(3)
C(4S)-C(3S)-H(3S1)	111.9
C(2S)-C(3S)-H(3S1)	111.9

C(4S)-C(3S)-H(3S2)	111.9
C(2S)-C(3S)-H(3S2)	111.9
H(3S1)-C(3S)-H(3S2)	109.6
C(3S)-C(4S)-O(1S)	109(4)
C(3S)-C(4S)-H(4S1)	109.8
O(1S)-C(4S)-H(4S1)	109.8
C(3S)-C(4S)-H(4S2)	109.8
O(1S)-C(4S)-H(4S2)	109.8
H(4S1)-C(4S)-H(4S2)	108.3
C(40)#4-O(1SA)-C(1SA)	119(8)
C(40)#4-O(1SA)-C(4SA)	87(7)
C(1SA)-O(1SA)-C(4SA)	98(4)
C(40)#4-O(1SA)-C(39)#4	55(4)
C(1SA)-O(1SA)-C(39)#4	75(7)
C(4SA)-O(1SA)-C(39)#4	126(7)
C(2SA)-C(1SA)-O(1SA)	110(4)
C(2SA)-C(1SA)-C(39)#4	143(7)
O(1SA)-C(1SA)-C(39)#4	55(5)
C(2SA)-C(1SA)-H(1S3)	109.8
O(1SA)-C(1SA)-H(1S3)	109.8
C(39)#4-C(1SA)-H(1S3)	107.1
C(2SA)-C(1SA)-H(1S4)	109.8
O(1SA)-C(1SA)-H(1S4)	109.8
C(39)#4-C(1SA)-H(1S4)	58.8
H(1S3)-C(1SA)-H(1S4)	108.2
C(1SA)-C(2SA)-C(3SA)	100(3)
C(1SA)-C(2SA)-H(2S3)	111.9
C(3SA)-C(2SA)-H(2S3)	111.9
C(1SA)-C(2SA)-H(2S4)	111.9
C(3SA)-C(2SA)-H(2S4)	111.9
H(2S3)-C(2SA)-H(2S4)	109.6
C(4SA)-C(3SA)-C(2SA)	99(3)
C(4SA)-C(3SA)-H(3S3)	111.9
C(2SA)-C(3SA)-H(3S3)	111.9
C(4SA)-C(3SA)-H(3S4)	111.9
C(2SA)-C(3SA)-H(3S4)	111.9

H(3S3)-C(3SA)-H(3S4)	109.6
C(3SA)-C(4SA)-O(1SA)	109(4)
C(3SA)-C(4SA)-C(40)#4	109(7)
O(1SA)-C(4SA)-C(40)#4	44(4)
C(3SA)-C(4SA)-H(4S3)	109.9
O(1SA)-C(4SA)-H(4S3)	109.9
C(40)#4-C(4SA)-H(4S3)	68.9
C(3SA)-C(4SA)-H(4S4)	109.9
O(1SA)-C(4SA)-H(4S4)	109.9
C(40)#4-C(4SA)-H(4S4)	138.9
H(4S3)-C(4SA)-H(4S4)	108.3
C(2X)-C(1X)-H(1X1)	109.5
C(2X)-C(1X)-H(1X2)	109.5
H(1X1)-C(1X)-H(1X2)	109.5
C(2X)-C(1X)-H(1X3)	109.5
H(1X1)-C(1X)-H(1X3)	109.5
H(1X2)-C(1X)-H(1X3)	109.5
C(3X)-C(2X)-C(1X)	123(4)
C(3X)-C(2X)-H(2X1)	106.6
C(1X)-C(2X)-H(2X1)	106.6
C(3X)-C(2X)-H(2X2)	106.6
C(1X)-C(2X)-H(2X2)	106.6
H(2X1)-C(2X)-H(2X2)	106.6
C(4X)-C(3X)-C(2X)	131(6)
C(4X)-C(3X)-H(3X1)	104.6
C(2X)-C(3X)-H(3X1)	104.6
C(4X)-C(3X)-H(3X2)	104.6
C(2X)-C(3X)-H(3X2)	104.6
H(3X1)-C(3X)-H(3X2)	105.7
C(3X)-C(4X)-C(5X)	123(5)
C(3X)-C(4X)-H(4X1)	106.6
C(5X)-C(4X)-H(4X1)	106.6
C(3X)-C(4X)-H(4X2)	106.6
C(5X)-C(4X)-H(4X2)	106.6
H(4X1)-C(4X)-H(4X2)	106.6
C(4X)-C(5X)-H(5X1)	109.5

C(4X)-C(5X)-H(5X2)	109.5
H(5X1)-C(5X)-H(5X2)	109.5
C(4X)-C(5X)-H(5X3)	109.5
H(5X1)-C(5X)-H(5X3)	109.5
H(5X2)-C(5X)-H(5X3)	109.5
C(2Y)-C(1Y)-H(1Y1)	109.5
C(2Y)-C(1Y)-H(1Y2)	109.5
H(1Y1)-C(1Y)-H(1Y2)	109.5
C(2Y)-C(1Y)-H(1Y3)	109.5
H(1Y1)-C(1Y)-H(1Y3)	109.5
H(1Y2)-C(1Y)-H(1Y3)	109.5
C(3Y)-C(2Y)-C(1Y)	123(5)
C(3Y)-C(2Y)-H(2Y1)	106.7
C(1Y)-C(2Y)-H(2Y1)	106.7
C(3Y)-C(2Y)-H(2Y2)	106.7
C(1Y)-C(2Y)-H(2Y2)	106.7
H(2Y1)-C(2Y)-H(2Y2)	106.6
C(4Y)-C(3Y)-C(2Y)	131(6)
C(4Y)-C(3Y)-H(3Y1)	104.6
C(2Y)-C(3Y)-H(3Y1)	104.6
C(4Y)-C(3Y)-H(3Y2)	104.6
C(2Y)-C(3Y)-H(3Y2)	104.6
H(3Y1)-C(3Y)-H(3Y2)	105.7
C(3Y)-C(4Y)-C(5Y)	123(5)
C(3Y)-C(4Y)-H(4Y1)	106.6
C(5Y)-C(4Y)-H(4Y1)	106.6
C(3Y)-C(4Y)-H(4Y2)	106.6
C(5Y)-C(4Y)-H(4Y2)	106.6
H(4Y1)-C(4Y)-H(4Y2)	106.5
C(4Y)-C(5Y)-H(5Y1)	109.5
C(4Y)-C(5Y)-H(5Y2)	109.5
H(5Y1)-C(5Y)-H(5Y2)	109.5
C(4Y)-C(5Y)-H(5Y3)	109.5
H(5Y1)-C(5Y)-H(5Y3)	109.5
H(5Y2)-C(5Y)-H(5Y3)	109.5
C(2T)-C(1T)-H(1T1)	109.5

C(2T)-C(1T)-H(1T2)	109.5
H(1T1)-C(1T)-H(1T2)	109.5
C(2T)-C(1T)-H(1T3)	109.5
H(1T1)-C(1T)-H(1T3)	109.5
H(1T2)-C(1T)-H(1T3)	109.5
C(3T)-C(2T)-C(1T)	123(5)
C(3T)-C(2T)-H(2T1)	106.6
C(1T)-C(2T)-H(2T1)	106.6
C(3T)-C(2T)-H(2T2)	106.6
C(1T)-C(2T)-H(2T2)	106.6
H(2T1)-C(2T)-H(2T2)	106.6
C(4T)-C(3T)-C(2T)	131(6)
C(4T)-C(3T)-H(3T1)	104.5
C(2T)-C(3T)-H(3T1)	104.5
C(4T)-C(3T)-H(3T2)	104.5
C(2T)-C(3T)-H(3T2)	104.5
H(3T1)-C(3T)-H(3T2)	105.6
C(3T)-C(4T)-C(5T)	123(4)
C(3T)-C(4T)-H(4T1)	106.6
C(5T)-C(4T)-H(4T1)	106.6
C(3T)-C(4T)-H(4T2)	106.6
C(5T)-C(4T)-H(4T2)	106.6
H(4T1)-C(4T)-H(4T2)	106.6
C(4T)-C(5T)-H(5T1)	109.5
C(4T)-C(5T)-H(5T2)	109.5
H(5T1)-C(5T)-H(5T2)	109.5
C(4T)-C(5T)-H(5T3)	109.5
H(5T1)-C(5T)-H(5T3)	109.5
H(5T2)-C(5T)-H(5T3)	109.5
C(2U)-C(1U)-H(1U1)	109.5
C(2U)-C(1U)-H(1U2)	109.5
H(1U1)-C(1U)-H(1U2)	109.5
C(2U)-C(1U)-H(1U3)	109.5
H(1U1)-C(1U)-H(1U3)	109.5
H(1U2)-C(1U)-H(1U3)	109.5
C(3U)-C(2U)-C(1U)	123(5)

C(3U)-C(2U)-H(2U1)	106.6
C(1U)-C(2U)-H(2U1)	106.6
C(3U)-C(2U)-H(2U2)	106.6
C(1U)-C(2U)-H(2U2)	106.6
H(2U1)-C(2U)-H(2U2)	106.5
C(2U)-C(3U)-C(4U)	131(6)
C(2U)-C(3U)-H(3U1)	104.5
C(4U)-C(3U)-H(3U1)	104.5
C(2U)-C(3U)-H(3U2)	104.5
C(4U)-C(3U)-H(3U2)	104.5
H(3U1)-C(3U)-H(3U2)	105.7
C(3U)-C(4U)-C(5U)	123(5)
C(3U)-C(4U)-H(4U1)	106.6
C(5U)-C(4U)-H(4U1)	106.6
C(3U)-C(4U)-H(4U2)	106.6
C(5U)-C(4U)-H(4U2)	106.6
H(4U1)-C(4U)-H(4U2)	106.6
C(4U)-C(5U)-H(5U1)	109.5
C(4U)-C(5U)-H(5U2)	109.5
H(5U1)-C(5U)-H(5U2)	109.5
C(4U)-C(5U)-H(5U3)	109.5
H(5U1)-C(5U)-H(5U3)	109.5
H(5U2)-C(5U)-H(5U3)	109.5
C(4V)-O(1V)-C(1V)	98(4)
C(2V)-C(1V)-O(1V)	109(4)
C(2V)-C(1V)-H(1V1)	109.9
O(1V)-C(1V)-H(1V1)	109.9
C(2V)-C(1V)-H(1V2)	109.9
O(1V)-C(1V)-H(1V2)	109.9
H(1V1)-C(1V)-H(1V2)	108.3
C(1V)-C(2V)-C(3V)	99(3)
C(1V)-C(2V)-H(2V1)	112.0
C(3V)-C(2V)-H(2V1)	111.9
C(1V)-C(2V)-H(2V2)	112.0
C(3V)-C(2V)-H(2V2)	112.0
H(2V1)-C(2V)-H(2V2)	109.6

C(4V)-C(3V)-C(2V)	100(3)
C(4V)-C(3V)-H(3V1)	111.9
C(2V)-C(3V)-H(3V1)	111.9
C(4V)-C(3V)-H(3V2)	111.9
C(2V)-C(3V)-H(3V2)	111.9
H(3V1)-C(3V)-H(3V2)	109.6
C(3V)-C(4V)-O(1V)	110(4)
C(3V)-C(4V)-H(4V1)	109.7
O(1V)-C(4V)-H(4V1)	109.7
C(3V)-C(4V)-H(4V2)	109.7
O(1V)-C(4V)-H(4V2)	109.7
H(4V1)-C(4V)-H(4V2)	108.2

Symmetry transformations used to generate equivalent atoms:

#1 y,-x+1/2,z #2 -y+1/2,x,z #3 y,-x+1/2,z-1

#4 -y+1/2,x,z+1

Table S1D. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1b**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	84(1)	50(1)	79(1)	8(1)	-12(1)	-3(1)
N(1)	90(3)	59(3)	69(4)	5(3)	0(3)	-7(2)
C(1)	119(6)	75(5)	69(4)	5(4)	7(4)	-11(4)
C(2)	131(7)	85(6)	82(5)	3(4)	28(5)	-5(5)
C(3)	115(6)	72(5)	101(6)	11(4)	33(5)	9(4)
C(4)	91(5)	55(4)	81(4)	7(3)	11(4)	-2(3)
C(5)	69(4)	50(4)	79(4)	5(3)	5(4)	1(3)
N(2)	59(3)	51(3)	78(3)	10(3)	-2(3)	3(3)
N(3)	65(3)	56(3)	107(4)	6(3)	-8(3)	-6(2)
C(6)	64(4)	76(5)	145(8)	-5(4)	-17(4)	-9(4)
C(7)	66(4)	81(6)	161(8)	4(5)	4(4)	-13(4)
C(8)	62(4)	75(5)	125(6)	5(4)	5(4)	-2(4)
C(9)	60(3)	56(4)	97(5)	10(3)	-4(3)	0(3)
C(10)	61(4)	58(4)	73(5)	4(3)	3(4)	3(3)
N(4)	58(3)	60(4)	75(4)	1(3)	6(3)	0(3)
N(5)	111(5)	56(4)	95(4)	9(3)	-27(3)	0(3)
C(11)	149(7)	73(4)	114(5)	-9(5)	-48(4)	5(4)
C(12)	177(8)	127(6)	179(9)	-15(7)	-97(6)	30(6)
C(13)	184(9)	159(8)	181(9)	-25(8)	-88(6)	24(7)
C(14)	169(9)	174(9)	180(10)	-39(8)	-63(7)	-6(6)
C(15)	192(10)	108(6)	150(8)	-45(6)	-45(6)	-17(5)
C(16)	185(9)	79(5)	149(7)	-18(5)	-59(6)	-20(5)
C(17)	201(9)	164(9)	121(6)	-38(6)	-28(5)	-27(7)
C(18)	206(10)	177(9)	132(7)	-43(7)	-34(7)	-22(7)
C(19)	235(12)	181(10)	173(9)	-20(9)	-68(7)	-14(8)
C(20)	212(11)	150(8)	166(8)	-60(8)	-30(8)	-14(7)
C(23)	200(20)	56(5)	158(16)	17(8)	-76(14)	-10(12)
C(24)	142(10)	129(14)	125(11)	72(9)	16(10)	31(13)
C(23A)	123(9)	75(12)	160(14)	28(12)	-3(11)	20(8)
C(24A)	137(12)	57(9)	128(15)	28(9)	-24(13)	-12(9)
C(21)	93(5)	53(3)	83(5)	9(3)	2(4)	-1(3)

C(22)	111(5)	58(4)	102(5)	20(3)	-16(4)	-2(4)
C(25)	123(6)	74(8)	99(8)	-1(8)	-23(5)	17(7)
C(26)	148(9)	76(9)	103(7)	3(8)	-33(6)	23(9)
C(27)	162(12)	102(11)	126(10)	12(11)	-51(7)	28(12)
C(28)	144(10)	106(11)	159(12)	14(13)	-45(9)	37(12)
C(29)	124(7)	107(11)	152(11)	17(12)	-19(9)	42(11)
C(30)	116(6)	78(9)	125(9)	14(9)	-15(7)	21(9)
C(25A)	164(11)	70(9)	100(5)	25(6)	-17(6)	-1(9)
C(26A)	185(12)	87(11)	106(7)	14(9)	-34(8)	-11(10)
C(27A)	218(15)	102(13)	107(8)	8(11)	-31(11)	-15(12)
C(28A)	243(17)	95(13)	115(10)	-1(12)	-22(10)	7(14)
C(29A)	224(15)	109(13)	105(10)	10(11)	-2(10)	16(13)
C(30A)	194(12)	93(12)	100(8)	23(10)	1(8)	26(11)
Mo(2)	66(1)	54(1)	72(1)	8(1)	5(1)	4(1)
N(6)	55(3)	53(3)	93(4)	7(3)	5(2)	3(2)
C(31)	59(4)	54(3)	110(6)	15(4)	10(3)	0(3)
C(32)	59(4)	62(4)	124(7)	17(4)	3(4)	-10(3)
C(33)	59(4)	63(4)	118(6)	11(4)	-6(4)	-2(3)
C(34)	57(4)	56(3)	102(5)	13(3)	0(3)	-2(3)
C(35)	65(4)	54(3)	90(5)	6(3)	-1(4)	0(3)
N(7)	70(4)	56(3)	91(4)	11(3)	-6(3)	-1(3)
N(8)	73(2)	62(4)	65(3)	9(3)	-5(2)	1(3)
C(36)	98(4)	72(5)	60(4)	8(3)	-7(3)	-1(4)
C(37)	97(5)	91(6)	83(5)	-9(4)	-31(4)	14(5)
C(38)	73(4)	97(6)	104(6)	-23(5)	-26(4)	11(4)
C(39)	67(3)	66(4)	78(4)	-2(3)	-14(3)	9(4)
C(40)	51(4)	57(4)	80(4)	5(3)	-10(3)	7(3)
N(9)	51(3)	69(4)	78(4)	0(3)	-8(3)	-1(3)
N(10)	77(4)	73(3)	80(3)	14(3)	15(3)	5(3)
C(41)	82(4)	80(4)	87(4)	23(3)	13(3)	-3(3)
C(42)	80(5)	87(7)	118(8)	27(6)	23(5)	-5(5)
C(43)	94(6)	95(8)	110(8)	27(5)	24(5)	-20(6)
C(44)	99(6)	87(6)	116(8)	35(5)	11(6)	-8(6)
C(45)	89(6)	91(5)	110(7)	37(5)	2(5)	7(5)
C(46)	75(7)	82(5)	104(7)	31(4)	9(5)	6(5)
C(47)	91(7)	109(7)	88(6)	30(5)	8(5)	-11(6)

C(48)	104(7)	116(7)	98(7)	36(5)	0(6)	-19(7)
C(49)	119(9)	118(8)	102(7)	28(6)	20(6)	-30(7)
C(50)	104(7)	118(7)	115(8)	40(6)	-7(6)	-4(6)
C(42A)	84(5)	95(7)	92(8)	25(6)	12(5)	5(6)
C(43A)	95(6)	104(8)	105(8)	36(5)	1(5)	-5(6)
C(44A)	101(9)	114(9)	89(8)	30(6)	0(6)	-26(8)
C(45A)	92(7)	96(8)	93(7)	21(5)	13(7)	-31(7)
C(46A)	75(7)	86(7)	92(7)	16(6)	15(6)	-18(7)
C(47A)	98(9)	79(5)	95(8)	21(5)	10(7)	-3(6)
C(48A)	96(7)	83(5)	104(8)	26(6)	12(6)	-6(7)
C(49A)	99(6)	99(7)	115(9)	30(6)	5(7)	0(7)
C(50A)	99(7)	88(8)	101(8)	19(7)	14(7)	-24(8)
C(53)	144(17)	65(5)	155(15)	-9(8)	62(14)	9(7)
C(54)	87(6)	106(12)	137(13)	-31(12)	33(7)	-13(8)
C(53A)	95(12)	176(17)	116(10)	-57(11)	24(8)	-5(10)
C(54A)	147(18)	86(11)	146(16)	21(11)	70(12)	43(10)
C(51)	70(4)	61(3)	86(4)	-3(3)	-2(3)	4(3)
C(52)	79(5)	69(4)	108(5)	-6(4)	20(4)	6(3)
C(55)	96(9)	153(11)	102(5)	-13(6)	27(5)	13(8)
C(56)	112(12)	226(15)	121(9)	-32(11)	10(8)	-9(10)
C(57)	145(14)	262(18)	127(11)	-28(14)	-1(9)	-14(13)
C(58)	177(16)	260(19)	130(11)	-12(13)	9(11)	-2(14)
C(59)	175(15)	231(17)	114(8)	15(12)	16(11)	-3(13)
C(60)	135(11)	176(13)	114(7)	15(9)	27(9)	13(10)
C(55A)	89(8)	84(8)	141(9)	-3(8)	28(6)	-3(6)
C(56A)	78(9)	101(11)	169(11)	-26(10)	28(9)	-4(7)
C(57A)	104(11)	123(13)	191(13)	-36(13)	43(11)	-28(8)
C(58A)	101(12)	136(15)	193(15)	-18(13)	44(11)	-15(10)
C(59A)	103(12)	146(14)	169(12)	3(12)	44(10)	-23(10)
C(60A)	99(10)	130(11)	145(9)	10(10)	36(8)	-13(8)
O(1S)	120(20)	59(13)	120(20)	11(16)	6(17)	1(14)
C(1S)	110(20)	64(17)	130(30)	12(17)	6(17)	5(16)
C(2S)	120(20)	67(17)	130(30)	14(18)	4(19)	7(16)
C(3S)	120(20)	60(13)	130(30)	16(17)	3(19)	5(18)
C(4S)	110(20)	61(14)	130(20)	15(16)	4(16)	2(16)
O(1SA)	130(30)	90(20)	130(30)	10(20)	0(20)	10(20)

C(1SA)	130(30)	80(20)	130(30)	10(20)	0(20)	10(20)
C(2SA)	120(20)	74(18)	130(30)	11(19)	1(19)	2(17)
C(3SA)	120(20)	77(18)	130(30)	9(19)	3(19)	1(18)
C(4SA)	130(30)	80(20)	130(30)	10(20)	0(20)	10(20)
C(1X)	130(40)	190(30)	40(30)	40(30)	-10(40)	-30(30)
C(2X)	130(30)	190(30)	48(15)	10(20)	-10(20)	-30(20)
C(3X)	130(30)	190(30)	47(16)	10(20)	-10(20)	-30(20)
C(4X)	130(30)	190(30)	44(16)	10(20)	-10(20)	-30(20)
C(5X)	130(40)	190(30)	60(40)	20(40)	-20(30)	-30(30)
C(1Y)	140(30)	190(30)	40(20)	20(30)	-10(30)	-30(30)
C(2Y)	130(30)	190(30)	48(16)	10(30)	0(30)	-30(30)
C(3Y)	130(30)	190(30)	47(14)	10(20)	-10(20)	-30(20)
C(4Y)	130(30)	190(30)	46(19)	10(20)	-10(30)	-30(20)
C(5Y)	130(40)	190(30)	50(30)	20(30)	-20(30)	-30(30)
C(1T)	114(9)	115(9)	128(10)	4(9)	6(9)	-31(9)
C(2T)	114(9)	115(9)	128(10)	4(9)	6(9)	-31(9)
C(3T)	114(9)	115(9)	128(10)	4(9)	6(9)	-31(9)
C(4T)	114(9)	115(9)	128(10)	4(9)	6(9)	-31(9)
C(5T)	114(9)	115(9)	128(10)	4(9)	6(9)	-31(9)
C(1U)	115(9)	115(9)	128(10)	5(9)	6(9)	-30(9)
C(2U)	115(9)	115(9)	128(10)	5(9)	6(9)	-30(9)
C(3U)	115(9)	115(9)	128(10)	5(9)	6(9)	-30(9)
C(4U)	115(9)	115(9)	128(10)	5(9)	6(9)	-30(9)
C(5U)	115(9)	115(9)	128(10)	5(9)	6(9)	-30(9)
O(1V)	126(16)	127(16)	131(12)	6(14)	6(13)	-23(14)
C(1V)	118(15)	122(16)	127(14)	9(13)	9(13)	-31(13)
C(2V)	117(14)	119(13)	126(14)	11(12)	10(13)	-31(12)
C(3V)	116(12)	117(12)	130(11)	6(11)	6(11)	-30(11)
C(4V)	117(13)	122(13)	130(12)	4(13)	6(11)	-30(11)

Table S1E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **1b**.

	x	y	z	U(eq)
H(1)	1104	2672	-1549	105
H(2)	1802	2181	-1620	119
H(3)	1887	1708	-933	115
H(6)	-691	2644	-466	114
H(7)	-1150	3007	113	123
H(8)	-642	3618	468	105
H(12A)	-544	3075	-1663	193
H(12B)	-842	2812	-1300	193
H(13)	-1255	2723	-1994	210
H(14A)	-1264	2128	-1461	209
H(14B)	-1348	1923	-1932	209
H(15)	-832	1432	-1585	180
H(16A)	-551	1994	-1048	165
H(16B)	-102	1782	-1288	165
H(17A)	317	2210	-1812	195
H(17B)	146	2715	-1972	195
H(18)	-82	2123	-2512	206
H(19A)	-539	2805	-2377	236
H(19B)	-852	2386	-2559	236
H(20A)	-128	1520	-1988	211
H(20B)	-580	1522	-2291	211
H(23A)	526	4551	-1125	206
H(23B)	923	4308	-840	206
H(23C)	391	4308	-679	206
H(24A)	773	4038	-1750	198
H(24B)	773	3482	-1688	198
H(24C)	1160	3795	-1452	198
H(23D)	16	4069	-738	179
H(23E)	-198	3749	-1111	179
H(23F)	-49	4278	-1211	179

H(24D)	858	4305	-769	161
H(24E)	794	4494	-1249	161
H(24F)	1183	4108	-1146	161
H(21A)	610	3581	-577	91
H(21B)	952	3369	-919	91
H(26)	156	3958	-1957	131
H(27)	-603	4008	-2246	156
H(28)	-1226	3979	-1737	164
H(29)	-1081	3946	-985	153
H(30)	-302	3774	-780	128
H(26A)	-98	3895	-1806	151
H(27A)	-17	3719	-2550	171
H(28A)	709	3414	-2766	181
H(29A)	1362	3334	-2305	175
H(30A)	1202	3498	-1568	155
H(31)	108	374	369	89
H(32)	-564	337	-127	98
H(33)	-614	1114	-509	96
H(36)	1429	1678	1359	92
H(37)	2273	1821	1410	108
H(38)	2649	1531	730	110
H(42A)	30	339	1272	114
H(42B)	115	741	1622	114
H(43)	-25	-11	1988	120
H(44A)	493	-624	1860	121
H(44B)	292	-453	1407	121
H(45)	1111	-580	1371	116
H(46A)	1283	193	1052	104
H(46B)	791	-6	887	104
H(47A)	941	1010	1795	115
H(47B)	1371	770	1549	115
H(48)	1298	441	2277	127
H(49A)	609	47	2451	136
H(49B)	477	565	2297	136
H(50A)	1606	-32	1721	135
H(50B)	1333	-347	2065	135

H(42C)	1351	741	1561	108
H(42D)	1396	348	1196	108
H(43A)	1542	6	1918	122
H(44C)	1005	523	2256	122
H(44D)	932	-8	2402	122
H(45A)	196	318	2277	112
H(46C)	46	626	1542	102
H(46D)	421	937	1796	102
H(47C)	676	4	856	109
H(47D)	176	137	1052	109
H(48A)	442	-632	1314	113
H(49C)	1243	-430	1324	125
H(49D)	1086	-649	1774	125
H(50C)	246	-468	2037	115
H(50D)	-88	-178	1720	115
H(53A)	460	2718	1009	182
H(53B)	-85	2707	1128	182
H(53C)	79	2620	643	182
H(54A)	-350	1852	644	165
H(54B)	-512	1959	1126	165
H(54C)	-249	1479	1016	165
H(53D)	740	2373	1339	193
H(53E)	604	1885	1558	193
H(53F)	283	2336	1634	193
H(54D)	225	2695	753	190
H(54E)	-216	2638	1064	190
H(54F)	-220	2399	600	190
H(51A)	811	2044	744	87
H(51B)	393	1938	432	87
H(56)	896	2425	1433	183
H(57)	1192	2389	2142	214
H(58)	751	1935	2637	227
H(59)	55	1537	2435	208
H(60)	-166	1596	1705	170
H(56A)	-365	1486	596	139
H(57A)	-1054	1068	772	167

H(58A)	-1208	973	1517	172
H(59A)	-789	1401	2049	167
H(60A)	-158	1863	1798	149
H(1S1)	1934	2241	10177	122
H(1S2)	2357	2511	10409	122
H(2S1)	2043	3027	10073	124
H(2S2)	1931	2690	9668	124
H(3S1)	2687	3077	9481	123
H(3S2)	2902	2947	9946	123
H(4S1)	3115	2407	9562	120
H(4S2)	2630	2398	9302	120
H(1S3)	2891	1719	10472	135
H(1S4)	3163	2191	10596	135
H(2S3)	2597	2436	10281	130
H(2S4)	2600	2010	9938	130
H(3S3)	3045	2651	9578	132
H(3S4)	3364	2725	10002	132
H(4S3)	3746	2272	9633	138
H(4S4)	3288	1994	9477	138
H(1X1)	1515	3211	2395	180
H(1X2)	1191	2812	2598	180
H(1X3)	1283	2823	2092	180
H(2X1)	2168	2631	2243	147
H(2X2)	2047	2576	2738	147
H(3X1)	1690	1926	2620	147
H(3X2)	1750	1984	2119	147
H(4X1)	2427	1736	2680	145
H(4X2)	2495	1802	2178	145
H(5X1)	2463	921	2333	187
H(5X2)	2019	1040	2039	187
H(5X3)	1956	973	2546	187
H(1Y1)	1920	3310	2363	182
H(1Y2)	1596	2949	2619	182
H(1Y3)	1627	2923	2107	182
H(2Y1)	2503	2664	2175	148
H(2Y2)	2452	2666	2683	148

H(3Y1)	2091	2033	2693	147
H(3Y2)	1976	2051	2198	147
H(4Y1)	2832	1832	2502	148
H(4Y2)	2635	1770	2029	148
H(5Y1)	2712	962	2414	188
H(5Y2)	2188	1032	2244	188
H(5Y3)	2307	1115	2740	188
H(1T1)	8693	2174	6774	178
H(1T2)	9121	2315	6469	178
H(1T3)	8772	1905	6329	178
H(2T1)	8105	2509	6227	143
H(2T2)	8441	2918	6381	143
H(3T1)	8798	2934	5788	143
H(3T2)	8562	2465	5631	143
H(4T1)	8277	2888	5215	143
H(4T2)	8336	3338	5508	143
H(5T1)	7463	3252	5340	178
H(5T2)	7516	3182	5848	178
H(5T3)	7456	2737	5542	178
H(1U1)	8461	2579	6707	179
H(1U2)	8874	2531	6363	179
H(1U3)	8428	2194	6335	179
H(2U1)	7914	2935	6157	143
H(2U2)	8379	3238	6136	143
H(3U1)	8420	2603	5561	143
H(3U2)	8447	3153	5525	143
H(4U1)	7821	2557	5258	143
H(4U2)	7993	3042	5068	143
H(5U1)	7126	3146	5184	179
H(5U2)	7356	3462	5552	179
H(5U3)	7155	2954	5666	179
H(1V1)	9013	2468	6591	147
H(1V2)	8763	2007	6775	147
H(2V1)	8403	1895	6214	145
H(2V2)	8915	2067	6059	145
H(3V1)	8638	2894	6014	145

H(3V2)	8248	2595	5756	145
H(4V1)	7826	2541	6269	148
H(4V2)	8037	3057	6327	148

Table S2A. Crystal data and structure refinement for **2a**.

Identification code	X8_10007	
Empirical formula	C65.50 H68 Mo N2 O	
Formula weight	995.16	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 11.3417(8) Å	α= 91.909(2)°
	b = 12.1241(9) Å	β= 105.359(2)°
	c = 19.6415(15) Å	γ = 96.352(2)°
Volume	2582.9(3) $Å^3$	
Z	2	
Density (calculated)	1.280 Mg/m^3	
Absorption coefficient	0.299 mm^{-1}	
F(000)	1050	
Crystal size	0.15 x 0.03 x 0.02 mm^3	
Theta range for data collection	1.69 to 29.57°	
Index ranges	-15<=h<=15, -16<=k<=16, -27<=l<=27	
Reflections collected	79093	
Independent reflections	14466 [R(int) = 0.0536]	
Completeness to theta = 29.57°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9940 and 0.9565	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14466 / 221 / 703	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0432, wR2 = 0.0980	
R indices (all data)	R1 = 0.0587, wR2 = 0.1048	
Largest diff. peak and hole	1.038 and -0.738 e.$Å^{-3}$	

Table S2B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	9137(1)	9532(1)	2629(1)	20(1)
C(1)	7620(2)	8742(2)	2652(1)	24(1)
C(2)	6567(2)	8687(2)	2988(1)	24(1)
C(3)	5765(3)	9587(2)	2681(2)	40(1)
C(4)	7031(3)	8923(2)	3792(1)	35(1)
C(5)	5842(2)	7520(2)	2828(1)	25(1)
C(6)	4627(2)	7338(2)	2427(1)	33(1)
C(7)	3998(3)	6264(3)	2284(1)	46(1)
C(8)	4574(3)	5374(2)	2532(2)	49(1)
C(9)	5796(3)	5533(2)	2935(2)	46(1)
C(10)	6424(3)	6600(2)	3081(1)	34(1)
N(1)	9356(2)	10554(1)	3288(1)	24(1)
C(11)	9533(2)	11584(2)	3728(1)	25(1)
C(12)	8337(2)	12127(2)	3555(1)	30(1)
C(13)	9908(3)	11347(2)	4515(1)	33(1)
C(14)	10558(2)	12371(2)	3559(1)	29(1)
C(15)	8536(3)	13229(2)	4010(1)	34(1)
C(16)	8896(3)	12989(2)	4790(1)	41(1)
C(17)	10087(3)	12457(2)	4963(1)	42(1)
C(18)	11121(3)	13235(2)	4796(1)	44(1)
C(19)	10750(3)	13474(2)	4010(1)	34(1)
C(20)	9555(3)	14009(2)	3840(1)	35(1)
N(2)	10241(2)	8312(1)	2955(1)	24(1)
C(21)	9878(2)	7190(2)	3019(1)	26(1)
C(22)	10877(2)	6632(2)	3181(1)	30(1)
C(23)	11930(2)	7421(2)	3230(1)	33(1)
C(24)	11520(2)	8437(2)	3094(1)	25(1)
C(25)	12269(2)	9526(2)	3131(1)	25(1)
C(26)	12482(2)	9983(2)	2525(1)	26(1)
C(27)	13263(2)	10981(2)	2593(1)	30(1)
C(28)	13840(2)	11525(2)	3249(1)	33(1)

C(29)	13623(3)	11054(2)	3847(1)	35(1)
C(30)	12849(2)	10065(2)	3799(1)	32(1)
C(31)	11933(2)	9400(2)	1803(1)	32(1)
C(32)	14698(3)	12588(2)	3323(2)	49(1)
C(33)	12662(3)	9567(2)	4462(1)	47(1)
O(1)	9034(1)	10064(1)	1701(1)	20(1)
C(41)	8362(2)	10281(2)	1046(1)	18(1)
C(42)	8465(2)	11383(2)	839(1)	18(1)
C(51)	9358(2)	12272(2)	1308(1)	19(1)
C(52)	10616(2)	12192(2)	1494(1)	23(1)
C(53)	11453(2)	13054(2)	1890(1)	26(1)
C(54)	11042(2)	14002(2)	2115(1)	25(1)
C(55)	9797(2)	14084(2)	1944(1)	22(1)
C(56)	8954(2)	13229(2)	1541(1)	20(1)
C(43)	7714(2)	11620(2)	184(1)	19(1)
C(61)	7770(2)	12770(2)	-71(1)	19(1)
C(62)	8745(2)	13200(2)	-325(1)	26(1)
C(63)	8797(2)	14271(2)	-559(1)	29(1)
C(64)	7891(2)	14924(2)	-531(1)	28(1)
C(65)	6917(2)	14511(2)	-279(1)	26(1)
C(66)	6847(2)	13429(2)	-56(1)	23(1)
C(44)	6921(2)	10774(2)	-253(1)	19(1)
C(45)	6855(2)	9666(2)	-68(1)	18(1)
C(71)	6035(2)	8802(2)	-589(1)	18(1)
C(72)	4861(2)	9009(2)	-967(1)	21(1)
C(73)	4088(2)	8227(2)	-1465(1)	24(1)
C(74)	4477(2)	7208(2)	-1589(1)	25(1)
C(75)	5635(2)	6994(2)	-1225(1)	24(1)
C(76)	6421(2)	7780(2)	-735(1)	21(1)
C(46)	7574(2)	9416(2)	597(1)	17(1)
C(81)	7500(2)	8269(2)	848(1)	19(1)
C(82)	6380(2)	7714(2)	895(1)	21(1)
C(83)	6321(2)	6645(2)	1136(1)	26(1)
C(84)	7371(2)	6121(2)	1323(1)	28(1)
C(85)	8487(2)	6661(2)	1274(1)	26(1)
C(86)	8548(2)	7733(2)	1043(1)	22(1)

C(1X)	3679(12)	5948(13)	4765(7)	69(3)
C(2X)	4835(15)	5959(16)	4610(10)	102(4)
C(3X)	5643(14)	5189(16)	4894(8)	76(3)
C(4X)	5736(12)	4657(11)	5536(6)	69(3)
C(5X)	5380(20)	3481(11)	5504(11)	79(4)
C(1Y)	3890(20)	4820(30)	5265(13)	106(6)
C(2Y)	4687(17)	5240(20)	4860(12)	81(4)
C(3Y)	5914(15)	4960(20)	5068(14)	79(3)
C(4Y)	6178(17)	4101(17)	5541(12)	72(4)
C(5Y)	5330(30)	3115(18)	5445(15)	72(6)

Table S2C. Bond lengths [Å] and angles [°] for **2a**.

Mo(1)-N(1)	1.7099(17)
Mo(1)-C(1)	1.886(2)
Mo(1)-O(1)	1.9334(14)
Mo(1)-N(2)	2.0527(19)
C(1)-C(2)	1.507(3)
C(1)-H(1)	0.971(16)
C(2)-C(4)	1.533(3)
C(2)-C(5)	1.534(3)
C(2)-C(3)	1.535(3)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-C(6)	1.384(3)
C(5)-C(10)	1.397(3)
C(6)-C(7)	1.395(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.361(5)
C(7)-H(7)	0.9500
C(8)-C(9)	1.391(5)
C(8)-H(8)	0.9500
C(9)-C(10)	1.387(3)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
N(1)-C(11)	1.459(2)
C(11)-C(14)	1.534(3)
C(11)-C(12)	1.535(3)
C(11)-C(13)	1.537(3)
C(12)-C(15)	1.543(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(17)	1.547(3)

C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(19)	1.542(3)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.524(4)
C(15)-C(20)	1.525(3)
C(15)-H(15)	1.0000
C(16)-C(17)	1.523(4)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.535(4)
C(17)-H(17)	1.0000
C(18)-C(19)	1.534(4)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.530(4)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
N(2)-C(24)	1.392(3)
N(2)-C(21)	1.396(3)
C(21)-C(22)	1.355(3)
C(21)-H(21)	0.9500
C(22)-C(23)	1.425(3)
C(22)-H(22)	0.9500
C(23)-C(24)	1.374(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.478(3)
C(25)-C(26)	1.396(3)
C(25)-C(30)	1.404(3)
C(26)-C(27)	1.398(3)
C(26)-C(31)	1.506(3)
C(27)-C(28)	1.387(3)
C(27)-H(27)	0.9500
C(28)-C(29)	1.391(3)

C(28)-C(32)	1.505(3)
C(29)-C(30)	1.390(3)
C(29)-H(29)	0.9500
C(30)-C(33)	1.508(3)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
O(1)-C(41)	1.360(2)
C(41)-C(46)	1.411(3)
C(41)-C(42)	1.411(3)
C(42)-C(43)	1.401(3)
C(42)-C(51)	1.495(3)
C(51)-C(52)	1.391(3)
C(51)-C(56)	1.400(3)
C(52)-C(53)	1.391(3)
C(52)-H(52)	0.9500
C(53)-C(54)	1.388(3)
C(53)-H(53)	0.9500
C(54)-C(55)	1.378(3)
C(54)-H(54)	0.9500
C(55)-C(56)	1.392(3)
C(55)-H(55)	0.9500
C(56)-H(56)	0.9500
C(43)-C(44)	1.388(3)
C(43)-C(61)	1.497(3)
C(61)-C(62)	1.388(3)
C(61)-C(66)	1.390(3)
C(62)-C(63)	1.393(3)
C(62)-H(62)	0.9500
C(63)-C(64)	1.377(3)

C(63)-H(63)	0.9500
C(64)-C(65)	1.378(3)
C(64)-H(64)	0.9500
C(65)-C(66)	1.398(3)
C(65)-H(65)	0.9500
C(66)-H(66)	0.9500
C(44)-C(45)	1.403(3)
C(44)-H(44)	0.9500
C(45)-C(46)	1.407(3)
C(45)-C(71)	1.490(3)
C(71)-C(72)	1.396(3)
C(71)-C(76)	1.403(3)
C(72)-C(73)	1.387(3)
C(72)-H(72)	0.9500
C(73)-C(74)	1.393(3)
C(73)-H(73)	0.9500
C(74)-C(75)	1.376(3)
C(74)-H(74)	0.9500
C(75)-C(76)	1.388(3)
C(75)-H(75)	0.9500
C(76)-H(76)	0.9500
C(46)-C(81)	1.492(3)
C(81)-C(86)	1.389(3)
C(81)-C(82)	1.397(3)
C(82)-C(83)	1.396(3)
C(82)-H(82)	0.9500
C(83)-C(84)	1.381(3)
C(83)-H(83)	0.9500
C(84)-C(85)	1.387(3)
C(84)-H(84)	0.9500
C(85)-C(86)	1.391(3)
C(85)-H(85)	0.9500
C(86)-H(86)	0.9500
C(1X)-C(2X)	1.421(9)
C(1X)-H(1X1)	0.9800
C(1X)-H(1X2)	0.9800

C(1X)-H(1X3)	0.9800
C(2X)-C(3X)	1.405(9)
C(2X)-H(2X1)	0.9900
C(2X)-H(2X2)	0.9900
C(3X)-C(4X)	1.420(9)
C(3X)-H(3X1)	0.9900
C(3X)-H(3X2)	0.9900
C(4X)-C(5X)	1.434(9)
C(4X)-H(4X1)	0.9900
C(4X)-H(4X2)	0.9900
C(5X)-H(5X1)	0.9800
C(5X)-H(5X2)	0.9800
C(5X)-H(5X3)	0.9800
C(1Y)-C(2Y)	1.420(9)
C(1Y)-H(1Y1)	0.9800
C(1Y)-H(1Y2)	0.9800
C(1Y)-H(1Y3)	0.9800
C(2Y)-C(3Y)	1.423(9)
C(2Y)-H(2Y1)	0.9900
C(2Y)-H(2Y2)	0.9900
C(3Y)-C(4Y)	1.423(9)
C(3Y)-H(3Y1)	0.9900
C(3Y)-H(3Y2)	0.9900
C(4Y)-C(5Y)	1.424(9)
C(4Y)-H(4Y1)	0.9900
C(4Y)-H(4Y2)	0.9900
C(5Y)-H(5Y1)	0.9800
C(5Y)-H(5Y2)	0.9800
C(5Y)-H(5Y3)	0.9800

N(1)-Mo(1)-C(1)	101.96(9)
N(1)-Mo(1)-O(1)	114.72(7)
C(1)-Mo(1)-O(1)	110.45(8)
N(1)-Mo(1)-N(2)	111.01(8)
C(1)-Mo(1)-N(2)	98.33(8)
O(1)-Mo(1)-N(2)	117.88(7)

C(2)-C(1)-Mo(1)	145.64(15)
C(2)-C(1)-H(1)	114.4(15)
Mo(1)-C(1)-H(1)	99.6(15)
C(1)-C(2)-C(4)	111.37(19)
C(1)-C(2)-C(5)	108.99(17)
C(4)-C(2)-C(5)	108.89(18)
C(1)-C(2)-C(3)	107.49(19)
C(4)-C(2)-C(3)	108.3(2)
C(5)-C(2)-C(3)	111.81(19)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(6)-C(5)-C(10)	118.3(2)
C(6)-C(5)-C(2)	122.2(2)
C(10)-C(5)-C(2)	119.5(2)
C(5)-C(6)-C(7)	120.8(3)
C(5)-C(6)-H(6)	119.6
C(7)-C(6)-H(6)	119.6
C(8)-C(7)-C(6)	120.5(3)
C(8)-C(7)-H(7)	119.8
C(6)-C(7)-H(7)	119.8
C(7)-C(8)-C(9)	119.9(2)
C(7)-C(8)-H(8)	120.1
C(9)-C(8)-H(8)	120.1
C(10)-C(9)-C(8)	119.8(3)
C(10)-C(9)-H(9)	120.1
C(8)-C(9)-H(9)	120.1

C(9)-C(10)-C(5)	120.8(3)
C(9)-C(10)-H(10)	119.6
C(5)-C(10)-H(10)	119.6
C(11)-N(1)-Mo(1)	167.81(15)
N(1)-C(11)-C(14)	108.05(17)
N(1)-C(11)-C(12)	109.62(17)
C(14)-C(11)-C(12)	109.22(18)
N(1)-C(11)-C(13)	110.21(17)
C(14)-C(11)-C(13)	109.65(19)
C(12)-C(11)-C(13)	110.06(19)
C(11)-C(12)-C(15)	109.49(19)
C(11)-C(12)-H(12A)	109.8
C(15)-C(12)-H(12A)	109.8
C(11)-C(12)-H(12B)	109.8
C(15)-C(12)-H(12B)	109.8
H(12A)-C(12)-H(12B)	108.2
C(11)-C(13)-C(17)	108.65(19)
C(11)-C(13)-H(13A)	110.0
C(17)-C(13)-H(13A)	110.0
C(11)-C(13)-H(13B)	110.0
C(17)-C(13)-H(13B)	110.0
H(13A)-C(13)-H(13B)	108.3
C(11)-C(14)-C(19)	109.02(19)
C(11)-C(14)-H(14A)	109.9
C(19)-C(14)-H(14A)	109.9
C(11)-C(14)-H(14B)	109.9
C(19)-C(14)-H(14B)	109.9
H(14A)-C(14)-H(14B)	108.3
C(16)-C(15)-C(20)	110.2(2)
C(16)-C(15)-C(12)	109.18(19)
C(20)-C(15)-C(12)	109.0(2)
C(16)-C(15)-H(15)	109.5
C(20)-C(15)-H(15)	109.5
C(12)-C(15)-H(15)	109.5
C(17)-C(16)-C(15)	109.8(2)
C(17)-C(16)-H(16A)	109.7

C(15)-C(16)-H(16A)	109.7
C(17)-C(16)-H(16B)	109.7
C(15)-C(16)-H(16B)	109.7
H(16A)-C(16)-H(16B)	108.2
C(16)-C(17)-C(18)	110.0(2)
C(16)-C(17)-C(13)	110.2(2)
C(18)-C(17)-C(13)	108.5(2)
C(16)-C(17)-H(17)	109.4
C(18)-C(17)-H(17)	109.4
C(13)-C(17)-H(17)	109.4
C(19)-C(18)-C(17)	109.6(2)
C(19)-C(18)-H(18A)	109.8
C(17)-C(18)-H(18A)	109.8
C(19)-C(18)-H(18B)	109.8
C(17)-C(18)-H(18B)	109.8
H(18A)-C(18)-H(18B)	108.2
C(20)-C(19)-C(18)	109.8(2)
C(20)-C(19)-C(14)	109.7(2)
C(18)-C(19)-C(14)	109.0(2)
C(20)-C(19)-H(19)	109.5
C(18)-C(19)-H(19)	109.5
C(14)-C(19)-H(19)	109.5
C(15)-C(20)-C(19)	109.6(2)
C(15)-C(20)-H(20A)	109.7
C(19)-C(20)-H(20A)	109.7
C(15)-C(20)-H(20B)	109.7
C(19)-C(20)-H(20B)	109.7
H(20A)-C(20)-H(20B)	108.2
C(24)-N(2)-C(21)	106.47(18)
C(24)-N(2)-Mo(1)	125.43(14)
C(21)-N(2)-Mo(1)	127.86(15)
C(22)-C(21)-N(2)	110.0(2)
C(22)-C(21)-H(21)	125.0
N(2)-C(21)-H(21)	125.0
C(21)-C(22)-C(23)	107.1(2)
C(21)-C(22)-H(22)	126.4

C(23)-C(22)-H(22)	126.4
C(24)-C(23)-C(22)	107.3(2)
C(24)-C(23)-H(23)	126.3
C(22)-C(23)-H(23)	126.3
C(23)-C(24)-N(2)	109.1(2)
C(23)-C(24)-C(25)	127.7(2)
N(2)-C(24)-C(25)	123.13(19)
C(26)-C(25)-C(30)	119.8(2)
C(26)-C(25)-C(24)	121.45(19)
C(30)-C(25)-C(24)	118.58(19)
C(25)-C(26)-C(27)	119.3(2)
C(25)-C(26)-C(31)	121.5(2)
C(27)-C(26)-C(31)	119.2(2)
C(28)-C(27)-C(26)	121.6(2)
C(28)-C(27)-H(27)	119.2
C(26)-C(27)-H(27)	119.2
C(27)-C(28)-C(29)	118.3(2)
C(27)-C(28)-C(32)	121.7(2)
C(29)-C(28)-C(32)	120.1(2)
C(30)-C(29)-C(28)	121.7(2)
C(30)-C(29)-H(29)	119.2
C(28)-C(29)-H(29)	119.2
C(29)-C(30)-C(25)	119.4(2)
C(29)-C(30)-C(33)	120.0(2)
C(25)-C(30)-C(33)	120.6(2)
C(26)-C(31)-H(31A)	109.5
C(26)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(26)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(28)-C(32)-H(32A)	109.5
C(28)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(28)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5

H(32B)-C(32)-H(32C)	109.5
C(30)-C(33)-H(33A)	109.5
C(30)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(30)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(41)-O(1)-Mo(1)	150.88(13)
O(1)-C(41)-C(46)	119.89(17)
O(1)-C(41)-C(42)	118.47(16)
C(46)-C(41)-C(42)	121.63(17)
C(43)-C(42)-C(41)	118.40(17)
C(43)-C(42)-C(51)	120.98(17)
C(41)-C(42)-C(51)	120.62(17)
C(52)-C(51)-C(56)	118.49(18)
C(52)-C(51)-C(42)	120.71(17)
C(56)-C(51)-C(42)	120.73(19)
C(53)-C(52)-C(51)	120.64(19)
C(53)-C(52)-H(52)	119.7
C(51)-C(52)-H(52)	119.7
C(54)-C(53)-C(52)	120.4(2)
C(54)-C(53)-H(53)	119.8
C(52)-C(53)-H(53)	119.8
C(55)-C(54)-C(53)	119.53(19)
C(55)-C(54)-H(54)	120.2
C(53)-C(54)-H(54)	120.2
C(54)-C(55)-C(56)	120.45(19)
C(54)-C(55)-H(55)	119.8
C(56)-C(55)-H(55)	119.8
C(55)-C(56)-C(51)	120.5(2)
C(55)-C(56)-H(56)	119.7
C(51)-C(56)-H(56)	119.7
C(44)-C(43)-C(42)	119.99(18)
C(44)-C(43)-C(61)	118.58(17)
C(42)-C(43)-C(61)	121.41(17)
C(62)-C(61)-C(66)	118.78(19)

C(62)-C(61)-C(43)	120.60(19)
C(66)-C(61)-C(43)	120.61(18)
C(61)-C(62)-C(63)	120.5(2)
C(61)-C(62)-H(62)	119.8
C(63)-C(62)-H(62)	119.8
C(64)-C(63)-C(62)	120.3(2)
C(64)-C(63)-H(63)	119.8
C(62)-C(63)-H(63)	119.8
C(63)-C(64)-C(65)	119.9(2)
C(63)-C(64)-H(64)	120.1
C(65)-C(64)-H(64)	120.1
C(64)-C(65)-C(66)	120.1(2)
C(64)-C(65)-H(65)	120.0
C(66)-C(65)-H(65)	120.0
C(61)-C(66)-C(65)	120.4(2)
C(61)-C(66)-H(66)	119.8
C(65)-C(66)-H(66)	119.8
C(43)-C(44)-C(45)	122.08(18)
C(43)-C(44)-H(44)	119.0
C(45)-C(44)-H(44)	119.0
C(44)-C(45)-C(46)	118.78(17)
C(44)-C(45)-C(71)	118.37(17)
C(46)-C(45)-C(71)	122.84(17)
C(72)-C(71)-C(76)	118.00(17)
C(72)-C(71)-C(45)	120.11(17)
C(76)-C(71)-C(45)	121.85(18)
C(73)-C(72)-C(71)	121.33(19)
C(73)-C(72)-H(72)	119.3
C(71)-C(72)-H(72)	119.3
C(72)-C(73)-C(74)	119.8(2)
C(72)-C(73)-H(73)	120.1
C(74)-C(73)-H(73)	120.1
C(75)-C(74)-C(73)	119.57(19)
C(75)-C(74)-H(74)	120.2
C(73)-C(74)-H(74)	120.2
C(74)-C(75)-C(76)	120.93(19)

