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A series of organopolymolybdate polymers linked by dual fuses: metal-organic moiety and organic ligand through Mo-N bonds

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ELECTRONIC SUPPLEMENTARY INFORMATION

Table S1. Selected Bond Lengths (Å) and Bond Angles (°) for Compounds **1**–**3**.

		Compound **1**	
Mo(3)-N(6)#1	2.269(4)	Cu(1)-N(1)	1.927(4)
Cu(1)-N(5)#2	1.929(4)	Cu(1)-OW1	2.278(5)
Cu(1)-O(7)	2.331(4)	Cu(2)-N(7)	1.876(4)
Cu(2)-N(2)#3	1.891(4)	Cu(2)-O(4)	2.342(4)
Cu(2)-O(8)	2.763(4)	N(1)-Cu(1)-N(5)#2	166.65(18)
OW1-Cu(1)-O(7)	107.0(2)	N(7)-Cu(2)-N(2)#3	167.76(18)
O(4)-Cu(2)-O(8)	139.0(3)		
Symmetry codes for **1**: #1 x,y+1,z #2 -x-1,-y-1,-z #3 -x,-y,-z+1			
		Compound **2**	
Mo(3)-N(1)	2.245(4)	Cu(1)-N(6)#1	1.977(4)
Cu(1)-O(7)#3	2.000(3)	Cu(1)-OW1#3	2.398(4)
Cu(2)-N(7)	2.021(4)	Cu(2)-N(10)	2.031(4)
Cu(2)-O(13)#1	2.373(3)	N(6)#1-Cu(1)-N(6)#2	180.00(2)
N(6)#1-Cu(1)-O(7)	89.96(16)	N(7)-Cu(2)-N(10)	89.30(18)
N(7)#1-Cu(2)-N(7)	180.00(1)	N(7)-Cu(2)-O(13)#1	89.63(15)
Symmetry codes for **2**: #1 -x,-y+1,-z+2 #2 x,y-1,z+1 #3 -x,-y,-z+3			
		Compound **3**	
Mo(2)-N(3)	2.272(5)	OW1-Cu(1)	2.277(5)
OW2-Cu(1)	1.996(4)	O(7)-Cu(1)	1.977(4)
Cu(1)-N(6)#1	1.945(5)	Cu(1)-N(1)	1.976(5)
N(6)#1-Cu(1)-N(1)	167.1(2)	N(1)-Cu(1)-O(7)	84.77(18)
N(1)-Cu(1)-OW2	94.08(19)	O(7)-Cu(1)-OW2	175.65(18)
Symmetry code for **3**: #1 -x+1,-y,-z-1			

Fig. S1. The schematic view of the 3D framework of compound **1** (green: γ-Mo_8 anion; orange: 2D layer; pink: the b-type bte ligand).

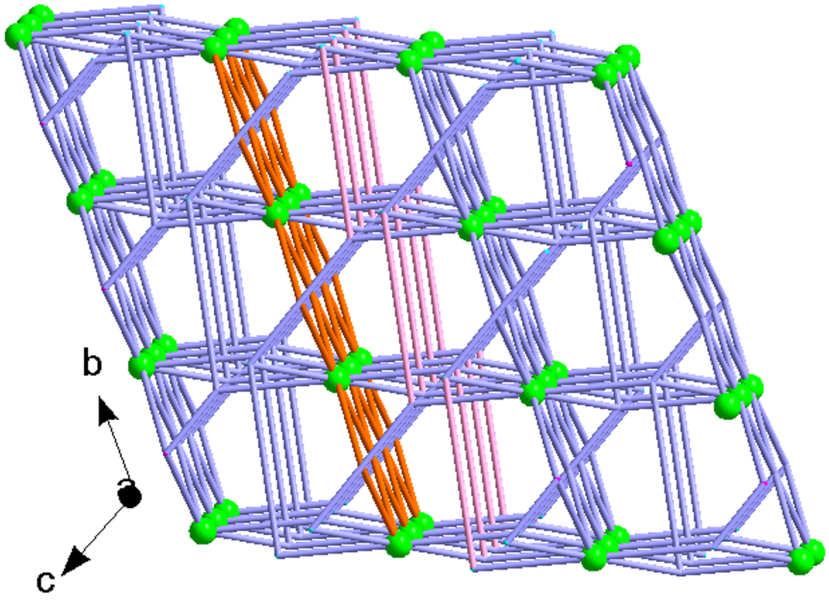

Fig. S2. The inorganic line (a) and the metal-organic line (b) in compound **2**.

