Electronic Supplementary Material (ESI) for CrystEngComm

Two Octamolybdate-Based Complexes: Hydrothermal Synthesis, Structural Characterization and Properties

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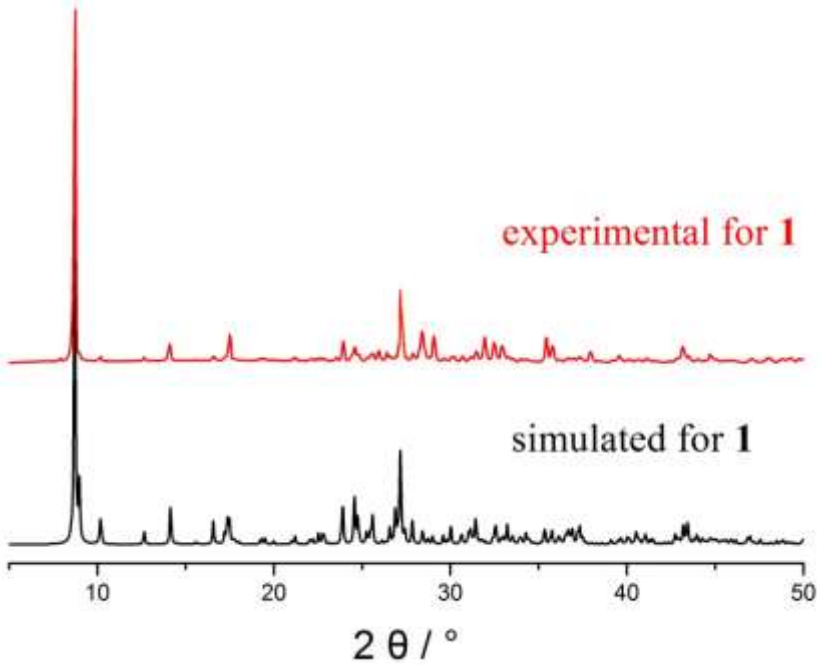

Fig. S1 The simulated and experimental powder X-ray diffraction patterns for compounds **1**.

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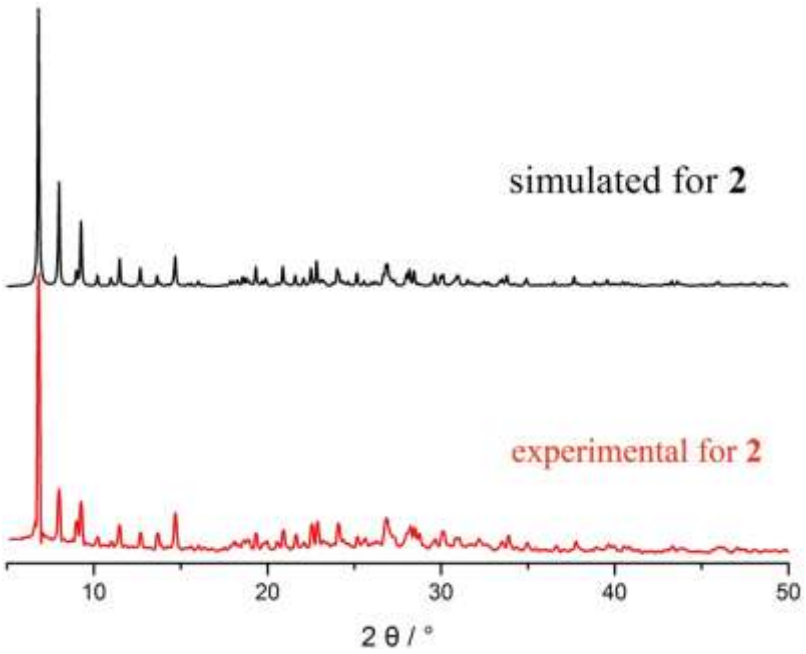

Fig. S2 The simulated and experimental powder X-ray diffraction patterns for compounds **2**.

