Supporting Information

A Triply Bonded Dimolybdenum Hydride Complex with Acid, Base and Radical Activity.

Celedonio M. Alvarez,[a] M. Angeles Alvarez,[a] M. Esther García,[a] Alberto Ramos,[a] Miguel A. Ruiz,*[a] Maurizio Lanfranchi[b] and Antonio Tiripicchio[b]

[a] *Departamento de Química Orgánica e Inorgánica/IUQOEM, Universidad de Oviedo, E-33071 Oviedo, Spain. E-mail: mara@fq.uniovi.es*

[b] *Dipartimento di Chimica Generale ed Inorganica, Chimica Analitica, Chimica Fisica, Universitá di Parma, Parco Area delle Scienze 17/A, I-43100 Parma, Italy*

- Preparative Procedures and Spectroscopic Data for New Compounds.
- Structure Solution and Refinements for compounds **1**, **3**, **4** and **6**.
- Crystallographic Data for compounds **1**, **3**, **4** and **6**.
- CIF files for compounds **1**, **3**, **4** and **6**.

General Procedures and Starting Materials

All manipulations and reactions were carried out under a nitrogen (99.9995%) atmosphere using standard Schlenk techniques. Solvents were purified according to literature procedures, and distilled prior to use. Petroleum ether refers to that fraction distilling in the range 65-70 ºC. Compound **1** was prepared as described previously, and all other reagents were obtained from the usual commercial suppliers and used as received, unless otherwise stated. Chromatographic separations were carried out using jacketed columns cooled by tap water (ca. 15 ºC). Commercial aluminium oxide (activity I, 150 mesh) was degassed under vacuum prior to use. The latter was mixed under nitrogen with the appropriate amount of water to reach the activity desired. Filtrations were performed using diatomaceous earth. IR stretching frequencies of CO ligands were measured in solution and are referred to as ν(CO) (solvent). Nuclear Magnetic Resonance (NMR) spectra were routinely recorded at 300.13 (^{1}H), 121.50 (^{31}P{^{1}H}) or 75.47 MHz (^{13}C{^{1}H}) at 290 K in CD_2Cl_2 solutions unless otherwise stated. Chemical shifts (δ) are given in ppm, relative to internal tetramethylsilane (TMS) or external 85% aqueous H_3PO_4 solutions (^{31}P). Coupling constants (*J*) are given in Hertz.

Preparative Procedures and Spectroscopic Data for New Compounds

[$Mo_2Cp_2(\mu$-HCN^{t}Bu)(μ-PCy_2)$(CO)_2$] (3). Compound **1** (0.040 g, 0.069 mmol) in dichloromethane (10 mL) was stirred with CN^{t}Bu (1.5 mL of a 0.05 M solution in petroleum ether, 0.075 mmol) for 1 minute to give a yellow solution. Solvent was then removed under vacuum and the residue dissolved in dichloromethane/petroleum ether (1:4) and chromatographed on an alumina column (activity IV) at 15ºC. Elution with the same solvent mixture gave a yellow fraction. Removal of solvents from the latter yielded compound **3** as a yellow microcrystalline solid (0.042 g, 92%). The crystals used in the X-ray study were grown by slow diffusion of a layer of petroleum ether into a diethylether solution of the complex at -20ºC. Anal. calcd for $C_{29}H_{42}Mo_2NO_2P$: C, 52.48; H, 6.38; N, 2.11. Found: C, 52.24; H, 6.21; N, 1.90. ν(CO) (CH_2Cl_2): 1851(m, sh), 1823(vs) cm^{-1}. ^{31}P{^{1}H} NMR (121.52 MHz, CD_2Cl_2): δ 155.2 (s, μ-P) ppm. ^{1}H NMR (300.13 MHz, CD_2Cl_2): δ 5.32, 5.27 (2 x s, 2 x 5H, Cp), 3.72 (d, J_{HP} = 1.5 Hz, 1H, HCN), 2.30-1.10 (m, 22H, Cy), 0.90 (s, 9H, Me) ppm. ^{13}C{^{1}H} NMR (C_6D_6): δ 242.1 (d, J_{CP} = 9, CO), 238.2 (d, J_{CP} = 8, CO), 92.3, 88.2 (2 x s, Cp), 63.6 (d, J_{CP} = 33, HCN), 54.0 [s, C^1(^{t}Bu)], 49.3 [d, J_{CP} = 13, C^1(Cy)], 44.8 [d, J_{CP} = C^1(Cy)], 35.9, 34.4, 33.6 [3 x s, C^{2,6}(Cy)], 34.1 [d, J_{CP} = 4, C^{2,6}(Cy)], 31.0 [s, C^2(^{t}Bu)], 28.9-28.1 [4 x d, C^{3,5}(Cy)], 26.9, 26.6 [2 x s, C^4(Cy)] ppm.

[$Mo_2Cp_2(\mu$-$SnPh_3$)(μ-PCy_2)$(CO)_2$] (4). Compound **1** (0.030 g, 0.05 mmol) and $HSnPh_3$ (0.025 g, 0.07 mmol) were stirred in toluene (10 mL) for 2 h to give a brown solution. Solvent was then removed from the solution under vacuum and the residue dissolved in petroleum ether and chromatographed on an alumina column (activity IV) at 15ºC. Elution with the same solvent gave a brown fraction. Removal of solvents from the latter under vacuum gave compound **4** as a brown powder (0.042 g, 91%). The crystals used in the X-ray study were grown by slow diffusion of a layer of petroleum ether into a concentrated toluene solution of the complex at -20ºC. Anal. calcd for $C_{42}H_{47}Mo_2O_2PSn$: C, 54.51; H, 5.12. Found: C, 54.79; H, 5.42. ν(CO) (CH_2Cl_2): 1864(m), 1809(vs) cm^{-1}. ^{31}P{^{1}H} NMR (81.03 MHz, CD_2Cl_2): δ 248.6 (s, $J_{P117Sn} \approx J_{P119Sn}$ = 86, μ-P) ppm. ^{1}H NMR (200.13 MHz, CD_2Cl_2): δ 7.80-7.10 (m, 15H, Ph), 4.64 (s, 10H, Cp), 2.80-1.10 (m, 22H, Cy) ppm. ^{13}C{^{1}H} NMR (100.63 MHz, CD_2Cl_2, 213K): δ 247.1 (d, J_{CP} = 11, CO), 145.5 [s, C^1(Ph)], 137.6 [s, C^2(Ph)], 128.2 [s, C^3(Ph)], 127.5 [s, C^4(Ph)], 89.3 (s, Cp), 48.8 [d, J_{CP} = 16, C^1(Cy)], 33.6, 31.2 [2 x s, C^{2,6}(Cy)], 27.8 [d, J_{CP} = 11, C^{3,5}(Cy)], 27.6 [d, J_{CP} = 14, C^{5,3} (Cy)], 26.1 [s, C^4(Cy)] ppm.

[$MnMo_2(\mu_3$-H)(μ-PCy_2)$(CO)_4$] (5). A THF solution of [MnCp'$(CO)_2$(THF)] (Cp' = C_5H_4Me) was prepared from [MnCp'$(CO)_3$] (50 μL, 0.3 mmol) according to literature procedures.[1] Compound **1** (0.030 g, 0.05 mmol) was then added to this solution, and the mixture was stirred for 30 min. Solvent was then removed from the solution under vacuum to yield a brown residue which was extracted with dichloromethane/petroleum ether (1:4). The extracts were then chromatographed on an alumina column (activity IV) at -20ºC. Elution with the same solvent mixture gave a green fraction. Removal of solvents from the latter under vacuum gave compound **5** (0.023 g, 60%) as a green solid. Anal. calcd for $C_{32}H_{40}MnMo_2O_4P$: C, 50.15; H, 5.26. Found: C, 50.38; H, 5.40. ν(CO) (CH_2Cl_2): 1915(vs), 1875(m, sh), 1851(s), 1833(m, sh) cm^{-1}. ^{31}P{^{1}H} NMR (121.50 MHz, C_6D_6): δ 167.5 (s, μ-P) ppm. ^{1}H NMR (300.09 MHz, C_6D_6): δ 5.13 (s, 10H, Cp), 4.28 (s, 1H, C_5H_4), 4.19 (s, 2H, C_5H_4), 4.13 (s, 1H, C_5H_4), 3.00-0.80 (m, 22H, Cy), 1.93 (s, 3H, Me), -15.82 (s, 1H, μ-H) ppm. ^{13}C{^{1}H} NMR (75.48 MHz, C_6D_6): δ 244.4 (d, J_{CP} = 12, MoCO), 235.0, 233.4 (2 x s, 2 x MnCO), 97.5 [s, C^1(Cp')], 89.7 (s, Cp), 83.2, 82.1, 81.5, 81.3 [4 x s, C$^{2-5}$(Cp')], 51.4 [s, br, C^1(Cy)], 33.9 [d, J_{CP} = 3, C^{2,6}(Cy)], 33.1 [s, C^{6,2}(Cy)], 28.5 [d, J_{CP} = 12, C^{3,5}(Cy)], 28.2 [d, J_{CP} = 10, C^{5,3}(Cy)], 26.6 [s, C^4(Cy)], 14.2 (s, Me) ppm.

[$Mo_3Cp_3(\mu$-PCy_2)(μ_3-CO)$(CO)_4$] (6). A toluene solution (10 mL) of compound **1** (0.030 g, 0.05 mmol) and [$Mo_2Cp_2(CO)_6$] (0.050 g, 0.1 mmol) was placed in a jacketed Pyrex Schlenk tube refrigerated with tap water, and was irradiated with visible light for 5 h using a conventional 200 W lamp. Solvent was then removed from the solution under vacuum, the residue was extracted with dichloromethane/petroleum ether (1:4) and the extracts were chromatographed on an alumina column (activity IV) at -20ºC. Elution with dichloromethane/petroleum ether (1:1) gave a brown fraction. Removal of solvents from the latter under vacuum gave compound **6** (0.025 g, 61%) as a dark brown solid. The crystals used in the X-ray study were grown by slow diffusion of a layer of petroleum ether and

diethyl ether into a toluene solution of the complex at -20ºC. Anal. calcd for $C_{32}H_{37}Mo_3O_5P$: C, 46.85; H, 4.55. Found: C, 47.13, H, 4.82. ν(CO) (CH_2Cl_2): 1954(vs), 1915(m), 1890(m), 1866(m), 1814(w) cm^{-1}. $^{31}P\{^1H\}$ NMR (81.04 MHz, $CDCl_3$): δ 178.3 (s, μ-P) ppm. ^1H NMR (200.13 MHz, $CDCl_3$): δ 5.31 (s, 5H, Cp), 5.07 (s, 10H, Cp), 2.50-1.00 (m, 22H, Cy) ppm.

X-Ray Structural Studies

X-Ray Structure Determination of Compounds 1 and 3.

Suitable crystals of **1** were grown by slow diffusion of a layer of petroleum ether into a toluene solution of the complex at -20 ºC. Accurate unit-cell parameters of **1** and **3** were determined by least-squares refinement of the setting angles of 22 (**1**) and 24 (**3**) randomly distributed and carefully centred reflections with θ in the range 7-13° (**1**) and 10-20° (**3**) respectively. The data collections were performed at 293 K on a Philips PW 1100 diffractometer with graphite-monochromated Mo-K_α radiation (λ = 0.71073 Å) by using $\theta/2\theta$ scan mode. No decay was observed. The structures were solved by direct metods (SIR97)[2] and refined by least squares against F_o^2 (SHELXL-97)[3] using the WinGX software package.[4] All the non-hydrogen atoms were refined anisotropically. For **1** the two Cp rings and only one Cy ring were found disordered and distributed in two positions with an occupancy factor of ca. 0.60 and 0.40 respectively. All the hydrogen atoms were introduced from geometrical calculations and refined using a riding model except for the hydride H1 atom of **1,** which was found and refined isotropically.

X-Ray Structure Determination of Compounds 4 and 6.

The X-ray intensity data were collected on a Smart-CCD-1000 BRUKER diffractometer using graphite-monochromated Mo-K_α radiation at 120 K. Cell dimensions and orientation matrixes were initially determined from least-squares refinements on reflections measured in 3 sets of 30 exposures collected in 3 diferent ω regions and eventually refined against all reflections. The software SMART[5] was used for collecting frames of data, indexing reflections, and determining lattice parameters. The collected frames were then processed for integration by the software SAINT,[5] and a multi-scan absorption correction was applied with SADABS.[6] The structures were solved by Patterson interpretation and phase expansion using DIRDIF,[7] and refined with full-matrix least squares on F^2 using SHELXL97.[3] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were geometrically located, and they were given an overall isotropic thermal parameter. The final refinements on F^2 proceeded by full-matrix least-squares calculations using anisotropic thermal parameters for all the non-hydrogen atoms.

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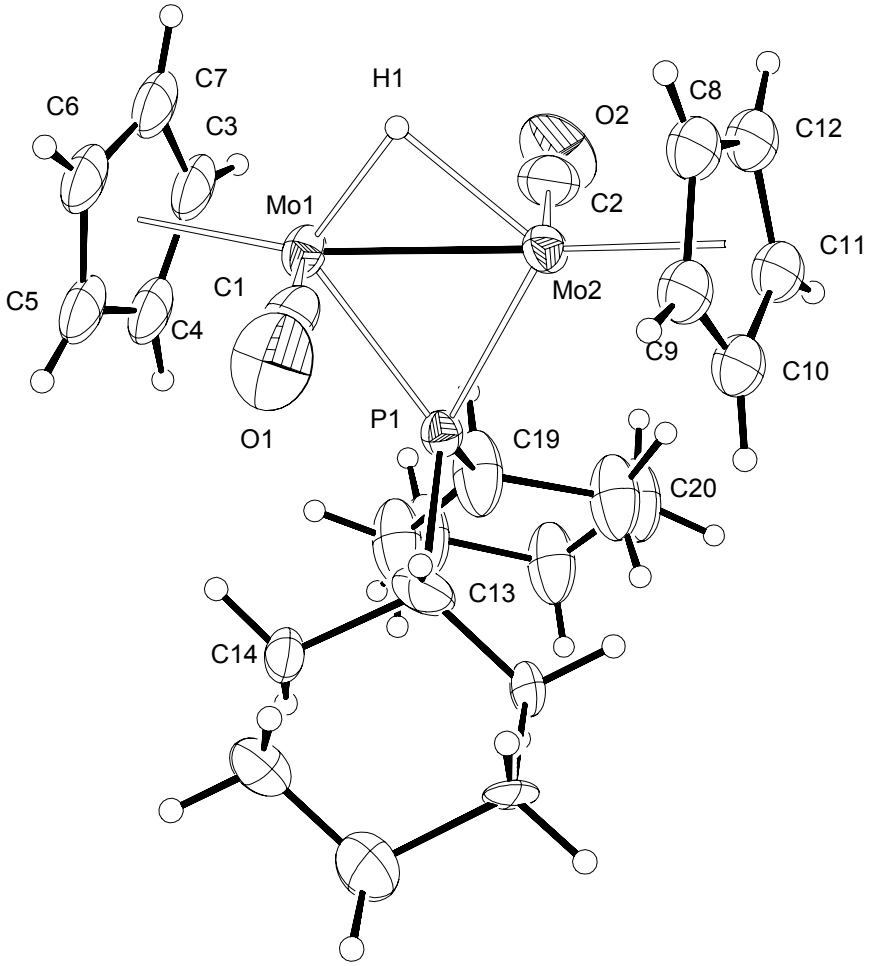

Figure S1: ORTEP view of the molecular structure of compound **1**.

Table S1: Crystal Data for Compound **1**.

Compound	**1**
mol formula	$C_{24}H_{33}O_2Mo_2P$
mol wt	576.38
cryst syst,space group	Monoclinic, *C2/c*
crystal color	Dark-brown
crystal shape	prism
radiation (λ, Å)	MoKα(λ=0.71073Å)
a, Å	35.081(12)
b, Å	8.798(3)
c, Å	16.104(6)
α, deg	90
β, deg	103.27(2)
γ, deg	90
V, Å^3	4838(3)
Z	8
calcd density, gcm^{-3}	1.583
μ, cm^{-1}	11.198
Diffractometer	Philips PW1100
temperature, K	293
θ limits, deg	3.03 - 25
total data	4256
unique total data	4256
unique data used	1798 [$(F_O)^2>2\sigma(F_O)^2$]
R[a]	0.0585
R_W[b]	0.1121
GOF	0.874
Octants collected	41, 40; 0, 10 ; 0,19
Nb of variables	176
$\Delta\sigma$ (mean)	0.001
$\Delta\rho$(max, min), e/Å^3	0.842, -0.539

[a] $R = \Sigma||F_O| - |F_C|| / \Sigma|F_O|$. [b] $R_W = [\Sigma w(|F_O|^2 - |F_C|^2)^2 / \Sigma w|F_O|^2]^{1/2}$. $w = 1/[\sigma^2(F_o^2) + (0.0536P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$.

Table S2. Fractional Atomic Coordinates for Compound **1**.

