Self-assembly of a novel multicomponent polyoxometalate-based tetrahedral supercluster with high catalytic activity for thioether oxidation

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Experimental details.

Experimental details.

1. Materials and general methods:

All chemical materials were commercially purchased without further purification. Infrared(IR) spectra (KBr pellet) were performed on a Varian 640 FTIR FT-IR infrared spectrophotometer in the range of 400-4000 cm^{-1} (Fig. S2). Powder X-ray diffraction (PXRD) patterns were recorded on a D/teX Ultra diffractometer with Cu Kα radiation (λ = 1.5418 Å). Simulated XRD data were simulated by the Mercury Software with the step of 0.02° from 5° to 50°. Thermogravimetric analyses were conducted using a Hitachi TG/DTA7200 analyzer in an N_2-flow atmosphere with a heating rate of 10 °C/min at a temperature of 25-800 °C. X-ray photoelectron spectrum (XPS) was measured using a Thermomo Scientific K-Alpha photoelectron spectrometer. The catalytic reaction was analyzed by using a Shimadzu Tech-comp GC-7900 gas chromatograph (GC) with a flame ionization detector equipped with a TM-5 Sil capillary column. The quantitative analyses of Mo, Co and Pb elements and the filtrate after the removal of the catalyst were achieved by Perkin Elmer NexION 300X inductively coupled plasma optical emission spectrometer (ICP).

2. Synthesis

Synthesis of 1: A mixture of $Na_2MoO_4·2H_2O$ (0.500g, 2.067 mmol), $CoCl_2·6H_2O$ (0.200 g, 0.841 mmol), $Pb(OAc)_2·3H_2O$ (0.100g, 0.264 mmol), H_3PO_4 (0.56 ml, 10 mmol), benzimidazole (0.118 g, 1 mmol) were dissolved in a mixed solution of $EtOH/H_2O$ (6mL, v:v = 1:5). After being stirred for 35 min at room temperature and then adjusted with 1 M NaOH solution to pH=1.9, Then the above mixture was placed into a 25 ml Teflon reactor and heated at 160 °C for 4 days, finally cooled to room temperature. Black block crystals of **1** were isolated. Yield: ~ 82 mg (16.32 % based on $Na_2MoO_4·2H_2O$). IR (KBr pellet, cm^{-1}, Fig. S2): 3543(w),3143(s), 2969(w), 2865(w), 2364(w), 1615(m), 1543(w), 1506(w),1448(m), 1370(w), 1234(m),1112(w), 1048(s), 994(s), 812(w), 753(s), 622(m), 572(m), 482(m).

3. X-ray crystallography

The intensity data of the compound were collected on a Bruker Apex CCD II area detector diffractometer with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) at 173 K. Absorption corrections were applied using multiscan techniques. The structure was solved by direct methods and refined by full-matrix least-squares techniques using the SHELXL program[1-3]. The contribution of disordered solvent molecules to the overall intensity data of structure was treated using the SQUEEZE method in PLATON. Crystallographic data for compound **1** is summarized in Table S1. The bond length (Å) and angle (deg) range of compound **1** is listed in Table S2-S3. BVS result of compound **1** is listed in Table S4. The crystallographic data have been deposited with the Cambridge Crystallographic Data Centre (CCDC) as entry 2166179.

4. Catalytic oxidation of thioether

The substrate thioether (0.5 mmol), powder catalyst **1** ($3×10^{-4}$ mmol), EtOH as solvent (3 ml), tert-butyl hydroperoxide (TBHP, 0.65 mmol, 70% aqueous solution), and internal standard naphthalene (15 mg) were added into the sealed reaction vessel at room temperature and stirred for 60 min under 60 °C. The yield of the product was determined by GC. At the end of the reaction, the mixture was rinsed with EtOH, and the remaining powder was dried in the air and used in the cycle reaction.

Table S1. Crystal data and structure refinement for compound **1**.

Compound **1**	
Empirical formula	$C_{84}H_{342}Co_{12}Mo_{80}N_{24}O_{489}P_{36}Pb_4$
Formula weight	19839.84
Crystal system	Monoclinic
Space group	C2/c
T (K)	173
a (Å)	30.9076(13)
b (Å)	57.925(2)
c (Å)	32.2149(16)
α(°)	90
β(°)	109.355(2)
γ (°)	90
V (Å^3)	54416(4)
Z	4
D_c (Mg m^{-3})	2.136
μ (mm^{-1})	3.555
F(000)	32720
Reflections collected / unique	292167 / 48305 [R(int) = 0.0624]
Data / restraints / parameters	48305 / 714 / 2658
GOF	1.033
R index [I > 2σ(I)]	R_1 = 0.0444, wR_2 = 0.1081
R (all data)	R_1 = 0.0632, wR_2 = 0.1191

$R_1 = \Sigma||F_o| - |F_c|| / \Sigma|F_o|$; $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$

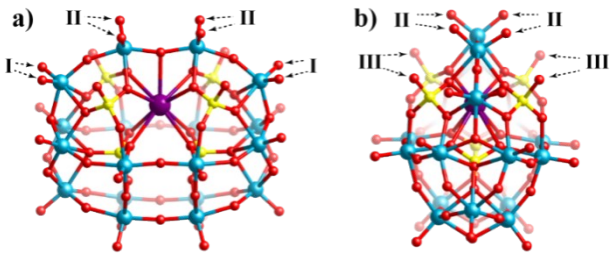


Fig. S1.a) –b) Potential active coordination sites for P_6Mo_{18}.

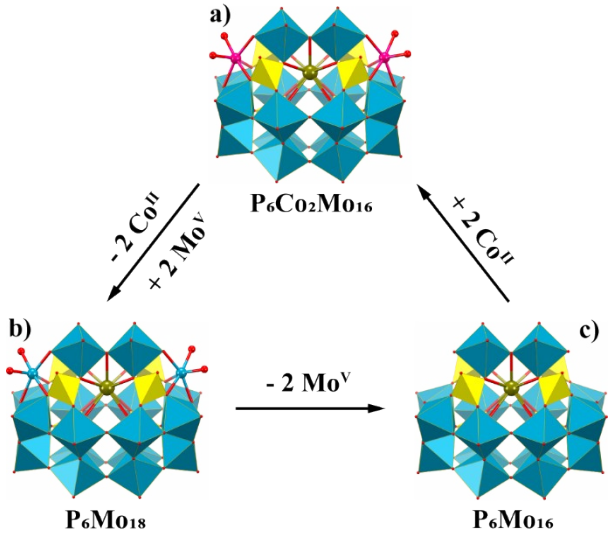


Fig. S2 a)– c) Structural correlation in the novel $P_6Co_2Mo_{16}$, classical P_6Mo_{18}, and isolated P_6Mo_{16}. MoO_6: wathet blue octahedra; PO_4: yellow tetrahedron; Mo, wathet blue spheres; Co, pink spheres; O, red spheres; Pb, dark yellow spheres.

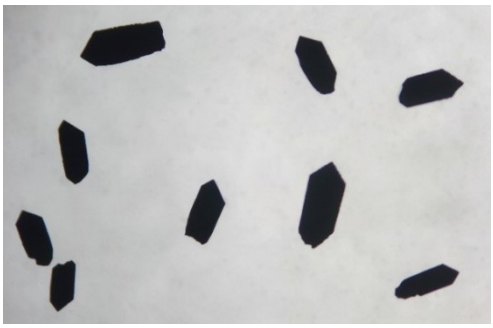


Fig. S3 Crystals of **1** under an optical microscope (Magnification information: 4.5*10)

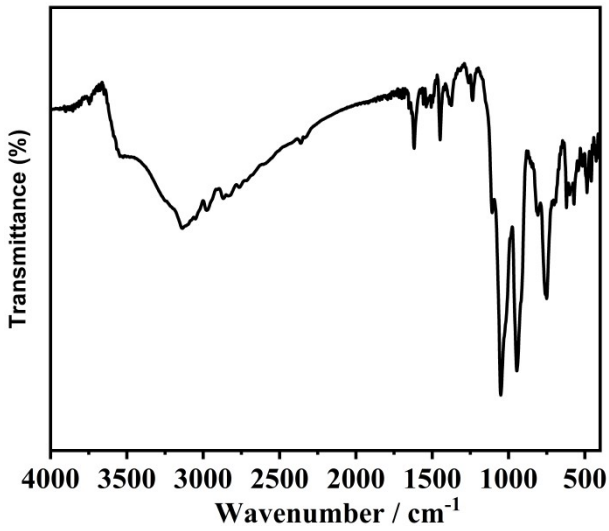


Fig. S4 IR spectrum of **1**

The FT-IR spectrum of **1** was recorded in the range of 4000–500 cm^{-1} using KBr pellets. Strong

bands located at 3543 and 1615cm^{-1} are assigned to ν(O–H) stretching and bending vibrations of water molecules. The peaks at 1048, 994, 812, and 753cm^{-1} are attributed to ν(P–O_a), ν(Mo=$O_{terminal}$), and ν(Mo–O_{bridge}) vibrations, respectively. The peaks located at 572 and 622 cm^{-1} can be attributed to ν(Mo–O). The peaks at 1448cm^{-1} is attributed to ν(C-N) vibrations.

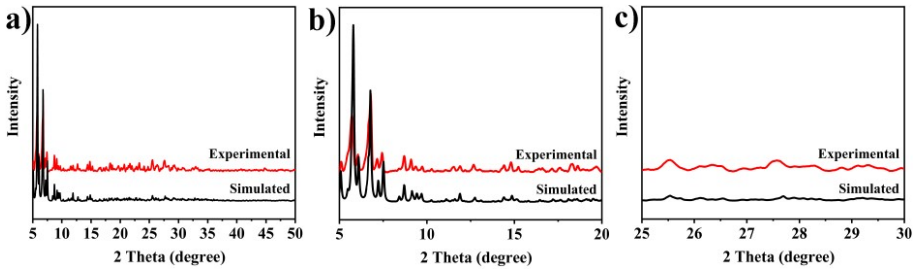


Fig. S5. Simulated and experimental PXRD patterns of **1** in the characteristic regions of a) 5-50 degree; b) 5-20 degree; c) 25-30 degree.

The phase purity of **1** was determined by the good consistency between the experimental and simulated PXRD patterns. The difference in intensity between the experimental and simulated PXRD patterns may be due to the change in the preferred orientation of the powder samples during the acquisition of the experimental PXRD patterns.

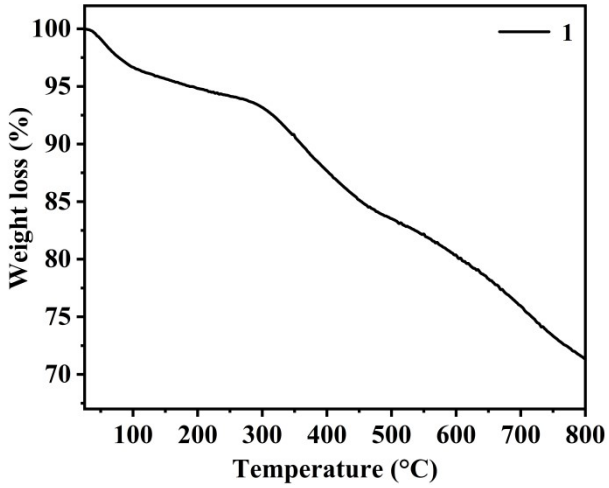


Fig. S6. The TG curve of **1**.

For the sake of exploring the thermal stability of compound **1**, the TG measurement was carried out from 25 to 800 °C under an N_2 atmosphere at a heating rate of 10 °C min^{-1}. The TG curve suggests that compound **1** undergoes a two-step weight loss (Figure S5). The first weight loss from 25 to 157 °C of 4.52 % (calcd. 4.45 %) is attributed to the liberation of 49 lattice water molecules. Upon heating to 390 °C, the second weight loss of 7.22 % (calcd. 7.26 %) is attributed to 80 lattice water molecules.