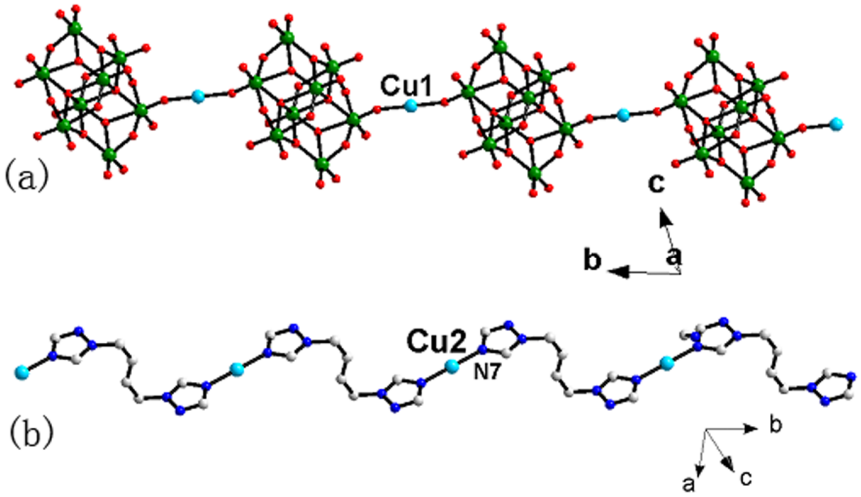

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Fig. S3. The new channel-like chain connects with each other through sharing the Cu1 ions to construct a 2D layer in compound **2**, viewing along the *a* (a) and *b* (b) axises.

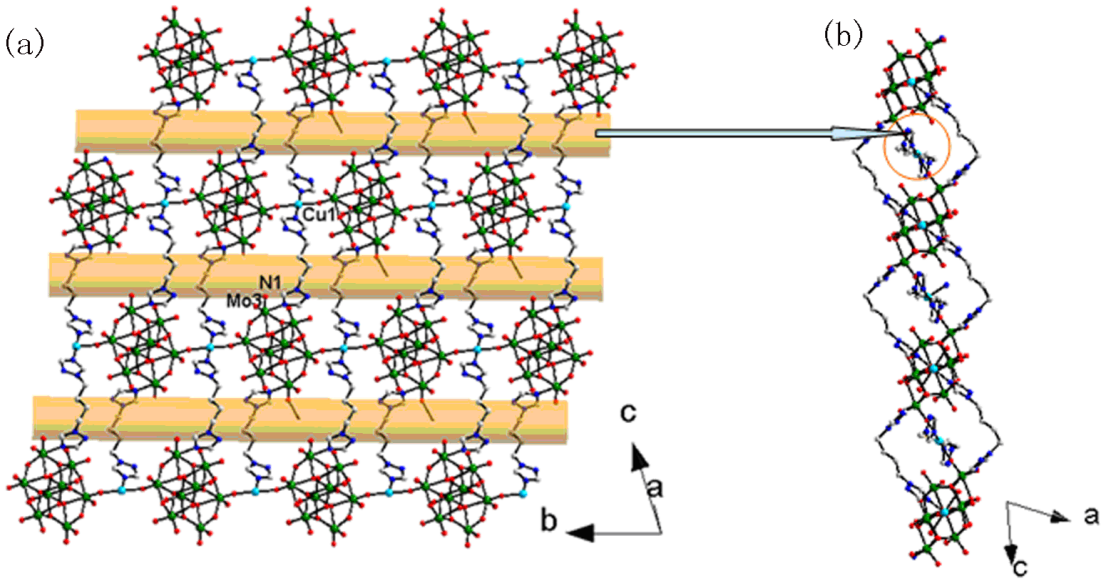

Fig. S4. The γ-Mo_8 anion in compounds **1**–**3** including six [MoO_6] and two [MoO_5] clusters.

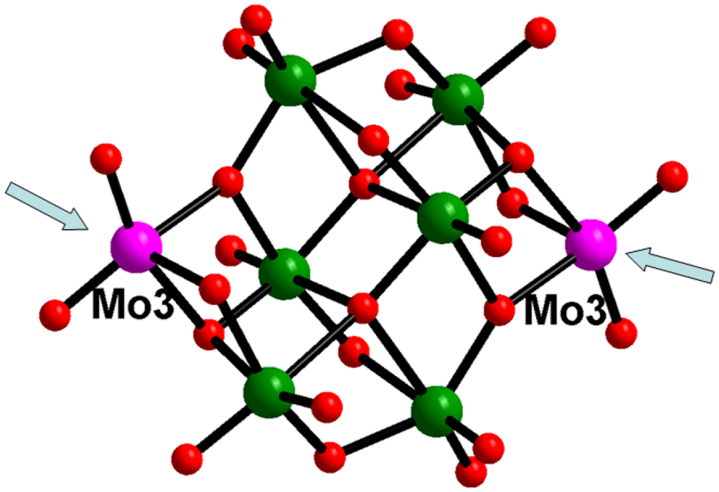

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Fig. S5. IR spectra of compounds **1–3**.

