

Supporting Information

Table S1. X-ray crystallographic data for **1-3**.

	1	2	3
formula	H ₁₅₂ Cu ₈ Mo ₃₀ N ₂₀ O ₁₆₉ V ₁₀	H ₁₄₄ Cu ₁₁ Mo ₃₀ N ₁₀ NaO ₁₈₁ V ₉	H ₁₄₅ Cu _{8.5} Mo ₂₃ N _{9.5} Na _{0.5} O _{158.5} V ₉
<i>M_r</i> [g]	7033.34	7239.84	6031.92
crystal system	triclinic	Monoclinic	Orthorhombic
space group	<i>P</i> $\bar{1}$	C2/c	Pnmm
<i>Z</i>	1	4	4
<i>a</i> [Å]	14.7333 (3)	53.884(5)	28.2107(14)
<i>b</i> [Å]	17.2359 (6)	13.9563(11)	23.9375(12)
<i>c</i> [Å]	18.2871 (4)	26.848(2)	26.1899 (13)
α [°]	96.789 (2)°	90	90
β [°]	98.188 (2)°	104.181(2)	90
γ [°]	93.537 (2)°	90	90
<i>V</i> [Å ³]	4549.7 (2)	19575(3)	17685.9 (15)
ρ_{calcd} [g cm ⁻³]	2.567	2.457	2.188
μ [mm ⁻¹]	3.504	3.536	3.120
Reflections collected	15926	17200	15938
Radiation type	MoK α	MoK α	MoK α
<i>R</i> ₁ [<i>I</i> >2 σ (<i>I</i>)] ^[a]	0.0453	0.0663	0.0657
<i>wR</i> ₂ [all data] ^[b]	0.135	0.215	0.1569
GOF on <i>F</i> ²	1.053	1.004	1.061

[a] $R_1 = \sum |F_o| - |F_c| / \sum |F_c|$; [b] $wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$ with $1/w = \sigma^2 F_o^2 + aP^2 + bP$ and $P = F_o^2 + 2F_c^2/3$.

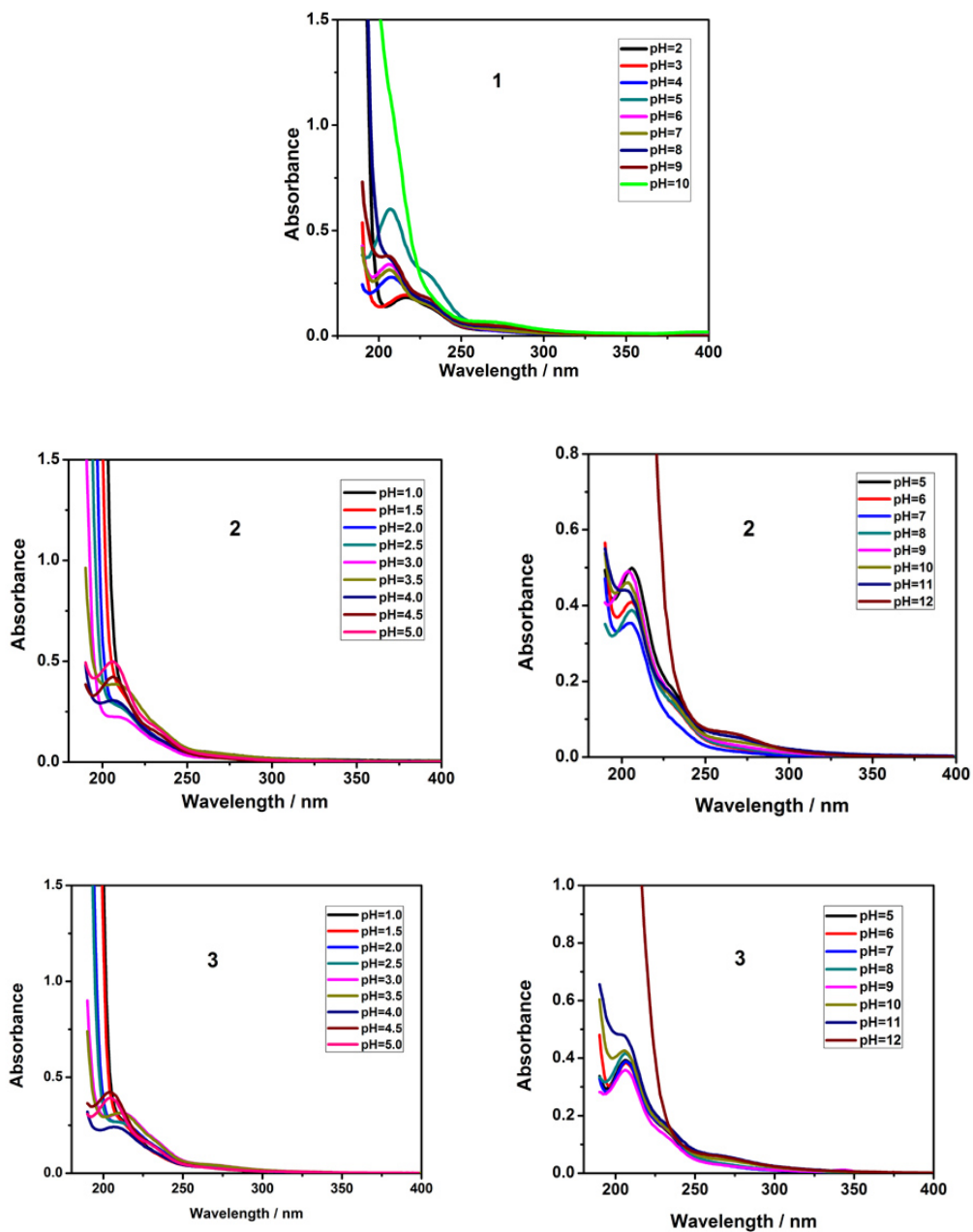
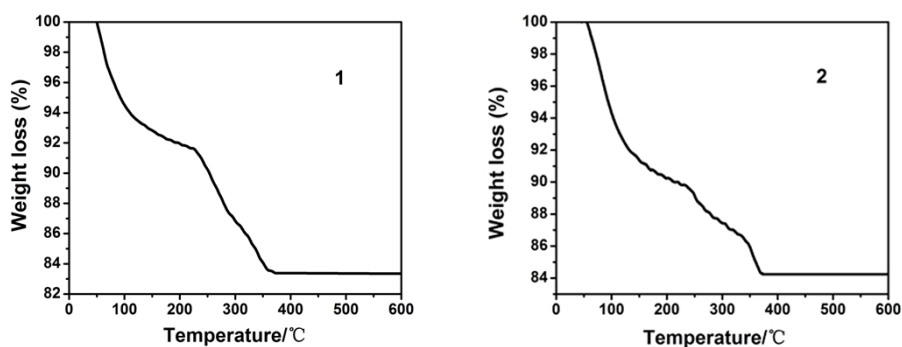


Figure S1. Influence of the pH values on the stability of **1**, **2** and **3** in aqueous solution: (a) The UV spectral evolution in pH=1-5 ; (b) The UV spectral evolution in pH =5-10.



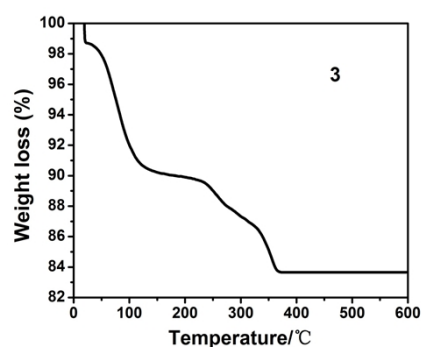


Figure S2. TG curves for compounds 1–3.