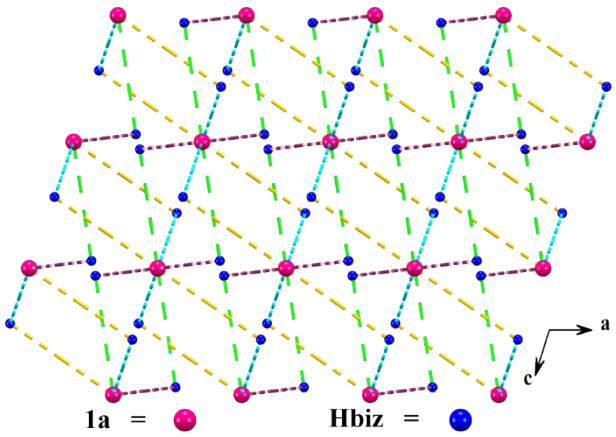


Fig. S7 The simplified diagram of 3D supramolecular framework of compound **1** (The pink ball represents cluster 1a; the blue ball represents Hbiz ligand).

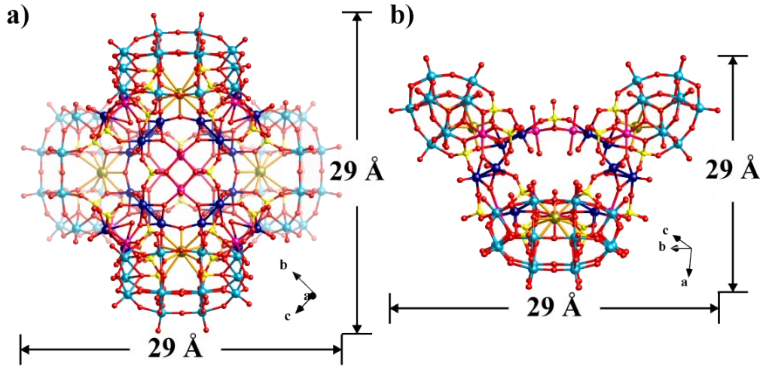


Fig. S8. a)–b) Ball-and-stick model and dimension of **1a** established by X-ray crystallography. H atoms are omitted for clarity. Atoms colored wathet blue, dark blue, pink, dark yellow, yellow, and red, correspond to Mo^{V}, Mo^{VI}, Co, Pb, P, and O.

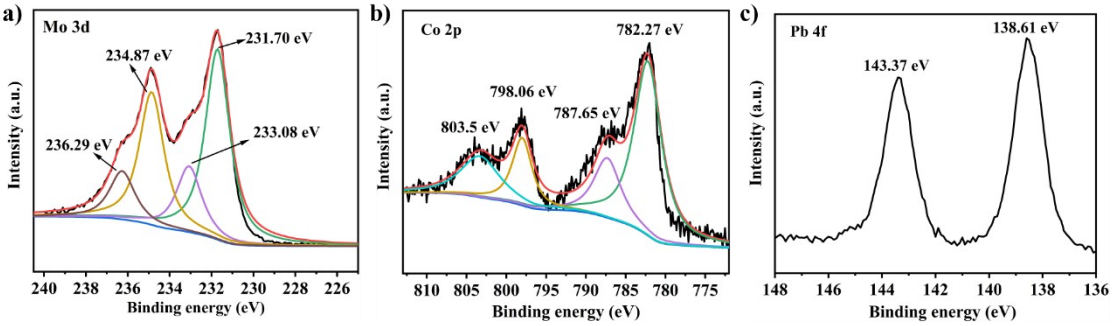


Fig. S9. The XPS pattern for a) Mo; b) Co; c) Pb.

The XPS studies on **1** were conducted to identify the oxidation states of Mo, Co, and Pb atoms. The XPS spectrum for Mo atoms displays two peaks at 233.08 and 231.70 eV in the energy region of Mo $3d_{5/2}$, and two peaks at 236.29 and 234.87 eV in the energy region of Mo $3d_{3/2}$. The peaks at 231.70 and 234.87 eV are typical for the Mo^{V} ions;[4] whereas the Mo^{VI} ions are labeled with the characteristic peaks at 236.29 and 233.08 eV,[5] illustrating that Mo^{VI} ions in the starting materials are partially reduced to Mo^{V} ions in the synthetic procedure.

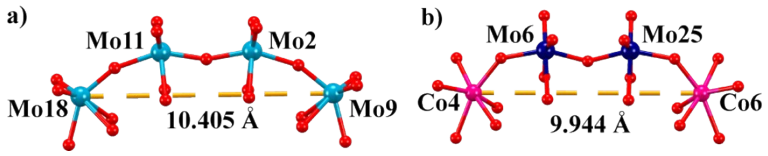


Fig. S10. a) The distance between the two metal atoms at the bottom of the basket handle of P_6Mo_{18}; b) The distance between the two metal atoms at the bottom of the basket handle of $P_6Co_2Mo_{16}$.

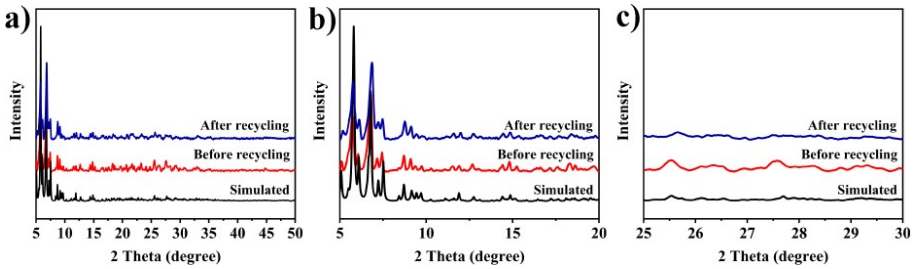


Fig. S11. PXRD spectra of **1** before and after five runs catalytic reactions in the characteristic regions of a) 5-50 degree; b) 5-20 degree; c) 25-30 degree.

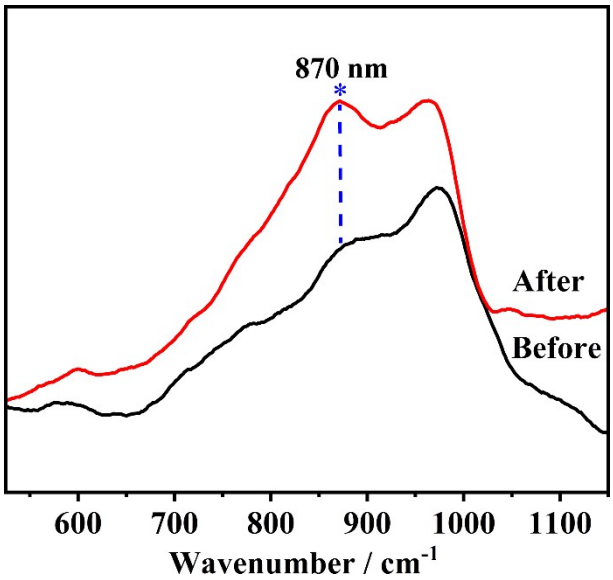


Fig. S12. Raman spectra of **1** before and after treating with TBHP.

Table S2. The bond angle (deg) range in compound **1**.

Bond	Angle (°)	Bond	Angle (°)	Bond	Angle (°)	Bond	Angle (°)
O(8)-Pb(1)-O(29)	88.89(15)	O(26)-Mo(12)-O(9)	85.95(19)	O(133)-Mo(25)-O(69)	104.1(3)	O(166)-Mo(39)-O(116)	155.9(3)
O(13)-Pb(1)-O(8)	123.26(16)	O(41)-Mo(12)-O(9)	72.56(19)	O(133)-Mo(25)-O(96)	99.8(3)	O(166)-Mo(39)-O(126)	95.1(3)
O(13)-Pb(1)-O(14)	91.13(16)	O(41)-Mo(12)-O(26)	76.5(2)	O(133)-Mo(25)-O(169)	172.0(3)	O(166)-Mo(39)-O(139)	88.2(3)
O(13)-Pb(1)-O(29)	63.31(16)	O(47)-Mo(12)-O(9)	83.9(2)	O(133)-Mo(25)-O(179)	96.1(3)	O(177)-Mo(39)-O(90)	164.5(3)
O(14)-Pb(1)-O(8)	63.46(16)	O(47)-Mo(12)-O(26)	85.0(2)	O(169)-Mo(25)-Mo(34)	87.11(15)	O(177)-Mo(39)-O(116)	96.6(3)
O(14)-Pb(1)-O(29)	123.74(16)	O(47)-Mo(12)-O(41)	150.8(2)	O(179)-Mo(25)-Mo(34)	135.57(16)	O(177)-Mo(39)-O(126)	104.4(3)
O(22)-Pb(1)-O(8)	60.20(15)	O(47)-Mo(12)-O(75)	97.7(2)	O(179)-Mo(25)-O(169)	75.9(2)	O(177)-Mo(39)-O(139)	96.6(3)
O(22)-Pb(1)-O(13)	63.06(16)	O(75)-Mo(12)-O(9)	74.8(2)	O(87)-Mo(26)-O(31)	79.3(2)	O(177)-Mo(39)-O(166)	104.6(3)
O(22)-Pb(1)-O(14)	63.51(16)	O(75)-Mo(12)-O(26)	160.1(2)	O(88)-Mo(26)-O(31)	72.5(2)	O(110)-Mo(40)-O(90)	73.1(2)
O(22)-Pb(1)-O(29)	60.24(16)	O(75)-Mo(12)-O(41)	92.7(2)	O(88)-Mo(26)-O(87)	83.6(2)	O(110)-Mo(40)-O(180)	77.0(2)
O(32)-Pb(2)-O(34)	62.98(17)	O(100)-Mo(12)-O(9)	171.7(2)	O(141)-Mo(26)-O(31)	169.4(3)	O(116)-Mo(40)-O(90)	75.3(3)
O(32)-Pb(2)-O(49)	63.15(17)	O(100)-Mo(12)-O(26)	97.8(2)	O(141)-Mo(26)-O(87)	92.0(3)	O(116)-Mo(40)-O(110)	91.5(3)
O(32)-Pb(2)-O(169)	90.80(18)	O(100)-Mo(12)-O(41)	101.0(2)	O(141)-Mo(26)-O(88)	100.8(3)	O(116)-Mo(40)-O(180)	160.5(3)
O(32)-Pb(2)-O(179)	122.62(17)	O(100)-Mo(12)-O(47)	103.7(3)	O(141)-Mo(26)-O(161)	100.7(3)	O(149)-Mo(40)-O(90)	83.4(3)
O(34)-Pb(2)-O(49)	59.33(18)	O(100)-Mo(12)-O(75)	100.6(3)	O(141)-Mo(26)-O(167)	100.3(3)	O(149)-Mo(40)-O(110)	151.0(3)
O(34)-Pb(2)-O(169)	63.65(18)	O(30)-Mo(13)-Mo(16)	49.12(16)	O(161)-Mo(26)-O(31)	88.0(2)	O(149)-Mo(40)-O(116)	98.9(3)
O(34)-Pb(2)-O(179)	59.65(16)	O(30)-Mo(13)-O(65)	153.7(2)	O(161)-Mo(26)-O(87)	167.3(2)	O(149)-Mo(40)-O(180)	84.8(2)
O(169)-Pb(2)-O(49)	122.97(17)	O(30)-Mo(13)-O(84)	86.7(2)	O(161)-Mo(26)-O(88)	92.4(2)	O(154)-Mo(40)-O(90)	171.0(3)
O(169)-Pb(2)-O(179)	63.53(18)	O(30)-Mo(13)-O(170)	68.7(2)	O(161)-Mo(26)-O(167)	91.2(3)	O(154)-Mo(40)-O(110)	99.8(3)
O(179)-Pb(2)-O(49)	88.12(17)	O(50)-Mo(13)-Mo(16)	49.02(15)	O(167)-Mo(26)-O(31)	85.5(2)	O(154)-Mo(40)-O(116)	99.7(3)
O(6)-Mo(1)-Mo(3)	48.56(14)	O(50)-Mo(13)-O(30)	98.1(2)	O(167)-Mo(26)-O(87)	88.1(2)	O(154)-Mo(40)-O(149)	105.0(3)
O(6)-Mo(1)-O(8)	87.40(19)	O(50)-Mo(13)-O(65)	86.0(2)	O(167)-Mo(26)-O(88)	157.5(2)	O(154)-Mo(40)-O(180)	97.8(3)
O(6)-Mo(1)-O(14)	81.18(19)	O(50)-Mo(13)-O(84)	146.8(2)	O(62)-Mo(27)-O(83)	83.3(2)	O(180)-Mo(40)-O(90)	86.2(2)

