

Supplement Materials

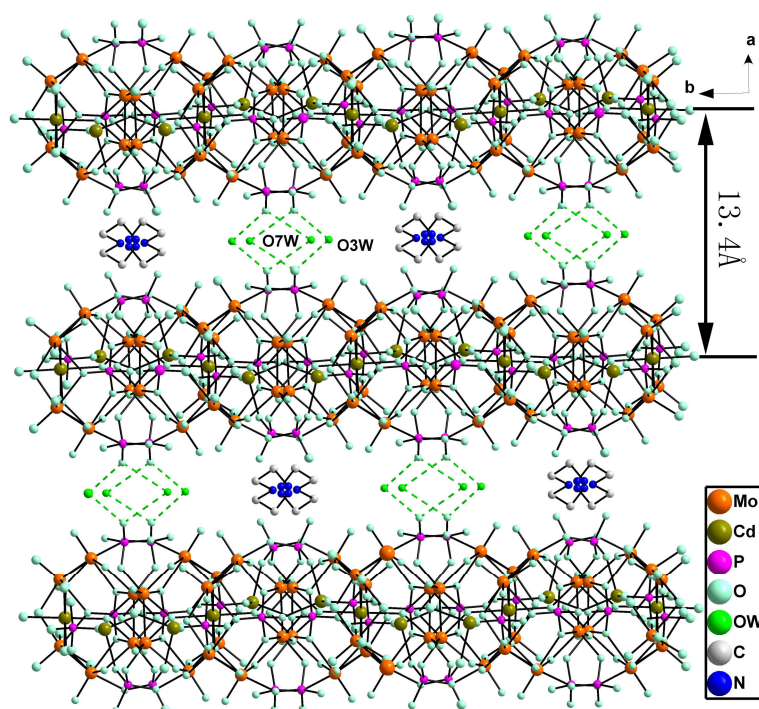


Fig. S1 Packing of **1** down the *b* axis, showing the inter-sheet hydrogen bonds and the dien molecules filled in the interlayer. [Symmetry code: (A) *x*, *y*, 1+*z*].

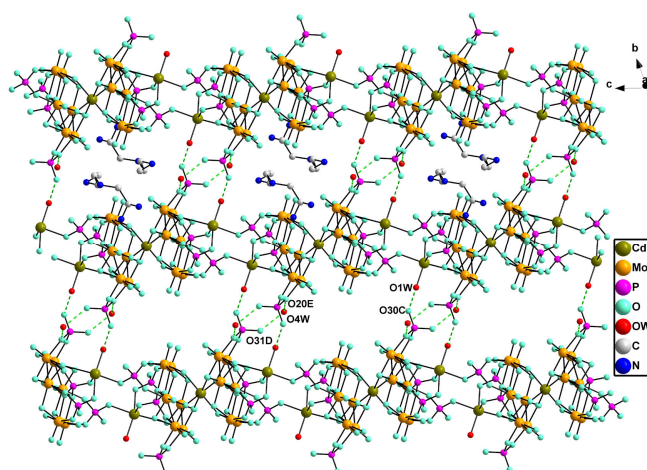


Fig. S2 View of the supramolecular framework of **2** with the 1-D tunnels filled by dien molecules.

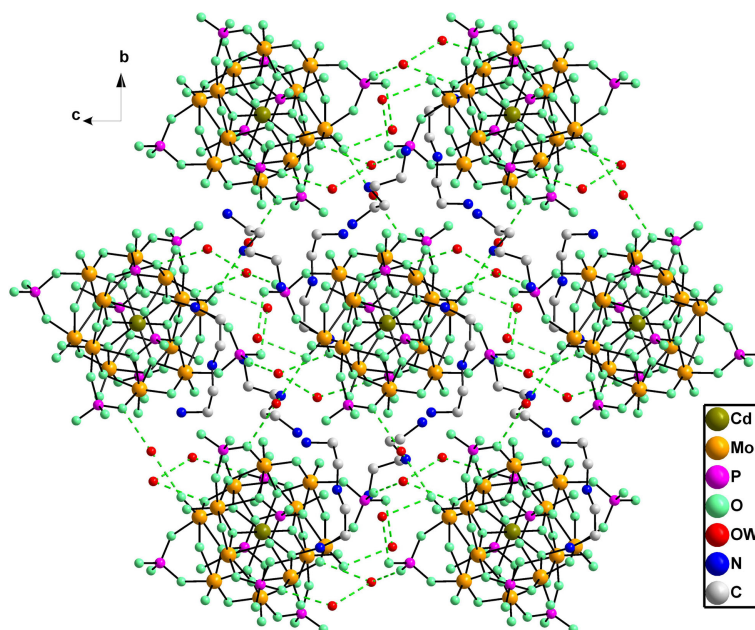


Fig. S3 View of 3-D supramolecular network for **4**, showing the dien molecules lie in these tunnels.

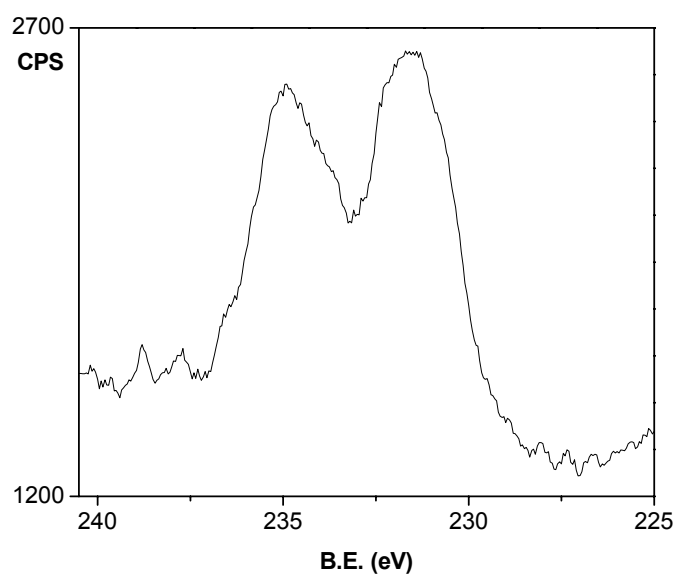


Fig. S4 XPS for Mo in compound **1**.

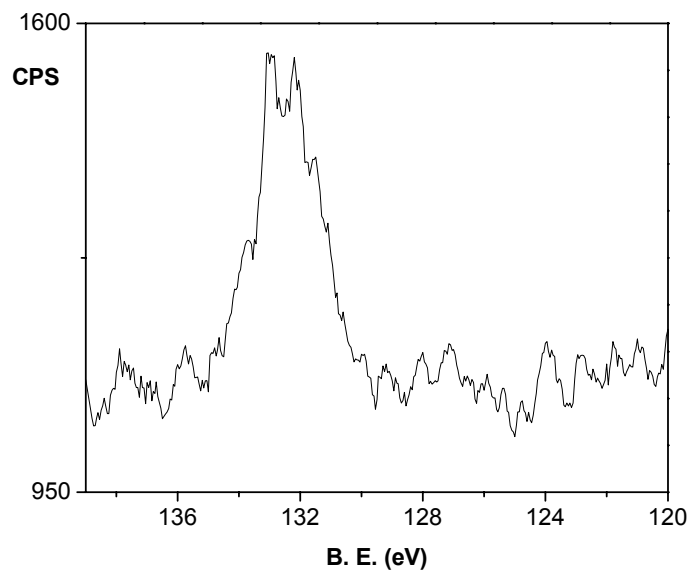


Fig. S5 XPS for P in compound **1**.

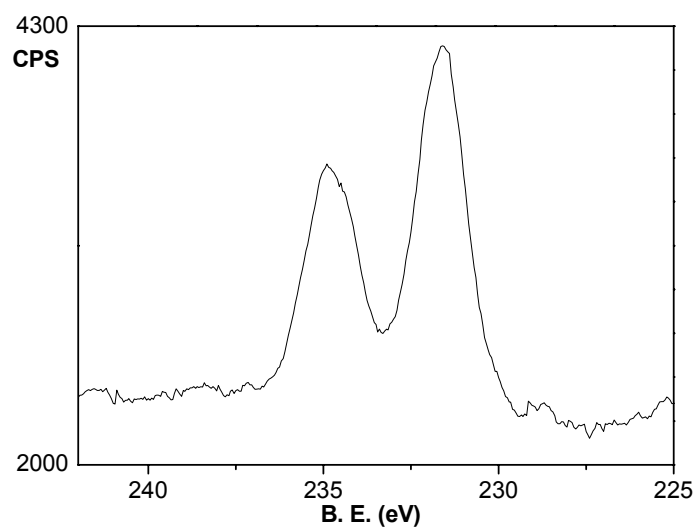


Fig. S6 XPS for Mo in compound **2**.

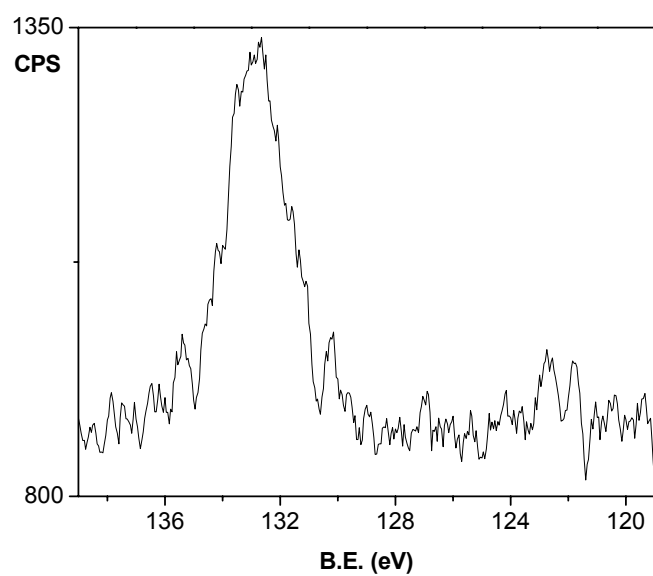


Fig. S7 XPS for P in compound **2**.

