

Assembly of Two New Polyoxometalate-Templated Supramolecular Compounds by Utilizing a Ligand with Combination of Rigidity and Flexibility

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Table 1. Selected bond length (ranges) (Å) and bond angles (deg) for compounds **1**
and **2**

Compound 1			
P—O	1.465(18)–1.595(16)	Cu1-N2	1.864(13)
W—O _a	2.422(17)–2.473(19)	Cu2-N5	1.864(13)
W—O _b	1.859(13)–1.927(11)	N7-Cu1-N2	176.2(6)
W—O _t	1.634(10)–1.680(9)	N5-Cu2-N5	180.000(6)
Cu1-N7	1.892(14)		
Compound 2			
P—O	1.465(8) to 1.574(8)	Cu2-N5	1.855(6)
Mo—O _a	2.397(9)–2.507(8)	Cu2-N8	1.874(7)
Mo—O _b	1.871(6)–1.928(6)	N4-Cu1-N4	180.000(2)
Mo—O _t	1.639(5)–1.664(5)	N5-Cu2-N8	174.5(3)
Cu1-N4	1.873(7)		

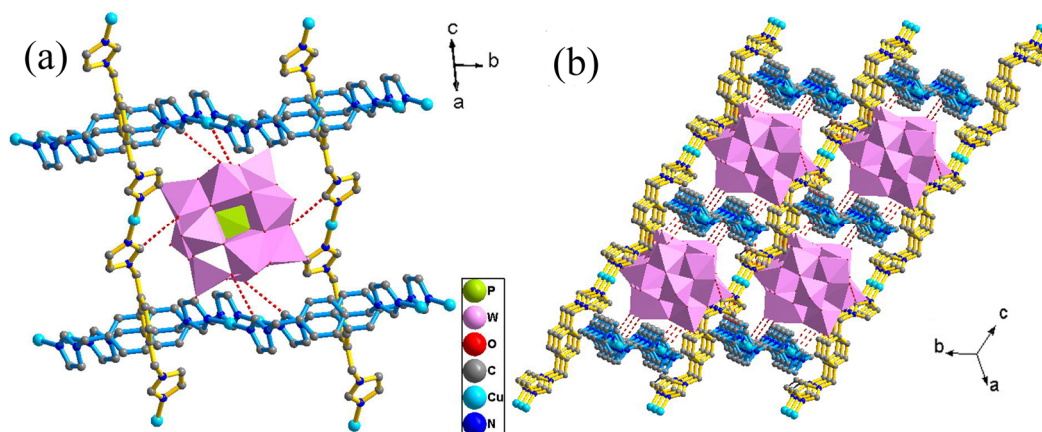


Fig. S1. (a) The hydrogen bonding around the polyanion and (b) in the 3D supramolecular framework of compound **1**. The hydrogen atoms are omitted for clarity. (The hydrogen bonding are shown in red dashed.)

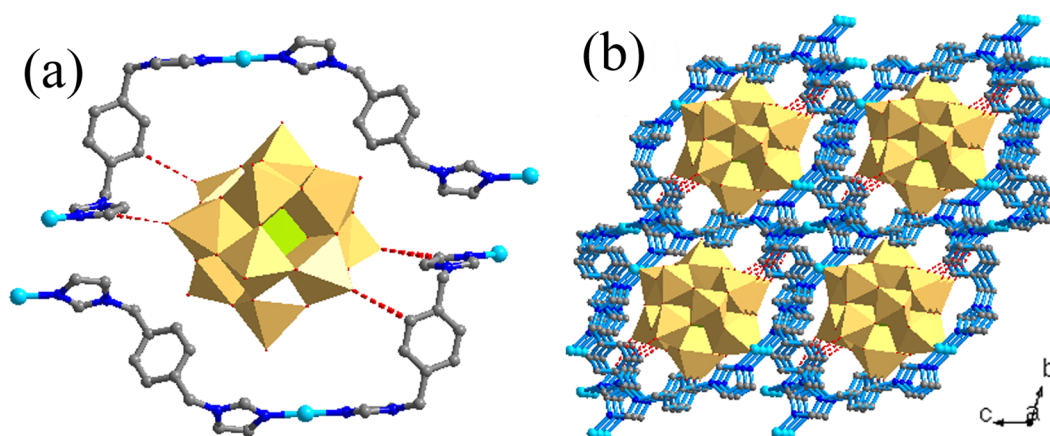


Fig. S2. (a) The hydrogen bonding around the polyanion and (b) in the 3D supramolecular framework of compound **2**. The hydrogen atoms are omitted for clarity. (The hydrogen bonding are shown in red dashed.)