O(8)-Mo(1)-Mo(3)	135.22(13)	O(50)-Mo(13)-O(170)	68.4(2)	O(111)-Mo(27)-O(62)	76.0(2)	O(5)-Co(1)-O(7)	173.7(2)
O(8)-Mo(1)-O(14)	75.51(19)	O(65)-Mo(13)-Mo(16)	130.24(15)	O(111)-Mo(27)-O(83)	72.9(2)	O(5)-Co(1)-O(19)	73.21(19)
O(14)-Mo(1)-Mo(3)	88.18(13)	O(65)-Mo(13)-O(84)	76.4(2)	O(123)-Mo(27)-O(62)	159.1(3)	O(6)-Co(1)-O(5)	89.36(19)
O(16)-Mo(1)-Mo(3)	48.37(15)	O(65)-Mo(13)-O(170)	89.2(2)	O(123)-Mo(27)-O(83)	76.3(2)	O(6)-Co(1)-O(7)	87.04(19)
O(16)-Mo(1)-O(6)	95.8(2)	O(84)-Mo(13)-Mo(16)	127.99(15)	O(123)-Mo(27)-O(111)	93.6(3)	O(6)-Co(1)-O(11)	103.5(2)
O(16)-Mo(1)-O(8)	159.4(2)	O(84)-Mo(13)-O(170)	83.2(2)	O(123)-Mo(27)-O(178)	98.7(3)	O(6)-Co(1)-O(19)	162.2(2)
O(16)-Mo(1)-O(14)	84.9(2)	O(128)-Mo(13)-Mo(16)	107.2(2)	O(168)-Mo(27)-O(62)	97.6(3)	O(11)-Co(1)-O(5)	92.7(2)
O(22)-Mo(1)-Mo(3)	138.13(15)	O(128)-Mo(13)-O(30)	100.7(3)	O(168)-Mo(27)-O(83)	172.4(3)	O(11)-Co(1)-O(7)	83.13(19)
O(22)-Mo(1)-O(6)	155.9(2)	O(128)-Mo(13)-O(50)	104.4(3)	O(168)-Mo(27)-O(111)	100.0(3)	O(11)-Co(1)-O(19)	74.3(2)
O(22)-Mo(1)-O(8)	78.5(2)	O(128)-Mo(13)-O(65)	103.4(2)	O(168)-Mo(27)-O(123)	102.1(3)	O(19)-Co(1)-O(7)	109.96(19)
O(22)-Mo(1)-O(14)	76.5(2)	O(128)-Mo(13)-O(84)	106.9(2)	O(168)-Mo(27)-O(178)	103.5(3)	O(46)-Co(1)-O(5)	92.8(2)
O(22)-Mo(1)-O(16)	91.1(2)	O(128)-Mo(13)-O(170)	165.3(2)	O(178)-Mo(27)-O(62)	83.3(2)	O(46)-Co(1)-O(6)	97.4(2)
O(76)-Mo(1)-Mo(3)	99.15(19)	O(170)-Mo(13)-Mo(16)	58.26(13)	O(178)-Mo(27)-O(83)	84.1(2)	O(46)-Co(1)-O(7)	92.7(2)
O(76)-Mo(1)-O(6)	99.7(2)	O(15)-Mo(14)-O(9)	83.58(18)	O(178)-Mo(27)-O(111)	150.4(3)	O(46)-Co(1)-O(11)	158.4(2)
O(76)-Mo(1)-O(8)	95.5(2)	O(35)-Mo(14)-O(9)	83.9(2)	O(57)-Mo(28)-O(20)	78.4(2)	O(46)-Co(1)-O(19)	87.4(2)
O(76)-Mo(1)-O(14)	171.0(2)	O(35)-Mo(14)-O(15)	83.2(2)	O(98)-Mo(28)-O(20)	85.4(2)	O(15)-Co(2)-O(26)	92.79(19)
O(76)-Mo(1)-O(16)	103.9(2)	O(35)-Mo(14)-O(41)	149.6(2)	O(98)-Mo(28)-O(57)	92.5(2)	O(15)-Co(2)-O(41)	73.17(19)
O(76)-Mo(1)-O(22)	101.0(2)	O(35)-Mo(14)-O(82)	98.6(2)	O(98)-Mo(28)-O(102)	92.8(3)	O(15)-Co(2)-O(50)	83.38(19)
O(13)-Mo(2)-Mo(7)	87.97(12)	O(41)-Mo(14)-O(9)	72.59(19)	O(98)-Mo(28)-O(178)	167.9(3)	O(24)-Co(2)-O(15)	103.1(2)
O(18)-Mo(2)-Mo(7)	48.44(15)	O(41)-Mo(14)-O(15)	75.4(2)	O(102)-Mo(28)-O(20)	84.8(2)	O(24)-Co(2)-O(26)	88.2(2)
O(18)-Mo(2)-O(13)	84.8(2)	O(68)-Mo(14)-O(9)	172.7(2)	O(102)-Mo(28)-O(57)	162.0(2)	O(24)-Co(2)-O(41)	158.8(2)
O(18)-Mo(2)-O(24)	95.9(2)	O(68)-Mo(14)-O(15)	98.0(2)	O(102)-Mo(28)-O(178)	88.0(2)	O(24)-Co(2)-O(50)	85.6(2)
O(18)-Mo(2)-O(29)	159.9(2)	O(68)-Mo(14)-O(35)	103.3(2)	O(143)-Mo(28)-O(20)	172.8(3)	O(26)-Co(2)-O(50)	171.7(2)
O(22)-Mo(2)-Mo(7)	137.92(15)	O(68)-Mo(14)-O(41)	100.9(2)	O(143)-Mo(28)-O(57)	95.7(3)	O(41)-Co(2)-O(26)	71.4(2)
O(22)-Mo(2)-O(13)	76.2(2)	O(68)-Mo(14)-O(82)	102.5(3)	O(143)-Mo(28)-O(98)	99.1(3)	O(41)-Co(2)-O(50)	114.2(2)
O(22)-Mo(2)-O(18)	90.9(2)	O(82)-Mo(14)-O(9)	75.2(2)	O(143)-Mo(28)-O(102)	100.5(3)	O(80)-Co(2)-O(15)	158.2(2)

O(22)-Mo(2)-O(24)	155.4(2)	O(82)-Mo(14)-O(15)	158.3(2)	O(143)-Mo(28)-O(178)	92.6(3)	O(80)-Co(2)-O(24)	97.5(2)
O(22)-Mo(2)-O(29)	78.7(2)	O(82)-Mo(14)-O(41)	93.8(2)	O(178)-Mo(28)-O(20)	82.6(2)	O(80)-Co(2)-O(26)	95.0(2)
O(24)-Mo(2)-Mo(7)	48.59(14)	O(40)-Mo(15)-O(4)	80.9(2)	O(178)-Mo(28)-O(57)	83.2(2)	O(80)-Co(2)-O(41)	90.1(2)
O(24)-Mo(2)-O(13)	80.96(19)	O(64)-Mo(15)-O(4)	85.7(2)	O(103)-Mo(29)-O(101)	84.5(2)	O(80)-Co(2)-O(50)	91.2(2)
O(24)-Mo(2)-O(29)	87.3(2)	O(64)-Mo(15)-O(40)	94.7(2)	O(103)-Mo(29)-O(126)	89.1(2)	O(16)-Co(3)-O(61)	168.3(2)
O(29)-Mo(2)-Mo(7)	135.21(14)	O(64)-Mo(15)-O(167)	95.1(2)	O(103)-Mo(29)-O(137)	156.5(3)	O(16)-Co(3)-O(78)	90.00(19)
O(29)-Mo(2)-O(13)	76.09(19)	O(64)-Mo(15)-O(175)	167.1(2)	O(126)-Mo(29)-O(101)	78.8(2)	O(18)-Co(3)-O(16)	100.72(19)
O(77)-Mo(2)-Mo(7)	99.19(18)	O(117)-Mo(15)-O(4)	171.1(2)	O(137)-Mo(29)-O(101)	72.3(2)	O(18)-Co(3)-O(61)	90.9(2)
O(77)-Mo(2)-O(13)	171.7(2)	O(117)-Mo(15)-O(40)	91.8(2)	O(137)-Mo(29)-O(126)	83.0(3)	O(18)-Co(3)-O(78)	169.0(2)
O(77)-Mo(2)-O(18)	103.1(2)	O(117)-Mo(15)-O(64)	100.1(3)	O(150)-Mo(29)-O(101)	170.5(3)	O(18)-Co(3)-O(160)	93.0(3)
O(77)-Mo(2)-O(22)	100.9(2)	O(117)-Mo(15)-O(167)	100.4(3)	O(150)-Mo(29)-O(103)	101.0(3)	O(61)-Co(3)-O(78)	78.3(2)
O(77)-Mo(2)-O(24)	100.6(2)	O(117)-Mo(15)-O(175)	92.0(2)	O(150)-Mo(29)-O(126)	93.4(3)	O(121)-Co(3)-O(16)	88.5(2)
O(77)-Mo(2)-O(29)	95.8(2)	O(167)-Mo(15)-O(4)	85.7(2)	O(150)-Mo(29)-O(137)	101.6(3)	O(121)-Co(3)-O(18)	88.3(2)
O(6)-Mo(3)-Mo(1)	49.14(14)	O(167)-Mo(15)-O(40)	162.7(2)	O(150)-Mo(29)-O(163)	99.7(3)	O(121)-Co(3)-O(61)	89.9(2)
O(6)-Mo(3)-O(25)	81.8(2)	O(167)-Mo(15)-O(175)	87.1(2)	O(163)-Mo(29)-O(101)	87.8(2)	O(121)-Co(3)-O(78)	89.5(2)
O(6)-Mo(3)-O(43)	162.3(2)	O(175)-Mo(15)-O(4)	81.7(2)	O(163)-Mo(29)-O(103)	91.5(3)	O(121)-Co(3)-O(160)	178.5(3)
O(6)-Mo(3)-O(54)	87.6(2)	O(175)-Mo(15)-O(40)	80.2(2)	O(163)-Mo(29)-O(126)	166.5(3)	O(160)-Co(3)-O(16)	92.1(3)
O(16)-Mo(3)-Mo(1)	47.79(14)	O(30)-Mo(16)-Mo(13)	49.29(15)	O(163)-Mo(29)-O(137)	91.1(3)	O(160)-Co(3)-O(61)	89.3(3)
O(16)-Mo(3)-O(6)	95.8(2)	O(30)-Mo(16)-O(81)	148.3(2)	O(92)-Mo(30)-O(39)	85.8(2)	O(160)-Co(3)-O(78)	89.2(3)
O(16)-Mo(3)-O(25)	84.7(2)	O(30)-Mo(16)-O(85)	85.7(2)	O(92)-Mo(30)-O(93)	95.2(2)	O(21)-Co(4)-O(30)	85.6(2)
O(16)-Mo(3)-O(43)	88.8(2)	O(30)-Mo(16)-O(170)	69.7(2)	O(92)-Mo(30)-O(149)	166.7(3)	O(21)-Co(4)-O(37)	89.2(2)
O(16)-Mo(3)-O(54)	164.5(2)	O(50)-Mo(16)-Mo(13)	49.15(15)	O(93)-Mo(30)-O(39)	80.2(2)	O(21)-Co(4)-O(111)	160.4(2)
O(25)-Mo(3)-Mo(1)	88.52(13)	O(50)-Mo(16)-O(30)	98.4(2)	O(103)-Mo(30)-O(39)	85.6(3)	O(37)-Co(4)-O(30)	172.6(2)
O(43)-Mo(3)-Mo(1)	136.34(15)	O(50)-Mo(16)-O(81)	86.8(2)	O(103)-Mo(30)-O(92)	93.3(3)	O(62)-Co(4)-O(21)	103.1(2)
O(43)-Mo(3)-O(25)	81.6(2)	O(50)-Mo(16)-O(85)	154.0(2)	O(103)-Mo(30)-O(93)	162.9(3)	O(62)-Co(4)-O(30)	83.5(2)
O(43)-Mo(3)-O(54)	83.7(2)	O(50)-Mo(16)-O(170)	69.4(2)	O(103)-Mo(30)-O(149)	88.4(2)	O(62)-Co(4)-O(37)	92.6(2)