Atom	X/a	Y/b	Z/c
C1	0.5689(3)	0.4713(16)	0.0822(8)
C2	0.5667(2)	0.0270(8)	-0.0126(4)
C3_C	0.5648(2)	0.3664(8)	-0.1635(4)
C4_C	0.5967(2)	0.4613(8)	-0.1249(4)
C5_C	0.5817(2)	0.5847(8)	-0.0854(4)
C6_C	0.5405(2)	0.5661(8)	-0.0995(4)
C7_C	0.5301(2)	0.4312(8)	-0.1478(4)
C8A_	0.5331(2)	0.0014(8)	0.1594(4)
C9A_	0.5479(2)	0.1284(8)	0.2113(4)
C10A	0.5891(2)	0.1107(8)	0.2396(4)
C11A	0.5998(2)	-0.0272(8)	0.2051(4)
C12A	0.5652(2)	-0.0948(8)	0.1556(4)
C19	0.6602(2)	0.1365(8)	0.0102(4)
C20	0.6745(4)	-0.0163(13)	0.0534(9)
C21	0.6931(4)	-0.1189(14)	-0.0027(9)
C22	0.7191(4)	-0.0440(14)	-0.0454(9)
C23	0.7039(4)	0.1005(14)	-0.0903(9)
C24	0.6874(4)	0.204814)	-0.0323(9)
O1	0.5689(3)	0.5508(12)	0.1411(7)
O2	0.5692(3)	-0.0518(12)	-0.0707(6)
P1	0.6283(1)	0.2483(4)	0.0638(16)
Mo1	0.56917(3)	0.3550(1)	-0.01833(6)
Mo2	0.56905(3)	0.14346(13)	0.08783(6)
C8_B	0.53001(3)	0.06304(13)	0.18134(6)
C9_B	0.56455(3)	0.12685(13)	0.23321(6)
C10_	0.59677(3)	0.03546(13)	0.22449(6)
C11_	0.58214(3)	-0.08483(13)	0.16723(6)
C12_	0.54088(3)	-0.06778(13)	0.14056(6)
C3A_	0.58891(3)	0.37693(13)	-0.15226(6)
C4A_	0.59745(3)	0.51653(13)	-0.10762(6)
C5A_	0.56152(3)	0.58143(13)	-0.09885(6)
C6A_	0.53077(3)	0.48194(13)	-0.13808(6)
C7A_	0.54769(3)	0.35555(13)	-0.17109(6)
C13_	0.66050(3)	0.35976(13)	0.15029(6)
C14_	0.67710(3)	0.50725(13)	0.11495(6)
C15_	0.68772(3)	0.62727(13)	0.20786(6)
C16_	0.71864(3)	0.54708(13)	0.26641(6)
C17_	0.69925(3)	0.40209(13)	0.30223(6)
C18_	0.69014(3)	0.28459(13)	0.21429(6)
C13A	0.66050(3)	0.35976(13)	0.15029(6)
C14A	0.66830(3)	0.52968(13)	0.12789(6)
C15A	0.70757(3)	0.58393(13)	0.18316(6)
C16A	0.71864(3)	0.54708(13)	0.26641(6)
C17A	0.71213(3)	0.37348(13)	0.28436(6)
C18A	0.66250(3)	0.32863(13)	0.23242(6)
H1	0.529(3)	0.246(12)	0.015(5)

Table S3. Bond Lengths [Å] for Compound **1**

C1	- O1	1.177(17)	Mo1	- Mo2	2.5278(17)
C1	- MO1	1.918(13)	Mo1	- C3A_	2.4196(17)
C2	- O2	1.183(12)	Mo1	- C4A_	2.3930(17)
C2	- MO2	1.900(6)	Mo1	- C5A_	2.3584(17)
C3_C	- C4_C	1.419(9)	Mo1	- C6A_	2.3640(15)
C3_C	- C7_C	1.42(1)	Mo1	- C7A_	2.4018(16)
C3_C	- MO1	2.30(7)	Mo1	- H1	1.88(9)
C4_C	- C5_C	1.42(1)	Mo2	- C8_B	2.3645(17)
C4_C	- MO1	2.349(7)	Mo2	- C9_B	2.3869(17)
C5_C	- C6_C	1.419(9)	Mo2	- C10_	2.3894(15)
C5_C	- MO1	2.379(7)	Mo2	- C11_	2.3686(17)
C6_C	- C7_C	1.420(9)	Mo2	- C12_	2.3531(17)
C6_C	- MO1	2.359(7)	Mo2	- H1	1.84(8)
C7_C	- MO1	2.316(6)	C8_B	- C9_B	1.4200(14)
C8A_	- C9A_	1.420(9)	C8_B	- C12_	1.4200(16)
C8A_	- C12A	1.42(1)	C9_B	- C10_	1.4201(16)
C8A_	- MO2	2.268(7)	C10_	- C11_	1.4200(15)
C9A_	- C10A	1.419(9)	C11_	- C12_	1.4201(15)
C9A_	- MO2	2.280(7)	C3A_	- C4A_	1.4199(16)
C10A	- C11A	1.42(1)	C3A_	- C7A_	1.4202(15)
C10A	- MO2	2.399(6)	C4A_	- C5A_	1.4200(16)
C11A	- C12A	1.419(9)	C5A_	- C6A_	1.4199(15)
C11A	- MO2	2.459(6)	C6A_	- C7A_	1.4200(16)
C12A	- MO2	2.381(7)	C13_	- C14_	1.5808(17)
C19	- C20	1.543(14)	C13_	- C18_	1.4453(14)
C19	- C24	1.427(16)	C14_	- C15_	1.7990(15)
C19	- P1	1.845(8)	C15_	- C16_	1.4470(14)
C20	- C21	1.52(2)	C16_	- C17_	1.6133(17)
C21	- C22	1.42(2)	C17_	- C18_	1.7230(15)
C22	- C23	1.498(18)	C13A	- C18A	1.3367(15)
C23	- C24	1.51(2)	C14A	- C15A	1.5346(14)
P1	- MO1	2.382(3)	C15A	- C16A	1.3469(14)
P1	- MO2	2.385(3)	C16A	- C17A	1.5807(17)
P1	- C13_	1.858(3)	C17A	- C18A	1.7939(15)
P1	- C13A	1.858(3)			

Table S4. Bond Angles [°] for Compound **1**.

O1 - C1 - Mo1	175.8(11)	C1 - Mo1 - C7_C	119.3(4)
O2 - C2 - Mo2	172.7(7)	C1 - Mo1 - P1	85.1(4)
C4_C - C3_C - C7_C	108.0(6)	C1 - Mo1 - Mo2	79.7(4)
C4_C - C3_C - Mo1	73.7(4)	C1 - Mo1 - C3A_	140.2(4)
C7_C - C3_C - Mo1	72.4(4)	C1 - Mo1 - C4A_	105.9(4)
C3_C - C4_C - C5_C	108.0(6)	C1 - Mo1 - C5A_	89.5(4)
C3_C - C4_C - Mo1	70.8(4)	C1 - Mo1 - C6A_	108.9(4)
C5_C - C4_C - Mo1	73.7(4)	C1 - Mo1 - C7A_	143.4(4)
C4_C - C5_C - C6_C	108.0(6)	C1 - Mo1 - H1	83(3)
C4_C - C5_C - Mo1	71.4(4)	C3_C - Mo1 - C4_C	35.5(2)
C6_C - C5_C - Mo1	71.8(4)	C3_C - Mo1 - C5_C	58.7(2)
C5_C - C6_C - C7_C	108.0(6)	C3_C - Mo1 - C6_C	58.9(2)
C5_C - C6_C - Mo1	73.3(4)	C3_C - Mo1 - C7_C	35.8(2)
C7_C - C6_C - Mo1	70.7(4)	C3_C - Mo1 - P1	115.2(2)
C3_C - C7_C - C6_C	108.0(6)	C3_C - Mo1 - Mo2	135.0(2)
C3_C - C7_C - Mo1	71.9(4)	C3_C - Mo1 - H1	116(3)
C6_C - C7_C - Mo1	74.0(4)	C4_C - Mo1 - C5_C	35.0(2)
C6_C - C7_C - C5A_	23.6(3)	C4_C - Mo1 - C6_C	58.4(2)
C9A_ - C8A_ - C12A	108.0(6)	C4_C - Mo1 - C7_C	59.0(2)
C9A_ - C8A_ - Mo2	72.3(4)	C4_C - Mo1 - P1	96.4(2)
C12A - C8A_ - Mo2	76.6(4)	C4_C - Mo1 - Mo2	148.4(2)
C8A_ - C9A_ - C10A	108.0(4)	C4_C - Mo1 - H1	150(3)
C8A_ - C9A_ - Mo2	71.4(4)	C5_C - Mo1 - C6_C	34.9(2)
C10A - C9A_ - Mo2	77.0(4)	C5_C - Mo1 - C7_C	58.6(2)
Mo2 - C9A_ - C8_B	84.0(4)	C5_C - Mo1 - P1	111.0(2)
C9A_ - C10A - C11A	108.0(6)	C5_C - Mo1 - Mo2	164.0(2)
C9A_ - C10A - Mo2	67.8(4)	C5_C - Mo1 - H1	142(3)
C11A - C10A - Mo2	75.3(4)	C6_C - Mo1 - C7_C	35.3(2)
C10A - C11A - C12A	108.0(6)	C6_C - Mo1 - P1	145.5(2)
C10A - C11A - Mo2	70.7(4)	C6_C - Mo1 - Mo2	152.6(2)
C12A - C11A - Mo2	69.9(4)	C6_C - Mo1 - H1	108(3)
C11A - H11A - C10_	24.4(4)	C7_C - Mo1 - P1	150.9(2)
C8A_ - C12A - C11A	108.0(6)	C7_C - Mo1 - Mo2	136.8(2)
C8A_ - C12A - Mo2	67.9(4)	C7_C - Mo1 - H1	94(3)
C11A - C12A - Mo2	76.0(4)	P1 - Mo1 - Mo2	58.0(1)
C20 - C19 - C24	113.5(8)	P1 - Mo1 - C3A_	97.8(1)
C20 - C19 - P1	115.0(6)	P1 - Mo1 - C4A_	98.0(1)
C24 - C19 - P1	122.9(7)	P1 - Mo1 - C5A_	127.8(1)
C19 - C20 - C21	112.8(9)	P1 - Mo1 - C6A_	154.1(1)
C20 - C21 - C22	114.9(12)	P1 - Mo1 - C7A_	126.7(1)
C21 - C22 - C23	115.4(11)	P1 - Mo1 - H1	104(3)
C22 - C23 - C24	111.0(11)	Mo2 - Mo1 - C3A_	135.0(1)
C19 - C24 - C23	115.6(11)	Mo2 - Mo1 - C4A_	155.4(1)
C19 - P1 - Mo1	119.6(3)	Mo2 - Mo1 - C5A_	167.5(1)
C19 - P1 - Mo2	121.0(3)	Mo2 - Mo1 - C6A_	144.1(1)
C19 - P1 - C13_	107.6(3)	Mo2 - Mo1 - C7A_	130.2(1)
C19 - P1 - C13A	107.6(2)	Mo2 - Mo1 - H1	46(3)
Mo1 - P1 - Mo2	64.03(1)	C3A_ - Mo1 - C4A_	34.31(4)
Mo1 - P1 - C13_	120.7(1)	C3A_ - Mo1 - C5A_	57.47(4)
Mo1 - P1 - C13A	120.7(1)	C3A_ - Mo1 - C6A_	57.40(4)
Mo2 - P1 - C13_	119.0(1)	C3A_ - Mo1 - C7A_	34.26(4)
Mo2 - P1 - C13A	119.0(1)	C3A_ - Mo1 - H1	133(3)
C1 - Mo1 - C3_C	145.0(4)	C4A_ - Mo1 - C5A_	34.77(4)
C1 - Mo1 - C4_C	119.2(4)	C4A_ - Mo1 - C6A_	57.76(4)
C1 - Mo1 - C5_C	88.1(4)	C4A_ - Mo1 - C7A_	57.26(4)
C1 - Mo1 - C6_C	87.9(4)	C4A_ - Mo1 - H1	156(3)

C5A_	Mo1	C6A_	35.00(4)
C5A_	Mo1	C7A_	57.71(4)
C5A_	Mo1	H1	126(3)
C6A_	Mo1	C7A_	34.66(4)
C6A_	Mo1	H1	98.69(3)
C7A_	Mo1	H1	102(3)
C2	Mo2	P1	86.5(2)
C2	Mo2	Mo1	80.1(2)
C2	Mo2	C10_	119.9(2)
C2	Mo2	C11_	88.1(2)
C2	Mo2	C12_	86.7(2)
C2	Mo2	H1	81(3)
C8A_	Mo2	C9A_	36.4(2)
C8A_	Mo2	C10A	58.9(2)
C8A_	Mo2	C11A	58.0(2)
C8A_	Mo2	C12A	35.5(2)
C8A_	Mo2	P1	154.4(2)
C8A_	Mo2	Mo1	146.8(2)
C8A_	Mo2	H1	99(3)
C9A_	Mo2	C10A	35.2(2)
C9A_	Mo2	C11A	57.8(2)
C9A_	Mo2	C12A	59.0(2)
C9A_	Mo2	P1	129.4(2)
C9A_	Mo2	Mo1	133.2(2)
C9A_	Mo2	H1	103(3)
C10A	Mo2	C11A	34.0(2)
C10A	Mo2	C12A	57.4(2)
C10A	Mo2	P1	98.6(2)
C10A	Mo2	Mo1	137.0(2)
C10A	Mo2	H1	135(3)
C11A	Mo2	C12A	34.1(2)
C11A	Mo2	P1	96.7(2)
C11A	Mo2	Mo1	154.2(2)
C11A	Mo2	H1	157(3)
C12A	Mo2	P1	123.9(2)
C12A	Mo2	Mo1	165.3(2)
C12A	Mo2	H1	127(3)
P1	Mo2	Mo1	57.9(1)
P1	Mo2	C8_B	150.8(1)
P1	Mo2	C9_B	116.1(1)
P1	Mo2	C10_	96.8(1)
P1	Mo2	C11_	110.3(1)
P1	Mo2	C12_	144.8(1)
P1	Mo2	H1	106(1)
Mo1	Mo2	C8_B	137.9(1)
Mo1	Mo2	C9_B	134.0(1)
Mo1	Mo2	C10_	148.5(1)
Mo1	Mo2	C11_	163.6(1)
Mo1	Mo2	C12_	153.1(1)
Mo1	Mo2	H1	48(3)
C8_B	Mo2	C9_B	34.78(4)
C8_B	Mo2	C10_	57.80(4)
C8_B	Mo2	C11_	58.08(4)
C8_B	Mo2	C12_	35.03(4)
C8_B	Mo2	H1	94(3)
C9_B	Mo2	C10_	34.59(4)
C9_B	Mo2	C11_	57.78(4)
C9_B	Mo2	C12_	57.99(4)
C9_B	Mo2	H1	116(3)
C10_	Mo2	C11_	34.73(4)
C10_	Mo2	C12_	57.95(4)
C10_	Mo2	H1	150(3)
C11_	Mo2	C12_	35.00(4)
C11_	Mo2	H1	141(3)
C12_	Mo2	H1	107(3)
Mo2	C8_B	C9_B	73.47(7)
Mo2	C8_B	C12_	72.04(7)
H8_B	C8_B	C9_B	126.0(1)
H8_B	C8_B	C12_	126.0(1)
C9_B	C8_B	C12_	108.0(1)
Mo2	C9_B	C8_B	71.7(1)
Mo2	C9_B	C10_	72.8(1)
C8_B	C9_B	C10_	108.0(1)
Mo2	C10_	C9_B	72.6(1)
Mo2	C10_	C11_	71.8(1)
C9_B	C10_	C11_	108.0(1)
Mo1	C4A_	C3A_	73.9(1)
Mo1	C4A_	C5A_	71.3(1)
C3A_	C4A_	C5A_	108.0(1)
C4_C	C5A_	C5_C	51.1(1)
C4_C	C5A_	C6_C	129.5(6)
C4_C	C5A_	C7_C	81.1(3)
Mo1	C5A_	C4A_	73.1(1)
Mo1	C5A_	C6A_	72.7(1)
C4A_	C5A_	C6A_	108.0(1)
Mo1	C6A_	C5A_	72.3(1)
Mo1	C6A_	C7A_	74.1(1)
C5A_	C6A_	C7A_	108.0(1)
Mo1	C7A_	C3A_	73.6(1)
Mo1	C7A_	C6A_	71.2(1)
C3A_	C7A_	C6A_	108.0(1)
P1	C13_	C14_	112.0(1)
P1	C13_	C18_	120.4(1)
P1	C13_	C14A	115.9(1)
P1	C13_	C18A	121.2(1)
C14_	C13_	C18_	111.6(1)
C13_	C14_	C15_	101.9(1)
C14_	C15_	C16_	103.7(1)
C15_	C16_	C17_	107.7(1)
C16_	C17_	C18_	101.2(1)
C16A	C17_	C18A	113.4(1)
C13_	C18_	C17_	106.2(1)
P1	C13A	C14A	115.9(1)
P1	C13A	C18A	121.2(1)
C14A	C13A	C18A	116.6(1)
C13A	C14A	C15A	110.0(1)
C14A	C15A	C16A	121.2(1)
C15A	C16A	C17A	113.2(1)
C16A	C17A	C18A	107.0(1)
C13A	C18A	C17A	104.0(1)
Mo1	H1	Mo2	85(4)