C(74)-C(75)-H(75)	119.5
C(76)-C(75)-H(75)	119.5
C(75)-C(76)-C(71)	120.4(2)
C(75)-C(76)-H(76)	119.8
C(71)-C(76)-H(76)	119.8
C(45)-C(46)-C(41)	119.00(17)
C(45)-C(46)-C(81)	121.83(17)
C(41)-C(46)-C(81)	119.14(17)
C(86)-C(81)-C(82)	118.64(19)
C(86)-C(81)-C(46)	120.46(19)
C(82)-C(81)-C(46)	120.90(18)
C(83)-C(82)-C(81)	120.5(2)
C(83)-C(82)-H(82)	119.8
C(81)-C(82)-H(82)	119.8
C(84)-C(83)-C(82)	120.1(2)
C(84)-C(83)-H(83)	119.9
C(82)-C(83)-H(83)	119.9
C(83)-C(84)-C(85)	120.0(2)
C(83)-C(84)-H(84)	120.0
C(85)-C(84)-H(84)	120.0
C(84)-C(85)-C(86)	119.9(2)
C(84)-C(85)-H(85)	120.1
C(86)-C(85)-H(85)	120.1
C(81)-C(86)-C(85)	120.9(2)
C(81)-C(86)-H(86)	119.5
C(85)-C(86)-H(86)	119.5
C(2X)-C(1X)-H(1X1)	109.5
C(2X)-C(1X)-H(1X2)	109.5
H(1X1)-C(1X)-H(1X2)	109.5
C(2X)-C(1X)-H(1X3)	109.5
H(1X1)-C(1X)-H(1X3)	109.5
H(1X2)-C(1X)-H(1X3)	109.5
C(3X)-C(2X)-C(1X)	120.8(11)
C(3X)-C(2X)-H(2X1)	107.1
C(1X)-C(2X)-H(2X1)	107.1
C(3X)-C(2X)-H(2X2)	107.1

C(1X)-C(2X)-H(2X2)	107.1
H(2X1)-C(2X)-H(2X2)	106.8
C(2X)-C(3X)-C(4X)	127.3(11)
C(2X)-C(3X)-H(3X1)	105.5
C(4X)-C(3X)-H(3X1)	105.5
C(2X)-C(3X)-H(3X2)	105.5
C(4X)-C(3X)-H(3X2)	105.5
H(3X1)-C(3X)-H(3X2)	106.1
C(3X)-C(4X)-C(5X)	118.8(11)
C(3X)-C(4X)-H(4X1)	107.6
C(5X)-C(4X)-H(4X1)	107.6
C(3X)-C(4X)-H(4X2)	107.6
C(5X)-C(4X)-H(4X2)	107.6
H(4X1)-C(4X)-H(4X2)	107.1
C(4X)-C(5X)-H(5X1)	109.5
C(4X)-C(5X)-H(5X2)	109.5
H(5X1)-C(5X)-H(5X2)	109.5
C(4X)-C(5X)-H(5X3)	109.5
H(5X1)-C(5X)-H(5X3)	109.5
H(5X2)-C(5X)-H(5X3)	109.5
C(2Y)-C(1Y)-H(1Y1)	109.5
C(2Y)-C(1Y)-H(1Y2)	109.5
H(1Y1)-C(1Y)-H(1Y2)	109.5
C(2Y)-C(1Y)-H(1Y3)	109.5
H(1Y1)-C(1Y)-H(1Y3)	109.5
H(1Y2)-C(1Y)-H(1Y3)	109.5
C(1Y)-C(2Y)-C(3Y)	116.5(11)
C(1Y)-C(2Y)-H(2Y1)	108.2
C(3Y)-C(2Y)-H(2Y1)	108.2
C(1Y)-C(2Y)-H(2Y2)	108.2
C(3Y)-C(2Y)-H(2Y2)	108.2
H(2Y1)-C(2Y)-H(2Y2)	107.3
C(2Y)-C(3Y)-C(4Y)	118.5(11)
C(2Y)-C(3Y)-H(3Y1)	107.7
C(4Y)-C(3Y)-H(3Y1)	107.7
C(2Y)-C(3Y)-H(3Y2)	107.7

C(4Y)-C(3Y)-H(3Y2)	107.7
H(3Y1)-C(3Y)-H(3Y2)	107.1
C(3Y)-C(4Y)-C(5Y)	119.3(11)
C(3Y)-C(4Y)-H(4Y1)	107.5
C(5Y)-C(4Y)-H(4Y1)	107.5
C(3Y)-C(4Y)-H(4Y2)	107.5
C(5Y)-C(4Y)-H(4Y2)	107.5
H(4Y1)-C(4Y)-H(4Y2)	107.0
C(4Y)-C(5Y)-H(5Y1)	109.5
C(4Y)-C(5Y)-H(5Y2)	109.5
H(5Y1)-C(5Y)-H(5Y2)	109.5
C(4Y)-C(5Y)-H(5Y3)	109.5
H(5Y1)-C(5Y)-H(5Y3)	109.5
H(5Y2)-C(5Y)-H(5Y3)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S2D. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2a**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	28(1)	15(1)	15(1)	1(1)	4(1)	0(1)
C(1)	33(1)	18(1)	18(1)	2(1)	5(1)	1(1)
C(2)	28(1)	19(1)	22(1)	1(1)	7(1)	-1(1)
C(3)	37(2)	25(1)	59(2)	8(1)	14(1)	6(1)
C(4)	44(2)	33(1)	25(1)	-6(1)	14(1)	-11(1)
C(5)	31(1)	22(1)	23(1)	-4(1)	11(1)	-5(1)
C(6)	33(1)	38(1)	28(1)	-3(1)	11(1)	-4(1)
C(7)	43(2)	54(2)	36(1)	-14(1)	16(1)	-21(1)
C(8)	66(2)	32(1)	51(2)	-17(1)	35(2)	-22(1)
C(9)	65(2)	21(1)	60(2)	2(1)	34(2)	1(1)
C(10)	40(1)	24(1)	39(1)	3(1)	15(1)	0(1)
N(1)	33(1)	19(1)	20(1)	1(1)	7(1)	-3(1)
C(11)	39(1)	16(1)	16(1)	0(1)	6(1)	-3(1)
C(12)	40(1)	21(1)	28(1)	-2(1)	10(1)	-2(1)
C(13)	54(2)	21(1)	20(1)	1(1)	9(1)	-5(1)
C(14)	38(1)	20(1)	27(1)	0(1)	10(1)	-5(1)
C(15)	50(2)	20(1)	35(1)	-2(1)	18(1)	1(1)
C(16)	72(2)	22(1)	32(1)	-6(1)	25(1)	-6(1)
C(17)	76(2)	26(1)	18(1)	-3(1)	8(1)	-7(1)
C(18)	60(2)	30(1)	32(1)	-9(1)	2(1)	-10(1)
C(19)	45(2)	22(1)	32(1)	-2(1)	11(1)	-10(1)
C(20)	54(2)	19(1)	31(1)	-2(1)	14(1)	-4(1)
N(2)	32(1)	18(1)	19(1)	1(1)	4(1)	0(1)
C(21)	32(1)	18(1)	25(1)	0(1)	4(1)	0(1)
C(22)	41(1)	18(1)	29(1)	0(1)	8(1)	2(1)
C(23)	36(1)	26(1)	39(1)	3(1)	12(1)	7(1)
C(24)	32(1)	22(1)	21(1)	0(1)	9(1)	1(1)
C(25)	30(1)	22(1)	25(1)	2(1)	11(1)	0(1)
C(26)	28(1)	29(1)	23(1)	5(1)	10(1)	8(1)
C(27)	35(1)	29(1)	32(1)	10(1)	16(1)	5(1)
C(28)	34(1)	28(1)	40(1)	4(1)	14(1)	-1(1)

C(29)	44(2)	29(1)	30(1)	-3(1)	9(1)	-6(1)
C(30)	43(1)	28(1)	26(1)	0(1)	14(1)	-4(1)
C(31)	36(1)	39(1)	23(1)	4(1)	12(1)	8(1)
C(32)	56(2)	35(1)	53(2)	5(1)	20(1)	-13(1)
C(33)	76(2)	39(1)	25(1)	-2(1)	20(1)	-14(1)
O(1)	26(1)	18(1)	16(1)	2(1)	4(1)	1(1)
C(41)	22(1)	15(1)	16(1)	1(1)	6(1)	3(1)
C(42)	24(1)	15(1)	18(1)	0(1)	8(1)	1(1)
C(51)	27(1)	14(1)	16(1)	3(1)	7(1)	0(1)
C(52)	27(1)	18(1)	27(1)	2(1)	11(1)	1(1)
C(53)	23(1)	23(1)	32(1)	4(1)	9(1)	-3(1)
C(54)	31(1)	19(1)	24(1)	2(1)	8(1)	-6(1)
C(55)	33(1)	14(1)	19(1)	2(1)	7(1)	0(1)
C(56)	25(1)	16(1)	18(1)	3(1)	5(1)	2(1)
C(43)	24(1)	16(1)	18(1)	1(1)	9(1)	4(1)
C(61)	26(1)	16(1)	14(1)	0(1)	5(1)	1(1)
C(62)	32(1)	22(1)	27(1)	4(1)	13(1)	4(1)
C(63)	33(1)	26(1)	29(1)	8(1)	12(1)	-2(1)
C(64)	39(1)	18(1)	26(1)	6(1)	5(1)	-1(1)
C(65)	33(1)	21(1)	25(1)	3(1)	4(1)	8(1)
C(66)	27(1)	20(1)	21(1)	4(1)	7(1)	2(1)
C(44)	23(1)	17(1)	16(1)	2(1)	5(1)	4(1)
C(45)	23(1)	16(1)	16(1)	-1(1)	7(1)	2(1)
C(71)	26(1)	15(1)	13(1)	0(1)	7(1)	1(1)
C(72)	27(1)	19(1)	17(1)	1(1)	8(1)	3(1)
C(73)	24(1)	26(1)	19(1)	0(1)	5(1)	1(1)
C(74)	34(1)	22(1)	18(1)	-4(1)	8(1)	-5(1)
C(75)	35(1)	16(1)	21(1)	-1(1)	10(1)	2(1)
C(76)	27(1)	19(1)	17(1)	0(1)	6(1)	4(1)
C(46)	22(1)	14(1)	17(1)	1(1)	8(1)	3(1)
C(81)	28(1)	14(1)	13(1)	-1(1)	4(1)	2(1)
C(82)	26(1)	18(1)	18(1)	0(1)	4(1)	2(1)
C(83)	33(1)	20(1)	22(1)	0(1)	6(1)	-4(1)
C(84)	42(1)	15(1)	26(1)	3(1)	6(1)	2(1)
C(85)	34(1)	18(1)	26(1)	2(1)	4(1)	9(1)
C(86)	27(1)	18(1)	20(1)	0(1)	6(1)	3(1)

C(1X)	82(7)	82(8)	34(5)	-11(6)	-3(5)	19(6)
C(2X)	97(7)	128(9)	79(7)	2(6)	18(6)	15(6)
C(3X)	57(6)	107(7)	63(6)	3(5)	21(5)	-10(5)
C(4X)	43(6)	99(8)	54(5)	-8(6)	9(5)	-24(5)
C(5X)	91(9)	74(8)	56(7)	9(7)	-21(7)	43(7)
C(1Y)	84(9)	141(13)	79(11)	-24(11)	22(9)	-38(11)
C(2Y)	76(7)	104(8)	58(7)	8(6)	9(6)	6(6)
C(3Y)	62(6)	100(8)	60(6)	11(6)	-1(6)	-16(6)
C(4Y)	51(7)	88(9)	60(6)	6(7)	-3(6)	-16(5)
C(5Y)	70(9)	64(10)	51(8)	-17(8)	-24(8)	-14(9)

Table S2E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **2a**.

	x	y	z	U(eq)
H(1)	7490(20)	8223(18)	2243(11)	28
H(3A)	6258	10319	2794	60
H(3B)	5065	9568	2887	60
H(3C)	5460	9450	2166	60
H(4A)	7589	8385	3994	52
H(4B)	6329	8859	3997	52
H(4C)	7472	9677	3900	52
H(6)	4215	7951	2248	40
H(7)	3162	6154	2012	55
H(8)	4142	4644	2430	59
H(9)	6200	4914	3110	55
H(10)	7259	6706	3355	40
H(12A)	7666	11618	3653	36
H(12B)	8096	12273	3047	36
H(13A)	10685	11005	4627	39
H(13B)	9260	10823	4624	39
H(14A)	10327	12514	3050	35
H(14B)	11333	12026	3664	35
H(15)	7755	13580	3899	41
H(16A)	9012	13691	5086	50
H(16B)	8231	12483	4896	50
H(17)	10325	12312	5477	51
H(18A)	11273	13940	5092	53
H(18B)	11891	12883	4905	53
H(19)	11419	13990	3904	41
H(20A)	9681	14724	4123	42
H(20B)	9314	14161	3333	42
H(21)	9052	6867	2958	31
H(22)	10875	5859	3248	36
H(23)	12762	7272	3338	40

H(27)	13402	11293	2180	36
H(29)	14014	11416	4299	42
H(31A)	12002	8603	1829	47
H(31B)	12377	9708	1473	47
H(31C)	11062	9510	1636	47
H(32A)	14947	12683	2885	73
H(32B)	15430	12556	3718	73
H(32C)	14277	13218	3414	73
H(33A)	13148	8944	4570	71
H(33B)	11788	9300	4389	71
H(33C)	12929	10134	4857	71
H(52)	10906	11542	1349	28
H(53)	12310	12994	2008	31
H(54)	11616	14591	2384	30
H(55)	9512	14727	2102	26
H(56)	8098	13295	1424	24
H(62)	9383	12760	-339	31
H(63)	9461	14553	-740	35
H(64)	7937	15659	-684	34
H(65)	6292	14961	-258	32
H(66)	6164	13141	107	27
H(44)	6408	10951	-692	22
H(72)	4586	9699	-881	25
H(73)	3296	8387	-1720	28
H(74)	3946	6663	-1923	30
H(75)	5900	6298	-1310	28
H(76)	7225	7626	-497	25
H(82)	5652	8067	761	25
H(83)	5558	6277	1173	31
H(84)	7329	5392	1484	34
H(85)	9209	6299	1398	31
H(86)	9317	8104	1018	27
H(1X1)	3316	6622	4603	104
H(1X2)	3799	5924	5277	104
H(1X3)	3126	5291	4523	104
H(2X1)	4666	5870	4089	123

H(2X2)	5289	6711	4758	123
H(3X1)	6480	5567	4932	92
H(3X2)	5489	4580	4521	92
H(4X1)	5233	5021	5798	83
H(4X2)	6604	4809	5824	83
H(5X1)	5448	3241	5983	118
H(5X2)	5918	3093	5289	118
H(5X3)	4523	3305	5217	118
H(1Y1)	3070	5046	5072	159
H(1Y2)	4220	5109	5758	159
H(1Y3)	3823	4002	5243	159
H(2Y1)	4726	6056	4880	98
H(2Y2)	4315	4960	4361	98
H(3Y1)	6463	5643	5288	95
H(3Y2)	6142	4748	4633	95
H(4Y1)	6284	4428	6025	86
H(4Y2)	6983	3877	5523	86
H(5Y1)	5636	2611	5812	107
H(5Y2)	5236	2749	4978	107
H(5Y3)	4527	3307	5477	107

Table S3A. Crystal data and structure refinement for **2b**.

Identification code	10243	
Empirical formula	C59 H74 Br2 Mo N2 O2 Si	
Formula weight	1127.05	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1$	
Unit cell dimensions	a = 10.4204(6) Å	α= 90°
	b = 18.2373(10) Å	β= 102.8630(10)°
	c = 14.6979(8) Å	γ = 90°
Volume	2723.1(3) $Å^3$	
Z	2	
Density (calculated)	1.375 Mg/m^3	
Absorption coefficient	1.773 mm^{-1}	
F(000)	1168	
Crystal size	0.30 x 0.15 x 0.10 mm^3	
Theta range for data collection	1.42 to 29.57°	
Index ranges	-14<=h<=14, -25<=k<=25, -20<=l<=20	
Reflections collected	73176	
Independent reflections	15310 [R(int) = 0.0563]	
Completeness to theta = 29.57°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8426 and 0.6183	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15310 / 2 / 617	
Goodness-of-fit on F^2	0.999	
Final R indices [I>2sigma(I)]	R1 = 0.0281, wR2 = 0.0568	
R indices (all data)	R1 = 0.0342, wR2 = 0.0589	
Absolute structure parameter	-0.006(3)	
Largest diff. peak and hole	0.389 and -0.283 $e.Å^{-3}$	

Table S3B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	1512(1)	9595(1)	2594(1)	13(1)
C(1)	211(2)	10267(1)	2769(2)	16(1)
C(2)	-1183(2)	10538(1)	2384(2)	17(1)
C(3)	-1131(2)	11389(1)	2411(2)	24(1)
C(4)	-2039(2)	10286(1)	3044(2)	23(1)
C(5)	-1722(2)	10319(1)	1362(2)	16(1)
C(6)	-2963(2)	10006(1)	1050(2)	21(1)
C(7)	-3471(2)	9877(1)	96(2)	24(1)
C(8)	-2753(2)	10059(1)	-545(2)	25(1)
C(9)	-1509(2)	10357(1)	-243(2)	22(1)
C(10)	-996(2)	10486(1)	694(2)	19(1)
N(1)	586(2)	9026(1)	1783(1)	15(1)
C(11)	-128(2)	8375(1)	1385(2)	15(1)
C(12)	829(2)	7723(1)	1582(2)	23(1)
C(13)	-1261(2)	8238(1)	1880(2)	21(1)
C(14)	-674(2)	8459(1)	333(2)	20(1)
C(15)	92(3)	7022(1)	1195(2)	32(1)
C(16)	-1049(3)	6886(1)	1679(2)	35(1)
C(17)	-1991(2)	7538(1)	1498(2)	24(1)
C(18)	-2543(2)	7622(1)	443(2)	24(1)
C(19)	-1411(2)	7753(1)	-46(2)	23(1)
C(20)	-458(3)	7104(2)	141(2)	34(1)
N(2)	2477(2)	10313(1)	1893(1)	16(1)
C(21)	2560(2)	11067(1)	2022(2)	18(1)
C(22)	3447(2)	11355(1)	1569(2)	21(1)
C(23)	3935(2)	10767(1)	1120(2)	24(1)
C(24)	3341(2)	10135(1)	1329(2)	17(1)
C(25)	3479(2)	9366(1)	1036(2)	17(1)
C(26)	4281(2)	8867(1)	1635(2)	18(1)
C(27)	4388(2)	8149(1)	1328(2)	21(1)
C(28)	3722(2)	7906(1)	454(2)	23(1)

C(29)	2944(2)	8412(1)	-127(2)	23(1)
C(30)	2814(2)	9136(1)	138(2)	20(1)
C(31)	5020(2)	9092(1)	2589(2)	22(1)
C(32)	3821(3)	7116(1)	158(2)	30(1)
C(33)	1963(2)	9661(2)	-517(2)	30(1)
O(1)	2239(1)	8949(1)	3654(1)	16(1)
C(41)	2795(2)	8960(1)	4571(2)	14(1)
C(42)	3424(2)	9587(1)	4998(1)	16(1)
Br(1)	-1168(1)	6388(1)	4757(1)	20(1)
C(43)	3981(2)	9619(1)	5938(2)	19(1)
C(44)	3965(2)	8999(1)	6492(2)	19(1)
C(45)	4570(2)	9049(1)	7530(2)	25(1)
C(46)	4998(2)	8309(1)	7965(2)	26(1)
C(47)	3877(2)	7764(2)	7690(2)	25(1)
C(48)	3508(2)	7644(1)	6642(2)	21(1)
C(49)	3398(2)	8350(1)	6082(2)	16(1)
C(50)	2789(2)	8335(1)	5125(2)	13(1)
C(51)	2159(2)	7644(1)	4682(2)	14(1)
C(52)	954(2)	7408(1)	4868(2)	13(1)
O(2)	398(1)	7782(1)	5492(1)	15(1)
Si(1)	-709(1)	8453(1)	5419(1)	15(1)
C(53)	423(2)	6750(1)	4494(2)	15(1)
Br(2)	3510(1)	10409(1)	4214(1)	19(1)
C(54)	1036(2)	6329(1)	3929(2)	17(1)
C(55)	2231(2)	6551(1)	3744(2)	16(1)
C(56)	2889(2)	6064(1)	3144(2)	22(1)
C(57)	3948(2)	6452(1)	2771(2)	22(1)
C(58)	4854(2)	6871(1)	3554(2)	22(1)
C(59)	4091(2)	7473(1)	3928(2)	19(1)
C(60)	2796(2)	7211(1)	4123(2)	14(1)
C(61)	-2167(2)	8295(1)	4447(2)	26(1)
C(62)	40(2)	9351(1)	5241(2)	23(1)
C(63)	-1167(2)	8415(1)	6586(2)	19(1)
C(64)	-1926(2)	7709(1)	6687(2)	24(1)
C(65)	-2038(3)	9075(2)	6693(2)	38(1)
C(66)	79(3)	8437(2)	7375(2)	33(1)

Table S3C. Bond lengths [Å] and angles [°] for **2b**.

Mo(1)-N(1)	1.7074(18)
Mo(1)-C(1)	1.888(2)
Mo(1)-O(1)	1.9654(15)
Mo(1)-N(2)	2.0608(18)
C(1)-C(2)	1.519(3)
C(1)-H(1)	0.959(16)
C(2)-C(4)	1.528(3)
C(2)-C(5)	1.535(3)
C(2)-C(3)	1.554(3)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-C(6)	1.395(3)
C(5)-C(10)	1.399(3)
C(6)-C(7)	1.403(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.368(4)
C(7)-H(7)	0.9500
C(8)-C(9)	1.384(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.382(3)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
N(1)-C(11)	1.453(3)
C(11)-C(14)	1.532(3)
C(11)-C(12)	1.538(3)
C(11)-C(13)	1.539(3)
C(12)-C(15)	1.534(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(17)	1.528(3)

C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(19)	1.539(3)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(20)	1.535(4)
C(15)-C(16)	1.536(4)
C(15)-H(15)	1.0000
C(16)-C(17)	1.527(4)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.538(3)
C(17)-H(17)	1.0000
C(18)-C(19)	1.530(3)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.530(4)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
N(2)-C(21)	1.388(3)
N(2)-C(24)	1.391(3)
C(21)-C(22)	1.359(3)
C(21)-H(21)	0.9500
C(22)-C(23)	1.412(3)
C(22)-H(22)	0.9500
C(23)-C(24)	1.374(3)
C(23)-H(23)	0.9500
C(24)-C(25)	1.483(3)
C(25)-C(26)	1.406(3)
C(25)-C(30)	1.410(3)
C(26)-C(27)	1.397(3)
C(26)-C(31)	1.500(3)
C(27)-C(28)	1.390(3)
C(27)-H(27)	0.9500
C(28)-C(29)	1.390(3)

C(28)-C(32)	1.515(3)
C(29)-C(30)	1.392(3)
C(29)-H(29)	0.9500
C(30)-C(33)	1.500(3)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
O(1)-C(41)	1.344(3)
C(41)-C(42)	1.395(3)
C(41)-C(50)	1.402(3)
C(42)-C(43)	1.376(3)
C(42)-Br(2)	1.906(2)
Br(1)-C(53)	1.902(2)
C(43)-C(44)	1.395(3)
C(43)-H(43)	0.9500
C(44)-C(49)	1.399(3)
C(44)-C(45)	1.518(3)
C(45)-C(46)	1.518(4)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-C(47)	1.518(3)
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-C(48)	1.519(3)
C(47)-H(47A)	0.9900
C(47)-H(47B)	0.9900
C(48)-C(49)	1.518(3)
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(49)-C(50)	1.408(3)

C(50)-C(51)	1.501(3)
C(51)-C(60)	1.408(3)
C(51)-C(52)	1.410(3)
C(52)-O(2)	1.370(2)
C(52)-C(53)	1.384(3)
O(2)-Si(1)	1.6696(16)
Si(1)-C(62)	1.858(2)
Si(1)-C(61)	1.862(3)
Si(1)-C(63)	1.882(2)
C(53)-C(54)	1.386(3)
C(54)-C(55)	1.392(3)
C(54)-H(54)	0.9500
C(55)-C(60)	1.399(3)
C(55)-C(56)	1.519(3)
C(56)-C(57)	1.514(3)
C(56)-H(56A)	0.9900
C(56)-H(56B)	0.9900
C(57)-C(58)	1.521(3)
C(57)-H(57A)	0.9900
C(57)-H(57B)	0.9900
C(58)-C(59)	1.527(3)
C(58)-H(58A)	0.9900
C(58)-H(58B)	0.9900
C(59)-C(60)	1.518(3)
C(59)-H(59A)	0.9900
C(59)-H(59B)	0.9900
C(61)-H(61A)	0.9800
C(61)-H(61B)	0.9800
C(61)-H(61C)	0.9800
C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800
C(63)-C(64)	1.535(3)
C(63)-C(65)	1.536(3)
C(63)-C(66)	1.537(4)
C(64)-H(64A)	0.9800

C(64)-H(64B)	0.9800
C(64)-H(64C)	0.9800
C(65)-H(65A)	0.9800
C(65)-H(65B)	0.9800
C(65)-H(65C)	0.9800
C(66)-H(66A)	0.9800
C(66)-H(66B)	0.9800
C(66)-H(66C)	0.9800

N(1)-Mo(1)-C(1)	100.23(9)
N(1)-Mo(1)-O(1)	104.34(7)
C(1)-Mo(1)-O(1)	116.26(8)
N(1)-Mo(1)-N(2)	107.49(8)
C(1)-Mo(1)-N(2)	95.78(8)
O(1)-Mo(1)-N(2)	129.20(7)
C(2)-C(1)-Mo(1)	144.77(16)
C(2)-C(1)-H(1)	110.3(14)
Mo(1)-C(1)-H(1)	104.9(14)
C(1)-C(2)-C(4)	108.11(18)
C(1)-C(2)-C(5)	113.01(17)
C(4)-C(2)-C(5)	113.89(18)
C(1)-C(2)-C(3)	106.93(18)
C(4)-C(2)-C(3)	107.83(19)
C(5)-C(2)-C(3)	106.72(18)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5

C(6)-C(5)-C(10)	117.7(2)
C(6)-C(5)-C(2)	122.6(2)
C(10)-C(5)-C(2)	119.52(19)
C(5)-C(6)-C(7)	120.9(2)
C(5)-C(6)-H(6)	119.5
C(7)-C(6)-H(6)	119.5
C(8)-C(7)-C(6)	120.3(2)
C(8)-C(7)-H(7)	119.9
C(6)-C(7)-H(7)	119.9
C(7)-C(8)-C(9)	119.4(2)
C(7)-C(8)-H(8)	120.3
C(9)-C(8)-H(8)	120.3
C(10)-C(9)-C(8)	120.9(2)
C(10)-C(9)-H(9)	119.6
C(8)-C(9)-H(9)	119.6
C(9)-C(10)-C(5)	120.8(2)
C(9)-C(10)-H(10)	119.6
C(5)-C(10)-H(10)	119.6
C(11)-N(1)-Mo(1)	159.50(15)
N(1)-C(11)-C(14)	111.49(18)
N(1)-C(11)-C(12)	107.66(17)
C(14)-C(11)-C(12)	110.32(18)
N(1)-C(11)-C(13)	108.68(17)
C(14)-C(11)-C(13)	110.02(18)
C(12)-C(11)-C(13)	108.60(18)
C(15)-C(12)-C(11)	108.92(18)
C(15)-C(12)-H(12A)	109.9
C(11)-C(12)-H(12A)	109.9
C(15)-C(12)-H(12B)	109.9
C(11)-C(12)-H(12B)	109.9
H(12A)-C(12)-H(12B)	108.3
C(17)-C(13)-C(11)	109.49(19)
C(17)-C(13)-H(13A)	109.8
C(11)-C(13)-H(13A)	109.8
C(17)-C(13)-H(13B)	109.8
C(11)-C(13)-H(13B)	109.8

H(13A)-C(13)-H(13B)	108.2
C(11)-C(14)-C(19)	108.92(19)
C(11)-C(14)-H(14A)	109.9
C(19)-C(14)-H(14A)	109.9
C(11)-C(14)-H(14B)	109.9
C(19)-C(14)-H(14B)	109.9
H(14A)-C(14)-H(14B)	108.3
C(12)-C(15)-C(20)	109.7(2)
C(12)-C(15)-C(16)	109.8(2)
C(20)-C(15)-C(16)	109.3(2)
C(12)-C(15)-H(15)	109.4
C(20)-C(15)-H(15)	109.4
C(16)-C(15)-H(15)	109.4
C(17)-C(16)-C(15)	109.1(2)
C(17)-C(16)-H(16A)	109.9
C(15)-C(16)-H(16A)	109.9
C(17)-C(16)-H(16B)	109.9
C(15)-C(16)-H(16B)	109.9
H(16A)-C(16)-H(16B)	108.3
C(16)-C(17)-C(13)	109.8(2)
C(16)-C(17)-C(18)	109.6(2)
C(13)-C(17)-C(18)	109.32(19)
C(16)-C(17)-H(17)	109.4
C(13)-C(17)-H(17)	109.4
C(18)-C(17)-H(17)	109.4
C(19)-C(18)-C(17)	109.53(19)
C(19)-C(18)-H(18A)	109.8
C(17)-C(18)-H(18A)	109.8
C(19)-C(18)-H(18B)	109.8
C(17)-C(18)-H(18B)	109.8
H(18A)-C(18)-H(18B)	108.2
C(18)-C(19)-C(20)	109.5(2)
C(18)-C(19)-C(14)	109.62(19)
C(20)-C(19)-C(14)	109.32(19)
C(18)-C(19)-H(19)	109.5
C(20)-C(19)-H(19)	109.5

C(14)-C(19)-H(19)	109.5
C(19)-C(20)-C(15)	109.7(2)
C(19)-C(20)-H(20A)	109.7
C(15)-C(20)-H(20A)	109.7
C(19)-C(20)-H(20B)	109.7
C(15)-C(20)-H(20B)	109.7
H(20A)-C(20)-H(20B)	108.2
C(21)-N(2)-C(24)	106.44(18)
C(21)-N(2)-Mo(1)	125.72(14)
C(24)-N(2)-Mo(1)	127.04(14)
C(22)-C(21)-N(2)	110.2(2)
C(22)-C(21)-H(21)	124.9
N(2)-C(21)-H(21)	124.9
C(21)-C(22)-C(23)	106.8(2)
C(21)-C(22)-H(22)	126.6
C(23)-C(22)-H(22)	126.6
C(24)-C(23)-C(22)	107.8(2)
C(24)-C(23)-H(23)	126.1
C(22)-C(23)-H(23)	126.1
C(23)-C(24)-N(2)	108.73(19)
C(23)-C(24)-C(25)	130.5(2)
N(2)-C(24)-C(25)	120.71(19)
C(26)-C(25)-C(30)	119.5(2)
C(26)-C(25)-C(24)	120.9(2)
C(30)-C(25)-C(24)	119.6(2)
C(27)-C(26)-C(25)	118.9(2)
C(27)-C(26)-C(31)	119.9(2)
C(25)-C(26)-C(31)	121.2(2)
C(28)-C(27)-C(26)	122.6(2)
C(28)-C(27)-H(27)	118.7
C(26)-C(27)-H(27)	118.7
C(29)-C(28)-C(27)	117.2(2)
C(29)-C(28)-C(32)	121.6(2)
C(27)-C(28)-C(32)	121.2(2)
C(28)-C(29)-C(30)	122.6(2)
C(28)-C(29)-H(29)	118.7

C(30)-C(29)-H(29)	118.7
C(29)-C(30)-C(25)	119.1(2)
C(29)-C(30)-C(33)	120.4(2)
C(25)-C(30)-C(33)	120.5(2)
C(26)-C(31)-H(31A)	109.5
C(26)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(26)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(28)-C(32)-H(32A)	109.5
C(28)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(28)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(30)-C(33)-H(33A)	109.5
C(30)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(30)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(41)-O(1)-Mo(1)	142.25(14)
O(1)-C(41)-C(42)	121.18(19)
O(1)-C(41)-C(50)	120.92(19)
C(42)-C(41)-C(50)	117.89(19)
C(43)-C(42)-C(41)	122.5(2)
C(43)-C(42)-Br(2)	120.49(18)
C(41)-C(42)-Br(2)	116.96(15)
C(42)-C(43)-C(44)	119.6(2)
C(42)-C(43)-H(43)	120.2
C(44)-C(43)-H(43)	120.2
C(43)-C(44)-C(49)	119.5(2)
C(43)-C(44)-C(45)	118.8(2)
C(49)-C(44)-C(45)	121.7(2)
C(46)-C(45)-C(44)	112.8(2)

C(46)-C(45)-H(45A)	109.0
C(44)-C(45)-H(45A)	109.0
C(46)-C(45)-H(45B)	109.0
C(44)-C(45)-H(45B)	109.0
H(45A)-C(45)-H(45B)	107.8
C(45)-C(46)-C(47)	109.5(2)
C(45)-C(46)-H(46A)	109.8
C(47)-C(46)-H(46A)	109.8
C(45)-C(46)-H(46B)	109.8
C(47)-C(46)-H(46B)	109.8
H(46A)-C(46)-H(46B)	108.2
C(46)-C(47)-C(48)	111.7(2)
C(46)-C(47)-H(47A)	109.3
C(48)-C(47)-H(47A)	109.3
C(46)-C(47)-H(47B)	109.3
C(48)-C(47)-H(47B)	109.3
H(47A)-C(47)-H(47B)	107.9
C(49)-C(48)-C(47)	113.6(2)
C(49)-C(48)-H(48A)	108.8
C(47)-C(48)-H(48A)	108.8
C(49)-C(48)-H(48B)	108.8
C(47)-C(48)-H(48B)	108.8
H(48A)-C(48)-H(48B)	107.7
C(44)-C(49)-C(50)	120.0(2)
C(44)-C(49)-C(48)	120.7(2)
C(50)-C(49)-C(48)	119.2(2)
C(41)-C(50)-C(49)	120.31(19)
C(41)-C(50)-C(51)	119.33(18)
C(49)-C(50)-C(51)	120.34(19)
C(60)-C(51)-C(52)	119.89(19)
C(60)-C(51)-C(50)	120.41(18)
C(52)-C(51)-C(50)	119.62(19)
O(2)-C(52)-C(53)	120.38(18)
O(2)-C(52)-C(51)	120.37(19)
C(53)-C(52)-C(51)	118.83(19)
C(52)-O(2)-Si(1)	135.32(14)

O(2)-Si(1)-C(62)	110.46(9)
O(2)-Si(1)-C(61)	111.68(10)
C(62)-Si(1)-C(61)	108.98(12)
O(2)-Si(1)-C(63)	103.12(9)
C(62)-Si(1)-C(63)	111.14(11)
C(61)-Si(1)-C(63)	111.39(11)
C(52)-C(53)-C(54)	121.38(19)
C(52)-C(53)-Br(1)	120.66(16)
C(54)-C(53)-Br(1)	117.96(16)
C(53)-C(54)-C(55)	120.5(2)
C(53)-C(54)-H(54)	119.7
C(55)-C(54)-H(54)	119.7
C(54)-C(55)-C(60)	119.17(19)
C(54)-C(55)-C(56)	118.8(2)
C(60)-C(55)-C(56)	122.00(19)
C(57)-C(56)-C(55)	113.35(19)
C(57)-C(56)-H(56A)	108.9
C(55)-C(56)-H(56A)	108.9
C(57)-C(56)-H(56B)	108.9
C(55)-C(56)-H(56B)	108.9
H(56A)-C(56)-H(56B)	107.7
C(56)-C(57)-C(58)	109.90(19)
C(56)-C(57)-H(57A)	109.7
C(58)-C(57)-H(57A)	109.7
C(56)-C(57)-H(57B)	109.7
C(58)-C(57)-H(57B)	109.7
H(57A)-C(57)-H(57B)	108.2
C(57)-C(58)-C(59)	110.38(18)
C(57)-C(58)-H(58A)	109.6
C(59)-C(58)-H(58A)	109.6
C(57)-C(58)-H(58B)	109.6
C(59)-C(58)-H(58B)	109.6
H(58A)-C(58)-H(58B)	108.1
C(60)-C(59)-C(58)	113.41(18)
C(60)-C(59)-H(59A)	108.9
C(58)-C(59)-H(59A)	108.9

C(60)-C(59)-H(59B)	108.9
C(58)-C(59)-H(59B)	108.9
H(59A)-C(59)-H(59B)	107.7
C(55)-C(60)-C(51)	120.19(19)
C(55)-C(60)-C(59)	120.56(19)
C(51)-C(60)-C(59)	119.25(19)
Si(1)-C(61)-H(61A)	109.5
Si(1)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
Si(1)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
Si(1)-C(62)-H(62A)	109.5
Si(1)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
Si(1)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(64)-C(63)-C(65)	108.55(19)
C(64)-C(63)-C(66)	108.4(2)
C(65)-C(63)-C(66)	108.8(2)
C(64)-C(63)-Si(1)	111.05(16)
C(65)-C(63)-Si(1)	109.88(17)
C(66)-C(63)-Si(1)	110.11(16)
C(63)-C(64)-H(64A)	109.5
C(63)-C(64)-H(64B)	109.5
H(64A)-C(64)-H(64B)	109.5
C(63)-C(64)-H(64C)	109.5
H(64A)-C(64)-H(64C)	109.5
H(64B)-C(64)-H(64C)	109.5
C(63)-C(65)-H(65A)	109.5
C(63)-C(65)-H(65B)	109.5
H(65A)-C(65)-H(65B)	109.5
C(63)-C(65)-H(65C)	109.5
H(65A)-C(65)-H(65C)	109.5
H(65B)-C(65)-H(65C)	109.5

C(63)-C(66)-H(66A)	109.5
C(63)-C(66)-H(66B)	109.5
H(66A)-C(66)-H(66B)	109.5
C(63)-C(66)-H(66C)	109.5
H(66A)-C(66)-H(66C)	109.5
H(66B)-C(66)-H(66C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S3D. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2b**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	14(1)	12(1)	12(1)	0(1)	2(1)	-1(1)
C(1)	18(1)	14(1)	14(1)	0(1)	3(1)	-1(1)
C(2)	18(1)	14(1)	19(1)	-1(1)	3(1)	0(1)
C(3)	26(1)	17(1)	28(1)	-3(1)	2(1)	3(1)
C(4)	22(1)	30(1)	20(1)	-2(1)	7(1)	1(1)
C(5)	18(1)	10(1)	19(1)	0(1)	1(1)	1(1)
C(6)	18(1)	21(1)	23(1)	0(1)	2(1)	0(1)
C(7)	18(1)	22(1)	27(1)	-4(1)	-2(1)	-1(1)
C(8)	27(1)	23(1)	19(1)	2(1)	-3(1)	4(1)
C(9)	25(1)	21(1)	21(1)	5(1)	6(1)	2(1)
C(10)	19(1)	14(1)	24(1)	3(1)	3(1)	0(1)
N(1)	18(1)	13(1)	14(1)	-2(1)	3(1)	-1(1)
C(11)	17(1)	14(1)	13(1)	-2(1)	1(1)	-1(1)
C(12)	20(1)	17(1)	29(1)	-4(1)	-1(1)	5(1)
C(13)	21(1)	24(1)	18(1)	-1(1)	6(1)	-2(1)
C(14)	20(1)	26(1)	14(1)	-2(1)	4(1)	-2(1)
C(15)	26(1)	16(1)	46(2)	-9(1)	-9(1)	4(1)
C(16)	40(2)	17(1)	42(2)	6(1)	-7(1)	-7(1)
C(17)	23(1)	20(1)	26(1)	1(1)	3(1)	-8(1)
C(18)	19(1)	23(1)	27(1)	-5(1)	-1(1)	-3(1)
C(19)	21(1)	28(1)	17(1)	-8(1)	0(1)	-2(1)
C(20)	26(1)	33(2)	42(2)	-23(1)	4(1)	1(1)
N(2)	17(1)	15(1)	14(1)	-1(1)	3(1)	-2(1)
C(21)	21(1)	13(1)	19(1)	-2(1)	2(1)	-2(1)
C(22)	20(1)	17(1)	26(1)	4(1)	1(1)	-4(1)
C(23)	23(1)	22(1)	28(1)	3(1)	12(1)	-3(1)
C(24)	16(1)	19(1)	14(1)	2(1)	3(1)	0(1)
C(25)	15(1)	19(1)	18(1)	1(1)	6(1)	-2(1)
C(26)	17(1)	19(1)	20(1)	3(1)	8(1)	-1(1)
C(27)	19(1)	18(1)	26(1)	5(1)	10(1)	2(1)
C(28)	23(1)	22(1)	29(1)	-2(1)	15(1)	-2(1)

C(29)	24(1)	28(1)	19(1)	-6(1)	9(1)	-2(1)
C(30)	18(1)	26(1)	19(1)	-1(1)	7(1)	-1(1)
C(31)	20(1)	22(1)	23(1)	6(1)	2(1)	-1(1)
C(32)	39(2)	22(1)	33(2)	-6(1)	15(1)	2(1)
C(33)	31(1)	35(2)	22(1)	0(1)	0(1)	3(1)
O(1)	19(1)	15(1)	13(1)	-2(1)	1(1)	-2(1)
C(41)	14(1)	16(1)	12(1)	0(1)	2(1)	1(1)
C(42)	15(1)	13(1)	20(1)	2(1)	5(1)	0(1)
Br(1)	19(1)	17(1)	28(1)	-2(1)	9(1)	-5(1)
C(43)	18(1)	17(1)	20(1)	-4(1)	2(1)	-3(1)
C(44)	17(1)	23(1)	15(1)	-3(1)	0(1)	0(1)
C(45)	26(1)	29(1)	15(1)	-4(1)	-5(1)	-2(1)
C(46)	24(1)	34(1)	16(1)	1(1)	-3(1)	0(1)
C(47)	23(1)	33(1)	17(1)	7(1)	2(1)	1(1)
C(48)	21(1)	25(1)	14(1)	4(1)	0(1)	0(1)
C(49)	13(1)	18(1)	15(1)	1(1)	1(1)	2(1)
C(50)	11(1)	13(1)	15(1)	-1(1)	3(1)	-2(1)
C(51)	14(1)	13(1)	12(1)	2(1)	0(1)	1(1)
C(52)	16(1)	12(1)	11(1)	1(1)	4(1)	2(1)
O(2)	15(1)	16(1)	16(1)	-1(1)	6(1)	1(1)
Si(1)	15(1)	14(1)	16(1)	2(1)	5(1)	1(1)
C(53)	14(1)	14(1)	16(1)	2(1)	3(1)	-2(1)
Br(2)	21(1)	14(1)	22(1)	1(1)	5(1)	-3(1)
C(54)	19(1)	12(1)	20(1)	1(1)	4(1)	-1(1)
C(55)	19(1)	15(1)	15(1)	2(1)	4(1)	2(1)
C(56)	26(1)	15(1)	26(1)	-4(1)	11(1)	0(1)
C(57)	26(1)	20(1)	24(1)	-3(1)	12(1)	1(1)
C(58)	19(1)	22(1)	26(1)	2(1)	10(1)	3(1)
C(59)	17(1)	18(1)	23(1)	-2(1)	8(1)	-2(1)
C(60)	16(1)	13(1)	14(1)	2(1)	3(1)	1(1)
C(61)	23(1)	30(1)	20(1)	3(1)	0(1)	2(1)
C(62)	26(1)	15(1)	31(1)	3(1)	13(1)	2(1)
C(63)	23(1)	16(1)	20(1)	0(1)	9(1)	2(1)
C(64)	30(1)	21(1)	25(1)	4(1)	13(1)	1(1)
C(65)	49(2)	23(1)	52(2)	1(1)	33(2)	10(1)
C(66)	39(2)	39(2)	21(1)	-4(1)	10(1)	-4(1)

Table S3E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **2b**.

	x	y	z	U(eq)
H(1)	620(20)	10547(12)	3307(13)	19
H(3A)	-2014	11587	2159	36
H(3B)	-528	11564	2033	36
H(3C)	-820	11554	3057	36
H(4A)	-2087	9749	3041	35
H(4B)	-2927	10489	2837	35
H(4C)	-1654	10458	3678	35
H(6)	-3471	9878	1488	26
H(7)	-4317	9662	-105	29
H(8)	-3106	9983	-1191	30
H(9)	-1001	10473	-685	27
H(10)	-141	10691	888	23
H(12A)	1577	7805	1281	27
H(12B)	1181	7673	2263	27
H(13A)	-906	8188	2560	25
H(13B)	-1877	8659	1775	25
H(14A)	56	8548	16	24
H(14B)	-1281	8883	210	24
H(15)	712	6596	1313	39
H(16A)	-1522	6432	1434	42
H(16B)	-703	6825	2359	42
H(17)	-2733	7453	1815	28
H(18A)	-3029	7173	192	28
H(18B)	-3163	8041	324	28
H(19)	-1770	7803	-733	27
H(20A)	274	7185	-177	41
H(20B)	-922	6649	-111	41
H(21)	2068	11341	2375	22
H(22)	3691	11856	1556	26
H(23)	4562	10801	742	28

H(27)	4937	7814	1732	25
H(29)	2483	8258	-729	28
H(31A)	5191	9621	2596	33
H(31B)	5857	8826	2749	33
H(31C)	4494	8976	3046	33
H(32A)	2937	6902	-19	46
H(32B)	4351	6836	678	46
H(32C)	4240	7097	-376	46
H(33A)	1496	9396	-1072	45
H(33B)	2515	10044	-702	45
H(33C)	1324	9887	-204	45
H(43)	4375	10061	6209	22
H(45A)	5342	9379	7629	30
H(45B)	3919	9267	7849	30
H(46A)	5245	8356	8653	31
H(46B)	5776	8132	7747	31
H(47A)	3099	7947	7904	30
H(47B)	4141	7290	8005	30
H(48A)	4180	7326	6460	25
H(48B)	2655	7382	6480	25
H(54)	639	5886	3666	20
H(56A)	3284	5636	3519	26
H(56B)	2211	5878	2612	26
H(57A)	3538	6797	2270	27
H(57B)	4465	6089	2502	27
H(58A)	5584	7092	3318	26
H(58B)	5238	6528	4065	26
H(59A)	4646	7671	4511	23
H(59B)	3913	7877	3468	23
H(61A)	-1876	8229	3862	38
H(61B)	-2759	8718	4391	38
H(61C)	-2633	7854	4577	38
H(62A)	850	9420	5721	35
H(62B)	-581	9746	5285	35
H(62C)	247	9361	4622	35
H(64A)	-1409	7284	6575	36

H(64B)	-2771	7712	6232	36
H(64C)	-2083	7682	7319	36
H(65A)	-2279	9050	7300	57
H(65B)	-2838	9066	6194	57
H(65C)	-1553	9530	6653	57
H(66A)	-170	8427	7980	49
H(66B)	572	8888	7325	49
H(66C)	631	8011	7324	49

Table S4A. Crystal data and structure refinement for **2c**.

Identification code	X8_10082	
Empirical formula	C71 H96 Mo N2 O Si0.50	
Formula weight	1103.48	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 41.846(2) Å	α= 90°
	b = 14.9408(7) Å	β= 96.4610(10)°
	c = 20.0700(10) Å	γ = 90°
Volume	12468.2(11) $Å^3$	
Z	8	
Density (calculated)	1.176 Mg/m^3	
Absorption coefficient	0.263 mm^{-1}	
F(000)	4744	
Crystal size	0.20 x 0.20 x 0.10 mm^3	
Theta range for data collection	1.45 to 30.31°	
Index ranges	-59<=h<=59, -21<=k<=21, -28<=l<=28	
Reflections collected	145253	
Independent reflections	18713 [R(int) = 0.0718]	
Completeness to theta = 30.31°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9742 and 0.9492	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	18713 / 1384 / 1020	
Goodness-of-fit on F^2	1.017	
Final R indices [I>2sigma(I)]	R1 = 0.0367, wR2 = 0.0800	
R indices (all data)	R1 = 0.0582, wR2 = 0.0903	
Largest diff. peak and hole	0.439 and -0.498 e.$Å^{-3}$	

Table S4B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2c**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	3512(1)	7227(1)	8754(1)	18(1)
C(1)	3434(1)	8036(1)	9435(1)	24(1)
C(2)	3239(1)	8198(1)	10019(1)	30(1)
C(3)	2932(1)	7621(1)	9946(1)	40(1)
C(4)	3441(1)	7923(1)	10672(1)	36(1)
C(5)	3142(1)	9187(1)	10001(1)	30(1)
C(6)	2952(1)	9521(1)	9440(1)	37(1)
C(7)	2864(1)	10413(2)	9392(1)	46(1)
C(8)	2967(1)	10999(2)	9907(1)	47(1)
C(9)	3155(1)	10684(2)	10464(1)	44(1)
C(10)	3241(1)	9785(1)	10515(1)	35(1)
N(1)	3303(1)	6300(1)	8956(1)	23(1)
C(11)	3214(1)	5391(1)	9124(1)	23(1)
C(12)	3336(1)	4762(1)	8603(1)	27(1)
C(13)	2848(1)	5298(1)	9102(1)	27(1)
C(14)	3376(1)	5142(1)	9823(1)	31(1)
C(15)	3249(1)	3793(1)	8756(1)	33(1)
C(16)	2884(1)	3704(1)	8734(1)	34(1)
C(17)	2765(1)	4324(1)	9259(1)	31(1)
C(18)	2924(1)	4079(1)	9957(1)	38(1)
C(19)	3288(1)	4165(1)	9975(1)	37(1)
C(20)	3409(1)	3543(1)	9454(1)	40(1)
N(2)	3247(1)	7843(1)	7959(1)	22(1)
C(21)	3221(1)	8771(1)	7895(1)	27(1)
C(22)	3050(1)	8984(1)	7299(1)	30(1)
C(23)	2959(1)	8168(1)	6973(1)	31(1)
C(24)	3081(1)	7483(1)	7381(1)	24(1)
C(25)	3036(1)	6513(1)	7242(1)	23(1)
C(26)	3268(1)	6024(1)	6946(1)	26(1)
C(31)	3579(1)	6454(1)	6815(1)	35(1)
C(27)	3203(1)	5137(1)	6756(1)	29(1)

C(28)	2913(1)	4730(1)	6856(1)	30(1)
C(32)	2846(1)	3771(1)	6646(1)	44(1)
C(29)	2688(1)	5220(1)	7156(1)	29(1)
C(30)	2744(1)	6110(1)	7350(1)	26(1)
C(33)	2492(1)	6631(1)	7664(1)	34(1)
O(1)	3962(1)	7151(9)	8685(8)	18(1)
C(41)	4282(2)	7263(4)	8659(8)	17(1)
C(42)	4493(1)	6536(3)	8790(3)	18(1)
C(51)	4390(3)	5629(4)	9004(3)	17(1)
C(52)	4308(2)	4958(3)	8526(2)	19(1)
C(57)	4274(1)	5166(2)	7781(2)	27(1)
C(58)	4035(1)	4557(3)	7365(2)	32(1)
C(59)	4598(1)	5130(3)	7500(2)	50(1)
C(53)	4269(1)	4086(3)	8749(2)	22(1)
C(54)	4306(1)	3859(2)	9420(2)	23(1)
C(60)	4291(1)	2876(2)	9621(2)	32(1)
C(61)	4191(1)	2722(2)	10308(2)	43(1)
C(62)	4614(1)	2416(2)	9561(2)	42(1)
C(55)	4372(2)	4537(3)	9886(2)	25(1)
C(56)	4417(3)	5420(4)	9690(3)	21(1)
C(63)	4495(2)	6139(3)	10220(3)	25(1)
C(64)	4768(2)	5855(4)	10755(4)	34(1)
C(65)	4190(1)	6384(3)	10539(2)	45(1)
C(43)	4819(1)	6660(3)	8738(2)	25(1)
C(44)	4938(1)	7478(2)	8560(2)	30(1)
C(45)	4730(1)	8196(3)	8464(2)	27(1)
C(46)	4403(1)	8113(3)	8520(2)	20(1)
C(71)	4198(2)	8940(4)	8459(2)	18(1)
C(72)	4074(2)	9237(5)	7817(2)	18(1)
C(77)	4127(2)	8713(5)	7190(2)	19(1)
C(78)	3830(2)	8754(7)	6663(4)	25(1)
C(79)	4421(2)	9080(8)	6882(3)	28(1)
C(73)	3911(3)	10056(5)	7757(3)	20(1)
C(74)	3874(3)	10579(5)	8312(3)	22(1)
C(80)	3694(1)	11468(4)	8227(4)	26(1)
C(81)	3340(1)	11290(2)	7922(2)	38(1)

C(82)	3853(1)	12070(2)	7760(2)	38(1)
C(75)	3984(3)	10258(5)	8944(3)	21(1)
C(76)	4152(2)	9446(5)	9027(2)	20(1)
C(83)	4293(2)	9146(5)	9727(2)	26(1)
C(84)	4112(2)	9528(9)	10285(4)	32(1)
C(85)	4647(1)	9416(4)	9869(3)	40(1)
O(1A)	3952(3)	7110(20)	8620(20)	18(1)
C(41A)	4276(4)	7179(11)	8600(20)	17(1)
C(42A)	4470(3)	6415(8)	8709(9)	18(1)
C(51A)	4378(8)	5571(10)	9042(7)	20(2)
C(52A)	4294(4)	4792(7)	8649(4)	19(2)
C(57A)	4271(2)	4827(5)	7898(4)	26(1)
C(58A)	3985(2)	4291(6)	7544(4)	33(2)
C(59A)	4588(2)	4491(7)	7665(4)	50(2)
C(53A)	4254(3)	4004(6)	8985(5)	23(2)
C(54A)	4300(3)	3943(6)	9664(4)	28(2)
C(60A)	4266(2)	3009(5)	9979(4)	34(2)
C(61A)	4208(2)	3063(6)	10706(5)	60(3)
C(62A)	4568(2)	2459(5)	9915(5)	43(2)
C(55A)	4363(5)	4706(7)	10040(5)	25(2)
C(56A)	4412(7)	5540(9)	9745(6)	23(2)
C(63A)	4503(4)	6348(9)	10180(8)	32(3)
C(64A)	4791(4)	6129(9)	10703(10)	39(3)
C(65A)	4223(3)	6683(7)	10538(6)	38(3)
C(43A)	4789(3)	6484(7)	8574(5)	21(2)
C(44A)	4906(2)	7264(5)	8318(4)	24(1)
C(45A)	4714(2)	8020(6)	8242(4)	20(2)
C(46A)	4396(3)	8000(8)	8395(8)	20(1)
C(71A)	4204(5)	8849(11)	8321(5)	15(2)
C(72A)	4099(5)	9200(12)	7689(6)	14(2)
C(77A)	4144(4)	8741(12)	7040(6)	17(2)
C(78A)	3838(5)	8720(20)	6546(10)	26(3)
C(79A)	4426(5)	9130(20)	6724(8)	23(3)
C(73A)	3944(7)	10031(14)	7655(8)	20(2)
C(74A)	3866(6)	10490(14)	8211(8)	21(2)
C(80A)	3673(4)	11343(11)	8191(9)	27(2)

C(81A)	3358(2)	11298(4)	8520(4)	42(2)
C(82A)	3624(2)	11840(4)	7548(4)	41(2)
C(75A)	3996(7)	10152(13)	8828(7)	22(2)
C(76A)	4156(6)	9333(12)	8900(6)	18(2)
C(83A)	4288(4)	9015(12)	9601(6)	24(2)
C(84A)	4132(6)	9410(20)	10171(9)	30(3)
C(85A)	4654(4)	9158(11)	9725(8)	38(3)
Si(1S)	5044(1)	8502(1)	2599(1)	26(1)
C(1S)	4850(2)	9297(5)	3147(4)	28(1)
C(2S)	4768(1)	7536(3)	2396(2)	42(1)
C(3S)	5133(3)	9052(5)	1814(5)	45(2)
C(4S)	5426(1)	8087(3)	3069(2)	44(1)

Table S4C. Bond lengths [Å] and angles [°] for **2c**.