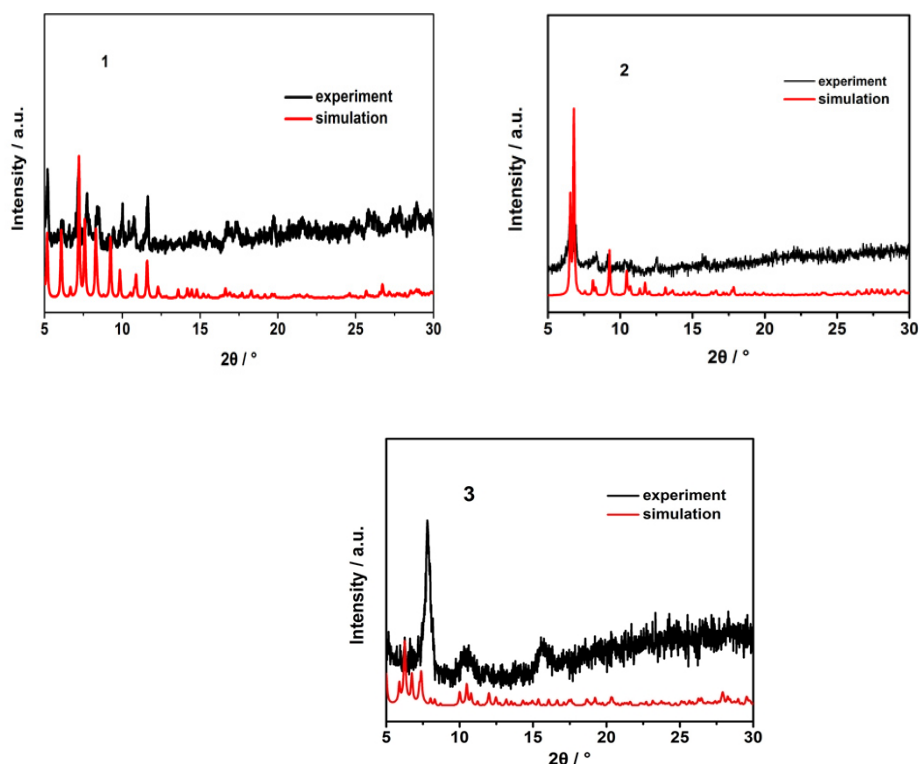


Fig S3. The PXRD pattern and simulated pattern of 1-3.

FT-IR Spectroscopy

The IR spectrum of **1** exhibits very strong bands at 908 and 856 cm^{-1} for characteristics of $\nu(\text{V}=\text{O})$ and $\nu(\text{Mo}=\text{O})$ and strong bands at 796 and 715 cm^{-1} for characteristics of $\nu(\text{M}-\text{O}-\text{M})$ ($\text{M} = \text{Mo}$ or V). Bands at 676 cm^{-1} are likely due to $\nu_{\text{as}}(\text{M}-(\mu_3\text{O}))$ ($\text{M} = \text{Mo}$ or V) mode (Fig. S4, ESI†). The bands at 3432 and 1628 cm^{-1} are ascribed to water molecules, respectively. The band at 3145 cm^{-1} ascribed to the N–H stretching vibration of ammonium ion. The IR spectra of complexes **2–3** are similar to that of compound **1**.

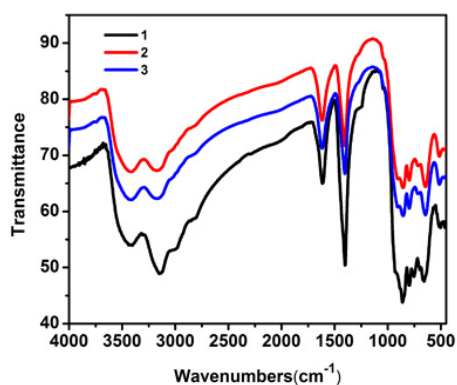


Fig S4. The IR spectra of 1–3.

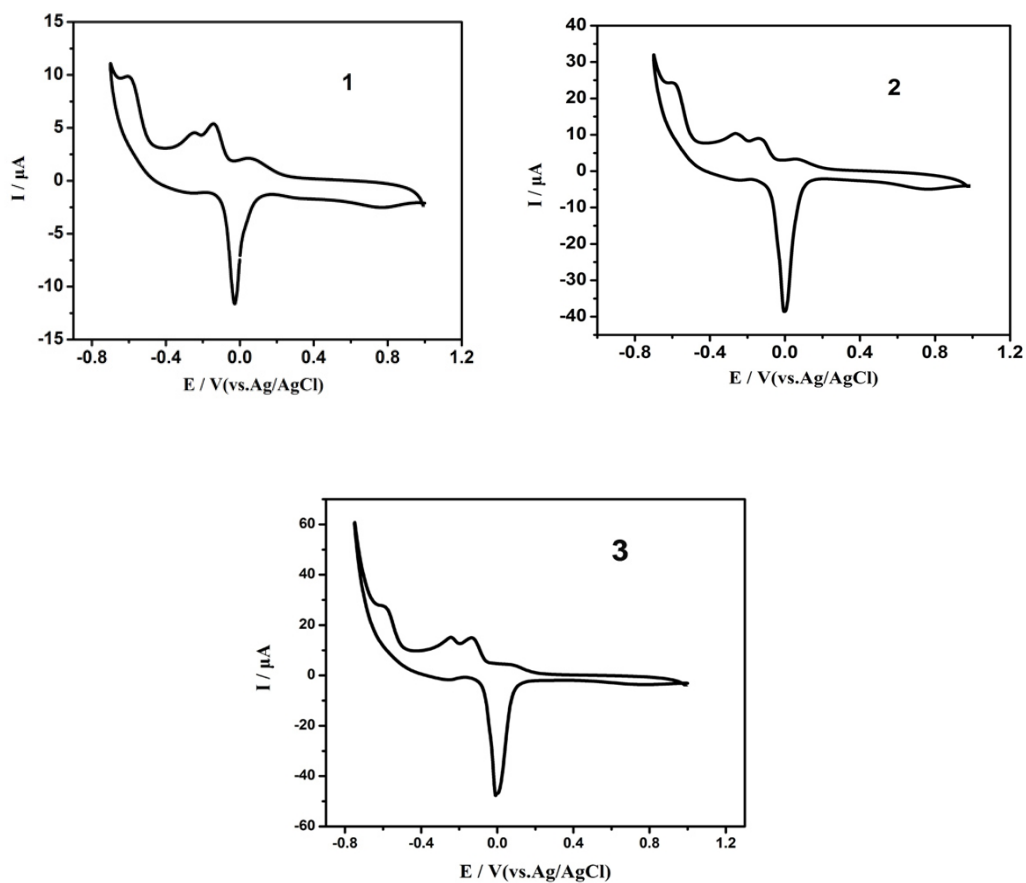


Figure S5. Cyclic voltammograms of compounds 1–3 in 0.4M $\text{CH}_3\text{COONa}+\text{CH}_3\text{COOH}$ buffer solution (pH=4.5) at a scan rate of 10 mV s^{-1}

Table S2. Selected bond lengths [\AA] and bond angles ($^\circ$) for the compound 1.