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for compound **1**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

Atom	U11	U22	U33	U23	U13	U12
C1	48(8)	69(11)	62(9)	78(8)	21(7)	26(7)
C2	56(9)	79(12)	65(10)	10(9)	8(8)	-13(8)
C3_C	72(8)	78(9)	63(9)	43(7)	20(6)	22(7)
C4_C	72(8)	78(9)	63(9)	43(7)	20(6)	22(7)
C5_C	72(8)	78(9)	63(9)	43 (7)	20(6)	22(7)
C6_C	72(8)	78(9)	63(9)	43(7)	20(6)	22(7)
C7_C	72(8)	78 (9)	63(8)	43(7)	20(6)	22(7)
C8A_	89(14)	86(16)	41(12)	-5(12)	3(9)	-24(12)
C9A_	89(14)	86(16)	41(12)	-5(12)	3(9)	-24(12)
C10A	89(14)	86(16)	41(12)	-5(12)	3(9)	-24(12)
C11A	89(14)	86(16)	41(12)	-5(12)	3(9)	-24(12)
C12A	89(14)	86(16)	41(12)	-5(12)	3(9)	-24(12
C19	111(5)	59(5)	124(5)	28(4)	75(4)	34(4)
C20	111(5)	59(5)	124(5)	28(4)	75(4)	34(4))
C21	111(5)	59(5)	124(5)	28(4)	75(4)	34(4)
C22	111(5)	59(5)	124(5)	28(4)	75(4)	34(4)
C23	111(5)	9(5)	124(5)	28(4)	75(4)	34(4)
C24	111(5)	59(5)	124(5)	28(4)	75(4)	34(4))
O1	135(10)	82(8)	103(8)	-26(7)	51(7)	39(7)
O2	145(10)	90(8)	81(7)	-42(7)	42(7)	-38(7)
P1	43(2)	36(2)	33(2)	2(2)	11(1)	0(2)
Mo1	46(1)	45(1)	41(1)	8(1)	16(1)	10(1)
Mo2	45(1)	44(1)	37(1)	4(1)	10(1)	-8(1)
C8_B	78(8)	76(9)	44(7)	16(6)	7(5)	-12(6)
C9_B	78(8)	76(9)	44(7)	16(6)	7(5)	-12(6)
C10_	78(8)	76(9)	44(7)	16(6)	7(5)	-12(6)
C11_	78(8)	76(9)	44(7)	16(6)	7(5)	-12(6)
C12_	78(8)	76(9)	44(7)	16(6)	7(5)	-12(6)
C3A_	87(13)	78(14)	68(14)	16(12)	30(10)	12(11)
C4A_	87(13)	78(14)	68(14)	16(12)	30(10)	12(11)
C5A_	87(13)	78(14)	68(14)	16(12)	30(10)	12(11)
C6A_	87(13)	78(14)	68(14)	16(12)	30(10)	12(11)
C7A_	87(13)	78(14)	68(14)	16(12)	30(10)	12(11)
C13_	82(10)	77(11)	71(9)	3(9)	-13(8)	-46(9)
C14_	47(13)	38(15)	57(15)	16(12)	14(12)	8(12)
C15_	73(17)	50(15)	101(20)	-4(17)	3(14)	-20(14)
C16_	154(18)	68(13)	128(16)	16(12)	-41(13)	-42(12)
C17_	50(13)	44(15)	51(13)	-9(12)	-33(11)	-16(11)
C18_	60(14)	21(11)	58(14)	10(10)	8(11)	1(9)
C13A	82(10)	77(11)	71(9)	3(9)	-13(7)	-46(9)
C14A	24(17)	72(29)	37(20)	-20(20)	25(16)	-14(17)
C15A	111(34)	31(21)	55(23)	-12(18)	24(23)	-27(22)
C16A	154(18)	68(13)	128(16)	16(12)	-41(13)	-42(12)
C17A	81(26)	79(32)	47(21)	-16(23)	31(20)	-7(25)
C18A	127(31)	20(19)	25(16)	-16(14)	12(18)	3(19)
H1	66(32)					

Table S6. Fractional Hydrogen Coordinates for Compound **1**.

atom	x/a	y/b	z/c
H3_C	0.56640	0.27747	-0.19374
H4_C	0.62288	0.44536	-0.12546
H5_C	0.59628	0.66380	-0.05549
H6_C	0.52337	0.63092	-0.08053
H7_C	0.50490	0.39215	-0.16597
H8A_	0.50704	-0.01579	0.13261
H9A_	0.53315	0.20899	0.22448
H10A	0.60604	0.17772	0.27450
H11A	0.62497	-0.06638	0.21355
H12A	0.56379	-0.18597	0.12585
H19	0.64063	0.09945	-0.03924
H20A	0.69344	0.00345	0.10636
H20B	0.65244	-0.06900	0.06717
H21A	0.70742	-0.19907	0.03260
H21B	0.67244	-0.16642	-0.04508
H22A	0.72550	-0.11354	-0.08690
H22B	0.74320	-0.02136	-0.00396
H23A	0.68357	0.07684	-0.14055
H23B	0.72494	0.15201	-0.10884
H24A	0.70902	0.24568	0.01047
H24B	0.67452	0.28948	-0.06600
H8_B	0.50472	0.10038	0.17516
H9_B	0.56585	0.21331	0.26697
H10_	0.62287	0.05155	0.25153
H11_	0.59698	-0.16134	0.15019
H12_	0.52395	-0.13116	0.10298
H3A_	0.60710	0.31106	-0.16664
H4A_	0.62223	0.55815	-0.08763
H5A_	0.55864	0.67302	-0.07212
H6A_	0.50421	0.49692	-0.14155
H7A_	0.53416	0.27322	-0.19997
H13_	0.64233	0.40008	0.18284
H14A	0.65773	0.55315	0.06902
H14B	0.70056	0.48505	0.09495
H15A	0.69647	0.72689	0.19429
H15B	0.66486	0.63901	0.23164
H16A	0.73087	0.61323	0.31314
H16B	0.73850	0.51402	0.23723
H17A	0.67527	0.42937	0.31890
H17B	0.71727	0.35565	0.35028
H18A	0.71378	0.26965	0.19373
H18B	0.68083	0.18631	0.22848
H13A	0.68573	0.31646	0.14608
H14C	0.66879	0.53730	0.06805
H14D	0.64733	0.59392	0.13789
H15C	0.72791	0.54776	0.15620
H15D	0.70770	0.69399	0.17973
H16C	0.70394	0.60844	0.29821
H16D	0.74617	0.57136	0.28702
H17C	0.71652	0.35540	0.34524
H17D	0.73016	0.31078	0.26186
H18C	0.65684	0.22230	0.24009
H18D	0.64421	0.39077	0.25447
H1	0.529(3)	0.246(12)	0.015(5)

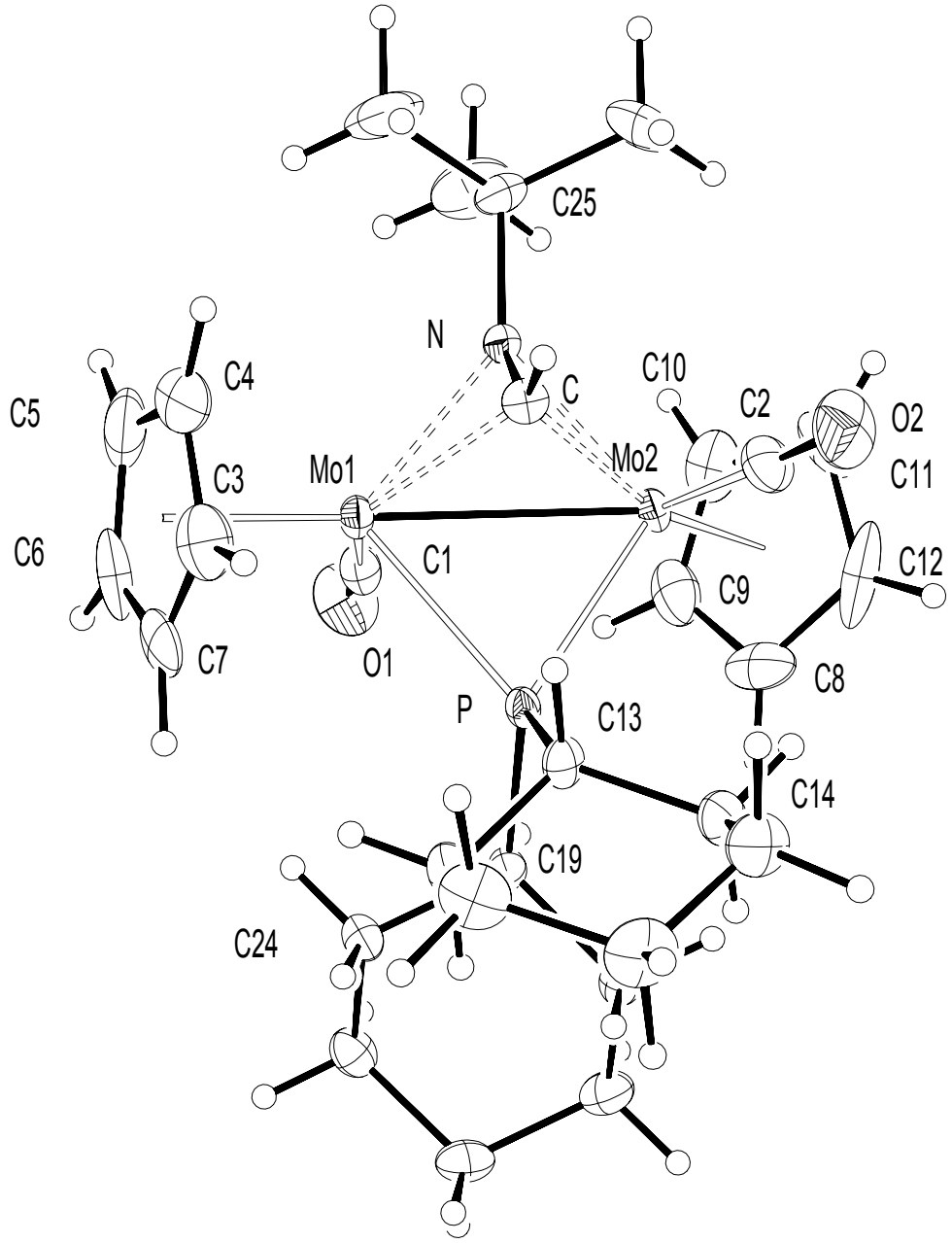

Figure S2: ORTEP view of the molecular structure of compound **3**.

Table S7: Crystal data for Compounds **3**.

Compound	**3**
mol formula	$C_{29}H_{42}O_2Mo_2PN$
mol wt	659.49
cryst syst,space group	Triclinic, *P-1*
crystal color	Yellow-orange
crystal shape	prism
crystal size, mm^3	0.40 × 0.35 × 0.30
radiation (λ, Å)	MoKα(λ=0.71073Å)
a, Å	10.100(6)
b, Å	11.745(7)
c, Å	13.815(9)
α, deg	105.90(2)
β, deg	98.26(2)
γ, deg	107.56(2)
V, $Å^3$	1456.2(15)
Z	2
calcd density, gcm^{-3}	1.504
μ, cm^{-1}	9.41
Diffractometer	Philips PW1100
temperature, K	293
θ limits, deg	3.1-24
total data	4240
unique total data	4240
unique data used	3772 [$(F_O)^2>2\sigma(F_O)^2$]
R[a]	0.058
R_W[b]	0.063
GOF	1.072
Octants collected	-11,11 ; -13,12 ; 0,15
Nb of variables	316
$\Delta\sigma$ (mean)	0.001
$\Delta\rho$(max, min), e/$Å^3$	2.116, -1.996

[a] $R = \Sigma||F_O| - |F_C|| / \Sigma|F_O|$. [b] $R_W = [\Sigma w(|F_O|^2 - |F_C|^2)^2 / \Sigma w|F_O|^2]^{1/2}$. $w = 1/[\sigma^2(F_o^2) + (0.1563P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$.

Table S8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C	4670(6)	6434(5)	6305(4)	30(1)
C(1)	5905(6)	8817(6)	8794(4)	38(1)
C(2)	2240(7)	5886(6)	5592(4)	46(1)
C(3)	6618(9)	5532(7)	7934(6)	61(2)
C(4)	7549(10)	6319(10)	7501(7)	72(3)
C(5)	8247(8)	7514(10)	8328(9)	83(3)
C(6)	7729(9)	7403(9)	9192(7)	78(3)
C(7)	6755(8)	6207(7)	8943(6)	58(2)
C(8)	1744(9)	8236(8)	7634(7)	66(2)
C(9)	2988(9)	9226(8)	7867(6)	57(2)
C(10)	3243(8)	9438(6)	7012(6)	57(2)
C(11)	2178(9)	8612(8)	6159(5)	62(2)
C(12)	1186(8)	7774(7)	6533(9)	86(3)
C(13)	2546(5)	4491(5)	7517(4)	31(1)
C(14)	917(6)	3960(5)	7070(4)	39(1)
C(15)	361(7)	2529(6)	6541(5)	54(2)
C(16)	797(7)	1850(5)	7249(5)	54(2)
C(17)	2414(8)	2377(6)	7708(5)	54(2)
C(18)	2933(6)	3809(5)	8251(4)	38(1)
C(19)	2957(5)	6878(5)	9300(4)	27(1)
C(20)	1382(6)	6301(5)	9330(4)	33(1)
C(21)	1102(7)	6979(6)	10350(5)	43(1)
C(22)	2075(6)	6901(6)	11268(4)	42(1)
C(23)	3639(6)	7458(5)	11256(4)	38(1)
C(24)	3938(6)	6826(5)	10234(4)	33(1)
C(25)	6119(6)	8292(6)	5814(5)	44(1)
C(26)	5084(11)	7912(12)	4764(7)	92(3)
C(27)	7339(10)	7786(11)	5634(8)	88(3)
C(28)	6715(10)	9714(7)	6353(8)	81(3)
N	5365(4)	7719(4)	6500(3)	30(1)
O(1)	6116(6)	9779(4)	9410(4)	68(1)
O(2)	1617(5)	5021(5)	4832(4)	71(2)
P	3398(1)	6256(1)	8033(1)	23(1)
Mo(1)	5806(1)	7179(1)	7873(1)	25(1)
Mo(2)	3260(1)	7363(1)	6788(1)	24(1)

Table S9. Bond lengths [Å] for compound **3**.

C-N	1.388(7)	C(11)-Mo(2)	2.343(6)
C-Mo(1)	2.101(6)	C(12)-Mo(2)	2.288(7)
C-Mo(2)	2.115(6)	C(13)-C(18)	1.530(8)
C(1)-O(1)	1.149(7)	C(13)-C(14)	1.535(8)
C(1)-Mo(1)	1.959(6)	C(13)-P	1.867(5)
C(2)-O(2)	1.171(7)	C(14)-C(15)	1.522(8)
C(2)-Mo(2)	1.914(6)	C(15)-C(16)	1.517(10)
C(3)-C(7)	1.366(11)	C(16)-C(17)	1.527(10)
C(3)-C(4)	1.426(12)	C(17)-C(18)	1.526(8)
C(3)-Mo(1)	2.335(7)	C(19)-C(24)	1.537(7)
C(4)-C(5)	1.437(14)	C(19)-C(20)	1.542(7)
C(4)-Mo(1)	2.330(7)	C(19)-P	1.874(5)
C(5)-C(6)	1.392(13)	C(20)-C(21)	1.528(8)
C(5)-Mo(1)	2.337(8)	C(21)-C(22)	1.530(9)
C(6)-C(7)	1.365(11)	C(22)-C(23)	1.522(8)
C(6)-Mo(1)	2.361(7)	C(23)-C(24)	1.523(8)
C(7)-Mo(1)	2.363(6)	C(25)-N	1.475(7)
C(8)-C(9)	1.353(12)	C(25)-C(28)	1.514(10)
C(8)-C(12)	1.429(12)	C(25)-C(26)	1.526(11)
C(8)-Mo(2)	2.359(6)	C(25)-C(27)	1.543(10)
C(9)-C(10)	1.316(11)	N-Mo(2)	2.157(4)
C(9)-Mo(2)	2.404(7)	N-Mo(1)	2.187(4)
C(10)-C(11)	1.366(10)	P-Mo(1)	2.4163(19)
C(10)-Mo(2)	2.377(6)	P-Mo(2)	2.4363(17)
C(11)-C(12)	1.439(13)	Mo(1)-Mo(2)	2.8831(15)

Table S10. Bond Angles [°] for Compound **3**.