Mo(1)-N(1)	1.7127(13)
Mo(1)-C(1)	1.8811(16)
Mo(1)-O(1A)	1.901(12)
Mo(1)-O(1)	1.909(5)
Mo(1)-N(2)	2.0551(13)
C(1)-C(2)	1.520(2)
C(1)-H(1)	0.990(19)
C(2)-C(5)	1.532(3)
C(2)-C(4)	1.535(3)
C(2)-C(3)	1.542(2)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-C(10)	1.393(2)
C(5)-C(6)	1.397(3)
C(6)-C(7)	1.384(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.386(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.375(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.392(3)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
N(1)-C(11)	1.457(2)
C(11)-C(14)	1.534(2)
C(11)-C(12)	1.535(2)
C(11)-C(13)	1.536(2)
C(12)-C(15)	1.533(2)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900

C(13)-C(17)	1.537(2)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(19)	1.544(2)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.529(2)
C(15)-C(20)	1.529(3)
C(15)-H(15)	1.0000
C(16)-C(17)	1.527(3)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.527(3)
C(17)-H(17)	1.0000
C(18)-C(19)	1.526(3)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.527(3)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
N(2)-C(24)	1.391(2)
N(2)-C(21)	1.395(2)
C(21)-C(22)	1.361(2)
C(21)-H(21)	0.9500
C(22)-C(23)	1.417(3)
C(22)-H(22)	0.9500
C(23)-C(24)	1.372(2)
C(23)-H(23)	0.9500
C(24)-C(25)	1.484(2)
C(25)-C(26)	1.399(2)
C(25)-C(30)	1.402(2)
C(26)-C(27)	1.397(2)
C(26)-C(31)	1.504(2)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800

C(31)-H(31C)	0.9800
C(27)-C(28)	1.392(2)
C(27)-H(27)	0.9500
C(28)-C(29)	1.383(3)
C(28)-C(32)	1.510(2)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(29)-C(30)	1.397(2)
C(29)-H(29)	0.9500
C(30)-C(33)	1.505(2)
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
O(1)-C(41)	1.356(5)
C(41)-C(46)	1.406(5)
C(41)-C(42)	1.406(5)
C(42)-C(43)	1.392(5)
C(42)-C(51)	1.499(5)
C(51)-C(52)	1.403(5)
C(51)-C(56)	1.404(5)
C(52)-C(53)	1.392(4)
C(52)-C(57)	1.519(4)
C(57)-C(59)	1.524(4)
C(57)-C(58)	1.527(4)
C(57)-H(57)	1.0000
C(58)-H(58A)	0.9800
C(58)-H(58B)	0.9800
C(58)-H(58C)	0.9800
C(59)-H(59A)	0.9800
C(59)-H(59B)	0.9800
C(59)-H(59C)	0.9800
C(53)-C(54)	1.381(4)
C(53)-H(53)	0.9500
C(54)-C(55)	1.385(4)
C(54)-C(60)	1.527(4)

C(60)-C(61)	1.503(4)
C(60)-C(62)	1.532(4)
C(60)-H(60)	1.0000
C(61)-H(61A)	0.9800
C(61)-H(61B)	0.9800
C(61)-H(61C)	0.9800
C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800
C(55)-C(56)	1.396(5)
C(55)-H(55)	0.9500
C(56)-C(63)	1.522(5)
C(63)-C(65)	1.534(6)
C(63)-C(64)	1.536(5)
C(63)-H(63)	1.0000
C(64)-H(64A)	0.9800
C(64)-H(64B)	0.9800
C(64)-H(64C)	0.9800
C(65)-H(65A)	0.9800
C(65)-H(65B)	0.9800
C(65)-H(65C)	0.9800
C(43)-C(44)	1.383(5)
C(43)-H(43)	0.9500
C(44)-C(45)	1.383(4)
C(44)-H(44)	0.9500
C(45)-C(46)	1.393(5)
C(45)-H(45)	0.9500
C(46)-C(71)	1.500(4)
C(71)-C(76)	1.399(4)
C(71)-C(72)	1.406(5)
C(72)-C(73)	1.400(5)
C(72)-C(77)	1.519(5)
C(77)-C(79)	1.537(5)
C(77)-C(78)	1.538(5)
C(77)-H(77)	1.0000
C(78)-H(78A)	0.9800

C(78)-H(78B)	0.9800
C(78)-H(78C)	0.9800
C(79)-H(79A)	0.9800
C(79)-H(79B)	0.9800
C(79)-H(79C)	0.9800
C(73)-C(74)	1.383(5)
C(73)-H(73)	0.9500
C(74)-C(75)	1.386(5)
C(74)-C(80)	1.527(5)
C(80)-C(82)	1.507(6)
C(80)-C(81)	1.561(7)
C(80)-H(80)	1.0000
C(81)-H(81A)	0.9800
C(81)-H(81B)	0.9800
C(81)-H(81C)	0.9800
C(82)-H(82A)	0.9800
C(82)-H(82B)	0.9800
C(82)-H(82C)	0.9800
C(75)-C(76)	1.402(5)
C(75)-H(75)	0.9500
C(76)-C(83)	1.529(5)
C(83)-C(84)	1.530(5)
C(83)-C(85)	1.531(6)
C(83)-H(83)	1.0000
C(84)-H(84A)	0.9800
C(84)-H(84B)	0.9800
C(84)-H(84C)	0.9800
C(85)-H(85A)	0.9800
C(85)-H(85B)	0.9800
C(85)-H(85C)	0.9800
O(1A)-C(41A)	1.362(12)
C(41A)-C(42A)	1.404(12)
C(41A)-C(46A)	1.407(12)
C(42A)-C(43A)	1.395(12)
C(42A)-C(51A)	1.497(11)
C(51A)-C(56A)	1.404(12)

C(51A)-C(52A)	1.427(11)
C(52A)-C(53A)	1.376(9)
C(52A)-C(57A)	1.502(9)
C(57A)-C(59A)	1.539(9)
C(57A)-C(58A)	1.544(10)
C(57A)-H(57A)	1.0000
C(58A)-H(58D)	0.9800
C(58A)-H(58E)	0.9800
C(58A)-H(58F)	0.9800
C(59A)-H(59D)	0.9800
C(59A)-H(59E)	0.9800
C(59A)-H(59F)	0.9800
C(53A)-C(54A)	1.357(9)
C(53A)-H(53A)	0.9500
C(54A)-C(55A)	1.377(10)
C(54A)-C(60A)	1.546(9)
C(60A)-C(61A)	1.507(10)
C(60A)-C(62A)	1.525(9)
C(60A)-H(60A)	1.0000
C(61A)-H(61D)	0.9800
C(61A)-H(61E)	0.9800
C(61A)-H(61F)	0.9800
C(62A)-H(62D)	0.9800
C(62A)-H(62E)	0.9800
C(62A)-H(62F)	0.9800
C(55A)-C(56A)	1.405(11)
C(55A)-H(55A)	0.9500
C(56A)-C(63A)	1.514(11)
C(63A)-C(65A)	1.525(13)
C(63A)-C(64A)	1.544(13)
C(63A)-H(63A)	1.0000
C(64A)-H(64D)	0.9800
C(64A)-H(64E)	0.9800
C(64A)-H(64F)	0.9800
C(65A)-H(65D)	0.9800
C(65A)-H(65E)	0.9800

C(65A)-H(65F)	0.9800
C(43A)-C(44A)	1.385(10)
C(43A)-H(43A)	0.9500
C(44A)-C(45A)	1.385(10)
C(44A)-H(44A)	0.9500
C(45A)-C(46A)	1.397(11)
C(45A)-H(45A)	0.9500
C(46A)-C(71A)	1.500(11)
C(71A)-C(72A)	1.396(10)
C(71A)-C(76A)	1.403(9)
C(72A)-C(73A)	1.399(12)
C(72A)-C(77A)	1.503(10)
C(77A)-C(79A)	1.517(12)
C(77A)-C(78A)	1.529(13)
C(77A)-H(77A)	1.0000
C(78A)-H(78D)	0.9800
C(78A)-H(78E)	0.9800
C(78A)-H(78F)	0.9800
C(79A)-H(79D)	0.9800
C(79A)-H(79E)	0.9800
C(79A)-H(79F)	0.9800
C(73A)-C(74A)	1.380(11)
C(73A)-H(73A)	0.9500
C(74A)-C(75A)	1.391(12)
C(74A)-C(80A)	1.507(12)
C(80A)-C(82A)	1.482(13)
C(80A)-C(81A)	1.543(13)
C(80A)-H(80A)	1.0000
C(81A)-H(81D)	0.9800
C(81A)-H(81E)	0.9800
C(81A)-H(81F)	0.9800
C(82A)-H(82D)	0.9800
C(82A)-H(82E)	0.9800
C(82A)-H(82F)	0.9800
C(75A)-C(76A)	1.395(11)
C(75A)-H(75A)	0.9500

C(76A)-C(83A)	1.528(11)
C(83A)-C(84A)	1.504(11)
C(83A)-C(85A)	1.536(13)
C(83A)-H(83A)	1.0000
C(84A)-H(84D)	0.9800
C(84A)-H(84E)	0.9800
C(84A)-H(84F)	0.9800
C(85A)-H(85D)	0.9800
C(85A)-H(85E)	0.9800
C(85A)-H(85F)	0.9800
Si(1S)-C(3S)	1.852(8)
Si(1S)-C(2S)	1.865(4)
Si(1S)-C(4S)	1.865(4)
Si(1S)-C(1S)	1.866(6)
C(1S)-H(1S1)	0.9800
C(1S)-H(1S2)	0.9800
C(1S)-H(1S3)	0.9800
C(2S)-H(2S1)	0.9800
C(2S)-H(2S2)	0.9800
C(2S)-H(2S3)	0.9800
C(3S)-H(3S1)	0.9800
C(3S)-H(3S2)	0.9800
C(3S)-H(3S3)	0.9800
C(4S)-H(4S1)	0.9800
C(4S)-H(4S2)	0.9800
C(4S)-H(4S3)	0.9800

N(1)-Mo(1)-C(1)	102.22(7)
N(1)-Mo(1)-O(1A)	119.2(11)
C(1)-Mo(1)-O(1A)	114.5(11)
N(1)-Mo(1)-O(1)	120.3(4)
C(1)-Mo(1)-O(1)	110.2(4)
O(1A)-Mo(1)-O(1)	4.6(16)
N(1)-Mo(1)-N(2)	107.46(6)
C(1)-Mo(1)-N(2)	98.86(6)
O(1A)-Mo(1)-N(2)	112.2(12)

O(1)-Mo(1)-N(2)	115.0(5)
C(2)-C(1)-Mo(1)	144.53(12)
C(2)-C(1)-H(1)	115.5(11)
Mo(1)-C(1)-H(1)	100.0(11)
C(1)-C(2)-C(5)	107.36(15)
C(1)-C(2)-C(4)	108.91(14)
C(5)-C(2)-C(4)	113.38(15)
C(1)-C(2)-C(3)	110.69(14)
C(5)-C(2)-C(3)	108.78(15)
C(4)-C(2)-C(3)	107.74(16)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(10)-C(5)-C(6)	117.57(18)
C(10)-C(5)-C(2)	123.15(17)
C(6)-C(5)-C(2)	119.27(15)
C(7)-C(6)-C(5)	121.61(18)
C(7)-C(6)-H(6)	119.2
C(5)-C(6)-H(6)	119.2
C(6)-C(7)-C(8)	119.9(2)
C(6)-C(7)-H(7)	120.1
C(8)-C(7)-H(7)	120.1
C(9)-C(8)-C(7)	119.5(2)
C(9)-C(8)-H(8)	120.2
C(7)-C(8)-H(8)	120.2
C(8)-C(9)-C(10)	120.64(18)
C(8)-C(9)-H(9)	119.7

C(10)-C(9)-H(9)	119.7
C(9)-C(10)-C(5)	120.79(19)
C(9)-C(10)-H(10)	119.6
C(5)-C(10)-H(10)	119.6
C(11)-N(1)-Mo(1)	163.58(11)
N(1)-C(11)-C(14)	109.83(13)
N(1)-C(11)-C(12)	107.51(13)
C(14)-C(11)-C(12)	109.20(14)
N(1)-C(11)-C(13)	110.96(13)
C(14)-C(11)-C(13)	109.86(14)
C(12)-C(11)-C(13)	109.44(13)
C(15)-C(12)-C(11)	109.69(14)
C(15)-C(12)-H(12A)	109.7
C(11)-C(12)-H(12A)	109.7
C(15)-C(12)-H(12B)	109.7
C(11)-C(12)-H(12B)	109.7
H(12A)-C(12)-H(12B)	108.2
C(11)-C(13)-C(17)	109.13(14)
C(11)-C(13)-H(13A)	109.9
C(17)-C(13)-H(13A)	109.9
C(11)-C(13)-H(13B)	109.9
C(17)-C(13)-H(13B)	109.9
H(13A)-C(13)-H(13B)	108.3
C(11)-C(14)-C(19)	108.63(14)
C(11)-C(14)-H(14A)	110.0
C(19)-C(14)-H(14A)	110.0
C(11)-C(14)-H(14B)	110.0
C(19)-C(14)-H(14B)	110.0
H(14A)-C(14)-H(14B)	108.3
C(16)-C(15)-C(20)	109.87(16)
C(16)-C(15)-C(12)	109.59(15)
C(20)-C(15)-C(12)	108.94(15)
C(16)-C(15)-H(15)	109.5
C(20)-C(15)-H(15)	109.5
C(12)-C(15)-H(15)	109.5
C(17)-C(16)-C(15)	109.27(15)

C(17)-C(16)-H(16A)	109.8
C(15)-C(16)-H(16A)	109.8
C(17)-C(16)-H(16B)	109.8
C(15)-C(16)-H(16B)	109.8
H(16A)-C(16)-H(16B)	108.3
C(18)-C(17)-C(16)	110.18(16)
C(18)-C(17)-C(13)	109.18(14)
C(16)-C(17)-C(13)	109.56(15)
C(18)-C(17)-H(17)	109.3
C(16)-C(17)-H(17)	109.3
C(13)-C(17)-H(17)	109.3
C(19)-C(18)-C(17)	109.50(15)
C(19)-C(18)-H(18A)	109.8
C(17)-C(18)-H(18A)	109.8
C(19)-C(18)-H(18B)	109.8
C(17)-C(18)-H(18B)	109.8
H(18A)-C(18)-H(18B)	108.2
C(18)-C(19)-C(20)	109.86(16)
C(18)-C(19)-C(14)	109.44(16)
C(20)-C(19)-C(14)	109.65(16)
C(18)-C(19)-H(19)	109.3
C(20)-C(19)-H(19)	109.3
C(14)-C(19)-H(19)	109.3
C(19)-C(20)-C(15)	109.50(15)
C(19)-C(20)-H(20A)	109.8
C(15)-C(20)-H(20A)	109.8
C(19)-C(20)-H(20B)	109.8
C(15)-C(20)-H(20B)	109.8
H(20A)-C(20)-H(20B)	108.2
C(24)-N(2)-C(21)	106.37(13)
C(24)-N(2)-Mo(1)	130.49(11)
C(21)-N(2)-Mo(1)	123.01(11)
C(22)-C(21)-N(2)	109.90(15)
C(22)-C(21)-H(21)	125.1
N(2)-C(21)-H(21)	125.0
C(21)-C(22)-C(23)	107.01(15)

C(21)-C(22)-H(22)	126.5
C(23)-C(22)-H(22)	126.5
C(24)-C(23)-C(22)	107.62(15)
C(24)-C(23)-H(23)	126.2
C(22)-C(23)-H(23)	126.2
C(23)-C(24)-N(2)	109.09(15)
C(23)-C(24)-C(25)	125.81(15)
N(2)-C(24)-C(25)	125.07(14)
C(26)-C(25)-C(30)	119.96(15)
C(26)-C(25)-C(24)	120.66(14)
C(30)-C(25)-C(24)	119.08(15)
C(27)-C(26)-C(25)	119.28(15)
C(27)-C(26)-C(31)	120.26(16)
C(25)-C(26)-C(31)	120.44(15)
C(26)-C(31)-H(31A)	109.5
C(26)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(26)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(28)-C(27)-C(26)	121.37(17)
C(28)-C(27)-H(27)	119.3
C(26)-C(27)-H(27)	119.3
C(29)-C(28)-C(27)	118.62(16)
C(29)-C(28)-C(32)	120.72(17)
C(27)-C(28)-C(32)	120.65(18)
C(28)-C(32)-H(32A)	109.5
C(28)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(28)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(28)-C(29)-C(30)	121.59(16)
C(28)-C(29)-H(29)	119.2
C(30)-C(29)-H(29)	119.2
C(29)-C(30)-C(25)	119.18(16)

C(29)-C(30)-C(33)	120.43(15)
C(25)-C(30)-C(33)	120.39(15)
C(30)-C(33)-H(33A)	109.5
C(30)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(30)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(41)-O(1)-Mo(1)	169.3(10)
O(1)-C(41)-C(46)	119.8(7)
O(1)-C(41)-C(42)	119.9(6)
C(46)-C(41)-C(42)	120.3(4)
C(43)-C(42)-C(41)	118.8(4)
C(43)-C(42)-C(51)	117.2(6)
C(41)-C(42)-C(51)	123.9(6)
C(52)-C(51)-C(56)	119.8(4)
C(52)-C(51)-C(42)	120.5(4)
C(56)-C(51)-C(42)	119.2(4)
C(53)-C(52)-C(51)	118.5(3)
C(53)-C(52)-C(57)	120.4(3)
C(51)-C(52)-C(57)	121.0(3)
C(52)-C(57)-C(59)	111.7(4)
C(52)-C(57)-C(58)	113.5(3)
C(59)-C(57)-C(58)	109.3(3)
C(52)-C(57)-H(57)	107.4
C(59)-C(57)-H(57)	107.4
C(58)-C(57)-H(57)	107.4
C(57)-C(58)-H(58A)	109.5
C(57)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
C(57)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5
C(57)-C(59)-H(59A)	109.5
C(57)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	109.5

C(57)-C(59)-H(59C)	109.5
H(59A)-C(59)-H(59C)	109.5
H(59B)-C(59)-H(59C)	109.5
C(54)-C(53)-C(52)	122.6(3)
C(54)-C(53)-H(53)	118.7
C(52)-C(53)-H(53)	118.7
C(53)-C(54)-C(55)	118.1(3)
C(53)-C(54)-C(60)	119.4(3)
C(55)-C(54)-C(60)	122.4(3)
C(61)-C(60)-C(54)	114.4(3)
C(61)-C(60)-C(62)	110.0(3)
C(54)-C(60)-C(62)	110.3(3)
C(61)-C(60)-H(60)	107.2
C(54)-C(60)-H(60)	107.2
C(62)-C(60)-H(60)	107.2
C(60)-C(61)-H(61A)	109.5
C(60)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
C(60)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
C(60)-C(62)-H(62A)	109.5
C(60)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
C(60)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(54)-C(55)-C(56)	121.6(4)
C(54)-C(55)-H(55)	119.2
C(56)-C(55)-H(55)	119.2
C(55)-C(56)-C(51)	119.3(4)
C(55)-C(56)-C(63)	119.7(4)
C(51)-C(56)-C(63)	121.0(4)
C(56)-C(63)-C(65)	109.6(5)
C(56)-C(63)-C(64)	112.2(5)
C(65)-C(63)-C(64)	111.1(5)

C(56)-C(63)-H(63)	107.9
C(65)-C(63)-H(63)	107.9
C(64)-C(63)-H(63)	107.9
C(63)-C(64)-H(64A)	109.5
C(63)-C(64)-H(64B)	109.5
H(64A)-C(64)-H(64B)	109.5
C(63)-C(64)-H(64C)	109.5
H(64A)-C(64)-H(64C)	109.5
H(64B)-C(64)-H(64C)	109.5
C(63)-C(65)-H(65A)	109.5
C(63)-C(65)-H(65B)	109.5
H(65A)-C(65)-H(65B)	109.5
C(63)-C(65)-H(65C)	109.5
H(65A)-C(65)-H(65C)	109.5
H(65B)-C(65)-H(65C)	109.5
C(44)-C(43)-C(42)	121.5(4)
C(44)-C(43)-H(43)	119.2
C(42)-C(43)-H(43)	119.2
C(45)-C(44)-C(43)	118.8(3)
C(45)-C(44)-H(44)	120.6
C(43)-C(44)-H(44)	120.6
C(44)-C(45)-C(46)	122.0(3)
C(44)-C(45)-H(45)	119.0
C(46)-C(45)-H(45)	119.0
C(45)-C(46)-C(41)	118.3(4)
C(45)-C(46)-C(71)	118.5(5)
C(41)-C(46)-C(71)	123.1(5)
C(76)-C(71)-C(72)	120.3(3)
C(76)-C(71)-C(46)	120.6(3)
C(72)-C(71)-C(46)	118.9(4)
C(73)-C(72)-C(71)	118.7(4)
C(73)-C(72)-C(77)	119.6(4)
C(71)-C(72)-C(77)	121.6(4)
C(72)-C(77)-C(79)	110.3(4)
C(72)-C(77)-C(78)	111.5(5)
C(79)-C(77)-C(78)	109.2(5)

C(72)-C(77)-H(77)	108.6
C(79)-C(77)-H(77)	108.6
C(78)-C(77)-H(77)	108.6
C(77)-C(78)-H(78A)	109.5
C(77)-C(78)-H(78B)	109.5
H(78A)-C(78)-H(78B)	109.5
C(77)-C(78)-H(78C)	109.5
H(78A)-C(78)-H(78C)	109.5
H(78B)-C(78)-H(78C)	109.5
C(77)-C(79)-H(79A)	109.5
C(77)-C(79)-H(79B)	109.5
H(79A)-C(79)-H(79B)	109.5
C(77)-C(79)-H(79C)	109.5
H(79A)-C(79)-H(79C)	109.5
H(79B)-C(79)-H(79C)	109.5
C(74)-C(73)-C(72)	121.5(4)
C(74)-C(73)-H(73)	119.3
C(72)-C(73)-H(73)	119.3
C(73)-C(74)-C(75)	119.1(4)
C(73)-C(74)-C(80)	120.0(5)
C(75)-C(74)-C(80)	120.7(5)
C(82)-C(80)-C(74)	110.0(5)
C(82)-C(80)-C(81)	108.8(4)
C(74)-C(80)-C(81)	109.3(6)
C(82)-C(80)-H(80)	109.6
C(74)-C(80)-H(80)	109.6
C(81)-C(80)-H(80)	109.6
C(80)-C(81)-H(81A)	109.5
C(80)-C(81)-H(81B)	109.5
H(81A)-C(81)-H(81B)	109.5
C(80)-C(81)-H(81C)	109.5
H(81A)-C(81)-H(81C)	109.5
H(81B)-C(81)-H(81C)	109.5
C(80)-C(82)-H(82A)	109.5
C(80)-C(82)-H(82B)	109.5
H(82A)-C(82)-H(82B)	109.5

C(80)-C(82)-H(82C)	109.5
H(82A)-C(82)-H(82C)	109.5
H(82B)-C(82)-H(82C)	109.5
C(74)-C(75)-C(76)	121.1(4)
C(74)-C(75)-H(75)	119.4
C(76)-C(75)-H(75)	119.4
C(71)-C(76)-C(75)	119.0(4)
C(71)-C(76)-C(83)	121.0(4)
C(75)-C(76)-C(83)	119.9(4)
C(76)-C(83)-C(84)	113.1(5)
C(76)-C(83)-C(85)	111.1(5)
C(84)-C(83)-C(85)	108.2(5)
C(76)-C(83)-H(83)	108.1
C(84)-C(83)-H(83)	108.1
C(85)-C(83)-H(83)	108.1
C(83)-C(84)-H(84A)	109.5
C(83)-C(84)-H(84B)	109.5
H(84A)-C(84)-H(84B)	109.5
C(83)-C(84)-H(84C)	109.5
H(84A)-C(84)-H(84C)	109.5
H(84B)-C(84)-H(84C)	109.5
C(83)-C(85)-H(85A)	109.5
C(83)-C(85)-H(85B)	109.5
H(85A)-C(85)-H(85B)	109.5
C(83)-C(85)-H(85C)	109.5
H(85A)-C(85)-H(85C)	109.5
H(85B)-C(85)-H(85C)	109.5
C(41A)-O(1A)-Mo(1)	168(3)
O(1A)-C(41A)-C(42A)	119.5(16)
O(1A)-C(41A)-C(46A)	117.7(17)
C(42A)-C(41A)-C(46A)	122.3(11)
C(43A)-C(42A)-C(41A)	117.3(10)
C(43A)-C(42A)-C(51A)	116.7(15)
C(41A)-C(42A)-C(51A)	125.4(15)
C(56A)-C(51A)-C(52A)	121.2(10)
C(56A)-C(51A)-C(42A)	118.4(12)

C(52A)-C(51A)-C(42A)	120.0(11)
C(53A)-C(52A)-C(51A)	117.6(9)
C(53A)-C(52A)-C(57A)	121.6(8)
C(51A)-C(52A)-C(57A)	120.7(8)
C(52A)-C(57A)-C(59A)	109.5(9)
C(52A)-C(57A)-C(58A)	113.8(8)
C(59A)-C(57A)-C(58A)	109.9(6)
C(52A)-C(57A)-H(57A)	107.8
C(59A)-C(57A)-H(57A)	107.8
C(58A)-C(57A)-H(57A)	107.8
C(57A)-C(58A)-H(58D)	109.5
C(57A)-C(58A)-H(58E)	109.5
H(58D)-C(58A)-H(58E)	109.5
C(57A)-C(58A)-H(58F)	109.5
H(58D)-C(58A)-H(58F)	109.5
H(58E)-C(58A)-H(58F)	109.5
C(57A)-C(59A)-H(59D)	109.5
C(57A)-C(59A)-H(59E)	109.5
H(59D)-C(59A)-H(59E)	109.5
C(57A)-C(59A)-H(59F)	109.5
H(59D)-C(59A)-H(59F)	109.5
H(59E)-C(59A)-H(59F)	109.5
C(54A)-C(53A)-C(52A)	122.5(8)
C(54A)-C(53A)-H(53A)	118.7
C(52A)-C(53A)-H(53A)	118.7
C(53A)-C(54A)-C(55A)	119.5(8)
C(53A)-C(54A)-C(60A)	117.6(8)
C(55A)-C(54A)-C(60A)	122.9(8)
C(61A)-C(60A)-C(62A)	109.5(6)
C(61A)-C(60A)-C(54A)	112.4(7)
C(62A)-C(60A)-C(54A)	109.6(7)
C(61A)-C(60A)-H(60A)	108.4
C(62A)-C(60A)-H(60A)	108.4
C(54A)-C(60A)-H(60A)	108.4
C(60A)-C(61A)-H(61D)	109.5
C(60A)-C(61A)-H(61E)	109.5

H(61D)-C(61A)-H(61E)	109.5
C(60A)-C(61A)-H(61F)	109.5
H(61D)-C(61A)-H(61F)	109.5
H(61E)-C(61A)-H(61F)	109.5
C(60A)-C(62A)-H(62D)	109.5
C(60A)-C(62A)-H(62E)	109.5
H(62D)-C(62A)-H(62E)	109.5
C(60A)-C(62A)-H(62F)	109.5
H(62D)-C(62A)-H(62F)	109.5
H(62E)-C(62A)-H(62F)	109.5
C(54A)-C(55A)-C(56A)	122.0(9)
C(54A)-C(55A)-H(55A)	119.0
C(56A)-C(55A)-H(55A)	119.0
C(51A)-C(56A)-C(55A)	116.8(10)
C(51A)-C(56A)-C(63A)	123.0(11)
C(55A)-C(56A)-C(63A)	120.2(10)
C(56A)-C(63A)-C(65A)	112.1(13)
C(56A)-C(63A)-C(64A)	110.5(12)
C(65A)-C(63A)-C(64A)	109.5(13)
C(56A)-C(63A)-H(63A)	108.2
C(65A)-C(63A)-H(63A)	108.2
C(64A)-C(63A)-H(63A)	108.2
C(63A)-C(64A)-H(64D)	109.5
C(63A)-C(64A)-H(64E)	109.5
H(64D)-C(64A)-H(64E)	109.5
C(63A)-C(64A)-H(64F)	109.5
H(64D)-C(64A)-H(64F)	109.5
H(64E)-C(64A)-H(64F)	109.5
C(63A)-C(65A)-H(65D)	109.5
C(63A)-C(65A)-H(65E)	109.5
H(65D)-C(65A)-H(65E)	109.5
C(63A)-C(65A)-H(65F)	109.5
H(65D)-C(65A)-H(65F)	109.5
H(65E)-C(65A)-H(65F)	109.5
C(44A)-C(43A)-C(42A)	121.4(10)
C(44A)-C(43A)-H(43A)	119.3

C(42A)-C(43A)-H(43A)	119.3
C(45A)-C(44A)-C(43A)	120.1(8)
C(45A)-C(44A)-H(44A)	120.0
C(43A)-C(44A)-H(44A)	120.0
C(44A)-C(45A)-C(46A)	120.9(8)
C(44A)-C(45A)-H(45A)	119.5
C(46A)-C(45A)-H(45A)	119.5
C(45A)-C(46A)-C(41A)	117.7(10)
C(45A)-C(46A)-C(71A)	118.2(12)
C(41A)-C(46A)-C(71A)	124.1(12)
C(72A)-C(71A)-C(76A)	119.9(9)
C(72A)-C(71A)-C(46A)	121.2(9)
C(76A)-C(71A)-C(46A)	118.6(9)
C(71A)-C(72A)-C(73A)	118.4(10)
C(71A)-C(72A)-C(77A)	123.9(10)
C(73A)-C(72A)-C(77A)	117.7(10)
C(72A)-C(77A)-C(79A)	111.5(11)
C(72A)-C(77A)-C(78A)	113.2(12)
C(79A)-C(77A)-C(78A)	111.7(13)
C(72A)-C(77A)-H(77A)	106.6
C(79A)-C(77A)-H(77A)	106.6
C(78A)-C(77A)-H(77A)	106.6
C(77A)-C(78A)-H(78D)	109.5
C(77A)-C(78A)-H(78E)	109.5
H(78D)-C(78A)-H(78E)	109.5
C(77A)-C(78A)-H(78F)	109.5
H(78D)-C(78A)-H(78F)	109.5
H(78E)-C(78A)-H(78F)	109.5
C(77A)-C(79A)-H(79D)	109.5
C(77A)-C(79A)-H(79E)	109.5
H(79D)-C(79A)-H(79E)	109.5
C(77A)-C(79A)-H(79F)	109.5
H(79D)-C(79A)-H(79F)	109.5
H(79E)-C(79A)-H(79F)	109.5
C(74A)-C(73A)-C(72A)	123.5(12)
C(74A)-C(73A)-H(73A)	118.2

C(72A)-C(73A)-H(73A)	118.2
C(73A)-C(74A)-C(75A)	115.8(11)
C(73A)-C(74A)-C(80A)	125.0(12)
C(75A)-C(74A)-C(80A)	119.0(12)
C(82A)-C(80A)-C(74A)	118.0(12)
C(82A)-C(80A)-C(81A)	110.7(10)
C(74A)-C(80A)-C(81A)	115.6(14)
C(82A)-C(80A)-H(80A)	103.5
C(74A)-C(80A)-H(80A)	103.5
C(81A)-C(80A)-H(80A)	103.5
C(80A)-C(81A)-H(81D)	109.5
C(80A)-C(81A)-H(81E)	109.5
H(81D)-C(81A)-H(81E)	109.5
C(80A)-C(81A)-H(81F)	109.5
H(81D)-C(81A)-H(81F)	109.5
H(81E)-C(81A)-H(81F)	109.5
C(80A)-C(82A)-H(82D)	109.5
C(80A)-C(82A)-H(82E)	109.5
H(82D)-C(82A)-H(82E)	109.5
C(80A)-C(82A)-H(82F)	109.5
H(82D)-C(82A)-H(82F)	109.5
H(82E)-C(82A)-H(82F)	109.5
C(74A)-C(75A)-C(76A)	123.1(10)
C(74A)-C(75A)-H(75A)	118.5
C(76A)-C(75A)-H(75A)	118.5
C(75A)-C(76A)-C(71A)	118.6(9)
C(75A)-C(76A)-C(83A)	119.2(10)
C(71A)-C(76A)-C(83A)	122.1(9)
C(84A)-C(83A)-C(76A)	115.7(12)
C(84A)-C(83A)-C(85A)	109.4(12)
C(76A)-C(83A)-C(85A)	110.9(13)
C(84A)-C(83A)-H(83A)	106.8
C(76A)-C(83A)-H(83A)	106.8
C(85A)-C(83A)-H(83A)	106.8
C(83A)-C(84A)-H(84D)	109.5
C(83A)-C(84A)-H(84E)	109.5

H(84D)-C(84A)-H(84E)	109.5
C(83A)-C(84A)-H(84F)	109.5
H(84D)-C(84A)-H(84F)	109.5
H(84E)-C(84A)-H(84F)	109.5
C(83A)-C(85A)-H(85D)	109.5
C(83A)-C(85A)-H(85E)	109.5
H(85D)-C(85A)-H(85E)	109.5
C(83A)-C(85A)-H(85F)	109.5
H(85D)-C(85A)-H(85F)	109.5
H(85E)-C(85A)-H(85F)	109.5
C(3S)-Si(1S)-C(2S)	109.7(3)
C(3S)-Si(1S)-C(4S)	109.6(4)
C(2S)-Si(1S)-C(4S)	109.1(2)
C(3S)-Si(1S)-C(1S)	111.2(2)
C(2S)-Si(1S)-C(1S)	108.8(3)
C(4S)-Si(1S)-C(1S)	108.5(3)

Symmetry transformations used to generate equivalent atoms:

Table S4D. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2c**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	15(1)	17(1)	21(1)	-1(1)	1(1)	-2(1)
C(1)	17(1)	25(1)	30(1)	-3(1)	2(1)	-3(1)
C(2)	24(1)	34(1)	32(1)	-9(1)	7(1)	-6(1)
C(3)	30(1)	50(1)	44(1)	-13(1)	17(1)	-14(1)
C(4)	38(1)	41(1)	30(1)	-2(1)	9(1)	-4(1)
C(5)	20(1)	39(1)	31(1)	-13(1)	5(1)	-3(1)
C(6)	29(1)	46(1)	35(1)	-17(1)	-2(1)	1(1)
C(7)	36(1)	53(1)	45(1)	-13(1)	-5(1)	13(1)
C(8)	37(1)	44(1)	58(1)	-18(1)	-1(1)	11(1)
C(9)	32(1)	46(1)	51(1)	-27(1)	-4(1)	6(1)
C(10)	25(1)	45(1)	35(1)	-18(1)	-1(1)	2(1)
N(1)	21(1)	23(1)	23(1)	1(1)	0(1)	-5(1)
C(11)	22(1)	22(1)	25(1)	5(1)	-3(1)	-6(1)
C(12)	25(1)	23(1)	32(1)	0(1)	1(1)	-4(1)
C(13)	22(1)	27(1)	31(1)	3(1)	1(1)	-5(1)
C(14)	30(1)	34(1)	28(1)	7(1)	-6(1)	-10(1)
C(15)	32(1)	22(1)	44(1)	-2(1)	1(1)	-3(1)
C(16)	35(1)	24(1)	41(1)	4(1)	-4(1)	-9(1)
C(17)	25(1)	31(1)	36(1)	6(1)	-1(1)	-10(1)
C(18)	38(1)	35(1)	39(1)	11(1)	0(1)	-13(1)
C(19)	37(1)	36(1)	35(1)	15(1)	-10(1)	-12(1)
C(20)	33(1)	25(1)	60(1)	14(1)	-6(1)	-3(1)
N(2)	20(1)	18(1)	28(1)	1(1)	0(1)	-2(1)
C(21)	24(1)	19(1)	38(1)	1(1)	6(1)	-1(1)
C(22)	25(1)	22(1)	43(1)	9(1)	4(1)	4(1)
C(23)	25(1)	29(1)	36(1)	9(1)	-6(1)	0(1)
C(24)	19(1)	24(1)	27(1)	4(1)	-3(1)	-2(1)
C(25)	24(1)	22(1)	22(1)	3(1)	-6(1)	-3(1)
C(26)	28(1)	27(1)	22(1)	1(1)	-2(1)	-4(1)
C(31)	32(1)	37(1)	38(1)	-4(1)	7(1)	-6(1)
C(27)	34(1)	29(1)	23(1)	-2(1)	-1(1)	-1(1)

C(28)	37(1)	25(1)	26(1)	-1(1)	-8(1)	-6(1)
C(32)	55(1)	30(1)	46(1)	-8(1)	-4(1)	-10(1)
C(29)	27(1)	28(1)	30(1)	4(1)	-8(1)	-8(1)
C(30)	23(1)	26(1)	26(1)	5(1)	-7(1)	-2(1)
C(33)	24(1)	29(1)	50(1)	6(1)	2(1)	0(1)
O(1)	16(1)	20(1)	19(3)	0(2)	0(1)	0(1)
C(41)	16(1)	19(1)	17(3)	1(2)	1(1)	0(1)
C(42)	19(1)	17(1)	18(2)	1(1)	0(1)	0(1)
C(51)	16(2)	17(2)	18(1)	4(1)	1(2)	3(2)
C(52)	19(1)	16(2)	22(1)	3(1)	1(1)	3(1)
C(57)	37(1)	24(2)	18(1)	1(1)	2(1)	2(1)
C(58)	39(2)	31(2)	24(2)	-1(1)	-2(1)	5(1)
C(59)	52(2)	66(2)	34(2)	-13(2)	18(1)	-9(2)
C(53)	24(1)	20(1)	22(2)	0(1)	-4(2)	1(1)
C(54)	21(1)	18(1)	29(2)	4(1)	-6(2)	-2(1)
C(60)	34(1)	21(1)	41(2)	10(1)	-5(1)	-7(1)
C(61)	36(1)	38(2)	55(2)	26(2)	3(1)	-2(1)
C(62)	49(2)	16(1)	61(2)	9(2)	6(2)	5(1)
C(55)	29(2)	26(2)	20(2)	6(1)	0(2)	-2(2)
C(56)	21(2)	22(2)	19(1)	-2(1)	-2(1)	0(2)
C(63)	30(2)	24(2)	21(2)	-1(1)	-1(1)	1(1)
C(64)	33(2)	37(3)	28(2)	-7(2)	-9(1)	2(2)
C(65)	36(2)	56(3)	40(2)	-26(2)	-5(1)	11(2)
C(43)	19(1)	19(2)	38(3)	5(2)	1(2)	3(1)
C(44)	15(1)	24(2)	50(2)	12(1)	2(1)	0(1)
C(45)	20(1)	21(2)	40(2)	10(1)	2(2)	-1(1)
C(46)	19(1)	18(1)	24(2)	3(1)	0(1)	1(1)
C(71)	16(1)	15(2)	21(2)	4(2)	0(2)	1(1)
C(72)	16(2)	17(1)	21(2)	-1(2)	3(2)	-1(1)
C(77)	18(1)	18(1)	20(2)	5(2)	0(2)	0(1)
C(78)	28(2)	25(2)	21(3)	2(2)	-1(2)	-3(2)
C(79)	26(2)	29(2)	30(3)	-6(3)	8(2)	3(1)
C(73)	16(2)	18(2)	24(2)	5(2)	-1(2)	3(1)
C(74)	20(2)	16(2)	27(2)	-4(2)	-2(2)	-2(2)
C(80)	19(1)	13(2)	43(2)	-2(2)	-7(1)	-1(1)
C(81)	23(1)	23(1)	66(2)	-3(1)	-2(1)	4(1)

C(82)	35(1)	16(1)	62(2)	1(1)	4(1)	0(1)
C(75)	20(2)	21(2)	22(2)	-4(2)	0(2)	1(1)
C(76)	19(1)	21(2)	19(2)	-3(1)	0(2)	-3(1)
C(83)	31(2)	28(2)	18(2)	4(2)	-6(2)	1(1)
C(84)	36(2)	37(4)	21(3)	-6(2)	1(2)	-5(2)
C(85)	27(1)	59(4)	30(3)	4(2)	-8(2)	-2(2)
O(1A)	16(1)	20(1)	19(3)	0(2)	0(1)	0(1)
C(41A)	16(1)	19(1)	17(3)	1(2)	1(1)	0(1)
C(42A)	19(1)	17(1)	18(2)	1(1)	0(1)	0(1)
C(51A)	20(5)	13(3)	26(3)	6(2)	5(4)	-2(3)
C(52A)	20(3)	18(3)	19(3)	6(2)	-2(3)	3(3)
C(57A)	34(3)	18(4)	27(3)	3(2)	6(2)	4(3)
C(58A)	34(3)	38(5)	26(4)	-3(3)	-3(3)	3(3)
C(59A)	32(3)	77(6)	41(4)	-30(4)	5(3)	1(4)
C(53A)	27(3)	10(3)	30(4)	6(3)	-7(4)	3(2)
C(54A)	28(3)	28(3)	27(4)	14(3)	-8(4)	-2(3)
C(60A)	29(3)	31(3)	40(4)	21(3)	-3(3)	-3(2)
C(61A)	72(6)	50(5)	66(5)	42(4)	44(5)	20(4)
C(62A)	55(4)	31(4)	44(5)	8(4)	11(4)	11(3)
C(55A)	22(3)	31(4)	22(4)	9(3)	-5(4)	-3(4)
C(56A)	28(4)	21(3)	21(3)	8(3)	5(4)	1(4)
C(63A)	39(4)	32(5)	23(4)	-4(4)	-3(3)	0(4)
C(64A)	44(5)	45(8)	27(5)	-6(6)	-3(3)	5(6)
C(43A)	22(3)	21(4)	23(4)	5(3)	7(3)	2(3)
C(44A)	16(3)	23(3)	34(4)	3(3)	5(3)	1(2)
C(45A)	22(2)	19(3)	20(4)	5(3)	3(3)	-1(2)
C(46A)	19(1)	18(1)	24(2)	3(1)	0(1)	1(1)
C(71A)	15(3)	18(3)	12(3)	-8(3)	3(3)	-4(2)
C(72A)	13(3)	17(3)	13(3)	7(3)	6(3)	0(2)
C(77A)	34(4)	12(3)	7(4)	5(3)	7(3)	3(3)
C(78A)	19(3)	44(6)	17(5)	-6(4)	5(3)	2(4)
C(79A)	24(3)	31(5)	16(6)	-4(5)	11(4)	-4(3)
C(73A)	19(5)	23(3)	19(4)	-3(3)	8(3)	-2(3)
C(74A)	19(3)	17(4)	25(4)	-5(3)	-7(3)	0(3)
C(80A)	35(4)	12(4)	33(4)	-8(3)	-1(3)	-9(3)
C(81A)	38(3)	20(3)	70(5)	5(3)	10(3)	12(3)

C(82A)	53(4)	23(3)	47(4)	2(3)	1(3)	14(3)
C(75A)	26(4)	23(4)	17(3)	-17(3)	5(4)	-2(3)
C(76A)	20(3)	20(4)	15(3)	0(3)	0(4)	1(3)
C(83A)	29(3)	33(5)	11(3)	-7(3)	2(3)	-12(3)
C(84A)	45(6)	30(7)	15(5)	-8(5)	-5(4)	-10(5)
C(85A)	36(3)	52(8)	21(5)	-1(4)	-12(3)	-6(5)
Si(1S)	28(1)	21(1)	30(1)	-1(1)	2(1)	1(1)
C(1S)	27(2)	25(3)	30(3)	-2(2)	5(2)	3(2)
C(2S)	42(2)	40(2)	44(2)	-16(2)	10(2)	-12(2)
C(3S)	59(4)	35(5)	42(3)	-1(3)	11(3)	-3(3)
C(4S)	38(2)	31(2)	60(3)	0(2)	-4(2)	9(2)

Table S4E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for **2c**.

	x	y	z	U(eq)
H(1)	3585(4)	8520(13)	9348(9)	29
H(3A)	2807	7744	9512	60
H(3B)	2801	7767	10308	60
H(3C)	2990	6986	9972	60
H(4A)	3493	7284	10655	54
H(4B)	3319	8036	11052	54
H(4C)	3641	8272	10727	54
H(6)	2880	9126	9083	45
H(7)	2733	10624	9006	55
H(8)	2908	11613	9875	56
H(9)	3226	11085	10817	53
H(10)	3369	9577	10906	43
H(12A)	3237	4928	8148	32
H(12B)	3572	4820	8614	32
H(13A)	2743	5466	8653	32
H(13B)	2767	5703	9437	32
H(14A)	3301	5548	10164	38
H(14B)	3612	5205	9838	38
H(15)	3328	3385	8415	40
H(16A)	2780	3866	8283	41
H(16B)	2827	3077	8827	41
H(17)	2526	4262	9248	37
H(18A)	2846	4484	10295	45
H(18B)	2867	3458	10068	45
H(19)	3392	3997	10431	45
H(20A)	3358	2915	9556	48
H(20B)	3646	3598	9467	48
H(21)	3310	9191	8220	32
H(22)	3002	9570	7133	36
H(23)	2835	8105	6549	37

H(31A)	3535	6974	6522	53
H(31B)	3710	6022	6598	53
H(31C)	3696	6648	7241	53
H(27)	3360	4805	6554	35
H(32A)	2653	3560	6831	66
H(32B)	3030	3396	6815	66
H(32C)	2813	3735	6155	66
H(29)	2490	4945	7233	35
H(33A)	2592	6939	8066	51
H(33B)	2326	6222	7789	51
H(33C)	2394	7073	7343	51
H(57)	4192	5792	7723	32
H(58A)	4112	3938	7401	48
H(58B)	4016	4746	6895	48
H(58C)	3825	4598	7534	48
H(59A)	4750	5530	7760	74
H(59B)	4570	5320	7030	74
H(59C)	4680	4516	7530	74
H(53)	4216	3629	8426	27
H(60)	4126	2580	9293	39
H(61A)	4365	2910	10648	65
H(61B)	4146	2085	10366	65
H(61C)	3997	3072	10359	65
H(62A)	4668	2477	9101	63
H(62B)	4597	1780	9672	63
H(62C)	4781	2696	9872	63
H(55)	4388	4397	10351	30
H(63)	4568	6685	9991	30
H(64A)	4698	5338	11003	50
H(64B)	4821	6352	11066	50
H(64C)	4958	5692	10538	50
H(65A)	4031	6639	10196	67
H(65B)	4244	6824	10896	67
H(65C)	4102	5845	10727	67
H(43)	4963	6171	8826	30
H(44)	5160	7545	8506	36

H(45)	4813	8764	8356	32
H(77)	4169	8073	7317	22
H(78A)	3639	8572	6870	37
H(78B)	3861	8349	6292	37
H(78C)	3802	9367	6493	37
H(79A)	4392	9722	6794	42
H(79B)	4443	8767	6460	42
H(79C)	4615	8985	7195	42
H(73)	3823	10256	7325	24
H(80)	3695	11765	8674	31
H(81A)	3339	11040	7470	56
H(81B)	3219	11853	7898	56
H(81C)	3239	10864	8206	56
H(82A)	4082	12132	7922	57
H(82B)	3750	12660	7746	57
H(82C)	3830	11809	7309	57
H(75)	3944	10594	9329	26
H(83)	4280	8478	9747	32
H(84A)	4159	10169	10338	48
H(84B)	4181	9218	10707	48
H(84C)	3880	9443	10169	48
H(85A)	4770	9138	9537	59
H(85B)	4732	9214	10319	59
H(85C)	4665	10069	9843	59
H(57A)	4243	5467	7758	31
H(58D)	4008	3658	7667	50
H(58E)	3981	4354	7057	50
H(58F)	3783	4522	7683	50
H(59D)	4760	4920	7801	75
H(59E)	4562	4431	7176	75
H(59F)	4643	3907	7870	75
H(53A)	4192	3483	8732	28
H(60A)	4078	2697	9726	41
H(61D)	4353	3509	10936	89
H(61E)	4250	2477	10919	89
H(61F)	3984	3236	10737	89

H(62D)	4727	2831	9722	65
H(62E)	4513	1943	9623	65
H(62F)	4658	2249	10360	65
H(55A)	4374	4667	10515	30
H(63A)	4568	6840	9886	38
H(64D)	4887	6686	10890	59
H(64E)	4953	5793	10487	59
H(64F)	4718	5768	11064	59
H(65D)	4021	6616	10241	58
H(65E)	4256	7316	10654	58
H(65F)	4211	6334	10947	58
H(43A)	4928	5986	8659	26
H(44A)	5119	7281	8195	29
H(45A)	4799	8559	8084	24
H(77A)	4200	8104	7154	21
H(78D)	3653	8583	6787	39
H(78E)	3859	8260	6206	39
H(78F)	3806	9305	6328	39
H(79D)	4390	9770	6640	35
H(79E)	4447	8823	6300	35
H(79F)	4624	9048	7029	35
H(73A)	3890	10294	7226	24
H(80A)	3811	11755	8492	32
H(81D)	3222	10815	8314	63
H(81E)	3243	11869	8455	63
H(81F)	3407	11181	9001	63
H(82D)	3823	11832	7334	62
H(82E)	3564	12460	7634	62
H(82F)	3451	11556	7251	62
H(75A)	3975	10496	9219	26
H(83A)	4251	8354	9613	29
H(84D)	4196	10041	10230	46
H(84E)	4200	9081	10584	46
H(84F)	3897	9375	10072	46
H(85D)	4761	8753	9438	56
H(85E)	4728	9035	10197	56

H(85F)	4704	9779	9620	56
H(1S1)	4987	9826	3233	41
H(1S2)	4821	9003	3572	41
H(1S3)	4640	9479	2922	41
H(2S1)	4567	7750	2152	62
H(2S2)	4723	7243	2812	62
H(2S3)	4870	7107	2116	62
H(3S1)	4934	9296	1579	67
H(3S2)	5225	8613	1526	67
H(3S3)	5287	9539	1921	67
H(4S1)	5512	7599	2818	66
H(4S2)	5382	7869	3510	66
H(4S3)	5582	8577	3125	66

Table S5A. Crystal data and structure refinement for **3**(PMe_3).