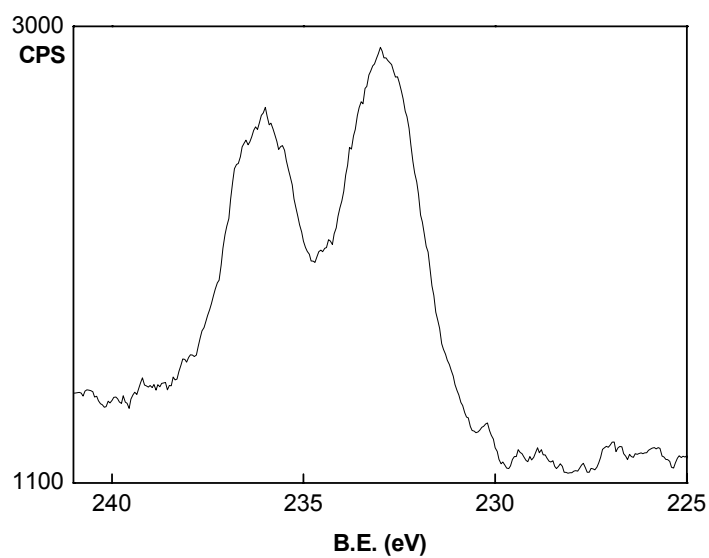


Fig. S8 XPS for Mo in compound **3**.

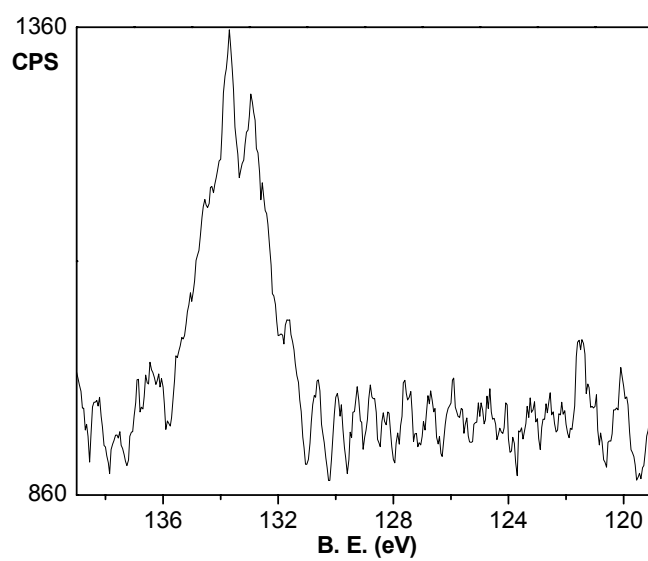


Fig. S9 XPS for P in compound **3**.

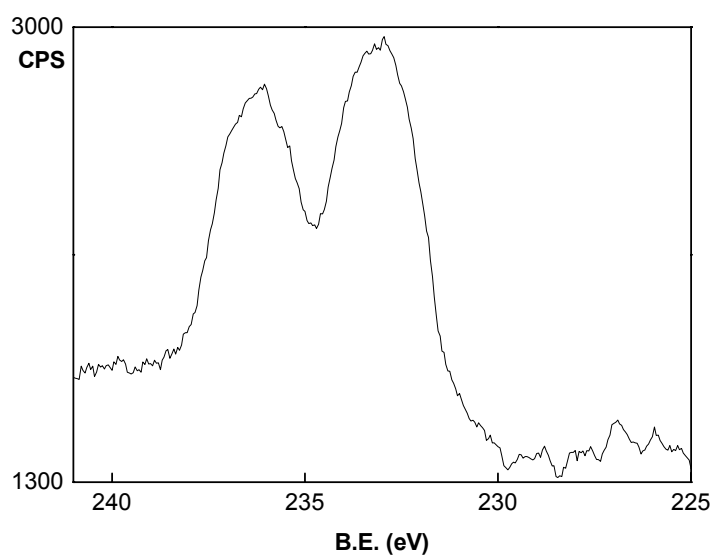


Fig. S10 XPS for Mo in compound 4.

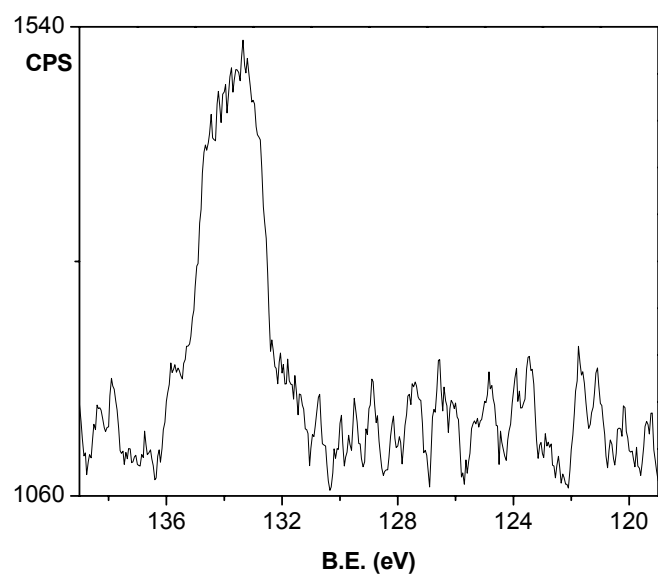


Fig. S11 XPS for P in compounds 4

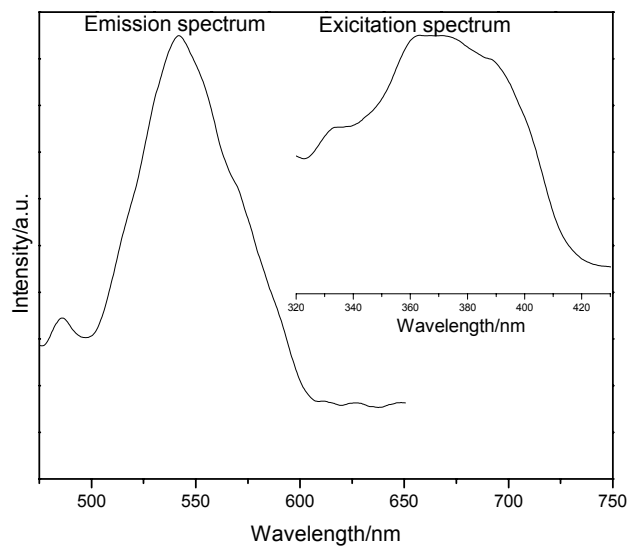


Fig. S12 Solid-state emission spectra of compounds **1** at room temperature.

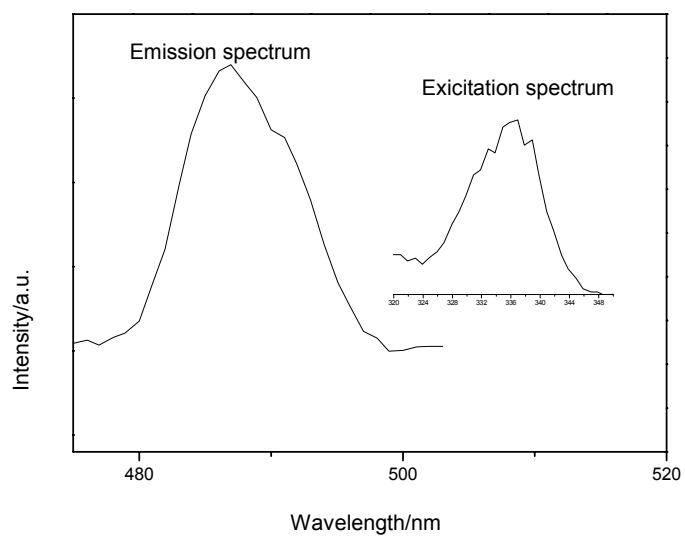


Fig. S13 Solid-state emission spectra of compounds **2** at room temperature.

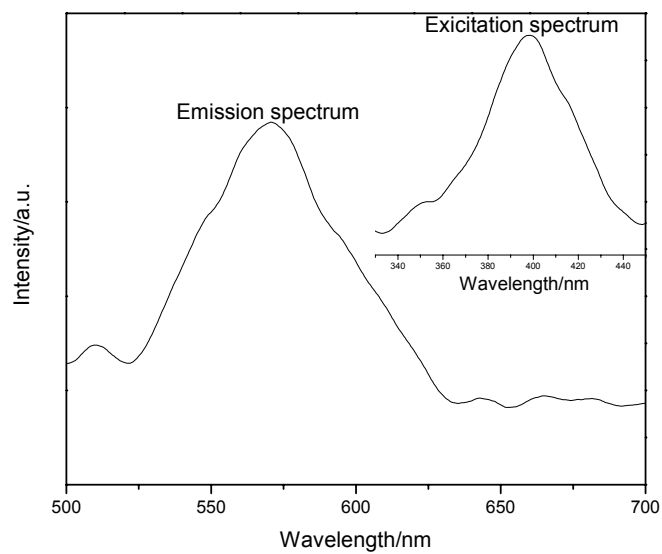


Fig. S14 Solid-state emission spectra of compounds **3** at room temperature.

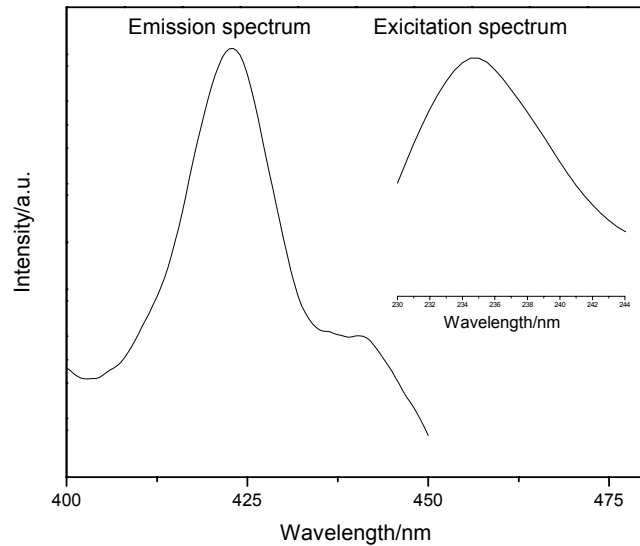


Fig. S15 Solid-state emission spectra of compounds **4** at room temperature.