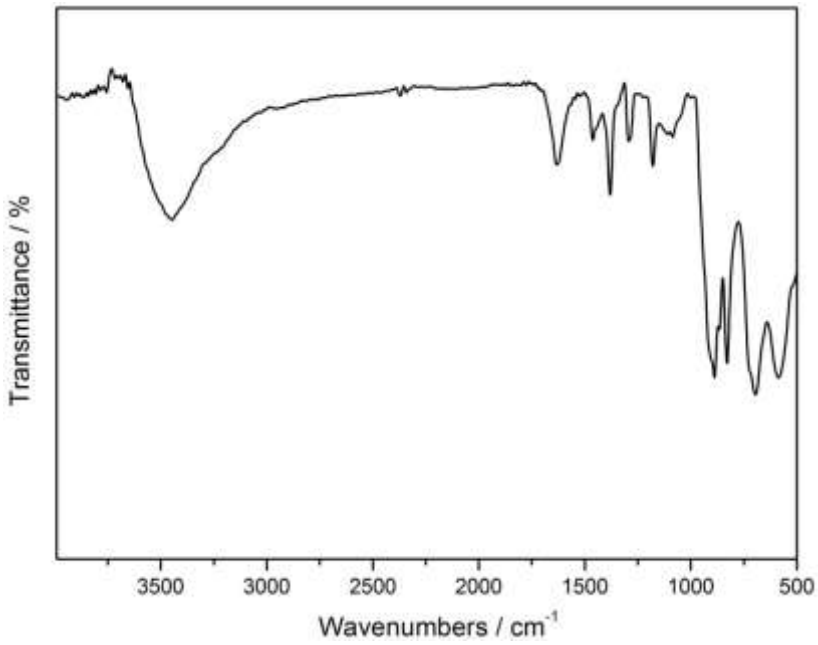

Figure. S3 The IR spectra of compound **1.**

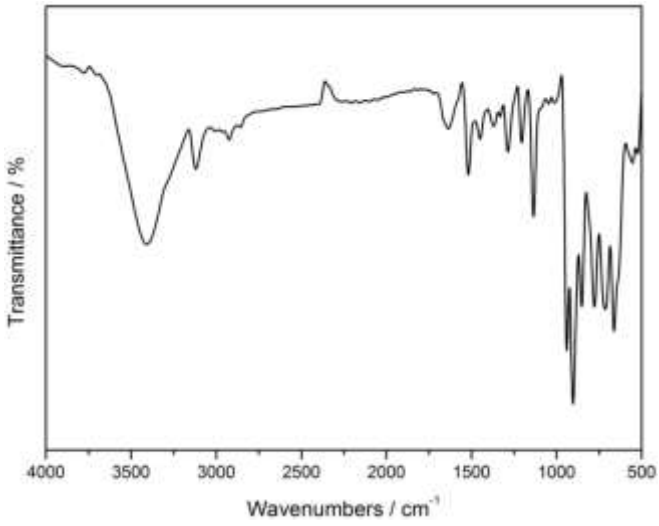

Fig. S4 The IR spectra of compound **2.**

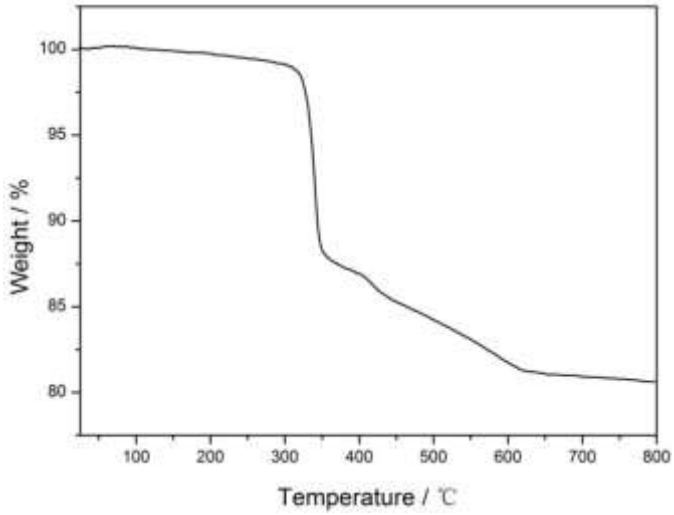

Fig. S5 The TG curve of compound **1**.

