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Two novel octamolybdate-based frameworks decorated by flexible bis-pyridyl-bis-amide ligands with different spacer lengths

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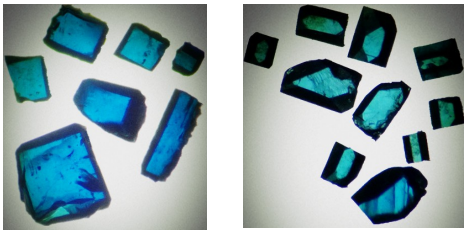

Fig. S1 Crystal photo of compounds **1** and **2**.

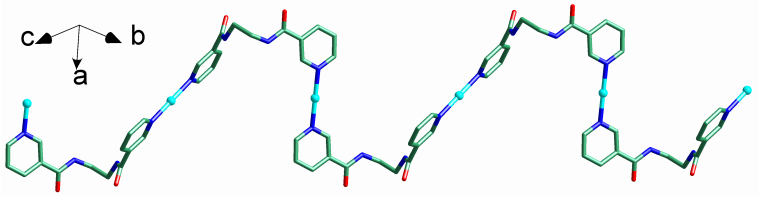

Fig. S2 The 1D chain formed by ligand L_1 and the Cu^{II} ions in **1**.

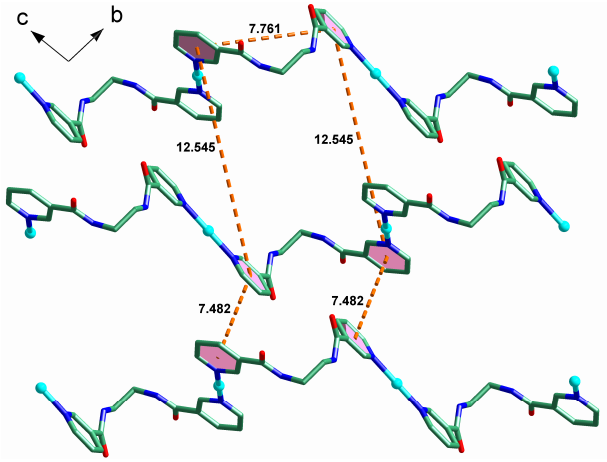

Fig. S3 The adjacent 1D chains are stagger–peaked with each other to form different cavities.

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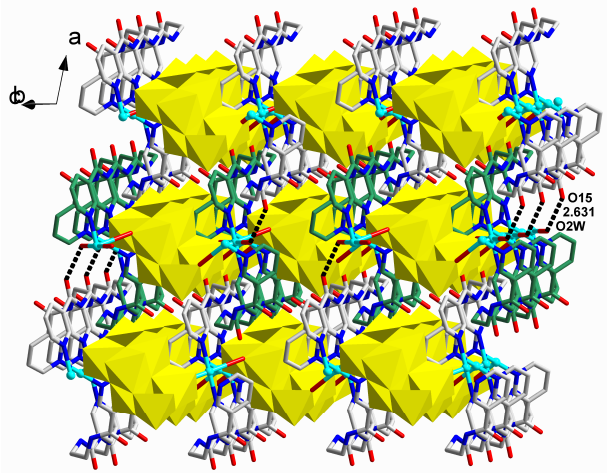


Fig. S4 The 3D supramolecular structure of compound **1**.

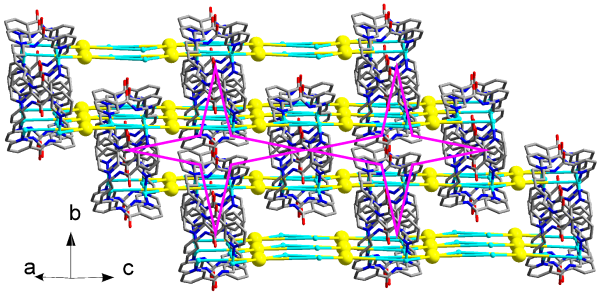
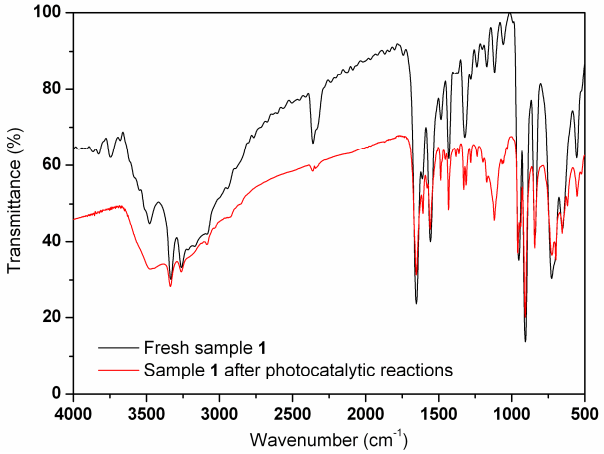


Fig. S5 The 3D framework of **2**. The yellow ball represents the Mo_8 polyanion.