O(54)-Mo(3)-Mo(1)	136.55(15)	O(81)-Mo(16)-Mo(13)	128.75(16)	O(146)-Mo(30)-O(39)	172.0(3)	O(62)-Co(4)-O(111)	74.2(2)
O(54)-Mo(3)-O(25)	80.8(2)	O(81)-Mo(16)-O(170)	83.3(2)	O(146)-Mo(30)-O(92)	99.0(3)	O(63)-Co(4)-O(21)	96.8(2)
O(114)-Mo(3)-Mo(1)	98.11(19)	O(85)-Mo(16)-Mo(13)	130.35(16)	O(146)-Mo(30)-O(93)	92.9(3)	O(63)-Co(4)-O(30)	91.3(2)
O(114)-Mo(3)-O(6)	100.5(2)	O(85)-Mo(16)-O(81)	77.0(2)	O(146)-Mo(30)-O(103)	100.4(3)	O(63)-Co(4)-O(37)	94.6(2)
O(114)-Mo(3)-O(16)	101.7(2)	O(85)-Mo(16)-O(170)	88.4(2)	O(146)-Mo(30)-O(149)	93.7(3)	O(63)-Co(4)-O(62)	158.9(2)
O(114)-Mo(3)-O(25)	172.9(2)	O(138)-Mo(16)-Mo(13)	108.0(2)	O(149)-Mo(30)-O(39)	81.1(2)	O(63)-Co(4)-O(111)	89.3(2)
O(114)-Mo(3)-O(43)	95.2(2)	O(138)-Mo(16)-O(30)	103.9(3)	O(149)-Mo(30)-O(93)	80.1(2)	O(111)-Co(4)-O(30)	112.9(2)
O(114)-Mo(3)-O(54)	92.5(2)	O(138)-Mo(16)-O(50)	102.1(3)	O(97)-Mo(31)-O(59)	77.7(2)	O(111)-Co(4)-O(37)	71.7(2)
O(10)-Mo(4)-O(2)	78.50(19)	O(138)-Mo(16)-O(81)	105.5(3)	O(98)-Mo(31)-O(59)	85.7(2)	O(36)-Co(5)-O(61)#1	169.7(2)
O(28)-Mo(4)-O(2)	84.5(2)	O(138)-Mo(16)-O(85)	101.8(3)	O(98)-Mo(31)-O(97)	92.6(2)	O(36)-Co(5)-O(69)	97.7(2)
O(28)-Mo(4)-O(10)	162.1(2)	O(138)-Mo(16)-O(170)	167.7(2)	O(98)-Mo(31)-O(135)	93.2(3)	O(36)-Co(5)-O(78)#1	91.9(2)
O(28)-Mo(4)-O(35)	88.8(2)	O(170)-Mo(16)-Mo(13)	59.85(13)	O(98)-Mo(31)-O(136)	167.1(3)	O(36)-Co(5)-O(132)	92.5(2)
O(28)-Mo(4)-O(38)	91.3(2)	O(5)-Mo(17)-O(48)	85.40(19)	O(135)-Mo(31)-O(59)	84.9(2)	O(61)#1-Co(5)-O(78)#1	77.9(2)
O(35)-Mo(4)-O(2)	83.7(2)	O(19)-Mo(17)-O(5)	76.7(2)	O(135)-Mo(31)-O(97)	161.2(3)	O(69)-Co(5)-O(61)#1	92.4(2)
O(35)-Mo(4)-O(10)	83.9(2)	O(19)-Mo(17)-O(48)	72.5(2)	O(135)-Mo(31)-O(136)	87.7(3)	O(69)-Co(5)-O(78)#1	170.1(2)
O(38)-Mo(4)-O(2)	84.3(2)	O(70)-Mo(17)-O(5)	159.6(2)	O(136)-Mo(31)-O(59)	81.6(2)	O(122)-Co(5)-O(36)	88.5(2)
O(38)-Mo(4)-O(10)	92.4(2)	O(70)-Mo(17)-O(19)	91.3(2)	O(136)-Mo(31)-O(97)	82.8(2)	O(122)-Co(5)-O(61)#1	89.6(2)
O(38)-Mo(4)-O(35)	167.9(2)	O(70)-Mo(17)-O(48)	75.2(2)	O(155)-Mo(31)-O(59)	170.9(3)	O(122)-Co(5)-O(69)	88.3(2)
O(74)-Mo(4)-O(2)	174.1(2)	O(118)-Mo(17)-O(5)	97.0(2)	O(155)-Mo(31)-O(97)	94.5(3)	O(122)-Co(5)-O(78)#1	89.5(2)
O(74)-Mo(4)-O(10)	95.6(2)	O(118)-Mo(17)-O(19)	99.7(2)	O(155)-Mo(31)-O(98)	99.6(3)	O(122)-Co(5)-O(132)	178.8(3)
O(74)-Mo(4)-O(28)	101.4(2)	O(118)-Mo(17)-O(48)	171.1(2)	O(155)-Mo(31)-O(135)	102.1(3)	O(132)-Co(5)-O(61)#1	89.3(2)
O(74)-Mo(4)-O(35)	95.4(2)	O(118)-Mo(17)-O(70)	101.3(3)	O(155)-Mo(31)-O(136)	92.7(3)	O(132)-Co(5)-O(69)	92.2(3)
O(74)-Mo(4)-O(38)	96.4(2)	O(118)-Mo(17)-O(175)	104.2(3)	O(105)-Mo(32)-O(60)	79.7(2)	O(132)-Co(5)-O(78)#1	89.8(2)
O(21)-Mo(5)-Mo(6)	49.06(15)	O(175)-Mo(17)-O(5)	85.2(2)	O(112)-Mo(32)-O(60)	72.4(2)	O(86)-Co(6)-O(110)	74.4(3)
O(21)-Mo(5)-O(56)	86.9(2)	O(175)-Mo(17)-O(19)	151.6(2)	O(112)-Mo(32)-O(105)	82.4(2)	O(86)-Co(6)-O(125)	82.3(2)
O(21)-Mo(5)-O(58)	82.4(2)	O(175)-Mo(17)-O(48)	84.5(2)	O(134)-Mo(32)-O(60)	169.4(3)	O(86)-Co(6)-O(180)	94.0(2)

O(21)-Mo(5)-O(72)#1	161.1(2)	O(175)-Mo(17)-O(70)	98.8(2)	O(134)-Mo(32)-O(105)	92.6(3)	O(96)-Co(6)-O(86)	103.8(2)
O(36)-Mo(5)-Mo(6)	48.27(16)	O(75)-Mo(18)-O(9)	71.50(19)	O(134)-Mo(32)-O(112)	99.6(3)	O(96)-Co(6)-O(110)	161.0(2)
O(36)-Mo(5)-O(21)	96.2(2)	O(82)-Mo(18)-O(9)	72.48(19)	O(134)-Mo(32)-O(163)	99.4(3)	O(96)-Co(6)-O(125)	86.1(2)
O(36)-Mo(5)-O(56)	165.6(2)	O(82)-Mo(18)-O(75)	80.7(2)	O(134)-Mo(32)-O(174)	102.1(3)	O(96)-Co(6)-O(180)	89.2(2)
O(36)-Mo(5)-O(58)	85.8(2)	O(94)-Mo(18)-O(9)	86.4(2)	O(163)-Mo(32)-O(60)	87.9(2)	O(110)-Co(6)-O(125)	112.1(2)
O(36)-Mo(5)-O(72)#1	88.4(2)	O(94)-Mo(18)-O(75)	157.7(2)	O(163)-Mo(32)-O(105)	167.5(3)	O(110)-Co(6)-O(180)	72.2(2)
O(56)-Mo(5)-Mo(6)	135.92(14)	O(94)-Mo(18)-O(82)	89.8(2)	O(163)-Mo(32)-O(112)	92.0(3)	O(127)-Co(6)-O(86)	157.2(2)
O(56)-Mo(5)-O(58)	80.65(19)	O(94)-Mo(18)-O(104)	94.0(2)	O(163)-Mo(32)-O(174)	91.3(3)	O(127)-Co(6)-O(96)	97.4(2)
O(58)-Mo(5)-Mo(6)	89.58(13)	O(104)-Mo(18)-O(9)	85.6(2)	O(174)-Mo(32)-O(60)	85.2(2)	O(127)-Co(6)-O(110)	88.2(2)
O(72)#1-Mo(5)-Mo(6)	136.21(15)	O(104)-Mo(18)-O(75)	87.7(2)	O(174)-Mo(32)-O(105)	89.7(2)	O(127)-Co(6)-O(125)	91.0(3)
O(72)#1-Mo(5)-O(56)	84.3(2)	O(104)-Mo(18)-O(82)	157.5(2)	O(174)-Mo(32)-O(112)	157.2(2)	O(127)-Co(6)-O(180)	94.6(3)
O(72)#1-Mo(5)-O(58)	79.7(2)	O(130)-Mo(18)-O(9)	166.3(2)	O(99)-Mo(33)-O(83)	71.8(2)	O(180)-Co(6)-O(125)	173.1(2)
O(120)-Mo(5)-Mo(6)	98.80(18)	O(130)-Mo(18)-O(75)	98.5(3)	O(99)-Mo(33)-O(123)	79.2(2)	O(8)-P(1)-O(11)	108.9(3)
O(120)-Mo(5)-O(21)	101.2(3)	O(130)-Mo(18)-O(82)	97.0(3)	O(105)-Mo(33)-O(83)	86.3(2)	O(8)-P(1)-O(17)	110.8(3)
O(120)-Mo(5)-O(36)	101.6(2)	O(130)-Mo(18)-O(94)	102.7(3)	O(105)-Mo(33)-O(99)	89.7(3)	O(8)-P(1)-O(52)	109.2(3)
O(120)-Mo(5)-O(56)	91.5(2)	O(130)-Mo(18)-O(104)	103.7(3)	O(105)-Mo(33)-O(123)	157.7(3)	O(17)-P(1)-O(11)	111.1(3)
O(120)-Mo(5)-O(58)	171.3(2)	O(28)-Mo(19)-O(12)	87.1(2)	O(105)-Mo(33)-O(176)	95.3(3)	O(17)-P(1)-O(52)	106.5(3)
O(120)-Mo(5)-O(72)#1	95.8(2)	O(28)-Mo(19)-O(51)	92.3(2)	O(123)-Mo(33)-O(83)	71.9(2)	O(52)-P(1)-O(11)	110.2(3)
O(21)-Mo(6)-Mo(5)	48.63(16)	O(28)-Mo(19)-O(53)	159.1(2)	O(171)-Mo(33)-O(83)	165.4(3)	O(1)-P(2)-O(9)	109.9(3)
O(21)-Mo(6)-O(32)	81.0(2)	O(28)-Mo(19)-O(94)	90.5(2)	O(171)-Mo(33)-O(99)	97.3(3)	O(1)-P(2)-O(12)	111.3(3)
O(21)-Mo(6)-O(49)	87.9(2)	O(51)-Mo(19)-O(12)	85.5(2)	O(171)-Mo(33)-O(105)	103.7(3)	O(2)-P(2)-O(1)	109.2(3)
O(32)-Mo(6)-Mo(5)	87.65(13)	O(51)-Mo(19)-O(53)	89.1(2)	O(171)-Mo(33)-O(123)	96.9(3)	O(2)-P(2)-O(9)	108.8(3)
O(34)-Mo(6)-Mo(5)	137.51(17)	O(51)-Mo(19)-O(94)	164.7(2)	O(171)-Mo(33)-O(176)	103.3(3)	O(2)-P(2)-O(12)	110.5(3)
O(34)-Mo(6)-O(21)	155.7(2)	O(53)-Mo(19)-O(12)	72.2(2)	O(176)-Mo(33)-O(83)	86.0(2)	O(12)-P(2)-O(9)	107.1(3)
O(34)-Mo(6)-O(32)	76.3(2)	O(94)-Mo(19)-O(12)	79.6(2)	O(176)-Mo(33)-O(99)	157.0(2)	O(10)-P(3)-O(15)	111.5(3)
O(34)-Mo(6)-O(36)	90.6(2)	O(94)-Mo(19)-O(53)	83.0(2)	O(176)-Mo(33)-O(123)	88.1(3)	O(10)-P(3)-O(29)	109.8(3)