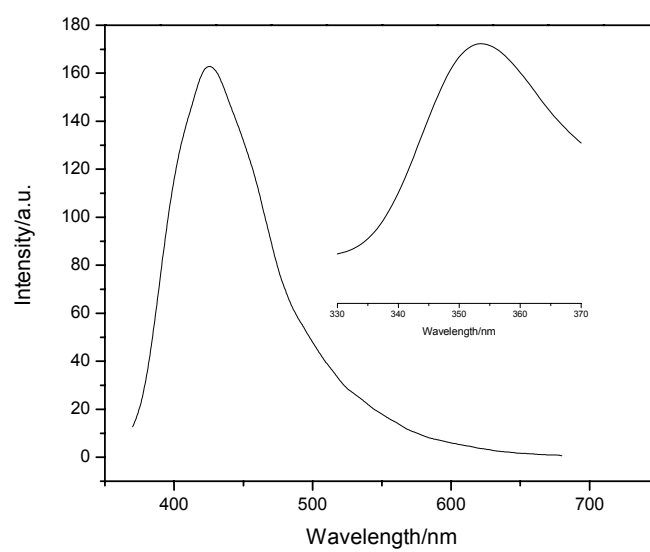


Fig. S16 Emission spectrum of dien at room temperature.

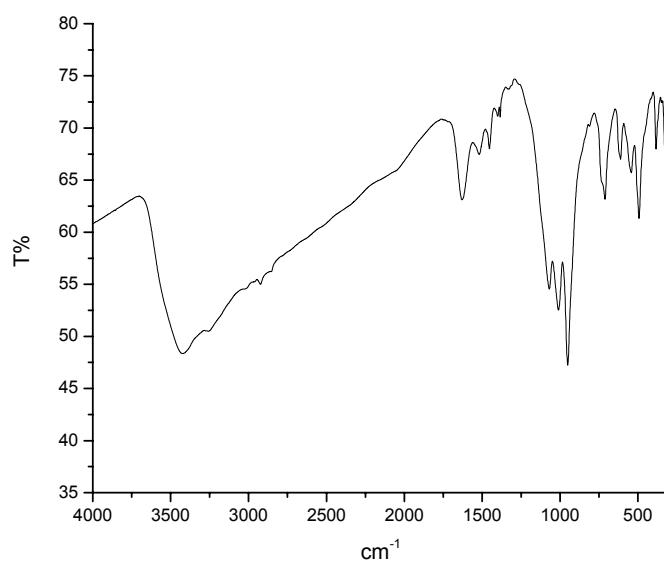


Fig. S17. IR spectrum of compound **1**.

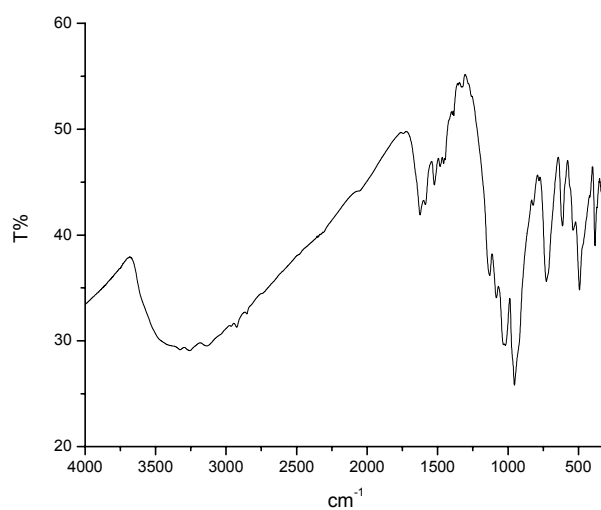


Fig. S18. IR spectrum of compound **2**.

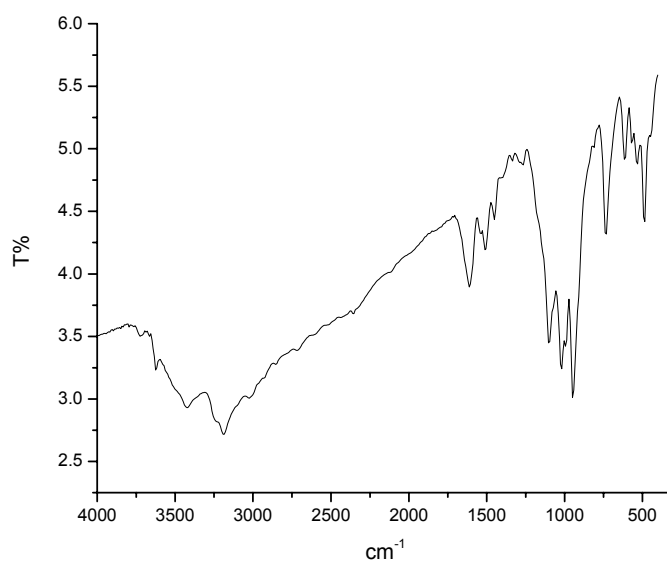


Fig. S19. IR spectrum of compound **3**.

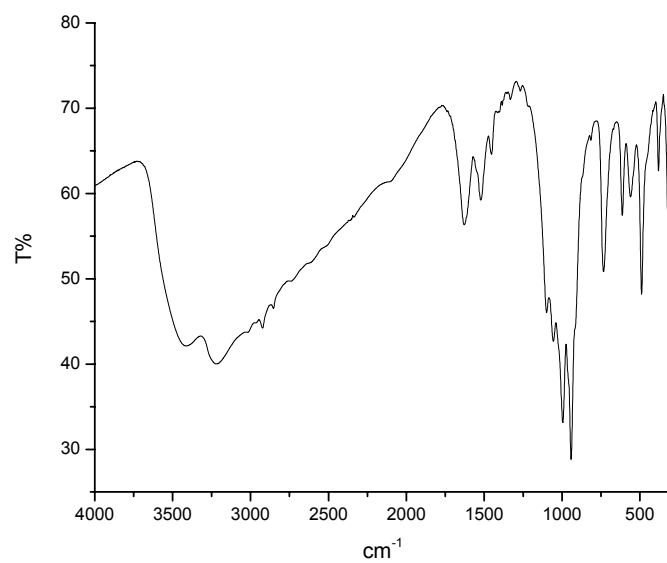


Fig. S20. IR spectrum of compound **4**.

Table S1 Selected bond lengths (Å) and angles (°) for **1-4**.

Compound 1			
Mo(1)-O(31)	1.675(12)	Cd(1)-O(4)#1	2.276(8)
Mo(1)-O(12)	1.930(9)	Cd(1)-O(4)	2.276(8)
Mo(1)-O(4)	1.984(8)	Cd(2)-N(1)	2.143(18)
Mo(1)-O(22)	2.034(10)	Cd(2)-O(19)	2.200(9)
Mo(1)-O(8)	2.111(9)	Cd(2)-O(26)#2	2.206(12)
Mo(1)-O(10)	2.291(11)	Cd(2)-N(2)	2.281(14)
Mo(1)-Mo(6)	2.6089(18)	Cd(2)-O(5W)	2.186(16)
Mo(2)-O(30)	1.666(9)	Cd(2)-O(6)	2.323(8)
Mo(2)-O(11)	1.946(11)	P(1)-O(6)	1.507(10)
Mo(2)-O(2)	1.992(8)	P(1)-O(10)	1.526(11)
Mo(2)-O(21)	2.045(9)	P(1)-O(7)	1.526(9)
Mo(2)-O(8)	2.116(11)	P(1)-O(5)	1.558(9)
Mo(2)-O(10)	2.273(9)	P(2)-O(16)	1.500(12)
Mo(2)-Mo(3)	2.5932(19)	P(2)-O(27)	1.506(10)
Mo(3)-O(9)	1.660(9)	P(2)-O(28)	1.539(10)
Mo(3)-O(11)	1.935(8)	P(2)-O(19)	1.563(11)
Mo(3)-O(2)	1.949(11)	P(3)-O(24)	1.488(13)
Mo(3)-O(15)	2.042(11)	P(3)-O(23)	1.490(14)
Mo(3)-O(13)	2.109(9)	P(3)-O(21)	1.537(11)
Mo(3)-O(7)	2.318(8)	P(3)-O(22)	1.542(11)
Mo(4)-O(14)	1.680(9)	P(4)-O(26)	1.501(10)
Mo(4)-O(17)	1.945(9)	P(4)-O(25)	1.514(11)
Mo(4)-O(1)	1.986(11)	P(4)-O(15)	1.523(12)
Mo(4)-O(20)	2.039(11)	P(4)-O(20)	1.586(10)
Mo(4)-O(13)	2.130(9)	Mo(6)-O(18)	1.677(10)
Mo(4)-O(7)	2.283(8)	Mo(6)-O(12)	1.947(9)
Mo(4)-Mo(5)	2.6084(16)	Mo(6)-O(4)	1.967(9)
Mo(5)-O(29)	1.686(9)	Mo(6)-O(16)	2.058(10)
Mo(5)-O(1)	1.955(9)	Mo(6)-O(3)	2.133(8)
Mo(5)-O(17)	1.970(11)	Mo(6)-O(5)	2.303(10)
Mo(5)-O(28)	2.039(9)	Cd(1)-O(1)	2.254(10)
Mo(5)-O(3)	2.104(10)	Cd(1)-O(1)#1	2.254(10)
Mo(5)-O(5)	2.244(8)	Cd(1)-O(2)	2.262(9)
Cd(1)-O(2)#1	2.262(9)		
O(31)-Mo(1)-O(12)	107.2(4)	O(1)-Cd(1)-O(2)#1	84.3(4)
O(31)-Mo(1)-O(4)	100.5(5)	O(1)#1-Cd(1)-O(2)#1	95.7(4)
O(12)-Mo(1)-O(4)	94.7(4)	O(2)-Cd(1)-O(2)#1	180.0(5)
O(31)-Mo(1)-O(22)	97.5(5)	O(1)-Cd(1)-O(4)#1	82.9(3)
O(12)-Mo(1)-O(22)	85.8(4)	O(1)#1-Cd(1)-O(4)#1	97.1(3)
O(4)-Mo(1)-O(22)	161.0(4)	O(2)-Cd(1)-O(4)#1	81.8(3)
O(31)-Mo(1)-O(8)	97.7(5)	O(2)#1-Cd(1)-O(4)#1	98.2(3)