Identification code	11015	
Empirical formula	C60 H85 F3 Mo N O4 P S	
Formula weight	1100.26	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 11.9252(15) Å	α= 90°
	b = 23.200(3) Å	β= 99.781(2)°
	c = 20.709(3) Å	γ = 90°
Volume	5646.0(13) $Å^3$	
Z	4	
Density (calculated)	1.294 Mg/m^3	
Absorption coefficient	0.353 mm^{-1}	
F(000)	2336	
Crystal size	0.30 x 0.20 x 0.15 mm^3	
Theta range for data collection	1.33 to 30.32°	
Index ranges	-16<=h<=16, -32<=k<=32, -29<=l<=29	
Reflections collected	156288	
Independent reflections	16915 [R(int) = 0.0730]	
Completeness to theta = 30.32°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9489 and 0.9014	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16915 / 56 / 677	
Goodness-of-fit on F^2	1.041	
Final R indices [I>2sigma(I)]	R1 = 0.0345, wR2 = 0.0790	
R indices (all data)	R1 = 0.0473, wR2 = 0.0864	
Largest diff. peak and hole	0.577 and -0.750 e.$Å^{-3}$	

Table S5B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3**(PMe_3). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	9270(1)	2159(1)	8590(1)	12(1)
C(1)	8757(1)	2919(1)	8708(1)	15(1)
C(2)	7843(1)	3301(1)	8913(1)	17(1)
C(3)	8406(2)	3718(1)	9456(1)	24(1)
C(4)	6958(1)	2942(1)	9186(1)	22(1)
C(5)	7329(1)	3642(1)	8294(1)	19(1)
C(6)	8019(2)	4021(1)	8009(1)	23(1)
C(7)	7607(2)	4314(1)	7433(1)	30(1)
C(8)	6501(2)	4233(1)	7122(1)	35(1)
C(9)	5800(2)	3867(1)	7400(1)	35(1)
C(10)	6205(1)	3576(1)	7981(1)	26(1)
N(1)	8304(1)	1740(1)	8927(1)	15(1)
C(11)	7619(1)	1291(1)	9162(1)	14(1)
C(12)	7889(1)	1263(1)	9918(1)	20(1)
C(13)	6342(1)	1425(1)	8961(1)	20(1)
C(14)	7885(1)	707(1)	8874(1)	18(1)
C(15)	7169(2)	781(1)	10160(1)	23(1)
C(16)	5903(2)	914(1)	9951(1)	25(1)
C(17)	5624(1)	947(1)	9203(1)	23(1)
C(18)	5891(2)	369(1)	8906(1)	24(1)
C(19)	7159(2)	233(1)	9116(1)	21(1)
C(20)	7444(2)	202(1)	9866(1)	26(1)
O(1)	10469(1)	2286(1)	8024(1)	13(1)
C(21)	11612(1)	2316(1)	8080(1)	12(1)
C(22)	12209(1)	1868(1)	7819(1)	12(1)
C(31)	11614(1)	1426(1)	7349(1)	13(1)
C(32)	11424(1)	1558(1)	6673(1)	15(1)
C(37)	11808(1)	2131(1)	6420(1)	18(1)
C(38)	12947(2)	2063(1)	6178(1)	26(1)
C(39)	10923(2)	2399(1)	5883(1)	23(1)
C(33)	10912(1)	1142(1)	6225(1)	17(1)

C(34)	10581(1)	605(1)	6425(1)	17(1)
C(40)	9974(2)	171(1)	5939(1)	22(1)
C(41)	8742(2)	87(1)	6034(1)	30(1)
C(42)	10586(2)	-413(1)	5987(1)	33(1)
C(35)	10797(1)	481(1)	7093(1)	16(1)
C(36)	11312(1)	877(1)	7557(1)	14(1)
C(43)	11604(1)	696(1)	8270(1)	16(1)
C(44)	12789(1)	422(1)	8393(1)	22(1)
C(45)	10739(1)	271(1)	8473(1)	22(1)
C(23)	13396(1)	1878(1)	7932(1)	16(1)
C(24)	13996(1)	2331(1)	8269(1)	17(1)
C(25)	13401(1)	2798(1)	8456(1)	15(1)
C(26)	12209(1)	2810(1)	8352(1)	12(1)
C(51)	11673(1)	3380(1)	8473(1)	13(1)
C(52)	11286(1)	3747(1)	7933(1)	14(1)
C(57)	11273(1)	3547(1)	7230(1)	15(1)
C(58)	10380(1)	3856(1)	6726(1)	20(1)
C(59)	12457(1)	3616(1)	7040(1)	22(1)
C(53)	10984(1)	4314(1)	8048(1)	17(1)
C(54)	11045(1)	4537(1)	8679(1)	19(1)
C(60)	10765(2)	5165(1)	8808(1)	27(1)
C(61)	10939(7)	5567(4)	8246(4)	30(2)
C(62)	9523(11)	5231(5)	8873(12)	70(4)
C(61A)	10740(20)	5563(5)	8243(6)	80(4)
C(62A)	9717(14)	5216(7)	9106(11)	67(4)
C(55)	11398(1)	4166(1)	9202(1)	18(1)
C(56)	11718(1)	3595(1)	9114(1)	15(1)
C(63)	12149(1)	3228(1)	9711(1)	17(1)
C(64)	11326(2)	3222(1)	10205(1)	23(1)
C(65)	13330(2)	3431(1)	10050(1)	25(1)
P(1)	8102(1)	2125(1)	7467(1)	15(1)
C(66)	8424(2)	1481(1)	7039(1)	23(1)
C(67)	6559(1)	2123(1)	7348(1)	26(1)
C(68)	8408(2)	2716(1)	6955(1)	24(1)
O(2)	10763(1)	1976(1)	9320(1)	19(1)
S(1)	10953(1)	1605(1)	9914(1)	17(1)

O(3)	10608(1)	1020(1)	9780(1)	26(1)
O(4)	10654(1)	1875(1)	10480(1)	27(1)
C(69)	12514(1)	1558(1)	10088(1)	22(1)
F(1)	12818(1)	1192(1)	10583(1)	40(1)
F(2)	13005(1)	2060(1)	10270(1)	26(1)
F(3)	12936(1)	1368(1)	9577(1)	43(1)

Table S5C. Bond lengths [Å] and angles [°] for **3**(PMe_3).

Mo(1)-N(1)	1.7413(13)
Mo(1)-C(1)	1.8951(16)
Mo(1)-O(1)	2.0180(11)
Mo(1)-O(2)	2.1721(11)
Mo(1)-P(1)	2.5012(5)
C(1)-C(2)	1.521(2)
C(1)-H(1)	0.957(14)
C(2)-C(4)	1.525(2)
C(2)-C(5)	1.543(2)
C(2)-C(3)	1.547(2)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-C(10)	1.395(2)
C(5)-C(6)	1.402(2)
C(6)-C(7)	1.386(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.379(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.382(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.393(3)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
N(1)-C(11)	1.4574(19)
C(11)-C(14)	1.534(2)
C(11)-C(13)	1.541(2)
C(11)-C(12)	1.545(2)
C(12)-C(15)	1.543(2)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900

C(13)-C(17)	1.537(2)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(19)	1.535(2)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.530(3)
C(15)-C(20)	1.533(3)
C(15)-H(15)	1.0000
C(16)-C(17)	1.531(3)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.529(3)
C(17)-H(17)	1.0000
C(18)-C(19)	1.534(3)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.535(2)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
O(1)-C(21)	1.3499(16)
C(21)-C(26)	1.415(2)
C(21)-C(22)	1.418(2)
C(22)-C(23)	1.395(2)
C(22)-C(31)	1.505(2)
C(31)-C(36)	1.411(2)
C(31)-C(32)	1.414(2)
C(32)-C(33)	1.404(2)
C(32)-C(37)	1.527(2)
C(37)-C(39)	1.529(2)
C(37)-C(38)	1.534(2)
C(37)-H(37)	1.0000
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800

C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(33)-C(34)	1.391(2)
C(33)-H(33)	0.9500
C(34)-C(35)	1.393(2)
C(34)-C(40)	1.517(2)
C(40)-C(41)	1.527(3)
C(40)-C(42)	1.535(3)
C(40)-H(40)	1.0000
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(35)-C(36)	1.396(2)
C(35)-H(35)	0.9500
C(36)-C(43)	1.517(2)
C(43)-C(44)	1.531(2)
C(43)-C(45)	1.536(2)
C(43)-H(43)	1.0000
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(23)-C(24)	1.390(2)
C(23)-H(23)	0.9500
C(24)-C(25)	1.385(2)
C(24)-H(24)	0.9500
C(25)-C(26)	1.402(2)
C(25)-H(25)	0.9500
C(26)-C(51)	1.508(2)
C(51)-C(56)	1.410(2)

C(51)-C(52)	1.419(2)
C(52)-C(53)	1.396(2)
C(52)-C(57)	1.526(2)
C(57)-C(58)	1.536(2)
C(57)-C(59)	1.537(2)
C(57)-H(57)	1.0000
C(58)-H(58A)	0.9800
C(58)-H(58B)	0.9800
C(58)-H(58C)	0.9800
C(59)-H(59A)	0.9800
C(59)-H(59B)	0.9800
C(59)-H(59C)	0.9800
C(53)-C(54)	1.396(2)
C(53)-H(53)	0.9500
C(54)-C(55)	1.392(2)
C(54)-C(60)	1.527(2)
C(60)-C(61A)	1.488(10)
C(60)-C(62A)	1.488(9)
C(60)-C(62)	1.517(9)
C(60)-C(61)	1.533(7)
C(60)-H(60A)	1.0000
C(60)-H(60B)	1.0000
C(61)-H(61A)	0.9800
C(61)-H(61B)	0.9800
C(61)-H(61C)	0.9800
C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800
C(61A)-H(61D)	0.9800
C(61A)-H(61E)	0.9800
C(61A)-H(61F)	0.9800
C(62A)-H(62D)	0.9800
C(62A)-H(62E)	0.9800
C(62A)-H(62F)	0.9800
C(55)-C(56)	1.397(2)
C(55)-H(55)	0.9500

C(56)-C(63)	1.518(2)
C(63)-C(64)	1.532(2)
C(63)-C(65)	1.537(2)
C(63)-H(63)	1.0000
C(64)-H(64A)	0.9800
C(64)-H(64B)	0.9800
C(64)-H(64C)	0.9800
C(65)-H(65A)	0.9800
C(65)-H(65B)	0.9800
C(65)-H(65C)	0.9800
P(1)-C(68)	1.8071(18)
P(1)-C(66)	1.8118(18)
P(1)-C(67)	1.8153(17)
C(66)-H(66A)	0.9800
C(66)-H(66B)	0.9800
C(66)-H(66C)	0.9800
C(67)-H(67A)	0.9800
C(67)-H(67B)	0.9800
C(67)-H(67C)	0.9800
C(68)-H(68A)	0.9800
C(68)-H(68B)	0.9800
C(68)-H(68C)	0.9800
O(2)-S(1)	1.4872(12)
S(1)-O(4)	1.4273(13)
S(1)-O(3)	1.4324(13)
S(1)-C(69)	1.8388(17)
C(69)-F(3)	1.322(2)
C(69)-F(2)	1.3298(19)
C(69)-F(1)	1.332(2)

N(1)-Mo(1)-C(1)	102.59(6)
N(1)-Mo(1)-O(1)	153.63(5)
C(1)-Mo(1)-O(1)	102.44(6)
N(1)-Mo(1)-O(2)	97.54(5)
C(1)-Mo(1)-O(2)	109.68(6)
O(1)-Mo(1)-O(2)	81.68(4)

N(1)-Mo(1)-P(1)	93.06(4)
C(1)-Mo(1)-P(1)	90.46(5)
O(1)-Mo(1)-P(1)	78.57(3)
O(2)-Mo(1)-P(1)	154.41(3)
C(2)-C(1)-Mo(1)	147.17(12)
C(2)-C(1)-H(1)	113.8(12)
Mo(1)-C(1)-H(1)	98.9(12)
C(1)-C(2)-C(4)	111.11(13)
C(1)-C(2)-C(5)	105.64(13)
C(4)-C(2)-C(5)	112.73(13)
C(1)-C(2)-C(3)	108.87(13)
C(4)-C(2)-C(3)	108.28(14)
C(5)-C(2)-C(3)	110.15(13)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(10)-C(5)-C(6)	117.38(16)
C(10)-C(5)-C(2)	122.96(15)
C(6)-C(5)-C(2)	119.61(15)
C(7)-C(6)-C(5)	121.44(17)
C(7)-C(6)-H(6)	119.3
C(5)-C(6)-H(6)	119.3
C(8)-C(7)-C(6)	120.38(18)
C(8)-C(7)-H(7)	119.8
C(6)-C(7)-H(7)	119.8
C(7)-C(8)-C(9)	119.16(18)
C(7)-C(8)-H(8)	120.4

C(9)-C(8)-H(8)	120.4
C(8)-C(9)-C(10)	120.78(18)
C(8)-C(9)-H(9)	119.6
C(10)-C(9)-H(9)	119.6
C(9)-C(10)-C(5)	120.84(17)
C(9)-C(10)-H(10)	119.6
C(5)-C(10)-H(10)	119.6
C(11)-N(1)-Mo(1)	168.35(11)
N(1)-C(11)-C(14)	109.67(12)
N(1)-C(11)-C(13)	110.49(12)
C(14)-C(11)-C(13)	109.47(13)
N(1)-C(11)-C(12)	109.68(12)
C(14)-C(11)-C(12)	109.58(13)
C(13)-C(11)-C(12)	107.94(13)
C(15)-C(12)-C(11)	109.14(13)
C(15)-C(12)-H(12A)	109.9
C(11)-C(12)-H(12A)	109.9
C(15)-C(12)-H(12B)	109.9
C(11)-C(12)-H(12B)	109.9
H(12A)-C(12)-H(12B)	108.3
C(17)-C(13)-C(11)	110.26(13)
C(17)-C(13)-H(13A)	109.6
C(11)-C(13)-H(13A)	109.6
C(17)-C(13)-H(13B)	109.6
C(11)-C(13)-H(13B)	109.6
H(13A)-C(13)-H(13B)	108.1
C(11)-C(14)-C(19)	109.92(13)
C(11)-C(14)-H(14A)	109.7
C(19)-C(14)-H(14A)	109.7
C(11)-C(14)-H(14B)	109.7
C(19)-C(14)-H(14B)	109.7
H(14A)-C(14)-H(14B)	108.2
C(16)-C(15)-C(20)	109.41(14)
C(16)-C(15)-C(12)	109.84(14)
C(20)-C(15)-C(12)	109.71(14)
C(16)-C(15)-H(15)	109.3

C(20)-C(15)-H(15)	109.3
C(12)-C(15)-H(15)	109.3
C(15)-C(16)-C(17)	109.24(14)
C(15)-C(16)-H(16A)	109.8
C(17)-C(16)-H(16A)	109.8
C(15)-C(16)-H(16B)	109.8
C(17)-C(16)-H(16B)	109.8
H(16A)-C(16)-H(16B)	108.3
C(18)-C(17)-C(16)	109.82(15)
C(18)-C(17)-C(13)	109.68(14)
C(16)-C(17)-C(13)	109.14(14)
C(18)-C(17)-H(17)	109.4
C(16)-C(17)-H(17)	109.4
C(13)-C(17)-H(17)	109.4
C(17)-C(18)-C(19)	109.24(13)
C(17)-C(18)-H(18A)	109.8
C(19)-C(18)-H(18A)	109.8
C(17)-C(18)-H(18B)	109.8
C(19)-C(18)-H(18B)	109.8
H(18A)-C(18)-H(18B)	108.3
C(18)-C(19)-C(20)	109.50(14)
C(18)-C(19)-C(14)	110.10(14)
C(20)-C(19)-C(14)	108.87(14)
C(18)-C(19)-H(19)	109.4
C(20)-C(19)-H(19)	109.4
C(14)-C(19)-H(19)	109.4
C(15)-C(20)-C(19)	109.59(14)
C(15)-C(20)-H(20A)	109.8
C(19)-C(20)-H(20A)	109.8
C(15)-C(20)-H(20B)	109.8
C(19)-C(20)-H(20B)	109.8
H(20A)-C(20)-H(20B)	108.2
C(21)-O(1)-Mo(1)	139.66(9)
O(1)-C(21)-C(26)	120.58(13)
O(1)-C(21)-C(22)	119.62(13)
C(26)-C(21)-C(22)	119.64(13)

C(23)-C(22)-C(21)	118.97(13)
C(23)-C(22)-C(31)	118.27(13)
C(21)-C(22)-C(31)	122.21(12)
C(36)-C(31)-C(32)	119.46(13)
C(36)-C(31)-C(22)	122.22(13)
C(32)-C(31)-C(22)	118.19(13)
C(33)-C(32)-C(31)	118.97(14)
C(33)-C(32)-C(37)	119.58(14)
C(31)-C(32)-C(37)	121.40(13)
C(32)-C(37)-C(39)	113.21(13)
C(32)-C(37)-C(38)	110.85(13)
C(39)-C(37)-C(38)	110.11(14)
C(32)-C(37)-H(37)	107.5
C(39)-C(37)-H(37)	107.5
C(38)-C(37)-H(37)	107.5
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(34)-C(33)-C(32)	122.14(14)
C(34)-C(33)-H(33)	118.9
C(32)-C(33)-H(33)	118.9
C(33)-C(34)-C(35)	117.86(14)
C(33)-C(34)-C(40)	121.60(14)
C(35)-C(34)-C(40)	120.51(14)
C(34)-C(40)-C(41)	111.16(14)
C(34)-C(40)-C(42)	112.04(14)
C(41)-C(40)-C(42)	109.62(15)

C(34)-C(40)-H(40)	108.0
C(41)-C(40)-H(40)	108.0
C(42)-C(40)-H(40)	108.0
C(40)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(40)-C(42)-H(42A)	109.5
C(40)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(40)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(34)-C(35)-C(36)	122.25(15)
C(34)-C(35)-H(35)	118.9
C(36)-C(35)-H(35)	118.9
C(35)-C(36)-C(31)	119.27(14)
C(35)-C(36)-C(43)	119.37(14)
C(31)-C(36)-C(43)	121.25(13)
C(36)-C(43)-C(44)	109.20(13)
C(36)-C(43)-C(45)	112.97(13)
C(44)-C(43)-C(45)	109.36(13)
C(36)-C(43)-H(43)	108.4
C(44)-C(43)-H(43)	108.4
C(45)-C(43)-H(43)	108.4
C(43)-C(44)-H(44A)	109.5
C(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(43)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(43)-C(45)-H(45A)	109.5
C(43)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5

C(43)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(24)-C(23)-C(22)	121.25(14)
C(24)-C(23)-H(23)	119.4
C(22)-C(23)-H(23)	119.4
C(25)-C(24)-C(23)	119.08(14)
C(25)-C(24)-H(24)	120.5
C(23)-C(24)-H(24)	120.5
C(24)-C(25)-C(26)	121.85(14)
C(24)-C(25)-H(25)	119.1
C(26)-C(25)-H(25)	119.1
C(25)-C(26)-C(21)	118.23(13)
C(25)-C(26)-C(51)	116.10(13)
C(21)-C(26)-C(51)	125.29(12)
C(56)-C(51)-C(52)	118.99(13)
C(56)-C(51)-C(26)	121.18(13)
C(52)-C(51)-C(26)	119.02(13)
C(53)-C(52)-C(51)	119.32(14)
C(53)-C(52)-C(57)	119.24(13)
C(51)-C(52)-C(57)	121.30(13)
C(52)-C(57)-C(58)	113.60(13)
C(52)-C(57)-C(59)	110.57(13)
C(58)-C(57)-C(59)	109.77(13)
C(52)-C(57)-H(57)	107.6
C(58)-C(57)-H(57)	107.6
C(59)-C(57)-H(57)	107.6
C(57)-C(58)-H(58A)	109.5
C(57)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
C(57)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5
C(57)-C(59)-H(59A)	109.5
C(57)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	109.5

C(57)-C(59)-H(59C)	109.5
H(59A)-C(59)-H(59C)	109.5
H(59B)-C(59)-H(59C)	109.5
C(54)-C(53)-C(52)	122.38(14)
C(54)-C(53)-H(53)	118.8
C(52)-C(53)-H(53)	118.8
C(55)-C(54)-C(53)	117.32(14)
C(55)-C(54)-C(60)	120.03(15)
C(53)-C(54)-C(60)	122.64(15)
C(61A)-C(60)-C(62A)	111.9(8)
C(61A)-C(60)-C(62)	96.9(8)
C(61A)-C(60)-C(54)	115.4(6)
C(62A)-C(60)-C(54)	111.8(6)
C(62)-C(60)-C(54)	111.0(5)
C(62A)-C(60)-C(61)	119.8(8)
C(62)-C(60)-C(61)	105.4(8)
C(54)-C(60)-C(61)	112.6(4)
C(61A)-C(60)-H(60A)	114.4
C(62A)-C(60)-H(60A)	91.7
C(62)-C(60)-H(60A)	109.3
C(54)-C(60)-H(60A)	109.3
C(61)-C(60)-H(60A)	109.3
C(61A)-C(60)-H(60B)	105.6
C(62A)-C(60)-H(60B)	105.6
C(62)-C(60)-H(60B)	122.6
C(54)-C(60)-H(60B)	105.6
C(61)-C(60)-H(60B)	99.2
C(60)-C(61)-H(61A)	109.5
C(60)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
C(60)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
C(60)-C(62)-H(62A)	109.5
C(60)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5

C(60)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(60)-C(61A)-H(61D)	109.5
C(60)-C(61A)-H(61E)	109.5
H(61D)-C(61A)-H(61E)	109.5
C(60)-C(61A)-H(61F)	109.5
H(61D)-C(61A)-H(61F)	109.5
H(61E)-C(61A)-H(61F)	109.5
C(60)-C(62A)-H(62D)	109.5
C(60)-C(62A)-H(62E)	109.5
H(62D)-C(62A)-H(62E)	109.5
C(60)-C(62A)-H(62F)	109.5
H(62D)-C(62A)-H(62F)	109.5
H(62E)-C(62A)-H(62F)	109.5
C(54)-C(55)-C(56)	122.56(15)
C(54)-C(55)-H(55)	118.7
C(56)-C(55)-H(55)	118.7
C(55)-C(56)-C(51)	119.39(14)
C(55)-C(56)-C(63)	119.14(14)
C(51)-C(56)-C(63)	121.42(13)
C(56)-C(63)-C(64)	112.47(13)
C(56)-C(63)-C(65)	110.93(13)
C(64)-C(63)-C(65)	109.88(14)
C(56)-C(63)-H(63)	107.8
C(64)-C(63)-H(63)	107.8
C(65)-C(63)-H(63)	107.8
C(63)-C(64)-H(64A)	109.5
C(63)-C(64)-H(64B)	109.5
H(64A)-C(64)-H(64B)	109.5
C(63)-C(64)-H(64C)	109.5
H(64A)-C(64)-H(64C)	109.5
H(64B)-C(64)-H(64C)	109.5
C(63)-C(65)-H(65A)	109.5
C(63)-C(65)-H(65B)	109.5
H(65A)-C(65)-H(65B)	109.5

C(63)-C(65)-H(65C)	109.5
H(65A)-C(65)-H(65C)	109.5
H(65B)-C(65)-H(65C)	109.5
C(68)-P(1)-C(66)	104.99(9)
C(68)-P(1)-C(67)	102.92(9)
C(66)-P(1)-C(67)	103.06(9)
C(68)-P(1)-Mo(1)	112.69(6)
C(66)-P(1)-Mo(1)	110.47(6)
C(67)-P(1)-Mo(1)	121.16(6)
P(1)-C(66)-H(66A)	109.5
P(1)-C(66)-H(66B)	109.5
H(66A)-C(66)-H(66B)	109.5
P(1)-C(66)-H(66C)	109.5
H(66A)-C(66)-H(66C)	109.5
H(66B)-C(66)-H(66C)	109.5
P(1)-C(67)-H(67A)	109.5
P(1)-C(67)-H(67B)	109.5
H(67A)-C(67)-H(67B)	109.5
P(1)-C(67)-H(67C)	109.5
H(67A)-C(67)-H(67C)	109.5
H(67B)-C(67)-H(67C)	109.5
P(1)-C(68)-H(68A)	109.5
P(1)-C(68)-H(68B)	109.5
H(68A)-C(68)-H(68B)	109.5
P(1)-C(68)-H(68C)	109.5
H(68A)-C(68)-H(68C)	109.5
H(68B)-C(68)-H(68C)	109.5
S(1)-O(2)-Mo(1)	132.93(7)
O(4)-S(1)-O(3)	118.19(8)
O(4)-S(1)-O(2)	113.70(8)
O(3)-S(1)-O(2)	112.87(7)
O(4)-S(1)-C(69)	104.57(8)
O(3)-S(1)-C(69)	103.25(8)
O(2)-S(1)-C(69)	101.75(7)
F(3)-C(69)-F(2)	108.04(15)
F(3)-C(69)-F(1)	108.31(15)

F(2)-C(69)-F(1)	106.95(13)
F(3)-C(69)-S(1)	111.92(11)
F(2)-C(69)-S(1)	112.64(12)
F(1)-C(69)-S(1)	108.78(13)

Symmetry transformations used to generate equivalent atoms:

Table S5D. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3**(PMe_3). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	11(1)	12(1)	12(1)	1(1)	3(1)	0(1)
C(1)	16(1)	17(1)	15(1)	2(1)	4(1)	1(1)
C(2)	18(1)	14(1)	22(1)	1(1)	8(1)	2(1)
C(3)	26(1)	20(1)	26(1)	-2(1)	7(1)	1(1)
C(4)	22(1)	21(1)	25(1)	2(1)	11(1)	-2(1)
C(5)	19(1)	15(1)	25(1)	3(1)	8(1)	5(1)
C(6)	23(1)	20(1)	30(1)	6(1)	12(1)	4(1)
C(7)	30(1)	27(1)	38(1)	14(1)	17(1)	9(1)
C(8)	31(1)	39(1)	37(1)	20(1)	11(1)	16(1)
C(9)	21(1)	42(1)	42(1)	16(1)	4(1)	9(1)
C(10)	19(1)	24(1)	35(1)	8(1)	8(1)	4(1)
N(1)	13(1)	16(1)	15(1)	2(1)	2(1)	0(1)
C(11)	15(1)	14(1)	14(1)	2(1)	4(1)	-2(1)
C(12)	25(1)	20(1)	15(1)	-1(1)	5(1)	-6(1)
C(13)	14(1)	19(1)	27(1)	5(1)	4(1)	-1(1)
C(14)	23(1)	15(1)	17(1)	-1(1)	7(1)	0(1)
C(15)	35(1)	22(1)	13(1)	1(1)	7(1)	-8(1)
C(16)	33(1)	20(1)	26(1)	-5(1)	18(1)	-9(1)
C(17)	18(1)	22(1)	30(1)	1(1)	7(1)	-6(1)
C(18)	28(1)	22(1)	21(1)	-2(1)	7(1)	-11(1)
C(19)	32(1)	12(1)	21(1)	-2(1)	10(1)	-2(1)
C(20)	39(1)	16(1)	23(1)	6(1)	8(1)	-2(1)
O(1)	10(1)	14(1)	16(1)	0(1)	3(1)	0(1)
C(21)	12(1)	12(1)	10(1)	2(1)	1(1)	0(1)
C(22)	13(1)	11(1)	13(1)	0(1)	2(1)	0(1)
C(31)	12(1)	13(1)	14(1)	-2(1)	3(1)	0(1)
C(32)	16(1)	14(1)	15(1)	0(1)	4(1)	0(1)
C(37)	23(1)	15(1)	15(1)	0(1)	5(1)	-2(1)
C(38)	26(1)	26(1)	27(1)	4(1)	10(1)	-3(1)
C(39)	29(1)	18(1)	20(1)	4(1)	4(1)	1(1)
C(33)	21(1)	18(1)	13(1)	-1(1)	3(1)	0(1)

C(34)	19(1)	16(1)	16(1)	-5(1)	2(1)	0(1)
C(40)	29(1)	18(1)	17(1)	-5(1)	2(1)	-4(1)
C(41)	28(1)	24(1)	33(1)	-5(1)	-4(1)	-6(1)
C(42)	41(1)	23(1)	33(1)	-15(1)	2(1)	3(1)
C(35)	19(1)	13(1)	17(1)	-2(1)	2(1)	-1(1)
C(36)	15(1)	12(1)	15(1)	-1(1)	3(1)	0(1)
C(43)	19(1)	14(1)	15(1)	0(1)	2(1)	0(1)
C(44)	20(1)	22(1)	24(1)	6(1)	0(1)	0(1)
C(45)	22(1)	24(1)	19(1)	1(1)	5(1)	-3(1)
C(23)	14(1)	14(1)	20(1)	0(1)	3(1)	1(1)
C(24)	12(1)	15(1)	24(1)	0(1)	1(1)	0(1)
C(25)	14(1)	13(1)	19(1)	0(1)	0(1)	-3(1)
C(26)	13(1)	11(1)	13(1)	2(1)	2(1)	0(1)
C(51)	12(1)	11(1)	16(1)	0(1)	2(1)	-1(1)
C(52)	14(1)	13(1)	15(1)	0(1)	2(1)	0(1)
C(57)	19(1)	12(1)	15(1)	2(1)	3(1)	0(1)
C(58)	26(1)	18(1)	16(1)	3(1)	1(1)	4(1)
C(59)	23(1)	21(1)	22(1)	3(1)	9(1)	1(1)
C(53)	21(1)	13(1)	18(1)	3(1)	2(1)	1(1)
C(54)	24(1)	12(1)	21(1)	-1(1)	4(1)	1(1)
C(60)	43(1)	13(1)	24(1)	-2(1)	6(1)	6(1)
C(61)	46(4)	9(3)	38(3)	0(2)	16(2)	-4(2)
C(62)	67(4)	21(3)	141(12)	-11(5)	72(6)	-5(3)
C(61A)	168(12)	22(5)	64(7)	11(4)	65(7)	27(6)
C(62A)	98(7)	26(4)	94(9)	3(4)	69(7)	23(5)
C(55)	24(1)	14(1)	16(1)	-2(1)	3(1)	0(1)
C(56)	16(1)	13(1)	15(1)	0(1)	2(1)	-2(1)
C(63)	22(1)	13(1)	15(1)	0(1)	0(1)	-1(1)
C(64)	30(1)	22(1)	17(1)	3(1)	6(1)	3(1)
C(65)	26(1)	24(1)	21(1)	3(1)	-4(1)	-4(1)
P(1)	12(1)	19(1)	13(1)	1(1)	2(1)	0(1)
C(66)	24(1)	25(1)	19(1)	-4(1)	1(1)	2(1)
C(67)	14(1)	42(1)	21(1)	0(1)	2(1)	1(1)
C(68)	27(1)	28(1)	18(1)	6(1)	2(1)	-3(1)
O(2)	16(1)	23(1)	16(1)	4(1)	0(1)	-1(1)
S(1)	19(1)	15(1)	16(1)	1(1)	0(1)	0(1)

O(3)	27(1)	16(1)	33(1)	0(1)	-2(1)	-2(1)
O(4)	35(1)	28(1)	19(1)	-2(1)	7(1)	0(1)
C(69)	23(1)	17(1)	23(1)	-1(1)	-6(1)	1(1)
F(1)	37(1)	24(1)	51(1)	15(1)	-19(1)	-1(1)
F(2)	25(1)	18(1)	32(1)	1(1)	-6(1)	-2(1)
F(3)	21(1)	66(1)	41(1)	-27(1)	-2(1)	8(1)

Table S5E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3**(PMe_3).

	x	y	z	U(eq)
H(1)	9340(14)	3128(8)	8542(9)	18
H(3A)	8711	3497	9851	36
H(3B)	7838	3993	9558	36
H(3C)	9026	3926	9304	36
H(4A)	6604	2669	8852	33
H(4B)	6374	3198	9309	33
H(4C)	7329	2730	9573	33
H(6)	8786	4079	8214	28
H(7)	8090	4571	7252	36
H(8)	6224	4426	6722	42
H(9)	5034	3814	7192	42
H(10)	5709	3329	8167	31
H(12A)	8708	1182	10063	24
H(12B)	7711	1638	10106	24
H(13A)	6167	1799	9152	24
H(13B)	6151	1456	8478	24
H(14A)	8702	616	9010	22
H(14B)	7721	726	8390	22
H(15)	7351	758	10649	28
H(16A)	5718	1286	10143	30
H(16B)	5441	609	10113	30
H(17)	4798	1037	9065	27
H(18A)	5702	389	8423	28
H(18B)	5426	61	9060	28
H(19)	7335	-146	8926	26
H(20A)	6994	-108	10028	31
H(20B)	8261	112	10003	31
H(37)	11931	2406	6797	21
H(38A)	12867	1775	5827	39
H(38B)	13532	1937	6541	39

H(38C)	13169	2433	6010	39
H(39A)	10826	2154	5493	34
H(39B)	11181	2782	5773	34
H(39C)	10195	2434	6039	34
H(33)	10786	1230	5770	21
H(40)	9965	327	5488	26
H(41A)	8728	-101	6456	45
H(41B)	8342	-154	5679	45
H(41C)	8365	463	6026	45
H(42A)	11355	-363	5889	49
H(42B)	10161	-682	5671	49
H(42C)	10631	-568	6431	49
H(35)	10586	114	7237	20
H(43)	11621	1049	8549	19
H(44A)	12791	80	8116	33
H(44B)	12985	310	8855	33
H(44C)	13348	701	8288	33
H(45A)	9966	412	8316	32
H(45B)	10864	238	8952	32
H(45C)	10836	-108	8280	32
H(23)	13801	1570	7776	19
H(24)	14803	2320	8370	21
H(25)	13813	3119	8659	19
H(57)	11084	3126	7210	18
H(58A)	9645	3852	6877	30
H(58B)	10308	3657	6303	30
H(58C)	10618	4255	6676	30
H(59A)	12686	4022	7081	32
H(59B)	12431	3489	6586	32
H(59C)	13009	3381	7332	32
H(53)	10728	4557	7684	21
H(60A)	11254	5297	9223	32
H(60B)	11401	5303	9152	32
H(61A)	11738	5555	8190	45
H(61B)	10736	5962	8349	45
H(61C)	10454	5441	7840	45

H(62A)	9347	4971	9215	105
H(62B)	9042	5135	8455	105
H(62C)	9378	5630	8990	105
H(61D)	11437	5510	8055	120
H(61E)	10703	5962	8393	120
H(61F)	10077	5478	7910	120
H(62D)	9777	4960	9487	100
H(62E)	9053	5106	8782	100
H(62F)	9631	5615	9244	100
H(55)	11423	4305	9636	22
H(63)	12226	2823	9559	20
H(64A)	11266	3611	10380	34
H(64B)	11612	2957	10564	34
H(64C)	10575	3093	9986	34
H(65A)	13870	3398	9744	37
H(65B)	13588	3190	10436	37
H(65C)	13286	3834	10186	37
H(66A)	7982	1481	6595	34
H(66B)	8226	1140	7276	34
H(66C)	9238	1473	7016	34
H(67A)	6297	2444	7592	39
H(67B)	6294	1759	7508	39
H(67C)	6252	2166	6881	39
H(68A)	9232	2746	6973	37
H(68B)	8119	3076	7113	37
H(68C)	8038	2646	6502	37

Table S6A. Crystal data and structure refinement for **4**.

Identification code	X8_11002	
Empirical formula	C61 H79 Mo N3 O	
Formula weight	966.21	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 22.5368(13) Å	α= 90°
	b = 12.3855(7) Å	β= 106.3860(10)°
	c = 19.7104(12) Å	γ = 90°
Volume	5278.3(5) $Å^3$	
Z	4	
Density (calculated)	1.216 Mg/m^3	
Absorption coefficient	0.291 mm^{-1}	
F(000)	2064	
Crystal size	0.10 x 0.10 x 0.05 mm^3	
Theta range for data collection	1.88 to 29.13°	
Index ranges	-30<=h<=30, -16<=k<=16, -26<=l<=26	
Reflections collected	118187	
Independent reflections	14184 [R(int) = 0.0849]	
Completeness to theta = 29.13°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9856 and 0.9715	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14184 / 191 / 646	
Goodness-of-fit on F^2	1.127	
Final R indices [I>2sigma(I)]	R1 = 0.0622, wR2 = 0.1539	
R indices (all data)	R1 = 0.0817, wR2 = 0.1634	
Largest diff. peak and hole	0.750 and -0.726 e.$Å^{-3}$	

Table S6B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	7258(1)	870(1)	8623(1)	23(1)
Mo(1A)	7411(5)	559(9)	8508(2)	53(2)
C(1)	7367(2)	2105(3)	9203(2)	37(1)
C(2)	7728(2)	3154(3)	9363(2)	40(1)
C(3)	7411(2)	3897(3)	9794(3)	56(1)
C(4)	7694(2)	3698(4)	8659(2)	64(1)
C(5)	8398(2)	2977(3)	9802(2)	41(1)
C(6)	8616(2)	2009(3)	10111(2)	50(1)
C(7)	9219(2)	1894(4)	10538(2)	60(1)
C(8)	9612(2)	2754(5)	10646(3)	69(1)
C(9)	9409(2)	3715(5)	10329(3)	70(1)
C(10)	8808(2)	3855(4)	9914(3)	58(1)
N(1)	7893(1)	914(3)	8309(2)	42(1)
C(11)	8430(2)	779(4)	8042(2)	49(1)
C(12)	8486(2)	-394(4)	7837(3)	56(1)
C(13)	8352(2)	1500(4)	7387(2)	55(1)
C(14)	9012(2)	1145(6)	8619(3)	82(2)
C(15)	9048(2)	-530(5)	7559(3)	75(2)
C(16)	8970(3)	184(5)	6911(3)	77(2)
C(17)	8913(3)	1344(5)	7100(3)	76(2)
C(18)	9501(3)	1704(7)	7673(4)	106(2)
C(19)	9572(3)	1001(7)	8311(4)	97(2)
C(20)	9629(3)	-173(8)	8130(4)	108(3)
N(2)	6563(1)	1480(2)	7802(1)	31(1)
C(21)	6112(2)	2188(3)	7872(2)	38(1)
C(22)	5630(2)	2215(3)	7259(2)	44(1)
C(23)	5781(2)	1536(3)	6781(2)	43(1)
C(24)	6349(2)	1095(3)	7112(2)	35(1)
C(25)	6703(2)	403(3)	6803(2)	42(1)
N(3)	6984(2)	-142(3)	6537(2)	63(1)
O(1)	7060(1)	-398(2)	9063(1)	27(1)

C(31)	6955(1)	-1105(2)	9545(1)	23(1)
C(32)	6587(1)	-781(2)	9975(1)	25(1)
C(41)	6302(1)	318(2)	9907(1)	26(1)
C(42)	5781(1)	545(2)	9338(1)	24(1)
C(47)	5444(1)	-347(2)	8851(1)	28(1)
C(48)	4905(6)	-702(9)	9100(6)	59(3)
C(49)	5227(6)	-12(7)	8073(3)	45(2)
C(48A)	4772(5)	-433(16)	8908(10)	43(4)
C(49A)	5419(8)	-226(14)	8094(6)	30(3)
C(43)	5532(1)	1588(2)	9272(2)	27(1)
C(44)	5772(2)	2393(2)	9759(2)	29(1)
C(50)	5476(2)	3508(2)	9684(2)	33(1)
C(51)	5474(2)	4049(3)	8990(2)	44(1)
C(52)	4815(2)	3453(3)	9741(2)	43(1)
C(45)	6274(2)	2136(2)	10333(2)	30(1)
C(46)	6541(2)	1113(2)	10422(2)	31(1)
C(53)	7065(2)	858(3)	11078(2)	42(1)
C(54)	6818(4)	706(8)	11706(3)	54(2)
C(55)	7551(3)	1734(6)	11231(4)	56(2)
C(54A)	6979(6)	1281(14)	11762(5)	58(3)
C(55A)	7682(4)	1076(16)	11002(6)	73(5)
C(33)	6479(2)	-1529(3)	10455(2)	30(1)
C(34)	6735(2)	-2553(2)	10518(2)	31(1)
C(35)	7089(1)	-2854(2)	10084(2)	28(1)
C(36)	7203(1)	-2151(2)	9588(1)	24(1)
C(61)	7573(1)	-2518(2)	9106(2)	27(1)
C(62)	7271(1)	-2806(2)	8400(2)	28(1)
C(67)	6570(1)	-2767(3)	8131(2)	30(1)
C(68)	6321(2)	-2485(3)	7346(2)	44(1)
C(69)	6290(2)	-3808(3)	8293(2)	48(1)
C(63)	7626(2)	-3159(3)	7973(2)	37(1)
C(64)	8261(2)	-3255(4)	8219(2)	46(1)
C(70)	8666(2)	-3640(4)	7756(2)	60(1)
C(71)	8375(2)	-3472(6)	6979(3)	82(2)
C(72)	8874(3)	-4791(4)	7937(3)	85(2)
C(65)	8544(2)	-2996(4)	8925(2)	46(1)

C(66)	8217(2)	-2618(3)	9371(2)	37(1)
C(73)	8555(2)	-2259(3)	10118(2)	39(1)
C(74)	9064(2)	-3022(4)	10499(2)	68(1)
C(75)	8796(3)	-1126(4)	10107(2)	81(2)

Table S6C. Bond lengths [Å] and angles [°] for **4**.

Mo(1)-N(1)	1.714(3)
Mo(1)-C(1)	1.883(4)
Mo(1)-O(1)	1.906(2)
Mo(1)-N(2)	2.053(3)
C(1)-C(2)	1.518(5)
C(1)-H(1)	0.977(18)
C(2)-C(4)	1.525(5)
C(2)-C(5)	1.529(5)
C(2)-C(3)	1.556(6)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-C(6)	1.372(6)
C(5)-C(10)	1.403(5)
C(6)-C(7)	1.388(6)
C(6)-H(6)	0.9500
C(7)-C(8)	1.364(7)
C(7)-H(7)	0.9500
C(8)-C(9)	1.362(8)
C(8)-H(8)	0.9500
C(9)-C(10)	1.381(7)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
N(1)-C(11)	1.458(5)
C(11)-C(12)	1.523(6)
C(11)-C(13)	1.538(5)
C(11)-C(14)	1.543(6)
C(12)-C(15)	1.525(6)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(17)	1.535(6)

C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(19)	1.556(7)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.523(7)
C(15)-C(20)	1.531(9)
C(15)-H(15)	1.0000
C(16)-C(17)	1.499(8)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.546(9)
C(17)-H(17)	1.0000
C(18)-C(19)	1.500(10)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.512(10)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
N(2)-C(21)	1.380(4)
N(2)-C(24)	1.393(4)
C(21)-C(22)	1.378(5)
C(21)-H(21)	0.9500
C(22)-C(23)	1.376(6)
C(22)-H(22)	0.9500
C(23)-C(24)	1.374(5)
C(23)-H(23)	0.9500
C(24)-C(25)	1.419(5)
C(25)-N(3)	1.149(5)
O(1)-C(31)	1.361(3)
C(31)-C(32)	1.402(4)
C(31)-C(36)	1.404(4)
C(32)-C(33)	1.395(4)
C(32)-C(41)	1.495(4)
C(41)-C(42)	1.405(4)

C(41)-C(46)	1.407(4)
C(42)-C(43)	1.400(4)
C(42)-C(47)	1.519(4)
C(47)-C(49A)	1.485(10)
C(47)-C(48)	1.498(6)
C(47)-C(49)	1.531(6)
C(47)-C(48A)	1.555(11)
C(47)-H(47A)	1.0000
C(47)-H(47B)	1.0000
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(48A)-H(48D)	0.9800
C(48A)-H(48E)	0.9800
C(48A)-H(48F)	0.9800
C(49A)-H(49D)	0.9800
C(49A)-H(49E)	0.9800
C(49A)-H(49F)	0.9800
C(43)-C(44)	1.383(4)
C(43)-H(43)	0.9500
C(44)-C(45)	1.392(4)
C(44)-C(50)	1.523(4)
C(50)-C(51)	1.522(4)
C(50)-C(52)	1.528(5)
C(50)-H(50)	1.0000
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(45)-C(46)	1.392(4)
C(45)-H(45)	0.9500

C(46)-C(53)	1.517(4)
C(53)-C(55A)	1.465(9)
C(53)-C(54)	1.506(7)
C(53)-C(54A)	1.510(9)
C(53)-C(55)	1.511(7)
C(53)-H(53A)	1.0000
C(53)-H(53B)	1.0000
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(55)-H(55A)	0.9800
C(55)-H(55B)	0.9800
C(55)-H(55C)	0.9800
C(54A)-H(54D)	0.9800
C(54A)-H(54E)	0.9800
C(54A)-H(54F)	0.9800
C(55A)-H(55D)	0.9800
C(55A)-H(55E)	0.9800
C(55A)-H(55F)	0.9800
C(33)-C(34)	1.384(4)
C(33)-H(33)	0.9500
C(34)-C(35)	1.376(4)
C(34)-H(34)	0.9500
C(35)-C(36)	1.387(4)
C(35)-H(35)	0.9500
C(36)-C(61)	1.501(4)
C(61)-C(66)	1.402(4)
C(61)-C(62)	1.410(4)
C(62)-C(63)	1.387(4)
C(62)-C(67)	1.519(4)
C(67)-C(69)	1.509(5)
C(67)-C(68)	1.531(4)
C(67)-H(67)	1.0000
C(68)-H(68A)	0.9800
C(68)-H(68B)	0.9800
C(68)-H(68C)	0.9800

C(69)-H(69A)	0.9800
C(69)-H(69B)	0.9800
C(69)-H(69C)	0.9800
C(63)-C(64)	1.381(5)
C(63)-H(63)	0.9500
C(64)-C(65)	1.395(5)
C(64)-C(70)	1.536(5)
C(70)-C(71)	1.501(7)
C(70)-C(72)	1.512(8)
C(70)-H(70)	1.0000
C(71)-H(71A)	0.9800
C(71)-H(71B)	0.9800
C(71)-H(71C)	0.9800
C(72)-H(72A)	0.9800
C(72)-H(72B)	0.9800
C(72)-H(72C)	0.9800
C(65)-C(66)	1.379(5)
C(65)-H(65)	0.9500
C(66)-C(73)	1.520(4)
C(73)-C(75)	1.507(6)
C(73)-C(74)	1.514(6)
C(73)-H(73)	1.0000
C(74)-H(74A)	0.9800
C(74)-H(74B)	0.9800
C(74)-H(74C)	0.9800
C(75)-H(75A)	0.9800
C(75)-H(75B)	0.9800
C(75)-H(75C)	0.9800

N(1)-Mo(1)-C(1)	102.32(16)
N(1)-Mo(1)-O(1)	121.14(13)
C(1)-Mo(1)-O(1)	113.63(13)
N(1)-Mo(1)-N(2)	103.42(13)
C(1)-Mo(1)-N(2)	96.85(13)
O(1)-Mo(1)-N(2)	115.97(10)
C(2)-C(1)-Mo(1)	142.4(3)

C(2)-C(1)-H(1)	116(2)
Mo(1)-C(1)-H(1)	101(2)
C(1)-C(2)-C(4)	107.6(3)
C(1)-C(2)-C(5)	112.4(3)
C(4)-C(2)-C(5)	111.5(3)
C(1)-C(2)-C(3)	108.6(3)
C(4)-C(2)-C(3)	108.8(4)
C(5)-C(2)-C(3)	107.9(3)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(6)-C(5)-C(10)	118.0(4)
C(6)-C(5)-C(2)	123.3(3)
C(10)-C(5)-C(2)	118.6(4)
C(5)-C(6)-C(7)	121.7(4)
C(5)-C(6)-H(6)	119.1
C(7)-C(6)-H(6)	119.1
C(8)-C(7)-C(6)	119.8(5)
C(8)-C(7)-H(7)	120.1
C(6)-C(7)-H(7)	120.1
C(9)-C(8)-C(7)	119.4(4)
C(9)-C(8)-H(8)	120.3
C(7)-C(8)-H(8)	120.3
C(8)-C(9)-C(10)	121.9(5)
C(8)-C(9)-H(9)	119.1
C(10)-C(9)-H(9)	119.1
C(9)-C(10)-C(5)	119.2(5)

C(9)-C(10)-H(10)	120.4
C(5)-C(10)-H(10)	120.4
C(11)-N(1)-Mo(1)	171.6(3)
N(1)-C(11)-C(12)	110.2(3)
N(1)-C(11)-C(13)	109.1(3)
C(12)-C(11)-C(13)	109.3(4)
N(1)-C(11)-C(14)	108.6(3)
C(12)-C(11)-C(14)	111.0(4)
C(13)-C(11)-C(14)	108.7(4)
C(11)-C(12)-C(15)	109.9(4)
C(11)-C(12)-H(12A)	109.7
C(15)-C(12)-H(12A)	109.7
C(11)-C(12)-H(12B)	109.7
C(15)-C(12)-H(12B)	109.7
H(12A)-C(12)-H(12B)	108.2
C(17)-C(13)-C(11)	109.0(4)
C(17)-C(13)-H(13A)	109.9
C(11)-C(13)-H(13A)	109.9
C(17)-C(13)-H(13B)	109.9
C(11)-C(13)-H(13B)	109.9
H(13A)-C(13)-H(13B)	108.3
C(11)-C(14)-C(19)	107.1(4)
C(11)-C(14)-H(14A)	110.3
C(19)-C(14)-H(14A)	110.3
C(11)-C(14)-H(14B)	110.3
C(19)-C(14)-H(14B)	110.3
H(14A)-C(14)-H(14B)	108.6
C(16)-C(15)-C(12)	109.1(4)
C(16)-C(15)-C(20)	108.7(5)
C(12)-C(15)-C(20)	109.1(5)
C(16)-C(15)-H(15)	110.0
C(12)-C(15)-H(15)	110.0
C(20)-C(15)-H(15)	110.0
C(17)-C(16)-C(15)	110.3(5)
C(17)-C(16)-H(16A)	109.6
C(15)-C(16)-H(16A)	109.6

C(17)-C(16)-H(16B)	109.6
C(15)-C(16)-H(16B)	109.6
H(16A)-C(16)-H(16B)	108.1
C(16)-C(17)-C(13)	110.5(4)
C(16)-C(17)-C(18)	109.9(5)
C(13)-C(17)-C(18)	108.6(5)
C(16)-C(17)-H(17)	109.3
C(13)-C(17)-H(17)	109.3
C(18)-C(17)-H(17)	109.3
C(19)-C(18)-C(17)	108.3(5)
C(19)-C(18)-H(18A)	110.0
C(17)-C(18)-H(18A)	110.0
C(19)-C(18)-H(18B)	110.0
C(17)-C(18)-H(18B)	110.0
H(18A)-C(18)-H(18B)	108.4
C(18)-C(19)-C(20)	110.8(6)
C(18)-C(19)-C(14)	110.7(6)
C(20)-C(19)-C(14)	109.5(5)
C(18)-C(19)-H(19)	108.6
C(20)-C(19)-H(19)	108.6
C(14)-C(19)-H(19)	108.6
C(19)-C(20)-C(15)	109.9(5)
C(19)-C(20)-H(20A)	109.7
C(15)-C(20)-H(20A)	109.7
C(19)-C(20)-H(20B)	109.7
C(15)-C(20)-H(20B)	109.7
H(20A)-C(20)-H(20B)	108.2
C(21)-N(2)-C(24)	104.7(3)
C(21)-N(2)-Mo(1)	125.1(2)
C(24)-N(2)-Mo(1)	128.4(2)
C(22)-C(21)-N(2)	110.4(3)
C(22)-C(21)-H(21)	124.8
N(2)-C(21)-H(21)	124.8
C(23)-C(22)-C(21)	107.4(3)
C(23)-C(22)-H(22)	126.3
C(21)-C(22)-H(22)	126.3

C(24)-C(23)-C(22)	107.2(3)
C(24)-C(23)-H(23)	126.4
C(22)-C(23)-H(23)	126.4
C(23)-C(24)-N(2)	110.3(3)
C(23)-C(24)-C(25)	126.7(3)
N(2)-C(24)-C(25)	122.9(3)
N(3)-C(25)-C(24)	178.2(4)
C(31)-O(1)-Mo(1)	163.00(19)
O(1)-C(31)-C(32)	119.2(2)
O(1)-C(31)-C(36)	119.4(2)
C(32)-C(31)-C(36)	121.4(2)
C(33)-C(32)-C(31)	117.8(3)
C(33)-C(32)-C(41)	120.8(3)
C(31)-C(32)-C(41)	121.3(2)
C(42)-C(41)-C(46)	120.0(3)
C(42)-C(41)-C(32)	119.6(2)
C(46)-C(41)-C(32)	120.3(3)
C(43)-C(42)-C(41)	118.8(3)
C(43)-C(42)-C(47)	119.8(3)
C(41)-C(42)-C(47)	121.0(2)
C(49A)-C(47)-C(48)	123.7(7)
C(49A)-C(47)-C(42)	115.6(7)
C(48)-C(47)-C(42)	108.2(3)
C(48)-C(47)-C(49)	110.4(5)
C(42)-C(47)-C(49)	113.4(3)
C(49A)-C(47)-C(48A)	108.6(8)
C(42)-C(47)-C(48A)	109.1(7)
C(49)-C(47)-C(48A)	92.8(7)
C(49A)-C(47)-H(47A)	107.8
C(48)-C(47)-H(47A)	89.8
C(42)-C(47)-H(47A)	107.8
C(49)-C(47)-H(47A)	124.1
C(48A)-C(47)-H(47A)	107.8
C(49A)-C(47)-H(47B)	90.3
C(48)-C(47)-H(47B)	108.2
C(42)-C(47)-H(47B)	108.2