O(1)-Mo(5)	1.970(5)	Mo(1)-O(5)#1	1.775(5)
O(1)-Mo(3)	1.985(5)	O(6)-Cu(4)-O(14)#1	177.5(2)
O(1)-Mo(12)	2.245(5)	O(6)-Cu(4)-O(5)	90.2(2)

O(2)-Mo(12)	1.948(6)	O(14)#1-Cu(4)-O(5)	92.1(2)
O(2)-Mo(3)	2.197(5)	O(6)-Cu(4)-O(11)	90.7(2)
O(2)-Mo(6)	2.199(5)	O(14)#1-Cu(4)-O(11)	86.9(2)
O(3)-Mo(6)	1.973(5)	O(6)-Cu(4)-O(35)	88.1(2)
O(3)-Mo(2)	1.985(6)	O(14)#1-Cu(4)-O(35)	92.9(2)
O(3)-Mo(12)	2.183(5)	O(5)-Cu(4)-O(35)	92.9(2)
O(4)-Mo(3)	1.677(5)	O(11)-Cu(4)-O(35)	92.0(2)
O(5)-Mo(1)#1	1.775(5)	O(6)-Cu(4)-O(11)#1	91.01(19)
O(5)-Cu(4)	1.988(5)	O(14)#1-Cu(4)-O(11)#1	87.69(19)
O(6)-Mo(3)	1.756(5)	O(5)-Cu(4)-O(11)#1	93.9(2)
O(6)-Cu(4)	1.956(5)	O(11)-Cu(4)-O(11)#1	81.32(19)
O(7)-Mo(1)	1.777(5)	O(35)-Cu(4)-O(11)#1	173.20(18)
O(7)-Cu(3)	1.973(5)	O(38)-V(1)-O(24)	109.0(3)
O(8)-V(2)	1.772(5)	O(38)-V(1)-O(37)	109.4(3)
O(8)-Mo(1)	2.253(5)	O(24)-V(1)-O(37)	109.6(3)
O(8)-Mo(5)	2.350(4)	O(38)-V(1)-O(25)	106.9(3)
O(8)-Mo(2)	2.394(5)	O(24)-V(1)-O(25)	110.9(3)
O(9)-V(2)	1.680(5)	O(37)-V(1)-O(25)	111.0(3)
O(9)-Cu(3)	2.119(5)	O(11)-V(2)-O(9)	108.3(2)
O(9)-Cu(2)	2.285(5)	O(11)-V(2)-O(12)	107.6(3)
O(10)-Mo(4)	1.794(5)	O(9)-V(2)-O(12)	109.0(2)
O(10)-Cu(2)	1.946(5)	O(11)-V(2)-O(8)	109.8(2)
O(11)-V(2)	1.674(5)	O(9)-V(2)-O(8)	107.6(2)
O(11)-Cu(4)	2.017(5)	O(12)-V(2)-O(8)	114.3(2)
O(11)-Cu(4)#1	2.358(5)	O(47)-V(3)-O(15)	105.3(3)
O(12)-V(2)	1.754(5)	O(47)-V(3)-O(17)	110.6(3)
O(12)-Mo(4)	2.284(5)	O(15)-V(3)-O(17)	107.0(3)
O(12)-Mo(3)	2.347(5)	O(47)-V(3)-O(16)	112.4(3)
O(12)-Mo(6)	2.399(5)	O(15)-V(3)-O(16)	106.2(3)
O(14)-Mo(5)	1.761(5)	O(17)-V(3)-O(16)	114.6(2)
O(14)-Cu(4)#1	1.963(5)	O(31)-V(4)-O(57)	105.5(3)
O(15)-V(3)	1.660(5)	O(31)-V(4)-O(21)	105.8(3)
O(15)-Cu(3)	2.065(6)	O(57)-V(4)-O(21)	111.3(3)
O(16)-V(3)	1.815(5)	O(31)-V(4)-O(20)	106.9(3)
O(16)-Mo(15)	2.002(5)	O(57)-V(4)-O(20)	112.3(3)
O(16)-Mo(11)	2.282(5)	O(21)-V(4)-O(20)	114.2(3)
O(17)-V(3)	1.807(5)	O(69)-V(5)-O(70)	100.0(7)
O(17)-Mo(8)	2.009(5)	O(69)-V(5)-O(18)	106.6(4)
O(17)-Mo(9)	2.258(5)	O(70)-V(5)-O(18)	110.5(6)
O(18)-V(5)	1.882(5)	O(69)-V(5)-O(42)	105.5(4)
O(18)-Mo(9)	1.920(5)	O(70)-V(5)-O(42)	112.4(6)
O(18)-Mo(8)	2.127(5)	O(18)-V(5)-O(42)	119.7(3)
O(20)-V(4)	1.825(5)	O(72)-V(6)-O(71)	89.8(12)
O(20)-Mo(14)	1.983(5)	O(72)-V(6)-O(22)	109.0(7)

O(20)-Mo(7)	2.252(5)	O(71)-V(6)-O(22)	114.0(8)
O(21)-V(4)	1.823(5)	O(72)-V(6)-O(43)	112.9(7)
O(21)-Mo(10)	2.006(5)	O(71)-V(6)-O(43)	111.0(9)
O(21)-Mo(13)	2.254(5)	O(22)-V(6)-O(43)	117.0(3)
O(22)-Mo(11)	1.892(6)	O(68)-Cu(2)-O(23)	93.5(2)
O(22)-V(6)	1.898(7)	O(10)-Cu(2)-O(54)	92.3(2)
O(22)-Mo(15)	2.121(6)	O(68)-Cu(2)-O(54)	82.8(2)
O(23)-Mo(10)	1.732(5)	O(23)-Cu(2)-O(54)	173.6(2)
O(23)-Cu(2)	2.064(5)	O(10)-Cu(2)-O(31)	91.2(2)
O(24)-V(1)	1.723(5)	O(68)-Cu(2)-O(31)	96.2(2)
O(24)-Mo(9)	2.327(5)	O(23)-Cu(2)-O(31)	86.0(2)
O(24)-Mo(11)	2.348(5)	O(54)-Cu(2)-O(31)	89.2(2)
O(25)-V(1)	1.733(5)	O(10)-Cu(2)-O(9)	94.4(2)
O(25)-Mo(10)	2.326(5)	O(68)-Cu(2)-O(9)	78.51(19)
O(25)-Mo(15)	2.349(5)	O(23)-Cu(2)-O(9)	91.01(19)
O(26)-Mo(15)	1.733(5)	O(54)-Cu(2)-O(9)	93.35(19)
O(26)-Cu(3)	2.172(6)	O(31)-Cu(2)-O(9)	173.8(2)
O(27)-Mo(8)	1.718(5)	O(7)-Cu(3)-O(68)	169.9(2)
O(27)-Cu(1)	2.190(5)	O(7)-Cu(3)-O(15)	88.7(2)
O(28)-Mo(9)	1.711(5)	O(68)-Cu(3)-O(15)	96.9(2)
O(29)-Mo(5)	1.840(6)	O(7)-Cu(3)-O(9)	92.8(2)
O(29)-Mo(1)	2.109(5)	O(68)-Cu(3)-O(9)	82.5(2)
O(30)-Mo(3)	1.832(5)	O(15)-Cu(3)-O(9)	174.3(2)
O(30)-Mo(4)	2.094(5)	O(7)-Cu(3)-O(26)	97.1(2)
O(31)-V(4)	1.631(5)	O(68)-Cu(3)-O(26)	91.57(19)
O(31)-Cu(2)	2.173(6)	O(15)-Cu(3)-O(26)	87.1(2)
O(32)-Mo(14)	1.715(5)	O(9)-Cu(3)-O(26)	87.3(2)
O(32)-Cu(1)	2.121(5)	O(7)-Cu(3)-O(55)	91.7(2)
O(33)-Mo(14)	1.878(5)	O(68)-Cu(3)-O(55)	79.7(2)
O(33)-Mo(8)	1.896(5)	O(15)-Cu(3)-O(55)	92.0(2)
O(34)-Mo(5)	1.716(5)	O(9)-Cu(3)-O(55)	93.4(2)
O(35)-Mo(4)	1.736(5)	O(26)-Cu(3)-O(55)	171.1(2)
O(35)-Cu(4)	2.312(6)	V(1)-O(24)-Mo(9)	129.9(3)
O(36)-Mo(12)	1.978(6)	V(1)-O(24)-Mo(11)	129.0(3)
O(36)-Mo(2)	2.203(5)	V(1)-O(25)-Mo(10)	129.6(3)
O(36)-Mo(5)	2.216(5)	V(1)-O(25)-Mo(15)	129.5(3)
O(37)-V(1)	1.721(5)	V(4)-O(31)-Cu(2)	139.8(3)
O(37)-Mo(13)	2.326(5)	V(1)-O(37)-Mo(13)	128.9(3)
O(37)-Mo(7)	2.372(5)	V(1)-O(37)-Mo(7)	130.2(3)
O(38)-V(1)	1.676(5)	V(1)-O(38)-Mo(8)	132.9(3)
O(38)-Mo(8)	2.368(5)	V(1)-O(38)-Mo(14)	131.7(3)
O(38)-Mo(14)	2.376(5)	V(5)-O(42)-Mo(7)	136.0(3)
O(39)-Mo(9)	1.711(5)	V(5)-O(42)-Mo(14)	109.8(2)
O(40)-Mo(7)	1.930(5)	Mo(13)-O(43)-V(6)	132.7(3)