N-C-Mo(1)	74.5(3)	C(26)-C(25)-C(27)	108.1(8)
N-C-Mo(2)	72.7(3)	C-N-C(25)	126.4(5)
Mo(1)-C-Mo(2)	86.3(2)	C-N-Mo(2)	69.4(3)
O(1)-C(1)-Mo(1)	171.3(5)	C(25)-N-Mo(2)	135.4(3)
O(2)-C(2)-Mo(2)	176.6(6)	C-N-Mo(1)	67.8(3)
C(7)-C(3)-C(4)	109.0(8)	C(25)-N-Mo(1)	140.5(3)
C(7)-C(3)-Mo(1)	74.3(4)	Mo(2)-N-Mo(1)	83.16(14)
C(4)-C(3)-Mo(1)	72.0(4)	C(13)-P-C(19)	109.4(2)
C(3)-C(4)-C(5)	105.0(7)	C(13)-P-Mo(1)	117.33(18)
C(3)-C(4)-Mo(1)	72.4(4)	C(19)-P-Mo(1)	118.65(17)
C(5)-C(4)-Mo(1)	72.3(5)	C(13)-P-Mo(2)	116.77(17)
C(6)-C(5)-C(4)	107.7(7)	C(19)-P-Mo(2)	118.08(17)
C(6)-C(5)-Mo(1)	73.7(4)	Mo(1)-P-Mo(2)	72.90(4)
C(4)-C(5)-Mo(1)	71.8(4)	C(1)-Mo(1)-C	121.9(2)
C(7)-C(6)-C(5)	108.9(8)	C(1)-Mo(1)-N	91.5(2)
C(7)-C(6)-Mo(1)	73.3(4)	C-Mo(1)-N	37.69(19)
C(5)-C(6)-Mo(1)	71.8(4)	C(1)-Mo(1)-C(4)	132.9(3)
C(6)-C(7)-C(3)	109.4(8)	C-Mo(1)-C(4)	92.0(3)
C(6)-C(7)-Mo(1)	73.1(4)	N-Mo(1)-C(4)	100.3(2)
C(3)-C(7)-Mo(1)	71.9(4)	C(1)-Mo(1)-C(3)	139.4(3)
C(9)-C(8)-C(12)	107.8(7)	C-Mo(1)-C(3)	98.7(3)
C(9)-C(8)-Mo(2)	75.3(4)	N-Mo(1)-C(3)	125.4(2)
C(12)-C(8)-Mo(2)	69.4(4)	C(4)-Mo(1)-C(3)	35.6(3)
C(10)-C(9)-C(8)	109.8(7)	C(1)-Mo(1)-C(5)	97.1(3)
C(10)-C(9)-Mo(2)	72.9(4)	C-Mo(1)-C(5)	120.5(3)
C(8)-C(9)-Mo(2)	71.7(4)	N-Mo(1)-C(5)	108.9(3)
C(9)-C(10)-C(11)	111.5(7)	C(4)-Mo(1)-C(5)	35.9(4)
C(9)-C(10)-Mo(2)	75.2(4)	C(3)-Mo(1)-C(5)	58.2(3)
C(11)-C(10)-Mo(2)	71.8(4)	C(1)-Mo(1)-C(6)	84.4(3)
C(10)-C(11)-C(12)	105.9(7)	C-Mo(1)-C(6)	150.2(3)
C(10)-C(11)-Mo(2)	74.5(4)	N-Mo(1)-C(6)	141.2(3)
C(12)-C(11)-Mo(2)	69.8(4)	C(4)-Mo(1)-C(6)	58.3(3)
C(8)-C(12)-C(11)	104.9(6)	C(3)-Mo(1)-C(6)	56.7(3)
C(8)-C(12)-Mo(2)	74.8(4)	C(5)-Mo(1)-C(6)	34.5(3)
C(11)-C(12)-Mo(2)	74.0(4)	C(1)-Mo(1)-C(7)	106.5(3)
C(18)-C(13)-C(14)	109.5(4)	C-Mo(1)-C(7)	130.5(3)
C(18)-C(13)-P	115.3(3)	N-Mo(1)-C(7)	157.8(2)
C(14)-C(13)-P	115.6(4)	C(4)-Mo(1)-C(7)	57.9(3)
C(15)-C(14)-C(13)	111.3(5)	C(3)-Mo(1)-C(7)	33.8(3)
C(16)-C(15)-C(14)	112.5(5)	C(5)-Mo(1)-C(7)	57.0(3)
C(15)-C(16)-C(17)	111.8(5)	C(6)-Mo(1)-C(7)	33.6(3)
C(18)-C(17)-C(16)	110.2(5)	C(1)-Mo(1)-P	88.76(18)
C(17)-C(18)-C(13)	111.9(5)	C-Mo(1)-P	79.41(16)
C(24)-C(19)-C(20)	109.1(4)	N-Mo(1)-P	100.40(11)
C(24)-C(19)-P	113.6(4)	C(4)-Mo(1)-P	132.3(3)
C(20)-C(19)-P	116.0(3)	C(3)-Mo(1)-P	99.0(2)
C(21)-C(20)-C(19)	111.7(4)	C(5)-Mo(1)-P	149.9(2)
C(20)-C(21)-C(22)	110.1(5)	C(6)-Mo(1)-P	118.0(3)
C(23)-C(22)-C(21)	110.3(4)	C(7)-Mo(1)-P	93.0(2)
C(22)-C(23)-C(24)	112.3(4)	C(1)-Mo(1)-Mo(2)	80.38(17)
C(23)-C(24)-C(19)	111.7(5)	C-Mo(1)-Mo(2)	47.05(15)
N-C(25)-C(28)	107.4(5)	N-Mo(1)-Mo(2)	47.97(11)
N-C(25)-C(26)	109.8(5)	C(4)-Mo(1)-Mo(2)	139.0(2)
C(28)-C(25)-C(26)	111.7(7)	C(3)-Mo(1)-Mo(2)	135.5(2)
N-C(25)-C(27)	109.2(5)	C(5)-Mo(1)-Mo(2)	156.2(2)
C(28)-C(25)-C(27)	110.7(7)	C(6)-Mo(1)-Mo(2)	162.7(2)

C(7)-Mo(1)-Mo(2)	146.4(2)	C-Mo(2)-C(9)	147.5(3)
P-Mo(1)-Mo(2)	53.87(5)	N-Mo(2)-C(9)	113.1(2)
C(2)-Mo(2)-C	70.3(2)	C(12)-Mo(2)-C(9)	57.2(3)
C(2)-Mo(2)-N	97.9(2)	C(11)-Mo(2)-C(9)	55.6(3)
C-Mo(2)-N	37.89(19)	C(8)-Mo(2)-C(9)	33.0(3)
C(2)-Mo(2)-C(12)	84.0(3)	C(10)-Mo(2)-C(9)	31.9(3)
C-Mo(2)-C(12)	153.1(3)	C(2)-Mo(2)-P	96.7(2)
N-Mo(2)-C(12)	145.7(3)	C-Mo(2)-P	78.69(15)
C(2)-Mo(2)-C(11)	93.0(3)	N-Mo(2)-P	100.66(12)
C-Mo(2)-C(11)	134.7(2)	C(12)-Mo(2)-P	113.2(3)
N-Mo(2)-C(11)	109.7(3)	C(11)-Mo(2)-P	146.4(2)
C(12)-Mo(2)-C(11)	36.2(3)	C(8)-Mo(2)-P	88.90(17)
C(2)-Mo(2)-C(8)	113.3(3)	C(10)-Mo(2)-P	130.8(2)
C-Mo(2)-C(8)	167.5(2)	C(9)-Mo(2)-P	99.6(2)
N-Mo(2)-C(8)	146.1(3)	C(2)-Mo(2)-Mo(1)	111.5(2)
C(12)-Mo(2)-C(8)	35.8(3)	C-Mo(2)-Mo(1)	46.66(15)
C(11)-Mo(2)-C(8)	57.8(3)	N-Mo(2)-Mo(1)	48.87(12)
C(2)-Mo(2)-C(10)	126.2(3)	C(12)-Mo(2)-Mo(1)	159.2(3)
C-Mo(2)-C(10)	133.7(2)	C(11)-Mo(2)-Mo(1)	148.1(2)
N-Mo(2)-C(10)	96.4(2)	C(8)-Mo(2)-Mo(1)	123.5(2)
C(12)-Mo(2)-C(10)	57.4(3)	C(10)-Mo(2)-Mo(1)	116.82(18)
C(11)-Mo(2)-C(10)	33.6(3)	C(9)-Mo(2)-Mo(1)	106.45(18)
C(8)-Mo(2)-C(10)	54.9(3)	P-Mo(2)-Mo(1)	53.23(4)
C(2)-Mo(2)-C(9)	141.2(3)		

Table S11. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for compound **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U11	U22	U33	U23	U13	U12
C	33(3)	26(3)	32(3)	8(2)	9(2)	10(2)
C(1)	34(3)	37(3)	37(3)	12(3)	0(2)	10(3)
C(2)	48(4)	47(4)	33(3)	6(3)	3(3)	15(3)
C(3)	67(5)	54(4)	75(5)	26(4)	9(4)	40(4)
C(4)	79(6)	118(8)	73(5)	51(6)	37(5)	85(6)
C(5)	33(4)	99(7)	121(8)	69(7)	-6(4)	15(4)
C(6)	61(5)	82(6)	78(5)	20(5)	-31(4)	36(5)
C(7)	55(4)	71(5)	68(5)	45(4)	1(3)	39(4)
C(8)	80(6)	89(6)	92(6)	64(5)	62(5)	70(5)
C(9)	63(5)	63(5)	48(4)	7(3)	3(3)	41(4)
C(10)	55(4)	30(3)	85(5)	15(3)	6(4)	23(3)
C(11)	94(6)	77(5)	45(4)	31(4)	9(4)	65(5)
C(12)	31(4)	39(4)	149(9)	-3(5)	-31(5)	13(3)
C(13)	25(3)	24(3)	33(3)	5(2)	-2(2)	2(2)
C(14)	36(3)	31(3)	38(3)	9(2)	-1(2)	1(2)
C(15)	47(4)	41(4)	41(3)	-2(3)	-1(3)	-10(3)
C(16)	59(4)	16(3)	66(4)	6(3)	10(3)	-5(3)
C(17)	70(5)	34(3)	58(4)	13(3)	16(3)	19(3)
C(18)	41(3)	27(3)	40(3)	12(2)	-2(2)	8(2)
C(19)	26(3)	28(3)	27(3)	11(2)	2(2)	7(2)
C(20)	31(3)	30(3)	36(3)	12(2)	7(2)	11(2)
C(21)	41(3)	48(4)	48(3)	20(3)	23(3)	18(3)
C(22)	50(4)	42(3)	36(3)	12(2)	22(3)	14(3)
C(23)	42(3)	32(3)	33(3)	10(2)	3(2)	10(2)
C(24)	35(3)	37(3)	29(3)	13(2)	4(2)	15(2)
C(25)	35(3)	57(4)	50(3)	27(3)	23(3)	15(3)
C(26)	91(7)	144(9)	61(5)	73(6)	24(5)	31(6)
C(27)	81(6)	130(8)	120(8)	91(7)	77(6)	63(6)
C(28)	84(6)	55(5)	113(7)	43(5)	49(5)	12(4)
N	24(2)	40(3)	31(2)	20(2)	8(2)	14(2)
O(1)	87(4)	42(3)	54(3)	-5(2)	-1(3)	18(3)
O(2)	62(3)	60(3)	51(3)	-12(2)	-8(2)	6(3)
P	21(1)	21(1)	26(1)	10(1)	1(1)	5(1)
Mo(1)	21(1)	25(1)	28(1)	11(1)	2(1)	8(1)
Mo(2)	23(1)	22(1)	24(1)	9(1)	-2(1)	6(1)

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

	x	y	z	U(eq)
H(0)	4543	5670	5732	36
H(3)	6016	4695	7585	73
H(4)	7676	6105	6830	86
H(5)	8924	8232	8293	99
H(6)	8002	8040	9834	93
H(7)	6260	5900	9391	69
H(8)	1327	7914	8106	79
H(9)	3574	9688	8531	68
H(10)	4046	10070	6991	68
H(11)	2109	8594	5476	75
H(12)	363	7083	6143	103
H(13)	2944	4222	6925	37
H(14A)	450	4168	7625	47
H(14B)	679	4355	6571	47
H(15A)	-676	2219	6316	65
H(15B)	728	2332	5928	65
H(16A)	494	953	6858	65
H(16B)	314	1940	7808	65
H(17A)	2647	1975	8202	65
H(17B)	2897	2190	7159	65
H(18A)	3965	4134	8520	46
H(18B)	2506	3987	8834	46
H(19)	3145	7780	9418	33
H(20A)	763	6360	8755	39
H(20B)	1149	5410	9247	39
H(21A)	107	6589	10348	52
H(21B)	1284	7861	10420	52
H(22A)	1920	7364	11914	51
H(22B)	1839	6022	11229	51
H(23A)	4236	7359	11820	45
H(23B)	3896	8358	11372	45
H(24A)	3793	5947	10157	40
H(24B)	4930	7247	10246	40
H(26A)	4310	8211	4859	138
H(26B)	4709	7005	4452	138
H(26C)	5581	8282	4319	138
H(27A)	7997	8003	6288	132
H(27B)	7836	8160	5191	132
H(27C)	6944	6881	5311	132
H(28A)	7392	9922	6996	122
H(28B)	5947	10005	6491	122
H(28C)	7185	10119	5914	122

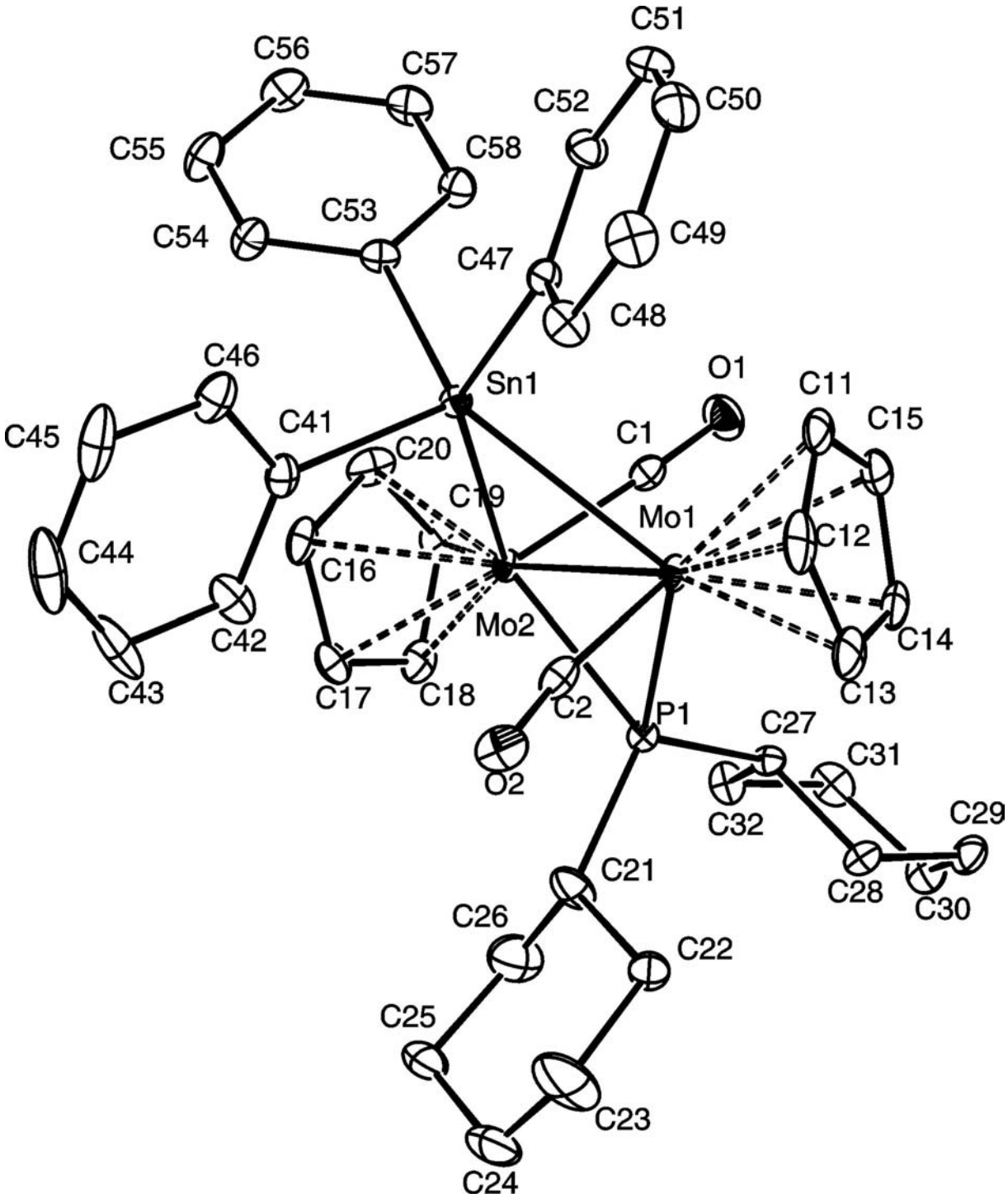

Figure S3: ORTEP view of the molecular structure of compound **4**. Ellipsoids represent 30% probability.