C(49)-C(47)-H(47B)	108.2
C(48A)-C(47)-H(47B)	124.4
C(47)-C(48)-H(48A)	109.5
C(47)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(47)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(47)-C(49)-H(49A)	109.5
C(47)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(47)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(47)-C(48A)-H(48D)	109.5
C(47)-C(48A)-H(48E)	109.5
H(48D)-C(48A)-H(48E)	109.5
C(47)-C(48A)-H(48F)	109.5
H(48D)-C(48A)-H(48F)	109.5
H(48E)-C(48A)-H(48F)	109.5
C(47)-C(49A)-H(49D)	109.5
C(47)-C(49A)-H(49E)	109.5
H(49D)-C(49A)-H(49E)	109.5
C(47)-C(49A)-H(49F)	109.5
H(49D)-C(49A)-H(49F)	109.5
H(49E)-C(49A)-H(49F)	109.5
C(44)-C(43)-C(42)	122.1(3)
C(44)-C(43)-H(43)	118.9
C(42)-C(43)-H(43)	118.9
C(43)-C(44)-C(45)	117.9(3)
C(43)-C(44)-C(50)	120.7(3)
C(45)-C(44)-C(50)	121.3(3)
C(51)-C(50)-C(44)	112.2(3)
C(51)-C(50)-C(52)	109.4(3)
C(44)-C(50)-C(52)	111.2(3)
C(51)-C(50)-H(50)	108.0

C(44)-C(50)-H(50)	108.0
C(52)-C(50)-H(50)	108.0
C(50)-C(51)-H(51A)	109.5
C(50)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(50)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(50)-C(52)-H(52A)	109.5
C(50)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(50)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(46)-C(45)-C(44)	122.3(3)
C(46)-C(45)-H(45)	118.8
C(44)-C(45)-H(45)	118.8
C(45)-C(46)-C(41)	118.7(3)
C(45)-C(46)-C(53)	120.2(3)
C(41)-C(46)-C(53)	121.1(3)
C(55A)-C(53)-C(54)	133.5(6)
C(55A)-C(53)-C(54A)	113.0(7)
C(54)-C(53)-C(55)	109.9(5)
C(54A)-C(53)-C(55)	80.8(7)
C(55A)-C(53)-C(46)	114.1(5)
C(54)-C(53)-C(46)	110.3(4)
C(54A)-C(53)-C(46)	115.0(5)
C(55)-C(53)-C(46)	111.5(4)
C(55A)-C(53)-H(53A)	70.1
C(54)-C(53)-H(53A)	108.4
C(54A)-C(53)-H(53A)	128.3
C(55)-C(53)-H(53A)	108.4
C(46)-C(53)-H(53A)	108.4
C(55A)-C(53)-H(53B)	104.4
C(54)-C(53)-H(53B)	76.8
C(54A)-C(53)-H(53B)	104.4

C(55)-C(53)-H(53B)	137.4
C(46)-C(53)-H(53B)	104.4
C(53)-C(54)-H(54A)	109.5
C(53)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(53)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(53)-C(55)-H(55A)	109.5
C(53)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5
C(53)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
C(53)-C(54A)-H(54D)	109.5
C(53)-C(54A)-H(54E)	109.5
H(54D)-C(54A)-H(54E)	109.5
C(53)-C(54A)-H(54F)	109.5
H(54D)-C(54A)-H(54F)	109.5
H(54E)-C(54A)-H(54F)	109.5
C(53)-C(55A)-H(55D)	109.5
C(53)-C(55A)-H(55E)	109.5
H(55D)-C(55A)-H(55E)	109.5
C(53)-C(55A)-H(55F)	109.5
H(55D)-C(55A)-H(55F)	109.5
H(55E)-C(55A)-H(55F)	109.5
C(34)-C(33)-C(32)	121.4(3)
C(34)-C(33)-H(33)	119.3
C(32)-C(33)-H(33)	119.3
C(35)-C(34)-C(33)	119.5(3)
C(35)-C(34)-H(34)	120.2
C(33)-C(34)-H(34)	120.2
C(34)-C(35)-C(36)	121.6(3)
C(34)-C(35)-H(35)	119.2
C(36)-C(35)-H(35)	119.2
C(35)-C(36)-C(31)	118.2(3)

C(35)-C(36)-C(61)	120.2(3)
C(31)-C(36)-C(61)	121.6(2)
C(66)-C(61)-C(62)	120.4(3)
C(66)-C(61)-C(36)	119.5(3)
C(62)-C(61)-C(36)	120.0(3)
C(63)-C(62)-C(61)	118.5(3)
C(63)-C(62)-C(67)	121.3(3)
C(61)-C(62)-C(67)	120.2(3)
C(69)-C(67)-C(62)	110.8(3)
C(69)-C(67)-C(68)	110.7(3)
C(62)-C(67)-C(68)	114.2(3)
C(69)-C(67)-H(67)	106.9
C(62)-C(67)-H(67)	106.9
C(68)-C(67)-H(67)	106.9
C(67)-C(68)-H(68A)	109.5
C(67)-C(68)-H(68B)	109.5
H(68A)-C(68)-H(68B)	109.5
C(67)-C(68)-H(68C)	109.5
H(68A)-C(68)-H(68C)	109.5
H(68B)-C(68)-H(68C)	109.5
C(67)-C(69)-H(69A)	109.5
C(67)-C(69)-H(69B)	109.5
H(69A)-C(69)-H(69B)	109.5
C(67)-C(69)-H(69C)	109.5
H(69A)-C(69)-H(69C)	109.5
H(69B)-C(69)-H(69C)	109.5
C(64)-C(63)-C(62)	122.2(3)
C(64)-C(63)-H(63)	118.9
C(62)-C(63)-H(63)	118.9
C(63)-C(64)-C(65)	117.9(3)
C(63)-C(64)-C(70)	123.3(3)
C(65)-C(64)-C(70)	118.9(3)
C(71)-C(70)-C(72)	112.9(5)
C(71)-C(70)-C(64)	113.6(4)
C(72)-C(70)-C(64)	110.5(4)
C(71)-C(70)-H(70)	106.4

C(72)-C(70)-H(70)	106.4
C(64)-C(70)-H(70)	106.4
C(70)-C(71)-H(71A)	109.5
C(70)-C(71)-H(71B)	109.5
H(71A)-C(71)-H(71B)	109.5
C(70)-C(71)-H(71C)	109.5
H(71A)-C(71)-H(71C)	109.5
H(71B)-C(71)-H(71C)	109.5
C(70)-C(72)-H(72A)	109.5
C(70)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5
C(70)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5
H(72B)-C(72)-H(72C)	109.5
C(66)-C(65)-C(64)	122.5(3)
C(66)-C(65)-H(65)	118.7
C(64)-C(65)-H(65)	118.7
C(65)-C(66)-C(61)	118.4(3)
C(65)-C(66)-C(73)	120.3(3)
C(61)-C(66)-C(73)	121.2(3)
C(75)-C(73)-C(74)	111.3(4)
C(75)-C(73)-C(66)	110.1(3)
C(74)-C(73)-C(66)	113.6(3)
C(75)-C(73)-H(73)	107.2
C(74)-C(73)-H(73)	107.2
C(66)-C(73)-H(73)	107.2
C(73)-C(74)-H(74A)	109.5
C(73)-C(74)-H(74B)	109.5
H(74A)-C(74)-H(74B)	109.5
C(73)-C(74)-H(74C)	109.5
H(74A)-C(74)-H(74C)	109.5
H(74B)-C(74)-H(74C)	109.5
C(73)-C(75)-H(75A)	109.5
C(73)-C(75)-H(75B)	109.5
H(75A)-C(75)-H(75B)	109.5
C(73)-C(75)-H(75C)	109.5

H(75A)-C(75)-H(75C)	109.5
H(75B)-C(75)-H(75C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S6D. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	28(1)	24(1)	18(1)	1(1)	8(1)	-2(1)
Mo(1A)	84(3)	48(3)	32(1)	7(2)	28(2)	-31(3)
C(1)	42(2)	36(2)	29(2)	1(1)	5(1)	-6(1)
C(2)	49(2)	34(2)	36(2)	-1(1)	8(2)	-6(1)
C(3)	52(2)	38(2)	80(3)	-8(2)	19(2)	-4(2)
C(4)	86(3)	49(2)	48(2)	12(2)	3(2)	-26(2)
C(5)	42(2)	49(2)	35(2)	-8(2)	15(2)	-6(2)
C(6)	49(2)	50(2)	42(2)	-2(2)	1(2)	-5(2)
C(7)	54(3)	66(3)	55(2)	-10(2)	6(2)	2(2)
C(8)	42(2)	92(4)	68(3)	-19(3)	9(2)	-5(2)
C(9)	53(3)	75(3)	80(3)	-14(3)	16(2)	-21(2)
C(10)	57(3)	55(2)	66(3)	-16(2)	22(2)	-17(2)
N(1)	42(2)	47(2)	39(2)	4(1)	15(1)	-5(1)
C(11)	41(2)	64(3)	46(2)	9(2)	20(2)	-4(2)
C(12)	57(3)	56(2)	67(3)	11(2)	35(2)	14(2)
C(13)	69(3)	53(2)	54(2)	11(2)	34(2)	-2(2)
C(14)	43(2)	143(6)	62(3)	-1(3)	19(2)	-17(3)
C(15)	66(3)	89(4)	85(4)	15(3)	45(3)	17(3)
C(16)	74(3)	98(4)	78(3)	11(3)	53(3)	10(3)
C(17)	83(4)	83(4)	80(4)	12(3)	53(3)	-8(3)
C(18)	78(4)	145(6)	118(5)	-16(5)	68(4)	-39(4)
C(19)	45(3)	159(7)	96(5)	-7(5)	32(3)	-20(4)
C(20)	63(4)	176(8)	99(5)	28(5)	49(4)	38(4)
N(2)	44(2)	26(1)	23(1)	2(1)	9(1)	-5(1)
C(21)	51(2)	30(2)	38(2)	2(1)	20(2)	0(1)
C(22)	45(2)	40(2)	48(2)	16(2)	14(2)	3(2)
C(23)	47(2)	49(2)	30(2)	12(2)	5(2)	-2(2)
C(24)	50(2)	33(2)	23(1)	4(1)	9(1)	-6(1)
C(25)	58(2)	35(2)	34(2)	-7(1)	13(2)	-8(2)
N(3)	80(3)	54(2)	62(2)	-25(2)	30(2)	-11(2)
O(1)	34(1)	27(1)	20(1)	6(1)	9(1)	-3(1)

C(31)	29(1)	25(1)	15(1)	2(1)	6(1)	-2(1)
C(32)	35(1)	22(1)	18(1)	1(1)	8(1)	2(1)
C(41)	39(2)	23(1)	17(1)	1(1)	10(1)	4(1)
C(42)	37(2)	22(1)	16(1)	0(1)	10(1)	0(1)
C(47)	41(2)	23(1)	19(1)	-2(1)	8(1)	2(1)
C(48)	96(6)	48(5)	53(5)	-32(4)	53(5)	-42(4)
C(49)	67(6)	38(3)	20(2)	1(2)	-2(2)	-10(4)
C(43)	37(2)	26(1)	20(1)	0(1)	9(1)	4(1)
C(44)	41(2)	24(1)	24(1)	-1(1)	14(1)	1(1)
C(50)	46(2)	23(1)	34(2)	-4(1)	15(1)	3(1)
C(51)	56(2)	28(2)	48(2)	6(2)	17(2)	9(2)
C(52)	45(2)	33(2)	51(2)	-10(2)	16(2)	2(1)
C(45)	42(2)	26(1)	23(1)	-6(1)	9(1)	-2(1)
C(46)	41(2)	30(2)	20(1)	-1(1)	5(1)	4(1)
C(53)	51(2)	41(2)	28(1)	-7(1)	-1(1)	8(2)
C(54)	82(6)	52(5)	19(3)	5(3)	1(3)	24(4)
C(55)	55(4)	42(4)	55(4)	-8(3)	-14(3)	5(3)
C(54A)	64(7)	76(9)	24(4)	-5(5)	-1(4)	3(6)
C(55A)	58(5)	126(14)	30(5)	14(6)	3(4)	0(7)
C(33)	40(2)	33(2)	21(1)	5(1)	14(1)	7(1)
C(34)	42(2)	28(1)	25(1)	8(1)	16(1)	4(1)
C(35)	35(2)	24(1)	28(1)	3(1)	11(1)	5(1)
C(36)	28(1)	26(1)	20(1)	-2(1)	8(1)	-2(1)
C(61)	31(2)	31(1)	22(1)	-5(1)	10(1)	-3(1)
C(62)	33(2)	31(2)	20(1)	-4(1)	8(1)	-3(1)
C(67)	30(2)	38(2)	22(1)	-3(1)	9(1)	-2(1)
C(68)	43(2)	55(2)	30(2)	2(2)	4(1)	-1(2)
C(69)	42(2)	46(2)	50(2)	8(2)	1(2)	-12(2)
C(63)	38(2)	49(2)	26(2)	-12(1)	11(1)	-2(1)
C(64)	39(2)	67(3)	36(2)	-16(2)	19(2)	-6(2)
C(70)	51(2)	84(3)	52(2)	-23(2)	26(2)	-9(2)
C(71)	66(3)	144(5)	52(3)	-26(3)	40(2)	-14(3)
C(72)	115(5)	65(3)	108(4)	-24(3)	86(4)	-10(3)
C(65)	30(2)	72(3)	38(2)	-12(2)	13(1)	-3(2)
C(66)	33(2)	49(2)	29(2)	-9(1)	7(1)	-1(1)
C(73)	31(2)	59(2)	28(2)	-10(2)	7(1)	-3(2)

C(74)	86(3)	70(3)	35(2)	-6(2)	-3(2)	12(3)
C(75)	120(5)	64(3)	39(2)	-8(2)	-9(3)	-28(3)

Table S6E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4**.

	x	y	z	U(eq)
H(1)	7053(14)	1990(30)	9449(19)	44
H(3A)	6978	4012	9526	85
H(3B)	7626	4593	9879	85
H(3C)	7430	3554	10247	85
H(4A)	7942	3289	8412	97
H(4B)	7855	4436	8745	97
H(4C)	7263	3720	8367	97
H(6)	8348	1401	10032	60
H(7)	9357	1219	10754	72
H(8)	10024	2684	10940	82
H(9)	9688	4306	10395	84
H(10)	8674	4537	9708	70
H(12A)	8108	-613	7469	68
H(12B)	8530	-864	8255	68
H(13A)	7968	1304	7019	66
H(13B)	8322	2267	7516	66
H(14A)	9069	699	9050	98
H(14B)	8972	1910	8744	98
H(15)	9089	-1303	7431	90
H(16A)	9332	97	6724	92
H(16B)	8596	-38	6537	92
H(17)	8860	1802	6669	91
H(18A)	9867	1630	7495	127
H(18B)	9463	2470	7799	127
H(19)	9957	1220	8681	117
H(20A)	9682	-622	8558	129
H(20B)	9997	-272	7957	129
H(21)	6130	2600	8284	46
H(22)	5261	2626	7181	53
H(23)	5539	1398	6310	52

H(47A)	5659	-1043	9023	34
H(47B)	5733	-973	8895	34
H(48A)	4630	-86	9090	89
H(48B)	5055	-978	9584	89
H(48C)	4679	-1272	8788	89
H(49A)	4909	548	8010	67
H(49B)	5055	-640	7781	67
H(49C)	5579	271	7928	67
H(48D)	4561	262	8782	65
H(48E)	4781	-622	9394	65
H(48F)	4548	-992	8584	65
H(49D)	5181	-823	7822	45
H(49E)	5840	-235	8046	45
H(49F)	5220	461	7915	45
H(43)	5186	1749	8881	33
H(50)	5724	3969	10079	40
H(51A)	5900	4115	8962	65
H(51B)	5289	4769	8968	65
H(51C)	5233	3612	8593	65
H(52A)	4560	3022	9350	64
H(52B)	4645	4184	9720	64
H(52C)	4816	3116	10192	64
H(45)	6440	2677	10675	36
H(53A)	7264	167	10994	50
H(53B)	7051	55	11124	50
H(54A)	7164	635	12136	81
H(54B)	6564	51	11641	81
H(54C)	6566	1331	11750	81
H(55A)	7919	1482	11593	84
H(55B)	7387	2380	11402	84
H(55C)	7662	1909	10797	84
H(54D)	7204	819	12154	87
H(54E)	6538	1280	11734	87
H(54F)	7140	2020	11842	87
H(55D)	7985	1080	11470	110
H(55E)	7683	1781	10777	110

H(55F)	7792	513	10710	110
H(33)	6224	-1332	10745	36
H(34)	6667	-3044	10858	37
H(35)	7259	-3561	10125	34
H(67)	6429	-2183	8400	36
H(68A)	6415	-3074	7060	66
H(68B)	6516	-1818	7248	66
H(68C)	5872	-2383	7225	66
H(69A)	6413	-4402	8033	73
H(69B)	5838	-3745	8149	73
H(69C)	6436	-3953	8802	73
H(63)	7425	-3342	7495	45
H(70)	9048	-3185	7888	72
H(71A)	8005	-3923	6821	124
H(71B)	8671	-3672	6719	124
H(71C)	8260	-2711	6890	124
H(72A)	8515	-5272	7807	127
H(72B)	9076	-4848	8446	127
H(72C)	9167	-4998	7675	127
H(65)	8979	-3083	9105	55
H(73)	8243	-2240	10392	47
H(74A)	9413	-2962	10297	102
H(74B)	8908	-3765	10445	102
H(74C)	9201	-2835	11003	102
H(75A)	9113	-1118	9854	122
H(75B)	8977	-876	10593	122
H(75C)	8455	-647	9867	122

Table S7A. Crystal data and structure refinement for **5**.

Identification code	X8_10084_t5	
Empirical formula	C_{60} H_{85} Mo N O_2	
Formula weight	948.23	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 12.0586(14) Å	α = 89.536(3)°
	b = 13.0094(14) Å	β = 88.685(3)°
	c = 37.249(4) Å	γ = 64.701(3)°
Volume	5281.5(10) $Å^3$	
Z	4	
Density (calculated)	1.193 Mg/m^3	
Absorption coefficient	0.290 mm^{-1}	
F(000)	2040	
Crystal size	0.15 x 0.10 x 0.10 mm^3	
Theta range for data collection	1.64 to 30.60°	
Index ranges	-17<=h<=17, -18<=k<=18, 0<=l<=53	
Reflections collected	33165	
Independent reflections	33171 [R(int) = 0.0799]	
Completeness to theta = 30.60°	97.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9716 and 0.9578	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	33171 / 896 / 1306	
Goodness-of-fit on F^2	1.088	
Final R indices [I>2sigma(I)]	R1 = 0.0586, wR2 = 0.1311	
R indices (all data)	R1 = 0.0712, wR2 = 0.1366	
Largest diff. peak and hole	1.338 and -1.105 $e.Å^{-3}$	

Table S7B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	7710(1)	1483(1)	8624(1)	15(1)
C(1)	8520(3)	113(3)	8876(1)	18(1)
C(2)	9188(3)	-1175(3)	8846(1)	18(1)
C(3)	9362(3)	-1548(3)	8451(1)	24(1)
C(4)	10469(3)	-1566(3)	9007(1)	23(1)
C(5)	8473(3)	-1727(3)	9055(1)	18(1)
C(6)	7403(3)	-1099(3)	9254(1)	21(1)
C(7)	6759(4)	-1622(3)	9434(1)	25(1)
C(8)	7175(4)	-2789(3)	9417(1)	27(1)
C(9)	8237(4)	-3429(3)	9221(1)	30(1)
C(10)	8881(3)	-2905(3)	9044(1)	23(1)
N(1)	7775(3)	1049(3)	8188(1)	20(1)
C(11)	7750(3)	915(3)	7799(1)	19(1)
C(12)	7340(5)	2083(3)	7623(1)	34(1)
C(13)	9003(4)	101(4)	7646(1)	32(1)
C(14)	6807(4)	450(4)	7715(1)	34(1)
C(15)	7316(5)	1970(4)	7205(1)	39(1)
C(16)	8566(5)	1157(4)	7068(1)	41(1)
C(17)	8943(4)	-22(4)	7230(1)	35(1)
C(18)	7997(4)	-454(4)	7166(1)	37(1)
C(19)	6736(5)	341(4)	7300(1)	40(1)
C(20)	6356(4)	1520(4)	7135(1)	42(1)
O(1)	6067(2)	2274(2)	8829(1)	17(1)
C(21)	5258(3)	2237(3)	9081(1)	14(1)
C(22)	5395(3)	2425(3)	9449(1)	16(1)
C(31)	6421(3)	2660(3)	9586(1)	22(1)
C(32)	7219(3)	1945(4)	9845(1)	25(1)
C(37)	7192(4)	846(4)	9981(1)	28(1)
C(38)	8448(4)	-180(4)	9961(1)	37(1)
C(39)	6696(4)	991(4)	10373(1)	34(1)
C(33)	8092(4)	2233(4)	9998(1)	32(1)

C(34)	8171(4)	3237(5)	9915(1)	36(1)
C(40)	9100(5)	3531(5)	10107(1)	46(1)
C(41)	10036(5)	3620(5)	9864(2)	51(1)
C(42)	8427(4)	4510(4)	10370(1)	35(1)
C(35)	7370(4)	3944(4)	9656(1)	33(1)
C(36)	6481(4)	3690(4)	9494(1)	26(1)
C(43)	5560(4)	4571(3)	9250(1)	26(1)
C(44)	4685(4)	5578(4)	9482(1)	38(1)
C(45)	6161(4)	4973(4)	8951(1)	31(1)
C(23)	4498(3)	2428(3)	9693(1)	18(1)
C(24)	3500(3)	2254(3)	9588(1)	17(1)
C(25)	3364(3)	2102(3)	9225(1)	17(1)
C(26)	4218(3)	2106(3)	8968(1)	14(1)
C(51)	3964(3)	2029(3)	8579(1)	16(1)
C(52)	4070(3)	991(3)	8432(1)	18(1)
C(57)	4593(4)	-112(3)	8643(1)	21(1)
C(58)	3804(4)	-758(4)	8637(1)	36(1)
C(59)	5903(4)	-840(3)	8507(1)	31(1)
C(53)	3726(3)	977(3)	8076(1)	21(1)
C(54)	3254(3)	1951(3)	7863(1)	24(1)
C(60)	2860(4)	1880(4)	7481(1)	31(1)
C(61)	1738(4)	1629(5)	7486(1)	43(1)
C(62)	2618(5)	2935(5)	7252(1)	44(1)
C(55)	3159(3)	2957(3)	8013(1)	24(1)
C(56)	3502(3)	3014(3)	8367(1)	20(1)
C(63)	3355(4)	4153(3)	8511(1)	25(1)
C(64)	4136(5)	4613(4)	8290(1)	40(1)
C(65)	2010(4)	5004(4)	8528(1)	39(1)
O(2)	8610(2)	2342(2)	8685(1)	19(1)
C(71)	9798(3)	2259(3)	8768(1)	24(1)
C(72)	10297(4)	1483(4)	9090(1)	27(1)
C(73)	9633(4)	3452(4)	8857(1)	36(1)
C(74)	10610(4)	1792(5)	8436(1)	41(1)
Mo(2)	2482(1)	3475(1)	3624(1)	15(1)
C(101)	1614(3)	4863(3)	3870(1)	18(1)
C(102)	963(3)	6143(3)	3833(1)	17(1)

C(103)	-348(3)	6540(3)	3998(1)	23(1)
C(104)	844(3)	6498(3)	3437(1)	22(1)
C(105)	1664(3)	6696(3)	4035(1)	17(1)
C(106)	2729(3)	6070(3)	4223(1)	19(1)
C(107)	3339(3)	6591(3)	4407(1)	23(1)
C(108)	2902(4)	7767(3)	4399(1)	27(1)
C(109)	1853(4)	8404(3)	4210(1)	31(1)
C(110)	1238(3)	7879(3)	4032(1)	25(1)
N(2)	2522(3)	3897(3)	3186(1)	20(1)
C(111)	2591(3)	3971(3)	2799(1)	17(1)
C(112)	3510(5)	2800(4)	2663(1)	38(1)
C(113)	1337(4)	4273(4)	2644(1)	36(1)
C(114)	3073(4)	4835(4)	2686(1)	33(1)
C(115)	3614(5)	2836(4)	2247(1)	47(1)
C(116)	2346(5)	3129(4)	2094(1)	41(1)
C(117)	1439(4)	4291(4)	2223(1)	39(1)
C(118)	1886(5)	5196(4)	2122(1)	51(1)
C(119)	3162(5)	4860(5)	2272(1)	43(1)
C(120)	4050(5)	3709(5)	2139(1)	47(1)
O(3)	4084(2)	2692(2)	3834(1)	17(1)
C(121)	4862(3)	2742(3)	4081(1)	14(1)
C(122)	5901(3)	2892(3)	3963(1)	14(1)
C(131)	6191(3)	2974(3)	3571(1)	16(1)
C(132)	6077(3)	4012(3)	3423(1)	17(1)
C(137)	5534(3)	5113(3)	3638(1)	19(1)
C(138)	6462(4)	5605(4)	3689(1)	29(1)
C(139)	4398(4)	5985(3)	3455(1)	29(1)
C(133)	6463(3)	4024(3)	3067(1)	20(1)
C(134)	6967(3)	3052(3)	2852(1)	21(1)
C(140)	7418(3)	3133(3)	2472(1)	26(1)
C(141)	8599(4)	3287(4)	2479(1)	35(1)
C(142)	7592(4)	2126(4)	2233(1)	38(1)
C(135)	7066(3)	2041(3)	3007(1)	21(1)
C(136)	6686(3)	1980(3)	3358(1)	18(1)
C(143)	6849(3)	833(3)	3504(1)	25(1)
C(144)	6133(4)	341(4)	3286(2)	38(1)

C(145)	8203(4)	5(3)	3522(1)	34(1)
C(123)	6721(3)	2906(3)	4217(1)	19(1)
C(124)	6558(3)	2750(3)	4582(1)	20(1)
C(125)	5552(3)	2565(3)	4690(1)	20(1)
C(126)	4691(3)	2557(3)	4448(1)	18(1)
C(151)	3618(7)	2379(6)	4595(3)	13(1)
C(152)	2774(5)	3128(4)	4846(2)	12(1)
C(157)	2802(6)	4228(5)	4968(2)	18(1)
C(158)	3221(8)	4116(6)	5365(2)	21(1)
C(159)	1552(6)	5254(5)	4948(2)	20(1)
C(153)	1872(4)	2841(4)	5000(1)	13(1)
C(154)	1798(4)	1836(4)	4926(1)	14(1)
C(160)	857(4)	1533(4)	5120(1)	16(1)
C(161)	1488(9)	490(11)	5362(3)	28(2)
C(162)	-4(4)	1350(4)	4861(1)	18(1)
C(155)	2637(5)	1110(4)	4680(2)	15(1)
C(156)	3545(5)	1348(4)	4511(2)	14(1)
C(163)	4500(6)	443(5)	4272(2)	15(1)
C(164)	3934(8)	46(10)	3970(2)	22(2)
C(165)	5330(7)	-570(6)	4501(2)	23(1)
C(51A)	3760(20)	2124(16)	4561(8)	16(2)
C(52A)	2890(13)	2778(11)	4825(4)	15(2)
C(57A)	2841(15)	3902(11)	4955(5)	20(2)
C(58A)	3350(20)	3785(15)	5334(6)	27(4)
C(59A)	1565(15)	4868(12)	4950(6)	26(3)
C(53A)	2045(11)	2402(10)	4972(3)	13(1)
C(54A)	2069(10)	1377(9)	4866(3)	11(2)
C(60A)	1211(9)	924(9)	5045(3)	16(1)
C(61A)	1650(30)	450(30)	5420(6)	27(4)
C(62A)	-128(9)	1805(8)	5044(3)	15(2)
C(55A)	2936(12)	732(11)	4616(4)	15(2)
C(56A)	3795(13)	1075(11)	4456(4)	14(1)
C(63A)	4761(15)	240(13)	4206(5)	20(3)
C(64A)	4180(20)	-120(20)	3900(6)	21(4)
C(65A)	5611(18)	-818(15)	4418(5)	24(3)
O(4)	1568(2)	2614(2)	3680(1)	20(1)

C(171)	376(3)	2695(3)	3773(1)	18(1)
C(172)	-151(3)	3481(3)	4097(1)	24(1)
C(173)	-424(4)	3124(4)	3447(1)	30(1)
C(174)	553(4)	1487(3)	3870(1)	27(1)

Table S7C. Bond lengths [Å] and angles [°] for **5**.

Mo(1)-N(1)	1.713(3)
Mo(1)-O(2)	1.879(2)
Mo(1)-C(1)	1.880(3)
Mo(1)-O(1)	1.941(2)
C(1)-C(2)	1.521(5)
C(1)-H(1)	0.972(18)
C(2)-C(5)	1.533(5)
C(2)-C(3)	1.534(5)
C(2)-C(4)	1.540(5)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-C(10)	1.395(5)
C(5)-C(6)	1.396(5)
C(6)-C(7)	1.393(5)
C(6)-H(6)	0.9500
C(7)-C(8)	1.381(5)
C(7)-H(7)	0.9500
C(8)-C(9)	1.387(6)
C(8)-H(8)	0.9500
C(9)-C(10)	1.387(5)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
N(1)-C(11)	1.463(4)
C(11)-C(13)	1.528(5)
C(11)-C(12)	1.531(5)
C(11)-C(14)	1.537(5)
C(12)-C(15)	1.565(7)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(17)	1.565(6)

C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(19)	1.561(7)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(16)	1.505(7)
C(15)-C(20)	1.532(7)
C(15)-H(15)	1.0000
C(16)-C(17)	1.525(6)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.495(7)
C(17)-H(17)	1.0000
C(18)-C(19)	1.504(7)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.529(7)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
O(1)-C(21)	1.353(4)
C(21)-C(26)	1.409(5)
C(21)-C(22)	1.420(4)
C(22)-C(23)	1.396(5)
C(22)-C(31)	1.497(5)
C(31)-C(36)	1.411(5)
C(31)-C(32)	1.411(5)
C(32)-C(33)	1.393(5)
C(32)-C(37)	1.524(6)
C(37)-C(38)	1.533(6)
C(37)-C(39)	1.548(6)
C(37)-H(37)	1.0000
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800

C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(33)-C(34)	1.382(7)
C(33)-H(33)	0.9500
C(34)-C(35)	1.406(7)
C(34)-C(40)	1.523(6)
C(40)-C(41)	1.471(8)
C(40)-C(42)	1.531(7)
C(40)-H(40)	1.0000
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(35)-C(36)	1.399(5)
C(35)-H(35)	0.9500
C(36)-C(43)	1.522(6)
C(43)-C(45)	1.522(5)
C(43)-C(44)	1.540(6)
C(43)-H(43)	1.0000
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(23)-C(24)	1.383(5)
C(23)-H(23)	0.9500
C(24)-C(25)	1.390(5)
C(24)-H(24)	0.9500
C(25)-C(26)	1.392(5)
C(25)-H(25)	0.9500
C(26)-C(51)	1.499(5)
C(51)-C(56)	1.404(5)
C(51)-C(52)	1.414(5)

C(52)-C(53)	1.403(5)
C(52)-C(57)	1.518(5)
C(57)-C(58)	1.516(5)
C(57)-C(59)	1.530(5)
C(57)-H(57)	1.0000
C(58)-H(58A)	0.9800
C(58)-H(58B)	0.9800
C(58)-H(58C)	0.9800
C(59)-H(59A)	0.9800
C(59)-H(59B)	0.9800
C(59)-H(59C)	0.9800
C(53)-C(54)	1.395(5)
C(53)-H(53)	0.9500
C(54)-C(55)	1.386(6)
C(54)-C(60)	1.527(5)
C(60)-C(61)	1.522(6)
C(60)-C(62)	1.530(7)
C(60)-H(60)	1.0000
C(61)-H(61A)	0.9800
C(61)-H(61B)	0.9800
C(61)-H(61C)	0.9800
C(62)-H(62A)	0.9800
C(62)-H(62B)	0.9800
C(62)-H(62C)	0.9800
C(55)-C(56)	1.401(5)
C(55)-H(55)	0.9500
C(56)-C(63)	1.518(5)
C(63)-C(65)	1.524(6)
C(63)-C(64)	1.536(6)
C(63)-H(63)	1.0000
C(64)-H(64A)	0.9800
C(64)-H(64B)	0.9800
C(64)-H(64C)	0.9800
C(65)-H(65A)	0.9800
C(65)-H(65B)	0.9800
C(65)-H(65C)	0.9800

O(2)-C(71)	1.431(4)
C(71)-C(73)	1.516(6)
C(71)-C(74)	1.517(6)
C(71)-C(72)	1.523(5)
C(72)-H(72A)	0.9800
C(72)-H(72B)	0.9800
C(72)-H(72C)	0.9800
C(73)-H(73A)	0.9800
C(73)-H(73B)	0.9800
C(73)-H(73C)	0.9800
C(74)-H(74A)	0.9800
C(74)-H(74B)	0.9800
C(74)-H(74C)	0.9800
Mo(2)-N(2)	1.724(3)
Mo(2)-O(4)	1.885(2)
Mo(2)-C(101)	1.888(3)
Mo(2)-O(3)	1.937(2)
C(101)-C(102)	1.514(5)
C(101)-H(101)	0.954(18)
C(102)-C(104)	1.535(5)
C(102)-C(105)	1.535(5)
C(102)-C(103)	1.550(5)
C(103)-H(10A)	0.9800
C(103)-H(10B)	0.9800
C(103)-H(10C)	0.9800
C(104)-H(10D)	0.9800
C(104)-H(10E)	0.9800
C(104)-H(10F)	0.9800
C(105)-C(106)	1.394(5)
C(105)-C(110)	1.400(5)
C(106)-C(107)	1.387(5)
C(106)-H(106)	0.9500
C(107)-C(108)	1.390(5)
C(107)-H(107)	0.9500
C(108)-C(109)	1.383(6)
C(108)-H(108)	0.9500

C(109)-C(110)	1.385(5)
C(109)-H(109)	0.9500
C(110)-H(110)	0.9500
N(2)-C(111)	1.448(4)
C(111)-C(113)	1.517(5)
C(111)-C(114)	1.522(5)
C(111)-C(112)	1.532(5)
C(112)-C(115)	1.555(6)
C(112)-H(11A)	0.9900
C(112)-H(11B)	0.9900
C(113)-C(117)	1.569(6)
C(113)-H(11C)	0.9900
C(113)-H(11D)	0.9900
C(114)-C(119)	1.545(6)
C(114)-H(11E)	0.9900
C(114)-H(11F)	0.9900
C(115)-C(120)	1.490(8)
C(115)-C(116)	1.531(7)
C(115)-H(115)	1.0000
C(116)-C(117)	1.512(7)
C(116)-H(11G)	0.9900
C(116)-H(11H)	0.9900
C(117)-C(118)	1.531(8)
C(117)-H(117)	1.0000
C(118)-C(119)	1.527(8)
C(118)-H(11I)	0.9900
C(118)-H(11J)	0.9900
C(119)-C(120)	1.500(8)
C(119)-H(119)	1.0000
C(120)-H(12C)	0.9900
C(120)-H(12D)	0.9900
O(3)-C(121)	1.352(4)
C(121)-C(122)	1.408(4)
C(121)-C(126)	1.413(5)
C(122)-C(123)	1.391(5)
C(122)-C(131)	1.505(4)

C(131)-C(132)	1.407(4)
C(131)-C(136)	1.411(4)
C(132)-C(133)	1.400(5)
C(132)-C(137)	1.520(5)
C(137)-C(138)	1.524(5)
C(137)-C(139)	1.526(5)
C(137)-H(137)	1.0000
C(138)-H(13C)	0.9800
C(138)-H(13D)	0.9800
C(138)-H(13E)	0.9800
C(139)-H(13F)	0.9800
C(139)-H(13G)	0.9800
C(139)-H(13H)	0.9800
C(133)-C(134)	1.395(5)
C(133)-H(133)	0.9500
C(134)-C(135)	1.390(5)
C(134)-C(140)	1.523(5)
C(140)-C(141)	1.521(6)
C(140)-C(142)	1.528(6)
C(140)-H(140)	1.0000
C(141)-H(14C)	0.9800
C(141)-H(14D)	0.9800
C(141)-H(14E)	0.9800
C(142)-H(14F)	0.9800
C(142)-H(14G)	0.9800
C(142)-H(14H)	0.9800
C(135)-C(136)	1.390(5)
C(135)-H(135)	0.9500
C(136)-C(143)	1.518(5)
C(143)-C(144)	1.526(5)
C(143)-C(145)	1.527(5)
C(143)-H(143)	1.0000
C(144)-H(14I)	0.9800
C(144)-H(14J)	0.9800
C(144)-H(14K)	0.9800
C(145)-H(14L)	0.9800

C(145)-H(14M)	0.9800
C(145)-H(14N)	0.9800
C(123)-C(124)	1.396(5)
C(123)-H(123)	0.9500
C(124)-C(125)	1.384(5)
C(124)-H(124)	0.9500
C(125)-C(126)	1.392(5)
C(125)-H(125)	0.9500
C(126)-C(151)	1.499(6)
C(126)-C(51A)	1.508(12)
C(151)-C(152)	1.408(6)
C(151)-C(156)	1.418(6)
C(152)-C(153)	1.404(6)
C(152)-C(157)	1.520(6)
C(157)-C(159)	1.530(7)
C(157)-C(158)	1.557(7)
C(157)-H(157)	1.0000
C(158)-H(15A)	0.9800
C(158)-H(15B)	0.9800
C(158)-H(15C)	0.9800
C(159)-H(15D)	0.9800
C(159)-H(15E)	0.9800
C(159)-H(15F)	0.9800
C(153)-C(154)	1.379(6)
C(153)-H(153)	0.9500
C(154)-C(155)	1.382(6)
C(154)-C(160)	1.517(5)
C(160)-C(162)	1.524(6)
C(160)-C(161)	1.538(8)
C(160)-H(160)	1.0000
C(161)-H(16C)	0.9800
C(161)-H(16D)	0.9800
C(161)-H(16E)	0.9800
C(162)-H(16F)	0.9800
C(162)-H(16G)	0.9800
C(162)-H(16H)	0.9800

C(155)-C(156)	1.396(6)
C(155)-H(155)	0.9500
C(156)-C(163)	1.523(6)
C(163)-C(164)	1.529(7)
C(163)-C(165)	1.536(7)
C(163)-H(163)	1.0000
C(164)-H(16I)	0.9800
C(164)-H(16J)	0.9800
C(164)-H(16K)	0.9800
C(165)-H(16L)	0.9800
C(165)-H(16M)	0.9800
C(165)-H(16N)	0.9800
C(51A)-C(56A)	1.404(11)
C(51A)-C(52A)	1.414(11)
C(52A)-C(53A)	1.404(11)
C(52A)-C(57A)	1.520(11)
C(57A)-C(59A)	1.515(12)
C(57A)-C(58A)	1.529(13)
C(57A)-H(57A)	1.0000
C(58A)-H(58D)	0.9800
C(58A)-H(58E)	0.9800
C(58A)-H(58F)	0.9800
C(59A)-H(59D)	0.9800
C(59A)-H(59E)	0.9800
C(59A)-H(59F)	0.9800
C(53A)-C(54A)	1.381(11)
C(53A)-H(53A)	0.9500
C(54A)-C(55A)	1.370(11)
C(54A)-C(60A)	1.532(10)
C(60A)-C(62A)	1.529(12)
C(60A)-C(61A)	1.530(13)
C(60A)-H(60A)	1.0000
C(61A)-H(61D)	0.9800
C(61A)-H(61E)	0.9800
C(61A)-H(61F)	0.9800
C(62A)-H(62D)	0.9800

C(62A)-H(62E)	0.9800
C(62A)-H(62F)	0.9800
C(55A)-C(56A)	1.411(11)
C(55A)-H(55A)	0.9500
C(56A)-C(63A)	1.513(11)
C(63A)-C(64A)	1.528(13)
C(63A)-C(65A)	1.544(13)
C(63A)-H(63A)	1.0000
C(64A)-H(64D)	0.9800
C(64A)-H(64E)	0.9800
C(64A)-H(64F)	0.9800
C(65A)-H(65D)	0.9800
C(65A)-H(65E)	0.9800
C(65A)-H(65F)	0.9800
O(4)-C(171)	1.430(4)
C(171)-C(173)	1.517(5)
C(171)-C(172)	1.530(5)
C(171)-C(174)	1.534(5)
C(172)-H(17A)	0.9800
C(172)-H(17B)	0.9800
C(172)-H(17C)	0.9800
C(173)-H(17D)	0.9800
C(173)-H(17E)	0.9800
C(173)-H(17F)	0.9800
C(174)-H(17G)	0.9800
C(174)-H(17H)	0.9800
C(174)-H(17I)	0.9800

N(1)-Mo(1)-O(2)	111.74(13)
N(1)-Mo(1)-C(1)	103.46(14)
O(2)-Mo(1)-C(1)	107.25(13)
N(1)-Mo(1)-O(1)	114.97(12)
O(2)-Mo(1)-O(1)	110.54(11)
C(1)-Mo(1)-O(1)	108.31(13)
C(2)-C(1)-Mo(1)	145.6(3)
C(2)-C(1)-H(1)	117(3)

Mo(1)-C(1)-H(1)	97(3)
C(1)-C(2)-C(5)	110.1(3)
C(1)-C(2)-C(3)	110.6(3)
C(5)-C(2)-C(3)	110.5(3)
C(1)-C(2)-C(4)	108.6(3)
C(5)-C(2)-C(4)	109.2(3)
C(3)-C(2)-C(4)	107.9(3)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(10)-C(5)-C(6)	117.5(3)
C(10)-C(5)-C(2)	119.7(3)
C(6)-C(5)-C(2)	122.8(3)
C(7)-C(6)-C(5)	121.5(3)
C(7)-C(6)-H(6)	119.3
C(5)-C(6)-H(6)	119.3
C(8)-C(7)-C(6)	119.9(4)
C(8)-C(7)-H(7)	120.0
C(6)-C(7)-H(7)	120.0
C(7)-C(8)-C(9)	119.5(3)
C(7)-C(8)-H(8)	120.3
C(9)-C(8)-H(8)	120.3
C(8)-C(9)-C(10)	120.4(4)
C(8)-C(9)-H(9)	119.8
C(10)-C(9)-H(9)	119.8
C(9)-C(10)-C(5)	121.2(4)
C(9)-C(10)-H(10)	119.4

C(5)-C(10)-H(10)	119.4
C(11)-N(1)-Mo(1)	168.7(3)
N(1)-C(11)-C(13)	111.8(3)
N(1)-C(11)-C(12)	108.8(3)
C(13)-C(11)-C(12)	109.8(3)
N(1)-C(11)-C(14)	108.9(3)
C(13)-C(11)-C(14)	109.0(3)
C(12)-C(11)-C(14)	108.4(3)
C(11)-C(12)-C(15)	110.1(3)
C(11)-C(12)-H(12A)	109.6
C(15)-C(12)-H(12A)	109.6
C(11)-C(12)-H(12B)	109.6
C(15)-C(12)-H(12B)	109.6
H(12A)-C(12)-H(12B)	108.1
C(11)-C(13)-C(17)	110.5(3)
C(11)-C(13)-H(13A)	109.6
C(17)-C(13)-H(13A)	109.6
C(11)-C(13)-H(13B)	109.6
C(17)-C(13)-H(13B)	109.6
H(13A)-C(13)-H(13B)	108.1
C(11)-C(14)-C(19)	109.6(3)
C(11)-C(14)-H(14A)	109.7
C(19)-C(14)-H(14A)	109.7
C(11)-C(14)-H(14B)	109.7
C(19)-C(14)-H(14B)	109.7
H(14A)-C(14)-H(14B)	108.2
C(16)-C(15)-C(20)	111.3(4)
C(16)-C(15)-C(12)	109.5(4)
C(20)-C(15)-C(12)	105.9(4)
C(16)-C(15)-H(15)	110.0
C(20)-C(15)-H(15)	110.0
C(12)-C(15)-H(15)	110.0
C(15)-C(16)-C(17)	111.0(4)
C(15)-C(16)-H(16A)	109.4
C(17)-C(16)-H(16A)	109.4
C(15)-C(16)-H(16B)	109.4

C(17)-C(16)-H(16B)	109.4
H(16A)-C(16)-H(16B)	108.0
C(18)-C(17)-C(16)	111.1(4)
C(18)-C(17)-C(13)	107.1(4)
C(16)-C(17)-C(13)	107.1(4)
C(18)-C(17)-H(17)	110.5
C(16)-C(17)-H(17)	110.5
C(13)-C(17)-H(17)	110.5
C(17)-C(18)-C(19)	113.2(4)
C(17)-C(18)-H(18A)	108.9
C(19)-C(18)-H(18A)	108.9
C(17)-C(18)-H(18B)	108.9
C(19)-C(18)-H(18B)	108.9
H(18A)-C(18)-H(18B)	107.8
C(18)-C(19)-C(20)	110.2(4)
C(18)-C(19)-C(14)	107.3(4)
C(20)-C(19)-C(14)	108.2(4)
C(18)-C(19)-H(19)	110.4
C(20)-C(19)-H(19)	110.4
C(14)-C(19)-H(19)	110.4
C(19)-C(20)-C(15)	110.7(4)
C(19)-C(20)-H(20A)	109.5
C(15)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
C(15)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	108.1
C(21)-O(1)-Mo(1)	145.2(2)
O(1)-C(21)-C(26)	118.7(3)
O(1)-C(21)-C(22)	120.7(3)
C(26)-C(21)-C(22)	120.4(3)
C(23)-C(22)-C(21)	118.0(3)
C(23)-C(22)-C(31)	118.4(3)
C(21)-C(22)-C(31)	123.6(3)
C(36)-C(31)-C(32)	119.4(3)
C(36)-C(31)-C(22)	119.5(3)
C(32)-C(31)-C(22)	120.5(3)

C(33)-C(32)-C(31)	120.0(4)
C(33)-C(32)-C(37)	115.8(4)
C(31)-C(32)-C(37)	124.1(3)
C(32)-C(37)-C(38)	113.4(4)
C(32)-C(37)-C(39)	110.5(4)
C(38)-C(37)-C(39)	108.9(3)
C(32)-C(37)-H(37)	108.0
C(38)-C(37)-H(37)	108.0
C(39)-C(37)-H(37)	108.0
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(34)-C(33)-C(32)	121.9(4)
C(34)-C(33)-H(33)	119.1
C(32)-C(33)-H(33)	119.1
C(33)-C(34)-C(35)	117.5(4)
C(33)-C(34)-C(40)	119.3(5)
C(35)-C(34)-C(40)	123.2(5)
C(41)-C(40)-C(34)	113.6(4)
C(41)-C(40)-C(42)	117.7(5)
C(34)-C(40)-C(42)	109.5(4)
C(41)-C(40)-H(40)	104.9
C(34)-C(40)-H(40)	104.9
C(42)-C(40)-H(40)	104.9
C(40)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5

C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(40)-C(42)-H(42A)	109.5
C(40)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(40)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(36)-C(35)-C(34)	122.7(4)
C(36)-C(35)-H(35)	118.6
C(34)-C(35)-H(35)	118.6
C(35)-C(36)-C(31)	118.3(4)
C(35)-C(36)-C(43)	118.8(4)
C(31)-C(36)-C(43)	122.7(3)
C(36)-C(43)-C(45)	113.3(3)
C(36)-C(43)-C(44)	108.6(3)
C(45)-C(43)-C(44)	111.0(3)
C(36)-C(43)-H(43)	107.9
C(45)-C(43)-H(43)	107.9
C(44)-C(43)-H(43)	107.9
C(43)-C(44)-H(44A)	109.5
C(43)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(43)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(43)-C(45)-H(45A)	109.5
C(43)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(43)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5
C(24)-C(23)-C(22)	122.1(3)
C(24)-C(23)-H(23)	119.0
C(22)-C(23)-H(23)	119.0

C(23)-C(24)-C(25)	119.1(3)
C(23)-C(24)-H(24)	120.5
C(25)-C(24)-H(24)	120.5
C(24)-C(25)-C(26)	121.4(3)
C(24)-C(25)-H(25)	119.3
C(26)-C(25)-H(25)	119.3
C(25)-C(26)-C(21)	118.9(3)
C(25)-C(26)-C(51)	118.6(3)
C(21)-C(26)-C(51)	122.4(3)
C(56)-C(51)-C(52)	119.2(3)
C(56)-C(51)-C(26)	120.0(3)
C(52)-C(51)-C(26)	120.5(3)
C(53)-C(52)-C(51)	118.8(3)
C(53)-C(52)-C(57)	119.2(3)
C(51)-C(52)-C(57)	122.0(3)
C(58)-C(57)-C(52)	113.7(3)
C(58)-C(57)-C(59)	111.9(3)
C(52)-C(57)-C(59)	109.0(3)
C(58)-C(57)-H(57)	107.3
C(52)-C(57)-H(57)	107.3
C(59)-C(57)-H(57)	107.3
C(57)-C(58)-H(58A)	109.5
C(57)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
C(57)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5
C(57)-C(59)-H(59A)	109.5
C(57)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	109.5
C(57)-C(59)-H(59C)	109.5
H(59A)-C(59)-H(59C)	109.5
H(59B)-C(59)-H(59C)	109.5
C(54)-C(53)-C(52)	122.6(3)
C(54)-C(53)-H(53)	118.7
C(52)-C(53)-H(53)	118.7

C(55)-C(54)-C(53)	117.5(3)
C(55)-C(54)-C(60)	122.7(4)
C(53)-C(54)-C(60)	119.8(4)
C(61)-C(60)-C(54)	110.5(3)
C(61)-C(60)-C(62)	109.9(4)
C(54)-C(60)-C(62)	114.2(4)
C(61)-C(60)-H(60)	107.3
C(54)-C(60)-H(60)	107.3
C(62)-C(60)-H(60)	107.3
C(60)-C(61)-H(61A)	109.5
C(60)-C(61)-H(61B)	109.5
H(61A)-C(61)-H(61B)	109.5
C(60)-C(61)-H(61C)	109.5
H(61A)-C(61)-H(61C)	109.5
H(61B)-C(61)-H(61C)	109.5
C(60)-C(62)-H(62A)	109.5
C(60)-C(62)-H(62B)	109.5
H(62A)-C(62)-H(62B)	109.5
C(60)-C(62)-H(62C)	109.5
H(62A)-C(62)-H(62C)	109.5
H(62B)-C(62)-H(62C)	109.5
C(54)-C(55)-C(56)	122.1(3)
C(54)-C(55)-H(55)	119.0
C(56)-C(55)-H(55)	119.0
C(55)-C(56)-C(51)	119.9(3)
C(55)-C(56)-C(63)	118.6(3)
C(51)-C(56)-C(63)	121.5(3)
C(56)-C(63)-C(65)	111.1(3)
C(56)-C(63)-C(64)	111.0(4)
C(65)-C(63)-C(64)	111.6(4)
C(56)-C(63)-H(63)	107.6
C(65)-C(63)-H(63)	107.6
C(64)-C(63)-H(63)	107.6
C(63)-C(64)-H(64A)	109.5
C(63)-C(64)-H(64B)	109.5
H(64A)-C(64)-H(64B)	109.5

C(63)-C(64)-H(64C)	109.5
H(64A)-C(64)-H(64C)	109.5
H(64B)-C(64)-H(64C)	109.5
C(63)-C(65)-H(65A)	109.5
C(63)-C(65)-H(65B)	109.5
H(65A)-C(65)-H(65B)	109.5
C(63)-C(65)-H(65C)	109.5
H(65A)-C(65)-H(65C)	109.5
H(65B)-C(65)-H(65C)	109.5
C(71)-O(2)-Mo(1)	143.3(2)
O(2)-C(71)-C(73)	106.7(3)
O(2)-C(71)-C(74)	107.0(3)
C(73)-C(71)-C(74)	111.7(4)
O(2)-C(71)-C(72)	109.8(3)
C(73)-C(71)-C(72)	110.0(4)
C(74)-C(71)-C(72)	111.5(4)
C(71)-C(72)-H(72A)	109.5
C(71)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5
C(71)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5
H(72B)-C(72)-H(72C)	109.5
C(71)-C(73)-H(73A)	109.5
C(71)-C(73)-H(73B)	109.5
H(73A)-C(73)-H(73B)	109.5
C(71)-C(73)-H(73C)	109.5
H(73A)-C(73)-H(73C)	109.5
H(73B)-C(73)-H(73C)	109.5
C(71)-C(74)-H(74A)	109.5
C(71)-C(74)-H(74B)	109.5
H(74A)-C(74)-H(74B)	109.5
C(71)-C(74)-H(74C)	109.5
H(74A)-C(74)-H(74C)	109.5
H(74B)-C(74)-H(74C)	109.5
N(2)-Mo(2)-O(4)	112.27(13)
N(2)-Mo(2)-C(101)	103.25(15)