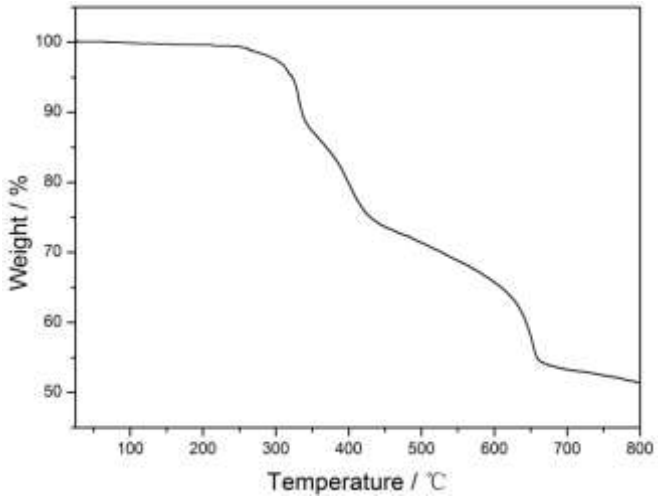

Fig. S6 The TG curve of compound **2**.

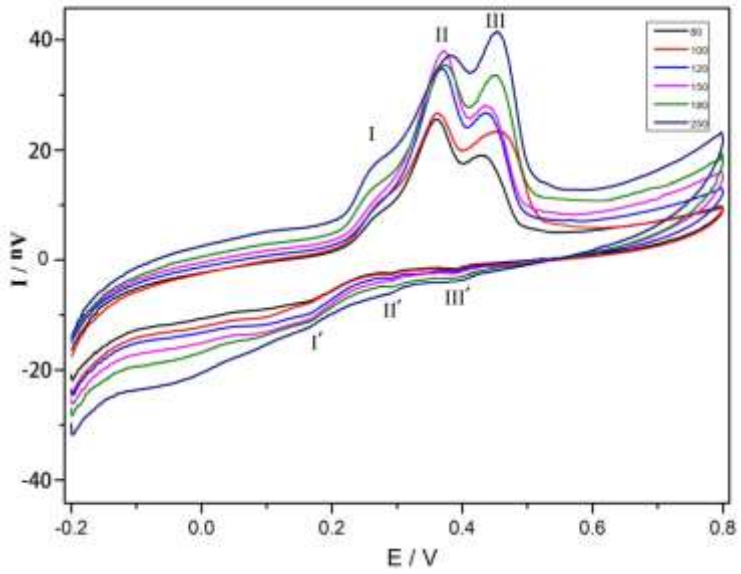

Fig. S7 Cyclic voltammograms of the **2**-CPE in 1 M H_2SO_4 aqueous solution at different scan rates (from inner to outer: 80, 100, 120, 150, 180, 250 mV s^{-1}).

Table. S1 Selected bonds distances (Å) for **1**

Mo(1)-O(2)	1.71(2)	Mo(4)-O(10)#1	2.32(2)	O(8)-Ag(3)#7	2.41(2)
Mo(1)-O(14)	1.758(17)	Mo(4)-O(7)	2.342(18)	O(10)-Mo(4)#1	2.32(2)
Mo(1)-O(10)	1.93(2)	Ag(3)-N(1)#2	2.41(2)	O(13)-Ag(1)#8	2.407(18)
Mo(1)-O(4)	1.934(16)	Ag(3)-O(2W)	2.41(2)	O(14)-Mo(2)#1	2.33(2)
Mo(1)-O(7)	2.195(16)	Ag(3)-O(8)#3	2.41(2)	S(2)-C(3)	1.77(3)
Mo(1)-O(7)#1	2.324(18)	Ag(3)-S(2)	2.609(6)	S(2)-Ag(1)#5	2.722(7)
Mo(1)-Mo(3)	3.210(3)	Ag(4)-N(3)	2.21(2)	S(1)-C(1)	1.68(2)
Mo(2)-O(1)	1.721(19)	Ag(4)-N(2)#2	2.349(19)	N(8)-C(3)	1.28(4)
Mo(2)-O(8)	1.75(2)	Ag(4)-S(2)	2.492(7)	N(8)-N(5)	1.30(4)
Mo(2)-O(5)	1.89(2)	Ag(4)-Ag(1)	2.961(3)	N(8)-C(4)	1.45(4)
Mo(2)-O(9)	1.937(19)	Ag(1)-O(13)#4	2.407(18)	N(7)-C(3)	1.31(3)
Mo(2)-O(14)#1	2.33(2)	Ag(1)-S(1)	2.589(7)	N(7)-N(6)	1.33(3)
Mo(3)-O(6)	1.679(19)	Ag(1)-O(11)	2.594(19)	N(3)-C(1)	1.36(3)
Mo(3)-O(13)	1.695(18)	Ag(1)-S(2)#5	2.722(7)	N(3)-N(2)	1.37(3)
Mo(3)-O(9)	1.908(17)	Ag(1)-S(2)	2.769(7)	N(6)-N(5)	1.31(3)
Mo(3)-O(10)	2.021(17)	Ag(1)-Ag(2)	2.941(4)	N(6)-Ag(2)#6	2.41(2)
Mo(3)-O(7)	2.236(17)	Ag(1)-Ag(1)#5	3.148(5)	N(4)-N(1)	1.35(3)
Mo(3)-O(4)#1	2.328(18)	Ag(2)-N(7)	2.21(2)	N(4)-C(1)	1.40(3)
Mo(4)-O(3)	1.707(18)	Ag(2)-N(6)#6	2.41(2)	N(4)-C(2)	1.44(3)
Mo(4)-O(11)	1.711(19)	Ag(2)-S(1)	2.504(9)	N(2)-N(1)	1.29(3)
Mo(4)-O(5)	1.92(2)	O(4)-Mo(3)#1	2.328(18)	N(2)-Ag(4)#2	2.349(19)
Mo(4)-O(4)	2.028(16)	O(7)-Mo(1)#1	2.324(18)	N(1)-Ag(3)#2	2.41(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1,-z; #2 -x+1,-y-1,-z; #3 x-1,y-1,z-1; #4 x-1,y-1,z; #5 -x+1,-y,-z;#6 -x+2,-y,-z; #7 x+1,y+1,z+1; #8 x+1,y+1,z