O(40)-Mo(13)	1.955(6)	V(6)-O(43)-Mo(10)	113.3(3)
O(41)-Mo(10)	1.902(6)	Cu(2)-O(54)-Cu(1)	92.3(2)
O(41)-Mo(15)	1.906(6)	Cu(1)-O(55)-Cu(3)	92.7(2)
O(42)-V(5)	1.916(6)	Cu(1)-O(68)-Cu(2)	103.0(2)
O(42)-Mo(7)	1.919(5)	Cu(1)-O(68)-Cu(3)	103.9(2)
O(42)-Mo(14)	2.116(5)	Cu(2)-O(68)-Cu(3)	106.3(2)
O(43)-Mo(13)	1.883(5)	O(68)-Cu(1)-O(61)	173.1(2)
O(43)-V(6)	1.896(7)	O(68)-Cu(1)-O(32)	96.30(19)
O(43)-Mo(10)	2.113(5)	O(61)-Cu(1)-O(32)	88.6(2)
O(44)-Mo(10)	1.680(6)	O(68)-Cu(1)-O(55)	81.34(19)
O(45)-Mo(2)	1.806(6)	O(61)-Cu(1)-O(55)	93.8(2)
O(45)-Mo(1)	2.113(5)	O(32)-Cu(1)-O(55)	177.6(2)
O(46)-Mo(1)	1.720(6)	O(68)-Cu(1)-O(27)	95.20(19)
O(47)-V(3)	1.627(6)	O(61)-Cu(1)-O(27)	89.9(2)
O(48)-Mo(15)	1.693(6)	O(32)-Cu(1)-O(27)	87.1(2)
O(49)-Mo(11)	1.938(5)	O(55)-Cu(1)-O(27)	92.7(2)
O(49)-Mo(9)	1.943(5)	O(68)-Cu(1)-O(54)	79.5(2)
O(50)-Mo(7)	1.696(6)	O(61)-Cu(1)-O(54)	95.3(3)
O(51)-Mo(13)	1.704(6)	O(32)-Cu(1)-O(54)	95.1(2)
O(52)-Mo(8)	1.665(5)	O(55)-Cu(1)-O(54)	84.8(2)
O(53)-Mo(14)	1.674(6)	O(27)-Cu(1)-O(54)	174.40(19)
O(54)-Mo(6)	1.784(5)	O(10)-Cu(2)-O(68)	171.1(2)
O(54)-Cu(2)	2.070(5)	O(10)-Cu(2)-O(23)	92.0(2)
O(54)-Cu(1)	2.222(6)	Mo(5)-O(14)-Cu(4)#1	135.8(3)
O(55)-Mo(2)	1.782(5)	V(3)-O(15)-Cu(3)	140.4(3)
O(55)-Cu(1)	2.137(6)	V(3)-O(16)-Mo(15)	138.7(3)
O(55)-Cu(3)	2.178(5)	V(3)-O(16)-Mo(11)	117.4(3)
O(56)-Mo(7)	1.707(6)	V(3)-O(17)-Mo(8)	138.9(3)
O(57)-V(4)	1.641(6)	V(3)-O(17)-Mo(9)	116.8(3)
O(58)-Mo(13)	1.716(6)	V(5)-O(18)-Mo(9)	136.7(3)
O(59)-Mo(11)	1.710(6)	V(5)-O(18)-Mo(8)	110.1(3)
O(60)-Mo(11)	1.709(6)	V(4)-O(20)-Mo(14)	137.4(3)
O(61)-Cu(1)	1.987(6)	V(4)-O(20)-Mo(7)	117.2(2)
O(62)-Mo(4)	1.705(6)	V(4)-O(21)-Mo(10)	137.5(3)
O(63)-Mo(12)	1.705(6)	V(4)-O(21)-Mo(13)	117.7(3)
O(64)-Mo(6)	1.702(6)	Mo(11)-O(22)-V(6)	134.5(3)
O(65)-Mo(2)	1.706(5)	V(6)-O(22)-Mo(15)	112.8(3)
O(66)-Mo(6)	1.808(6)	V(2)-O(11)-Cu(4)	128.4(3)
O(66)-Mo(4)	2.164(6)	V(2)-O(11)-Cu(4)#1	118.8(2)
O(67)-Mo(12)	1.707(6)	Cu(4)-O(11)-Cu(4)#1	98.68(19)
O(68)-Cu(1)	1.968(5)	V(2)-O(12)-Mo(4)	126.1(2)
O(68)-Cu(2)	1.989(5)	V(2)-O(12)-Mo(3)	116.4(2)
O(68)-Cu(3)	1.997(5)	V(2)-O(12)-Mo(6)	121.8(2)
O(69)-V(5)	1.511(9)	V(2)-O(9)-Cu(2)	118.3(3)

O(70)-V(5)	1.620(14)	Cu(3)-O(9)-Cu(2)	92.72(19)
O(71)-V(6)	1.58(2)	V(2)-O(9)-Cu(3)	123.1(3)
O(72)-V(6)	1.515(18)	V(2)-O(8)-Mo(1)	125.7(2)
Cu(4)-O(14)#1	1.963(5)	V(2)-O(8)-Mo(5)	118.2(2)
Cu(4)-O(11)#1	2.358(5)	V(2)-O(8)-Mo(2)	120.1(2)

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

Table S3. Selected bond lengths [Å] and bond angles (°) for the compound 2.