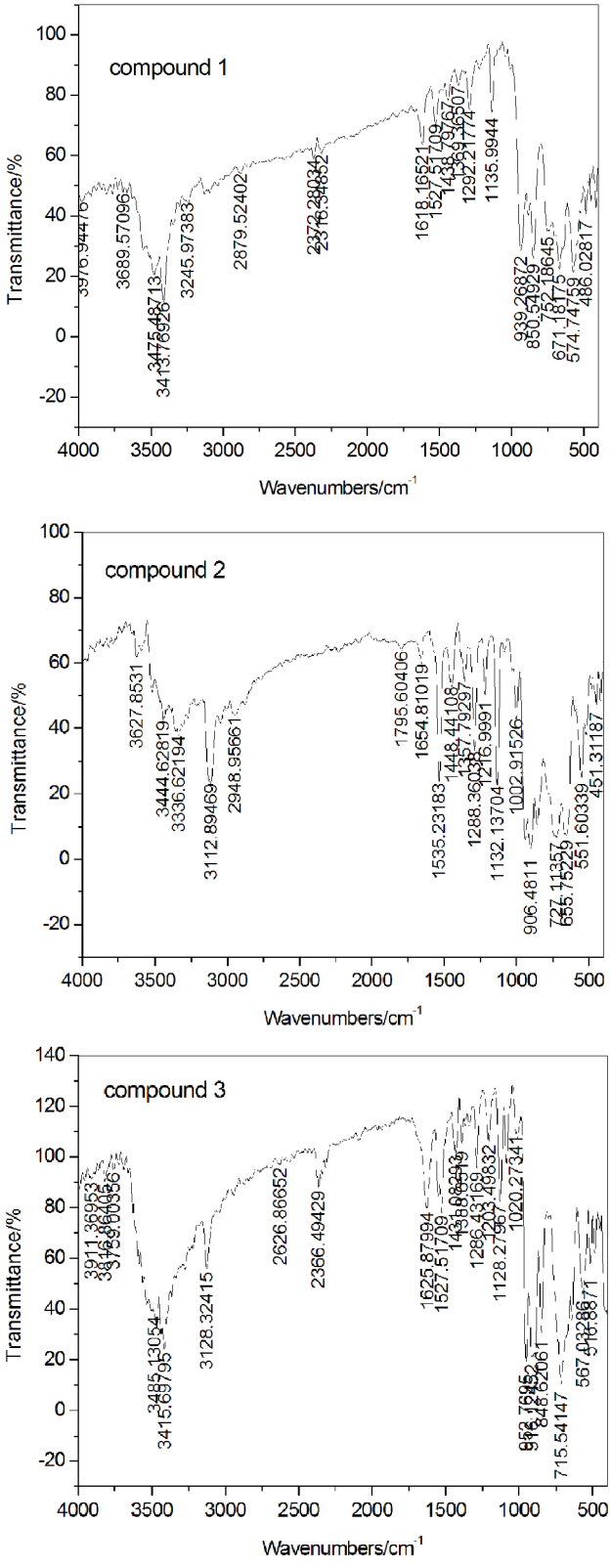

Fig. S6. The simulative (blue line) and experimental (black line) powder X-ray diffraction patterns for compounds **1**–**3**.