O(12)-Mo(1)-O(8)	154.5(4)	O(1)-Cd(1)-O(4)	97.1(3)
O(4)-Mo(1)-O(8)	85.9(3)	O(1)#1-Cd(1)-O(4)	82.9(3)
O(22)-Mo(1)-O(8)	85.5(4)	O(2)-Cd(1)-O(4)	98.2(3)
O(31)-Mo(1)-O(10)	167.9(4)	O(2)#1-Cd(1)-O(4)	81.8(3)
O(12)-Mo(1)-O(10)	83.9(4)	O(4)#1-Cd(1)-O(4)	179.999(1)
O(4)-Mo(1)-O(10)	82.8(4)	N(1)-Cd(2)-O(19)	165.7(6)
O(22)-Mo(1)-O(10)	78.4(4)	N(1)-Cd(2)-O(26)#2	96.8(7)
O(8)-Mo(1)-O(10)	70.8(4)	O(19)-Cd(2)-O(26)#2	91.4(4)
O(31)-Mo(1)-Mo(6)	100.6(3)	N(1)-Cd(2)-N(2)	77.8(6)
O(12)-Mo(1)-Mo(6)	48.0(3)	O(19)-Cd(2)-N(2)	88.5(5)
O(4)-Mo(1)-Mo(6)	48.4(2)	O(26)#2-Cd(2)-N(2)	109.3(6)
O(22)-Mo(1)-Mo(6)	133.6(3)	N(1)-Cd(2)-O(5W)	143.2(7)
O(8)-Mo(1)-Mo(6)	133.0(2)	O(19)-Cd(2)-O(5W)	51.0(6)
O(10)-Mo(1)-Mo(6)	90.3(2)	O(26)#2-Cd(2)-O(5W)	61.7(6)
O(30)-Mo(2)-O(11)	104.3(5)	N(2)-Cd(2)-O(5W)	135.7(6)
O(30)-Mo(2)-O(2)	100.9(4)	N(1)-Cd(2)-O(6)	96.0(5)
O(11)-Mo(2)-O(2)	94.6(4)	O(19)-Cd(2)-O(6)	96.6(3)
O(30)-Mo(2)-O(21)	97.5(4)	O(26)#2-Cd(2)-O(6)	83.3(4)
O(11)-Mo(2)-O(21)	85.9(4)	N(2)-Cd(2)-O(6)	166.3(6)
O(2)-Mo(2)-O(21)	160.9(4)	O(5W)-Cd(2)-O(6)	54.6(5)
O(30)-Mo(2)-O(8)	99.7(5)	O(6)-P(1)-O(10)	110.9(5)
O(11)-Mo(2)-O(8)	155.3(4)	O(6)-P(1)-O(7)	111.7(6)
O(2)-Mo(2)-O(8)	86.5(4)	O(10)-P(1)-O(7)	107.0(5)
O(21)-Mo(2)-O(8)	85.3(4)	O(6)-P(1)-O(5)	110.4(5)
O(30)-Mo(2)-O(10)	170.7(5)	O(10)-P(1)-O(5)	107.4(6)
O(11)-Mo(2)-O(10)	84.7(4)	O(7)-P(1)-O(5)	109.3(5)
O(2)-Mo(2)-O(10)	80.1(3)	O(16)-P(2)-O(27)	108.0(6)
O(21)-Mo(2)-O(10)	80.9(3)	O(16)-P(2)-O(28)	110.7(6)
O(8)-Mo(2)-O(10)	71.1(4)	O(27)-P(2)-O(28)	106.7(5)
O(30)-Mo(2)-Mo(3)	99.1(4)	O(16)-P(2)-O(19)	109.5(6)
O(11)-Mo(2)-Mo(3)	47.9(3)	O(27)-P(2)-O(19)	113.0(6)
O(2)-Mo(2)-Mo(3)	48.2(3)	O(28)-P(2)-O(19)	109.0(6)
O(21)-Mo(2)-Mo(3)	133.4(4)	O(24)-P(3)-O(23)	112.6(8)
O(8)-Mo(2)-Mo(3)	133.4(2)	O(24)-P(3)-O(21)	108.4(9)
O(10)-Mo(2)-Mo(3)	88.4(2)	O(23)-P(3)-O(21)	107.9(7)
O(9)-Mo(3)-O(11)	105.5(4)	O(24)-P(3)-O(22)	109.4(7)
O(9)-Mo(3)-O(2)	101.3(5)	O(23)-P(3)-O(22)	107.8(8)
O(11)-Mo(3)-O(2)	96.3(4)	O(21)-P(3)-O(22)	110.7(6)
O(9)-Mo(3)-O(15)	96.4(5)	O(26)-P(4)-O(25)	113.1(7)
O(11)-Mo(3)-O(15)	86.8(4)	O(26)-P(4)-O(15)	107.7(6)
O(2)-Mo(3)-O(15)	160.4(4)	O(25)-P(4)-O(15)	109.3(6)
O(9)-Mo(3)-O(13)	98.3(4)	O(26)-P(4)-O(20)	109.3(6)
O(11)-Mo(3)-O(13)	155.6(4)	O(25)-P(4)-O(20)	108.1(6)
O(2)-Mo(3)-O(13)	83.8(4)	O(15)-P(4)-O(20)	109.3(6)

O(15)-Mo(3)-O(13)	85.4(4)	O(1)-Mo(5)-O(5)	81.7(3)
O(9)-Mo(3)-O(7)	170.5(4)	O(17)-Mo(5)-O(5)	83.3(4)
O(11)-Mo(3)-O(7)	83.3(3)	O(28)-Mo(5)-O(5)	80.9(3)
O(2)-Mo(3)-O(7)	80.9(4)	O(3)-Mo(5)-O(5)	72.7(3)
O(15)-Mo(3)-O(7)	80.2(4)	O(29)-Mo(5)-Mo(4)	102.3(3)
O(13)-Mo(3)-O(7)	72.6(3)	O(1)-Mo(5)-Mo(4)	49.1(3)
O(9)-Mo(3)-Mo(2)	100.5(4)	O(17)-Mo(5)-Mo(4)	47.8(3)
O(11)-Mo(3)-Mo(2)	48.3(3)	O(28)-Mo(5)-Mo(4)	132.9(3)
O(2)-Mo(3)-Mo(2)	49.6(2)	O(3)-Mo(5)-Mo(4)	133.8(2)
O(15)-Mo(3)-Mo(2)	134.7(3)	O(5)-Mo(5)-Mo(4)	88.4(2)
O(13)-Mo(3)-Mo(2)	132.2(3)	O(18)-Mo(6)-O(12)	107.3(4)
O(7)-Mo(3)-Mo(2)	88.1(2)	O(18)-Mo(6)-O(4)	101.6(5)
O(14)-Mo(4)-O(17)	106.0(4)	O(12)-Mo(6)-O(4)	94.8(4)
O(14)-Mo(4)-O(1)	99.9(5)	O(18)-Mo(6)-O(16)	96.3(4)
O(17)-Mo(4)-O(1)	95.3(4)	O(12)-Mo(6)-O(16)	87.0(4)
O(14)-Mo(4)-O(20)	96.2(5)	O(4)-Mo(6)-O(16)	160.5(4)
O(17)-Mo(4)-O(20)	86.8(4)	O(18)-Mo(6)-O(3)	100.4(4)
O(1)-Mo(4)-O(20)	162.5(4)	O(12)-Mo(6)-O(3)	151.6(4)
O(14)-Mo(4)-O(13)	98.2(4)	O(4)-Mo(6)-O(3)	85.6(3)
O(17)-Mo(4)-O(13)	155.1(3)	O(16)-Mo(6)-O(3)	83.7(4)
O(1)-Mo(4)-O(13)	86.0(4)	O(18)-Mo(6)-O(5)	171.0(4)
O(20)-Mo(4)-O(13)	85.0(4)	O(12)-Mo(6)-O(5)	81.0(4)
O(14)-Mo(4)-O(7)	170.3(4)	O(4)-Mo(6)-O(5)	80.8(4)
O(17)-Mo(4)-O(7)	82.4(3)	O(16)-Mo(6)-O(5)	80.3(4)
O(1)-Mo(4)-O(7)	83.7(4)	O(3)-Mo(6)-O(5)	71.0(3)
O(20)-Mo(4)-O(7)	79.3(4)	O(18)-Mo(6)-Mo(1)	101.5(3)
O(13)-Mo(4)-O(7)	73.0(3)	O(12)-Mo(6)-Mo(1)	47.4(3)
O(14)-Mo(4)-Mo(5)	99.9(3)	O(4)-Mo(6)-Mo(1)	49.0(2)
O(17)-Mo(4)-Mo(5)	48.6(3)	O(16)-Mo(6)-Mo(1)	134.2(3)
O(1)-Mo(4)-Mo(5)	48.1(3)	O(3)-Mo(6)-Mo(1)	132.6(2)
O(20)-Mo(4)-Mo(5)	135.2(3)	O(5)-Mo(6)-Mo(1)	86.6(2)
O(13)-Mo(4)-Mo(5)	132.7(3)	O(1)-Cd(1)-O(1)#1	179.998(1)
O(7)-Mo(4)-Mo(5)	89.2(2)	O(1)-Cd(1)-O(2)	95.7(4)
O(29)-Mo(5)-O(1)	101.4(4)	O(1)#1-Cd(1)-O(2)	84.3(4)
O(29)-Mo(5)-O(17)	107.5(5)	O(17)-Mo(5)-O(28)	85.3(4)
O(1)-Mo(5)-O(17)	95.5(4)	O(29)-Mo(5)-O(3)	96.1(4)
O(29)-Mo(5)-O(28)	95.2(4)	O(1)-Mo(5)-O(3)	86.0(4)
O(1)-Mo(5)-O(28)	162.3(4)	O(17)-Mo(5)-O(3)	155.5(3)
O(29)-Mo(5)-O(5)	168.3(4)	O(28)-Mo(5)-O(3)	86.2(4)
Compound 2			
Cd(1)-O(13)	2.258(4)	Mo(3)-O(23)	1.675(4)
Cd(1)-O(13)#1	2.258(4)	Mo(3)-O(6)	1.942(4)
Cd(1)-O(14)#1	2.269(3)	Mo(3)-O(11)	1.965(3)
Cd(1)-O(14)	2.269(3)	Mo(3)-O(4)	2.070(4)