Mo(1)-O(22)	1.705(9)	O(11)-V(4)-O(2)	105.7(4)
Mo(1)-O(17)	1.741(8)	O(50)-V(4)-O(2)	111.9(4)
Mo(1)-O(23)	1.921(8)	O(11)-V(4)-O(3)	106.0(4)
Mo(1)-O(3)	1.988(8)	O(50)-V(4)-O(3)	113.4(4)
Mo(1)-O(9)	2.061(8)	O(2)-V(4)-O(3)	111.8(4)
Mo(1)-O(14)	2.347(8)	O(1B)-V(5)-O(1A)	104.4(8)
Mo(1)-Na(1)	3.71(4)	O(1B)-V(5)-O(4)	109.3(7)
Mo(2)-O(20)	1.691(10)	O(1A)-V(5)-O(4)	109.8(6)
Mo(2)-O(10)	1.699(9)	O(1B)-V(5)-O(5)	110.8(7)
Mo(2)-O(9)	1.867(8)	O(1A)-V(5)-O(5)	107.1(6)
Mo(2)-O(29)	1.942(8)	O(4)-V(5)-O(5)	114.9(4)
Mo(2)-O(3)	2.294(8)	O(44)-Cu(1)-O(17)	92.7(3)
Mo(2)-O(21)	2.304(8)	O(19)-Cu(1)-O(17)	92.1(3)
Mo(3)-O(28)	1.659(8)	O(44)-Cu(1)-O(15)	95.6(4)
Mo(3)-O(13)	1.720(8)	O(19)-Cu(1)-O(15)	79.9(4)
Mo(3)-O(27)	1.897(8)	O(44)-Cu(1)-O(11)	88.3(3)
Mo(3)-O(2)	1.985(8)	O(19)-Cu(1)-O(11)	98.0(3)
Mo(3)-O(4)	2.135(8)	O(17)-Cu(1)-O(11)	85.0(3)
Mo(3)-O(24)	2.333(8)	O(15)-Cu(1)-O(11)	93.0(3)
Mo(4)-O(51)	1.684(9)	O(44)-Cu(1)-O(12)	92.9(3)
Mo(4)-O(18)	1.736(8)	O(19)-Cu(1)-O(12)	81.4(3)
Mo(4)-O(23)	1.906(9)	O(17)-Cu(1)-O(12)	87.2(3)
Mo(4)-O(26)	2.019(8)	O(15)-Cu(1)-O(12)	94.6(3)
Mo(4)-O(6)	2.070(8)	O(19)-Cu(2)-O(30)	97.0(3)
Mo(4)-O(14)	2.348(8)	O(52)-Cu(2)-O(30)	87.7(4)
Mo(5)-O(25)	1.713(9)	O(19)-Cu(2)-O(15)	79.2(3)
Mo(5)-O(41)	1.735(10)	O(52)-Cu(2)-O(15)	96.2(4)
Mo(5)-O(5)	1.927(9)	O(19)-Cu(2)-O(13)	96.5(3)
Mo(5)-O(58)	1.946(8)	O(52)-Cu(2)-O(13)	86.9(4)
Mo(5)-O(8)	2.232(8)	O(30)-Cu(2)-O(13)	83.9(3)
Mo(5)-O(1)	2.329(8)	O(15)-Cu(2)-O(13)	95.7(3)
Mo(6)-O(49)	1.705(9)	O(19)-Cu(2)-O(54)	77.8(3)
Mo(6)-O(7)	1.717(8)	O(52)-Cu(2)-O(54)	98.7(4)
Mo(6)-O(29)	1.921(8)	O(30)-Cu(2)-O(54)	96.2(3)
Mo(6)-O(4)	1.946(8)	O(15)-Cu(2)-O(54)	83.8(3)
Mo(6)-O(2)	2.286(8)	O(33)-Cu(3)-O(18)	92.0(4)

Mo(6)-O(21)	2.325(8)	O(33)-Cu(3)-O(54)	93.6(4)
Mo(8)-O(39)	1.687(10)	O(18)-Cu(3)-O(19)	90.8(3)
Mo(8)-O(67)	1.714(10)	O(54)-Cu(3)-O(19)	84.2(3)
Mo(8)-O(6)	1.887(9)	O(33)-Cu(3)-O(31)	92.0(4)
Mo(8)-O(58)	1.947(10)	O(18)-Cu(3)-O(31)	87.4(3)
Mo(8)-O(26)	2.250(8)	O(54)-Cu(3)-O(31)	88.6(4)
Mo(8)-O(1)	2.327(8)	O(19)-Cu(3)-O(31)	96.1(3)
Mo(8)-Na(1)	3.59(6)	O(33)-Cu(3)-O(12)	91.9(3)
Mo(9)-O(42)	1.636(9)	O(18)-Cu(3)-O(12)	87.5(3)
Mo(9)-O(30)	1.703(8)	O(54)-Cu(3)-O(12)	96.1(3)
Mo(9)-O(27)	1.906(8)	O(19)-Cu(3)-O(12)	80.2(3)
Mo(9)-O(8)	2.013(8)	O(40)-Cu(4)-O(38)	88.4(3)
Mo(9)-O(5)	2.138(8)	O(61)#1-Cu(4)-O(38)	89.8(3)
Mo(9)-O(24)	2.321(9)	O(40)-Cu(4)-O(53)#1	91.6(4)
Mo(10)-O(47)	1.705(10)	O(61)#1-Cu(4)-O(53)#1	89.9(4)
Mo(10)-O(48)	1.778(11)	O(40)-Cu(4)-O(59)	90.4(4)
Mo(10)-O(15)	1.829(8)	O(61)#1-Cu(4)-O(59)	92.7(4)
Mo(10)-O(56)	1.968(10)	O(38)-Cu(4)-O(59)	92.6(3)
Mo(10)-O(55)	2.203(9)	O(53)#1-Cu(4)-O(59)	93.1(4)
Mo(10)-O(32)	2.379(8)	O(40)-Cu(4)-O(38)#1	89.2(4)
Mo(11)-O(63)	1.739(12)	O(61)#1-Cu(4)-O(38)#1	87.5(4)
Mo(11)-O(53)	1.749(9)	O(38)-Cu(4)-O(38)#1	80.4(3)
Mo(11)-O(44)	1.799(8)	O(53)#1-Cu(4)-O(38)#1	94.0(3)
Mo(11)-O(62)	2.083(9)	O(3B)-Cu(6)-O(16)#2	80.0(10)
Mo(11)-O(48)	2.118(9)	O(3B)-Cu(6)-O(50)	100.1(10)
Mo(11)-O(32)	2.260(9)	O(3B)-Cu(6)-O(2W)	156.4(12)
Mo(12)-O(46)	1.679(10)	O(16)#2-Cu(6)-O(2W)	90.4(5)
Mo(12)-O(61)	1.755(8)	O(50)-Cu(6)-O(2W)	90.2(5)
Mo(12)-O(62)	1.813(11)	O(16)#2-Cu(6)-O(3W)	88.4(6)
Mo(12)-O(57)	1.969(11)	O(50)-Cu(6)-O(3W)	91.0(6)
Mo(12)-O(55)	2.208(9)	O(3B)-Cu(6)-O(4W)	71.7(11)
Mo(12)-O(32)	2.330(8)	O(16)#2-Cu(6)-O(4W)	92.9(6)
Mo(13)-O(34)	1.702(12)	O(50)-Cu(6)-O(4W)	89.0(5)
Mo(13)-O(59)	1.757(9)	O(2W)-Cu(6)-O(4W)	87.5(6)
Mo(13)-O(33)	1.800(9)	O(3W)-Cu(6)-O(4W)	92.6(8)
Mo(13)-O(35)	2.094(11)	O(3B)-Cu(6)-O(1W)	110.4(10)
Mo(13)-O(64)	2.117(11)	O(16)#2-Cu(6)-O(1W)	85.1(4)
Mo(13)-O(43)	2.267(10)	O(50)-Cu(6)-O(1W)	93.1(4)
Mo(14)-O(37)	1.727(10)	O(2W)-Cu(6)-O(1W)	89.9(5)
Mo(14)-O(54)	1.781(8)	O(3W)-Cu(6)-O(1W)	90.0(7)
Mo(14)-O(64)	1.801(12)	O(4W)-Cu(6)-O(1W)	176.7(5)
Mo(14)-O(56)	1.989(10)	O(6)-Cu(5)-O(23W)	161.1(12)
Mo(14)-O(36)	2.226(10)	O(6)-Cu(5)-O(9)	106.8(6)
Mo(14)-O(43)	2.384(8)	O(23W)-Cu(5)-O(9)	87.0(10)