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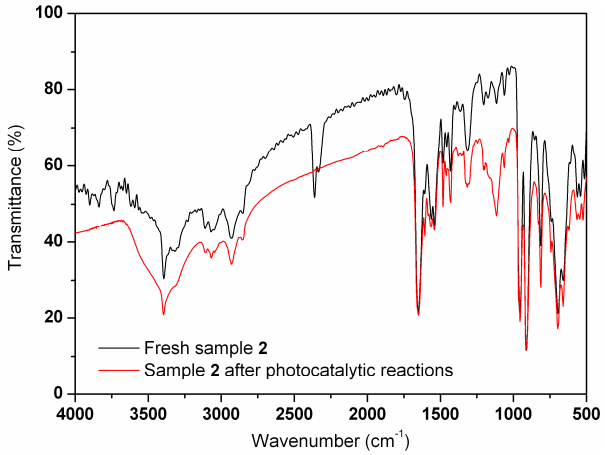


Fig. S6 IR spectra of samples **1** and **2** before and after photocatalytic reactions.

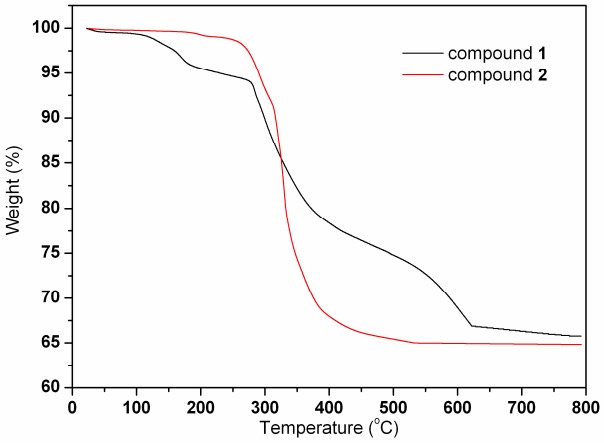
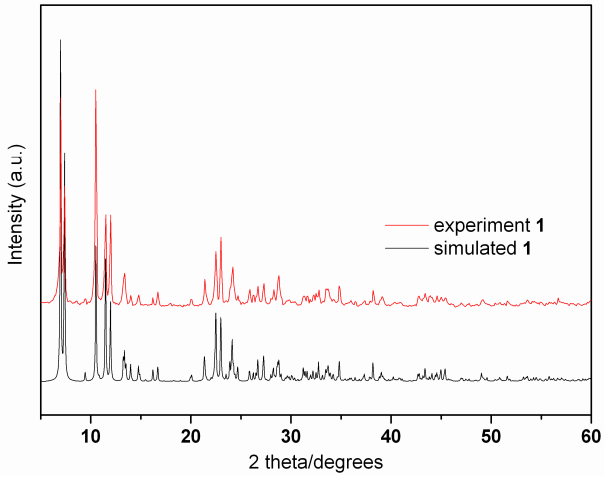


Fig. S7 The TG curves of compounds **1** and **2**.



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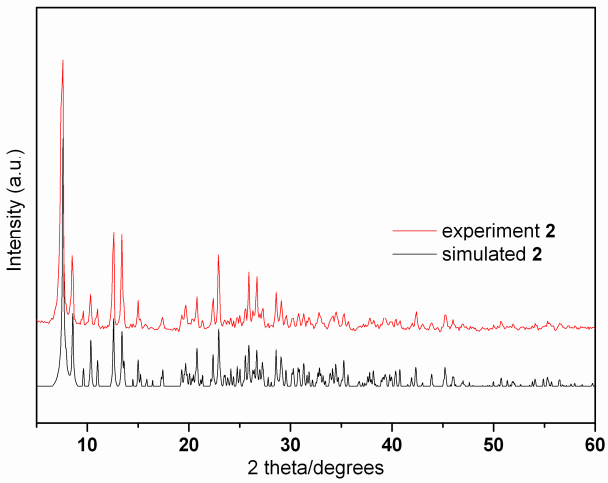

Figure S8 The simulated (black line) and experimental (red line) powder X-ray diffraction patterns for compounds **1** and **2**. The diffraction peaks of both simulated and experimental patterns mach well in positions, thus indicating that the phase purities of the compounds **1** and **2** are well.