Cd(1)-O(11)	2.279(4)	Mo(3)-O(5)	2.102(4)
Cd(1)-O(11)#1	2.279(4)	Mo(3)-O(7)	2.280(3)
Cd(2)-N(1)	2.230(5)	Mo(4)-O(26)	1.682(4)
Cd(2)-O(1)	2.237(3)	Mo(4)-O(8)	1.946(4)
Cd(2)-O(27)	2.272(4)	Mo(4)-O(13)	1.970(4)
Cd(2)-O(1W)	2.339(4)	Mo(4)-O(21)	2.027(4)
Cd(2)-O(2)#2	2.348(4)	Mo(4)-O(15)	2.120(4)
Cd(2)-O(19)	2.819(4)	Mo(4)-O(10)	2.278(4)
Mo(1)-O(25)	1.676(4)	Mo(4)-Mo(6)	2.6017(9)
Mo(1)-O(6)	1.939(4)	Mo(5)-O(17)	1.682(4)
Mo(1)-O(11)	1.976(3)	Mo(5)-O(19)	1.945(4)
Mo(1)-O(24)	2.035(4)	Mo(5)-O(14)	1.964(3)
Mo(1)-O(12)	2.126(4)	Mo(5)-O(20)	2.038(4)
Mo(1)-O(9)	2.256(4)	Mo(5)-O(15)	2.103(4)
Mo(1)-Mo(3)	2.6160(8)	Mo(5)-O(10)	2.273(4)
Mo(2)-O(16)	1.685(4)	Mo(6)-O(22)	1.673(4)
Mo(2)-O(19)	1.931(4)	Mo(6)-O(8)	1.938(4)
Mo(2)-O(14)	1.964(3)	Mo(6)-O(13)	1.960(4)
Mo(2)-O(18)	2.036(4)	Mo(6)-O(3)	2.058(4)
Mo(2)-O(12)	2.128(4)	Mo(6)-O(5)	2.124(4)
Mo(2)-O(9)	2.244(4)	Mo(6)-O(7)	2.313(3)
Mo(2)-Mo(5)	2.6076(13)	P(1)-O(1)	1.499(4)
P(3)-O(29)	1.519(4)	P(1)-O(10)	1.549(4)
P(3)-O(27)	1.522(4)	P(1)-O(7)	1.550(4)
P(3)-O(18)	1.545(4)	P(1)-O(9)	1.558(4)
P(3)-O(24)	1.550(4)	P(2)-O(2)	1.520(4)
P(4)-O(30)	1.502(4)	P(2)-O(3)	1.526(4)
P(4)-O(31)	1.512(5)	P(2)-O(4)	1.531(4)
P(4)-O(21)	1.544(4)	P(2)-O(28)	1.564(4)
P(4)-O(20)	1.554(4)	O(2)-Cd(2)#2	2.348(4)
O(13)-Cd(1)-O(13)#1	180.00(13)	O(9)-Mo(2)-Mo(5)	88.54(9)
O(13)-Cd(1)-O(14)#1	82.27(13)	O(23)-Mo(3)-O(6)	105.28(18)
O(13)#1-Cd(1)-O(14)#1	97.73(13)	O(23)-Mo(3)-O(11)	101.92(17)
O(13)-Cd(1)-O(14)	97.73(13)	O(6)-Mo(3)-O(11)	94.93(15)
O(13)#1-Cd(1)-O(14)	82.27(13)	O(23)-Mo(3)-O(4)	94.81(17)
O(14)#1-Cd(1)-O(14)	180.000(2)	O(6)-Mo(3)-O(4)	87.76(15)
O(13)-Cd(1)-O(11)	95.64(13)	O(11)-Mo(3)-O(4)	161.66(14)
O(13)#1-Cd(1)-O(11)	84.36(13)	O(23)-Mo(3)-O(5)	97.39(17)
O(14)#1-Cd(1)-O(11)	82.77(13)	O(6)-Mo(3)-O(5)	156.29(14)
O(14)-Cd(1)-O(11)	97.23(13)	O(11)-Mo(3)-O(5)	86.98(14)
O(13)-Cd(1)-O(11)#1	84.36(13)	O(4)-Mo(3)-O(5)	83.45(15)
O(13)#1-Cd(1)-O(11)#1	95.64(13)	O(23)-Mo(3)-O(7)	169.20(16)
O(14)#1-Cd(1)-O(11)#1	97.23(13)	O(6)-Mo(3)-O(7)	83.59(14)

O(14)-Cd(1)-O(11)#1	82.77(13)	O(11)-Mo(3)-O(7)	83.12(14)
O(11)-Cd(1)-O(11)#1	180.0	O(4)-Mo(3)-O(7)	79.16(14)
N(1)-Cd(2)-O(1)	154.23(16)	O(5)-Mo(3)-O(7)	73.16(13)
N(1)-Cd(2)-O(27)	100.11(17)	O(23)-Mo(3)-Mo(1)	101.51(14)
O(1)-Cd(2)-O(27)	95.29(14)	O(6)-Mo(3)-Mo(1)	47.58(11)
N(1)-Cd(2)-O(1W)	81.97(17)	O(11)-Mo(3)-Mo(1)	48.60(10)
O(1)-Cd(2)-O(1W)	88.09(14)	O(4)-Mo(3)-Mo(1)	135.00(11)
O(27)-Cd(2)-O(1W)	165.90(15)	O(5)-Mo(3)-Mo(1)	134.29(10)
N(1)-Cd(2)-O(2)#2	122.92(16)	O(7)-Mo(3)-Mo(1)	89.01(9)
O(1)-Cd(2)-O(2)#2	79.49(13)	O(26)-Mo(4)-O(8)	106.43(19)
O(27)-Cd(2)-O(2)#2	81.94(14)	O(26)-Mo(4)-O(13)	99.71(18)
O(1W)-Cd(2)-O(2)#2	85.24(15)	O(8)-Mo(4)-O(13)	94.79(15)
N(1)-Cd(2)-O(19)	72.94(15)	O(26)-Mo(4)-O(21)	95.9(2)
O(1)-Cd(2)-O(19)	84.03(12)	O(8)-Mo(4)-O(21)	87.73(17)
O(27)-Cd(2)-O(19)	100.67(13)	O(13)-Mo(4)-O(21)	162.76(16)
O(1W)-Cd(2)-O(19)	93.29(14)	O(26)-Mo(4)-O(15)	98.09(18)
O(2)#2-Cd(2)-O(19)	163.50(12)	O(8)-Mo(4)-O(15)	154.72(15)
O(25)-Mo(1)-O(6)	105.86(18)	O(13)-Mo(4)-O(15)	86.91(14)
O(25)-Mo(1)-O(11)	101.40(17)	O(21)-Mo(4)-O(15)	83.68(16)
O(6)-Mo(1)-O(11)	94.65(15)	O(26)-Mo(4)-O(10)	169.73(17)
O(25)-Mo(1)-O(24)	96.46(18)	O(8)-Mo(4)-O(10)	83.76(14)
O(6)-Mo(1)-O(24)	86.43(15)	O(13)-Mo(4)-O(10)	80.35(14)
O(11)-Mo(1)-O(24)	161.06(15)	O(21)-Mo(4)-O(10)	82.98(16)
O(25)-Mo(1)-O(12)	97.64(17)	O(15)-Mo(4)-O(10)	71.64(13)
O(6)-Mo(1)-O(12)	155.63(14)	O(26)-Mo(4)-Mo(6)	100.10(15)
O(11)-Mo(1)-O(12)	86.83(14)	O(8)-Mo(4)-Mo(6)	47.82(11)
O(24)-Mo(1)-O(12)	84.58(15)	O(13)-Mo(4)-Mo(6)	48.38(11)
O(25)-Mo(1)-O(9)	168.57(17)	O(21)-Mo(4)-Mo(6)	135.38(13)
O(6)-Mo(1)-O(9)	85.20(14)	O(15)-Mo(4)-Mo(6)	133.84(10)
O(11)-Mo(1)-O(9)	80.20(14)	O(10)-Mo(4)-Mo(6)	87.66(9)
O(24)-Mo(1)-O(9)	81.05(14)	O(17)-Mo(5)-O(19)	106.98(19)
O(12)-Mo(1)-O(9)	71.06(13)	O(17)-Mo(5)-O(14)	101.51(18)
O(25)-Mo(1)-Mo(3)	101.53(14)	O(19)-Mo(5)-O(14)	94.19(15)
O(6)-Mo(1)-Mo(3)	47.66(11)	O(17)-Mo(5)-O(20)	94.98(19)
O(11)-Mo(1)-Mo(3)	48.23(10)	O(19)-Mo(5)-O(20)	87.87(17)
O(24)-Mo(1)-Mo(3)	133.66(11)	O(14)-Mo(5)-O(20)	161.97(16)
O(12)-Mo(1)-Mo(3)	133.64(10)	O(17)-Mo(5)-O(15)	98.16(18)
O(9)-Mo(1)-Mo(3)	88.03(9)	O(19)-Mo(5)-O(15)	154.19(15)
O(16)-Mo(2)-O(19)	108.71(18)	O(14)-Mo(5)-O(15)	86.28(14)
O(16)-Mo(2)-O(14)	101.19(17)	O(20)-Mo(5)-O(15)	84.19(16)
O(19)-Mo(2)-O(14)	94.66(15)	O(17)-Mo(5)-O(10)	169.42(18)
O(16)-Mo(2)-O(18)	95.24(18)	O(19)-Mo(5)-O(10)	82.45(15)
O(19)-Mo(2)-O(18)	86.78(17)	O(14)-Mo(5)-O(10)	82.18(14)
O(14)-Mo(2)-O(18)	162.06(15)	O(20)-Mo(5)-O(10)	80.34(15)