Mo(15)-O(45)	1.697(10)	O(6)-Cu(5)-O(24W)	83.3(10)
Mo(15)-O(40)	1.770(8)	O(23W)-Cu(5)-O(24W)	80.0(10)
Mo(15)-O(35)	1.803(13)	O(9)-Cu(5)-O(24W)	161.3(12)
Mo(15)-O(57)	1.978(10)	O(6)-Cu(5)-O(22W)	101.9(10)
Mo(15)-O(36)	2.213(9)	O(23W)-Cu(5)-O(22W)	87.2(10)
Mo(15)-O(43)	2.325(8)	O(9)-Cu(5)-O(22W)	102.6(10)
Mo(16)-O(65)	1.704(10)	O(24W)-Cu(5)-O(22W)	90.3(10)
Mo(16)-O(66)	1.711(9)	O(23W)-Na(1)-O(24W)	93(2)
Mo(16)-O(36)	1.902(13)	O(23W)-Na(1)-O(6)	162(3)
Mo(16)-O(55)	1.969(13)	O(24W)-Na(1)-O(6)	88(3)
Mo(16)-O(56)	2.174(9)	O(23W)-Na(1)-O(22W)	95(3)
Mo(16)-O(57)	2.230(8)	O(24W)-Na(1)-O(22W)	104(2)
V(1)-O(24)	1.693(9)	O(6)-Na(1)-O(22W)	102(3)
V(1)-O(1)	1.716(8)	O(23W)-Na(1)-O(9)	81(2)
V(1)-O(14)	1.722(7)	O(24W)-Na(1)-O(9)	160(3)
V(1)-O(21)	1.723(8)	O(6)-Na(1)-O(9)	91.3(14)
V(2)-O(31)	1.595(9)	O(22W)-Na(1)-O(9)	97(2)
V(2)-O(16)	1.657(9)	O(23W)-Na(1)-O(23)	99(2)
V(2)-O(8)	1.794(8)	O(24W)-Na(1)-O(23)	101(3)
V(2)-O(26)	1.815(9)	O(6)-Na(1)-O(23)	63.9(13)
V(3)-O(12)	1.658(8)	O(22W)-Na(1)-O(23)	151(2)
V(3)-O(38)	1.667(8)	O(9)-Na(1)-O(23)	61.1(9)
V(3)-O(43)	1.758(9)	V(1)-O(1)-Mo(8)	127.4(4)
V(3)-O(32)	1.779(9)	V(1)-O(1)-Mo(5)	130.8(4)
V(4)-O(11)	1.622(8)	V(4)-O(2)-Mo(3)	138.6(4)
V(4)-O(50)	1.657(9)	V(4)-O(2)-Mo(6)	116.6(4)
V(4)-O(2)	1.800(8)	V(4)-O(3)-Mo(1)	139.4(4)
V(4)-O(3)	1.818(8)	V(4)-O(3)-Mo(2)	117.9(4)
V(5)-O(1B)	1.583(15)	V(5)-O(4)-Mo(6)	131.3(5)
V(5)-O(1A)	1.621(16)	V(5)-O(4)-Mo(3)	116.1(4)
V(5)-O(4)	1.861(9)	Mo(5)-O(5)-V(5)	130.8(5)
V(5)-O(5)	1.942(9)	V(5)-O(5)-Mo(9)	115.7(4)
Cu(1)-O(44)	1.933(8)	Cu(5)-O(6)-Mo(4)	111.7(6)
Cu(1)-O(19)	1.966(8)	V(2)-O(8)-Mo(9)	138.5(5)
Cu(1)-O(17)	2.025(8)	V(2)-O(8)-Mo(5)	117.8(4)
Cu(1)-O(15)	2.034(8)	V(4)-O(11)-Cu(1)	137.6(5)
Cu(1)-O(11)	2.255(8)	V(3)-O(12)-Cu(3)	119.4(4)
Cu(1)-O(12)	2.259(8)	V(3)-O(12)-Cu(1)	119.3(4)
Cu(1)-Cu(2)	3.042(2)	Cu(3)-O(12)-Cu(1)	90.7(3)
Cu(2)-O(19)	1.943(8)	V(1)-O(14)-Mo(1)	127.8(4)
Cu(2)-O(52)	1.973(9)	V(1)-O(14)-Mo(4)	128.3(4)
Cu(2)-O(30)	2.076(8)	Mo(10)-O(15)-Cu(2)	133.5(5)
Cu(2)-O(15)	2.085(9)	Cu(1)-O(15)-Cu(2)	95.2(4)
Cu(2)-O(13)	2.252(8)	Cu(2)-O(19)-Cu(1)	102.2(4)

Cu(2)-O(54)	2.324(9)	Cu(2)-O(19)-Cu(3)	103.8(3)
Cu(3)-O(33)	1.945(8)	Cu(1)-O(19)-Cu(3)	107.6(3)
Cu(3)-O(18)	1.996(9)	V(1)-O(21)-Mo(2)	129.2(4)
Cu(3)-O(54)	2.004(9)	V(1)-O(21)-Mo(6)	130.3(4)
Cu(3)-O(19)	2.019(7)	V(1)-O(24)-Mo(9)	131.6(4)
Cu(3)-O(31)	2.233(8)	V(1)-O(24)-Mo(3)	132.3(4)
Cu(3)-O(12)	2.260(8)	V(2)-O(26)-Mo(4)	139.4(5)
Cu(4)-O(40)	1.953(8)	V(2)-O(26)-Mo(8)	117.9(4)
Cu(4)-O(61)#1	1.963(8)	V(2)-O(31)-Cu(3)	136.6(5)
Cu(4)-O(38)	2.104(9)	V(3)-O(32)-Mo(11)	125.2(4)
Cu(4)-O(53)#1	2.117(10)	V(3)-O(32)-Mo(12)	116.6(4)
Cu(4)-O(59)	2.144(11)	V(3)-O(32)-Mo(10)	121.2(4)
Cu(4)-O(38)#1	2.208(10)	V(3)-O(38)-Cu(4)#1	122.3(6)
Cu(6)-O(3B)	1.55(2)	Cu(4)-O(38)-Cu(4)#1	99.6(3)
Cu(6)-O(16)#2	1.908(9)	Mo(15)-O(40)-Cu(4)	137.1(5)
Cu(6)-O(50)	1.930(9)	V(3)-O(43)-Mo(13)	125.7(4)
Cu(6)-O(2W)	2.091(13)	V(3)-O(43)-Mo(15)	116.1(4)
Cu(6)-O(3W)	2.158(18)	V(3)-O(43)-Mo(14)	121.9(4)
Cu(6)-O(4W)	2.273(19)	Cu(3)-O(54)-Cu(2)	91.9(3)
Cu(6)-O(1W)	2.343(13)	O(24)-V(1)-O(14)	104.8(4)
Cu(5)-O(6)	1.91(2)	O(1)-V(1)-O(14)	112.7(4)
Cu(5)-O(23W)	2.00(3)	O(24)-V(1)-O(21)	109.3(4)
Cu(5)-O(9)	2.016(15)	O(1)-V(1)-O(21)	108.9(4)
Cu(5)-O(24W)	2.21(3)	O(14)-V(1)-O(21)	111.9(4)
Cu(5)-O(22W)	2.34(3)	O(31)-V(2)-O(16)	108.1(5)
O(16)-Cu(6)#3	1.908(9)	O(31)-V(2)-O(8)	106.6(4)
O(38)-Cu(4)#1	2.208(10)	O(16)-V(2)-O(8)	111.2(4)
O(53)-Cu(4)#1	2.117(10)	O(31)-V(2)-O(26)	106.6(4)
O(61)-Cu(4)#1	1.963(8)	O(16)-V(2)-O(26)	113.2(5)
O(24)-V(1)-O(1)	109.0(4)	O(8)-V(2)-O(26)	110.7(4)
O(12)-V(3)-O(32)	108.4(4)	O(12)-V(3)-O(38)	108.0(4)
O(38)-V(3)-O(32)	110.0(5)	O(12)-V(3)-O(43)	108.0(4)
O(43)-V(3)-O(32)	114.1(4)	O(38)-V(3)-O(43)	108.2(4)
O(11)-V(4)-O(50)	107.5(4)		

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

Table S4. Selected bond lengths [Å] and bond angles (°) for the compound **3**.