Table. S2 Selected bonds distances (Å) for **2**

Ag(1)-N(2)	2.143(6)	Mo(4)-O(9)	2.111(8)	N(1)-C(17)	1.317(10)
Ag(1)-N(6)#1	2.150(6)	Mo(4)-O(3)	2.367(10)	N(1)-Ag(2A)#3	2.266(7)
Ag(1)-O(7)#2	2.512(10)	Mo(5)-O(1)	0.800(16)	N(6)-C(16)	1.319(11)
Ag(2A)-Ag(2A)#3	0.600(3)	Mo(5)-O(23)	1.680(15)	N(6)-C(15)	1.332(11)
Ag(2A)-N(1)	2.076(7)	Mo(5)-O(22)	1.726(14)	N(6)-Ag(1)#1	2.150(6)
Ag(2A)-N(1)#3	2.266(7)	Mo(5)-O(16)	1.912(10)	N(5)-C(16)	1.304(10)
Ag(2A)-O(22)	2.471(12)	Mo(5)-O(9)	2.089(7)	N(5)-N(4)	1.358(10)
Ag(2A)-O(9)	2.504(8)	Mo(5)-O(15)	2.207(10)	N(5)-C(12)	1.484(10)
Ag(2A)-Mo(5)	3.000(3)	Mo(5)-O(2)	2.243(15)	C(2)-C(3)	1.386(11)
Ag(3)-Ag(3)#4	1.155(4)	Mo(5)-O(19)#7	2.267(10)	C(2)-C(1)	1.397(13)
Ag(3)-N(8)#5	2.125(10)	Mo(5)-O(17)#7	2.391(10)	C(2)-C(11)	1.525(13)
Ag(3)-N(8)#6	2.284(13)	Mo(5)-O(18)	2.450(10)	C(3)-C(4)	1.393(13)
Mo(1)-O(7)	1.601(10)	Mo(5)-Mo(7)	3.218(2)	C(3)-C(8)	1.517(13)
Mo(1)-O(21)	1.638(11)	Mo(3)-O(9)	1.616(8)	C(12)-C(4)	1.513(11)
Mo(1)-O(17)	1.632(9)	Mo(3)-O(14)	1.693(10)	C(1)-C(6)	1.392(13)
Mo(1)-O(10)	1.869(6)	Mo(3)-O(6)	1.686(15)	C(1)-C(7)	1.555(12)
Mo(1)-O(13)	1.911(11)	Mo(3)-O(11)	1.867(12)	N(4)-C(15)	1.303(12)
Mo(1)-O(19)	1.897(9)	Mo(3)-O(3)	1.990(9)	C(6)-C(5)	1.403(12)
Mo(1)-O(18)	2.002(9)	Mo(3)-O(13)	2.169(11)	C(6)-C(10)	1.549(13)
Mo(1)-O(3)	2.084(10)	Mo(3)-O(20)	2.291(13)	C(4)-C(5)	1.414(13)
Mo(1)-O(18)#7	2.482(9)	Mo(3)-O(18)	2.328(9)	C(5)-C(9)	1.546(15)
Mo(1)-Mo(2)	2.9958(17)	Mo(3)-O(24)	2.393(18)	N(9)-C(14)	1.327(14)
Mo(1)-Mo(3)	3.2214(16)	Mo(3)-O(10)#7	2.501(7)	N(9)-N(7)	1.342(16)
Mo(2)-O(15)	1.517(10)	Mo(7)-O(16)	1.520(10)	N(9)-C(10)	1.483(12)