O(4)-Mo(2)-C(101)	107.39(13)
N(2)-Mo(2)-O(3)	114.05(12)
O(4)-Mo(2)-O(3)	110.65(10)
C(101)-Mo(2)-O(3)	108.70(12)
C(102)-C(101)-Mo(2)	145.2(3)
C(102)-C(101)-H(101)	113(3)
Mo(2)-C(101)-H(101)	102(3)
C(101)-C(102)-C(104)	111.1(3)
C(101)-C(102)-C(105)	109.7(3)
C(104)-C(102)-C(105)	110.2(3)
C(101)-C(102)-C(103)	107.9(3)
C(104)-C(102)-C(103)	108.1(3)
C(105)-C(102)-C(103)	109.9(3)
C(102)-C(103)-H(10A)	109.5
C(102)-C(103)-H(10B)	109.5
H(10A)-C(103)-H(10B)	109.5
C(102)-C(103)-H(10C)	109.5
H(10A)-C(103)-H(10C)	109.5
H(10B)-C(103)-H(10C)	109.5
C(102)-C(104)-H(10D)	109.5
C(102)-C(104)-H(10E)	109.5
H(10D)-C(104)-H(10E)	109.5
C(102)-C(104)-H(10F)	109.5
H(10D)-C(104)-H(10F)	109.5
H(10E)-C(104)-H(10F)	109.5
C(106)-C(105)-C(110)	117.4(3)
C(106)-C(105)-C(102)	123.0(3)
C(110)-C(105)-C(102)	119.7(3)
C(107)-C(106)-C(105)	121.9(3)
C(107)-C(106)-H(106)	119.1
C(105)-C(106)-H(106)	119.1
C(106)-C(107)-C(108)	119.7(3)
C(106)-C(107)-H(107)	120.1
C(108)-C(107)-H(107)	120.1
C(109)-C(108)-C(107)	119.4(3)
C(109)-C(108)-H(108)	120.3

C(107)-C(108)-H(108)	120.3
C(108)-C(109)-C(110)	120.6(4)
C(108)-C(109)-H(109)	119.7
C(110)-C(109)-H(109)	119.7
C(109)-C(110)-C(105)	121.1(3)
C(109)-C(110)-H(110)	119.5
C(105)-C(110)-H(110)	119.5
C(111)-N(2)-Mo(2)	165.8(3)
N(2)-C(111)-C(113)	109.7(3)
N(2)-C(111)-C(114)	111.0(3)
C(113)-C(111)-C(114)	110.9(3)
N(2)-C(111)-C(112)	106.9(3)
C(113)-C(111)-C(112)	110.3(3)
C(114)-C(111)-C(112)	107.9(3)
C(111)-C(112)-C(115)	108.8(3)
C(111)-C(112)-H(11A)	109.9
C(115)-C(112)-H(11A)	109.9
C(111)-C(112)-H(11B)	109.9
C(115)-C(112)-H(11B)	109.9
H(11A)-C(112)-H(11B)	108.3
C(111)-C(113)-C(117)	109.1(3)
C(111)-C(113)-H(11C)	109.9
C(117)-C(113)-H(11C)	109.9
C(111)-C(113)-H(11D)	109.9
C(117)-C(113)-H(11D)	109.9
H(11C)-C(113)-H(11D)	108.3
C(111)-C(114)-C(119)	109.1(3)
C(111)-C(114)-H(11E)	109.9
C(119)-C(114)-H(11E)	109.9
C(111)-C(114)-H(11F)	109.9
C(119)-C(114)-H(11F)	109.9
H(11E)-C(114)-H(11F)	108.3
C(120)-C(115)-C(116)	110.5(4)
C(120)-C(115)-C(112)	109.7(4)
C(116)-C(115)-C(112)	108.2(4)
C(120)-C(115)-H(115)	109.5

C(116)-C(115)-H(115)	109.5
C(112)-C(115)-H(115)	109.5
C(117)-C(116)-C(115)	110.2(4)
C(117)-C(116)-H(11G)	109.6
C(115)-C(116)-H(11G)	109.6
C(117)-C(116)-H(11H)	109.6
C(115)-C(116)-H(11H)	109.6
H(11G)-C(116)-H(11H)	108.1
C(116)-C(117)-C(118)	110.9(4)
C(116)-C(117)-C(113)	108.7(4)
C(118)-C(117)-C(113)	107.3(4)
C(116)-C(117)-H(117)	110.0
C(118)-C(117)-H(117)	110.0
C(113)-C(117)-H(117)	110.0
C(119)-C(118)-C(117)	109.5(4)
C(119)-C(118)-H(11I)	109.8
C(117)-C(118)-H(11I)	109.8
C(119)-C(118)-H(11J)	109.8
C(117)-C(118)-H(11J)	109.8
H(11I)-C(118)-H(11J)	108.2
C(120)-C(119)-C(118)	111.3(4)
C(120)-C(119)-C(114)	109.0(4)
C(118)-C(119)-C(114)	108.7(4)
C(120)-C(119)-H(119)	109.3
C(118)-C(119)-H(119)	109.3
C(114)-C(119)-H(119)	109.3
C(115)-C(120)-C(119)	110.2(4)
C(115)-C(120)-H(12C)	109.6
C(119)-C(120)-H(12C)	109.6
C(115)-C(120)-H(12D)	109.6
C(119)-C(120)-H(12D)	109.6
H(12C)-C(120)-H(12D)	108.1
C(121)-O(3)-Mo(2)	145.6(2)
O(3)-C(121)-C(122)	118.6(3)
O(3)-C(121)-C(126)	120.7(3)
C(122)-C(121)-C(126)	120.5(3)

C(123)-C(122)-C(121)	118.5(3)
C(123)-C(122)-C(131)	118.8(3)
C(121)-C(122)-C(131)	122.6(3)
C(132)-C(131)-C(136)	119.5(3)
C(132)-C(131)-C(122)	120.6(3)
C(136)-C(131)-C(122)	119.6(3)
C(133)-C(132)-C(131)	118.5(3)
C(133)-C(132)-C(137)	119.6(3)
C(131)-C(132)-C(137)	121.9(3)
C(132)-C(137)-C(138)	111.9(3)
C(132)-C(137)-C(139)	110.3(3)
C(138)-C(137)-C(139)	110.0(3)
C(132)-C(137)-H(137)	108.2
C(138)-C(137)-H(137)	108.2
C(139)-C(137)-H(137)	108.2
C(137)-C(138)-H(13C)	109.5
C(137)-C(138)-H(13D)	109.5
H(13C)-C(138)-H(13D)	109.5
C(137)-C(138)-H(13E)	109.5
H(13C)-C(138)-H(13E)	109.5
H(13D)-C(138)-H(13E)	109.5
C(137)-C(139)-H(13F)	109.5
C(137)-C(139)-H(13G)	109.5
H(13F)-C(139)-H(13G)	109.5
C(137)-C(139)-H(13H)	109.5
H(13F)-C(139)-H(13H)	109.5
H(13G)-C(139)-H(13H)	109.5
C(134)-C(133)-C(132)	123.1(3)
C(134)-C(133)-H(133)	118.5
C(132)-C(133)-H(133)	118.5
C(135)-C(134)-C(133)	116.9(3)
C(135)-C(134)-C(140)	123.6(3)
C(133)-C(134)-C(140)	119.5(3)
C(141)-C(140)-C(134)	110.8(3)
C(141)-C(140)-C(142)	110.1(3)
C(134)-C(140)-C(142)	113.8(3)

C(141)-C(140)-H(140)	107.3
C(134)-C(140)-H(140)	107.3
C(142)-C(140)-H(140)	107.3
C(140)-C(141)-H(14C)	109.5
C(140)-C(141)-H(14D)	109.5
H(14C)-C(141)-H(14D)	109.5
C(140)-C(141)-H(14E)	109.5
H(14C)-C(141)-H(14E)	109.5
H(14D)-C(141)-H(14E)	109.5
C(140)-C(142)-H(14F)	109.5
C(140)-C(142)-H(14G)	109.5
H(14F)-C(142)-H(14G)	109.5
C(140)-C(142)-H(14H)	109.5
H(14F)-C(142)-H(14H)	109.5
H(14G)-C(142)-H(14H)	109.5
C(134)-C(135)-C(136)	122.6(3)
C(134)-C(135)-H(135)	118.7
C(136)-C(135)-H(135)	118.7
C(135)-C(136)-C(131)	119.4(3)
C(135)-C(136)-C(143)	118.6(3)
C(131)-C(136)-C(143)	122.0(3)
C(136)-C(143)-C(144)	111.1(3)
C(136)-C(143)-C(145)	111.5(3)
C(144)-C(143)-C(145)	111.3(3)
C(136)-C(143)-H(143)	107.6
C(144)-C(143)-H(143)	107.6
C(145)-C(143)-H(143)	107.6
C(143)-C(144)-H(14I)	109.5
C(143)-C(144)-H(14J)	109.5
H(14I)-C(144)-H(14J)	109.5
C(143)-C(144)-H(14K)	109.5
H(14I)-C(144)-H(14K)	109.5
H(14J)-C(144)-H(14K)	109.5
C(143)-C(145)-H(14L)	109.5
C(143)-C(145)-H(14M)	109.5
H(14L)-C(145)-H(14M)	109.5

C(143)-C(145)-H(14N)	109.5
H(14L)-C(145)-H(14N)	109.5
H(14M)-C(145)-H(14N)	109.5
C(122)-C(123)-C(124)	122.0(3)
C(122)-C(123)-H(123)	119.0
C(124)-C(123)-H(123)	119.0
C(125)-C(124)-C(123)	118.2(3)
C(125)-C(124)-H(124)	120.9
C(123)-C(124)-H(124)	120.9
C(124)-C(125)-C(126)	122.4(3)
C(124)-C(125)-H(125)	118.8
C(126)-C(125)-H(125)	118.8
C(125)-C(126)-C(121)	118.3(3)
C(125)-C(126)-C(151)	118.1(5)
C(121)-C(126)-C(151)	123.7(5)
C(125)-C(126)-C(51A)	120.7(13)
C(121)-C(126)-C(51A)	119.9(12)
C(151)-C(126)-C(51A)	12.5(5)
C(152)-C(151)-C(156)	119.0(4)
C(152)-C(151)-C(126)	122.2(4)
C(156)-C(151)-C(126)	118.3(4)
C(153)-C(152)-C(151)	118.9(4)
C(153)-C(152)-C(157)	117.5(4)
C(151)-C(152)-C(157)	123.6(4)
C(152)-C(157)-C(159)	113.0(5)
C(152)-C(157)-C(158)	110.1(5)
C(159)-C(157)-C(158)	107.6(5)
C(152)-C(157)-H(157)	108.7
C(159)-C(157)-H(157)	108.7
C(158)-C(157)-H(157)	108.7
C(157)-C(158)-H(15A)	109.5
C(157)-C(158)-H(15B)	109.5
H(15A)-C(158)-H(15B)	109.5
C(157)-C(158)-H(15C)	109.5
H(15A)-C(158)-H(15C)	109.5
H(15B)-C(158)-H(15C)	109.5

C(157)-C(159)-H(15D)	109.5
C(157)-C(159)-H(15E)	109.5
H(15D)-C(159)-H(15E)	109.5
C(157)-C(159)-H(15F)	109.5
H(15D)-C(159)-H(15F)	109.5
H(15E)-C(159)-H(15F)	109.5
C(154)-C(153)-C(152)	122.8(4)
C(154)-C(153)-H(153)	118.6
C(152)-C(153)-H(153)	118.6
C(153)-C(154)-C(155)	117.3(4)
C(153)-C(154)-C(160)	120.6(4)
C(155)-C(154)-C(160)	122.0(4)
C(154)-C(160)-C(162)	112.3(4)
C(154)-C(160)-C(161)	110.8(5)
C(162)-C(160)-C(161)	111.0(6)
C(154)-C(160)-H(160)	107.5
C(162)-C(160)-H(160)	107.5
C(161)-C(160)-H(160)	107.5
C(160)-C(161)-H(16C)	109.5
C(160)-C(161)-H(16D)	109.5
H(16C)-C(161)-H(16D)	109.5
C(160)-C(161)-H(16E)	109.5
H(16C)-C(161)-H(16E)	109.5
H(16D)-C(161)-H(16E)	109.5
C(160)-C(162)-H(16F)	109.5
C(160)-C(162)-H(16G)	109.5
H(16F)-C(162)-H(16G)	109.5
C(160)-C(162)-H(16H)	109.5
H(16F)-C(162)-H(16H)	109.5
H(16G)-C(162)-H(16H)	109.5
C(154)-C(155)-C(156)	123.0(4)
C(154)-C(155)-H(155)	118.5
C(156)-C(155)-H(155)	118.5
C(155)-C(156)-C(151)	118.9(4)
C(155)-C(156)-C(163)	118.8(4)
C(151)-C(156)-C(163)	122.1(4)

C(156)-C(163)-C(164)	113.0(5)
C(156)-C(163)-C(165)	109.9(5)
C(164)-C(163)-C(165)	110.7(6)
C(156)-C(163)-H(163)	107.7
C(164)-C(163)-H(163)	107.7
C(165)-C(163)-H(163)	107.7
C(163)-C(164)-H(16I)	109.5
C(163)-C(164)-H(16J)	109.5
H(16I)-C(164)-H(16J)	109.5
C(163)-C(164)-H(16K)	109.5
H(16I)-C(164)-H(16K)	109.5
H(16J)-C(164)-H(16K)	109.5
C(163)-C(165)-H(16L)	109.5
C(163)-C(165)-H(16M)	109.5
H(16L)-C(165)-H(16M)	109.5
C(163)-C(165)-H(16N)	109.5
H(16L)-C(165)-H(16N)	109.5
H(16M)-C(165)-H(16N)	109.5
C(56A)-C(51A)-C(52A)	119.2(10)
C(56A)-C(51A)-C(126)	124.8(9)
C(52A)-C(51A)-C(126)	115.5(9)
C(53A)-C(52A)-C(51A)	120.3(9)
C(53A)-C(52A)-C(57A)	118.7(10)
C(51A)-C(52A)-C(57A)	121.1(10)
C(59A)-C(57A)-C(52A)	113.3(11)
C(59A)-C(57A)-C(58A)	109.4(13)
C(52A)-C(57A)-C(58A)	110.9(11)
C(59A)-C(57A)-H(57A)	107.7
C(52A)-C(57A)-H(57A)	107.7
C(58A)-C(57A)-H(57A)	107.7
C(57A)-C(58A)-H(58D)	109.5
C(57A)-C(58A)-H(58E)	109.5
H(58D)-C(58A)-H(58E)	109.5
C(57A)-C(58A)-H(58F)	109.5
H(58D)-C(58A)-H(58F)	109.5
H(58E)-C(58A)-H(58F)	109.5

C(57A)-C(59A)-H(59D)	109.5
C(57A)-C(59A)-H(59E)	109.5
H(59D)-C(59A)-H(59E)	109.5
C(57A)-C(59A)-H(59F)	109.5
H(59D)-C(59A)-H(59F)	109.5
H(59E)-C(59A)-H(59F)	109.5
C(54A)-C(53A)-C(52A)	120.6(9)
C(54A)-C(53A)-H(53A)	119.7
C(52A)-C(53A)-H(53A)	119.7
C(55A)-C(54A)-C(53A)	118.8(9)
C(55A)-C(54A)-C(60A)	120.4(9)
C(53A)-C(54A)-C(60A)	120.6(9)
C(62A)-C(60A)-C(61A)	112.9(14)
C(62A)-C(60A)-C(54A)	111.9(8)
C(61A)-C(60A)-C(54A)	111.3(12)
C(62A)-C(60A)-H(60A)	106.7
C(61A)-C(60A)-H(60A)	106.7
C(54A)-C(60A)-H(60A)	106.7
C(60A)-C(61A)-H(61D)	109.5
C(60A)-C(61A)-H(61E)	109.5
H(61D)-C(61A)-H(61E)	109.5
C(60A)-C(61A)-H(61F)	109.5
H(61D)-C(61A)-H(61F)	109.5
H(61E)-C(61A)-H(61F)	109.5
C(60A)-C(62A)-H(62D)	109.5
C(60A)-C(62A)-H(62E)	109.5
H(62D)-C(62A)-H(62E)	109.5
C(60A)-C(62A)-H(62F)	109.5
H(62D)-C(62A)-H(62F)	109.5
H(62E)-C(62A)-H(62F)	109.5
C(54A)-C(55A)-C(56A)	123.1(10)
C(54A)-C(55A)-H(55A)	118.5
C(56A)-C(55A)-H(55A)	118.5
C(51A)-C(56A)-C(55A)	118.0(9)
C(51A)-C(56A)-C(63A)	124.4(10)
C(55A)-C(56A)-C(63A)	117.4(10)

C(56A)-C(63A)-C(64A)	111.6(11)
C(56A)-C(63A)-C(65A)	109.9(12)
C(64A)-C(63A)-C(65A)	109.5(14)
C(56A)-C(63A)-H(63A)	108.6
C(64A)-C(63A)-H(63A)	108.6
C(65A)-C(63A)-H(63A)	108.6
C(63A)-C(64A)-H(64D)	109.5
C(63A)-C(64A)-H(64E)	109.5
H(64D)-C(64A)-H(64E)	109.5
C(63A)-C(64A)-H(64F)	109.5
H(64D)-C(64A)-H(64F)	109.5
H(64E)-C(64A)-H(64F)	109.5
C(63A)-C(65A)-H(65D)	109.5
C(63A)-C(65A)-H(65E)	109.5
H(65D)-C(65A)-H(65E)	109.5
C(63A)-C(65A)-H(65F)	109.5
H(65D)-C(65A)-H(65F)	109.5
H(65E)-C(65A)-H(65F)	109.5
C(171)-O(4)-Mo(2)	143.1(2)
O(4)-C(171)-C(173)	108.0(3)
O(4)-C(171)-C(172)	109.9(3)
C(173)-C(171)-C(172)	112.0(3)
O(4)-C(171)-C(174)	106.2(3)
C(173)-C(171)-C(174)	110.7(3)
C(172)-C(171)-C(174)	109.9(3)
C(171)-C(172)-H(17A)	109.5
C(171)-C(172)-H(17B)	109.5
H(17A)-C(172)-H(17B)	109.5
C(171)-C(172)-H(17C)	109.5
H(17A)-C(172)-H(17C)	109.5
H(17B)-C(172)-H(17C)	109.5
C(171)-C(173)-H(17D)	109.5
C(171)-C(173)-H(17E)	109.5
H(17D)-C(173)-H(17E)	109.5
C(171)-C(173)-H(17F)	109.5
H(17D)-C(173)-H(17F)	109.5

H(17E)-C(173)-H(17F)	109.5
C(171)-C(174)-H(17G)	109.5
C(171)-C(174)-H(17H)	109.5
H(17G)-C(174)-H(17H)	109.5
C(171)-C(174)-H(17I)	109.5
H(17G)-C(174)-H(17I)	109.5
H(17H)-C(174)-H(17I)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S7D. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	15(1)	17(1)	13(1)	0(1)	1(1)	-8(1)
C(1)	20(2)	22(2)	14(2)	-1(1)	1(1)	-12(1)
C(2)	17(2)	19(2)	16(2)	1(1)	3(1)	-7(1)
C(3)	22(2)	22(2)	23(2)	4(1)	4(1)	-5(1)
C(4)	18(2)	25(2)	28(2)	7(1)	-2(1)	-10(1)
C(5)	19(2)	23(2)	14(2)	0(1)	1(1)	-10(1)
C(6)	23(2)	20(2)	20(2)	-2(1)	3(1)	-10(1)
C(7)	28(2)	31(2)	22(2)	-7(2)	8(1)	-18(2)
C(8)	33(2)	29(2)	25(2)	2(2)	3(2)	-21(2)
C(9)	31(2)	22(2)	42(2)	0(2)	3(2)	-17(2)
C(10)	23(2)	22(2)	23(2)	-1(1)	4(1)	-9(1)
N(1)	20(2)	20(1)	16(1)	0(1)	2(1)	-6(1)
C(11)	21(2)	22(2)	14(2)	0(1)	2(1)	-8(1)
C(12)	49(3)	24(2)	30(2)	2(2)	-8(2)	-16(2)
C(13)	30(2)	36(2)	25(2)	4(2)	1(2)	-10(2)
C(14)	36(2)	43(2)	28(2)	-3(2)	2(2)	-21(2)
C(15)	51(3)	23(2)	39(3)	8(2)	-22(2)	-11(2)
C(16)	47(3)	48(3)	30(2)	12(2)	3(2)	-22(2)
C(17)	33(2)	30(2)	35(2)	-4(2)	-1(2)	-7(2)
C(18)	47(3)	36(2)	28(2)	0(2)	9(2)	-18(2)
C(19)	40(2)	41(2)	45(3)	-4(2)	-5(2)	-22(2)
C(20)	35(2)	40(2)	42(3)	7(2)	-3(2)	-7(2)
O(1)	17(1)	20(1)	13(1)	-2(1)	2(1)	-8(1)
C(21)	16(2)	15(1)	10(1)	-3(1)	3(1)	-6(1)
C(22)	18(2)	20(2)	12(2)	1(1)	1(1)	-10(1)
C(31)	22(2)	35(2)	12(2)	-6(1)	5(1)	-17(2)
C(32)	20(2)	48(2)	12(2)	-8(2)	3(1)	-20(2)
C(37)	25(2)	41(2)	18(2)	0(2)	-2(1)	-14(2)
C(38)	29(2)	52(3)	23(2)	6(2)	-6(2)	-10(2)
C(39)	32(2)	54(3)	19(2)	6(2)	-3(2)	-20(2)
C(33)	28(2)	64(3)	12(2)	-6(2)	1(1)	-27(2)

C(34)	30(2)	69(3)	20(2)	-19(2)	8(2)	-34(2)
C(40)	38(3)	73(4)	37(3)	-22(2)	5(2)	-34(3)
C(41)	33(3)	50(3)	74(4)	-25(3)	-1(2)	-22(2)
C(42)	34(2)	30(2)	42(3)	-9(2)	-11(2)	-15(2)
C(35)	38(2)	53(3)	25(2)	-13(2)	9(2)	-37(2)
C(36)	33(2)	38(2)	18(2)	-13(2)	7(1)	-26(2)
C(43)	34(2)	28(2)	25(2)	-7(2)	7(2)	-22(2)
C(44)	39(3)	42(2)	38(3)	-15(2)	13(2)	-23(2)
C(45)	40(2)	31(2)	30(2)	-4(2)	10(2)	-22(2)
C(23)	21(2)	25(2)	11(2)	-3(1)	4(1)	-12(1)
C(24)	17(2)	24(2)	13(2)	-3(1)	3(1)	-10(1)
C(25)	14(2)	23(2)	16(2)	0(1)	0(1)	-11(1)
C(26)	16(2)	14(1)	11(2)	-2(1)	1(1)	-6(1)
C(51)	13(2)	20(2)	16(2)	-4(1)	0(1)	-8(1)
C(52)	17(2)	24(2)	16(2)	-4(1)	2(1)	-11(1)
C(57)	30(2)	17(2)	18(2)	-3(1)	-1(1)	-11(1)
C(58)	41(3)	33(2)	43(3)	9(2)	-7(2)	-25(2)
C(59)	28(2)	27(2)	30(2)	-3(2)	-2(2)	-5(2)
C(53)	22(2)	26(2)	16(2)	-8(1)	0(1)	-10(1)
C(54)	18(2)	36(2)	16(2)	-3(1)	-1(1)	-11(1)
C(60)	29(2)	46(2)	15(2)	-7(2)	-2(1)	-13(2)
C(61)	33(2)	75(4)	26(2)	-9(2)	-5(2)	-29(2)
C(62)	51(3)	58(3)	18(2)	7(2)	-13(2)	-17(2)
C(55)	22(2)	31(2)	18(2)	5(1)	-4(1)	-12(1)
C(56)	20(2)	23(2)	18(2)	1(1)	-2(1)	-10(1)
C(63)	32(2)	23(2)	21(2)	3(1)	-8(1)	-12(2)
C(64)	51(3)	33(2)	44(3)	11(2)	-3(2)	-25(2)
C(65)	42(3)	29(2)	41(3)	-3(2)	-3(2)	-10(2)
O(2)	17(1)	20(1)	23(1)	2(1)	0(1)	-10(1)
C(71)	16(2)	31(2)	28(2)	8(2)	-4(1)	-12(1)
C(72)	26(2)	31(2)	29(2)	6(2)	-6(2)	-16(2)
C(73)	34(2)	35(2)	51(3)	17(2)	-18(2)	-26(2)
C(74)	28(2)	62(3)	30(2)	3(2)	8(2)	-16(2)
Mo(2)	12(1)	16(1)	18(1)	0(1)	-1(1)	-7(1)
C(101)	17(2)	18(2)	20(2)	0(1)	-3(1)	-10(1)
C(102)	14(2)	17(2)	19(2)	-3(1)	0(1)	-5(1)

C(103)	15(2)	22(2)	32(2)	-4(1)	2(1)	-8(1)
C(104)	26(2)	21(2)	14(2)	2(1)	-2(1)	-5(1)
C(105)	17(2)	16(2)	17(2)	0(1)	0(1)	-7(1)
C(106)	19(2)	18(2)	20(2)	0(1)	0(1)	-9(1)
C(107)	22(2)	23(2)	27(2)	1(1)	-4(1)	-12(1)
C(108)	33(2)	25(2)	31(2)	0(2)	-8(2)	-20(2)
C(109)	34(2)	19(2)	42(3)	4(2)	-9(2)	-14(2)
C(110)	20(2)	20(2)	37(2)	4(2)	-4(1)	-9(1)
N(2)	20(2)	20(1)	20(2)	1(1)	-3(1)	-9(1)
C(111)	20(2)	16(1)	16(2)	1(1)	-2(1)	-8(1)
C(112)	45(3)	32(2)	26(2)	-3(2)	-6(2)	-6(2)
C(113)	23(2)	55(3)	25(2)	2(2)	-3(2)	-14(2)
C(114)	45(2)	44(2)	20(2)	-1(2)	1(2)	-28(2)
C(115)	48(3)	41(2)	30(2)	-16(2)	-8(2)	2(2)
C(116)	48(3)	43(3)	32(2)	-10(2)	-1(2)	-20(2)
C(117)	28(2)	51(3)	28(2)	3(2)	-9(2)	-9(2)
C(118)	73(4)	36(2)	22(2)	7(2)	-16(2)	-1(2)
C(119)	64(3)	51(3)	24(2)	1(2)	3(2)	-36(3)
C(120)	34(2)	77(4)	24(2)	4(2)	5(2)	-19(2)
O(3)	12(1)	20(1)	22(1)	2(1)	-3(1)	-9(1)
C(121)	10(1)	13(1)	21(2)	2(1)	-4(1)	-5(1)
C(122)	11(2)	12(1)	20(2)	3(1)	-1(1)	-4(1)
C(131)	16(2)	19(2)	14(2)	0(1)	0(1)	-8(1)
C(132)	14(2)	17(2)	18(2)	1(1)	0(1)	-5(1)
C(137)	17(2)	19(2)	20(2)	2(1)	0(1)	-6(1)
C(138)	29(2)	28(2)	33(2)	-8(2)	4(2)	-15(2)
C(139)	27(2)	26(2)	24(2)	2(1)	-4(1)	-1(2)
C(133)	17(2)	22(2)	18(2)	4(1)	0(1)	-6(1)
C(134)	17(2)	25(2)	16(2)	1(1)	1(1)	-6(1)
C(140)	21(2)	33(2)	18(2)	1(1)	2(1)	-4(1)
C(141)	37(2)	44(2)	21(2)	6(2)	7(2)	-15(2)
C(142)	34(2)	53(3)	21(2)	-8(2)	5(2)	-14(2)
C(135)	22(2)	22(2)	18(2)	-2(1)	0(1)	-8(1)
C(136)	14(2)	16(2)	23(2)	0(1)	1(1)	-5(1)
C(143)	27(2)	17(2)	31(2)	-2(1)	7(1)	-10(1)
C(144)	39(2)	29(2)	55(3)	-6(2)	7(2)	-22(2)

C(145)	29(2)	22(2)	49(3)	7(2)	-6(2)	-8(2)
C(123)	15(2)	18(2)	26(2)	5(1)	-2(1)	-10(1)
C(124)	15(2)	24(2)	24(2)	4(1)	-4(1)	-12(1)
C(125)	17(2)	24(2)	20(2)	6(1)	-2(1)	-10(1)
C(126)	12(2)	20(2)	24(2)	5(1)	-1(1)	-9(1)
C(151)	9(3)	17(3)	16(3)	2(2)	0(2)	-6(3)
C(152)	11(2)	9(2)	16(2)	0(2)	-1(2)	-3(2)
C(157)	16(2)	17(3)	22(2)	-8(2)	1(2)	-9(2)
C(158)	20(3)	19(4)	20(3)	-10(2)	3(2)	-6(3)
C(159)	18(2)	15(2)	27(3)	-2(3)	4(2)	-7(2)
C(153)	10(2)	9(2)	19(2)	-1(2)	1(1)	-3(2)
C(154)	13(2)	14(2)	16(2)	-2(2)	4(2)	-7(2)
C(160)	15(2)	16(2)	21(2)	-6(2)	7(1)	-11(2)
C(161)	13(3)	35(4)	35(4)	13(3)	2(3)	-10(3)
C(162)	17(2)	24(2)	19(2)	-1(2)	3(2)	-14(2)
C(155)	14(2)	9(2)	21(3)	-1(2)	4(2)	-5(2)
C(156)	11(2)	16(2)	15(2)	-1(2)	3(1)	-5(2)
C(163)	12(3)	16(3)	18(3)	1(2)	4(2)	-7(2)
C(164)	18(4)	22(4)	26(4)	-5(2)	5(3)	-7(3)
C(165)	15(3)	19(3)	30(4)	-3(2)	2(2)	-2(2)
C(51A)	14(5)	13(5)	19(6)	1(4)	3(4)	-4(5)
C(52A)	18(5)	11(5)	16(5)	3(4)	0(3)	-7(4)
C(57A)	18(5)	17(5)	27(5)	-4(5)	5(4)	-10(4)
C(58A)	23(7)	13(9)	39(7)	-16(6)	-2(6)	0(7)
C(59A)	31(6)	13(6)	29(7)	-5(7)	-1(5)	-7(5)
C(53A)	10(2)	9(2)	19(2)	-1(2)	1(1)	-3(2)
C(54A)	13(4)	8(4)	14(4)	0(3)	2(3)	-6(3)
C(60A)	15(2)	16(2)	21(2)	-6(2)	7(1)	-11(2)
C(61A)	37(10)	18(8)	32(7)	15(6)	-4(6)	-18(7)
C(62A)	18(3)	10(4)	19(5)	-1(4)	6(4)	-8(3)
C(55A)	19(5)	14(5)	12(5)	-4(4)	5(3)	-8(4)
C(56A)	11(2)	16(2)	15(2)	-1(2)	3(1)	-5(2)
C(63A)	13(6)	13(5)	32(7)	-3(4)	7(4)	-3(4)
C(64A)	24(9)	13(8)	22(7)	-6(5)	9(6)	-5(7)
C(65A)	17(8)	18(6)	31(9)	3(6)	5(6)	-3(4)
O(4)	13(1)	21(1)	28(1)	1(1)	-2(1)	-9(1)

C(171)	13(2)	22(2)	22(2)	-3(1)	1(1)	-10(1)
C(172)	18(2)	24(2)	32(2)	-5(2)	5(1)	-11(1)
C(173)	17(2)	40(2)	34(2)	-2(2)	-6(2)	-12(2)
C(174)	30(2)	23(2)	33(2)	-4(2)	4(2)	-17(2)

Table S7E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **5**.

	x	y	z	U(eq)
H(1)	8450(40)	440(40)	9114(7)	21
H(3A)	8558	-1305	8342	36
H(3B)	9806	-2378	8437	36
H(3C)	9832	-1200	8323	36
H(4A)	10926	-1209	8876	35
H(4B)	10913	-2394	8988	35
H(4C)	10382	-1342	9261	35
H(6)	7108	-296	9267	25
H(7)	6034	-1178	9569	30
H(8)	6736	-3150	9538	32
H(9)	8526	-4231	9208	36
H(10)	9613	-3355	8913	27
H(12A)	7911	2416	7684	41
H(12B)	6511	2598	7714	41
H(13A)	9264	-653	7760	39
H(13B)	9617	393	7699	39
H(14A)	5992	970	7815	41
H(14B)	7052	-304	7829	41
H(15)	7069	2731	7090	47
H(16A)	9174	1447	7130	50
H(16B)	8558	1106	6803	50
H(17)	9760	-565	7130	42
H(18A)	8246	-1198	7286	44
H(18B)	7967	-576	6905	44
H(19)	6129	35	7242	48
H(20A)	5554	2051	7239	50
H(20B)	6263	1477	6873	50
H(37)	6618	679	9828	34
H(38A)	8796	-247	9717	55
H(38B)	8353	-873	10021	55

H(38C)	8999	-76	10131	55
H(39A)	7265	1121	10530	52
H(39B)	6619	301	10449	52
H(39C)	5890	1642	10388	52
H(33)	8649	1724	10164	38
H(40)	9562	2858	10261	55
H(41A)	10383	2951	9708	77
H(41B)	10690	3661	10007	77
H(41C)	9660	4308	9718	77
H(42A)	9028	4662	10506	52
H(42B)	7916	4301	10537	52
H(42C)	7907	5193	10237	52
H(35)	7435	4622	9589	39
H(43)	5064	4217	9136	32
H(44A)	4272	5305	9663	57
H(44B)	4071	6143	9329	57
H(44C)	5154	5928	9602	57
H(45A)	6645	5334	9056	47
H(45B)	5525	5524	8800	47
H(45C)	6700	4321	8805	47
H(23)	4577	2555	9940	22
H(24)	2915	2239	9760	21
H(25)	2673	1992	9151	20
H(57)	4643	88	8899	25
H(58A)	2971	-261	8721	54
H(58B)	4154	-1423	8794	54
H(58C)	3778	-1009	8391	54
H(59A)	5899	-970	8249	46
H(59B)	6230	-1572	8633	46
H(59C)	6419	-446	8554	46
H(53)	3818	275	7975	25
H(60)	3545	1222	7360	37
H(61A)	1900	952	7632	64
H(61B)	1557	1494	7240	64
H(61C)	1033	2279	7589	64
H(62A)	2438	2801	7006	66

H(62B)	3345	3090	7250	66
H(62C)	1915	3588	7355	66
H(55)	2852	3629	7872	28
H(63)	3664	4031	8762	30
H(64A)	5000	4064	8295	60
H(64B)	4044	5337	8392	60
H(64C)	3862	4730	8041	60
H(65A)	1686	5154	8285	59
H(65B)	1936	5715	8636	59
H(65C)	1542	4690	8674	59
H(72A)	9712	1767	9293	41
H(72B)	11083	1473	9157	41
H(72C)	10417	711	9029	41
H(73A)	9298	3948	8649	54
H(73B)	10429	3435	8915	54
H(73C)	9067	3743	9063	54
H(74A)	10657	1040	8378	62
H(74B)	11434	1726	8482	62
H(74C)	10263	2307	8234	62
H(101)	1540(40)	4610(40)	4107(7)	21
H(10A)	-820	6252	3852	35
H(10B)	-755	7373	4003	35
H(10C)	-296	6246	4243	35
H(10D)	1663	6256	3327	33
H(10E)	395	7327	3420	33
H(10F)	397	6139	3311	33
H(106)	3046	5264	4226	22
H(107)	4054	6145	4537	28
H(108)	3318	8131	4522	32
H(109)	1553	9208	4203	37
H(110)	515	8331	3906	30
H(11A)	3229	2216	2736	45
H(11B)	4322	2601	2769	45
H(11C)	747	5029	2733	43
H(11D)	1036	3706	2720	43
H(11E)	3893	4623	2788	40

H(11F)	2513	5597	2778	40
H(115)	4210	2074	2156	56
H(11G)	2400	3119	1829	49
H(11H)	2061	2551	2173	49
H(117)	619	4487	2117	46
H(11I)	1916	5265	1858	61
H(11J)	1310	5942	2222	61
H(119)	3466	5437	2197	51
H(12C)	4130	3722	1874	57
H(12D)	4867	3512	2241	57
H(137)	5278	4945	3880	23
H(13C)	7162	5062	3822	44
H(13D)	6074	6319	3824	44
H(13E)	6748	5750	3454	44
H(13F)	4637	6191	3222	44
H(13G)	4017	6665	3606	44
H(13H)	3812	5657	3419	44
H(133)	6379	4726	2966	24
H(140)	6781	3830	2360	32
H(14C)	8457	3976	2615	52
H(14D)	8861	3358	2233	52
H(14E)	9240	2627	2594	52
H(14F)	8261	1436	2324	57
H(14G)	7795	2272	1987	57
H(14H)	6832	2025	2234	57
H(135)	7408	1365	2867	26
H(143)	6503	954	3755	30
H(14I)	5260	867	3294	58
H(14J)	6242	-392	3388	58
H(14K)	6437	232	3037	58
H(14L)	8585	-81	3283	52
H(14M)	8276	-736	3607	52
H(14N)	8616	299	3689	52
H(123)	7413	3026	4140	23
H(124)	7123	2770	4752	24
H(125)	5445	2440	4937	24

H(157)	3404	4378	4813	21
H(15A)	2610	4018	5522	31
H(15B)	3302	4804	5435	31
H(15C)	4013	3455	5387	31
H(15D)	1236	5313	4705	30
H(15E)	1642	5948	5006	30
H(15F)	978	5157	5121	30
H(153)	1288	3361	5164	16
H(160)	346	2190	5278	19
H(16C)	2054	-153	5217	42
H(16D)	866	291	5477	42
H(16E)	1945	667	5547	42
H(16F)	-426	2039	4718	28
H(16G)	-610	1181	4998	28
H(16H)	471	711	4701	28
H(155)	2593	418	4623	18
H(163)	5026	782	4158	18
H(16I)	3379	-255	4074	34
H(16J)	4587	-550	3830	34
H(16K)	3473	690	3814	34
H(16L)	5628	-293	4704	35
H(16M)	6029	-1084	4354	35
H(16N)	4861	-980	4591	35
H(57A)	3380	4110	4791	24
H(58D)	3384	4495	5402	41
H(58E)	4173	3161	5338	41
H(58F)	2809	3623	5503	41
H(59D)	1420	5225	4712	38
H(59E)	1494	5433	5132	38
H(59F)	957	4570	5001	38
H(53A)	1451	2855	5146	16
H(60A)	1262	269	4896	19
H(61D)	1729	1041	5565	40
H(61E)	2440	-209	5399	40
H(61F)	1044	229	5535	40
H(62D)	-223	2459	5192	22

H(62E)	-653	1464	5143	22
H(62F)	-365	2056	4797	22
H(55A)	2959	21	4548	18
H(63A)	5265	614	4101	24
H(64D)	3661	-466	4000	31
H(64E)	4833	-681	3748	31
H(64F)	3688	542	3756	31
H(65D)	5707	-592	4661	36
H(65E)	6415	-1170	4296	36
H(65F)	5250	-1365	4431	36
H(17A)	429	3216	4294	35
H(17B)	-931	3475	4175	35
H(17C)	-290	4257	4031	35
H(17D)	-510	3889	3385	45
H(17E)	-1235	3152	3500	45
H(17F)	-43	2611	3244	45
H(17G)	978	970	3671	40
H(17H)	-250	1483	3914	40
H(17I)	1044	1236	4087	40

Table S8A. Crystal data and structure refinement for **6d**.

Identification code	X8_12044	
Empirical formula	C48 H55 F6 Mo N O2	
Formula weight	887.87	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 11.3519(5) Å	α =102.7680(10)°
	b = 11.6306(6) Å	β=95.3350(10)°
	c = 18.6057(9) Å	γ =112.9690(10)°
Volume	2161.43(18) $Å^3$	
Z	2	
Density (calculated)	1.364 Mg/m^3	
Absorption coefficient	0.368 mm^{-1}	
F(000)	924	
Crystal size	0.23 x 0.22 x 0.10 mm^3	
Theta range for data collection	1.98 to 31.15°	
Index ranges	-16<=h<=16, -16<=k<=16, 0<=l<=27	
Reflections collected	13841	
Independent reflections	13841 [R(int) = 0.0495]	
Completeness to theta = 31.15°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9641 and 0.9201	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13841 / 49 / 536	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0354, wR2 = 0.0943	
R indices (all data)	R1 = 0.0374, wR2 = 0.0958	
Largest diff. peak and hole	0.894 and -1.196 $e.Å^{-3}$	

Table S8B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6d**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	5542(1)	7350(1)	7261(1)	13(1)
C(1)	4669(2)	7814(2)	8007(1)	16(1)
C(2)	4325(2)	8912(2)	8378(1)	18(1)
C(3)	3821(2)	8675(2)	9100(1)	25(1)
C(4)	3218(2)	8885(2)	7828(1)	26(1)
C(5)	5518(2)	10226(2)	8608(1)	17(1)
C(6)	5456(2)	11350(2)	8495(1)	23(1)
C(7)	6536(2)	12548(2)	8760(1)	28(1)
C(8)	7695(2)	12650(2)	9142(1)	25(1)
C(9)	7773(2)	11537(2)	9257(1)	22(1)
C(10)	6697(2)	10342(2)	8991(1)	19(1)
N(1)	6158(1)	8726(1)	6977(1)	17(1)
C(11)	6801(2)	9772(2)	6648(1)	15(1)
C(12)	7504(2)	9297(2)	6062(1)	28(1)
C(13)	8196(2)	10393(2)	5704(1)	32(1)
C(14)	9184(2)	11597(2)	6311(1)	38(1)
C(15)	8476(2)	12065(2)	6886(1)	34(1)
C(16)	7808(2)	10970(2)	7252(1)	29(1)
C(17)	5790(2)	10121(2)	6259(1)	27(1)
C(18)	6483(2)	11207(2)	5895(1)	29(1)
C(19)	7175(2)	10736(2)	5319(1)	31(1)
C(20)	7461(2)	12401(2)	6500(1)	35(1)
O(1)	4244(1)	5909(1)	6455(1)	21(1)
C(21)	2975(2)	5362(2)	6056(1)	24(1)
C(22)	1954(2)	5178(2)	6572(1)	32(1)
C(23)	2821(2)	6244(2)	5580(1)	30(1)
F(1)	1624(2)	5738(2)	5148(1)	46(1)
F(2)	3678(2)	6477(2)	5133(1)	48(1)
F(3)	3000(1)	7391(1)	6026(1)	38(1)
C(24)	2757(2)	4018(2)	5543(1)	33(1)
F(4)	3571(2)	4113(2)	5082(1)	53(1)

F(5)	2870(2)	3271(1)	5962(1)	50(1)
F(6)	1538(2)	3381(1)	5125(1)	49(1)
O(2)	6874(1)	6922(1)	7686(1)	16(1)
C(31)	7618(1)	6815(1)	8254(1)	15(1)
C(32)	7041(2)	6126(2)	8756(1)	16(1)
C(33)	7846(2)	5971(2)	9307(1)	20(1)
C(34)	9190(2)	6473(2)	9360(1)	22(1)
C(35)	9753(2)	7181(2)	8873(1)	20(1)
C(36)	8982(2)	7366(2)	8319(1)	16(1)
C(41)	5605(2)	5600(2)	8724(1)	17(1)
C(42)	4727(2)	4582(2)	8106(1)	19(1)
C(43)	3384(2)	4140(2)	8094(1)	23(1)
C(44)	2897(2)	4682(2)	8668(1)	25(1)
C(45)	3786(2)	5675(2)	9279(1)	22(1)
C(46)	5134(2)	6140(2)	9321(1)	19(1)
C(47)	5189(2)	3947(2)	7465(1)	24(1)
C(48)	1447(2)	4226(2)	8630(1)	36(1)
C(49)	6034(2)	7227(2)	9999(1)	24(1)
C(51)	9624(1)	8154(2)	7816(1)	16(1)
C(52)	9637(2)	7535(2)	7078(1)	20(1)
C(53)	10339(2)	8288(2)	6643(1)	23(1)
C(54)	11018(2)	9630(2)	6919(1)	23(1)
C(55)	10960(2)	10228(2)	7641(1)	22(1)
C(56)	10276(2)	9511(2)	8097(1)	18(1)
C(57)	8933(2)	6078(2)	6766(1)	30(1)
C(58)	11840(2)	10411(2)	6454(1)	34(1)
C(59)	10277(2)	10199(2)	8884(1)	27(1)

Table S8C. Bond lengths [Å] and angles [°] for **6d**.