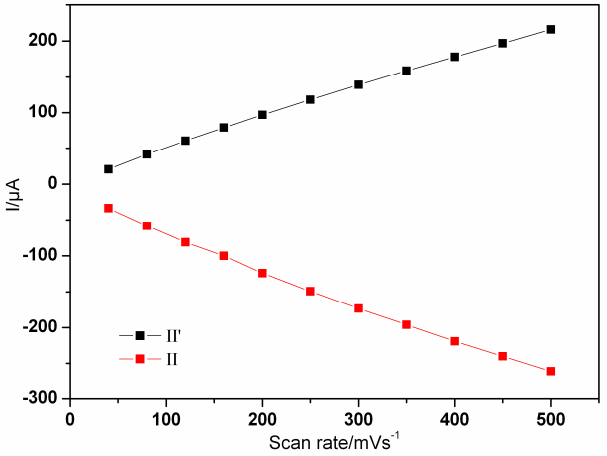

Fig. S9 The dependence of cathodic peak and anodic peak currents on scan rates of **1**–CPE.

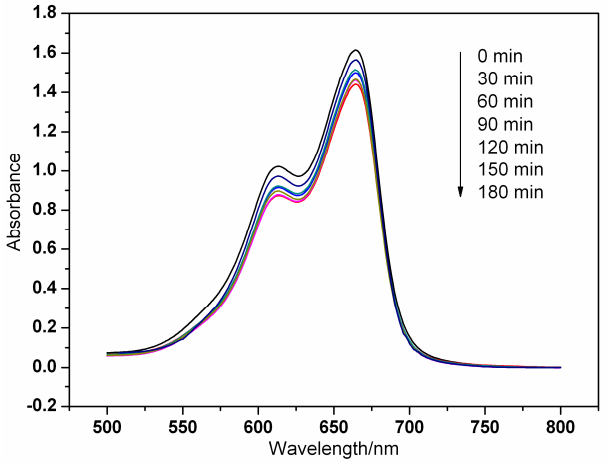

Fig. S10 Changes in the absorption spectra of the MB solution during the decomposition reaction under UV light irradiation without title compounds.

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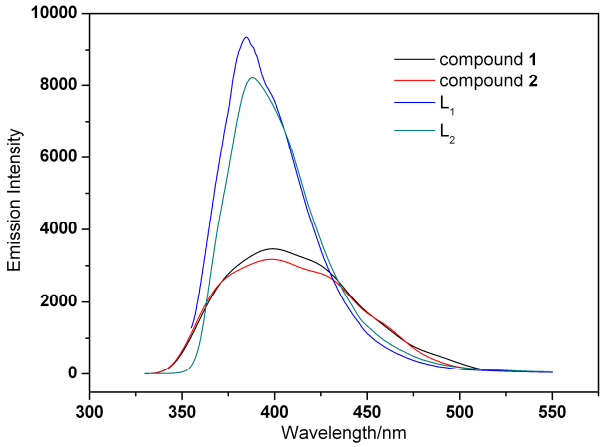

Fig. S11 Luminescence spectra of compounds **1**, **2** and the free L_1, L_2 ligands.

Table S1 Selected bond distances (Å) and angles (°) for compounds **1** and **2**.