O(34)-Mo(6)-O(49)	78.4(2)	O(109)-Mo(19)-O(12)	168.5(2)	O(69)-Mo(34)-Mo(25)	48.63(16)	O(10)-P(3)-O(65)	108.1(3)
O(36)-Mo(6)-Mo(5)	48.42(15)	O(109)-Mo(19)-O(28)	103.2(2)	O(69)-Mo(34)-O(96)	96.3(2)	O(29)-P(3)-O(15)	108.9(3)
O(36)-Mo(6)-O(21)	95.9(2)	O(109)-Mo(19)-O(51)	99.0(3)	O(69)-Mo(34)-O(119)	85.2(2)	O(29)-P(3)-O(65)	109.0(3)
O(36)-Mo(6)-O(32)	84.6(2)	O(109)-Mo(19)-O(53)	97.2(3)	O(69)-Mo(34)-O(153)#1	87.7(2)	O(65)-P(3)-O(15)	109.6(3)
O(36)-Mo(6)-O(49)	159.7(2)	O(109)-Mo(19)-O(94)	95.1(3)	O(69)-Mo(34)-O(164)	165.7(3)	O(3)-P(4)-O(4)	108.7(3)
O(49)-Mo(6)-Mo(5)	135.78(15)	O(42)-Mo(20)-O(23)	80.6(2)	O(96)-Mo(34)-Mo(25)	48.86(17)	O(3)-P(4)-O(31)	110.2(3)
O(49)-Mo(6)-O(32)	76.2(2)	O(92)-Mo(20)-O(23)	85.5(2)	O(96)-Mo(34)-O(119)	82.7(2)	O(3)-P(4)-O(48)	110.0(3)
O(89)-Mo(6)-Mo(5)	98.87(19)	O(92)-Mo(20)-O(42)	94.6(2)	O(96)-Mo(34)-O(153)#1	161.4(3)	O(4)-P(4)-O(31)	111.7(3)
O(89)-Mo(6)-O(21)	99.3(2)	O(92)-Mo(20)-O(106)	167.4(2)	O(96)-Mo(34)-O(164)	86.3(2)	O(4)-P(4)-O(48)	109.3(3)
O(89)-Mo(6)-O(32)	171.6(2)	O(92)-Mo(20)-O(174)	93.3(2)	O(119)-Mo(34)-Mo(25)	89.68(16)	O(31)-P(4)-O(48)	106.8(3)
O(89)-Mo(6)-O(34)	101.9(2)	O(106)-Mo(20)-O(23)	82.1(2)	O(144)-Mo(34)-Mo(25)	98.2(2)	O(13)-P(5)-O(26)	108.8(3)
O(89)-Mo(6)-O(36)	103.6(3)	O(106)-Mo(20)-O(42)	81.0(2)	O(144)-Mo(34)-O(69)	101.3(3)	O(13)-P(5)-O(27)	109.0(3)
O(89)-Mo(6)-O(49)	95.4(2)	O(173)-Mo(20)-O(23)	171.2(2)	O(144)-Mo(34)-O(96)	101.1(3)	O(13)-P(5)-O(44)	109.5(3)
O(18)-Mo(7)-Mo(2)	47.81(15)	O(173)-Mo(20)-O(42)	91.9(2)	O(144)-Mo(34)-O(119)	172.0(3)	O(27)-P(5)-O(26)	110.7(3)
O(18)-Mo(7)-O(24)	95.5(2)	O(173)-Mo(20)-O(92)	99.9(3)	O(144)-Mo(34)-O(153)#1	95.9(3)	O(44)-P(5)-O(26)	109.1(3)
O(18)-Mo(7)-O(44)	84.7(2)	O(173)-Mo(20)-O(106)	92.2(3)	O(144)-Mo(34)-O(164)	92.0(3)	O(44)-P(5)-O(27)	109.8(3)
O(18)-Mo(7)-O(71)	165.5(2)	O(173)-Mo(20)-O(174)	101.1(3)	O(153)#1-Mo(34)-Mo(25)	135.89(17)	O(32)-P(6)-O(37)	108.8(3)
O(18)-Mo(7)-O(162)	89.4(2)	O(174)-Mo(20)-O(23)	85.4(2)	O(153)#1-Mo(34)-O(119)	79.5(2)	O(32)-P(6)-O(42)	110.0(3)
O(24)-Mo(7)-Mo(2)	48.88(15)	O(174)-Mo(20)-O(42)	163.3(2)	O(153)#1-Mo(34)-O(164)	85.7(2)	O(42)-P(6)-O(37)	110.4(3)
O(24)-Mo(7)-O(44)	81.8(2)	O(174)-Mo(20)-O(106)	88.1(2)	O(164)-Mo(34)-Mo(25)	135.06(18)	O(58)-P(6)-O(32)	109.4(3)
O(24)-Mo(7)-O(71)	87.3(2)	O(33)-Mo(21)-O(12)	86.8(2)	O(164)-Mo(34)-O(119)	81.1(2)	O(58)-P(6)-O(37)	108.8(3)
O(24)-Mo(7)-O(162)	162.8(2)	O(33)-Mo(21)-O(53)	159.1(2)	O(135)-Mo(35)-O(101)	86.0(2)	O(58)-P(6)-O(42)	109.4(3)
O(44)-Mo(7)-Mo(2)	88.57(13)	O(33)-Mo(21)-O(104)	90.5(2)	O(135)-Mo(35)-O(137)	157.5(3)	O(56)-P(7)-O(84)	110.7(3)
O(71)-Mo(7)-Mo(2)	136.16(15)	O(33)-Mo(21)-O(161)	91.7(2)	O(135)-Mo(35)-O(166)	87.9(3)	O(56)-P(7)-O(91)	103.4(3)
O(71)-Mo(7)-O(44)	81.6(2)	O(53)-Mo(21)-O(12)	72.4(2)	O(137)-Mo(35)-O(101)	72.0(2)	O(63)-P(7)-O(56)	113.9(3)
O(95)-Mo(7)-Mo(2)	97.68(18)	O(104)-Mo(21)-O(12)	80.0(2)	O(137)-Mo(35)-O(166)	83.5(3)	O(63)-P(7)-O(84)	111.7(3)

O(95)-Mo(7)-O(18)	100.9(2)	O(104)-Mo(21)-O(53)	84.4(2)	O(147)-Mo(35)-O(101)	87.5(2)	O(63)-P(7)-O(91)	109.2(3)
O(95)-Mo(7)-O(24)	100.8(2)	O(129)-Mo(21)-O(12)	168.8(3)	O(147)-Mo(35)-O(135)	92.4(3)	O(84)-P(7)-O(91)	107.4(3)
O(95)-Mo(7)-O(44)	173.4(2)	O(129)-Mo(21)-O(33)	102.2(3)	O(147)-Mo(35)-O(137)	91.3(3)	O(43)-P(8)-O(140)	105.6(3)
O(95)-Mo(7)-O(71)	92.5(2)	O(129)-Mo(21)-O(53)	98.3(3)	O(147)-Mo(35)-O(166)	166.4(2)	O(72)-P(8)-O(43)	110.5(3)
O(95)-Mo(7)-O(162)	94.4(2)	O(129)-Mo(21)-O(104)	93.1(3)	O(151)-Mo(35)-O(101)	168.8(3)	O(72)-P(8)-O(78)	112.9(3)
O(162)-Mo(7)-Mo(2)	136.98(16)	O(129)-Mo(21)-O(161)	99.7(3)	O(151)-Mo(35)-O(135)	102.0(3)	O(72)-P(8)-O(140)	106.3(3)
O(162)-Mo(7)-O(44)	82.2(2)	O(161)-Mo(21)-O(12)	86.4(2)	O(151)-Mo(35)-O(137)	99.2(3)	O(78)-P(8)-O(43)	112.8(3)
O(162)-Mo(7)-O(71)	84.0(2)	O(161)-Mo(21)-O(53)	88.7(2)	O(151)-Mo(35)-O(147)	99.9(3)	O(78)-P(8)-O(140)	108.2(3)
O(17)-Mo(8)-O(3)	77.50(19)	O(161)-Mo(21)-O(104)	166.2(2)	O(151)-Mo(35)-O(166)	93.4(3)	O(14)-P(9)-O(5)	109.3(3)
O(17)-Mo(8)-O(45)	82.8(2)	O(51)-Mo(22)-O(31)	86.6(2)	O(166)-Mo(35)-O(101)	79.0(2)	O(14)-P(9)-O(25)	109.8(3)
O(38)-Mo(8)-O(3)	86.5(2)	O(51)-Mo(22)-O(66)	90.4(2)	O(102)-Mo(36)-O(60)	85.5(2)	O(14)-P(9)-O(40)	109.3(3)
O(38)-Mo(8)-O(17)	92.6(2)	O(51)-Mo(22)-O(73)	165.7(2)	O(102)-Mo(36)-O(112)	157.1(2)	O(25)-P(9)-O(5)	108.7(3)
O(38)-Mo(8)-O(45)	168.3(2)	O(51)-Mo(22)-O(88)	92.4(2)	O(102)-Mo(36)-O(176)	88.9(3)	O(25)-P(9)-O(40)	109.9(3)
O(38)-Mo(8)-O(66)	94.6(2)	O(66)-Mo(22)-O(31)	86.0(2)	O(112)-Mo(36)-O(60)	71.9(2)	O(40)-P(9)-O(5)	109.8(3)
O(45)-Mo(8)-O(3)	82.0(2)	O(66)-Mo(22)-O(73)	88.1(2)	O(112)-Mo(36)-O(176)	83.3(3)	O(46)-P(10)-O(54)	113.9(3)
O(66)-Mo(8)-O(3)	85.0(2)	O(66)-Mo(22)-O(88)	157.6(2)	O(145)-Mo(36)-O(60)	169.8(3)	O(46)-P(10)-O(67)	112.1(3)
O(66)-Mo(8)-O(17)	160.6(2)	O(73)-Mo(22)-O(31)	79.1(2)	O(145)-Mo(36)-O(102)	102.4(3)	O(46)-P(10)-O(79)	105.1(3)
O(66)-Mo(8)-O(45)	86.5(2)	O(88)-Mo(22)-O(31)	72.1(2)	O(145)-Mo(36)-O(112)	99.6(3)	O(54)-P(10)-O(67)	110.7(3)
O(108)-Mo(8)-O(3)	170.6(2)	O(88)-Mo(22)-O(73)	83.8(2)	O(145)-Mo(36)-O(147)	100.4(3)	O(54)-P(10)-O(79)	107.6(3)
O(108)-Mo(8)-O(17)	95.6(2)	O(172)-Mo(22)-O(31)	169.0(2)	O(145)-Mo(36)-O(176)	93.7(3)	O(67)-P(10)-O(79)	107.0(3)
O(108)-Mo(8)-O(38)	100.2(2)	O(172)-Mo(22)-O(51)	101.5(3)	O(147)-Mo(36)-O(60)	85.6(2)	O(20)-P(11)-O(23)	108.7(3)
O(108)-Mo(8)-O(45)	90.9(2)	O(172)-Mo(22)-O(66)	101.3(3)	O(147)-Mo(36)-O(102)	91.6(3)	O(20)-P(11)-O(60)	110.6(3)
O(108)-Mo(8)-O(66)	100.7(2)	O(172)-Mo(22)-O(73)	92.8(3)	O(147)-Mo(36)-O(112)	90.8(3)	O(20)-P(11)-O(83)	109.0(3)
O(11)-Mo(9)-O(48)	82.28(18)	O(172)-Mo(22)-O(88)	99.9(3)	O(147)-Mo(36)-O(176)	165.5(3)	O(23)-P(11)-O(60)	111.3(3)
O(19)-Mo(9)-O(11)	76.5(2)	O(55)-Mo(23)-O(48)	72.13(19)	O(176)-Mo(36)-O(60)	79.9(2)	O(23)-P(11)-O(83)	109.9(3)
O(19)-Mo(9)-O(48)	72.9(2)	O(70)-Mo(23)-O(48)	71.83(19)	O(86)-Mo(37)-O(90)	83.6(2)	O(60)-P(11)-O(83)	107.1(3)