Mo(1)-N(1)	1.7028(14)
Mo(1)-C(1)	1.8821(16)
Mo(1)-O(2)	1.9230(11)
Mo(1)-O(1)	1.9444(12)
C(1)-C(2)	1.521(2)
C(1)-H(1)	0.940(16)
C(2)-C(5)	1.529(2)
C(2)-C(4)	1.530(2)
C(2)-C(3)	1.546(2)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-C(6)	1.395(2)
C(5)-C(10)	1.399(2)
C(6)-C(7)	1.393(3)
C(6)-H(6)	0.9500
C(7)-C(8)	1.384(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.393(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.388(2)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
N(1)-C(11)	1.4523(19)
C(11)-C(16)	1.529(2)
C(11)-C(17)	1.532(2)
C(11)-C(12)	1.539(2)
C(12)-C(13)	1.542(3)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900
C(13)-C(14)	1.529(3)

C(13)-C(19)	1.532(3)
C(13)-H(13)	1.0000
C(14)-C(15)	1.526(4)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(20)	1.523(3)
C(15)-C(16)	1.545(3)
C(15)-H(15)	1.0000
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.541(3)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-C(20)	1.516(3)
C(18)-C(19)	1.516(3)
C(18)-H(18)	1.0000
C(19)-H(19A)	0.9900
C(19)-H(19B)	0.9900
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
O(1)-C(21)	1.382(2)
C(21)-C(23)	1.542(3)
C(21)-C(24)	1.552(3)
C(21)-C(22)	1.555(3)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-F(2)	1.324(3)
C(23)-F(3)	1.334(2)
C(23)-F(1)	1.343(2)
C(24)-F(4)	1.309(3)
C(24)-F(5)	1.322(2)
C(24)-F(6)	1.347(2)
O(2)-C(31)	1.3484(18)
C(31)-C(32)	1.407(2)
C(31)-C(36)	1.408(2)

C(32)-C(33)	1.398(2)
C(32)-C(41)	1.491(2)
C(33)-C(34)	1.390(2)
C(33)-H(33)	0.9500
C(34)-C(35)	1.390(2)
C(34)-H(34)	0.9500
C(35)-C(36)	1.398(2)
C(35)-H(35)	0.9500
C(36)-C(51)	1.493(2)
C(41)-C(46)	1.406(2)
C(41)-C(42)	1.408(2)
C(42)-C(43)	1.402(2)
C(42)-C(47)	1.508(2)
C(43)-C(44)	1.389(3)
C(43)-H(43)	0.9500
C(44)-C(45)	1.393(3)
C(44)-C(48)	1.509(3)
C(45)-C(46)	1.398(2)
C(45)-H(45)	0.9500
C(46)-C(49)	1.511(2)
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(51)-C(56)	1.402(2)
C(51)-C(52)	1.407(2)
C(52)-C(53)	1.393(2)
C(52)-C(57)	1.506(3)
C(53)-C(54)	1.388(3)
C(53)-H(53)	0.9500
C(54)-C(55)	1.389(3)

C(54)-C(58)	1.512(2)
C(55)-C(56)	1.396(2)
C(55)-H(55)	0.9500
C(56)-C(59)	1.505(2)
C(57)-H(57A)	0.9800
C(57)-H(57B)	0.9800
C(57)-H(57C)	0.9800
C(58)-H(58A)	0.9800
C(58)-H(58B)	0.9800
C(58)-H(58C)	0.9800
C(59)-H(59A)	0.9800
C(59)-H(59B)	0.9800
C(59)-H(59C)	0.9800

N(1)-Mo(1)-C(1)	101.82(7)
N(1)-Mo(1)-O(2)	113.06(6)
C(1)-Mo(1)-O(2)	110.11(6)
N(1)-Mo(1)-O(1)	110.90(6)
C(1)-Mo(1)-O(1)	107.81(6)
O(2)-Mo(1)-O(1)	112.50(5)
C(2)-C(1)-Mo(1)	141.90(12)
C(2)-C(1)-H(1)	117.4(15)
Mo(1)-C(1)-H(1)	100.6(14)
C(1)-C(2)-C(5)	111.46(13)
C(1)-C(2)-C(4)	107.55(14)
C(5)-C(2)-C(4)	112.43(14)
C(1)-C(2)-C(3)	109.61(14)
C(5)-C(2)-C(3)	107.48(13)
C(4)-C(2)-C(3)	108.25(14)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-H(4A)	109.5

C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(6)-C(5)-C(10)	117.92(15)
C(6)-C(5)-C(2)	122.32(15)
C(10)-C(5)-C(2)	119.61(14)
C(7)-C(6)-C(5)	120.84(17)
C(7)-C(6)-H(6)	119.6
C(5)-C(6)-H(6)	119.6
C(8)-C(7)-C(6)	120.63(17)
C(8)-C(7)-H(7)	119.7
C(6)-C(7)-H(7)	119.7
C(7)-C(8)-C(9)	119.23(17)
C(7)-C(8)-H(8)	120.4
C(9)-C(8)-H(8)	120.4
C(10)-C(9)-C(8)	120.05(16)
C(10)-C(9)-H(9)	120.0
C(8)-C(9)-H(9)	120.0
C(9)-C(10)-C(5)	121.33(16)
C(9)-C(10)-H(10)	119.3
C(5)-C(10)-H(10)	119.3
C(11)-N(1)-Mo(1)	169.14(12)
N(1)-C(11)-C(16)	110.46(13)
N(1)-C(11)-C(17)	110.00(13)
C(16)-C(11)-C(17)	109.94(15)
N(1)-C(11)-C(12)	108.12(13)
C(16)-C(11)-C(12)	109.00(15)
C(17)-C(11)-C(12)	109.29(14)
C(11)-C(12)-C(13)	109.09(15)
C(11)-C(12)-H(12A)	109.9
C(13)-C(12)-H(12A)	109.9
C(11)-C(12)-H(12B)	109.9
C(13)-C(12)-H(12B)	109.9
H(12A)-C(12)-H(12B)	108.3

C(14)-C(13)-C(19)	109.32(18)
C(14)-C(13)-C(12)	109.84(17)
C(19)-C(13)-C(12)	109.00(17)
C(14)-C(13)-H(13)	109.6
C(19)-C(13)-H(13)	109.6
C(12)-C(13)-H(13)	109.6
C(15)-C(14)-C(13)	109.45(16)
C(15)-C(14)-H(14A)	109.8
C(13)-C(14)-H(14A)	109.8
C(15)-C(14)-H(14B)	109.8
C(13)-C(14)-H(14B)	109.8
H(14A)-C(14)-H(14B)	108.2
C(20)-C(15)-C(14)	109.93(17)
C(20)-C(15)-C(16)	110.12(18)
C(14)-C(15)-C(16)	108.58(19)
C(20)-C(15)-H(15)	109.4
C(14)-C(15)-H(15)	109.4
C(16)-C(15)-H(15)	109.4
C(11)-C(16)-C(15)	109.31(14)
C(11)-C(16)-H(16A)	109.8
C(15)-C(16)-H(16A)	109.8
C(11)-C(16)-H(16B)	109.8
C(15)-C(16)-H(16B)	109.8
H(16A)-C(16)-H(16B)	108.3
C(11)-C(17)-C(18)	109.37(14)
C(11)-C(17)-H(17A)	109.8
C(18)-C(17)-H(17A)	109.8
C(11)-C(17)-H(17B)	109.8
C(18)-C(17)-H(17B)	109.8
H(17A)-C(17)-H(17B)	108.2
C(20)-C(18)-C(19)	110.11(17)
C(20)-C(18)-C(17)	109.33(17)
C(19)-C(18)-C(17)	109.45(17)
C(20)-C(18)-H(18)	109.3
C(19)-C(18)-H(18)	109.3
C(17)-C(18)-H(18)	109.3

C(18)-C(19)-C(13)	109.80(15)
C(18)-C(19)-H(19A)	109.7
C(13)-C(19)-H(19A)	109.7
C(18)-C(19)-H(19B)	109.7
C(13)-C(19)-H(19B)	109.7
H(19A)-C(19)-H(19B)	108.2
C(18)-C(20)-C(15)	109.54(16)
C(18)-C(20)-H(20A)	109.8
C(15)-C(20)-H(20A)	109.8
C(18)-C(20)-H(20B)	109.8
C(15)-C(20)-H(20B)	109.8
H(20A)-C(20)-H(20B)	108.2
C(21)-O(1)-Mo(1)	145.23(12)
O(1)-C(21)-C(23)	109.30(15)
O(1)-C(21)-C(24)	105.78(16)
C(23)-C(21)-C(24)	110.77(16)
O(1)-C(21)-C(22)	112.76(15)
C(23)-C(21)-C(22)	108.46(17)
C(24)-C(21)-C(22)	109.77(16)
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
F(2)-C(23)-F(3)	107.27(17)
F(2)-C(23)-F(1)	107.67(17)
F(3)-C(23)-F(1)	106.48(18)
F(2)-C(23)-C(21)	112.48(18)
F(3)-C(23)-C(21)	110.17(16)
F(1)-C(23)-C(21)	112.45(16)
F(4)-C(24)-F(5)	109.6(2)
F(4)-C(24)-F(6)	107.52(18)
F(5)-C(24)-F(6)	105.77(17)
F(4)-C(24)-C(21)	112.62(17)
F(5)-C(24)-C(21)	109.75(17)

F(6)-C(24)-C(21)	111.35(19)
C(31)-O(2)-Mo(1)	154.38(10)
O(2)-C(31)-C(32)	120.77(13)
O(2)-C(31)-C(36)	118.67(13)
C(32)-C(31)-C(36)	120.52(14)
C(33)-C(32)-C(31)	118.76(14)
C(33)-C(32)-C(41)	119.93(14)
C(31)-C(32)-C(41)	121.29(13)
C(34)-C(33)-C(32)	121.19(15)
C(34)-C(33)-H(33)	119.4
C(32)-C(33)-H(33)	119.4
C(35)-C(34)-C(33)	119.58(15)
C(35)-C(34)-H(34)	120.2
C(33)-C(34)-H(34)	120.2
C(34)-C(35)-C(36)	120.92(15)
C(34)-C(35)-H(35)	119.5
C(36)-C(35)-H(35)	119.5
C(35)-C(36)-C(31)	118.98(14)
C(35)-C(36)-C(51)	119.39(14)
C(31)-C(36)-C(51)	121.63(13)
C(46)-C(41)-C(42)	120.10(15)
C(46)-C(41)-C(32)	119.05(14)
C(42)-C(41)-C(32)	120.84(15)
C(43)-C(42)-C(41)	118.75(16)
C(43)-C(42)-C(47)	119.25(15)
C(41)-C(42)-C(47)	121.99(15)
C(44)-C(43)-C(42)	122.02(16)
C(44)-C(43)-H(43)	119.0
C(42)-C(43)-H(43)	119.0
C(43)-C(44)-C(45)	118.17(16)
C(43)-C(44)-C(48)	121.23(18)
C(45)-C(44)-C(48)	120.59(19)
C(44)-C(45)-C(46)	121.93(17)
C(44)-C(45)-H(45)	119.0
C(46)-C(45)-H(45)	119.0
C(45)-C(46)-C(41)	119.00(16)

C(45)-C(46)-C(49)	118.76(16)
C(41)-C(46)-C(49)	122.23(15)
C(42)-C(47)-H(47A)	109.5
C(42)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(42)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(44)-C(48)-H(48A)	109.5
C(44)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(44)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(46)-C(49)-H(49A)	109.5
C(46)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(46)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(56)-C(51)-C(52)	120.04(14)
C(56)-C(51)-C(36)	119.58(14)
C(52)-C(51)-C(36)	120.29(14)
C(53)-C(52)-C(51)	119.03(16)
C(53)-C(52)-C(57)	120.31(16)
C(51)-C(52)-C(57)	120.64(15)
C(54)-C(53)-C(52)	121.69(16)
C(54)-C(53)-H(53)	119.2
C(52)-C(53)-H(53)	119.2
C(53)-C(54)-C(55)	118.51(16)
C(53)-C(54)-C(58)	120.50(17)
C(55)-C(54)-C(58)	120.96(18)
C(54)-C(55)-C(56)	121.68(17)
C(54)-C(55)-H(55)	119.2
C(56)-C(55)-H(55)	119.2
C(55)-C(56)-C(51)	119.01(15)

C(55)-C(56)-C(59)	119.74(15)
C(51)-C(56)-C(59)	121.24(14)
C(52)-C(57)-H(57A)	109.5
C(52)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	109.5
C(52)-C(57)-H(57C)	109.5
H(57A)-C(57)-H(57C)	109.5
H(57B)-C(57)-H(57C)	109.5
C(54)-C(58)-H(58A)	109.5
C(54)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
C(54)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5
C(56)-C(59)-H(59A)	109.5
C(56)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	109.5
C(56)-C(59)-H(59C)	109.5
H(59A)-C(59)-H(59C)	109.5
H(59B)-C(59)-H(59C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S8D. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **6d**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	12(1)	13(1)	13(1)	3(1)	1(1)	5(1)
C(1)	14(1)	17(1)	17(1)	5(1)	2(1)	6(1)
C(2)	16(1)	20(1)	18(1)	5(1)	5(1)	10(1)
C(3)	26(1)	27(1)	25(1)	7(1)	13(1)	12(1)
C(4)	19(1)	30(1)	30(1)	4(1)	0(1)	15(1)
C(5)	19(1)	18(1)	14(1)	3(1)	4(1)	10(1)
C(6)	28(1)	22(1)	22(1)	5(1)	3(1)	15(1)
C(7)	39(1)	18(1)	25(1)	3(1)	2(1)	15(1)
C(8)	30(1)	17(1)	22(1)	0(1)	2(1)	7(1)
C(9)	22(1)	21(1)	19(1)	1(1)	1(1)	8(1)
C(10)	20(1)	17(1)	18(1)	3(1)	2(1)	8(1)
N(1)	19(1)	17(1)	17(1)	6(1)	4(1)	8(1)
C(11)	17(1)	15(1)	14(1)	5(1)	3(1)	7(1)
C(12)	41(1)	26(1)	27(1)	13(1)	18(1)	21(1)
C(13)	45(1)	36(1)	31(1)	20(1)	23(1)	25(1)
C(14)	20(1)	50(1)	48(1)	32(1)	9(1)	9(1)
C(15)	33(1)	25(1)	26(1)	6(1)	-4(1)	-5(1)
C(16)	32(1)	24(1)	18(1)	6(1)	-1(1)	1(1)
C(17)	21(1)	30(1)	37(1)	20(1)	6(1)	12(1)
C(18)	26(1)	30(1)	39(1)	22(1)	7(1)	14(1)
C(19)	37(1)	29(1)	21(1)	13(1)	2(1)	6(1)
C(20)	50(1)	20(1)	37(1)	11(1)	15(1)	15(1)
O(1)	19(1)	19(1)	18(1)	0(1)	-3(1)	6(1)
C(21)	23(1)	20(1)	22(1)	5(1)	-6(1)	3(1)
C(22)	25(1)	37(1)	29(1)	11(1)	3(1)	7(1)
C(23)	30(1)	28(1)	25(1)	8(1)	-4(1)	7(1)
F(1)	42(1)	42(1)	39(1)	10(1)	-19(1)	10(1)
F(2)	58(1)	57(1)	39(1)	28(1)	20(1)	24(1)
F(3)	44(1)	30(1)	36(1)	6(1)	-6(1)	17(1)
C(24)	38(1)	20(1)	26(1)	2(1)	-7(1)	2(1)
F(4)	61(1)	34(1)	47(1)	-9(1)	16(1)	12(1)

F(5)	72(1)	21(1)	44(1)	6(1)	-16(1)	13(1)
F(6)	46(1)	31(1)	41(1)	0(1)	-21(1)	-2(1)
O(2)	15(1)	18(1)	16(1)	7(1)	3(1)	8(1)
C(31)	15(1)	13(1)	16(1)	3(1)	1(1)	6(1)
C(32)	15(1)	14(1)	18(1)	5(1)	1(1)	5(1)
C(33)	19(1)	18(1)	21(1)	8(1)	0(1)	5(1)
C(34)	18(1)	22(1)	24(1)	10(1)	-2(1)	6(1)
C(35)	15(1)	21(1)	24(1)	8(1)	0(1)	6(1)
C(36)	16(1)	15(1)	18(1)	5(1)	3(1)	7(1)
C(41)	15(1)	16(1)	18(1)	8(1)	2(1)	4(1)
C(42)	19(1)	16(1)	21(1)	7(1)	1(1)	5(1)
C(43)	17(1)	20(1)	26(1)	9(1)	-1(1)	2(1)
C(44)	16(1)	29(1)	30(1)	16(1)	4(1)	6(1)
C(45)	20(1)	27(1)	24(1)	14(1)	8(1)	9(1)
C(46)	18(1)	19(1)	18(1)	9(1)	3(1)	6(1)
C(47)	24(1)	18(1)	24(1)	2(1)	0(1)	7(1)
C(48)	16(1)	48(1)	42(1)	20(1)	6(1)	7(1)
C(49)	26(1)	25(1)	20(1)	4(1)	3(1)	9(1)
C(51)	13(1)	19(1)	17(1)	6(1)	3(1)	8(1)
C(52)	17(1)	22(1)	18(1)	3(1)	2(1)	9(1)
C(53)	20(1)	35(1)	17(1)	7(1)	5(1)	14(1)
C(54)	20(1)	32(1)	24(1)	15(1)	10(1)	14(1)
C(55)	20(1)	21(1)	29(1)	12(1)	10(1)	11(1)
C(56)	18(1)	19(1)	20(1)	6(1)	7(1)	10(1)
C(57)	30(1)	24(1)	25(1)	-4(1)	3(1)	8(1)
C(58)	37(1)	44(1)	35(1)	23(1)	22(1)	20(1)
C(59)	34(1)	20(1)	26(1)	3(1)	14(1)	9(1)

Table S8E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **6d**.

	x	y	z	U(eq)
H(1)	4340(20)	7045(18)	8156(13)	19
H(3A)	3072	7824	8974	38
H(3B)	3553	9357	9323	38
H(3C)	4518	8692	9461	38
H(4A)	3538	9096	7381	39
H(4B)	2914	9526	8071	39
H(4C)	2495	8015	7680	39
H(6)	4668	11296	8235	28
H(7)	6477	13303	8677	33
H(8)	8428	13471	9323	30
H(9)	8564	11595	9517	26
H(10)	6762	9589	9071	22
H(12A)	6863	8517	5668	33
H(12B)	8152	9057	6307	33
H(13)	8657	10092	5323	38
H(14A)	9846	11382	6564	45
H(14B)	9638	12296	6080	45
H(15)	9123	12855	7282	41
H(16A)	8471	10746	7496	34
H(16B)	7373	11268	7642	34
H(17A)	5327	10420	6631	32
H(17B)	5137	9344	5869	32
H(18)	5822	11433	5640	35
H(19A)	7606	11424	5076	37
H(19B)	6531	9959	4925	37
H(20A)	7004	12705	6874	42
H(20B)	7895	13110	6271	42
H(22A)	2058	4641	6890	48
H(22B)	1072	4747	6262	48
H(22C)	2090	6029	6891	48

H(33)	7467	5514	9652	24
H(34)	9722	6334	9726	27
H(35)	10675	7543	8918	24
H(43)	2789	3449	7679	28
H(45)	3466	6046	9679	27
H(47A)	5002	4210	7018	35
H(47B)	4733	2999	7355	35
H(47C)	6131	4218	7605	35
H(48A)	1109	4645	8314	55
H(48B)	1282	4459	9138	55
H(48C)	1008	3280	8415	55
H(49A)	6364	6863	10355	37
H(49B)	5553	7690	10243	37
H(49C)	6768	7834	9840	37
H(53)	10353	7872	6146	28
H(55)	11396	11149	7828	26
H(57A)	9157	5807	6280	45
H(57B)	7989	5814	6698	45
H(57C)	9196	5665	7117	45
H(58A)	12118	11341	6691	52
H(58B)	11325	10169	5947	52
H(58C)	12611	10231	6420	52
H(59A)	10855	10058	9245	41
H(59B)	9388	9855	8980	41
H(59C)	10588	11134	8939	41

Table S9A. Crystal data and structure refinement for **7b**.

Identification code	X8_12055	
Empirical formula	C47 H52 F6 Mo N2 O	
Formula weight	870.85	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 20.7835(19) Å	α= 90°
	b = 10.8355(10) Å	β= 104.390(2)°
	c = 19.7836(18) Å	γ = 90°
Volume	4315.5(7) $Å^3$	
Z	4	
Density (calculated)	1.340 Mg/m^3	
Absorption coefficient	0.366 mm^{-1}	
F(000)	1808	
Crystal size	0.06 x 0.05 x 0.02 mm^3	
Theta range for data collection	2.02 to 31.00°	
Index ranges	-30<=h<=30, -15<=k<=15, -28<=l<=28	
Reflections collected	205294	
Independent reflections	13705 [R(int) = 0.0537]	
Completeness to theta = 31.00°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9927 and 0.9783	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13705 / 2 / 531	
Goodness-of-fit on F^2	1.061	
Final R indices [I>2sigma(I)]	R1 = 0.0327, wR2 = 0.0786	
R indices (all data)	R1 = 0.0432, wR2 = 0.0836	
Largest diff. peak and hole	1.422 and -0.642 $e.Å^{-3}$	

Table S9B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **7b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	7395(1)	8313(1)	3074(1)	16(1)
C(1)	7551(1)	9186(1)	3923(1)	19(1)
C(2)	7841(1)	10356(2)	4300(1)	21(1)
C(3)	8288(1)	9988(2)	5018(1)	32(1)
C(4)	8278(1)	11026(2)	3898(1)	30(1)
C(5)	7248(1)	11136(1)	4375(1)	20(1)
C(6)	6870(1)	10785(2)	4836(1)	25(1)
C(7)	6291(1)	11412(2)	4856(1)	29(1)
C(8)	6081(1)	12408(2)	4419(1)	31(1)
C(9)	6456(1)	12792(2)	3979(1)	34(1)
C(10)	7035(1)	12163(2)	3954(1)	27(1)
O(1)	6457(1)	7857(1)	2805(1)	21(1)
C(21)	5880(1)	7951(2)	3036(1)	21(1)
C(22)	5809(1)	9174(2)	3391(1)	30(1)
C(23)	5884(1)	6883(2)	3547(1)	33(1)
F(1)	5340(1)	6856(1)	3795(1)	49(1)
F(2)	5938(1)	5780(1)	3276(1)	50(1)
F(3)	6406(1)	7006(1)	4103(1)	47(1)
C(24)	5288(1)	7810(2)	2390(1)	26(1)
F(4)	4705(1)	7979(1)	2548(1)	39(1)
F(5)	5260(1)	6713(1)	2083(1)	40(1)
F(6)	5328(1)	8654(1)	1911(1)	41(1)
N(1)	7666(1)	9370(1)	2554(1)	20(1)
C(11)	7810(1)	10209(2)	2080(1)	23(1)
C(12)	8467(1)	10586(2)	2158(1)	31(1)
C(13)	8623(1)	11422(2)	1695(1)	43(1)
C(14)	8125(1)	11857(2)	1147(1)	47(1)
C(15)	7472(1)	11476(2)	1064(1)	38(1)
C(16)	7294(1)	10658(2)	1528(1)	27(1)
C(17)	6581(1)	10306(2)	1484(1)	28(1)
C(18)	6302(1)	11160(2)	1956(1)	36(1)

C(19)	6125(1)	10323(2)	744(1)	45(1)
N(2)	8048(1)	6957(1)	3401(1)	20(1)
C(31)	8480(1)	6305(1)	3087(1)	20(1)
C(32)	9129(1)	6048(2)	3488(1)	22(1)
C(41)	9343(1)	6504(2)	4223(1)	21(1)
C(42)	9165(1)	5850(2)	4763(1)	22(1)
C(43)	9352(1)	6320(2)	5440(1)	24(1)
C(44)	9727(1)	7388(2)	5602(1)	26(1)
C(45)	9898(1)	8022(2)	5062(1)	27(1)
C(46)	9706(1)	7610(2)	4375(1)	24(1)
C(47)	8784(1)	4656(2)	4621(1)	27(1)
C(48)	9950(1)	7842(2)	6345(1)	35(1)
C(49)	9870(1)	8364(2)	3801(1)	32(1)
C(33)	9562(1)	5383(2)	3194(1)	31(1)
C(34)	9365(1)	4953(2)	2513(1)	36(1)
C(35)	8726(1)	5204(2)	2121(1)	31(1)
C(36)	8277(1)	5884(2)	2393(1)	22(1)
C(51)	7598(1)	6118(2)	1942(1)	23(1)
C(52)	7059(1)	5404(2)	2022(1)	27(1)
C(53)	6439(1)	5569(2)	1558(1)	30(1)
C(54)	6342(1)	6414(2)	1017(1)	30(1)
C(55)	6882(1)	7114(2)	941(1)	27(1)
C(56)	7510(1)	6975(2)	1391(1)	23(1)
C(57)	7150(1)	4445(2)	2590(1)	36(1)
C(58)	5670(1)	6580(2)	513(1)	40(1)
C(59)	8090(1)	7699(2)	1264(1)	27(1)

Table S9C. Bond lengths [Å] and angles [°] for **7b**.

Mo(1)-N(1)	1.7261(13)
Mo(1)-C(1)	1.8833(16)
Mo(1)-O(1)	1.9518(11)
Mo(1)-N(2)	1.9950(13)
C(1)-C(2)	1.518(2)
C(1)-H(1)	0.977(14)
C(2)-C(4)	1.530(2)
C(2)-C(5)	1.533(2)
C(2)-C(3)	1.543(2)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-C(10)	1.394(2)
C(5)-C(6)	1.396(2)
C(6)-C(7)	1.392(2)
C(6)-H(6)	0.9500
C(7)-C(8)	1.384(3)
C(7)-H(7)	0.9500
C(8)-C(9)	1.370(3)
C(8)-H(8)	0.9500
C(9)-C(10)	1.393(3)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
O(1)-C(21)	1.3903(19)
C(21)-C(22)	1.524(2)
C(21)-C(23)	1.534(2)
C(21)-C(24)	1.547(2)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-F(2)	1.326(2)

C(23)-F(1)	1.340(2)
C(23)-F(3)	1.346(2)
C(24)-F(5)	1.329(2)
C(24)-F(6)	1.334(2)
C(24)-F(4)	1.3367(19)
N(1)-C(11)	1.390(2)
C(11)-C(12)	1.398(2)
C(11)-C(16)	1.412(2)
C(12)-C(13)	1.383(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.383(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.388(3)
C(14)-H(14)	0.9500
C(15)-C(16)	1.391(2)
C(15)-H(15)	0.9500
C(16)-C(17)	1.512(3)
C(17)-C(18)	1.529(3)
C(17)-C(19)	1.533(3)
C(17)-H(17)	1.0000
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
N(2)-C(31)	1.4041(19)
N(2)-H(2)	0.853(15)
C(31)-C(36)	1.409(2)
C(31)-C(32)	1.411(2)
C(32)-C(33)	1.388(2)
C(32)-C(41)	1.495(2)
C(41)-C(42)	1.406(2)
C(41)-C(46)	1.408(2)
C(42)-C(43)	1.394(2)
C(42)-C(47)	1.507(2)

C(43)-C(44)	1.388(3)
C(43)-H(43)	0.9500
C(44)-C(45)	1.389(3)
C(44)-C(48)	1.510(3)
C(45)-C(46)	1.391(2)
C(45)-H(45)	0.9500
C(46)-C(49)	1.507(2)
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
C(33)-C(34)	1.387(3)
C(33)-H(33)	0.9500
C(34)-C(35)	1.388(3)
C(34)-H(34)	0.9500
C(35)-C(36)	1.398(2)
C(35)-H(35)	0.9500
C(36)-C(51)	1.491(2)
C(51)-C(52)	1.403(2)
C(51)-C(56)	1.408(2)
C(52)-C(53)	1.394(3)
C(52)-C(57)	1.508(3)
C(53)-C(54)	1.386(3)
C(53)-H(53)	0.9500
C(54)-C(55)	1.394(3)
C(54)-C(58)	1.511(3)
C(55)-C(56)	1.393(2)
C(55)-H(55)	0.9500
C(56)-C(59)	1.512(2)
C(57)-H(57A)	0.9800
C(57)-H(57B)	0.9800

C(57)-H(57C)	0.9800
C(58)-H(58A)	0.9800
C(58)-H(58B)	0.9800
C(58)-H(58C)	0.9800
C(59)-H(59A)	0.9800
C(59)-H(59B)	0.9800
C(59)-H(59C)	0.9800

N(1)-Mo(1)-C(1)	100.88(7)
N(1)-Mo(1)-O(1)	117.20(6)
C(1)-Mo(1)-O(1)	108.03(6)
N(1)-Mo(1)-N(2)	112.67(6)
C(1)-Mo(1)-N(2)	97.41(6)
O(1)-Mo(1)-N(2)	117.02(5)
C(2)-C(1)-Mo(1)	144.78(12)
C(2)-C(1)-H(1)	112.7(12)
Mo(1)-C(1)-H(1)	102.5(12)
C(1)-C(2)-C(4)	110.82(13)
C(1)-C(2)-C(5)	106.07(12)
C(4)-C(2)-C(5)	112.58(14)
C(1)-C(2)-C(3)	108.14(14)
C(4)-C(2)-C(3)	107.64(15)
C(5)-C(2)-C(3)	111.54(13)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(10)-C(5)-C(6)	117.45(15)

C(10)-C(5)-C(2)	121.74(15)
C(6)-C(5)-C(2)	120.64(14)
C(7)-C(6)-C(5)	121.07(16)
C(7)-C(6)-H(6)	119.5
C(5)-C(6)-H(6)	119.5
C(8)-C(7)-C(6)	120.27(17)
C(8)-C(7)-H(7)	119.9
C(6)-C(7)-H(7)	119.9
C(9)-C(8)-C(7)	119.51(17)
C(9)-C(8)-H(8)	120.2
C(7)-C(8)-H(8)	120.2
C(8)-C(9)-C(10)	120.42(17)
C(8)-C(9)-H(9)	119.8
C(10)-C(9)-H(9)	119.8
C(9)-C(10)-C(5)	121.23(17)
C(9)-C(10)-H(10)	119.4
C(5)-C(10)-H(10)	119.4
C(21)-O(1)-Mo(1)	140.93(10)
O(1)-C(21)-C(22)	113.95(13)
O(1)-C(21)-C(23)	107.28(14)
C(22)-C(21)-C(23)	109.79(15)
O(1)-C(21)-C(24)	107.15(13)
C(22)-C(21)-C(24)	108.55(14)
C(23)-C(21)-C(24)	110.05(14)
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
F(2)-C(23)-F(1)	106.96(16)
F(2)-C(23)-F(3)	106.76(17)
F(1)-C(23)-F(3)	106.40(16)
F(2)-C(23)-C(21)	113.70(16)
F(1)-C(23)-C(21)	112.97(16)
F(3)-C(23)-C(21)	109.62(15)

F(5)-C(24)-F(6)	106.93(15)
F(5)-C(24)-F(4)	106.91(14)
F(6)-C(24)-F(4)	106.99(15)
F(5)-C(24)-C(21)	113.66(15)
F(6)-C(24)-C(21)	110.05(14)
F(4)-C(24)-C(21)	111.95(14)
C(11)-N(1)-Mo(1)	173.09(12)
N(1)-C(11)-C(12)	118.88(16)
N(1)-C(11)-C(16)	119.86(15)
C(12)-C(11)-C(16)	121.25(15)
C(13)-C(12)-C(11)	120.05(19)
C(13)-C(12)-H(12)	120.0
C(11)-C(12)-H(12)	120.0
C(14)-C(13)-C(12)	119.4(2)
C(14)-C(13)-H(13)	120.3
C(12)-C(13)-H(13)	120.3
C(13)-C(14)-C(15)	120.65(19)
C(13)-C(14)-H(14)	119.7
C(15)-C(14)-H(14)	119.7
C(14)-C(15)-C(16)	121.6(2)
C(14)-C(15)-H(15)	119.2
C(16)-C(15)-H(15)	119.2
C(15)-C(16)-C(11)	117.00(17)
C(15)-C(16)-C(17)	122.72(17)
C(11)-C(16)-C(17)	120.19(15)
C(16)-C(17)-C(18)	109.08(15)
C(16)-C(17)-C(19)	114.64(16)
C(18)-C(17)-C(19)	109.78(17)
C(16)-C(17)-H(17)	107.7
C(18)-C(17)-H(17)	107.7
C(19)-C(17)-H(17)	107.7
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5

H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(31)-N(2)-Mo(1)	133.32(11)
C(31)-N(2)-H(2)	109.5(14)
Mo(1)-N(2)-H(2)	111.6(14)
N(2)-C(31)-C(36)	121.59(14)
N(2)-C(31)-C(32)	118.60(14)
C(36)-C(31)-C(32)	119.79(14)
C(33)-C(32)-C(31)	119.70(15)
C(33)-C(32)-C(41)	120.81(15)
C(31)-C(32)-C(41)	119.49(14)
C(42)-C(41)-C(46)	119.55(15)
C(42)-C(41)-C(32)	120.16(15)
C(46)-C(41)-C(32)	120.26(14)
C(43)-C(42)-C(41)	118.90(15)
C(43)-C(42)-C(47)	120.05(15)
C(41)-C(42)-C(47)	121.05(15)
C(44)-C(43)-C(42)	122.22(16)
C(44)-C(43)-H(43)	118.9
C(42)-C(43)-H(43)	118.9
C(43)-C(44)-C(45)	118.09(16)
C(43)-C(44)-C(48)	121.06(17)
C(45)-C(44)-C(48)	120.85(17)
C(44)-C(45)-C(46)	121.72(16)
C(44)-C(45)-H(45)	119.1
C(46)-C(45)-H(45)	119.1
C(45)-C(46)-C(41)	119.46(15)
C(45)-C(46)-C(49)	119.88(16)
C(41)-C(46)-C(49)	120.64(16)
C(42)-C(47)-H(47A)	109.5
C(42)-C(47)-H(47B)	109.5

H(47A)-C(47)-H(47B)	109.5
C(42)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(44)-C(48)-H(48A)	109.5
C(44)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(44)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(46)-C(49)-H(49A)	109.5
C(46)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(46)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(34)-C(33)-C(32)	121.05(17)
C(34)-C(33)-H(33)	119.5
C(32)-C(33)-H(33)	119.5
C(33)-C(34)-C(35)	119.15(16)
C(33)-C(34)-H(34)	120.4
C(35)-C(34)-H(34)	120.4
C(34)-C(35)-C(36)	121.70(16)
C(34)-C(35)-H(35)	119.2
C(36)-C(35)-H(35)	119.2
C(35)-C(36)-C(31)	118.61(15)
C(35)-C(36)-C(51)	118.82(15)
C(31)-C(36)-C(51)	122.56(14)
C(52)-C(51)-C(56)	119.71(16)
C(52)-C(51)-C(36)	120.15(15)
C(56)-C(51)-C(36)	119.85(15)
C(53)-C(52)-C(51)	119.29(16)
C(53)-C(52)-C(57)	120.20(17)
C(51)-C(52)-C(57)	120.49(17)
C(54)-C(53)-C(52)	121.77(17)
C(54)-C(53)-H(53)	119.1

C(52)-C(53)-H(53)	119.1
C(53)-C(54)-C(55)	118.44(17)
C(53)-C(54)-C(58)	121.47(18)
C(55)-C(54)-C(58)	120.08(18)
C(56)-C(55)-C(54)	121.54(17)
C(56)-C(55)-H(55)	119.2
C(54)-C(55)-H(55)	119.2
C(55)-C(56)-C(51)	119.25(16)
C(55)-C(56)-C(59)	119.76(15)
C(51)-C(56)-C(59)	120.93(15)
C(52)-C(57)-H(57A)	109.5
C(52)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	109.5
C(52)-C(57)-H(57C)	109.5
H(57A)-C(57)-H(57C)	109.5
H(57B)-C(57)-H(57C)	109.5
C(54)-C(58)-H(58A)	109.5
C(54)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
C(54)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5
C(56)-C(59)-H(59A)	109.5
C(56)-C(59)-H(59B)	109.5
H(59A)-C(59)-H(59B)	109.5
C(56)-C(59)-H(59C)	109.5
H(59A)-C(59)-H(59C)	109.5
H(59B)-C(59)-H(59C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S9D. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **7b**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	15(1)	14(1)	17(1)	0(1)	2(1)	0(1)
C(1)	18(1)	18(1)	22(1)	0(1)	2(1)	2(1)
C(2)	19(1)	20(1)	23(1)	-4(1)	1(1)	1(1)
C(3)	27(1)	32(1)	30(1)	-9(1)	-6(1)	9(1)
C(4)	25(1)	27(1)	41(1)	-10(1)	12(1)	-8(1)
C(5)	19(1)	18(1)	20(1)	-4(1)	0(1)	0(1)
C(6)	28(1)	21(1)	25(1)	-2(1)	5(1)	0(1)
C(7)	26(1)	32(1)	31(1)	-9(1)	9(1)	-4(1)
C(8)	23(1)	34(1)	33(1)	-12(1)	-1(1)	8(1)
C(9)	37(1)	30(1)	30(1)	1(1)	1(1)	13(1)
C(10)	30(1)	26(1)	24(1)	2(1)	4(1)	5(1)
O(1)	16(1)	23(1)	24(1)	-3(1)	3(1)	-2(1)
C(21)	16(1)	24(1)	22(1)	-1(1)	2(1)	-3(1)
C(22)	21(1)	34(1)	36(1)	-12(1)	7(1)	-1(1)
C(23)	28(1)	40(1)	28(1)	4(1)	2(1)	-9(1)
F(1)	37(1)	74(1)	38(1)	12(1)	12(1)	-19(1)
F(2)	67(1)	27(1)	54(1)	10(1)	9(1)	-6(1)
F(3)	37(1)	61(1)	33(1)	18(1)	-8(1)	-15(1)
C(24)	20(1)	31(1)	26(1)	0(1)	2(1)	-4(1)
F(4)	16(1)	59(1)	38(1)	-4(1)	3(1)	-3(1)
F(5)	32(1)	41(1)	40(1)	-15(1)	-3(1)	-6(1)
F(6)	31(1)	52(1)	33(1)	16(1)	-4(1)	-9(1)
N(1)	21(1)	18(1)	21(1)	1(1)	4(1)	0(1)
C(11)	27(1)	18(1)	25(1)	4(1)	10(1)	0(1)
C(12)	28(1)	28(1)	40(1)	6(1)	12(1)	-2(1)
C(13)	36(1)	36(1)	62(1)	14(1)	23(1)	-2(1)
C(14)	52(1)	40(1)	59(1)	25(1)	30(1)	5(1)
C(15)	45(1)	33(1)	39(1)	17(1)	16(1)	8(1)
C(16)	31(1)	23(1)	27(1)	6(1)	9(1)	4(1)
C(17)	29(1)	24(1)	28(1)	7(1)	2(1)	3(1)
C(18)	28(1)	32(1)	49(1)	-1(1)	10(1)	4(1)

C(19)	46(1)	46(1)	35(1)	13(1)	-5(1)	-3(1)
N(2)	21(1)	19(1)	17(1)	1(1)	3(1)	5(1)
C(31)	24(1)	16(1)	21(1)	2(1)	7(1)	4(1)
C(32)	24(1)	21(1)	20(1)	5(1)	5(1)	7(1)
C(41)	19(1)	22(1)	22(1)	4(1)	3(1)	7(1)
C(42)	20(1)	22(1)	22(1)	5(1)	3(1)	6(1)
C(43)	23(1)	26(1)	21(1)	4(1)	4(1)	7(1)
C(44)	23(1)	28(1)	25(1)	0(1)	0(1)	7(1)
C(45)	21(1)	24(1)	32(1)	1(1)	2(1)	3(1)
C(46)	20(1)	22(1)	28(1)	5(1)	6(1)	5(1)
C(47)	30(1)	24(1)	27(1)	4(1)	7(1)	0(1)
C(48)	40(1)	35(1)	27(1)	-4(1)	1(1)	1(1)
C(49)	35(1)	27(1)	37(1)	7(1)	16(1)	3(1)
C(33)	31(1)	38(1)	25(1)	7(1)	8(1)	17(1)
C(34)	42(1)	41(1)	26(1)	4(1)	13(1)	23(1)
C(35)	41(1)	32(1)	20(1)	0(1)	8(1)	13(1)
C(36)	28(1)	20(1)	21(1)	2(1)	7(1)	5(1)
C(51)	27(1)	21(1)	20(1)	-1(1)	6(1)	3(1)
C(52)	34(1)	25(1)	22(1)	-3(1)	7(1)	-3(1)
C(53)	30(1)	34(1)	27(1)	-8(1)	9(1)	-6(1)
C(54)	28(1)	38(1)	22(1)	-8(1)	3(1)	2(1)
C(55)	30(1)	31(1)	20(1)	0(1)	5(1)	5(1)
C(56)	27(1)	23(1)	19(1)	-2(1)	6(1)	3(1)
C(57)	46(1)	30(1)	33(1)	4(1)	11(1)	-9(1)
C(58)	27(1)	59(1)	30(1)	-6(1)	0(1)	2(1)
C(59)	29(1)	26(1)	26(1)	3(1)	8(1)	2(1)

Table S9E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **7b**.

	x	y	z	U(eq)
H(1)	7373(10)	8628(17)	4219(9)	23
H(3A)	8019	9565	5290	49
H(3B)	8486	10731	5268	49
H(3C)	8640	9436	4952	49
H(4A)	8656	10502	3876	45
H(4B)	8440	11800	4136	45
H(4C)	8017	11207	3424	45
H(6)	7011	10107	5142	30
H(7)	6038	11155	5170	35
H(8)	5679	12823	4424	38
H(9)	6321	13491	3688	40
H(10)	7289	12438	3645	33
H(22A)	6185	9282	3798	46
H(22B)	5393	9175	3541	46
H(22C)	5802	9853	3062	46
H(12)	8808	10267	2530	38
H(13)	9068	11695	1754	51
H(14)	8231	12423	824	57
H(15)	7139	11782	681	46
H(17)	6580	9447	1669	33
H(18A)	6577	11102	2435	54
H(18B)	5846	10913	1945	54
H(18C)	6303	12012	1791	54
H(19A)	6045	11178	585	67
H(19B)	5701	9928	746	67
H(19C)	6338	9873	428	67
H(2)	8211(10)	6988(19)	3841(8)	23
H(43)	9217	5896	5802	29
H(45)	10154	8756	5164	32
H(47A)	9071	4012	4507	41

H(47B)	8396	4768	4228	41
H(47C)	8638	4412	5036	41
H(48A)	9669	7475	6623	53
H(48B)	9911	8743	6353	53
H(48C)	10413	7604	6542	53
H(49A)	10124	9096	4002	48
H(49B)	9458	8621	3470	48
H(49C)	10136	7865	3557	48
H(33)	10000	5219	3463	37
H(34)	9664	4493	2318	43
H(35)	8591	4906	1655	37
H(53)	6074	5088	1615	36
H(55)	6821	7698	572	33
H(57A)	6725	4036	2568	54
H(57B)	7308	4844	3046	54
H(57C)	7477	3832	2526	54
H(58A)	5551	7457	482	60
H(58B)	5336	6113	679	60
H(58C)	5688	6277	51	60
H(59A)	8345	7177	1020	40
H(59B)	8378	7963	1712	40
H(59C)	7926	8426	979	40

Table S10A. Crystal data and structure refinement for **8**.

Identification code	X8_11109_t5	
Empirical formula	C48 H54 F6 Mo N O	
Formula weight	870.86	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	$P\bar{1}$	
Unit cell dimensions	a = 10.6178(9) Å	α= 109.268(2)°
	b = 18.8500(16) Å	β= 96.928(2)°
	c = 22.2527(19) Å	γ = 90.162(2)°
Volume	4169.3(6) $Å^3$	
Z	4	
Density (calculated)	1.387 Mg/m^3	
Absorption coefficient	0.379 mm^{-1}	
F(000)	1812	
Crystal size	0.20 x 0.15 x 0.05 mm^3	
Theta range for data collection	1.15 to 30.62°	
Index ranges	-15<=h<=15, -26<=k<=25, 0<=l<=31	
Reflections collected	23776	
Independent reflections	23776 [R(int) = 0.0958]	
Completeness to theta = 25.00°	98.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9813 and 0.9281	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	23538 / 3839 / 1265	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0764, wR2 = 0.1836	
R indices (all data)	R1 = 0.1030, wR2 = 0.2015	
Largest diff. peak and hole	3.265 and -2.969 e.$Å^{-3}$	

Table S10B. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **8**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	9647(1)	2208(1)	2858(1)	13(1)
C(1)	11149(5)	2541(3)	2631(3)	18(1)
C(2)	11739(5)	2706(3)	2099(3)	18(1)
C(3)	11249(6)	3451(3)	2059(3)	21(1)
C(4)	13201(5)	2815(4)	2292(3)	28(1)
C(5)	11528(5)	2058(3)	1465(3)	21(1)
C(6)	11330(7)	2184(4)	877(3)	36(2)
C(7)	11244(8)	1580(4)	301(3)	46(2)
C(8)	11362(8)	859(4)	297(3)	39(2)
C(9)	11552(6)	727(3)	879(3)	28(1)
C(10)	11624(5)	1315(3)	1450(3)	21(1)
N(1)	8745(4)	1866(2)	2128(2)	17(1)
C(11)	7831(5)	1813(3)	1563(2)	14(1)
C(12)	7925(5)	2526(3)	1387(2)	18(1)
C(13)	6485(5)	1717(3)	1731(3)	18(1)
C(14)	8084(5)	1137(3)	987(2)	20(1)
C(15)	6935(5)	2477(3)	808(3)	19(1)
C(16)	5593(5)	2372(3)	977(3)	23(1)
C(17)	5507(5)	1659(3)	1145(3)	22(1)
C(18)	5771(6)	981(3)	568(3)	25(1)
C(19)	7106(5)	1086(3)	409(3)	22(1)
C(20)	7197(5)	1807(3)	238(3)	24(1)
C(21)	10260(5)	1234(3)	3127(2)	15(1)
C(22)	9595(5)	534(3)	2915(2)	17(1)
C(31)	8322(5)	355(3)	2508(3)	17(1)
C(32)	7209(5)	585(3)	2799(3)	20(1)
C(37)	7292(5)	1118(3)	3481(3)	24(1)
C(33)	6037(5)	310(3)	2451(3)	21(1)
C(34)	5910(5)	-187(3)	1817(3)	21(1)
C(38)	4617(6)	-443(4)	1444(3)	30(1)
C(35)	7027(5)	-404(3)	1543(3)	22(1)

C(36)	8209(5)	-154(3)	1878(3)	18(1)
C(39)	9393(6)	-411(3)	1563(3)	23(1)
C(23)	10038(5)	-61(3)	3115(3)	22(1)
C(24)	11150(6)	28(3)	3540(3)	25(1)
C(25)	11781(5)	731(3)	3787(3)	21(1)
C(26)	11344(5)	1321(3)	3587(2)	18(1)
C(41)	12041(5)	2064(3)	3918(3)	19(1)
C(42)	13198(5)	2222(3)	3737(3)	23(1)
C(47)	13795(6)	1627(4)	3233(3)	32(1)
C(43)	13797(6)	2938(4)	4042(3)	28(1)
C(44)	13315(6)	3476(4)	4525(3)	30(1)
C(48)	14003(8)	4235(4)	4856(4)	41(2)
C(45)	12216(7)	3306(3)	4735(3)	28(1)
C(46)	11567(5)	2597(3)	4434(3)	22(1)
C(49)	10439(6)	2403(4)	4711(3)	28(1)
O(1)	9004(11)	3007(5)	3538(5)	22(1)
C(51)	8501(7)	3690(4)	3814(3)	24(1)
C(52)	7185(7)	3706(5)	3447(3)	31(1)
F(1)	7258(5)	3677(3)	2848(2)	38(1)
F(2)	6478(5)	3104(3)	3414(3)	52(1)
F(3)	6572(5)	4314(3)	3726(3)	49(2)
C(53)	9381(8)	4326(5)	3773(4)	36(1)
F(4)	9521(5)	4274(4)	3167(3)	40(1)
F(5)	8952(12)	5007(5)	4055(7)	59(1)
F(6)	10547(5)	4319(3)	4056(3)	47(1)
C(54)	8395(10)	3800(6)	4519(4)	41(2)
O(1A)	8970(50)	3024(18)	3505(18)	22(1)
C(51A)	8440(20)	3713(14)	3726(9)	27(2)
C(52A)	7290(30)	3760(20)	3267(14)	31(1)
C(53A)	9450(20)	4347(16)	3839(12)	36(1)
F(4A)	9930(20)	4260(20)	3303(13)	40(1)
F(5A)	8950(50)	5018(18)	4040(30)	59(1)
F(6A)	10320(20)	4299(16)	4309(12)	47(1)
C(54A)	8125(18)	3847(11)	4412(9)	41(2)
F(7A)	7470(20)	4463(11)	4608(10)	48(3)
F(8A)	9226(19)	3952(13)	4803(9)	50(3)

F(9A)	7430(20)	3271(11)	4401(9)	43(4)
O(1B)	9160(90)	3050(50)	3540(30)	22(1)
C(51B)	8780(50)	3760(30)	3864(16)	26(2)
C(52B)	7380(50)	3800(30)	3620(20)	31(1)
F(1B)	7190(80)	3540(60)	2980(20)	38(1)
F(2B)	6660(60)	3360(50)	3830(40)	52(1)
F(3B)	6970(70)	4490(40)	3810(50)	49(2)
C(53B)	9590(80)	4340(70)	3710(40)	36(1)
C(54B)	9020(40)	3866(19)	4582(17)	41(2)
F(7B)	10210(40)	3702(15)	4730(30)	48(3)
F(8B)	8870(70)	4570(20)	4940(20)	50(3)
F(9B)	8260(40)	3400(30)	4730(30)	43(4)
Mo(2)	5727(1)	2788(1)	7149(1)	13(1)
C(101)	7322(5)	2449(3)	7372(2)	16(1)
C(102)	8206(5)	2288(3)	7893(3)	19(1)
C(103)	7686(6)	1537(3)	7939(3)	24(1)
C(104)	9553(5)	2166(3)	7689(3)	24(1)
C(105)	8338(5)	2936(3)	8532(3)	20(1)
C(106)	8421(5)	3679(3)	8542(3)	23(1)
C(107)	8686(5)	4279(3)	9117(3)	26(1)
C(108)	8863(6)	4142(4)	9693(3)	32(1)
C(109)	8772(7)	3406(4)	9697(3)	36(2)
C(110)	8508(6)	2805(4)	9124(3)	28(1)
N(2)	5175(4)	3110(2)	7879(2)	16(1)
C(111)	4545(5)	3185(3)	8443(2)	15(1)
C(112)	3138(5)	3287(3)	8291(3)	17(1)
C(113)	5126(5)	3869(3)	9017(2)	19(1)
C(114)	4732(5)	2477(3)	8635(3)	18(1)
C(115)	2449(5)	3359(3)	8871(3)	21(1)
C(116)	3021(5)	4038(3)	9438(3)	22(1)
C(117)	4435(5)	3944(3)	9602(3)	19(1)
C(118)	4603(5)	3232(3)	9786(2)	20(1)
C(119)	4044(5)	2544(3)	9217(2)	18(1)
C(120)	2630(5)	2637(3)	9058(3)	23(1)
C(121)	6224(5)	3752(3)	6880(2)	16(1)
C(122)	5679(5)	4463(3)	7097(2)	15(1)

C(131)	4600(5)	4647(3)	7491(2)	15(1)
C(132)	4795(5)	5144(3)	8128(3)	20(1)
C(137)	6108(6)	5406(3)	8460(3)	24(1)
C(133)	3733(5)	5391(3)	8455(3)	20(1)
C(134)	2504(5)	5164(3)	8155(3)	20(1)
C(138)	1379(6)	5420(4)	8513(3)	27(1)
C(135)	2334(5)	4680(3)	7529(3)	19(1)
C(136)	3360(5)	4408(3)	7192(2)	17(1)
C(139)	3106(6)	3878(3)	6509(3)	23(1)
C(123)	6044(5)	5055(3)	6897(3)	22(1)
C(124)	6934(6)	4974(3)	6478(3)	22(1)
C(125)	7411(6)	4279(3)	6226(3)	23(1)
C(126)	7079(5)	3666(3)	6415(3)	18(1)
C(141)	7597(5)	2927(3)	6087(3)	19(1)
C(142)	8840(5)	2765(4)	6269(3)	24(1)
C(147)	9697(6)	3352(4)	6765(3)	30(1)
C(143)	9286(6)	2065(4)	5962(3)	29(1)
C(144)	8539(7)	1523(3)	5467(3)	28(1)
C(148)	9041(8)	773(4)	5131(4)	38(2)
C(145)	7321(6)	1708(3)	5267(3)	25(1)
C(146)	6838(6)	2402(3)	5558(3)	22(1)
C(149)	5586(6)	2599(3)	5295(3)	27(1)
O(2)	4758(11)	1987(5)	6474(5)	23(1)
C(151)	4108(7)	1292(4)	6181(4)	28(1)
C(152)	5032(8)	668(4)	6183(4)	38(1)
F(101)	5525(6)	709(4)	6783(3)	44(1)
F(102)	4443(8)	-14(4)	5901(4)	58(2)
F(103)	5996(7)	694(4)	5887(4)	53(2)
C(153)	3002(7)	1275(4)	6556(3)	30(1)
F(104)	3366(5)	1314(3)	7154(2)	37(1)
F(105)	2232(6)	664(3)	6279(3)	48(2)
F(106)	2275(5)	1877(3)	6591(3)	48(1)
C(154)	3579(10)	1201(6)	5482(4)	44(2)
O(2C)	4760(40)	1977(16)	6483(15)	23(1)
C(51C)	4030(19)	1315(11)	6315(8)	32(2)
C(52C)	3060(30)	1410(18)	6791(14)	38(1)

C(53C)	4893(18)	667(12)	6325(9)	30(1)
F(4C)	5280(20)	757(15)	6943(9)	37(1)
F(5C)	4260(30)	6(14)	6058(13)	48(2)
F(6C)	5930(20)	665(17)	6068(14)	48(1)
C(54C)	3339(17)	1151(10)	5634(8)	44(2)
F(7C)	2657(17)	1734(10)	5624(10)	45(3)
F(8C)	2560(20)	553(12)	5485(11)	68(4)
F(9C)	4190(20)	1040(12)	5215(9)	54(3)
O(2D)	4700(50)	2070(30)	6430(18)	23(1)
C(51D)	4140(30)	1350(20)	6186(13)	34(2)
C(52D)	2830(40)	1360(20)	6403(18)	38(1)
F(1D)	2920(50)	1270(40)	6970(20)	44(1)
F(2D)	2030(40)	840(30)	5980(30)	58(2)
F(3D)	2340(50)	2030(30)	6450(30)	53(2)
C(53D)	5050(50)	820(40)	6400(30)	30(1)
C(54D)	4020(30)	1100(20)	5448(13)	44(2)
F(7D)	3980(50)	1690(20)	5250(20)	45(3)
F(8D)	3000(50)	640(30)	5180(20)	68(4)
F(9D)	5060(50)	720(30)	5290(20)	54(3)

Table S10C. Bond lengths [Å] and angles [°] for **8**.