O(16)-Mo(2)-O(12)	96.82(17)	O(15)-Mo(5)-O(10)	72.03(13)
O(19)-Mo(2)-O(12)	153.58(15)	O(17)-Mo(5)-Mo(2)	100.97(15)
O(14)-Mo(2)-O(12)	86.76(14)	O(19)-Mo(5)-Mo(2)	47.48(11)
O(18)-Mo(2)-O(12)	84.16(15)	O(14)-Mo(5)-Mo(2)	48.39(10)
O(16)-Mo(2)-O(9)	167.78(17)	O(20)-Mo(5)-Mo(2)	135.20(13)
O(19)-Mo(2)-O(9)	82.88(15)	O(15)-Mo(5)-Mo(2)	133.35(10)
O(14)-Mo(2)-O(9)	81.19(14)	O(10)-Mo(5)-Mo(2)	88.92(9)
O(18)-Mo(2)-O(9)	81.25(14)	O(22)-Mo(6)-O(8)	105.92(18)
O(12)-Mo(2)-O(9)	71.24(13)	O(22)-Mo(6)-O(13)	102.24(18)
O(16)-Mo(2)-Mo(5)	102.05(15)	O(8)-Mo(6)-O(13)	95.37(15)
O(19)-Mo(2)-Mo(5)	47.94(12)	O(22)-Mo(6)-O(3)	96.90(18)
O(14)-Mo(2)-Mo(5)	48.42(10)	O(8)-Mo(6)-O(3)	85.18(16)
O(18)-Mo(2)-Mo(5)	134.57(12)	O(13)-Mo(6)-O(3)	159.89(15)
O(12)-Mo(2)-Mo(5)	133.74(10)	O(22)-Mo(6)-O(5)	96.99(17)
O(1)-P(1)-O(10)	112.5(2)	O(8)-Mo(6)-O(5)	156.22(15)
O(1)-P(1)-O(7)	112.9(2)	O(13)-Mo(6)-O(5)	85.75(14)
O(10)-P(1)-O(7)	107.0(2)	O(3)-Mo(6)-O(5)	85.84(15)
O(1)-P(1)-O(9)	109.4(2)	O(22)-Mo(6)-O(7)	168.07(17)
O(10)-P(1)-O(9)	107.6(2)	O(8)-Mo(6)-O(7)	84.52(14)
O(7)-P(1)-O(9)	107.20(19)	O(13)-Mo(6)-O(7)	82.11(14)
O(2)-P(2)-O(3)	112.2(2)	O(3)-Mo(6)-O(7)	77.93(13)
O(2)-P(2)-O(4)	112.0(2)	O(5)-Mo(6)-O(7)	72.08(13)
O(3)-P(2)-O(4)	110.8(2)	O(22)-Mo(6)-Mo(4)	101.67(15)
O(2)-P(2)-O(28)	106.2(2)	O(8)-Mo(6)-Mo(4)	48.08(11)
O(3)-P(2)-O(28)	108.0(2)	O(13)-Mo(6)-Mo(4)	48.72(10)
O(4)-P(2)-O(28)	107.3(2)	O(3)-Mo(6)-Mo(4)	132.78(11)
O(29)-P(3)-O(27)	112.1(2)	O(5)-Mo(6)-Mo(4)	133.35(10)
O(29)-P(3)-O(18)	108.8(2)	O(7)-Mo(6)-Mo(4)	89.58(9)
O(27)-P(3)-O(18)	109.8(2)	O(31)-P(4)-O(21)	107.4(3)
O(29)-P(3)-O(24)	106.5(2)	O(30)-P(4)-O(20)	109.2(3)
O(27)-P(3)-O(24)	110.5(2)	O(31)-P(4)-O(20)	109.3(3)
O(18)-P(3)-O(24)	109.1(2)	O(21)-P(4)-O(20)	109.0(2)
O(30)-P(4)-O(31)	112.7(3)	O(30)-P(4)-O(21)	109.1(3)
Compound 3			
Mo(1)-O(23)	1.694(3)	Mo(6)-O(27)	1.682(3)
Mo(1)-O(22)	1.933(3)	Mo(6)-O(10)	1.938(3)
Mo(1)-O(2)	1.947(3)	Mo(6)-O(1)	1.960(3)
Mo(1)-O(24)	2.060(3)	Mo(6)-O(28)	2.065(3)
Mo(1)-O(15)	2.121(3)	Mo(6)-O(12)	2.120(3)
Mo(1)-O(13)	2.304(3)	Mo(6)-O(11)	2.273(3)
Mo(1)-Mo(3)	2.5914(11)	Na(1)-O(2)	2.242(3)
Mo(2)-O(17)	1.673(3)	Na(1)-O(2)#1	2.242(3)
Mo(2)-O(4)	1.941(3)	Na(1)-O(1)	2.261(3)
Mo(2)-O(3)	1.943(3)	Na(1)-O(1)#1	2.261(3)

Mo(2)-O(18)	2.084(3)	Na(1)-O(3)#1	2.354(3)
Mo(2)-O(16)	2.128(3)	Na(1)-O(3)	2.354(3)
Mo(2)-O(14)	2.306(3)	Na(2)-O(5)#2	2.419(4)
Mo(2)-Mo(4)	2.5932(9)	Na(2)-O(5)	2.419(4)
Mo(3)-O(21)	1.688(3)	Na(2)-O(6)#2	2.458(3)
Mo(3)-O(22)	1.937(3)	Na(2)-O(6)	2.458(3)
Mo(3)-O(2)	1.942(3)	Na(2)-O(4)	2.553(3)
Mo(3)-O(20)	2.081(3)	Na(2)-O(4)#2	2.553(3)
Mo(3)-O(16)	2.127(3)	Na(2)-P(1)#2	3.2642(15)
Mo(3)-O(14)	2.276(3)	Na(2)-P(1)	3.2642(15)
Mo(4)-O(31)	1.683(4)	Na(2)-P(2)#2	3.3934(17)
Mo(4)-O(4)	1.946(3)	Na(2)-P(2)	3.3934(17)
Mo(4)-O(3)	1.954(3)	P(1)-O(6)	1.513(3)
Mo(4)-O(29)	2.106(3)	P(1)-O(14)	1.551(3)
Mo(4)-O(12)	2.113(3)	P(1)-O(11)	1.550(3)
Mo(4)-O(11)	2.283(3)	P(1)-O(13)	1.551(3)
Mo(5)-O(26)	1.684(3)	P(2)-O(19)	1.500(3)
Mo(5)-O(10)	1.935(3)	P(2)-O(18)	1.520(4)
Mo(5)-O(1)	1.942(3)	P(2)-O(20)	1.530(4)
Mo(5)-O(25)	2.068(3)	P(2)-O(5)	1.581(4)
Mo(5)-O(15)	2.113(3)	P(3)-O(9)	1.523(4)
Mo(5)-O(13)	2.286(3)	P(3)-O(8)	1.523(3)
Mo(5)-Mo(6)	2.5734(10)	P(3)-O(24)	1.544(3)
P(4)-O(28)	1.544(4)	P(3)-O(25)	1.547(3)
P(4)-O(29)	1.553(3)	P(4)-O(30)	1.502(4)
P(4)-O(7)	1.565(4)		
O(23)-Mo(1)-O(22)	106.84(15)	O(10)-Mo(6)-O(11)	82.79(12)
O(23)-Mo(1)-O(2)	102.19(15)	O(1)-Mo(6)-O(11)	81.34(12)
O(22)-Mo(1)-O(2)	94.98(13)	O(28)-Mo(6)-O(11)	81.99(12)
O(23)-Mo(1)-O(24)	96.64(15)	O(12)-Mo(6)-O(11)	71.30(11)
O(22)-Mo(1)-O(24)	86.79(14)	O(2)-Na(1)-O(2)#1	179.999(1)
O(2)-Mo(1)-O(24)	159.66(13)	O(2)-Na(1)-O(1)	95.06(11)
O(23)-Mo(1)-O(15)	96.10(14)	O(2)#1-Na(1)-O(1)	84.94(11)
O(22)-Mo(1)-O(15)	156.43(13)	O(2)-Na(1)-O(1)#1	84.94(11)
O(2)-Mo(1)-O(15)	85.17(12)	O(2)#1-Na(1)-O(1)#1	95.06(11)
O(24)-Mo(1)-O(15)	85.25(13)	O(1)-Na(1)-O(1)#1	180.0
O(23)-Mo(1)-O(13)	167.68(13)	O(2)-Na(1)-O(3)#1	80.50(11)
O(22)-Mo(1)-O(13)	84.33(12)	O(2)#1-Na(1)-O(3)#1	99.50(11)
O(2)-Mo(1)-O(13)	81.54(12)	O(1)-Na(1)-O(3)#1	82.68(11)
O(24)-Mo(1)-O(13)	78.47(12)	O(1)#1-Na(1)-O(3)#1	97.32(12)
O(15)-Mo(1)-O(13)	72.35(11)	O(2)-Na(1)-O(3)	99.50(11)
O(23)-Mo(1)-Mo(3)	103.09(12)	O(2)#1-Na(1)-O(3)	80.50(11)
O(22)-Mo(1)-Mo(3)	48.04(9)	O(1)-Na(1)-O(3)	97.32(11)