O(45)-Mo(9)-O(11)	83.9(2)	O(70)-Mo(23)-O(55)	79.7(2)	O(110)-Mo(37)-O(86)	75.9(2)	O(49)-P(12)-O(57)	110.2(3)
O(45)-Mo(9)-O(19)	151.9(2)	O(73)-Mo(23)-O(48)	85.6(2)	O(110)-Mo(37)-O(90)	72.0(2)	O(49)-P(12)-O(62)	108.6(3)
O(45)-Mo(9)-O(48)	84.8(2)	O(73)-Mo(23)-O(55)	88.5(2)	O(136)-Mo(37)-O(86)	82.8(3)	O(49)-P(12)-O(85)	108.9(3)
O(45)-Mo(9)-O(55)	98.9(2)	O(73)-Mo(23)-O(70)	156.8(2)	O(136)-Mo(37)-O(90)	84.2(2)	O(57)-P(12)-O(62)	111.6(3)
O(55)-Mo(9)-O(11)	157.4(2)	O(73)-Mo(23)-O(87)	95.4(2)	O(136)-Mo(37)-O(110)	149.4(3)	O(57)-P(12)-O(85)	107.1(3)
O(55)-Mo(9)-O(19)	92.0(2)	O(87)-Mo(23)-O(48)	85.3(2)	O(136)-Mo(37)-O(139)	100.1(3)	O(85)-P(12)-O(62)	110.3(3)
O(55)-Mo(9)-O(48)	75.7(2)	O(87)-Mo(23)-O(55)	156.8(2)	O(139)-Mo(37)-O(86)	158.0(3)	O(71)-P(13)-O(81)	110.6(3)
O(113)-Mo(9)-O(11)	98.4(2)	O(87)-Mo(23)-O(70)	88.2(2)	O(139)-Mo(37)-O(90)	75.1(2)	O(71)-P(13)-O(159)	106.3(3)
O(113)-Mo(9)-O(19)	99.6(2)	O(107)-Mo(23)-O(48)	165.4(2)	O(139)-Mo(37)-O(110)	92.1(3)	O(80)-P(13)-O(71)	114.3(3)
O(113)-Mo(9)-O(45)	103.1(3)	O(107)-Mo(23)-O(55)	97.2(3)	O(148)-Mo(37)-O(86)	97.3(3)	O(80)-P(13)-O(81)	111.4(3)
O(113)-Mo(9)-O(48)	172.1(2)	O(107)-Mo(23)-O(70)	96.8(3)	O(148)-Mo(37)-O(90)	172.5(3)	O(80)-P(13)-O(159)	107.3(3)
O(113)-Mo(9)-O(55)	102.7(3)	O(107)-Mo(23)-O(73)	104.5(3)	O(148)-Mo(37)-O(110)	101.0(3)	O(81)-P(13)-O(159)	106.3(3)
O(27)-Mo(10)-O(1)	81.70(19)	O(107)-Mo(23)-O(87)	103.9(3)	O(148)-Mo(37)-O(136)	103.2(3)	O(61)-P(14)-O(153)	112.4(3)
O(33)-Mo(10)-O(1)	84.8(2)	O(37)-Mo(24)-O(83)	85.11(19)	O(148)-Mo(37)-O(139)	103.2(3)	O(61)-P(14)-O(157)	107.8(3)
O(33)-Mo(10)-O(27)	163.7(2)	O(99)-Mo(24)-O(37)	159.6(2)	O(125)#1-Mo(38)-Mo(38)	48.99(17)	O(61)-P(14)-O(162)	113.5(3)
O(33)-Mo(10)-O(47)	88.4(2)	O(99)-Mo(24)-O(83)	75.4(2)	O(125)-Mo(38)-Mo(38)#1	49.0(2)	O(153)-P(14)-O(157)	106.2(4)
O(33)-Mo(10)-O(64)	92.8(2)	O(99)-Mo(24)-O(111)	92.0(3)	O(125)-Mo(38)-O(125)#1	98.0(2)	O(153)-P(14)-O(162)	109.8(3)
O(47)-Mo(10)-O(1)	82.6(2)	O(106)-Mo(24)-O(37)	84.6(2)	O(125)-Mo(38)-O(131)#1	154.4(2)	O(162)-P(14)-O(157)	106.7(4)
O(47)-Mo(10)-O(27)	80.9(2)	O(106)-Mo(24)-O(83)	82.8(2)	O(125)#1-Mo(38)-O(131)#	86.0(3)	O(39)-P(15)-O(59)	108.9(3)
O(64)-Mo(10)-O(1)	83.9(2)	O(106)-Mo(24)-O(99)	98.5(3)	O(125)-Mo(38)-O(156)	69.31(19)	O(39)-P(15)-O(90)	109.9(3)
O(64)-Mo(10)-O(27)	94.8(2)	O(106)-Mo(24)-O(111)	149.8(2)	O(125)#1-Mo(38)-O(156)	69.30(18)	O(39)-P(15)-O(101)	110.8(3)
O(64)-Mo(10)-O(47)	166.2(2)	O(111)-Mo(24)-O(37)	76.3(2)	O(125)#1-Mo(38)-O(165)	147.7(2)	O(59)-P(15)-O(90)	109.2(3)
O(115)-Mo(10)-O(1)	174.2(2)	O(111)-Mo(24)-O(83)	72.5(2)	O(125)-Mo(38)-O(165)	87.7(3)	O(101)-P(15)-O(59)	111.1(4)
O(115)-Mo(10)-O(27)	92.6(2)	O(152)-Mo(24)-O(37)	97.3(2)	O(131)#1-Mo(38)-Mo(38)	130.2(2)	O(101)-P(15)-O(90)	107.0(3)
O(115)-Mo(10)-O(33)	100.7(3)	O(152)-Mo(24)-O(83)	173.4(3)	O(131)#1-Mo(38)-O(156)	88.9(2)	O(93)-P(16)-O(180)	109.9(3)
O(115)-Mo(10)-O(47)	95.7(3)	O(152)-Mo(24)-O(99)	101.4(3)	O(131)#1-Mo(38)-O(165)	76.2(3)	O(119)-P(16)-O(93)	110.0(4)

O(115)-Mo(10)-O(64)	97.5(3)	O(152)-Mo(24)-O(106)	103.5(3)	O(156)-Mo(38)-Mo(38)#1	58.87(11)	O(119)-P(16)-O(180)	108.9(3)
O(7)-Mo(11)-Mo(11)#1	48.80(15)	O(152)-Mo(24)-O(111)	102.0(3)	O(158)-Mo(38)-Mo(38)#1	108.1(2)	O(169)-P(16)-O(93)	109.9(3)
O(7)#1-Mo(11)-Mo(11)#1	48.60(15)	O(34)-Mo(25)-Mo(34)	137.60(17)	O(158)-Mo(38)-O(125)	101.4(3)	O(169)-P(16)-O(119)	109.4(3)
O(7)-Mo(11)-O(7)#1	97.4(2)	O(34)-Mo(25)-O(69)	90.7(2)	O(158)-Mo(38)-O(125)#1	104.0(3)	O(169)-P(16)-O(180)	108.8(4)
O(7)-Mo(11)-O(52)	86.6(2)	O(34)-Mo(25)-O(96)	155.6(2)	O(158)-Mo(38)-O(131)#1	102.2(3)	O(97)-P(17)-O(86)	111.6(4)
O(7)#1-Mo(11)-O(52)	153.2(2)	O(34)-Mo(25)-O(169)	76.7(2)	O(158)-Mo(38)-O(156)	166.9(3)	O(97)-P(17)-O(131)	106.7(4)
O(7)#1-Mo(11)-O(67)#1	88.1(2)	O(34)-Mo(25)-O(179)	78.2(2)	O(158)-Mo(38)-O(165)	106.0(3)	O(97)-P(17)-O(179)	110.7(3)
O(7)-Mo(11)-O(67)#1	147.4(2)	O(69)-Mo(25)-Mo(34)	48.23(17)	O(165)-Mo(38)-Mo(38)#1	128.81(18)	O(131)-P(17)-O(86)	110.4(4)
O(52)-Mo(11)-Mo(11)#1	129.98(15)	O(69)-Mo(25)-O(96)	96.1(2)	O(165)-Mo(38)-O(156)	83.4(2)	O(179)-P(17)-O(86)	108.2(3)
O(52)-Mo(11)-O(67)#1	75.2(2)	O(69)-Mo(25)-O(169)	83.7(2)	O(116)-Mo(39)-O(90)	71.5(2)	O(179)-P(17)-O(131)	109.1(3)
O(67)#1-Mo(11)-Mo(11)#	128.65(15)	O(69)-Mo(25)-O(179)	158.5(2)	O(116)-Mo(39)-O(139)	77.9(3)	O(127)-P(18)-O(142)	108.4(4)
O(124)-Mo(11)-Mo(11)#1	108.7(2)	O(96)-Mo(25)-Mo(34)	49.11(17)	O(126)-Mo(39)-O(90)	86.0(2)	O(127)-P(18)-O(164)	113.5(4)
O(124)-Mo(11)-O(7)	104.6(2)	O(96)-Mo(25)-O(169)	80.8(2)	O(126)-Mo(39)-O(116)	90.5(3)	O(127)-P(18)-O(165)	112.2(4)
O(124)-Mo(11)-O(7)#1	101.6(2)	O(96)-Mo(25)-O(179)	87.3(2)	O(126)-Mo(39)-O(139)	157.1(2)	O(164)-P(18)-O(142)	104.8(4)
O(124)-Mo(11)-O(52)	103.0(3)	O(133)-Mo(25)-Mo(34)	99.3(2)	O(139)-Mo(39)-O(90)	71.6(2)	O(164)-P(18)-O(165)	111.7(4)
O(124)-Mo(11)-O(67)#1	105.7(2)	O(133)-Mo(25)-O(34)	101.3(3)	O(166)-Mo(39)-O(90)	85.6(2)	O(165)-P(18)-O(142)	105.6(4)

Symmetry code: #1, -x+1,y,-z+3/2

Table S3. The bond length (Å) range in compound **1**.

Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)	Bond	Length (Å)
Pb(1)-O(8)	2.666(5)	Mo(13)-O(170)	2.506(6)	Mo(28)-O(178)	2.019(6)	Co(3)-O(160)	2.098(7)
Pb(1)-O(13)	2.484(5)	Mo(14)-O(9)	2.433(5)	Mo(29)-O(101)	2.277(6)	Co(4)-O(21)	2.069(5)
Pb(1)-O(14)	2.485(5)	Mo(14)-O(15)	2.156(5)	Mo(29)-O(103)	1.894(6)	Co(4)-O(30)	2.170(6)
Pb(1)-O(22)	2.474(5)	Mo(14)-O(35)	1.813(5)	Mo(29)-O(126)	2.066(6)	Co(4)-O(37)	2.158(6)
Pb(1)-O(29)	2.681(5)	Mo(14)-O(41)	1.948(5)	Mo(29)-O(137)	1.954(6)	Co(4)-O(62)	2.055(5)
Pb(2)-O(32)	2.472(5)	Mo(14)-O(68)	1.686(5)	Mo(29)-O(150)	1.678(6)	Co(4)-O(63)	1.988(5)
Pb(2)-O(34)	2.477(5)	Mo(14)-O(82)	1.825(5)	Mo(29)-O(163)	1.872(6)	Co(4)-O(111)	2.157(5)
Pb(2)-O(49)	2.705(6)	Mo(15)-O(4)	2.144(5)	Mo(30)-O(39)	2.141(6)	Co(5)-O(36)	2.080(6)
Pb(2)-O(169)	2.493(6)	Mo(15)-O(40)	2.075(5)	Mo(30)-O(92)	1.889(6)	Co(5)-O(61)#1	2.150(6)
Pb(2)-O(179)	2.673(6)	Mo(15)-O(64)	1.856(5)	Mo(30)-O(93)	2.087(6)	Co(5)-O(69)	2.091(5)
Mo(1)-Mo(3)	2.6095(9)	Mo(15)-O(117)	1.687(5)	Mo(30)-O(103)	1.878(6)	Co(5)-O(78)#1	2.167(5)
Mo(1)-O(6)	1.991(5)	Mo(15)-O(167)	1.873(6)	Mo(30)-O(146)	1.679(7)	Co(5)-O(122)	1.988(7)
Mo(1)-O(8)	2.154(5)	Mo(15)-O(175)	2.068(5)	Mo(30)-O(149)	2.066(6)	Co(5)-O(132)	2.089(6)
Mo(1)-O(14)	2.275(5)	Mo(16)-O(30)	1.954(5)	Mo(31)-O(59)	2.151(6)	Co(6)-O(86)	2.056(7)
Mo(1)-O(16)	1.944(5)	Mo(16)-O(50)	1.950(5)	Mo(31)-O(97)	2.049(6)	Co(6)-O(96)	2.051(6)
Mo(1)-O(22)	1.918(5)	Mo(16)-O(81)	2.057(5)	Mo(31)-O(98)	1.852(6)	Co(6)-O(110)	2.155(6)
Mo(1)-O(76)	1.685(5)	Mo(16)-O(85)	2.020(6)	Mo(31)-O(135)	1.881(6)	Co(6)-O(125)	2.199(6)
Mo(2)-Mo(7)	2.6058(9)	Mo(16)-O(138)	1.678(6)	Mo(31)-O(136)	2.032(7)	Co(6)-O(127)	2.003(7)
Mo(2)-O(13)	2.254(5)	Mo(16)-O(170)	2.465(6)	Mo(31)-O(155)	1.690(6)	Co(6)-O(180)	2.162(6)
Mo(2)-O(18)	1.942(5)	Mo(17)-O(5)	2.112(5)	Mo(32)-O(60)	2.263(6)	P(1)-O(8)	1.514(5)
Mo(2)-O(22)	1.930(5)	Mo(17)-O(19)	1.999(5)	Mo(32)-O(105)	2.075(6)	P(1)-O(11)	1.551(5)
Mo(2)-O(24)	1.980(5)	Mo(17)-O(48)	2.402(5)	Mo(32)-O(112)	1.968(6)	P(1)-O(17)	1.530(5)
Mo(2)-O(29)	2.151(5)	Mo(17)-O(70)	1.826(5)	Mo(32)-O(134)	1.688(6)	P(1)-O(52)	1.531(5)

Mo(2)-O(77)	1.686(5)	Mo(17)-O(118)	1.695(6)	Mo(32)-O(163)	1.869(6)	P(2)-O(1)	1.522(6)
Mo(3)-O(6)	1.974(5)	Mo(17)-O(175)	1.803(6)	Mo(32)-O(174)	1.888(6)	P(2)-O(2)	1.516(5)
Mo(3)-O(16)	1.962(5)	Mo(18)-O(9)	2.409(5)	Mo(33)-O(83)	2.409(5)	P(2)-O(9)	1.563(5)
Mo(3)-O(25)	2.278(5)	Mo(18)-O(75)	2.031(5)	Mo(33)-O(99)	2.051(6)	P(2)-O(12)	1.538(5)
Mo(3)-O(43)	2.068(5)	Mo(18)-O(82)	2.030(5)	Mo(33)-O(105)	1.789(7)	P(3)-O(10)	1.517(5)
Mo(3)-O(54)	2.106(5)	Mo(18)-O(94)	1.819(5)	Mo(33)-O(123)	2.077(6)	P(3)-O(15)	1.560(5)
Mo(3)-O(114)	1.682(6)	Mo(18)-O(104)	1.840(6)	Mo(33)-O(171)	1.689(6)	P(3)-O(29)	1.518(5)
Mo(4)-O(2)	2.153(5)	Mo(18)-O(130)	1.675(6)	Mo(33)-O(176)	1.812(6)	P(3)-O(65)	1.527(5)
Mo(4)-O(10)	2.042(5)	Mo(19)-O(12)	2.285(5)	Mo(34)-O(69)	1.944(6)	P(4)-O(3)	1.518(5)
Mo(4)-O(28)	1.882(5)	Mo(19)-O(28)	1.882(5)	Mo(34)-O(96)	1.975(6)	P(4)-O(4)	1.527(5)
Mo(4)-O(35)	1.993(5)	Mo(19)-O(51)	1.892(5)	Mo(34)-O(119)	2.282(6)	P(4)-O(31)	1.543(5)
Mo(4)-O(38)	1.913(5)	Mo(19)-O(53)	2.025(5)	Mo(34)-O(144)	1.668(6)	P(4)-O(48)	1.569(5)
Mo(4)-O(74)	1.697(5)	Mo(19)-O(94)	2.017(6)	Mo(34)-O(153)#1	2.068(7)	P(5)-O(13)	1.507(5)
Mo(5)-Mo(6)	2.5980(9)	Mo(19)-O(109)	1.667(6)	Mo(34)-O(164)	2.101(6)	P(5)-O(26)	1.560(6)
Mo(5)-O(21)	1.967(5)	Mo(20)-O(23)	2.147(5)	Mo(35)-O(101)	2.288(6)	P(5)-O(27)	1.535(5)
Mo(5)-O(36)	1.957(5)	Mo(20)-O(42)	2.083(5)	Mo(35)-O(135)	1.889(6)	P(5)-O(44)	1.518(6)
Mo(5)-O(56)	2.110(5)	Mo(20)-O(92)	1.880(6)	Mo(35)-O(137)	1.956(6)	P(6)-O(32)	1.526(5)
Mo(5)-O(58)	2.289(5)	Mo(20)-O(106)	2.040(6)	Mo(35)-O(147)	1.858(6)	P(6)-O(37)	1.558(6)
Mo(5)-O(72)#1	2.077(5)	Mo(20)-O(173)	1.680(6)	Mo(35)-O(151)	1.687(6)	P(6)-O(42)	1.547(6)
Mo(5)-O(120)	1.682(5)	Mo(20)-O(174)	1.885(6)	Mo(35)-O(166)	2.068(7)	P(6)-O(58)	1.524(5)
Mo(6)-O(21)	1.980(5)	Mo(21)-O(12)	2.270(5)	Mo(36)-O(60)	2.294(6)	P(7)-O(56)	1.530(6)
Mo(6)-O(32)	2.253(5)	Mo(21)-O(33)	1.882(6)	Mo(36)-O(102)	1.880(6)	P(7)-O(63)	1.511(5)
Mo(6)-O(34)	1.911(5)	Mo(21)-O(53)	2.036(6)	Mo(36)-O(112)	1.953(6)	P(7)-O(84)	1.541(5)
Mo(6)-O(36)	1.952(5)	Mo(21)-O(104)	2.033(6)	Mo(36)-O(145)	1.681(6)	P(7)-O(91)	1.580(5)
Mo(6)-O(49)	2.148(6)	Mo(21)-O(129)	1.689(5)	Mo(36)-O(147)	1.878(6)	P(8)-O(43)	1.521(5)
Mo(6)-O(89)	1.686(5)	Mo(21)-O(161)	1.884(6)	Mo(36)-O(176)	2.049(6)	P(8)-O(72)	1.510(6)

Mo(7)-O(18)	1.961(5)	Mo(22)-O(31)	2.284(5)	Mo(37)-O(86)	2.160(6)	P(8)-O(78)	1.521(5)
Mo(7)-O(24)	1.971(5)	Mo(22)-O(51)	1.847(5)	Mo(37)-O(90)	2.437(6)	P(8)-O(140)	1.583(6)
Mo(7)-O(44)	2.296(5)	Mo(22)-O(66)	1.904(5)	Mo(37)-O(110)	1.974(7)	P(9)-O(5)	1.564(5)
Mo(7)-O(71)	2.107(5)	Mo(22)-O(73)	2.072(5)	Mo(37)-O(136)	1.792(7)	P(9)-O(14)	1.511(5)
Mo(7)-O(95)	1.683(6)	Mo(22)-O(88)	1.935(6)	Mo(37)-O(139)	1.808(6)	P(9)-O(25)	1.520(6)
Mo(7)-O(162)	2.065(6)	Mo(22)-O(172)	1.678(6)	Mo(37)-O(148)	1.693(6)	P(9)-O(40)	1.545(5)
Mo(8)-O(3)	2.157(5)	Mo(23)-O(48)	2.404(5)	Mo(38)-Mo(38)#1	2.5639(17)	P(10)-O(46)	1.510(6)
Mo(8)-O(17)	2.034(5)	Mo(23)-O(55)	2.041(6)	Mo(38)-O(125)	1.954(6)	P(10)-O(54)	1.529(5)
Mo(8)-O(38)	1.827(5)	Mo(23)-O(70)	2.031(6)	Mo(38)-O(125)#1	1.954(7)	P(10)-O(67)	1.532(6)
Mo(8)-O(45)	2.061(5)	Mo(23)-O(73)	1.799(6)	Mo(38)-O(131)#1	2.000(6)	P(10)-O(79)	1.574(6)
Mo(8)-O(66)	1.874(5)	Mo(23)-O(87)	1.813(6)	Mo(38)-O(156)	2.480(8)	P(11)-O(20)	1.519(6)
Mo(8)-O(108)	1.697(5)	Mo(23)-O(107)	1.690(5)	Mo(38)-O(158)	1.671(6)	P(11)-O(23)	1.526(6)
Mo(9)-O(11)	2.137(5)	Mo(24)-O(37)	2.111(5)	Mo(38)-O(165)	2.067(7)	P(11)-O(60)	1.541(5)
Mo(9)-O(19)	1.977(5)	Mo(24)-O(83)	2.412(5)	Mo(39)-O(90)	2.397(5)	P(11)-O(83)	1.565(6)
Mo(9)-O(45)	1.804(5)	Mo(24)-O(99)	1.826(6)	Mo(39)-O(116)	2.047(7)	P(12)-O(49)	1.517(6)
Mo(9)-O(48)	2.400(5)	Mo(24)-O(106)	1.798(6)	Mo(39)-O(126)	1.807(6)	P(12)-O(57)	1.521(5)
Mo(9)-O(55)	1.829(5)	Mo(24)-O(111)	1.981(6)	Mo(39)-O(139)	2.083(7)	P(12)-O(62)	1.552(6)
Mo(9)-O(113)	1.681(5)	Mo(24)-O(152)	1.687(6)	Mo(39)-O(166)	1.804(7)	P(12)-O(85)	1.534(6)
Mo(10)-O(1)	2.159(5)	Mo(25)-Mo(34)	2.5873(11)	Mo(39)-O(177)	1.681(6)	P(13)-O(71)	1.524(6)
Mo(10)-O(27)	2.081(5)	Mo(25)-O(34)	1.918(6)	Mo(40)-O(90)	2.377(6)	P(13)-O(80)	1.515(6)
Mo(10)-O(33)	1.876(6)	Mo(25)-O(69)	1.956(6)	Mo(40)-O(110)	1.987(7)	P(13)-O(81)	1.534(6)
Mo(10)-O(47)	2.024(5)	Mo(25)-O(96)	1.967(6)	Mo(40)-O(116)	1.840(6)	P(13)-O(159)	1.572(5)
Mo(10)-O(64)	1.916(5)	Mo(25)-O(133)	1.693(6)	Mo(40)-O(149)	1.789(6)	P(14)-O(61)	1.521(6)
Mo(10)-O(115)	1.674(5)	Mo(25)-O(169)	2.281(5)	Mo(40)-O(154)	1.699(7)	P(14)-O(153)	1.533(6)
Mo(11)-Mo(11)#1	2.5704(13)	Mo(25)-O(179)	2.145(6)	Mo(40)-O(180)	2.096(6)	P(14)-O(157)	1.561(7)
Mo(11)-O(7)#1	1.951(5)	Mo(26)-O(31)	2.247(5)	Co(1)-O(5)	2.131(5)	P(14)-O(162)	1.534(6)