Mo(1)-O(33)	1.707(12)	O(15)-Cu(1)-O(23)	83.3(3)
Mo(1)-O(31)#1	1.791(8)	O(31)-Cu(1)-O(21)	91.5(3)
Mo(1)-O(31)	1.791(8)	O(14)-Cu(1)-O(21)	87.4(3)
Mo(1)-O(32)	2.100(8)	O(15)-Cu(1)-O(21)	98.9(3)
Mo(1)-O(32)#1	2.100(8)	O(23)-Cu(1)-O(21)	89.1(3)
Mo(1)-O(34)	2.265(11)	O(31)-Cu(1)-O(24)	91.3(3)

Mo(2)-O(57)	1.683(8)	O(14)-Cu(1)-O(24)	90.7(3)
Mo(2)-O(23)	1.772(7)	O(15)-Cu(1)-O(24)	78.6(3)
Mo(2)-O(32)	1.821(9)	O(23)-Cu(1)-O(24)	92.6(3)
Mo(2)-O(53)	1.989(9)	O(21)-Cu(1)-O(24)	176.7(3)
Mo(2)-O(55)	2.201(7)	O(15)-Cu(2)-O(42)	174.1(3)
Mo(2)-O(34)	2.366(7)	O(15)-Cu(2)-O(38)	94.7(3)
Mo(3)-O(49)	1.726(13)	O(42)-Cu(2)-O(38)	88.5(3)
Mo(3)-O(16)#1	1.783(7)	O(15)-Cu(2)-O(22)	82.1(3)
Mo(3)-O(16)	1.783(7)	O(42)-Cu(2)-O(22)	94.6(3)
Mo(3)-O(43)	2.114(8)	O(15)-Cu(2)-O(17)	95.5(3)
Mo(3)-O(43)#1	2.114(8)	O(42)-Cu(2)-O(17)	89.4(4)
Mo(3)-O(44)	2.262(11)	O(38)-Cu(2)-O(17)	88.9(3)
Mo(4)-O(56)	1.717(8)	O(22)-Cu(2)-O(17)	92.2(3)
Mo(4)-O(56)#1	1.717(8)	O(15)-Cu(2)-O(23)	79.1(3)
Mo(4)-O(55)	1.953(13)	O(42)-Cu(2)-O(23)	95.9(3)
Mo(4)-O(54)	1.966(13)	O(38)-Cu(2)-O(23)	92.5(3)
Mo(4)-O(53)#1	2.201(7)	O(22)-Cu(2)-O(23)	86.2(3)
Mo(4)-O(53)	2.201(7)	O(16)-Cu(3)-O(39)	93.9(3)
Mo(5)-O(35)	1.688(9)	O(15)-Cu(3)-O(39)	93.0(3)
Mo(5)-O(29)	1.705(8)	O(16)-Cu(3)-O(22)	93.3(3)
Mo(5)-O(4)	1.879(8)	O(15)-Cu(3)-O(22)	80.1(3)
Mo(5)-O(5)	1.966(8)	O(16)-Cu(3)-O(24)	91.6(3)
Mo(5)-O(20)	2.285(8)	O(15)-Cu(3)-O(24)	80.1(3)
Mo(5)-O(3)	2.327(8)	O(39)-Cu(3)-O(24)	89.8(3)
Mo(6)-O(50)	1.686(8)	O(22)-Cu(3)-O(24)	91.8(3)
Mo(6)-O(22)	1.793(8)	O(16)-Cu(3)-O(37)	89.2(3)
Mo(6)-O(43)	1.809(9)	O(15)-Cu(3)-O(37)	99.6(3)
Mo(6)-O(53)	1.966(9)	O(39)-Cu(3)-O(37)	85.6(3)
Mo(6)-O(54)	2.193(6)	O(22)-Cu(3)-O(37)	92.8(3)
Mo(6)-O(44)	2.371(7)	O(1W)-Cu(4)-O(3W)	178.4(4)
Mo(7)-O(46)	1.685(9)	O(1W)-Cu(4)-O(30)	88.7(4)
Mo(7)-O(14)	1.738(8)	O(3W)-Cu(4)-O(30)	89.9(4)
Mo(7)-O(13)	1.909(8)	O(1W)-Cu(4)-O(47)#2	90.5(4)
Mo(7)-O(20)	2.029(8)	O(3W)-Cu(4)-O(47)#2	90.9(4)
Mo(7)-O(4)	2.057(8)	O(1W)-Cu(4)-O(4W)	87.5(4)
Mo(7)-O(19)	2.336(8)	O(3W)-Cu(4)-O(4W)	93.3(4)
Mo(8)-O(45)	1.698(9)	O(30)-Cu(4)-O(4W)	89.3(4)
Mo(8)-O(28)	1.708(8)	O(47)#2-Cu(4)-O(4W)	89.8(4)
Mo(8)-O(5)	1.918(8)	O(1W)-Cu(4)-O(2W)	92.1(4)
Mo(8)-O(6)	1.950(8)	O(3W)-Cu(4)-O(2W)	87.1(4)
Mo(8)-O(8)	2.256(8)	O(30)-Cu(4)-O(2W)	90.8(4)
Mo(8)-O(3)	2.317(8)	O(47)#2-Cu(4)-O(2W)	90.2(4)
Mo(9)-O(12)	1.682(8)	O(4W)-Cu(4)-O(2W)	179.6(4)
Mo(9)-O(39)	1.735(9)	O(58)-Cu(5)-O(5W)	88.7(9)

Mo(9)-O(13)	1.899(8)	O(58)#3-Cu(5)-O(5W)	88.7(9)
Mo(9)-O(2)	2.026(8)	O(58)-Cu(5)-O(15W)	96.7(6)
Mo(9)-O(1)	2.074(8)	O(58)#3-Cu(5)-O(15W)	96.7(6)
Mo(9)-O(19)	2.327(8)	O(5W)-Cu(5)-O(15W)	103.6(18)
Mo(10)-O(26)	1.709(8)	O(58)-Cu(5)-O(14W)	87.8(9)
Mo(10)-O(40)	1.706(9)	O(58)#3-Cu(5)-O(14W)	87.8(9)
Mo(10)-O(1)	1.857(8)	O(5W)-Cu(5)-O(14W)	149.6(18)
Mo(10)-O(10)	1.970(9)	O(15W)-Cu(5)-O(14W)	107(2)
Mo(10)-O(2)	2.295(8)	O(58)-Na(1)-O(5W)	90(3)
Mo(10)-O(27)	2.314(8)	O(58)#3-Na(1)-O(5W)	90(3)
Mo(11)-O(41)	1.692(9)	O(58)-Na(1)-O(14W)	91(3)
Mo(11)-O(25)	1.699(8)	O(58)#3-Na(1)-O(14W)	91(3)
Mo(11)-O(10)	1.905(8)	O(5W)-Na(1)-O(14W)	166(4)
Mo(11)-O(7)	1.957(8)	O(58)-Na(1)-O(15W)	87.5(18)
Mo(11)-O(11)	2.255(8)	O(58)#3-Na(1)-O(15W)	87.5(18)
Mo(11)-O(27)	2.314(8)	O(5W)-Na(1)-O(15W)	94(3)
Mo(12)-O(48)	1.666(9)	O(14W)-Na(1)-O(15W)	99(4)
Mo(12)-O(17)	1.720(8)	O(24)#1-V(1)-O(24)	107.1(5)
Mo(12)-O(18)	1.906(8)	O(24)#1-V(1)-O(44)	109.3(4)
Mo(12)-O(11)	1.999(8)	O(24)-V(1)-O(44)	109.3(4)
Mo(12)-O(7)	2.177(8)	O(24)#1-V(1)-O(34)	110.1(4)
Mo(12)-O(9)	2.361(8)	O(24)-V(1)-O(34)	110.1(4)
Mo(13)-O(36)	1.640(8)	O(44)-V(1)-O(34)	110.7(5)
Mo(13)-O(38)	1.732(8)	O(9)-V(2)-O(19)	104.9(4)
Mo(13)-O(18)	1.904(8)	O(9)-V(2)-O(27)	110.5(4)
Mo(13)-O(8)	1.973(8)	O(19)-V(2)-O(27)	111.2(4)
Mo(13)-O(6)	2.158(8)	O(9)-V(2)-O(3)	110.6(4)
Mo(13)-O(9)	2.363(8)	O(19)-V(2)-O(3)	111.4(4)
Cu(1)-O(31)	1.993(8)	O(27)-V(2)-O(3)	108.1(3)
Cu(1)-O(14)	2.028(8)	O(37)-V(3)-O(30)	107.7(5)
Cu(1)-O(15)	2.022(8)	O(37)-V(3)-O(2)	106.8(4)
Cu(1)-O(23)	2.060(8)	O(30)-V(3)-O(2)	111.7(4)
Cu(1)-O(21)	2.203(9)	O(37)-V(3)-O(11)	108.6(4)
Cu(1)-O(24)	2.213(8)	O(30)-V(3)-O(11)	112.0(4)
Cu(2)-O(15)	1.954(7)	O(2)-V(3)-O(11)	109.9(4)
Cu(2)-O(42)	1.961(8)	O(21)-V(4)-O(47)	108.2(5)
Cu(2)-O(38)	2.032(8)	O(21)-V(4)-O(20)	106.1(4)
Cu(2)-O(22)	2.085(8)	O(47)-V(4)-O(20)	112.4(4)
Cu(2)-O(17)	2.226(9)	O(21)-V(4)-O(8)	107.5(4)
Cu(2)-O(23)	2.287(8)	O(47)-V(4)-O(8)	112.9(4)
Cu(3)-O(16)	1.968(8)	O(20)-V(4)-O(8)	109.3(4)
Cu(3)-O(15)	1.998(7)	Mo(10)-O(1)-V(5B)	131.9(6)
Cu(3)-O(39)	2.077(9)	V(5B)-O(1)-Mo(9)	112.7(6)
Cu(3)-O(22)	2.121(8)	V(3)-O(2)-Mo(9)	139.2(4)