Table 2. Hydrogen-bonding parameters in compounds **1** and **2**

Compounds	D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
1	C(1)-H(1A)...O(9) (i)	0.93	2.40	3.165(18)	138.9
	C(6)-H(6A)...O(14) (ii)	0.93	2.41	3.32(2)	165.4
	C(9)-H(9A)...O(3) (iii)	0.93	2.51	3.31(2)	143.6
	C(18)-H(18A)...O(15)(iv)	0.93	2.57	3.28(2)	133.1

	C(22)-H(22A)...O(10)(iv)	0.93	2.38	3.13(2)	138.3
	C(23)-H(23A)...O(2) (i)	0.93	2.33	2.92(2)	120.5
	C(24)-H(24A)...O(3) (v)	0.93	2.20	3.01(2)	144.9
2	C7-H7A...O16 (i)	0.93	2.59	3.201(10)	124.1
	C16-H16A...O18 (i)	0.93	2.54	3.358(12)	146.4

Symmetry transformations used to generate equivalent atoms:

Compound 1: (i) $x,y,z+1$; (ii) $-x+2,-y+2,-z$; (iii) $-x+1,-y+2,-z$; (iv) $-x+2,-y+2,-z+1$;

(v) $x+1,y,z+2$

Compound 2: (i) $x-1,y,z$

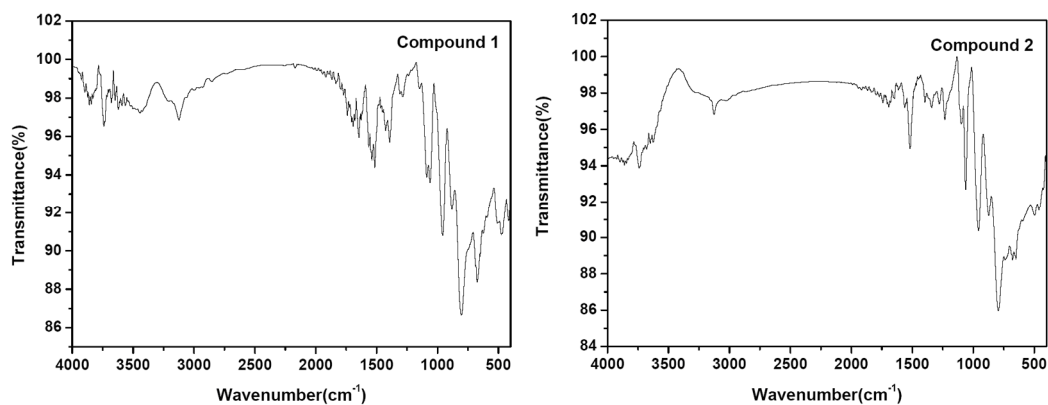


Fig. S3. IR spectra for compounds **1** and **2**.