Mo(2)-O(4)	1.705(10)	Mo(7)-O(8)	1.594(6)	N(8)-C(13)	1.27(3)
Mo(2)-O(10)	1.760(7)	Mo(7)-O(12)	1.698(11)	N(8)-C(14)	1.33(2)
Mo(2)-O(8)	1.809(6)	Mo(7)-O(11)#7	1.948(12)	N(8)-Ag(3)#5	2.125(10)
Mo(2)-O(16)	1.919(10)	Mo(7)-O(15)	1.928(10)	N(8)-Ag(3)#8	2.284(13)
Mo(2)-O(18)	2.351(9)	Mo(7)-O(3)#7	1.940(10)	C(14)-C(13)	2.05(3)
Mo(2)-O(17)#7	2.346(9)	Mo(7)-O(17)#7	2.322(9)	N(7)-C(13)	1.35(2)
Mo(2)-O(3)#7	2.403(10)	Mo(7)-O(10)	2.493(7)	O(19)-O(17)	1.749(14)
Mo(2)-Mo(6)	3.0015(19)	O(1)-O(22)	0.941(16)	O(19)-Mo(5)#7	2.267(10)
Mo(6)-O(23)	1.289(15)	O(2)-O(23)	0.765(15)	O(18)-O(17)#7	1.177(13)
Mo(6)-O(1)	1.704(17)	O(3)-O(11)	0.962(14)	O(18)-O(13)	1.525(14)
Mo(6)-O(2)	1.698(14)	O(3)-Mo(7)#7	1.940(10)	O(18)-Mo(1)#7	2.482(9)
Mo(6)-O(15)	1.906(9)	O(3)-Mo(2)#7	2.403(10)	O(17)-O(18)#7	1.177(13)
Mo(6)-O(9)	1.930(6)	O(4)-O(15)	1.605(15)	O(17)-Mo(6)#7	2.334(10)
Mo(6)-O(18)	1.943(9)	O(6)-O(24)	0.749(16)	O(17)-Mo(7)#7	2.322(9)
Mo(6)-O(16)	2.188(11)	O(7)-O(21)	1.092(15)	O(17)-Mo(2)#7	2.346(9)

Mo(6)-O(13)	2.262(11)	O(7)-Ag(1)#2	2.512(10)	O(17)-Mo(5)#7	2.391(10)
Mo(6)-O(17)#7	2.334(10)	O(10)-Mo(3)#7	2.501(7)	O(16)-O(15)	1.332(15)
Mo(4)-O(6)	1.067(14)	N(3)-C(18)	1.320(10)	O(16)-O(12)	1.502(16)
Mo(4)-O(14)	1.637(11)	N(3)-N(1)	1.364(9)	O(14)-O(20)	1.226(17)
Mo(4)-O(20)	1.684(14)	N(3)-C(11)	1.483(10)	O(11)-Mo(7)#7	1.948(12)
Mo(4)-O(24)	1.722(19)	N(2)-C(18)	1.332(10)		
Mo(4)-O(11)	1.852(12)	N(2)-C(17)	1.351(10)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y+2,-z+2; #2 -x,-y+1,-z+2; #3 -x+1,-y+1,-z+2; #4 -x+1,-y,-z+3; #5 -x,-y,-z+3; #6 x+1,y,z;#7 -x+1,-y,-z+2; #8 x-1,y,z