Table S13: Crystal data for Compound **4**.

Compound	**4**
mol formula	$C_{42}H_{47}O_2Mo_2PSn$
mol wt	925.34
cryst syst,space group	Triclinic, *P-1*
crystal color	brown
crystal shape	plate
crystal size, mm^3	$0.24 \times 0.20 \times 0.05$
radiation (λ, Å)	MoKα(λ=0.71073Å)
a, Å	8.974(2)
b, Å	12.207(3)
c, Å	17.457(4)
α, deg	94.374(4)
β, deg	97.325(4)
γ, deg	95.911(4)
V, $Å^3$	1878.9(8)
Z	2
calcd density, gcm^{-3}	1.636
μ, cm^{-1}	13.94
Diffractometer	Smart-CCD 1000 BRUKER
temperature, K	120
scan type	ω-scan
θ limits, deg	2.36-27.97
total data	23896
unique total data	8952
unique data used	6218 [$(F_O)^2>2\sigma(F_O)^2$]
R[a]	0.039
R_W[b]	0.073
GOF	1.077
Octants collected	-11,11;-16,16;0,23
Nb of variables	577
$\Delta\sigma$ (mean, max)	0.003, 0.079
$\Delta\rho$(max, min), e/$Å^3$	2.15, -1.14

[a] $R = \Sigma||F_O| - |F_C|| / \Sigma|F_O|$. [b] $R_W = [\Sigma w(|F_O|^2 - |F_C|^2)^2 / \Sigma w|F_O|^2]^{1/2}$. $w = 1/[\sigma^2(F_o^2) + (0.0245P)^2 + 4.5783P]$ where $P = (F_o^2 + 2F_c^2)/3$.

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	2082(1)	4763(1)	3287(1)	19(1)
Mo(2)	-156(1)	4430(1)	2185(1)	16(1)
Sn(1)	1918(1)	2732(1)	2273(1)	18(1)
P(1)	760(1)	6214(1)	2795(1)	17(1)
O(1)	-1525(4)	3911(3)	3666(2)	40(1)
O(2)	4390(4)	5450(3)	2185(2)	35(1)
C(1)	-883(5)	4112(4)	3142(3)	24(1)
C(2)	3460(5)	5146(4)	2549(3)	25(1)
C(11)	3135(7)	3900(5)	4358(3)	36(1)
C(12)	4270(7)	4631(5)	4136(3)	37(1)
C(13)	3841(7)	5721(6)	4248(3)	39(2)
C(14)	2452(6)	5628(5)	4539(3)	30(1)
C(15)	2033(7)	4507(5)	4611(3)	33(1)
C(16)	-953(6)	3673(4)	928(3)	28(1)
C(17)	-904(6)	4826(5)	920(3)	29(1)
C(18)	-1997(6)	5192(5)	1361(3)	29(1)
C(19)	-2714(6)	4257(5)	1641(3)	31(1)
C(20)	-2063(6)	3317(5)	1382(3)	33(1)
C(21)	1650(6)	7205(5)	2195(3)	35(1)
C(22)	3069(6)	7919(4)	2605(3)	29(1)
C(23)	3938(8)	8468(7)	2019(4)	80(3)
C(24)	3089(10)	8959(6)	1434(4)	74(3)
C(25)	1664(8)	8265(5)	1046(3)	48(2)
C(26)	688(8)	7796(6)	1671(4)	54(2)
C(27)	-316(5)	6958(4)	3464(3)	19(1)
C(28)	598(6)	7983(4)	3929(3)	25(1)
C(29)	-243(7)	8421(5)	4565(3)	31(1)
C(30)	-1789(7)	8696(5)	4233(4)	35(1)
C(31)	-2698(6)	7724(5)	3743(3)	33(1)
C(32)	-1849(6)	7250(5)	3106(3)	28(1)
C(41)	3113(5)	2768(4)	1268(3)	23(1)
C(42)	3074(6)	3626(5)	795(3)	33(1)
C(43)	3880(7)	3626(7)	162(3)	50(2)
C(44)	4700(7)	2771(8)	-7(4)	58(2)
C(45)	4735(7)	1908(7)	456(4)	48(2)
C(46)	3957(6)	1913(5)	1090(3)	32(1)
C(47)	3398(5)	1887(4)	3042(3)	22(1)
C(48)	4962(6)	2221(5)	3179(3)	29(1)
C(49)	5911(7)	1697(5)	3689(3)	36(1)
C(50)	5331(7)	843(5)	4074(3)	36(1)
C(51)	3810(7)	498(4)	3942(3)	32(1)
C(52)	2851(6)	1015(4)	3435(3)	27(1)
C(53)	82(5)	1412(4)	1931(3)	23(1)
C(54)	-171(6)	905(4)	1171(3)	27(1)
C(55)	-1411(6)	115(5)	929(3)	35(1)
C(56)	-2388(6)	-204(5)	1445(4)	36(1)
C(57)	-2149(6)	291(5)	2195(3)	33(1)
C(58)	-933(6)	1097(4)	2430(3)	27(1)

Table S15. Bond Lengths [Å] for compound **4**.

Mo(1)-C(2)	1.946(6)	C(25)-C(26)	1.588(8)
Mo(1)-C(13)	2.306(5)	C(25)-H(25A)	0.9700
Mo(1)-C(14)	2.323(5)	C(25)-H(25B)	0.9700
Mo(1)-C(12)	2.331(5)	C(26)-H(26A)	0.9700
Mo(1)-C(11)	2.357(5)	C(26)-H(26B)	0.9700
Mo(1)-C(15)	2.361(5)	C(27)-C(32)	1.526(7)
Mo(1)-P(1)	2.3854(13)	C(27)-C(28)	1.536(6)
Mo(1)-Mo(2)	2.5743(7)	C(27)-H(27)	0.83(5)
Mo(1)-Sn(1)	2.9139(7)	C(28)-C(29)	1.515(7)
Mo(2)-C(1)	1.922(5)	C(28)-H(28A)	1.01(5)
Mo(2)-C(16)	2.310(5)	C(28)-H(28B)	1.00(5)
Mo(2)-C(20)	2.314(5)	C(29)-C(30)	1.514(8)
Mo(2)-C(17)	2.327(5)	C(29)-H(29A)	0.90(5)
Mo(2)-C(19)	2.351(5)	C(29)-H(29B)	0.99(5)
Mo(2)-C(18)	2.363(5)	C(30)-C(31)	1.508(8)
Mo(2)-P(1)	2.3677(13)	C(30)-H(30A)	0.90(5)
Mo(2)-Sn(1)	2.9244(7)	C(30)-H(30B)	1.05(5)
Sn(1)-C(47)	2.162(5)	C(31)-C(32)	1.536(7)
Sn(1)-C(41)	2.170(5)	C(31)-H(31A)	1.05(5)
Sn(1)-C(53)	2.172(5)	C(31)-H(31B)	0.85(6)
P(1)-C(21)	1.844(5)	C(32)-H(32B)	0.99(5)
P(1)-C(27)	1.852(5)	C(32)-H(32A)	0.93(6)
O(1)-C(1)	1.169(6)	C(41)-C(42)	1.383(7)
O(2)-C(2)	1.161(6)	C(41)-C(46)	1.390(7)
C(11)-C(15)	1.391(8)	C(42)-C(43)	1.395(8)
C(11)-C(12)	1.397(9)	C(42)-H(42)	0.97(5)
C(11)-H(11)	0.90(5)	C(43)-C(44)	1.373(11)
C(12)-C(13)	1.428(9)	C(43)-H(43)	0.83(6)
C(12)-H(12)	0.94(5)	C(44)-C(45)	1.376(11)
C(13)-C(14)	1.402(8)	C(44)-H(44)	0.91(6)
C(13)-H(13)	0.84(6)	C(45)-C(46)	1.382(8)
C(14)-C(15)	1.401(8)	C(45)-H(45)	0.91(6)
C(14)-H(14)	0.88(5)	C(46)-H(46)	0.97(6)
C(15)-H(15)	0.93(5)	C(47)-C(52)	1.391(7)
C(16)-C(20)	1.405(8)	C(47)-C(48)	1.406(7)
C(16)-C(17)	1.405(7)	C(48)-C(49)	1.389(7)
C(16)-H(16)	0.91(5)	C(48)-H(48)	0.88(5)
C(17)-C(18)	1.408(7)	C(49)-C(50)	1.376(8)
C(17)-H(17)	0.96(5)	C(49)-H(49)	0.85(6)
C(18)-C(19)	1.405(8)	C(50)-C(51)	1.371(8)
C(18)-H(18)	0.96(6)	C(50)-H(50)	0.89(6)
C(19)-C(20)	1.410(8)	C(51)-C(52)	1.387(7)
C(19)-H(19)	0.92(5)	C(51)-H(51)	0.90(5)
C(20)-H(20)	0.93(5)	C(52)-H(52)	0.98(5)
C(21)-C(26)	1.460(8)	C(53)-C(58)	1.386(7)
C(21)-C(22)	1.529(7)	C(53)-C(54)	1.401(7)
C(21)-H(21)	0.9800	C(54)-C(55)	1.394(7)
C(22)-C(23)	1.519(8)	C(54)-H(54)	1.03(5)
C(22)-H(22A)	0.9700	C(55)-C(56)	1.385(8)
C(22)-H(22B)	0.9700	C(55)-H(55)	0.92(6)
C(23)-C(24)	1.403(10)	C(56)-C(57)	1.381(8)
C(23)-H(23A)	0.9700	C(56)-H(56)	0.98(6)
C(23)-H(23B)	0.9700	C(57)-C(58)	1.389(7)
C(24)-C(25)	1.510(9)	C(57)-H(57)	0.96(6)
C(24)-H(24A)	0.9700	C(58)-H(58)	0.82(5)
C(24)-H(24B)	0.9700		

Table S16. Bond Angles [°] for Compound **4**.

C(2)-Mo(1)-C(13)	87.9(2)	C(19)-Mo(2)-P(1)	113.72(14)
C(2)-Mo(1)-C(14)	121.0(2)	C(18)-Mo(2)-P(1)	90.34(13)
C(13)-Mo(1)-C(14)	35.3(2)	C(1)-Mo(2)-Mo(1)	71.22(15)
C(2)-Mo(1)-C(12)	85.1(2)	C(16)-Mo(2)-Mo(1)	145.01(13)
C(13)-Mo(1)-C(12)	35.9(2)	C(20)-Mo(2)-Mo(1)	153.03(14)
C(14)-Mo(1)-C(12)	58.7(2)	C(17)-Mo(2)-Mo(1)	142.41(14)
C(2)-Mo(1)-C(11)	115.2(2)	C(19)-Mo(2)-Mo(1)	155.66(15)
C(13)-Mo(1)-C(11)	58.5(2)	C(18)-Mo(2)-Mo(1)	147.87(13)
C(14)-Mo(1)-C(11)	57.97(19)	P(1)-Mo(2)-Mo(1)	57.54(3)
C(12)-Mo(1)-C(11)	34.7(2)	C(1)-Mo(2)-Sn(1)	93.42(14)
C(2)-Mo(1)-C(15)	142.0(2)	C(16)-Mo(2)-Sn(1)	85.99(13)
C(13)-Mo(1)-C(15)	58.1(2)	C(20)-Mo(2)-Sn(1)	94.48(14)
C(14)-Mo(1)-C(15)	34.80(19)	C(17)-Mo(2)-Sn(1)	112.87(13)
C(12)-Mo(1)-C(15)	57.7(2)	C(19)-Mo(2)-Sn(1)	128.77(14)
C(11)-Mo(1)-C(15)	34.29(19)	C(18)-Mo(2)-Sn(1)	144.42(13)
C(2)-Mo(1)-P(1)	84.47(14)	P(1)-Mo(2)-Sn(1)	117.42(4)
C(13)-Mo(1)-P(1)	101.65(17)	Mo(1)-Mo(2)-Sn(1)	63.627(17)
C(14)-Mo(1)-P(1)	91.98(14)	C(47)-Sn(1)-C(41)	101.03(18)
C(12)-Mo(1)-P(1)	136.52(16)	C(47)-Sn(1)-C(53)	99.57(18)
C(11)-Mo(1)-P(1)	149.26(14)	C(41)-Sn(1)-C(53)	103.55(18)
C(15)-Mo(1)-P(1)	116.44(14)	C(47)-Sn(1)-Mo(1)	96.80(12)
C(2)-Mo(1)-Mo(2)	90.50(14)	C(41)-Sn(1)-Mo(1)	118.30(13)
C(13)-Mo(1)-Mo(2)	158.51(17)	C(53)-Sn(1)-Mo(1)	130.78(13)
C(14)-Mo(1)-Mo(2)	134.70(14)	C(47)-Sn(1)-Mo(2)	144.98(12)
C(12)-Mo(1)-Mo(2)	164.97(15)	C(41)-Sn(1)-Mo(2)	108.13(13)
C(11)-Mo(1)-Mo(2)	139.78(16)	C(53)-Sn(1)-Mo(2)	92.15(12)
C(15)-Mo(1)-Mo(2)	127.41(15)	Mo(1)-Sn(1)-Mo(2)	52.327(16)
P(1)-Mo(1)-Mo(2)	56.88(3)	C(21)-P(1)-C(27)	109.4(3)
C(2)-Mo(1)-Sn(1)	76.35(14)	C(21)-P(1)-Mo(2)	116.86(19)
C(13)-Mo(1)-Sn(1)	135.81(17)	C(27)-P(1)-Mo(2)	121.75(16)
C(14)-Mo(1)-Sn(1)	148.44(14)	C(21)-P(1)-Mo(1)	120.73(19)
C(12)-Mo(1)-Sn(1)	100.93(15)	C(27)-P(1)-Mo(1)	117.03(17)
C(11)-Mo(1)-Sn(1)	91.29(13)	Mo(2)-P(1)-Mo(1)	65.59(4)
C(15)-Mo(1)-Sn(1)	114.94(14)	O(1)-C(1)-Mo(2)	170.5(4)
P(1)-Mo(1)-Sn(1)	117.20(4)	O(2)-C(2)-Mo(1)	171.6(4)
Mo(2)-Mo(1)-Sn(1)	64.045(16)	C(15)-C(11)-C(12)	108.5(5)
C(1)-Mo(2)-C(16)	131.0(2)	C(15)-C(11)-Mo(1)	73.0(3)
C(1)-Mo(2)-C(20)	96.2(2)	C(12)-C(11)-Mo(1)	71.7(3)
C(16)-Mo(2)-C(20)	35.4(2)	C(15)-C(11)-H(11)	127(4)
C(1)-Mo(2)-C(17)	143.6(2)	C(12)-C(11)-H(11)	124(4)
C(16)-Mo(2)-C(17)	35.29(18)	Mo(1)-C(11)-H(11)	121(3)
C(20)-Mo(2)-C(17)	58.7(2)	C(11)-C(12)-C(13)	107.4(5)
C(1)-Mo(2)-C(19)	86.2(2)	C(11)-C(12)-Mo(1)	73.7(3)
C(16)-Mo(2)-C(19)	58.30(19)	C(13)-C(12)-Mo(1)	71.1(3)
C(20)-Mo(2)-C(19)	35.16(19)	C(11)-C(12)-H(12)	131(3)
C(17)-Mo(2)-C(19)	57.9(2)	C(13)-C(12)-H(12)	122(3)
C(1)-Mo(2)-C(18)	110.9(2)	Mo(1)-C(12)-H(12)	121(3)
C(16)-Mo(2)-C(18)	58.51(18)	C(14)-C(13)-C(12)	107.5(6)
C(20)-Mo(2)-C(18)	58.54(19)	C(14)-C(13)-Mo(1)	73.0(3)
C(17)-Mo(2)-C(18)	34.94(18)	C(12)-C(13)-Mo(1)	73.0(3)
C(19)-Mo(2)-C(18)	34.67(19)	C(14)-C(13)-H(13)	120(4)
C(1)-Mo(2)-P(1)	86.93(14)	C(12)-C(13)-H(13)	132(4)
C(16)-Mo(2)-P(1)	135.96(14)	Mo(1)-C(13)-H(13)	117(4)
C(20)-Mo(2)-P(1)	147.77(14)	C(15)-C(14)-C(13)	107.9(5)
C(17)-Mo(2)-P(1)	101.40(14)	C(15)-C(14)-Mo(1)	74.1(3)