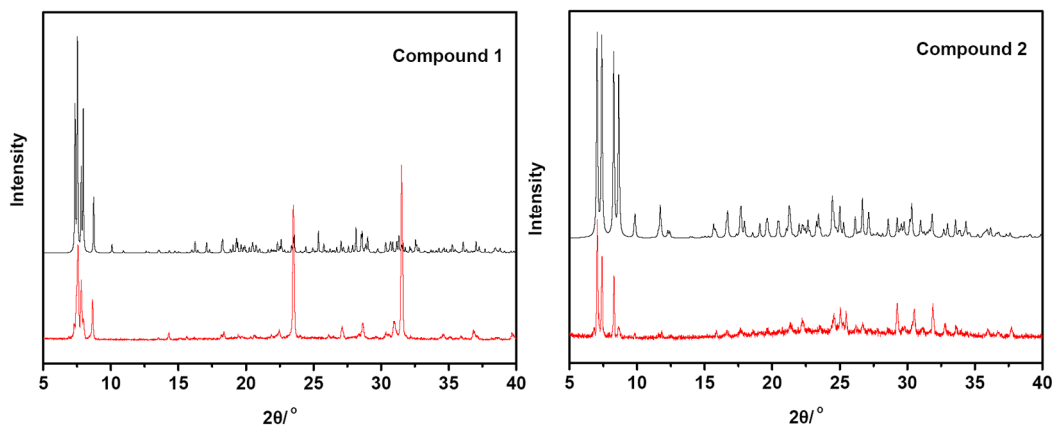


Fig. S4. The simulative (black line) and experimental (red line) powder X-ray diffraction patterns for compounds **1** and **2**.

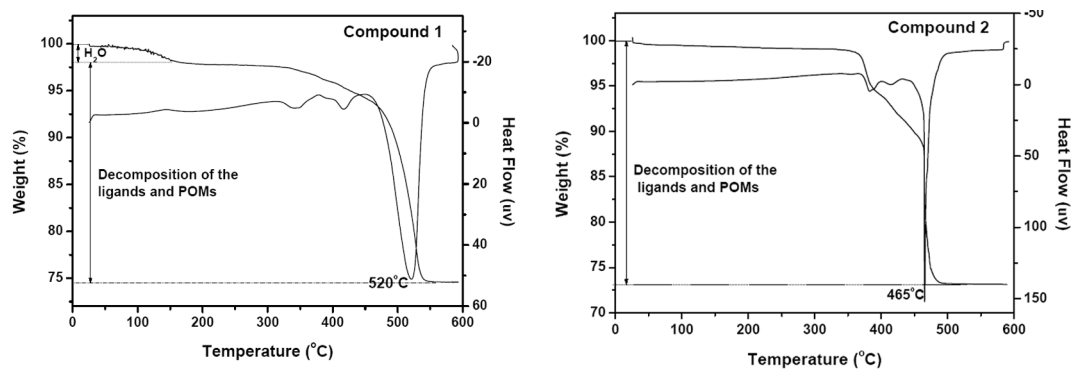


Fig. S5. TG and DTA curves of compounds 1 and 2.

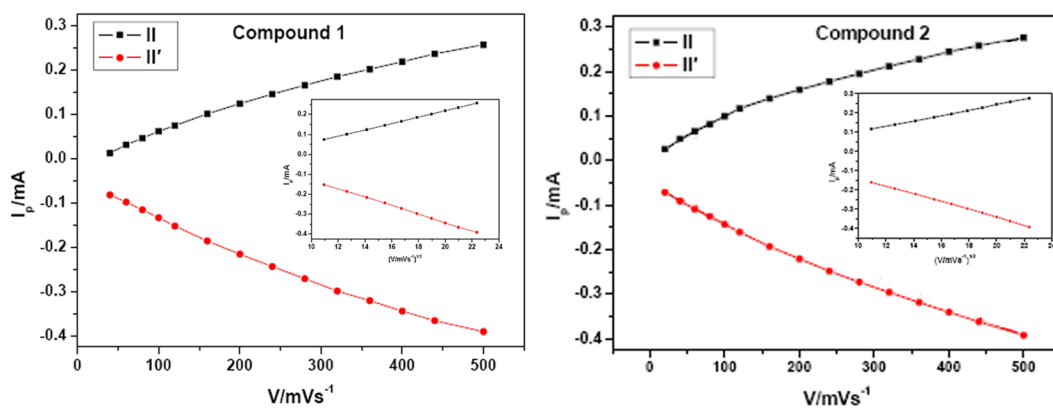


Fig. S6. The dependence of anodic peak (II) and cathodic peak (II') currents on scan rates for compound 1 and 2. The insets show the peak currents are proportional to the square root of the scan rates higher than 120 mV·s⁻¹.