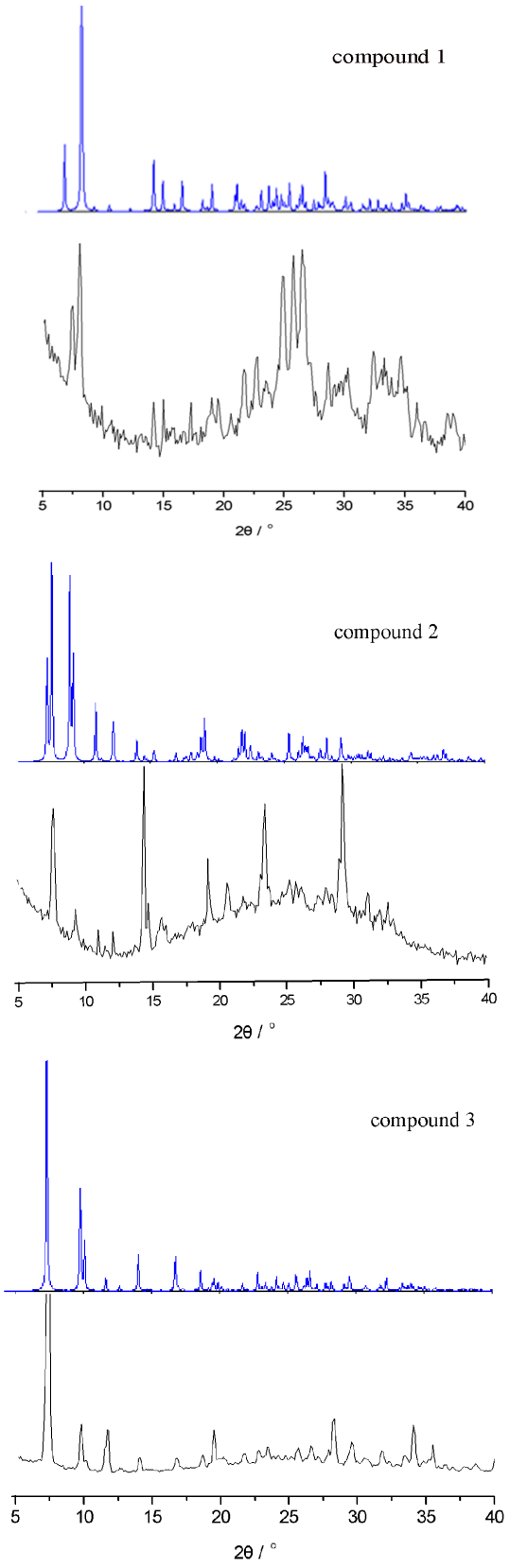

Fig. S7. The TG analyses of compounds **1–3**.

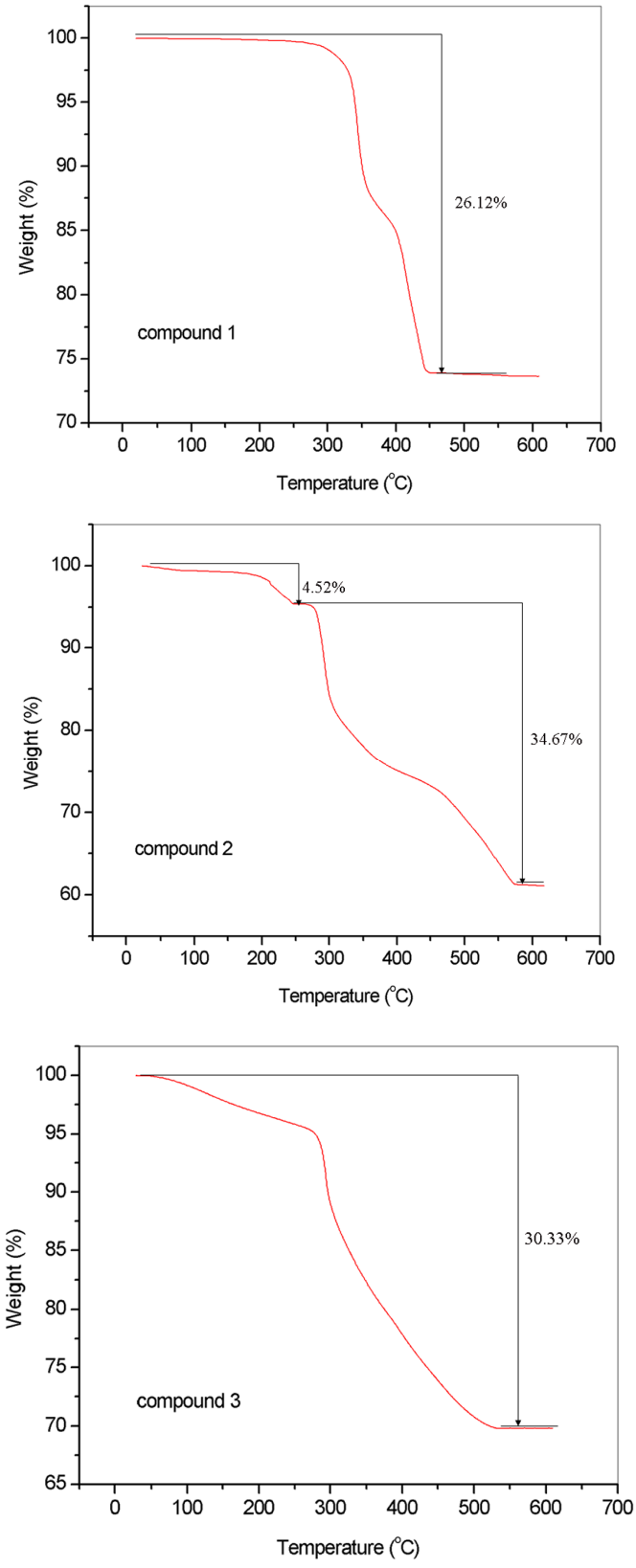

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Fig. S8. The cyclic voltammograms of the **2**– and **3**–CPEs in 1M H_2SO_4 at 100 $mV \cdot s^{-1}$.