Mo(1)-N(1)	1.703(4)
Mo(1)-C(1)	1.895(5)
Mo(1)-O(1B)	1.924(15)
Mo(1)-O(1A)	1.938(13)
Mo(1)-O(1)	1.943(5)
Mo(1)-C(21)	2.188(5)
C(1)-C(2)	1.521(7)
C(2)-C(5)	1.522(8)
C(2)-C(3)	1.526(7)
C(2)-C(4)	1.554(8)
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(5)-C(10)	1.394(8)
C(5)-C(6)	1.397(8)
C(6)-C(7)	1.399(9)
C(6)-H(6)	0.9500
C(7)-C(8)	1.363(10)
C(7)-H(7)	0.9500
C(8)-C(9)	1.389(9)
C(8)-H(8)	0.9500
C(9)-C(10)	1.377(8)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
N(1)-C(11)	1.468(6)
C(11)-C(12)	1.526(7)
C(11)-C(14)	1.531(7)
C(11)-C(13)	1.545(7)
C(12)-C(15)	1.537(7)
C(12)-H(12A)	0.9900
C(12)-H(12B)	0.9900

C(13)-C(17)	1.538(7)
C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(19)	1.530(8)
C(14)-H(14A)	0.9900
C(14)-H(14B)	0.9900
C(15)-C(20)	1.521(8)
C(15)-C(16)	1.545(7)
C(15)-H(15)	1.0000
C(16)-C(17)	1.513(7)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-C(18)	1.539(8)
C(17)-H(17)	1.0000
C(18)-C(19)	1.530(8)
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(20)	1.532(8)
C(19)-H(19)	1.0000
C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900
C(21)-C(22)	1.402(7)
C(21)-C(26)	1.416(7)
C(22)-C(23)	1.400(7)
C(22)-C(31)	1.505(8)
C(31)-C(36)	1.404(7)
C(31)-C(32)	1.417(8)
C(32)-C(33)	1.383(8)
C(32)-C(37)	1.510(8)
C(37)-H(37A)	0.9800
C(37)-H(37B)	0.9800
C(37)-H(37C)	0.9800
C(33)-C(34)	1.402(8)
C(33)-H(33)	0.9500
C(34)-C(35)	1.399(8)
C(34)-C(38)	1.505(8)

C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(35)-C(36)	1.375(8)
C(35)-H(35)	0.9500
C(36)-C(39)	1.516(8)
C(39)-H(39A)	0.9800
C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(23)-C(24)	1.393(8)
C(23)-H(23)	0.9500
C(24)-C(25)	1.390(8)
C(24)-H(24)	0.9500
C(25)-C(26)	1.389(8)
C(25)-H(25)	0.9500
C(26)-C(41)	1.494(8)
C(41)-C(42)	1.398(8)
C(41)-C(46)	1.402(8)
C(42)-C(43)	1.405(8)
C(42)-C(47)	1.504(8)
C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(43)-C(44)	1.364(9)
C(43)-H(43)	0.9500
C(44)-C(45)	1.382(9)
C(44)-C(48)	1.514(9)
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(45)-C(46)	1.415(8)
C(45)-H(45)	0.9500
C(46)-C(49)	1.507(8)
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800

O(1)-C(51)	1.373(7)
C(51)-C(54)	1.531(8)
C(51)-C(52)	1.537(8)
C(51)-C(53)	1.550(8)
C(52)-F(3)	1.324(8)
C(52)-F(1)	1.329(7)
C(52)-F(2)	1.336(8)
C(53)-F(6)	1.322(8)
C(53)-F(5)	1.339(8)
C(53)-F(4)	1.347(8)
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
O(1A)-C(51A)	1.378(14)
C(51A)-C(52A)	1.518(13)
C(51A)-C(54A)	1.539(13)
C(51A)-C(53A)	1.544(13)
C(52A)-H(52A)	0.9800
C(52A)-H(52B)	0.9800
C(52A)-H(52C)	0.9800
C(53A)-F(4A)	1.312(13)
C(53A)-F(5A)	1.329(13)
C(53A)-F(6A)	1.335(13)
C(54A)-F(9A)	1.303(13)
C(54A)-F(7A)	1.328(13)
C(54A)-F(8A)	1.343(13)
O(1B)-C(51B)	1.387(16)
C(51B)-C(52B)	1.529(13)
C(51B)-C(54B)	1.533(13)
C(51B)-C(53B)	1.535(14)
C(52B)-F(3B)	1.328(14)
C(52B)-F(2B)	1.331(14)
C(52B)-F(1B)	1.337(14)
C(53B)-H(53A)	0.9800
C(53B)-H(53B)	0.9800
C(53B)-H(53C)	0.9800

C(54B)-F(8B)	1.325(14)
C(54B)-F(9B)	1.330(14)
C(54B)-F(7B)	1.335(14)
Mo(2)-N(2)	1.714(4)
Mo(2)-C(101)	1.881(5)
Mo(2)-O(2C)	1.927(13)
Mo(2)-O(2)	1.928(6)
Mo(2)-O(2D)	1.930(15)
Mo(2)-C(121)	2.174(5)
C(101)-C(102)	1.514(7)
C(102)-C(105)	1.529(8)
C(102)-C(104)	1.547(7)
C(102)-C(103)	1.556(8)
C(103)-H(10A)	0.9800
C(103)-H(10B)	0.9800
C(103)-H(10C)	0.9800
C(104)-H(10D)	0.9800
C(104)-H(10E)	0.9800
C(104)-H(10F)	0.9800
C(105)-C(106)	1.396(8)
C(105)-C(110)	1.410(8)
C(106)-C(107)	1.397(8)
C(106)-H(106)	0.9500
C(107)-C(108)	1.379(9)
C(107)-H(107)	0.9500
C(108)-C(109)	1.395(9)
C(108)-H(108)	0.9500
C(109)-C(110)	1.394(9)
C(109)-H(109)	0.9500
C(110)-H(110)	0.9500
N(2)-C(111)	1.458(6)
C(111)-C(112)	1.519(7)
C(111)-C(114)	1.536(7)
C(111)-C(113)	1.546(7)
C(112)-C(115)	1.528(7)
C(112)-H(11A)	0.9900

C(112)-H(11B)	0.9900
C(113)-C(117)	1.536(7)
C(113)-H(11C)	0.9900
C(113)-H(11D)	0.9900
C(114)-C(119)	1.533(7)
C(114)-H(11E)	0.9900
C(114)-H(11F)	0.9900
C(115)-C(116)	1.531(8)
C(115)-C(120)	1.554(7)
C(115)-H(115)	1.0000
C(116)-C(117)	1.526(8)
C(116)-H(11G)	0.9900
C(116)-H(11H)	0.9900
C(117)-C(118)	1.533(7)
C(117)-H(117)	1.0000
C(118)-C(119)	1.538(7)
C(118)-H(11I)	0.9900
C(118)-H(11J)	0.9900
C(119)-C(120)	1.525(8)
C(119)-H(119)	1.0000
C(120)-H(12C)	0.9900
C(120)-H(12D)	0.9900
C(121)-C(122)	1.417(7)
C(121)-C(126)	1.427(7)
C(122)-C(123)	1.399(7)
C(122)-C(131)	1.499(7)
C(131)-C(136)	1.402(7)
C(131)-C(132)	1.408(7)
C(132)-C(133)	1.413(7)
C(132)-C(137)	1.496(8)
C(137)-H(13C)	0.9800
C(137)-H(13D)	0.9800
C(137)-H(13E)	0.9800
C(133)-C(134)	1.389(8)
C(133)-H(133)	0.9500
C(134)-C(135)	1.380(7)

C(134)-C(138)	1.507(8)
C(138)-H(13F)	0.9800
C(138)-H(13G)	0.9800
C(138)-H(13H)	0.9800
C(135)-C(136)	1.399(7)
C(135)-H(135)	0.9500
C(136)-C(139)	1.510(7)
C(139)-H(13I)	0.9800
C(139)-H(13J)	0.9800
C(139)-H(13K)	0.9800
C(123)-C(124)	1.381(8)
C(123)-H(123)	0.9500
C(124)-C(125)	1.370(8)
C(124)-H(124)	0.9500
C(125)-C(126)	1.411(7)
C(125)-H(125)	0.9500
C(126)-C(141)	1.485(8)
C(141)-C(142)	1.398(8)
C(141)-C(146)	1.419(8)
C(142)-C(143)	1.385(9)
C(142)-C(147)	1.489(8)
C(147)-H(14C)	0.9800
C(147)-H(14D)	0.9800
C(147)-H(14E)	0.9800
C(143)-C(144)	1.388(9)
C(143)-H(143)	0.9500
C(144)-C(145)	1.400(9)
C(144)-C(148)	1.498(9)
C(148)-H(14F)	0.9800
C(148)-H(14G)	0.9800
C(148)-H(14H)	0.9800
C(145)-C(146)	1.385(8)
C(145)-H(145)	0.9500
C(146)-C(149)	1.486(8)
C(149)-H(14I)	0.9800
C(149)-H(14J)	0.9800

C(149)-H(14K)	0.9800
O(2)-C(151)	1.393(7)
C(151)-C(153)	1.527(8)
C(151)-C(152)	1.535(9)
C(151)-C(154)	1.541(9)
C(152)-F(103)	1.291(8)
C(152)-F(102)	1.344(8)
C(152)-F(101)	1.352(9)
C(153)-F(104)	1.319(8)
C(153)-F(105)	1.334(8)
C(153)-F(106)	1.361(8)
C(154)-H(15A)	0.9800
C(154)-H(15B)	0.9800
C(154)-H(15C)	0.9800
O(2C)-C(51C)	1.383(14)
C(51C)-C(52C)	1.531(13)
C(51C)-C(54C)	1.533(13)
C(51C)-C(53C)	1.533(12)
C(52C)-H(52D)	0.9800
C(52C)-H(52E)	0.9800
C(52C)-H(52F)	0.9800
C(53C)-F(6C)	1.305(13)
C(53C)-F(5C)	1.328(13)
C(53C)-F(4C)	1.341(13)
C(54C)-F(8C)	1.322(13)
C(54C)-F(7C)	1.323(13)
C(54C)-F(9C)	1.343(13)
O(2D)-C(51D)	1.385(15)
C(51D)-C(52D)	1.525(13)
C(51D)-C(53D)	1.535(14)
C(51D)-C(54D)	1.540(13)
C(52D)-F(1D)	1.332(13)
C(52D)-F(2D)	1.335(14)
C(52D)-F(3D)	1.335(14)
C(53D)-H(53D)	0.9800
C(53D)-H(53E)	0.9800

C(53D)-H(53F)	0.9800
C(54D)-F(7D)	1.325(13)
C(54D)-F(8D)	1.327(13)
C(54D)-F(9D)	1.327(13)

N(1)-Mo(1)-C(1)	101.2(2)
N(1)-Mo(1)-O(1B)	122(2)
C(1)-Mo(1)-O(1B)	105(4)
N(1)-Mo(1)-O(1A)	116.7(15)
C(1)-Mo(1)-O(1A)	110.3(15)
O(1B)-Mo(1)-O(1A)	6(3)
N(1)-Mo(1)-O(1)	118.9(4)
C(1)-Mo(1)-O(1)	110.8(4)
O(1B)-Mo(1)-O(1)	5(4)
O(1A)-Mo(1)-O(1)	2.7(17)
N(1)-Mo(1)-C(21)	106.9(2)
C(1)-Mo(1)-C(21)	102.8(2)
O(1B)-Mo(1)-C(21)	116(3)
O(1A)-Mo(1)-C(21)	117.0(14)
O(1)-Mo(1)-C(21)	114.4(4)
C(2)-C(1)-Mo(1)	144.7(4)
C(1)-C(2)-C(5)	112.8(4)
C(1)-C(2)-C(3)	107.6(4)
C(5)-C(2)-C(3)	114.1(5)
C(1)-C(2)-C(4)	108.6(5)
C(5)-C(2)-C(4)	106.1(5)
C(3)-C(2)-C(4)	107.5(4)
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5

C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(10)-C(5)-C(6)	117.5(5)
C(10)-C(5)-C(2)	120.7(5)
C(6)-C(5)-C(2)	121.7(5)
C(5)-C(6)-C(7)	120.4(6)
C(5)-C(6)-H(6)	119.8
C(7)-C(6)-H(6)	119.8
C(8)-C(7)-C(6)	121.2(6)
C(8)-C(7)-H(7)	119.4
C(6)-C(7)-H(7)	119.4
C(7)-C(8)-C(9)	118.9(6)
C(7)-C(8)-H(8)	120.6
C(9)-C(8)-H(8)	120.6
C(10)-C(9)-C(8)	120.5(6)
C(10)-C(9)-H(9)	119.7
C(8)-C(9)-H(9)	119.7
C(9)-C(10)-C(5)	121.5(5)
C(9)-C(10)-H(10)	119.3
C(5)-C(10)-H(10)	119.3
C(11)-N(1)-Mo(1)	162.1(4)
N(1)-C(11)-C(12)	110.3(4)
N(1)-C(11)-C(14)	110.7(4)
C(12)-C(11)-C(14)	108.8(4)
N(1)-C(11)-C(13)	108.0(4)
C(12)-C(11)-C(13)	109.5(4)
C(14)-C(11)-C(13)	109.5(4)
C(11)-C(12)-C(15)	110.0(4)
C(11)-C(12)-H(12A)	109.7
C(15)-C(12)-H(12A)	109.7
C(11)-C(12)-H(12B)	109.7
C(15)-C(12)-H(12B)	109.7
H(12A)-C(12)-H(12B)	108.2
C(17)-C(13)-C(11)	109.0(4)
C(17)-C(13)-H(13A)	109.9

C(11)-C(13)-H(13A)	109.9
C(17)-C(13)-H(13B)	109.9
C(11)-C(13)-H(13B)	109.9
H(13A)-C(13)-H(13B)	108.3
C(19)-C(14)-C(11)	109.6(4)
C(19)-C(14)-H(14A)	109.7
C(11)-C(14)-H(14A)	109.7
C(19)-C(14)-H(14B)	109.7
C(11)-C(14)-H(14B)	109.7
H(14A)-C(14)-H(14B)	108.2
C(20)-C(15)-C(12)	109.0(4)
C(20)-C(15)-C(16)	109.5(5)
C(12)-C(15)-C(16)	109.3(4)
C(20)-C(15)-H(15)	109.7
C(12)-C(15)-H(15)	109.7
C(16)-C(15)-H(15)	109.7
C(17)-C(16)-C(15)	109.8(5)
C(17)-C(16)-H(16A)	109.7
C(15)-C(16)-H(16A)	109.7
C(17)-C(16)-H(16B)	109.7
C(15)-C(16)-H(16B)	109.7
H(16A)-C(16)-H(16B)	108.2
C(16)-C(17)-C(13)	109.6(4)
C(16)-C(17)-C(18)	109.3(5)
C(13)-C(17)-C(18)	109.9(5)
C(16)-C(17)-H(17)	109.3
C(13)-C(17)-H(17)	109.3
C(18)-C(17)-H(17)	109.3
C(19)-C(18)-C(17)	109.1(4)
C(19)-C(18)-H(18A)	109.9
C(17)-C(18)-H(18A)	109.9
C(19)-C(18)-H(18B)	109.9
C(17)-C(18)-H(18B)	109.9
H(18A)-C(18)-H(18B)	108.3
C(18)-C(19)-C(14)	109.6(4)
C(18)-C(19)-C(20)	109.6(5)

C(14)-C(19)-C(20)	109.9(5)
C(18)-C(19)-H(19)	109.2
C(14)-C(19)-H(19)	109.2
C(20)-C(19)-H(19)	109.2
C(15)-C(20)-C(19)	109.3(4)
C(15)-C(20)-H(20A)	109.8
C(19)-C(20)-H(20A)	109.8
C(15)-C(20)-H(20B)	109.8
C(19)-C(20)-H(20B)	109.8
H(20A)-C(20)-H(20B)	108.3
C(22)-C(21)-C(26)	116.4(5)
C(22)-C(21)-Mo(1)	124.6(4)
C(26)-C(21)-Mo(1)	118.8(4)
C(23)-C(22)-C(21)	121.4(5)
C(23)-C(22)-C(31)	113.1(5)
C(21)-C(22)-C(31)	125.4(5)
C(36)-C(31)-C(32)	119.2(5)
C(36)-C(31)-C(22)	120.4(5)
C(32)-C(31)-C(22)	119.3(5)
C(33)-C(32)-C(31)	119.1(5)
C(33)-C(32)-C(37)	120.1(5)
C(31)-C(32)-C(37)	120.8(5)
C(32)-C(37)-H(37A)	109.5
C(32)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(32)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(32)-C(33)-C(34)	122.3(5)
C(32)-C(33)-H(33)	118.9
C(34)-C(33)-H(33)	118.9
C(35)-C(34)-C(33)	117.3(5)
C(35)-C(34)-C(38)	122.0(5)
C(33)-C(34)-C(38)	120.7(5)
C(34)-C(38)-H(38A)	109.5
C(34)-C(38)-H(38B)	109.5

H(38A)-C(38)-H(38B)	109.5
C(34)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(36)-C(35)-C(34)	122.1(5)
C(36)-C(35)-H(35)	118.9
C(34)-C(35)-H(35)	118.9
C(35)-C(36)-C(31)	120.0(5)
C(35)-C(36)-C(39)	120.2(5)
C(31)-C(36)-C(39)	119.8(5)
C(36)-C(39)-H(39A)	109.5
C(36)-C(39)-H(39B)	109.5
H(39A)-C(39)-H(39B)	109.5
C(36)-C(39)-H(39C)	109.5
H(39A)-C(39)-H(39C)	109.5
H(39B)-C(39)-H(39C)	109.5
C(24)-C(23)-C(22)	120.8(5)
C(24)-C(23)-H(23)	119.6
C(22)-C(23)-H(23)	119.6
C(25)-C(24)-C(23)	118.7(5)
C(25)-C(24)-H(24)	120.6
C(23)-C(24)-H(24)	120.6
C(26)-C(25)-C(24)	120.3(5)
C(26)-C(25)-H(25)	119.8
C(24)-C(25)-H(25)	119.8
C(25)-C(26)-C(21)	122.1(5)
C(25)-C(26)-C(41)	115.8(5)
C(21)-C(26)-C(41)	122.0(5)
C(42)-C(41)-C(46)	119.3(5)
C(42)-C(41)-C(26)	120.7(5)
C(46)-C(41)-C(26)	120.0(5)
C(41)-C(42)-C(43)	118.9(6)
C(41)-C(42)-C(47)	120.1(5)
C(43)-C(42)-C(47)	120.9(5)
C(42)-C(47)-H(47A)	109.5
C(42)-C(47)-H(47B)	109.5

H(47A)-C(47)-H(47B)	109.5
C(42)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(44)-C(43)-C(42)	122.3(6)
C(44)-C(43)-H(43)	118.8
C(42)-C(43)-H(43)	118.8
C(43)-C(44)-C(45)	119.1(6)
C(43)-C(44)-C(48)	121.0(6)
C(45)-C(44)-C(48)	119.8(7)
C(44)-C(48)-H(48A)	109.5
C(44)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(44)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(44)-C(45)-C(46)	120.6(6)
C(44)-C(45)-H(45)	119.7
C(46)-C(45)-H(45)	119.7
C(41)-C(46)-C(45)	119.6(5)
C(41)-C(46)-C(49)	120.8(5)
C(45)-C(46)-C(49)	119.3(5)
C(46)-C(49)-H(49A)	109.5
C(46)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(46)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
C(51)-O(1)-Mo(1)	156.2(8)
O(1)-C(51)-C(54)	109.2(6)
O(1)-C(51)-C(52)	108.8(7)
C(54)-C(51)-C(52)	110.5(6)
O(1)-C(51)-C(53)	109.4(6)
C(54)-C(51)-C(53)	109.6(7)
C(52)-C(51)-C(53)	109.3(6)
F(3)-C(52)-F(1)	107.8(6)

F(3)-C(52)-F(2)	108.0(6)
F(1)-C(52)-F(2)	107.0(6)
F(3)-C(52)-C(51)	112.7(6)
F(1)-C(52)-C(51)	111.9(5)
F(2)-C(52)-C(51)	109.3(6)
F(6)-C(53)-F(5)	106.8(8)
F(6)-C(53)-F(4)	105.0(7)
F(5)-C(53)-F(4)	107.2(8)
F(6)-C(53)-C(51)	112.1(7)
F(5)-C(53)-C(51)	111.7(7)
F(4)-C(53)-C(51)	113.5(7)
C(51)-C(54)-H(54A)	109.5
C(51)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(51)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(51A)-O(1A)-Mo(1)	154(3)
O(1A)-C(51A)-C(52A)	110.8(18)
O(1A)-C(51A)-C(54A)	109.1(15)
C(52A)-C(51A)-C(54A)	113.0(15)
O(1A)-C(51A)-C(53A)	109.6(19)
C(52A)-C(51A)-C(53A)	112.2(15)
C(54A)-C(51A)-C(53A)	101.8(12)
C(51A)-C(52A)-H(52A)	109.5
C(51A)-C(52A)-H(52B)	109.5
H(52A)-C(52A)-H(52B)	109.5
C(51A)-C(52A)-H(52C)	109.5
H(52A)-C(52A)-H(52C)	109.5
H(52B)-C(52A)-H(52C)	109.5
F(4A)-C(53A)-F(5A)	110(2)
F(4A)-C(53A)-F(6A)	112.7(18)
F(5A)-C(53A)-F(6A)	108(2)
F(4A)-C(53A)-C(51A)	109.3(16)
F(5A)-C(53A)-C(51A)	111(2)
F(6A)-C(53A)-C(51A)	106.2(15)

F(9A)-C(54A)-F(7A)	108.7(16)
F(9A)-C(54A)-F(8A)	113.7(17)
F(7A)-C(54A)-F(8A)	108.1(15)
F(9A)-C(54A)-C(51A)	107.9(14)
F(7A)-C(54A)-C(51A)	110.5(15)
F(8A)-C(54A)-C(51A)	108.0(14)
C(51B)-O(1B)-Mo(1)	160(6)
O(1B)-C(51B)-C(52B)	107.4(19)
O(1B)-C(51B)-C(54B)	106.6(18)
C(52B)-C(51B)-C(54B)	113.3(17)
O(1B)-C(51B)-C(53B)	108(2)
C(52B)-C(51B)-C(53B)	110.8(18)
C(54B)-C(51B)-C(53B)	110.2(19)
F(3B)-C(52B)-F(2B)	108(2)
F(3B)-C(52B)-F(1B)	108(2)
F(2B)-C(52B)-F(1B)	107(2)
F(3B)-C(52B)-C(51B)	112(2)
F(2B)-C(52B)-C(51B)	110.4(19)
F(1B)-C(52B)-C(51B)	110(2)
C(51B)-C(53B)-H(53A)	109.5
C(51B)-C(53B)-H(53B)	109.5
H(53A)-C(53B)-H(53B)	109.5
C(51B)-C(53B)-H(53C)	109.5
H(53A)-C(53B)-H(53C)	109.5
H(53B)-C(53B)-H(53C)	109.5
F(8B)-C(54B)-F(9B)	110(2)
F(8B)-C(54B)-F(7B)	108(2)
F(9B)-C(54B)-F(7B)	107(2)
F(8B)-C(54B)-C(51B)	112(2)
F(9B)-C(54B)-C(51B)	111.0(19)
F(7B)-C(54B)-C(51B)	109.1(19)
N(2)-Mo(2)-C(101)	101.3(2)
N(2)-Mo(2)-O(2C)	117.4(13)
C(101)-Mo(2)-O(2C)	109.2(14)
N(2)-Mo(2)-O(2)	118.0(4)
C(101)-Mo(2)-O(2)	109.7(4)

O(2C)-Mo(2)-O(2)	1.0(14)
N(2)-Mo(2)-O(2D)	119.6(17)
C(101)-Mo(2)-O(2D)	114(2)
O(2C)-Mo(2)-O(2D)	7(2)
O(2)-Mo(2)-O(2D)	6(2)
N(2)-Mo(2)-C(121)	108.4(2)
C(101)-Mo(2)-C(121)	102.8(2)
O(2C)-Mo(2)-C(121)	115.8(11)
O(2)-Mo(2)-C(121)	114.8(4)
O(2D)-Mo(2)-C(121)	108.9(19)
C(102)-C(101)-Mo(2)	146.2(4)
C(101)-C(102)-C(105)	112.9(4)
C(101)-C(102)-C(104)	109.5(4)
C(105)-C(102)-C(104)	106.7(4)
C(101)-C(102)-C(103)	106.0(4)
C(105)-C(102)-C(103)	113.4(4)
C(104)-C(102)-C(103)	108.4(4)
C(102)-C(103)-H(10A)	109.5
C(102)-C(103)-H(10B)	109.5
H(10A)-C(103)-H(10B)	109.5
C(102)-C(103)-H(10C)	109.5
H(10A)-C(103)-H(10C)	109.5
H(10B)-C(103)-H(10C)	109.5
C(102)-C(104)-H(10D)	109.5
C(102)-C(104)-H(10E)	109.5
H(10D)-C(104)-H(10E)	109.5
C(102)-C(104)-H(10F)	109.5
H(10D)-C(104)-H(10F)	109.5
H(10E)-C(104)-H(10F)	109.5
C(106)-C(105)-C(110)	118.0(5)
C(106)-C(105)-C(102)	120.2(5)
C(110)-C(105)-C(102)	121.5(5)
C(105)-C(106)-C(107)	121.6(5)
C(105)-C(106)-H(106)	119.2
C(107)-C(106)-H(106)	119.2
C(108)-C(107)-C(106)	119.9(6)

C(108)-C(107)-H(107)	120.1
C(106)-C(107)-H(107)	120.1
C(107)-C(108)-C(109)	119.7(6)
C(107)-C(108)-H(108)	120.1
C(109)-C(108)-H(108)	120.1
C(110)-C(109)-C(108)	120.7(6)
C(110)-C(109)-H(109)	119.7
C(108)-C(109)-H(109)	119.7
C(109)-C(110)-C(105)	120.2(6)
C(109)-C(110)-H(110)	119.9
C(105)-C(110)-H(110)	119.9
C(111)-N(2)-Mo(2)	164.8(4)
N(2)-C(111)-C(112)	109.4(4)
N(2)-C(111)-C(114)	109.5(4)
C(112)-C(111)-C(114)	109.9(4)
N(2)-C(111)-C(113)	110.5(4)
C(112)-C(111)-C(113)	109.5(4)
C(114)-C(111)-C(113)	108.0(4)
C(111)-C(112)-C(115)	110.7(4)
C(111)-C(112)-H(11A)	109.5
C(115)-C(112)-H(11A)	109.5
C(111)-C(112)-H(11B)	109.5
C(115)-C(112)-H(11B)	109.5
H(11A)-C(112)-H(11B)	108.1
C(117)-C(113)-C(111)	109.6(4)
C(117)-C(113)-H(11C)	109.7
C(111)-C(113)-H(11C)	109.7
C(117)-C(113)-H(11D)	109.7
C(111)-C(113)-H(11D)	109.7
H(11C)-C(113)-H(11D)	108.2
C(119)-C(114)-C(111)	109.8(4)
C(119)-C(114)-H(11E)	109.7
C(111)-C(114)-H(11E)	109.7
C(119)-C(114)-H(11F)	109.7
C(111)-C(114)-H(11F)	109.7
H(11E)-C(114)-H(11F)	108.2

C(112)-C(115)-C(116)	109.3(4)
C(112)-C(115)-C(120)	109.1(4)
C(116)-C(115)-C(120)	108.8(4)
C(112)-C(115)-H(115)	109.9
C(116)-C(115)-H(115)	109.9
C(120)-C(115)-H(115)	109.9
C(117)-C(116)-C(115)	110.1(4)
C(117)-C(116)-H(11G)	109.6
C(115)-C(116)-H(11G)	109.6
C(117)-C(116)-H(11H)	109.6
C(115)-C(116)-H(11H)	109.6
H(11G)-C(116)-H(11H)	108.1
C(116)-C(117)-C(118)	109.0(4)
C(116)-C(117)-C(113)	109.9(4)
C(118)-C(117)-C(113)	109.2(4)
C(116)-C(117)-H(117)	109.5
C(118)-C(117)-H(117)	109.5
C(113)-C(117)-H(117)	109.5
C(117)-C(118)-C(119)	109.5(4)
C(117)-C(118)-H(11I)	109.8
C(119)-C(118)-H(11I)	109.8
C(117)-C(118)-H(11J)	109.8
C(119)-C(118)-H(11J)	109.8
H(11I)-C(118)-H(11J)	108.2
C(120)-C(119)-C(114)	110.1(4)
C(120)-C(119)-C(118)	109.2(5)
C(114)-C(119)-C(118)	109.4(4)
C(120)-C(119)-H(119)	109.4
C(114)-C(119)-H(119)	109.4
C(118)-C(119)-H(119)	109.4
C(119)-C(120)-C(115)	109.2(4)
C(119)-C(120)-H(12C)	109.8
C(115)-C(120)-H(12C)	109.8
C(119)-C(120)-H(12D)	109.8
C(115)-C(120)-H(12D)	109.8
H(12C)-C(120)-H(12D)	108.3

C(122)-C(121)-C(126)	116.0(4)
C(122)-C(121)-Mo(2)	124.5(3)
C(126)-C(121)-Mo(2)	119.3(4)
C(123)-C(122)-C(121)	121.1(5)
C(123)-C(122)-C(131)	112.9(5)
C(121)-C(122)-C(131)	125.8(4)
C(136)-C(131)-C(132)	119.6(5)
C(136)-C(131)-C(122)	119.1(5)
C(132)-C(131)-C(122)	120.6(5)
C(131)-C(132)-C(133)	119.1(5)
C(131)-C(132)-C(137)	120.8(5)
C(133)-C(132)-C(137)	120.1(5)
C(132)-C(137)-H(13C)	109.5
C(132)-C(137)-H(13D)	109.5
H(13C)-C(137)-H(13D)	109.5
C(132)-C(137)-H(13E)	109.5
H(13C)-C(137)-H(13E)	109.5
H(13D)-C(137)-H(13E)	109.5
C(134)-C(133)-C(132)	121.2(5)
C(134)-C(133)-H(133)	119.4
C(132)-C(133)-H(133)	119.4
C(135)-C(134)-C(133)	118.7(5)
C(135)-C(134)-C(138)	120.6(5)
C(133)-C(134)-C(138)	120.7(5)
C(134)-C(138)-H(13F)	109.5
C(134)-C(138)-H(13G)	109.5
H(13F)-C(138)-H(13G)	109.5
C(134)-C(138)-H(13H)	109.5
H(13F)-C(138)-H(13H)	109.5
H(13G)-C(138)-H(13H)	109.5
C(134)-C(135)-C(136)	122.0(5)
C(134)-C(135)-H(135)	119.0
C(136)-C(135)-H(135)	119.0
C(135)-C(136)-C(131)	119.3(5)
C(135)-C(136)-C(139)	119.3(5)
C(131)-C(136)-C(139)	121.4(5)

C(136)-C(139)-H(13I)	109.5
C(136)-C(139)-H(13J)	109.5
H(13I)-C(139)-H(13J)	109.5
C(136)-C(139)-H(13K)	109.5
H(13I)-C(139)-H(13K)	109.5
H(13J)-C(139)-H(13K)	109.5
C(124)-C(123)-C(122)	122.0(5)
C(124)-C(123)-H(123)	119.0
C(122)-C(123)-H(123)	119.0
C(125)-C(124)-C(123)	118.2(5)
C(125)-C(124)-H(124)	120.9
C(123)-C(124)-H(124)	120.9
C(124)-C(125)-C(126)	121.8(5)
C(124)-C(125)-H(125)	119.1
C(126)-C(125)-H(125)	119.1
C(125)-C(126)-C(121)	120.7(5)
C(125)-C(126)-C(141)	117.4(5)
C(121)-C(126)-C(141)	121.8(5)
C(142)-C(141)-C(146)	120.1(5)
C(142)-C(141)-C(126)	120.9(5)
C(146)-C(141)-C(126)	119.0(5)
C(143)-C(142)-C(141)	119.4(6)
C(143)-C(142)-C(147)	120.3(6)
C(141)-C(142)-C(147)	120.2(6)
C(142)-C(147)-H(14C)	109.5
C(142)-C(147)-H(14D)	109.5
H(14C)-C(147)-H(14D)	109.5
C(142)-C(147)-H(14E)	109.5
H(14C)-C(147)-H(14E)	109.5
H(14D)-C(147)-H(14E)	109.5
C(142)-C(143)-C(144)	121.7(6)
C(142)-C(143)-H(143)	119.1
C(144)-C(143)-H(143)	119.1
C(143)-C(144)-C(145)	118.2(6)
C(143)-C(144)-C(148)	121.2(7)
C(145)-C(144)-C(148)	120.5(6)

C(144)-C(148)-H(14F)	109.5
C(144)-C(148)-H(14G)	109.5
H(14F)-C(148)-H(14G)	109.5
C(144)-C(148)-H(14H)	109.5
H(14F)-C(148)-H(14H)	109.5
H(14G)-C(148)-H(14H)	109.5
C(146)-C(145)-C(144)	122.0(6)
C(146)-C(145)-H(145)	119.0
C(144)-C(145)-H(145)	119.0
C(145)-C(146)-C(141)	118.4(6)
C(145)-C(146)-C(149)	120.1(5)
C(141)-C(146)-C(149)	121.4(5)
C(146)-C(149)-H(14I)	109.5
C(146)-C(149)-H(14J)	109.5
H(14I)-C(149)-H(14J)	109.5
C(146)-C(149)-H(14K)	109.5
H(14I)-C(149)-H(14K)	109.5
H(14J)-C(149)-H(14K)	109.5
C(151)-O(2)-Mo(2)	157.5(8)
O(2)-C(151)-C(153)	107.4(7)
O(2)-C(151)-C(152)	108.8(7)
C(153)-C(151)-C(152)	112.2(6)
O(2)-C(151)-C(154)	110.2(7)
C(153)-C(151)-C(154)	109.0(6)
C(152)-C(151)-C(154)	109.2(7)
F(103)-C(152)-F(102)	107.7(7)
F(103)-C(152)-F(101)	105.5(7)
F(102)-C(152)-F(101)	107.3(7)
F(103)-C(152)-C(151)	112.8(7)
F(102)-C(152)-C(151)	110.7(7)
F(101)-C(152)-C(151)	112.4(6)
F(104)-C(153)-F(105)	107.8(6)
F(104)-C(153)-F(106)	105.9(6)
F(105)-C(153)-F(106)	106.4(7)
F(104)-C(153)-C(151)	113.4(6)
F(105)-C(153)-C(151)	112.7(6)

F(106)-C(153)-C(151)	110.1(6)
C(151)-C(154)-H(15A)	109.5
C(151)-C(154)-H(15B)	109.5
H(15A)-C(154)-H(15B)	109.5
C(151)-C(154)-H(15C)	109.5
H(15A)-C(154)-H(15C)	109.5
H(15B)-C(154)-H(15C)	109.5
C(51C)-O(2C)-Mo(2)	148(2)
O(2C)-C(51C)-C(52C)	108.8(17)
O(2C)-C(51C)-C(54C)	108.7(14)
C(52C)-C(51C)-C(54C)	110.0(15)
O(2C)-C(51C)-C(53C)	109.5(18)
C(52C)-C(51C)-C(53C)	110.7(15)
C(54C)-C(51C)-C(53C)	109.1(12)
C(51C)-C(52C)-H(52D)	109.5
C(51C)-C(52C)-H(52E)	109.5
H(52D)-C(52C)-H(52E)	109.5
C(51C)-C(52C)-H(52F)	109.5
H(52D)-C(52C)-H(52F)	109.5
H(52E)-C(52C)-H(52F)	109.5
F(6C)-C(53C)-F(5C)	110.0(17)
F(6C)-C(53C)-F(4C)	105.1(16)
F(5C)-C(53C)-F(4C)	108.4(17)
F(6C)-C(53C)-C(51C)	114.8(16)
F(5C)-C(53C)-C(51C)	111.1(16)
F(4C)-C(53C)-C(51C)	106.9(15)
F(8C)-C(54C)-F(7C)	108.4(16)
F(8C)-C(54C)-F(9C)	110.7(16)
F(7C)-C(54C)-F(9C)	109.9(16)
F(8C)-C(54C)-C(51C)	109.6(14)
F(7C)-C(54C)-C(51C)	108.4(14)
F(9C)-C(54C)-C(51C)	109.8(14)
C(51D)-O(2D)-Mo(2)	145(4)
O(2D)-C(51D)-C(52D)	108.7(19)
O(2D)-C(51D)-C(53D)	108.0(19)
C(52D)-C(51D)-C(53D)	114.2(18)

O(2D)-C(51D)-C(54D)	108.3(16)
C(52D)-C(51D)-C(54D)	110.0(15)
C(53D)-C(51D)-C(54D)	107.5(17)
F(1D)-C(52D)-F(2D)	110(2)
F(1D)-C(52D)-F(3D)	109(2)
F(2D)-C(52D)-F(3D)	107(2)
F(1D)-C(52D)-C(51D)	110.2(19)
F(2D)-C(52D)-C(51D)	111.9(19)
F(3D)-C(52D)-C(51D)	109.1(19)
C(51D)-C(53D)-H(53D)	109.5
C(51D)-C(53D)-H(53E)	109.5
H(53D)-C(53D)-H(53E)	109.5
C(51D)-C(53D)-H(53F)	109.5
H(53D)-C(53D)-H(53F)	109.5
H(53E)-C(53D)-H(53F)	109.5
F(7D)-C(54D)-F(8D)	110(2)
F(7D)-C(54D)-F(9D)	110(2)
F(8D)-C(54D)-F(9D)	110(2)
F(7D)-C(54D)-C(51D)	110.5(18)
F(8D)-C(54D)-C(51D)	111.7(19)
F(9D)-C(54D)-C(51D)	105.3(18)

Symmetry transformations used to generate equivalent atoms:

Table S10D. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **8**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	13(1)	13(1)	16(1)	8(1)	5(1)	1(1)
C(1)	15(2)	14(2)	25(3)	5(2)	9(2)	1(2)
C(2)	15(2)	18(3)	24(3)	10(2)	6(2)	-2(2)
C(3)	25(3)	10(2)	29(3)	4(2)	10(2)	2(2)
C(4)	19(3)	29(3)	39(3)	13(3)	9(2)	-3(2)
C(5)	20(3)	25(3)	21(3)	10(2)	10(2)	-1(2)
C(6)	59(5)	21(3)	35(4)	15(3)	18(3)	1(3)
C(7)	83(6)	36(4)	24(3)	12(3)	21(3)	7(4)
C(8)	68(5)	29(3)	21(3)	4(2)	20(3)	4(3)
C(9)	31(3)	16(3)	35(3)	3(2)	15(3)	3(2)
C(10)	21(3)	21(3)	24(3)	9(2)	9(2)	2(2)
N(1)	15(2)	20(2)	19(2)	12(2)	3(2)	-4(2)
C(11)	14(2)	15(2)	18(2)	12(2)	1(2)	1(2)
C(12)	13(2)	21(3)	22(3)	13(2)	2(2)	-3(2)
C(13)	16(2)	23(3)	20(3)	12(2)	2(2)	-1(2)
C(14)	22(3)	18(3)	22(3)	11(2)	4(2)	3(2)
C(15)	18(2)	18(3)	25(3)	13(2)	0(2)	-2(2)
C(16)	20(3)	24(3)	26(3)	13(2)	-2(2)	0(2)
C(17)	14(2)	24(3)	34(3)	17(2)	2(2)	-5(2)
C(18)	33(3)	18(3)	25(3)	11(2)	-3(2)	-3(2)
C(19)	25(3)	17(3)	21(3)	4(2)	2(2)	1(2)
C(20)	22(3)	27(3)	25(3)	15(2)	-1(2)	-2(2)
C(21)	16(2)	17(2)	16(2)	9(2)	7(2)	5(2)
C(22)	20(3)	18(3)	19(3)	10(2)	8(2)	2(2)
C(31)	24(3)	11(2)	21(3)	11(2)	5(2)	1(2)
C(32)	21(3)	16(3)	27(3)	10(2)	6(2)	0(2)
C(37)	19(3)	26(3)	24(3)	5(2)	8(2)	0(2)
C(33)	21(3)	15(3)	31(3)	11(2)	7(2)	-1(2)
C(34)	20(3)	15(3)	31(3)	15(2)	0(2)	-5(2)
C(38)	30(3)	23(3)	38(4)	11(3)	2(3)	-7(3)
C(35)	29(3)	8(2)	28(3)	7(2)	5(2)	0(2)

C(36)	24(3)	14(2)	19(3)	9(2)	6(2)	-2(2)
C(39)	29(3)	21(3)	18(3)	5(2)	8(2)	6(2)
C(23)	23(3)	18(3)	28(3)	13(2)	3(2)	3(2)
C(24)	29(3)	25(3)	29(3)	17(3)	5(2)	8(2)
C(25)	22(3)	24(3)	20(3)	11(2)	0(2)	5(2)
C(26)	16(2)	24(3)	14(2)	7(2)	4(2)	1(2)
C(41)	19(3)	21(3)	20(3)	11(2)	1(2)	1(2)
C(42)	18(3)	30(3)	21(3)	9(2)	-2(2)	-1(2)
C(47)	23(3)	40(4)	38(4)	18(3)	12(3)	12(3)
C(43)	18(3)	38(4)	33(3)	21(3)	-4(2)	-8(3)
C(44)	29(3)	33(4)	27(3)	14(3)	-9(2)	-8(3)
C(48)	46(4)	33(4)	46(4)	20(3)	-9(3)	-13(3)
C(45)	40(4)	21(3)	21(3)	7(2)	-1(3)	-2(3)
C(46)	21(3)	27(3)	19(3)	10(2)	4(2)	-1(2)
C(49)	37(4)	30(3)	23(3)	14(3)	14(3)	3(3)
O(1)	29(2)	17(2)	25(2)	9(2)	13(2)	6(2)
C(51)	23(2)	20(2)	30(3)	4(2)	10(2)	8(2)
C(52)	22(2)	39(3)	31(3)	8(3)	16(2)	11(2)
F(1)	44(3)	42(3)	29(2)	12(2)	3(2)	16(2)
F(2)	21(2)	64(3)	76(4)	28(3)	14(3)	-4(2)
F(3)	35(3)	53(3)	52(3)	8(3)	10(3)	31(2)
C(53)	34(3)	18(2)	53(3)	10(2)	-1(2)	4(2)
F(4)	31(3)	33(2)	73(3)	33(2)	18(3)	8(3)
F(5)	67(3)	13(2)	83(3)	0(2)	-1(3)	10(2)
F(6)	30(2)	39(3)	78(4)	31(3)	-1(2)	-8(2)
C(54)	47(4)	45(4)	32(2)	9(2)	15(2)	25(3)
O(1A)	29(2)	17(2)	25(2)	9(2)	13(2)	6(2)
C(51A)	28(4)	20(3)	34(4)	8(4)	10(3)	7(3)
C(52A)	22(2)	39(3)	31(3)	8(3)	16(2)	11(2)
C(53A)	34(3)	18(2)	53(3)	10(2)	-1(2)	4(2)
F(4A)	31(3)	33(2)	73(3)	33(2)	18(3)	8(3)
F(5A)	67(3)	13(2)	83(3)	0(2)	-1(3)	10(2)
F(6A)	30(2)	39(3)	78(4)	31(3)	-1(2)	-8(2)
C(54A)	47(4)	45(4)	32(2)	9(2)	15(2)	25(3)
F(7A)	48(6)	53(6)	34(6)	2(8)	7(6)	24(6)
F(8A)	58(7)	50(5)	33(5)	2(5)	4(6)	27(5)

F(9A)	56(7)	56(6)	20(7)	12(6)	22(6)	20(6)
O(1B)	29(2)	17(2)	25(2)	9(2)	13(2)	6(2)
C(51B)	23(3)	26(5)	32(4)	8(4)	14(4)	11(3)
C(52B)	22(2)	39(3)	31(3)	8(3)	16(2)	11(2)
F(1B)	44(3)	42(3)	29(2)	12(2)	3(2)	16(2)
F(2B)	21(2)	64(3)	76(4)	28(3)	14(3)	-4(2)
F(3B)	35(3)	53(3)	52(3)	8(3)	10(3)	31(2)
C(53B)	34(3)	18(2)	53(3)	10(2)	-1(2)	4(2)
C(54B)	47(4)	45(4)	32(2)	9(2)	15(2)	25(3)
F(7B)	48(6)	53(6)	34(6)	2(8)	7(6)	24(6)
F(8B)	58(7)	50(5)	33(5)	2(5)	4(6)	27(5)
F(9B)	56(7)	56(6)	20(7)	12(6)	22(6)	20(6)
Mo(2)	13(1)	13(1)	16(1)	7(1)	4(1)	-3(1)
C(101)	14(2)	18(3)	19(2)	8(2)	6(2)	-2(2)
C(102)	17(3)	20(3)	24(3)	10(2)	5(2)	2(2)
C(103)	25(3)	25(3)	30(3)	18(2)	9(2)	9(2)
C(104)	16(3)	29(3)	32(3)	14(3)	6(2)	6(2)
C(105)	14(2)	20(3)	27(3)	8(2)	4(2)	0(2)
C(106)	19(3)	23(3)	26(3)	7(2)	3(2)	-1(2)
C(107)	21(3)	26(3)	30(3)	8(2)	2(2)	-6(2)
C(108)	30(3)	31(3)	30(3)	5(3)	6(2)	-4(3)
C(109)	44(4)	40(4)	23(3)	13(3)	-2(3)	-9(3)
C(110)	31(3)	34(3)	19(3)	11(2)	1(2)	-5(3)
N(2)	14(2)	19(2)	20(2)	12(2)	6(2)	-1(2)
C(111)	13(2)	17(2)	18(2)	8(2)	4(2)	1(2)
C(112)	14(2)	19(3)	23(3)	11(2)	2(2)	3(2)
C(113)	24(3)	12(2)	23(3)	8(2)	5(2)	-1(2)
C(114)	21(2)	13(2)	23(3)	9(2)	6(2)	2(2)
C(115)	17(2)	29(3)	22(3)	15(2)	6(2)	3(2)
C(116)	22(3)	22(3)	29(3)	14(2)	12(2)	11(2)
C(117)	31(3)	11(2)	19(2)	8(2)	6(2)	2(2)
C(118)	25(3)	21(3)	17(2)	12(2)	1(2)	-1(2)
C(119)	24(3)	16(2)	21(2)	12(2)	7(2)	0(2)
C(120)	22(3)	25(3)	29(3)	18(2)	6(2)	-3(2)
C(121)	15(2)	17(3)	17(2)	7(2)	6(2)	-3(2)
C(122)	20(3)	12(2)	15(2)	6(2)	5(2)	-4(2)

C(131)	19(2)	11(2)	19(2)	9(2)	7(2)	0(2)
C(132)	24(3)	13(2)	24(3)	8(2)	5(2)	-5(2)
C(137)	23(3)	23(3)	28(3)	9(2)	8(2)	-3(2)
C(133)	29(3)	16(3)	19(2)	9(2)	8(2)	4(2)
C(134)	25(3)	13(2)	24(3)	9(2)	6(2)	4(2)
C(138)	24(3)	31(3)	29(3)	12(3)	9(2)	9(2)
C(135)	17(3)	19(3)	24(3)	10(2)	3(2)	0(2)
C(136)	21(3)	14(2)	18(2)	9(2)	4(2)	1(2)
C(139)	24(3)	24(3)	19(3)	4(2)	3(2)	-8(2)
C(123)	25(3)	13(3)	28(3)	8(2)	2(2)	-5(2)
C(124)	28(3)	17(3)	24(3)	10(2)	5(2)	-8(2)
C(125)	25(3)	26(3)	22(3)	10(2)	9(2)	-7(2)
C(126)	19(3)	17(3)	22(3)	10(2)	5(2)	-4(2)
C(141)	19(3)	23(3)	20(3)	11(2)	9(2)	-2(2)
C(142)	20(3)	33(3)	26(3)	13(3)	11(2)	-3(2)
C(147)	24(3)	35(4)	28(3)	6(3)	11(2)	-1(3)
C(143)	22(3)	34(4)	37(4)	16(3)	16(3)	4(3)
C(144)	40(4)	21(3)	30(3)	12(3)	18(3)	2(3)
C(148)	50(4)	23(3)	43(4)	8(3)	22(3)	7(3)
C(145)	31(3)	22(3)	23(3)	6(2)	10(2)	-7(2)
C(146)	28(3)	20(3)	20(3)	8(2)	10(2)	-3(2)
C(149)	30(3)	22(3)	27(3)	8(2)	0(2)	-4(3)
O(2)	21(2)	23(2)	24(2)	8(2)	1(2)	-7(2)
C(151)	29(3)	26(3)	27(3)	3(3)	6(2)	-17(2)
C(152)	45(3)	20(2)	49(3)	3(3)	27(2)	-10(2)
F(101)	33(3)	37(3)	67(3)	19(3)	18(2)	4(2)
F(102)	66(4)	25(2)	72(4)	-6(3)	34(3)	-23(2)
F(103)	58(3)	28(2)	87(5)	22(3)	51(3)	5(2)
C(153)	36(3)	24(2)	28(3)	2(2)	11(2)	-11(2)
F(104)	42(3)	39(3)	31(2)	16(2)	0(2)	-16(2)
F(105)	43(3)	46(3)	47(3)	4(2)	8(2)	-35(2)
F(106)	20(2)	55(3)	84(4)	39(3)	13(2)	4(2)
C(154)	49(4)	49(4)	30(2)	10(3)	2(2)	-28(3)
O(2C)	21(2)	23(2)	24(2)	8(2)	1(2)	-7(2)
C(51C)	24(4)	36(4)	32(4)	7(4)	6(3)	-11(3)
C(52C)	45(3)	20(2)	49(3)	3(3)	27(2)	-10(2)

C(53C)	36(3)	24(2)	28(3)	2(2)	11(2)	-11(2)
F(4C)	42(3)	39(3)	31(2)	16(2)	0(2)	-16(2)
F(5C)	43(3)	46(3)	47(3)	4(2)	8(2)	-35(2)
F(6C)	20(2)	55(3)	84(4)	39(3)	13(2)	4(2)
C(54C)	49(4)	49(4)	30(2)	10(3)	2(2)	-28(3)
F(7C)	38(7)	59(7)	38(8)	18(6)	-4(5)	-21(4)
F(8C)	76(8)	57(7)	55(8)	6(8)	-9(7)	-45(6)
F(9C)	79(7)	43(8)	34(6)	1(6)	22(6)	-12(5)
O(2D)	21(2)	23(2)	24(2)	8(2)	1(2)	-7(2)
C(51D)	39(4)	25(4)	34(4)	3(4)	8(3)	-7(3)
C(52D)	45(3)	20(2)	49(3)	3(3)	27(2)	-10(2)
F(1D)	33(3)	37(3)	67(3)	19(3)	18(2)	4(2)
F(2D)	66(4)	25(2)	72(4)	-6(3)	34(3)	-23(2)
F(3D)	58(3)	28(2)	87(5)	22(3)	51(3)	5(2)
C(53D)	36(3)	24(2)	28(3)	2(2)	11(2)	-11(2)
C(54D)	49(4)	49(4)	30(2)	10(3)	2(2)	-28(3)
F(7D)	38(7)	59(7)	38(8)	18(6)	-4(5)	-21(4)
F(8D)	76(8)	57(7)	55(8)	6(8)	-9(7)	-45(6)
F(9D)	79(7)	43(8)	34(6)	1(6)	22(6)	-12(5)

Table S10E. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **8**.

	x	y	z	U(eq)
H(3A)	11682	3599	1752	32
H(3B)	11416	3840	2483	32
H(3C)	10332	3394	1918	32
H(4A)	13548	2341	2312	42
H(4B)	13390	3206	2714	42
H(4C)	13587	2967	1972	42
H(6)	11254	2683	868	43
H(7)	11100	1674	-96	56
H(8)	11316	453	-97	47
H(9)	11632	227	883	33
H(10)	11743	1213	1843	25
H(12A)	8787	2589	1280	21
H(12B)	7777	2969	1757	21
H(13A)	6420	1256	1848	22
H(13B)	6315	2153	2102	22
H(14A)	8951	1192	882	24
H(14B)	8028	669	1095	24
H(15)	6992	2949	700	23
H(16A)	5416	2809	1346	27
H(16B)	4951	2340	607	27
H(17)	4634	1593	1250	27
H(18A)	5704	512	671	30
H(18B)	5136	942	192	30
H(19)	7280	646	34	26
H(20A)	8056	1872	127	28
H(20B)	6570	1771	-139	28
H(37A)	7490	1630	3491	35
H(37B)	7962	967	3751	35
H(37C)	6477	1103	3643	35
H(33)	5293	463	2649	25

H(38A)	4335	-88	1223	45
H(38B)	4013	-464	1739	45
H(38C)	4660	-944	1127	45
H(35)	6967	-734	1112	26
H(39A)	9891	-700	1793	34
H(39B)	9904	29	1576	34
H(39C)	9149	-728	1115	34
H(23)	9575	-531	2959	26
H(24)	11471	-383	3658	30
H(25)	12516	809	4095	26
H(47A)	14586	1835	3159	48
H(47B)	13208	1461	2833	48
H(47C)	13980	1198	3380	48
H(43)	14565	3052	3906	33
H(48A)	14722	4186	5158	62
H(48B)	13418	4593	5090	62
H(48C)	14315	4418	4535	62
H(45)	11894	3669	5084	33
H(49A)	9684	2307	4390	42
H(49B)	10296	2823	5093	42
H(49C)	10602	1952	4829	42
H(54A)	9241	3790	4746	62
H(54B)	7847	3394	4545	62
H(54C)	8029	4285	4717	62
H(52A)	7546	3687	2842	46
H(52B)	6938	4262	3427	46
H(52C)	6644	3377	3234	46
H(53A)	10476	4330	3896	54
H(53B)	9276	4843	3900	54
H(53C)	9544	4215	3247	54
H(10A)	6849	1611	8088	36
H(10B)	8270	1380	8242	36
H(10C)	7610	1148	7515	36
H(10D)	9502	1787	7260	36
H(10E)	10095	1992	7996	36
H(10F)	9915	2641	7681	36

H(106)	8293	3780	8148	28
H(107)	8745	4780	9112	31
H(108)	9046	4548	10085	38
H(109)	8890	3312	10093	43
H(110)	8443	2306	9133	33
H(11A)	2766	2850	7923	21
H(11B)	3024	3744	8168	21
H(11C)	6040	3801	9122	23
H(11D)	5042	4332	8902	23
H(11E)	4390	2027	8271	21
H(11F)	5649	2417	8741	21
H(115)	1524	3424	8764	25
H(11G)	2902	4503	9327	27
H(11H)	2580	4086	9816	27
H(117)	4801	4391	9970	23
H(11I)	4164	3277	10164	24
H(11J)	5516	3170	9900	24
H(119)	4163	2079	9337	22
H(12C)	2189	2678	9435	28
H(12D)	2258	2193	8698	28
H(13C)	6707	5022	8281	36
H(13D)	6131	5491	8920	36
H(13E)	6344	5877	8396	36
H(133)	3861	5717	8888	24
H(13F)	609	5351	8205	41
H(13G)	1513	5953	8772	41
H(13H)	1285	5123	8794	41
H(135)	1495	4527	7321	23
H(13I)	3589	4059	6236	35
H(13J)	2197	3857	6356	35
H(13K)	3367	3374	6492	35
H(123)	5669	5526	7055	26
H(124)	7209	5390	6368	27
H(125)	7980	4207	5914	28
H(14C)	9875	3760	6601	44
H(14D)	10494	3131	6866	44

H(14E)	9284	3553	7154	44
H(143)	10124	1952	6094	35
H(14F)	8397	376	5076	57
H(14G)	9809	693	5389	57
H(14H)	9246	759	4710	57
H(145)	6809	1347	4921	30
H(14I)	5299	2219	4878	40
H(14J)	5666	3092	5242	40
H(14K)	4966	2615	5592	40
H(15A)	4284	1207	5237	66
H(15B)	3028	1616	5477	66
H(15C)	3087	721	5288	66
H(52D)	2510	1819	6772	58
H(52E)	3512	1530	7226	58
H(52F)	2549	941	6680	58
H(53D)	5859	827	6230	45
H(53E)	4672	310	6245	45
H(53F)	5210	995	6873	45

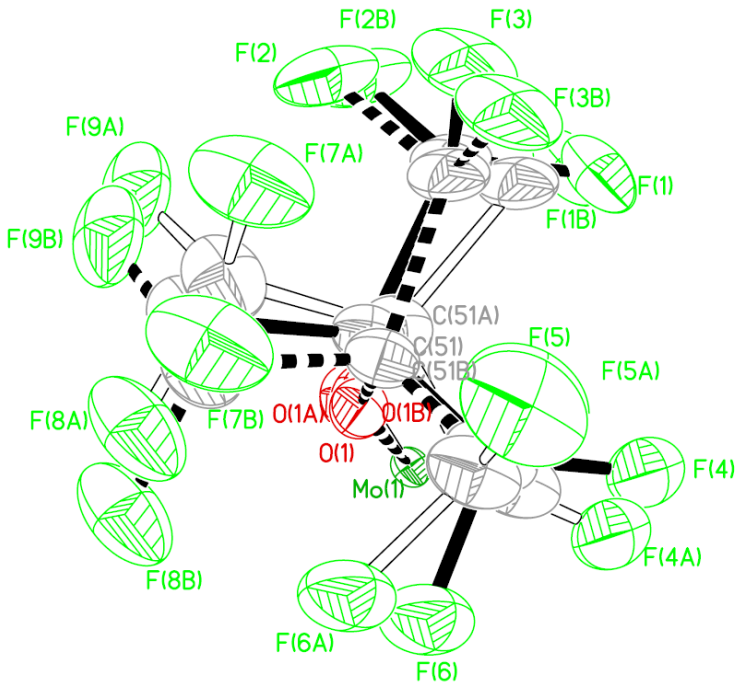

Figure S1. Front view of the three-part disorder of the alkoxide group of compound **8** (50% probability ellipsoids). Selected bond lengths (Å) and angles (^{o}) are shown. Mo(1)-O(1) = 1.940(6), Mo(1)-O(1A) = 1.933(14), Mo(1)-O(1B) = 1.928(15), Mo(1)-O(1)-C(51) = 155.6(9), Mo(1)-O(1A)-C(51A) = 153(3), Mo(1)-O(1B)-C(51B) = 158(7).

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