Cu(3)-O(24)	2.171(8)	V(3)-O(2)-Mo(10)	119.6(4)
Cu(3)-O(37)	2.191(10)	V(2)-O(3)-Mo(8)	129.8(4)
Cu(4)-O(1W)	1.964(9)	V(2)-O(3)-Mo(5)	128.2(4)
Cu(4)-O(3W)	1.980(9)	Mo(5)-O(4)-V(5B)	132.3(6)
Cu(4)-O(30)	2.023(9)	V(5B)-O(4)-Mo(7)	113.0(6)
Cu(4)-O(47)#2	2.026(9)	V(5)-O(6)-Mo(8)	136.2(4)
Cu(4)-O(4W)	2.304(13)	V(5)-O(6)-Mo(13)	114.0(4)
Cu(4)-O(2W)	2.342(12)	V(5)-O(7)-Mo(11)	137.6(5)
Cu(5)-O(58)	1.924(11)	V(5)-O(7)-Mo(12)	112.4(4)
Cu(5)-O(58)#3	1.924(11)	V(4)-O(8)-Mo(13)	139.0(4)
Cu(5)-O(5W)	2.05(4)	V(4)-O(8)-Mo(8)	116.6(4)
Cu(5)-O(15W)	2.21(5)	V(2)-O(9)-Mo(12)	132.2(4)
Cu(5)-O(14W)	2.10(4)	V(2)-O(9)-Mo(13)	130.8(4)
Na(1)-O(58)	1.913(11)	V(3)-O(11)-Mo(12)	135.2(4)
Na(1)-O(58)#3	1.913(11)	V(3)-O(11)-Mo(11)	119.2(4)
Na(1)-O(5W)	2.03(10)	Cu(2)-O(15)-Cu(3)	101.6(3)
Na(1)-O(14W)	2.00(10)	Cu(2)-O(15)-Cu(1)	104.0(3)
Na(1)-O(15W)	2.51(7)	Cu(3)-O(15)-Cu(1)	106.6(3)
V(1)-O(24)#1	1.664(7)	V(2)-O(19)-Mo(9)	129.0(4)
V(1)-O(24)	1.664(7)	V(2)-O(19)-Mo(7)	129.3(4)
V(1)-O(44)	1.759(11)	V(4)-O(20)-Mo(7)	140.7(4)
V(1)-O(34)	1.765(11)	V(4)-O(20)-Mo(5)	118.5(4)
V(2)-O(9)	1.681(8)	V(4)-O(21)-Cu(1)	135.2(5)
V(2)-O(19)	1.720(8)	Mo(6)-O(22)-Cu(3)	130.2(4)
V(2)-O(27)	1.716(8)	Cu(2)-O(22)-Cu(3)	93.5(3)
V(2)-O(3)	1.720(7)	Cu(1)-O(23)-Cu(2)	92.1(3)
V(3)-O(37)	1.631(9)	V(1)-O(24)-Cu(3)	122.6(4)
V(3)-O(30)	1.645(8)	V(1)-O(24)-Cu(1)	120.9(4)
V(3)-O(2)	1.794(9)	Cu(3)-O(24)-Cu(1)	94.7(3)
V(3)-O(11)	1.805(8)	V(2)-O(27)-Mo(10)	129.2(4)
V(4)-O(21)	1.622(8)	V(2)-O(27)-Mo(11)	129.4(4)
V(4)-O(47)	1.645(9)	V(1)-O(34)-Mo(1)	122.7(5)
V(4)-O(20)	1.800(8)	V(1)-O(34)-Mo(2)	120.6(3)
V(4)-O(8)	1.813(8)	V(1)-O(34)-Mo(2)#1	120.6(3)
O(1)-V(5B)	1.912(18)	V(1)-O(44)-Mo(3)	122.3(5)
O(4)-V(5B)	1.925(18)	V(1)-O(44)-Mo(6)	120.8(3)
O(6)-V(5)	1.848(8)	V(1)-O(44)-Mo(6)#1	120.8(3)
O(7)-V(5)	1.855(8)	O(59)-V(5)-O(58)	107.0(6)
O(34)-Mo(2)#1	2.366(7)	O(59)-V(5)-O(6)	106.0(5)
O(44)-Mo(6)#1	2.371(7)	O(58)-V(5)-O(6)	113.5(5)
O(47)-Cu(4)#4	2.026(9)	O(59)-V(5)-O(7)	105.1(5)
O(54)-Mo(6)#1	2.193(6)	O(58)-V(5)-O(7)	112.4(5)
O(55)-Mo(2)#1	2.201(7)	O(6)-V(5)-O(7)	112.2(4)
V(5)-O(59)	1.602(11)	O(59B)-V(5B)-O(58B)	106.5(11)

V(5)-O(58)	1.619(12)	O(59B)-V(5B)-O(1)	109.0(11)
V(5B)-O(59B)	1.605(15)	O(58B)-V(5B)-O(1)	108.6(11)
V(5B)-O(58B)	1.625(15)	O(59B)-V(5B)-O(4)	109.4(11)
O(31)-Cu(1)-O(14)	92.2(3)	O(58B)-V(5B)-O(4)	108.0(11)
O(14)-Cu(1)-O(15)	92.5(3)	O(1)-V(5B)-O(4)	115.0(9)
O(31)-Cu(1)-O(23)	92.8(3)		

Symmetry code for 3: #1 x,y,-z #2 x-1/2,-y+3/2,-z+1/2 #3 x,y,-z+1 #4 x+1/2, -y+3/2, -z+1/2