O(2)-Mo(1)-Mo(3)	48.14(9)	O(1)#1-Na(1)-O(3)	82.68(12)
O(24)-Mo(1)-Mo(3)	134.15(10)	O(3)#1-Na(1)-O(3)	180.00(14)
O(15)-Mo(1)-Mo(3)	132.05(9)	O(5)#2-Na(2)-O(5)	180.0
O(13)-Mo(1)-Mo(3)	88.19(8)	O(5)#2-Na(2)-O(6)#2	89.00(12)
O(17)-Mo(2)-O(4)	106.24(16)	O(5)-Na(2)-O(6)#2	91.00(12)
O(17)-Mo(2)-O(3)	103.19(15)	O(5)#2-Na(2)-O(6)	91.00(12)
O(4)-Mo(2)-O(3)	95.17(13)	O(5)-Na(2)-O(6)	89.00(12)
O(17)-Mo(2)-O(18)	94.27(16)	O(6)#2-Na(2)-O(6)	180.0
O(4)-Mo(2)-O(18)	86.58(14)	O(5)#2-Na(2)-O(4)	72.94(11)
O(3)-Mo(2)-O(18)	161.15(14)	O(5)-Na(2)-O(4)	107.06(11)
O(17)-Mo(2)-O(16)	100.13(16)	O(6)#2-Na(2)-O(4)	92.06(10)
O(4)-Mo(2)-O(16)	152.90(13)	O(6)-Na(2)-O(4)	87.94(10)
O(3)-Mo(2)-O(16)	84.66(13)	O(5)#2-Na(2)-O(4)#2	107.06(11)
O(18)-Mo(2)-O(16)	85.33(13)	O(5)-Na(2)-O(4)#2	72.94(11)
O(17)-Mo(2)-O(14)	168.11(14)	O(6)#2-Na(2)-O(4)#2	87.94(10)
O(4)-Mo(2)-O(14)	82.39(13)	O(6)-Na(2)-O(4)#2	92.06(10)
O(3)-Mo(2)-O(14)	83.78(12)	O(4)-Na(2)-O(4)#2	180.00(10)
O(18)-Mo(2)-O(14)	77.84(12)	O(6)-P(1)-O(14)	111.34(18)
O(16)-Mo(2)-O(14)	70.62(11)	O(6)-P(1)-O(11)	110.14(18)
O(21)-Mo(3)-O(22)	105.47(16)	O(14)-P(1)-O(11)	108.04(17)
O(21)-Mo(3)-O(2)	102.23(15)	O(6)-P(1)-O(13)	111.78(18)
O(22)-Mo(3)-O(2)	94.99(13)	O(14)-P(1)-O(13)	107.37(17)
O(21)-Mo(3)-O(20)	92.68(15)	O(11)-P(1)-O(13)	108.01(17)
O(22)-Mo(3)-O(20)	86.91(14)	O(6)-P(1)-Na(2)	45.66(13)
O(2)-Mo(3)-O(20)	163.82(13)	O(14)-P(1)-Na(2)	75.32(12)
O(21)-Mo(3)-O(16)	97.92(15)	O(11)-P(1)-Na(2)	96.78(12)
O(22)-Mo(3)-O(16)	155.26(13)	O(13)-P(1)-Na(2)	152.27(12)
O(2)-Mo(3)-O(16)	87.74(13)	O(19)-P(2)-O(18)	111.7(2)
O(20)-Mo(3)-O(16)	83.99(13)	O(19)-P(2)-O(20)	111.2(2)
O(21)-Mo(3)-O(14)	167.97(15)	O(18)-P(2)-O(20)	111.45(19)
O(22)-Mo(3)-O(14)	84.69(12)	O(19)-P(2)-O(5)	109.7(2)
O(2)-Mo(3)-O(14)	82.92(12)	O(18)-P(2)-O(5)	105.4(2)
O(20)-Mo(3)-O(14)	81.26(12)	O(20)-P(2)-O(5)	107.1(2)
O(16)-Mo(3)-O(14)	71.22(12)	O(9)-P(3)-O(8)	111.4(2)
O(31)-Mo(4)-O(4)	107.30(16)	O(9)-P(3)-O(24)	109.5(2)
O(31)-Mo(4)-O(3)	103.08(16)	O(8)-P(3)-O(24)	107.3(2)
O(4)-Mo(4)-O(3)	94.68(13)	O(9)-P(3)-O(25)	109.4(2)
O(31)-Mo(4)-O(29)	93.89(16)	O(8)-P(3)-O(25)	108.5(2)
O(4)-Mo(4)-O(29)	86.89(13)	O(24)-P(3)-O(25)	110.77(18)
O(3)-Mo(4)-O(29)	161.61(14)	O(30)-P(4)-O(28)	114.0(2)
O(31)-Mo(4)-O(12)	98.72(16)	O(30)-P(4)-O(29)	114.0(2)
O(4)-Mo(4)-O(12)	153.20(13)	O(28)-P(4)-O(29)	107.71(19)
O(3)-Mo(4)-O(12)	85.43(13)	O(30)-P(4)-O(7)	107.3(2)
O(29)-Mo(4)-O(12)	85.01(13)	O(28)-P(4)-O(7)	106.0(2)

O(31)-Mo(4)-O(11)	168.35(15)	O(29)-P(4)-O(7)	107.2(2)
O(4)-Mo(4)-O(11)	82.21(13)	O(27)-Mo(6)-O(10)	105.94(16)
O(3)-Mo(4)-O(11)	82.38(12)	O(27)-Mo(6)-O(1)	99.89(15)
O(29)-Mo(4)-O(11)	79.67(13)	O(10)-Mo(6)-O(1)	95.19(13)
O(12)-Mo(4)-O(11)	71.22(11)	O(27)-Mo(6)-O(28)	96.13(16)
O(26)-Mo(5)-O(10)	103.86(15)	O(10)-Mo(6)-O(28)	85.54(14)
O(26)-Mo(5)-O(1)	101.11(15)	O(1)-Mo(6)-O(28)	163.09(13)
O(10)-Mo(5)-O(1)	95.89(13)	O(27)-Mo(6)-O(12)	99.75(15)
O(26)-Mo(5)-O(25)	94.91(16)	O(10)-Mo(6)-O(12)	153.32(13)
O(10)-Mo(5)-O(25)	87.49(14)	O(1)-Mo(6)-O(12)	87.28(13)
O(1)-Mo(5)-O(25)	162.29(13)	O(28)-Mo(6)-O(12)	84.69(13)
O(26)-Mo(5)-O(15)	99.17(15)	O(27)-Mo(6)-O(11)	170.96(15)
O(10)-Mo(5)-O(15)	155.91(13)	O(10)-Mo(5)-O(13)	83.57(12)
O(1)-Mo(5)-O(15)	86.44(13)	O(1)-Mo(5)-O(13)	83.34(12)
O(25)-Mo(5)-O(15)	83.57(13)	O(25)-Mo(5)-O(13)	79.76(12)
O(26)-Mo(5)-O(13)	170.75(14)	O(15)-Mo(5)-O(13)	72.85(11)

Compound 4

Cd(1)-O(29)#1	2.2496(18)	Mo(5)-O(17)	1.680(2)
Cd(1)-O(29)	2.2497(18)	Mo(5)-O(27)	1.9303(19)
Cd(1)-O(28)	2.2728(18)	Mo(5)-O(20)	1.9718(18)
Cd(1)-O(28)#1	2.2728(18)	Mo(5)-O(31)	2.0528(19)
Cd(1)-O(20)#1	2.2750(18)	Mo(5)-O(13)	2.1267(19)
Cd(1)-O(20)	2.2750(18)	Mo(5)-O(8)	2.2806(18)
Mo(1)-O(24)	1.687(2)	Mo(6)-O(7)	1.677(2)
Mo(1)-O(22)	1.9318(19)	Mo(6)-O(3)	1.9397(19)
Mo(1)-O(29)	1.9749(18)	Mo(6)-O(28)	1.9643(18)
Mo(1)-O(25)	2.022(2)	Mo(6)-O(26)	2.0802(19)
Mo(1)-O(12)	2.1252(18)	Mo(6)-O(13)	2.1362(19)
Mo(1)-O(2)	2.2602(18)	Mo(6)-O(8)	2.2847(18)
Mo(1)-Mo(2)	2.6284(3)	P(1)-O(5)	1.509(2)
Mo(2)-O(15)	1.678(2)	P(1)-O(31)	1.534(2)
Mo(2)-O(22)	1.9509(19)	P(1)-O(26)	1.539(2)
Mo(2)-O(29)	1.9694(18)	P(1)-O(21)	1.560(2)
Mo(2)-O(11)	2.0698(19)	P(2)-O(14)	1.5118(19)
Mo(2)-O(18)	2.1012(19)	P(2)-O(16)	1.5433(19)
Mo(2)-O(16)	2.2944(18)	P(2)-O(2)	1.5505(19)
Mo(3)-O(9)	1.680(2)	P(2)-O(8)	1.5521(19)
Mo(3)-O(27)	1.9414(19)	P(3)-O(6)	1.502(2)
Mo(3)-O(20)	1.9715(18)	P(3)-O(23)	1.538(2)
Mo(3)-O(23)	2.041(2)	P(3)-O(11)	1.541(2)
Mo(3)-O(18)	2.1197(19)	P(3)-O(30)	1.568(2)
Mo(3)-O(16)	2.2874(18)	P(4)-O(1)	1.515(2)
Mo(3)-Mo(5)	2.6051(3)	P(4)-O(4)	1.522(2)
Mo(4)-O(10)	1.682(2)	P(4)-O(19)	1.557(2)