C(13)-C(14)-Mo(1)	71.7(3)
C(15)-C(14)-H(14)	125(3)
C(13)-C(14)-H(14)	127(3)
Mo(1)-C(14)-H(14)	122(3)
C(11)-C(15)-C(14)	108.6(6)
C(11)-C(15)-Mo(1)	72.7(3)
C(14)-C(15)-Mo(1)	71.1(3)
C(11)-C(15)-H(15)	129(3)
C(14)-C(15)-H(15)	122(3)
Mo(1)-C(15)-H(15)	118(3)
C(20)-C(16)-C(17)	108.0(5)
C(20)-C(16)-Mo(2)	72.5(3)
C(17)-C(16)-Mo(2)	73.0(3)
C(20)-C(16)-H(16)	124(3)
C(17)-C(16)-H(16)	128(3)
Mo(2)-C(16)-H(16)	121(3)
C(16)-C(17)-C(18)	108.5(5)
C(16)-C(17)-Mo(2)	71.7(3)
C(18)-C(17)-Mo(2)	73.9(3)
C(16)-C(17)-H(17)	126(3)
C(18)-C(17)-H(17)	126(3)
Mo(2)-C(17)-H(17)	121(3)
C(19)-C(18)-C(17)	107.2(5)
C(19)-C(18)-Mo(2)	72.2(3)
C(17)-C(18)-Mo(2)	71.1(3)
C(19)-C(18)-H(18)	124(4)
C(17)-C(18)-H(18)	129(4)
Mo(2)-C(18)-H(18)	122(4)
C(18)-C(19)-C(20)	108.7(5)
C(18)-C(19)-Mo(2)	73.1(3)
C(20)-C(19)-Mo(2)	71.0(3)
C(18)-C(19)-H(19)	127(3)
C(20)-C(19)-H(19)	123(3)
Mo(2)-C(19)-H(19)	115(3)
C(16)-C(20)-C(19)	107.5(5)
C(16)-C(20)-Mo(2)	72.1(3)
C(19)-C(20)-Mo(2)	73.9(3)
C(16)-C(20)-H(20)	126(3)
C(19)-C(20)-H(20)	127(3)
Mo(2)-C(20)-H(20)	122(3)
C(26)-C(21)-C(22)	113.6(5)
C(26)-C(21)-P(1)	119.1(4)
C(22)-C(21)-P(1)	115.0(4)
C(26)-C(21)-H(21)	101.8
C(22)-C(21)-H(21)	101.8
P(1)-C(21)-H(21)	101.8
C(23)-C(22)-C(21)	110.5(5)
C(23)-C(22)-H(22A)	109.6
C(21)-C(22)-H(22A)	109.6
C(23)-C(22)-H(22B)	109.6
C(21)-C(22)-H(22B)	109.6
H(22A)-C(22)-H(22B)	108.1
C(24)-C(23)-C(22)	116.7(6)
C(24)-C(23)-H(23A)	108.1
C(22)-C(23)-H(23A)	108.1
C(24)-C(23)-H(23B)	108.1
C(22)-C(23)-H(23B)	108.1
H(23A)-C(23)-H(23B)	107.3
C(23)-C(24)-C(25)	115.3(6)
C(23)-C(24)-H(24A)	108.5
C(25)-C(24)-H(24A)	108.5
C(23)-C(24)-H(24B)	108.5
C(25)-C(24)-H(24B)	108.5
H(24A)-C(24)-H(24B)	107.5
C(24)-C(25)-C(26)	110.9(5)
C(24)-C(25)-H(25A)	109.5
C(26)-C(25)-H(25A)	109.5
C(24)-C(25)-H(25B)	109.5
C(26)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	108.0
C(21)-C(26)-C(25)	108.2(5)
C(21)-C(26)-H(26A)	110.1
C(25)-C(26)-H(26A)	110.1
C(21)-C(26)-H(26B)	110.1
C(25)-C(26)-H(26B)	110.1
H(26A)-C(26)-H(26B)	108.4
C(32)-C(27)-C(28)	109.8(4)
C(32)-C(27)-P(1)	115.7(3)
C(28)-C(27)-P(1)	113.9(3)
C(32)-C(27)-H(27)	110(4)
C(28)-C(27)-H(27)	104(3)
P(1)-C(27)-H(27)	103(3)
C(29)-C(28)-C(27)	110.8(4)
C(29)-C(28)-H(28A)	109(3)
C(27)-C(28)-H(28A)	105(3)
C(29)-C(28)-H(28B)	111(3)
C(27)-C(28)-H(28B)	113(3)
H(28A)-C(28)-H(28B)	108(4)
C(30)-C(29)-C(28)	111.0(5)
C(30)-C(29)-H(29A)	110(3)
C(28)-C(29)-H(29A)	110(3)
C(30)-C(29)-H(29B)	110(3)
C(28)-C(29)-H(29B)	110(3)
H(29A)-C(29)-H(29B)	106(4)
C(31)-C(30)-C(29)	111.7(5)
C(31)-C(30)-H(30A)	114(3)
C(29)-C(30)-H(30A)	111(3)
C(31)-C(30)-H(30B)	111(3)
C(29)-C(30)-H(30B)	106(3)
H(30A)-C(30)-H(30B)	102(4)
C(30)-C(31)-C(32)	112.6(5)
C(30)-C(31)-H(31A)	110(2)
C(32)-C(31)-H(31A)	108(2)
C(30)-C(31)-H(31B)	111(4)
C(32)-C(31)-H(31B)	111(4)
H(31A)-C(31)-H(31B)	104(5)
C(27)-C(32)-C(31)	110.0(4)
C(27)-C(32)-H(32B)	112(3)
C(31)-C(32)-H(32B)	111(3)
C(27)-C(32)-H(32A)	112(4)
C(31)-C(32)-H(32A)	114(4)
H(32B)-C(32)-H(32A)	97(4)
C(42)-C(41)-C(46)	118.3(5)
C(42)-C(41)-Sn(1)	122.0(4)
C(46)-C(41)-Sn(1)	119.7(4)
C(41)-C(42)-C(43)	120.1(6)
C(41)-C(42)-H(42)	118(3)
C(43)-C(42)-H(42)	121(3)

C(44)-C(43)-C(42)	120.7(7)	C(50)-C(51)-C(52)	120.5(5)
C(44)-C(43)-H(43)	120(4)	C(50)-C(51)-H(51)	124(4)
C(42)-C(43)-H(43)	119(4)	C(52)-C(51)-H(51)	116(4)
C(43)-C(44)-C(45)	119.7(6)	C(51)-C(52)-C(47)	121.4(5)
C(43)-C(44)-H(44)	122(4)	C(51)-C(52)-H(52)	121(3)
C(45)-C(44)-H(44)	118(4)	C(47)-C(52)-H(52)	118(3)
C(44)-C(45)-C(46)	119.8(7)	C(58)-C(53)-C(54)	117.8(5)
C(44)-C(45)-H(45)	115(4)	C(58)-C(53)-Sn(1)	121.8(4)
C(46)-C(45)-H(45)	126(4)	C(54)-C(53)-Sn(1)	120.3(4)
C(45)-C(46)-C(41)	121.4(6)	C(55)-C(54)-C(53)	120.8(5)
C(45)-C(46)-H(46)	119(4)	C(55)-C(54)-H(54)	115(3)
C(41)-C(46)-H(46)	119(4)	C(53)-C(54)-H(54)	124(3)
C(52)-C(47)-C(48)	117.2(5)	C(56)-C(55)-C(54)	120.2(5)
C(52)-C(47)-Sn(1)	122.0(4)	C(56)-C(55)-H(55)	117(4)
C(48)-C(47)-Sn(1)	120.8(4)	C(54)-C(55)-H(55)	123(4)
C(49)-C(48)-C(47)	120.9(5)	C(57)-C(56)-C(55)	119.4(5)
C(49)-C(48)-H(48)	118(4)	C(57)-C(56)-H(56)	121(3)
C(47)-C(48)-H(48)	122(3)	C(55)-C(56)-H(56)	119(3)
C(50)-C(49)-C(48)	120.4(6)	C(56)-C(57)-C(58)	120.2(5)
C(50)-C(49)-H(49)	121(4)	C(56)-C(57)-H(57)	120(3)
C(48)-C(49)-H(49)	119(4)	C(58)-C(57)-H(57)	119(3)
C(51)-C(50)-C(49)	119.6(5)	C(53)-C(58)-C(57)	121.5(5)
C(51)-C(50)-H(50)	120(4)	C(53)-C(58)-H(58)	118(4)
C(49)-C(50)-H(50)	120(4)	C(57)-C(58)-H(58)	120(4)

Table S17. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for compound **4**. 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)	17(1)	22(1)	15(1)	-2(1)	-4(1)	5(1)
Mo(2)	13(1)	19(1)	16(1)	-1(1)	-2(1)	3(1)
Sn(1)	17(1)	18(1)	19(1)	1(1)	3(1)	3(1)
P(1)	14(1)	19(1)	20(1)	1(1)	2(1)	2(1)
O(1)	39(2)	49(2)	31(2)	7(2)	12(2)	-4(2)
O(2)	22(2)	34(2)	52(3)	0(2)	14(2)	4(2)
C(1)	22(3)	21(2)	28(3)	-2(2)	4(2)	3(2)
C(2)	17(2)	24(3)	31(3)	-7(2)	-5(2)	5(2)
C(11)	59(4)	31(3)	16(3)	-1(2)	-13(3)	18(3)
C(12)	29(3)	62(4)	18(3)	-6(3)	-14(2)	19(3)
C(13)	39(3)	49(4)	20(3)	-5(3)	-13(2)	-5(3)
C(14)	39(3)	34(3)	16(2)	-7(2)	-5(2)	12(3)
C(15)	43(3)	38(3)	17(3)	1(2)	-4(2)	5(3)
C(16)	25(3)	37(3)	20(3)	-8(2)	-9(2)	12(2)
C(17)	26(3)	41(3)	19(3)	9(2)	-4(2)	6(2)
C(18)	25(3)	34(3)	25(3)	-3(2)	-11(2)	7(2)
C(19)	14(2)	46(3)	33(3)	8(3)	-2(2)	6(2)
C(20)	18(3)	28(3)	46(3)	2(3)	-17(2)	-3(2)
C(21)	23(3)	50(4)	31(3)	15(3)	2(2)	-10(2)
C(22)	24(3)	32(3)	31(3)	2(2)	7(2)	-6(2)
C(23)	54(5)	112(7)	62(5)	36(5)	-2(4)	-48(5)
C(24)	106(7)	61(5)	46(4)	21(4)	8(4)	-40(5)
C(25)	69(5)	40(3)	31(3)	16(3)	0(3)	-10(3)
C(26)	57(4)	48(4)	58(4)	14(3)	5(4)	5(3)
C(27)	18(2)	16(2)	25(3)	2(2)	7(2)	5(2)
C(28)	24(3)	20(2)	30(3)	-2(2)	3(2)	0(2)
C(29)	39(3)	23(3)	30(3)	-5(2)	4(3)	8(2)
C(30)	38(3)	35(3)	37(3)	-2(3)	13(3)	19(3)
C(31)	22(3)	44(3)	39(3)	9(3)	9(3)	14(3)
C(32)	20(3)	39(3)	26(3)	3(2)	4(2)	9(2)
C(41)	17(2)	31(3)	20(2)	-4(2)	0(2)	-2(2)
C(42)	20(3)	51(4)	27(3)	13(3)	-1(2)	-1(2)
C(43)	27(3)	96(6)	23(3)	27(4)	-2(3)	-13(4)
C(44)	21(3)	127(7)	22(3)	-12(4)	4(3)	-7(4)
C(45)	22(3)	81(5)	35(4)	-30(4)	5(3)	1(3)
C(46)	22(3)	35(3)	37(3)	-11(3)	5(2)	-2(2)
C(47)	27(3)	20(2)	20(2)	1(2)	6(2)	5(2)
C(48)	21(3)	36(3)	30(3)	7(2)	3(2)	6(2)
C(49)	22(3)	48(4)	40(3)	5(3)	3(3)	12(3)
C(50)	42(4)	39(3)	31(3)	8(3)	2(3)	21(3)
C(51)	43(3)	23(3)	32(3)	10(2)	3(3)	6(2)
C(52)	28(3)	27(3)	26(3)	6(2)	-1(2)	4(2)
C(53)	21(2)	21(2)	28(3)	5(2)	3(2)	3(2)
C(54)	20(3)	29(3)	30(3)	-5(2)	7(2)	1(2)
C(55)	28(3)	36(3)	38(3)	-14(3)	3(3)	-3(2)
C(56)	24(3)	33(3)	48(4)	-2(3)	3(3)	-8(2)
C(57)	23(3)	36(3)	41(3)	9(3)	13(2)	-3(2)
C(58)	24(3)	30(3)	27(3)	1(2)	6(2)	2(2)

Table S18. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for Compound **4**.

	x	y	z	U(eq)
H(21)	2073	6713	1831	42
H(22A)	2783	8481	2964	35
H(22B)	3710	7463	2900	35
H(23A)	4694	9032	2298	95
H(23B)	4471	7917	1772	95
H(24A)	3725	9135	1041	89
H(24B)	2815	9650	1657	89
H(25A)	1929	7654	721	57
H(25B)	1069	8711	716	57
H(26A)	320	8399	1960	65
H(26B)	-176	7300	1416	65
H(32B)	-1750(50)	7770(40)	2710(30)	22(13)
H(17)	-250(60)	5290(40)	660(30)	27(14)
H(32A)	-2400(70)	6670(50)	2790(30)	44(17)
H(28A)	690(60)	8560(40)	3540(30)	30(14)
H(29A)	-340(50)	7910(40)	4910(30)	20(13)
H(54)	530(60)	1070(40)	760(30)	40(16)
H(52)	1760(60)	770(40)	3340(30)	29(14)
H(42)	2570(50)	4260(40)	950(30)	19(13)
H(31A)	-2970(50)	7090(40)	4090(30)	18(12)
H(29B)	360(60)	9090(40)	4860(30)	36(15)
H(27)	-440(60)	6510(40)	3790(30)	22(14)
H(48)	5380(60)	2750(40)	2940(30)	29(15)
H(15)	1120(60)	4260(40)	4770(30)	32(16)
H(30A)	-2270(60)	8980(40)	4610(30)	26(14)
H(11)	3140(60)	3160(40)	4340(30)	31(15)
H(14)	1940(50)	6170(40)	4680(30)	19(13)
H(28B)	1640(60)	7850(40)	4150(30)	30(14)
H(51)	3370(60)	-70(50)	4160(30)	38(16)
H(19)	-3400(60)	4240(40)	1990(30)	34(16)
H(58)	-790(60)	1390(40)	2880(30)	24(15)
H(20)	-2350(60)	2580(40)	1470(30)	29(14)
H(16)	-400(60)	3210(40)	690(30)	30(15)
H(57)	-2770(60)	40(40)	2570(30)	40(16)
H(12)	5180(60)	4500(40)	3950(30)	35(16)
H(49)	6840(70)	1940(50)	3780(40)	51(19)
H(18)	-2240(70)	5940(50)	1470(30)	49(18)
H(30B)	-1600(60)	9370(40)	3900(30)	30(14)
H(46)	3970(70)	1290(50)	1400(40)	52(19)
H(50)	5930(70)	560(50)	4440(40)	51(19)
H(56)	-3210(60)	-800(50)	1280(30)	44(17)
H(43)	3890(60)	4160(50)	-100(30)	35(17)
H(45)	5310(70)	1380(50)	310(30)	49(19)
H(55)	-1550(60)	-290(50)	450(30)	41(17)
H(31B)	-3560(70)	7890(50)	3550(40)	51(19)
H(13)	4240(70)	6340(50)	4150(30)	43(19)
H(44)	5150(70)	2720(50)	-440(40)	60(20)