Mo(11)-O(7)	1.944(5)	Mo(26)-O(87)	2.095(6)	Co(1)-O(6)	2.048(5)	P(15)-O(39)	1.524(6)
Mo(11)-O(52)	2.013(5)	Mo(26)-O(88)	1.959(6)	Co(1)-O(7)	2.162(5)	P(15)-O(59)	1.538(7)
Mo(11)-O(67)#1	2.054(5)	Mo(26)-O(141)	1.668(6)	Co(1)-O(11)	2.072(5)	P(15)-O(90)	1.573(6)
Mo(11)-O(124)	1.672(5)	Mo(26)-O(161)	1.855(6)	Co(1)-O(19)	2.150(5)	P(15)-O(101)	1.534(6)
Mo(12)-O(9)	2.411(5)	Mo(26)-O(167)	1.897(6)	Co(1)-O(46)	1.980(5)	P(16)-O(93)	1.536(7)
Mo(12)-O(26)	2.098(5)	Mo(27)-O(62)	2.167(5)	Co(2)-O(15)	2.062(5)	P(16)-O(119)	1.520(6)
Mo(12)-O(41)	1.982(5)	Mo(27)-O(83)	2.417(6)	Co(2)-O(24)	2.061(5)	P(16)-O(169)	1.494(6)
Mo(12)-O(47)	1.808(5)	Mo(27)-O(111)	1.953(6)	Co(2)-O(26)	2.173(5)	P(16)-O(180)	1.567(6)
Mo(12)-O(75)	1.817(6)	Mo(27)-O(123)	1.799(6)	Co(2)-O(41)	2.157(5)	P(17)-O(86)	1.546(7)
Mo(12)-O(100)	1.688(5)	Mo(27)-O(168)	1.690(6)	Co(2)-O(50)	2.198(5)	P(17)-O(97)	1.512(7)
Mo(13)-Mo(16)	2.5563(9)	Mo(27)-O(178)	1.820(6)	Co(2)-O(80)	1.961(5)	P(17)-O(131)	1.535(6)
Mo(13)-O(30)	1.959(5)	Mo(28)-O(20)	2.145(6)	Co(3)-O(16)	2.098(5)	P(17)-O(179)	1.526(6)
Mo(13)-O(50)	1.953(5)	Mo(28)-O(57)	2.051(5)	Co(3)-O(18)	2.093(5)	P(18)-O(127)	1.515(6)
Mo(13)-O(65)	2.018(5)	Mo(28)-O(98)	1.875(6)	Co(3)-O(61)	2.145(5)	P(18)-O(142)	1.561(7)
Mo(13)-O(84)	2.062(5)	Mo(28)-O(102)	1.885(6)	Co(3)-O(78)	2.154(5)	P(18)-O(164)	1.527(6)
Mo(13)-O(128)	1.669(6)	Mo(28)-O(143)	1.681(6)	Co(3)-O(121)	2.023(6)	P(18)-O(165)	1.535(7)

Symmetry code: #1, -x+1,y,-z+3/2

Table S4. Selected hydrogen bonding geometry (Å, °) for compound **1**.

D–H···A	D–H	H···A	D···A	D–H···A
N1–H1A···O45	0.88	2.16	2.987	156
N2–H2A···O106	0.88	2.52	3.018	117
N7–H7A···O116	0.88	1.93	2.775	161
N8–H8A···O138	0.88	2.10	2.927	155

Table S5. BVS values for Pb, Mo, and Co atoms in **1.**

Atom	BVS	Atom	BVS	Atom	BVS	Atom	BVS
Pb1	1.545	Mo5	5.131	Mo17	5.973	Mo29	5.895
Pb2	1.529	Mo6	5.433	Mo18	6.022	Mo30	5.781
Co1	2.029	Mo7	5.129	Mo19	5.850	Mo31	5.951
Co2	1.994	Mo8	5.986	Mo20	5.838	Mo32	5.834
Co3	1.959	Mo9	6.025	Mo21	5.726	Mo33	6.027
Co4	1.987	Mo10	5.790	Mo22	5.970	Mo34	5.241
Co5	1.970	Mo11	5.319	Mo23	6.085	Mo35	5.877
Co6	2.009	Mo12	6.065	Mo24	6.040	Mo36	5.918
Mo1	5.368	Mo13	5.246	Mo25	5.371	Mo37	6.034
Mo2	5.396	Mo14	5.999	Mo26	5.949	Mo38	5.290
Mo3	5.143	Mo15	5.868	Mo27	6.028	Mo39	6.049
Mo4	5.811	Mo16	5.259	Mo28	5.924	Mo40	6.012

Table S6. Comparison of POM-based crystalline heterogeneous catalytic systems for methyl phenyl sulfide oxidation.

Catalyst	Time (h)	Conv. (%)	Sel. (%)[a]	Ref.
Compound**1**	1.33	99.1	98.7	This work
$[Co_2L_{0.5}V_4O_{12}]$	4	99	100	S6
$\{Ni_4Se_7V_{10}\}$	1	96.4	100	S7
$[V_8O_{12}(CH_3O)_4(DAC)_4]$	8	90	97.8	S8
$[Co(HDTBA)V_2O_6]$	0.25	98	98	S9
$[Ni(DTBA)_2V_2O_6]$		100	98	
$\{Ru_3(trz)_6As_4W_{42}\}$	1	95.1	99	S10
$\{Ru_3(trz)_6As_2W_{21}\}$		68.2	99	
$\{Mn_6Se_8V_{20}\}$	1	96.2	97.8	S11
$\{Co_6Se_8V_{20}\}$		98.8	97.9	
$\{Zn_6Se_8V_{20}\}$		96.5	97.8	
$[Ni_2(1\text{-vIM})_7][V_4O_{12}]$	4	96.8	98.7	S12
$[Cu_2(1\text{-vIM})_8][V_4O_{12}]$		98.8	96.5	
$[Co(1\text{-vIM})][VO_3]_2$		91.5	98.5	
$[Co_4(1\text{-vIM})_{14}][V_4O_{12}]_2$		98.2	96.8	
$[Co][PMo_6(PABA)_3]_2$	0.33	99.5	98	S13
$[Mn][PMo_6(PABA)_3]_2$		96.3	97.1	
$[Ni][PMo_6(PABA)_3]_2$		98.3	97.6	

$[Zn][PMo_6(PABA)_3]_2$		97.3	97.4	
$[Cu_3(ptz)_4][Co_2Mo_{10}]$	4	99	100	S14
$[Cu(bim)_2]_2[Co_2Mo_{10}]$		98.4	95.2	
$[\{Cu_2(dpdo)_3\}_2\{Co_2Mo_{10}\}]$		94.8	95.1	
$(H_2bpp)_4\{CuCo_4Mo_{20}\}$		96.7	96.3	
$\{[Cu_8(dpyh)_4](\alpha-\gamma\text{-}Mo_8O_{26})\}(\beta\text{-}Mo_8O_{26})$	0.5	99	99	S15

[a]Selectivity to methyl phenyl sulfoxide.

Table S7. Oxidation of methyl phenyl sulfide to methyl phenyl sulfoxide catalyzed by compound **1** under different solvents[a].

Entry	Solvent (3 mL)	Conv. (%)	Sel. (%)[b]
1	EtOH	99.1	98.7
2	MeOH	72.8	>99
3	MeCN	24.3	100
4	1,4-Dioxane	73.4	98.6
5	dichloromethane	50.2	80.2

[a]Reaction conditions: 0.5 mmol of MPS; 0.3 μmol of catalyst; 0.65 mmol of TBHP; reaction temperature 60 °C, reaction time 80 min, and under nitrogen atmosphere. [b]Selectivity to sulfoxides, the byproduct was sulfone.

Table S8. Catalytic oxidation of methyl phenyl sulfide with different catalysts[a].

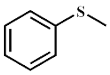
Entry	Catal.	Conv. (%)	Sel. (%)[b]
1	Compound 1	99.1	98.7
2	$Na_2MoO_4{\cdot}2H_2O$	75.1	87.3
3	$CoCl_2{\cdot}6H_2O$	55.4	93.5
4	$Pb(OAc)_2{\cdot}3H_2O$	18.1	99.3
5	biz	16.9	99.5
6	$Na_2MoO_4{\cdot}2H_2O$+ $CoCl_2{\cdot}6H_2O$+ $Pb(OAc)_2{\cdot}3H_2O$+ biz	71.5	86.2

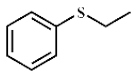
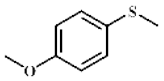
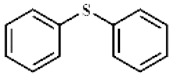
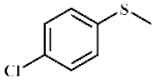
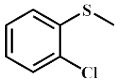
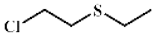
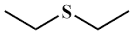
[a]Reaction conditions: 0.5 mmol of sulfide; 0.3 μmol of catalyst; 3 ml of EtOH; 0.65 mmol of TBHP; reaction temperature 60 °C, reaction time 80 min, and under nitrogen atmosphere. [b]Selectivity to sulfoxides, the byproduct was sulfone.

Table S9. ICP-MS analysis of the filtrate after the removal of the catalyst.

Entry	Test element	Element concentration of the test solution (μg/L)
1	Mo	12.483
2	Co	1.872
3	Pb	0.624

Table S10. Selective oxidation of various sulfides to sulfoxide[a].

Entry	Substrate	Temp.(°C)	Time(min)	Conv. (%)	Sel. (%)[b]
1		60	80	99.1	98.7

2		60	80	98.9	90.4
3		60	80	99.1	93.9
4		60	80	93.1	96.8
5		60	80	98.8	96.1
6		60	80	96.7	98.4
7[b]		60	80	99.1	99.0
8		60	80	97.8	98.6

[a]Reaction conditions: 0.5 mmol of sulfide; 0.3 μmol of catalyst; 3 ml of EtOH; 0.65 mmol of TBHP; reaction temperature 60 °C, reaction time 80 min, and under nitrogen atmosphere. [b]Selectivity to sulfoxides, the by product was sulfone.

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