Mo(4)-O(3)	1.9354(19)	P(4)-O(25)	1.558(2)
Mo(4)-O(28)	1.9689(19)	Mo(4)-O(12)	2.1316(18)
Mo(4)-O(19)	2.0270(19)	Mo(4)-O(2)	2.2571(18)
Mo(4)-Mo(6)	2.6006(3)		
O(29)#1-Cd(1)-O(29)	180.00(10)	O(17)-Mo(5)-O(27)	106.79(9)
O(29)#1-Cd(1)-O(28)	80.85(7)	O(17)-Mo(5)-O(20)	100.91(9)
O(29)-Cd(1)-O(28)	99.15(7)	O(27)-Mo(5)-O(20)	95.19(8)
O(29)#1-Cd(1)-O(28)#1	99.15(7)	O(17)-Mo(5)-O(31)	94.33(9)
O(29)-Cd(1)-O(28)#1	80.85(7)	O(27)-Mo(5)-O(31)	87.78(8)
O(28)-Cd(1)-O(28)#1	180.0	O(20)-Mo(5)-O(31)	162.86(8)
O(29)#1-Cd(1)-O(20)#1	96.51(6)	O(17)-Mo(5)-O(13)	96.64(9)
O(29)-Cd(1)-O(20)#1	83.49(6)	O(27)-Mo(5)-O(13)	155.46(8)
O(28)-Cd(1)-O(20)#1	83.19(7)	O(20)-Mo(5)-O(13)	87.30(7)
O(28)#1-Cd(1)-O(20)#1	96.81(7)	O(31)-Mo(5)-O(13)	83.18(8)
O(29)#1-Cd(1)-O(20)	83.49(6)	O(17)-Mo(5)-O(8)	168.76(9)
O(29)-Cd(1)-O(20)	96.50(6)	O(27)-Mo(5)-O(8)	83.81(7)
O(28)-Cd(1)-O(20)	96.81(7)	O(20)-Mo(5)-O(8)	81.42(7)
O(28)#1-Cd(1)-O(20)	83.19(7)	O(31)-Mo(5)-O(8)	82.14(7)
O(20)#1-Cd(1)-O(20)	180.0	O(13)-Mo(5)-O(8)	72.40(7)
O(24)-Mo(1)-O(22)	106.99(9)	O(7)-Mo(6)-O(3)	106.14(9)
O(24)-Mo(1)-O(29)	99.58(9)	O(7)-Mo(6)-O(28)	103.06(9)
O(22)-Mo(1)-O(29)	94.46(8)	O(3)-Mo(6)-O(28)	95.07(8)
O(24)-Mo(1)-O(25)	97.18(9)	O(7)-Mo(6)-O(26)	95.39(9)
O(22)-Mo(1)-O(25)	87.65(8)	O(3)-Mo(6)-O(26)	85.87(8)
O(29)-Mo(1)-O(25)	161.68(8)	O(28)-Mo(6)-O(26)	160.44(8)
O(24)-Mo(1)-O(12)	97.24(9)	O(7)-Mo(6)-O(13)	97.15(9)
O(22)-Mo(1)-O(12)	155.12(8)	O(3)-Mo(6)-O(13)	155.99(8)
O(29)-Mo(1)-O(12)	86.82(7)	O(28)-Mo(6)-O(13)	85.12(7)
O(25)-Mo(1)-O(12)	83.77(8)	O(26)-Mo(6)-O(13)	86.19(8)
O(24)-Mo(1)-O(2)	168.55(9)	O(7)-Mo(6)-O(8)	168.08(9)
O(22)-Mo(1)-O(2)	84.27(7)	O(3)-Mo(6)-O(8)	84.10(7)
O(29)-Mo(1)-O(2)	81.18(7)	O(28)-Mo(6)-O(8)	81.66(7)
O(25)-Mo(1)-O(2)	80.93(8)	O(26)-Mo(6)-O(8)	78.99(7)
O(12)-Mo(1)-O(2)	71.35(7)	O(13)-Mo(6)-O(8)	72.15(7)
O(15)-Mo(2)-O(22)	105.54(9)	O(5)-P(1)-O(31)	110.06(11)
O(15)-Mo(2)-O(29)	101.06(9)	O(5)-P(1)-O(26)	110.84(12)
O(22)-Mo(2)-O(29)	94.04(8)	O(31)-P(1)-O(26)	110.72(11)
O(15)-Mo(2)-O(11)	95.85(9)	O(5)-P(1)-O(21)	110.14(12)
O(22)-Mo(2)-O(11)	87.94(8)	O(31)-P(1)-O(21)	109.46(12)
O(29)-Mo(2)-O(11)	161.76(8)	O(26)-P(1)-O(21)	105.52(12)
O(15)-Mo(2)-O(18)	99.12(9)	O(14)-P(2)-O(16)	112.44(11)
O(22)-Mo(2)-O(18)	154.40(8)	O(14)-P(2)-O(2)	109.99(11)
O(29)-Mo(2)-O(18)	87.84(7)	O(16)-P(2)-O(2)	107.48(10)

O(11)-Mo(2)-O(18)	82.73(8)	O(14)-P(2)-O(8)	112.25(11)
O(15)-Mo(2)-O(16)	170.66(9)	O(16)-P(2)-O(8)	107.11(10)
O(22)-Mo(2)-O(16)	82.83(7)	O(2)-P(2)-O(8)	107.32(10)
O(29)-Mo(2)-O(16)	82.17(7)	O(6)-P(3)-O(23)	110.53(12)
O(11)-Mo(2)-O(16)	80.09(7)	O(6)-P(3)-O(11)	114.06(12)
O(18)-Mo(2)-O(16)	72.12(7)	O(23)-P(3)-O(11)	111.00(11)
O(9)-Mo(3)-O(27)	105.31(9)	O(6)-P(3)-O(30)	105.90(12)
O(9)-Mo(3)-O(20)	102.01(9)	O(23)-P(3)-O(30)	107.99(12)
O(27)-Mo(3)-O(20)	94.84(8)	O(11)-P(3)-O(30)	107.00(12)
O(9)-Mo(3)-O(23)	98.02(10)	O(1)-P(4)-O(4)	113.33(12)
O(27)-Mo(3)-O(23)	84.50(8)	O(1)-P(4)-O(19)	108.54(12)
O(20)-Mo(3)-O(23)	159.37(8)	O(4)-P(4)-O(19)	108.67(12)
O(9)-Mo(3)-O(18)	97.59(9)	O(1)-P(4)-O(25)	107.57(12)
O(27)-Mo(3)-O(18)	156.23(8)	O(4)-P(4)-O(25)	110.09(12)
O(20)-Mo(3)-O(18)	86.46(7)	O(19)-P(4)-O(25)	108.54(11)
O(23)-Mo(3)-O(18)	86.07(8)	O(10)-Mo(4)-O(3)	106.58(9)
O(9)-Mo(3)-O(16)	168.97(9)	O(10)-Mo(4)-O(28)	100.31(9)
O(27)-Mo(3)-O(16)	84.77(7)	O(3)-Mo(4)-O(28)	95.06(8)
O(20)-Mo(3)-O(16)	81.22(7)	O(10)-Mo(4)-O(19)	97.17(10)
O(23)-Mo(3)-O(16)	78.19(7)	O(3)-Mo(4)-O(19)	84.73(8)
O(18)-Mo(3)-O(16)	71.94(7)	O(28)-Mo(4)-O(19)	161.80(8)
O(9)-Mo(3)-Mo(5)	101.25(7)	O(10)-Mo(4)-O(12)	97.35(9)
O(27)-Mo(3)-Mo(5)	47.53(6)	O(3)-Mo(4)-O(12)	155.25(8)
O(20)-Mo(3)-Mo(5)	48.66(5)	O(28)-Mo(4)-O(12)	86.66(7)
O(23)-Mo(3)-Mo(5)	131.46(6)	O(19)-Mo(4)-O(12)	86.11(8)
O(18)-Mo(3)-Mo(5)	133.91(5)	O(10)-Mo(4)-O(2)	168.54(9)
O(16)-Mo(3)-Mo(5)	88.84(5)	O(3)-Mo(4)-O(2)	84.55(7)
O(19)-Mo(4)-O(2)	80.85(8)	O(28)-Mo(4)-O(2)	81.01(7)
O(12)-Mo(4)-O(2)	71.30(7)		

Symmetry transformations used to generate equivalent atoms: #1 $-x+1/2, -y+3/2, -z$; #2 $-x+1/2, y-1/2, -z+1/2$; #3 $-x+1/2, y+1/2, -z+1/2$; #4 $-x, y, -z+1/2$ for **1**; #1 $-x+2, -y+1, -z+1$, #2 $-x+2, -y+1, -z+2$ for **2**; #1 $-x, -y+2, -z+1$; #2 $-x, -y+2, -z+2$ for **3** and #1 $-x+2, -y+1, -z$ for **4**.

Table S2 Bond valence sums (Σs) for compounds **1-4**.

Compound	atom	Σs	atom	Σs	atom	Σs
1	Mo1	5.01	P1	5.18	O3	0.96
	Mo2	4.98	P2	5.21	O8	0.97
	Mo3	5.12	P3	5.31	O13	0.97
	Mo4	4.90	P4	5.06	O25	1.29
	Mo5	4.97			O27	1.34
	Mo6	4.85				
2	Mo1	4.99	P1	5.01	O5	0.99
	Mo2	5.01	P2	5.06	O12	0.94
	Mo3	4.97	P3	5.08	O15	0.99
	Mo4	4.97	P4	5.14	O31	1.32
	Mo5	5.01			O28	1.16
	Mo6	4.97			O29	1.31
3	Mo1	4.91	P1	4.98961	O12	0.98
	Mo2	5.03	P2	5.11562	O15	0.98
	Mo3	4.94	P3	5.09959	O16	0.94
	Mo4	4.88	P4	4.99717	O7	1.17
	Mo5	4.99			O9	1.34
	Mo6	4.98				
4	Mo1	5.08	P1	5.06678	O12	0.94
	Mo2	4.90	P2	5.00631	O13	0.93
	Mo3	4.96	P3	5.03866	O18	1.00
	Mo4	5.01	P4	5.02463	O21	1.17
	Mo5	4.94			O30	1.15
	Mo6	4.90				