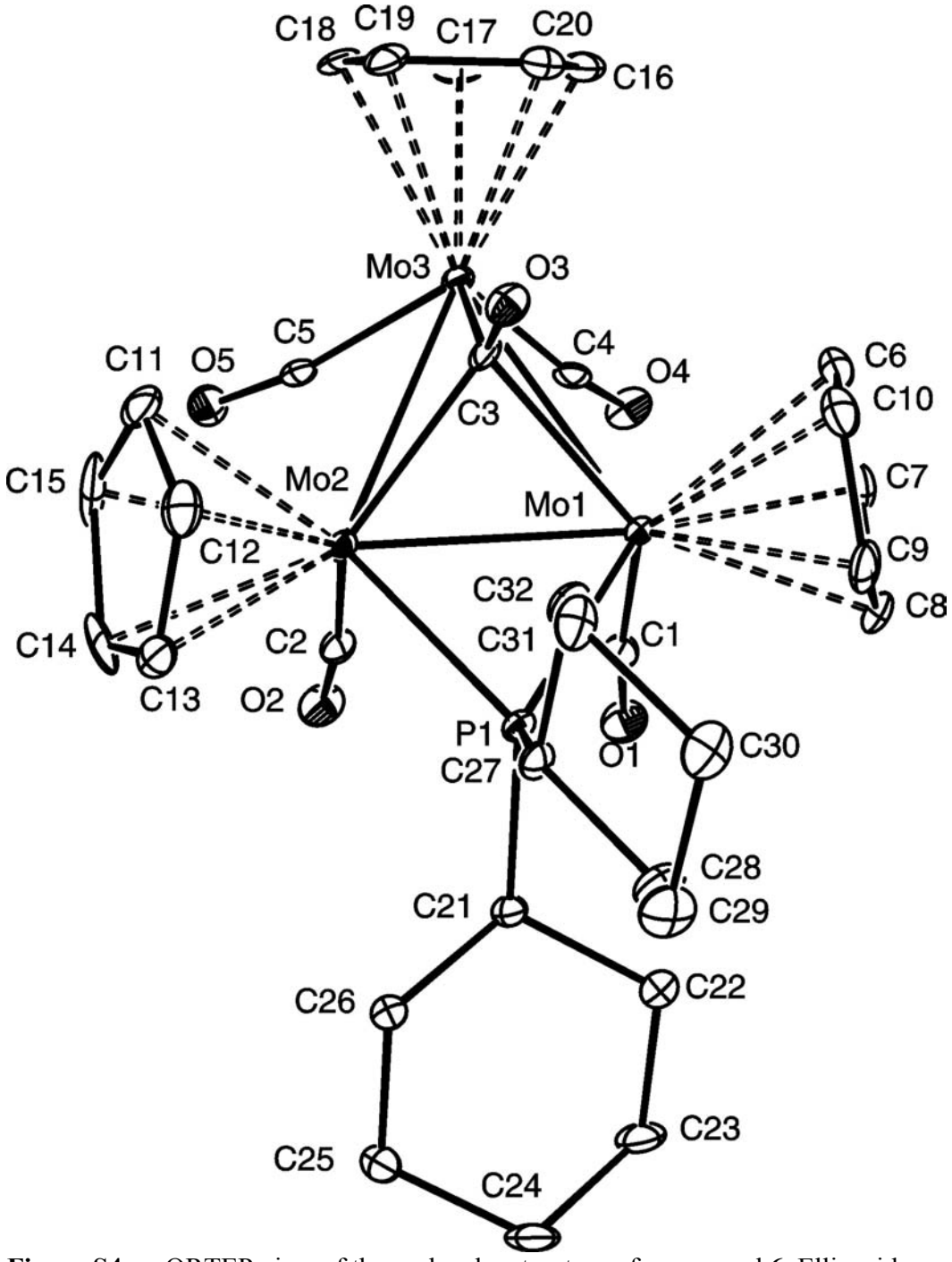

Figure S4: ORTEP view of the molecular structure of compound **6**. Ellipsoids represent 30% probability.

Table 19. Crystal data and structure refinement for compound **6**.

Empirical formula	$C_{32}H_{37}Mo_3O_5P$	
Formula weight	820.41	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 9.704(3) Å	α = 90°.
	b = 22.494(6) Å	β = 109.17(3)°.
	c = 14.465(4) Å	γ = 90°.
Volume	2982.4(15) Å^3	
Z	4	
Density (calculated)	1.827 Mg/m^3	
Absorption coefficient	1.336 mm^{-1}	
F(000)	1640	
Crystal size	0.22 x 0.18 x 0.18 mm^3	
θ range for data collection	1.74 to 28.26°.	
Index ranges	-12<=h<=12, 0<=k<=29, 0<=l<=18	
Reflections collected	7141	
Independent reflections	7141 [R(int) = 0.0000]	
Completeness to θ = 28.26°	96.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7949 and 0.7575	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7141 / 0 / 370	
Goodness-of-fit on F^2	1.120	
Final R indices [I>2σ(I)] [a]	R_1 = 0.0514, wR_2 = 0.1096	
R indices (all data) [a]	R_1 = 0.0818, wR_2 = 0.1214	
Largest diff. peak and hole	1.090 and -1.750 e.Å^{-3}	

[a] $R = \Sigma||F_O| - |F_C|| / \Sigma|F_O|$. $R_W = [\Sigma w(|F_O|^2 - |F_C|^2)^2 / \Sigma w|F_O|^2]^{1/2}$. $w = 1/[\sigma^2(F_o^2) + (0.0375P)^2 + 20.4280P]$ where $P = (F_o^2 + 2F_c^2)/3$.

Table 20. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **6**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	2203(1)	6386(1)	1392(1)	14(1)
Mo(2)	5041(1)	6065(1)	2350(1)	14(1)
Mo(3)	4405(1)	6651(1)	318(1)	14(1)
P(1)	3041(2)	5883(1)	2938(1)	14(1)
O(1)	2451(5)	7578(2)	2528(4)	29(1)
O(2)	5571(5)	7310(2)	3342(3)	28(1)
O(3)	3440(5)	5370(2)	541(3)	22(1)
O(4)	2836(5)	7844(2)	455(3)	26(1)
O(5)	7130(5)	7270(2)	1770(3)	25(1)
C(1)	2452(7)	7136(3)	2128(4)	21(1)
C(2)	5292(6)	6863(3)	2936(5)	21(1)
C(3)	3780(6)	5881(3)	812(4)	17(1)
C(4)	3341(7)	7374(3)	479(4)	19(1)
C(5)	6092(6)	7011(3)	1316(4)	17(1)
C(6)	434(7)	6479(3)	-168(5)	25(1)
C(7)	139(7)	6912(3)	429(5)	26(1)
C(8)	-210(7)	6610(3)	1195(5)	28(2)
C(9)	-127(7)	5992(3)	1032(5)	30(2)
C(10)	257(7)	5915(3)	187(5)	27(1)
C(11)	6936(8)	5504(4)	2119(5)	36(2)
C(12)	6244(7)	5143(3)	2630(5)	29(2)
C(13)	6445(7)	5401(3)	3546(5)	27(2)
C(14)	7262(7)	5917(3)	3621(5)	34(2)
C(15)	7563(7)	5975(4)	2721(7)	43(2)
C(16)	3393(8)	6711(3)	-1390(5)	27(2)
C(17)	4763(8)	6995(3)	-1098(5)	28(2)
C(18)	5850(7)	6561(3)	-700(5)	27(2)
C(19)	5146(7)	6013(3)	-725(5)	26(1)
C(20)	3611(7)	6115(3)	-1158(5)	24(1)
C(21)	3053(6)	6283(3)	4062(4)	17(1)
C(22)	1525(7)	6435(3)	4106(5)	23(1)
C(23)	1618(8)	6737(3)	5066(5)	30(2)
C(24)	2492(8)	6360(3)	5944(5)	31(2)
C(25)	4043(7)	6276(3)	5935(5)	24(1)
C(26)	4021(7)	5962(3)	4992(4)	21(1)
C(27)	2594(6)	5087(3)	3117(4)	17(1)
C(28)	1308(7)	4986(3)	3494(5)	26(1)
C(29)	1059(8)	4317(3)	3623(5)	30(2)
C(30)	793(7)	3979(3)	2672(5)	27(2)
C(31)	2085(7)	4068(3)	2310(5)	23(1)
C(32)	2351(7)	4727(3)	2177(5)	21(1)

Table 21. Bond Lengths [Å] for Compound **6**.

Mo(1)-C(1)	1.967(7)	C(13)-C(14)	1.390(10)
Mo(1)-C(3)	2.275(6)	C(13)-H(13)	0.9300
Mo(1)-C(8)	2.319(6)	C(14)-C(15)	1.430(11)
Mo(1)-C(9)	2.323(6)	C(14)-H(14)	0.9300
Mo(1)-C(7)	2.349(6)	C(15)-H(15)	0.9300
Mo(1)-C(6)	2.352(6)	C(16)-C(20)	1.383(9)
Mo(1)-C(10)	2.359(6)	C(16)-C(17)	1.409(10)
Mo(1)-P(1)	2.3989(17)	C(16)-H(16)	0.9300
Mo(1)-Mo(2)	2.7428(12)	C(17)-C(18)	1.414(10)
Mo(1)-Mo(3)	3.0846(11)	C(17)-H(17)	0.9300
Mo(2)-C(2)	1.965(7)	C(18)-C(19)	1.403(10)
Mo(2)-C(3)	2.197(6)	C(18)-H(18)	0.9300
Mo(2)-C(15)	2.335(6)	C(19)-C(20)	1.432(9)
Mo(2)-C(11)	2.343(7)	C(19)-H(19)	0.9300
Mo(2)-C(12)	2.349(6)	C(20)-H(20)	0.9300
Mo(2)-C(14)	2.353(6)	C(21)-C(26)	1.544(8)
Mo(2)-C(13)	2.353(6)	C(21)-C(22)	1.544(8)
Mo(2)-P(1)	2.3975(16)	C(21)-H(21)	0.9800
Mo(2)-Mo(3)	3.0935(10)	C(22)-C(23)	1.520(9)
Mo(3)-C(5)	1.966(6)	C(22)-H(22A)	0.9700
Mo(3)-C(4)	1.981(6)	C(22)-H(22B)	0.9700
Mo(3)-C(3)	2.042(6)	C(23)-C(24)	1.532(9)
Mo(3)-C(17)	2.320(6)	C(23)-H(23A)	0.9700
Mo(3)-C(16)	2.344(6)	C(23)-H(23B)	0.9700
Mo(3)-C(20)	2.350(6)	C(24)-C(25)	1.521(9)
Mo(3)-C(18)	2.352(6)	C(24)-H(24A)	0.9700
Mo(3)-C(19)	2.359(6)	C(24)-H(24B)	0.9700
P(1)-C(21)	1.855(6)	C(25)-C(26)	1.530(8)
P(1)-C(27)	1.880(6)	C(25)-H(25A)	0.9700
O(1)-C(1)	1.151(8)	C(25)-H(25B)	0.9700
O(2)-C(2)	1.153(7)	C(26)-H(26A)	0.9700
O(3)-C(3)	1.223(7)	C(26)-H(26B)	0.9700
O(4)-C(4)	1.160(7)	C(27)-C(32)	1.533(8)
O(5)-C(5)	1.163(7)	C(27)-C(28)	1.533(8)
C(6)-C(7)	1.391(9)	C(27)-H(27)	0.9800
C(6)-C(10)	1.400(9)	C(28)-C(29)	1.547(9)
C(6)-H(6)	0.9300	C(28)-H(28A)	0.9700
C(7)-C(8)	1.432(9)	C(28)-H(28B)	0.9700
C(7)-H(7)	0.9300	C(29)-C(30)	1.517(9)
C(8)-C(9)	1.418(10)	C(29)-H(29A)	0.9700
C(8)-H(8)	0.9300	C(29)-H(29B)	0.9700
C(9)-C(10)	1.401(10)	C(30)-C(31)	1.522(9)
C(9)-H(9)	0.9300	C(30)-H(30A)	0.9700
C(10)-H(10)	0.9300	C(30)-H(30B)	0.9700
C(11)-C(15)	1.381(12)	C(31)-C(32)	1.527(8)
C(11)-C(12)	1.408(10)	C(31)-H(31A)	0.9700
C(11)-H(11)	0.9300	C(31)-H(31B)	0.9700
C(12)-C(13)	1.400(10)	C(32)-H(32A)	0.9700
C(12)-H(12)	0.9300	C(32)-H(32B)	0.9700

Table 22. Bond Angles [°] for Compound **6**.

C(1)-Mo(1)-C(3)	130.5(2)	C(2)-Mo(2)-C(12)	138.4(3)
C(1)-Mo(1)-C(8)	79.6(3)	C(3)-Mo(2)-C(12)	95.0(2)
C(3)-Mo(1)-C(8)	146.9(2)	C(15)-Mo(2)-C(12)	57.3(3)
C(1)-Mo(1)-C(9)	112.7(3)	C(11)-Mo(2)-C(12)	34.9(2)
C(3)-Mo(1)-C(9)	116.7(2)	C(2)-Mo(2)-C(14)	80.8(3)
C(8)-Mo(1)-C(9)	35.6(3)	C(3)-Mo(2)-C(14)	145.8(2)
C(1)-Mo(1)-C(7)	79.6(2)	C(15)-Mo(2)-C(14)	35.5(3)
C(3)-Mo(1)-C(7)	125.4(2)	C(11)-Mo(2)-C(14)	58.3(3)
C(8)-Mo(1)-C(7)	35.7(2)	C(12)-Mo(2)-C(14)	57.6(2)
C(9)-Mo(1)-C(7)	58.8(2)	C(2)-Mo(2)-C(13)	107.6(3)
C(1)-Mo(1)-C(6)	111.4(2)	C(3)-Mo(2)-C(13)	128.3(2)
C(3)-Mo(1)-C(6)	93.4(2)	C(15)-Mo(2)-C(13)	57.7(2)
C(8)-Mo(1)-C(6)	58.3(2)	C(11)-Mo(2)-C(13)	58.0(2)
C(9)-Mo(1)-C(6)	58.0(2)	C(12)-Mo(2)-C(13)	34.6(2)
C(7)-Mo(1)-C(6)	34.4(2)	C(14)-Mo(2)-C(13)	34.4(2)
C(1)-Mo(1)-C(10)	135.4(2)	C(2)-Mo(2)-P(1)	90.16(17)
C(3)-Mo(1)-C(10)	88.6(2)	C(3)-Mo(2)-P(1)	94.60(16)
C(8)-Mo(1)-C(10)	58.4(2)	C(15)-Mo(2)-P(1)	144.4(2)
C(9)-Mo(1)-C(10)	34.8(2)	C(11)-Mo(2)-P(1)	136.3(2)
C(7)-Mo(1)-C(10)	57.9(2)	C(12)-Mo(2)-P(1)	101.66(18)
C(6)-Mo(1)-C(10)	34.6(2)	C(14)-Mo(2)-P(1)	109.8(2)
C(1)-Mo(1)-P(1)	87.45(17)	C(13)-Mo(2)-P(1)	88.35(17)
C(3)-Mo(1)-P(1)	92.56(15)	C(2)-Mo(2)-Mo(1)	86.52(18)
C(8)-Mo(1)-P(1)	103.65(18)	C(3)-Mo(2)-Mo(1)	53.48(14)
C(9)-Mo(1)-P(1)	92.02(18)	C(15)-Mo(2)-Mo(1)	160.33(18)
C(7)-Mo(1)-P(1)	138.79(17)	C(11)-Mo(2)-Mo(1)	140.8(2)
C(6)-Mo(1)-P(1)	148.60(17)	C(12)-Mo(2)-Mo(1)	132.77(17)
C(10)-Mo(1)-P(1)	114.91(17)	C(14)-Mo(2)-Mo(1)	160.5(2)
C(1)-Mo(1)-Mo(2)	91.57(18)	C(13)-Mo(2)-Mo(1)	141.43(17)
C(3)-Mo(1)-Mo(2)	50.90(15)	P(1)-Mo(2)-Mo(1)	55.14(4)
C(8)-Mo(1)-Mo(2)	157.65(17)	C(2)-Mo(2)-Mo(3)	88.79(18)
C(9)-Mo(1)-Mo(2)	138.99(17)	C(3)-Mo(2)-Mo(3)	41.20(16)
C(7)-Mo(1)-Mo(2)	162.09(16)	C(15)-Mo(2)-Mo(3)	97.05(19)
C(6)-Mo(1)-Mo(2)	143.46(17)	C(11)-Mo(2)-Mo(3)	90.89(17)
C(10)-Mo(1)-Mo(2)	133.06(17)	C(12)-Mo(2)-Mo(3)	118.24(18)
P(1)-Mo(1)-Mo(2)	55.10(4)	C(14)-Mo(2)-Mo(3)	130.5(2)
C(1)-Mo(1)-Mo(3)	97.17(18)	C(13)-Mo(2)-Mo(3)	148.90(16)
C(3)-Mo(1)-Mo(3)	41.44(15)	P(1)-Mo(2)-Mo(3)	118.56(5)
C(8)-Mo(1)-Mo(3)	137.28(18)	Mo(1)-Mo(2)-Mo(3)	63.48(3)
C(9)-Mo(1)-Mo(3)	138.20(18)	C(5)-Mo(3)-C(4)	85.2(2)
C(7)-Mo(1)-Mo(3)	101.60(17)	C(5)-Mo(3)-C(3)	111.3(2)
C(6)-Mo(1)-Mo(3)	84.71(17)	C(4)-Mo(3)-C(3)	115.5(2)
C(10)-Mo(1)-Mo(3)	103.51(18)	C(5)-Mo(3)-C(17)	100.4(2)
P(1)-Mo(1)-Mo(3)	118.84(5)	C(4)-Mo(3)-C(17)	93.7(2)
Mo(2)-Mo(1)-Mo(3)	63.81(3)	C(3)-Mo(3)-C(17)	137.8(2)
C(2)-Mo(2)-C(3)	123.9(2)	C(5)-Mo(3)-C(16)	135.2(2)
C(2)-Mo(2)-C(15)	90.4(3)	C(4)-Mo(3)-C(16)	91.3(2)
C(3)-Mo(2)-C(15)	114.2(3)	C(3)-Mo(3)-C(16)	110.4(2)
C(2)-Mo(2)-C(11)	124.2(3)	C(17)-Mo(3)-C(16)	35.2(2)
C(3)-Mo(2)-C(11)	87.5(2)	C(5)-Mo(3)-C(20)	145.4(2)
C(15)-Mo(2)-C(11)	34.3(3)	C(4)-Mo(3)-C(20)	120.0(2)

C(3)-Mo(3)-C(20)	80.5(2)	C(6)-C(7)-Mo(1)	72.9(4)
C(17)-Mo(3)-C(20)	57.9(2)	C(8)-C(7)-Mo(1)	71.0(3)
C(16)-Mo(3)-C(20)	34.3(2)	C(6)-C(7)-H(7)	126.3
C(5)-Mo(3)-C(18)	88.3(2)	C(8)-C(7)-H(7)	126.3
C(4)-Mo(3)-C(18)	125.8(2)	Mo(1)-C(7)-H(7)	121.5
C(3)-Mo(3)-C(18)	116.9(2)	C(9)-C(8)-C(7)	107.2(6)
C(17)-Mo(3)-C(18)	35.2(2)	C(9)-C(8)-Mo(1)	72.4(4)
C(16)-Mo(3)-C(18)	58.3(2)	C(7)-C(8)-Mo(1)	73.3(3)
C(20)-Mo(3)-C(18)	58.2(2)	C(9)-C(8)-H(8)	126.4
C(5)-Mo(3)-C(19)	111.4(2)	C(7)-C(8)-H(8)	126.4
C(4)-Mo(3)-C(19)	148.7(2)	Mo(1)-C(8)-H(8)	119.8
C(3)-Mo(3)-C(19)	84.0(2)	C(10)-C(9)-C(8)	108.1(6)
C(17)-Mo(3)-C(19)	58.2(2)	C(10)-C(9)-Mo(1)	74.0(4)
C(16)-Mo(3)-C(19)	58.1(2)	C(8)-C(9)-Mo(1)	72.1(4)
C(20)-Mo(3)-C(19)	35.4(2)	C(10)-C(9)-H(9)	125.9
C(18)-Mo(3)-C(19)	34.7(2)	C(8)-C(9)-H(9)	125.9
C(5)-Mo(3)-Mo(1)	104.91(16)	Mo(1)-C(9)-H(9)	119.8
C(4)-Mo(3)-Mo(1)	68.03(17)	C(6)-C(10)-C(9)	108.0(6)
C(3)-Mo(3)-Mo(1)	47.52(15)	C(6)-C(10)-Mo(1)	72.5(4)
C(17)-Mo(3)-Mo(1)	147.00(18)	C(9)-C(10)-Mo(1)	71.2(4)
C(16)-Mo(3)-Mo(1)	114.98(18)	C(6)-C(10)-H(10)	126.0
C(20)-Mo(3)-Mo(1)	106.44(17)	C(9)-C(10)-H(10)	126.0
C(18)-Mo(3)-Mo(1)	162.28(17)	Mo(1)-C(10)-H(10)	122.0
C(19)-Mo(3)-Mo(1)	127.69(17)	C(15)-C(11)-C(12)	107.4(6)
C(5)-Mo(3)-Mo(2)	67.61(17)	C(15)-C(11)-Mo(2)	72.5(4)
C(4)-Mo(3)-Mo(2)	100.81(17)	C(12)-C(11)-Mo(2)	72.8(4)
C(3)-Mo(3)-Mo(2)	45.14(17)	C(15)-C(11)-H(11)	126.3
C(17)-Mo(3)-Mo(2)	160.05(18)	C(12)-C(11)-H(11)	126.3
C(16)-Mo(3)-Mo(2)	155.52(18)	Mo(2)-C(11)-H(11)	120.3
C(20)-Mo(3)-Mo(2)	123.19(16)	C(13)-C(12)-C(11)	108.4(7)
C(18)-Mo(3)-Mo(2)	125.71(18)	C(13)-C(12)-Mo(2)	72.8(4)
C(19)-Mo(3)-Mo(2)	109.92(17)	C(11)-C(12)-Mo(2)	72.3(4)
Mo(1)-Mo(3)-Mo(2)	52.71(3)	C(13)-C(12)-H(12)	125.8
C(21)-P(1)-C(27)	106.1(3)	C(11)-C(12)-H(12)	125.8
C(21)-P(1)-Mo(2)	117.08(19)	Mo(2)-C(12)-H(12)	120.8
C(27)-P(1)-Mo(2)	117.51(19)	C(14)-C(13)-C(12)	108.6(6)
C(21)-P(1)-Mo(1)	119.4(2)	C(14)-C(13)-Mo(2)	72.8(4)
C(27)-P(1)-Mo(1)	123.7(2)	C(12)-C(13)-Mo(2)	72.5(4)
Mo(2)-P(1)-Mo(1)	69.76(5)	C(14)-C(13)-H(13)	125.7
O(1)-C(1)-Mo(1)	173.3(5)	C(12)-C(13)-H(13)	125.7
O(2)-C(2)-Mo(2)	173.2(6)	Mo(2)-C(13)-H(13)	120.7
O(3)-C(3)-Mo(3)	139.9(5)	C(13)-C(14)-C(15)	106.7(7)
O(3)-C(3)-Mo(2)	120.2(4)	C(13)-C(14)-Mo(2)	72.8(4)
Mo(3)-C(3)-Mo(2)	93.7(2)	C(15)-C(14)-Mo(2)	71.6(4)
O(3)-C(3)-Mo(1)	116.3(4)	C(13)-C(14)-H(14)	126.7
Mo(3)-C(3)-Mo(1)	91.0(2)	C(15)-C(14)-H(14)	126.7
Mo(2)-C(3)-Mo(1)	75.62(18)	Mo(2)-C(14)-H(14)	120.8
O(4)-C(4)-Mo(3)	167.3(5)	C(11)-C(15)-C(14)	108.9(6)
O(5)-C(5)-Mo(3)	168.3(5)	C(11)-C(15)-Mo(2)	73.2(4)
C(7)-C(6)-C(10)	109.3(6)	C(14)-C(15)-Mo(2)	72.9(4)
C(7)-C(6)-Mo(1)	72.7(4)	C(11)-C(15)-H(15)	125.5
C(10)-C(6)-Mo(1)	72.9(4)	C(14)-C(15)-H(15)	125.5
C(7)-C(6)-H(6)	125.3	Mo(2)-C(15)-H(15)	120.1
C(10)-C(6)-H(6)	125.3	C(20)-C(16)-C(17)	108.2(6)
Mo(1)-C(6)-H(6)	120.7	C(20)-C(16)-Mo(3)	73.1(4)
C(6)-C(7)-C(8)	107.4(6)	C(17)-C(16)-Mo(3)	71.5(4)

C(20)-C(16)-H(16)	125.9	H(24A)-C(24)-H(24B)	108.2
C(17)-C(16)-H(16)	125.9	C(24)-C(25)-C(26)	109.9(5)
Mo(3)-C(16)-H(16)	121.2	C(24)-C(25)-H(25A)	109.7
C(16)-C(17)-C(18)	108.3(6)	C(26)-C(25)-H(25A)	109.7
C(16)-C(17)-Mo(3)	73.4(4)	C(24)-C(25)-H(25B)	109.7
C(18)-C(17)-Mo(3)	73.6(4)	C(26)-C(25)-H(25B)	109.7
C(16)-C(17)-H(17)	125.9	H(25A)-C(25)-H(25B)	108.2
C(18)-C(17)-H(17)	125.9	C(25)-C(26)-C(21)	112.8(5)
Mo(3)-C(17)-H(17)	119.0	C(25)-C(26)-H(26A)	109.0
C(19)-C(18)-C(17)	107.7(6)	C(21)-C(26)-H(26A)	109.0
C(19)-C(18)-Mo(3)	72.9(3)	C(25)-C(26)-H(26B)	109.0
C(17)-C(18)-Mo(3)	71.2(3)	C(21)-C(26)-H(26B)	109.0
C(19)-C(18)-H(18)	126.1	H(26A)-C(26)-H(26B)	107.8
C(17)-C(18)-H(18)	126.1	C(32)-C(27)-C(28)	109.4(5)
Mo(3)-C(18)-H(18)	121.5	C(32)-C(27)-P(1)	110.9(4)
C(18)-C(19)-C(20)	107.4(6)	C(28)-C(27)-P(1)	116.1(4)
C(18)-C(19)-Mo(3)	72.4(4)	C(32)-C(27)-H(27)	106.6
C(20)-C(19)-Mo(3)	72.0(3)	C(28)-C(27)-H(27)	106.6
C(18)-C(19)-H(19)	126.3	P(1)-C(27)-H(27)	106.6
C(20)-C(19)-H(19)	126.3	C(27)-C(28)-C(29)	111.4(5)
Mo(3)-C(19)-H(19)	121.1	C(27)-C(28)-H(28A)	109.4
C(16)-C(20)-C(19)	108.3(6)	C(29)-C(28)-H(28A)	109.4
C(16)-C(20)-Mo(3)	72.6(4)	C(27)-C(28)-H(28B)	109.4
C(19)-C(20)-Mo(3)	72.6(4)	C(29)-C(28)-H(28B)	109.4
C(16)-C(20)-H(20)	125.8	H(28A)-C(28)-H(28B)	108.0
C(19)-C(20)-H(20)	125.8	C(30)-C(29)-C(28)	111.4(6)
Mo(3)-C(20)-H(20)	120.7	C(30)-C(29)-H(29A)	109.3
C(26)-C(21)-C(22)	112.7(5)	C(28)-C(29)-H(29A)	109.3
C(26)-C(21)-P(1)	111.3(4)	C(30)-C(29)-H(29B)	109.3
C(22)-C(21)-P(1)	114.5(4)	C(28)-C(29)-H(29B)	109.3
C(26)-C(21)-H(21)	105.8	H(29A)-C(29)-H(29B)	108.0
C(22)-C(21)-H(21)	105.8	C(29)-C(30)-C(31)	109.4(5)
P(1)-C(21)-H(21)	105.8	C(29)-C(30)-H(30A)	109.8
C(23)-C(22)-C(21)	111.5(5)	C(31)-C(30)-H(30A)	109.8
C(23)-C(22)-H(22A)	109.3	C(29)-C(30)-H(30B)	109.8
C(21)-C(22)-H(22A)	109.3	C(31)-C(30)-H(30B)	109.8
C(23)-C(22)-H(22B)	109.3	H(30A)-C(30)-H(30B)	108.2
C(21)-C(22)-H(22B)	109.3	C(30)-C(31)-C(32)	111.3(5)
H(22A)-C(22)-H(22B)	108.0	C(30)-C(31)-H(31A)	109.4
C(22)-C(23)-C(24)	111.1(6)	C(32)-C(31)-H(31A)	109.4
C(22)-C(23)-H(23A)	109.4	C(30)-C(31)-H(31B)	109.4
C(24)-C(23)-H(23A)	109.4	C(32)-C(31)-H(31B)	109.4
C(22)-C(23)-H(23B)	109.4	H(31A)-C(31)-H(31B)	108.0
C(24)-C(23)-H(23B)	109.4	C(31)-C(32)-C(27)	112.6(5)
H(23A)-C(23)-H(23B)	108.0	C(31)-C(32)-H(32A)	109.1
C(25)-C(24)-C(23)	110.0(5)	C(27)-C(32)-H(32A)	109.1
C(25)-C(24)-H(24A)	109.7	C(31)-C(32)-H(32B)	109.1
C(23)-C(24)-H(24A)	109.7	C(27)-C(32)-H(32B)	109.1
C(25)-C(24)-H(24B)	109.7	H(32A)-C(32)-H(32B)	107.8
C(23)-C(24)-H(24B)	109.7		

Table 23 Anisotropic displacement parameters ($Å^2 x\ 10^3$)for compound **6**. 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)	11(1)	18(1)	13(1)	0(1)	6(1)	1(1)
Mo(2)	11(1)	16(1)	15(1)	2(1)	6(1)	0(1)
Mo(3)	15(1)	16(1)	14(1)	0(1)	7(1)	1(1)
P(1)	14(1)	16(1)	16(1)	0(1)	8(1)	-1(1)
O(1)	33(3)	24(2)	32(3)	-3(2)	14(2)	3(2)
O(2)	28(3)	25(2)	34(3)	-14(2)	14(2)	-9(2)
O(3)	23(2)	17(2)	28(2)	-4(2)	12(2)	-1(2)
O(4)	33(3)	17(2)	34(3)	4(2)	18(2)	4(2)
O(5)	22(2)	29(2)	25(2)	5(2)	9(2)	-4(2)
C(1)	19(3)	26(3)	19(3)	9(3)	7(2)	4(2)
C(2)	16(3)	30(3)	21(3)	5(3)	10(2)	-2(2)
C(3)	14(3)	20(3)	20(3)	2(2)	10(2)	7(2)
C(4)	21(3)	26(3)	10(3)	2(2)	8(2)	-6(3)
C(5)	19(3)	20(3)	15(3)	1(2)	11(2)	0(2)
C(6)	17(3)	36(4)	19(3)	1(3)	1(2)	-2(3)
C(7)	15(3)	28(3)	29(4)	7(3)	1(3)	5(3)
C(8)	13(3)	45(4)	29(4)	-4(3)	10(3)	8(3)
C(9)	11(3)	43(4)	35(4)	14(3)	7(3)	-3(3)
C(10)	20(3)	26(3)	28(4)	-5(3)	-1(3)	-1(3)
C(11)	28(4)	57(5)	28(4)	17(3)	17(3)	26(4)
C(12)	23(3)	23(3)	39(4)	2(3)	6(3)	8(3)
C(13)	24(3)	33(4)	25(4)	16(3)	12(3)	14(3)
C(14)	25(4)	29(4)	31(4)	2(3)	-14(3)	15(3)
C(15)	9(3)	49(5)	69(6)	40(4)	9(3)	7(3)
C(16)	34(4)	34(4)	15(3)	-2(3)	10(3)	10(3)
C(17)	43(4)	30(4)	21(3)	1(3)	22(3)	-4(3)
C(18)	23(3)	46(4)	19(3)	-7(3)	17(3)	-4(3)
C(19)	30(3)	31(4)	21(3)	-4(3)	14(3)	11(3)
C(20)	28(3)	29(3)	16(3)	-4(3)	8(3)	1(3)
C(21)	17(3)	21(3)	15(3)	-3(2)	7(2)	-1(2)
C(22)	20(3)	29(3)	22(3)	-1(3)	9(3)	2(3)
C(23)	37(4)	38(4)	21(3)	1(3)	19(3)	11(3)
C(24)	43(4)	39(4)	16(3)	3(3)	18(3)	6(3)
C(25)	22(3)	31(3)	17(3)	1(3)	5(3)	-2(3)
C(26)	17(3)	28(3)	17(3)	2(2)	7(2)	0(2)
C(27)	13(3)	18(3)	20(3)	3(2)	8(2)	-3(2)
C(28)	29(4)	26(3)	32(4)	-4(3)	20(3)	-7(3)
C(29)	34(4)	26(4)	35(4)	3(3)	17(3)	-11(3)
C(30)	25(3)	18(3)	40(4)	-4(3)	13(3)	-9(3)
C(31)	18(3)	17(3)	34(4)	-5(3)	7(3)	-2(2)
C(32)	19(3)	19(3)	29(4)	-1(2)	13(3)	-4(2)

Table 24. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for compound **6**.

	x	y	z	U(eq)
H(6)	707	6554	-716	30
H(7)	163	7321	345	31
H(8)	-446	6787	1705	34
H(9)	-298	5689	1419	36
H(10)	373	5554	-90	32
H(11)	6966	5437	1491	43
H(12)	5738	4793	2398	35
H(13)	6092	5251	4024	32
H(14)	7556	6174	4153	41
H(15)	8094	6281	2567	52
H(16)	2496	6894	-1689	32
H(17)	4925	7399	-1157	34
H(18)	6851	6626	-463	32
H(19)	5594	5651	-502	31
H(20)	2884	5828	-1264	29
H(21)	3530	6665	4047	20
H(22A)	1028	6696	3566	28
H(22B)	956	6074	4037	28
H(23A)	642	6800	5090	36
H(23B)	2082	7122	5099	36
H(24A)	2511	6554	6546	37
H(24B)	2028	5975	5916	37
H(25A)	4596	6041	6497	28
H(25B)	4515	6660	5979	28
H(26A)	3666	5559	4996	25
H(26B)	5010	5938	4973	25
H(27)	3458	4919	3609	20
H(28A)	432	5157	3035	31
H(28B)	1500	5187	4117	31
H(29A)	1907	4153	4120	36
H(29B)	225	4268	3845	36
H(30A)	-92	4122	2185	33
H(30B)	671	3559	2777	33
H(31A)	1899	3864	1691	28
H(31B)	2952	3896	2777	28
H(32A)	1519	4888	1665	26
H(32B)	3200	4767	1969	26