Compound **1**			
Cu(1)–O(1W)	2.013(3)	Cu(1)–O(1W)#1	2.013(3)
Cu(1)–N(1)#1	2.017(3)	Cu(1)–N(1)	2.017(3)
Cu(1)–O(10)#1	2.364(3)	Cu(1)–O(10)	2.364(3)
Cu(2)–O(2W)	1.928(2)	Cu(2)–O(2W)#2	1.928(2)
Cu(2)–N(4)#2	2.016(3)	Cu(2)–N(4)	2.016(3)
Cu(2)–O(9)#4	2.601(2)	Cu(2)–O(9)#3	2.601(2)
O(1W)–Cu(1)–O(1W)#1	180.0	O(1W)–Cu(1)–N(1)#1	88.56(11)
O(1W)#1–Cu(1)–N(1)#1	91.44(11)	O(1W)–Cu(1)–N(1)	91.44(11)
O(1W)#1–Cu(1)–N(1)	88.56(11)	N(1)#1–Cu(1)–N(1)	180.0
O(1W)–Cu(1)–O(10)#1	91.17(11)	O(1W)–Cu(1)–O(10)	88.83(11)
O(1W)#1–Cu(1)–O(10)#1	88.83(11)	O(1W)#1–Cu(1)–O(10)	91.17(11)
N(1)#1–Cu(1)–O(10)#1	88.85(11)	N(1)#1–Cu(1)–O(10)	91.15(11)
N(1)–Cu(1)–O(10)#1	91.15(11)	N(1)–Cu(1)–O(10)	88.85(11)
O(10)#1–Cu(1)–O(10)	180	O(2W)–Cu(2)–N(4)	88.78(10)
O(2W)–Cu(2)–O(2W)#2	180	O(2W)#2–Cu(2)–N(4)	91.22(10)
O(2W)–Cu(2)–N(4)#2	91.22(10)	N(4)#2–Cu(2)–N(4)	180
O(2W)#2–Cu(2)–N(4)#2	88.78(10)	O(9)#3–Cu(2)–N(4)	93.61(11)
O(9)#3–Cu(2)–O(2W)#2	92.80(11)	O(9)#3–Cu(2)–N(4)#2	86.39(11)
O(9)#3–Cu(2)–O9	180	O(9)#3–Cu(2)–O2W	87.12(11)
O(9)#4–Cu(2)–N(4)#2	93.61(11)	O(9)#4–Cu(2)–O(2W)	92.80(11)
O(9)#4–Cu(2)–O2W#2	87.12(11)	O(9)#4–Cu(2)–N(4)	86.39(11)
Symmetry code for **1**: #1 $-x, -y+1, -z-2$; #2 $-x, -y, -z-1$; #3 $x, y, 1+z$; #4 $-x, -y, -2-z$			
Compound **2**			
Cu(1)–O(1W)	1.948(3)	Cu(1)–N(4)#2	2.013(3)
Cu(1)–O(12)#1	1.950(3)	Cu(1)–O(8)	2.418(3)
Cu(1)–N(1)	1.984(3)	Cu(1)–O(10)#1	2.620(3)
O(1W)–Cu(1)–O(12)#1	89.88(11)	N(1)–Cu(1)–N(4)#2	93.55(14)

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O(1W)–Cu(1)–N(1)	91.12(13)	O(1W)–Cu(1)–O(8)	89.01(11)
O(12)#1–Cu(1)–N(1)	175.57(13)	O(12)#1–Cu(1)–O(8)	92.90(10)
O(1W)–Cu(1)–N(4)#2	175.31(13)	N(1)–Cu(1)–O(8)	91.43(12)
O(12)#1–Cu(1)–N(4)#2	85.43(12)	N(4)#2–Cu(1)–O(8)	91.33(13)
O(12)#1–Cu(1)–O(10)#1	82.32(10)	O(1W)–Cu(1)–O(10)#1	79.58(10)
O(10)#1–Cu(1)–O(8)	167.58(10)	O(10)#1–Cu(1)–N(1)	93.62(12)
O(10)#1–Cu(1)–N(4)	99.66(13)		

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

Table S2 Ligand conformations and corresponding angles for L_1 and L_2.

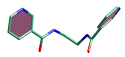
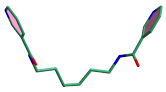
Compound	diagram	Torsion angle/°	Conformation	Dihedral angle/°
1		88.63 (C7 C8 N3 C9), 63.40 (N2 C7 C8 N3), －132.04 (C6 N2 C7 C8),	GGA *cis*	46.14 Plane 1: N1 C1 C2 C3 C4 C5 Plane 2: N4 C11 C10 C14 C13 C12
2		－94.06 (C13 N3 C12 C11), 175.56 (N3 C12 C11 C10), 162.49 (C12 C11 C10 C9), 22.55 (C11 C10 C9 C8), 169.43 (C10 C9 C8 C7), 177.77 (C9 C8 C7 N2), 103.07 (C8 C7 N2 C6),	AAAGAAA *cis*	59.30 Plane 1: N1 C1 C2 C3 C4 C5 Plane 2: N4 C15 C14 C18 C17 C16

Table S3 Selected hydrogen-bonding geometry (Å, °) for compound **1**.

D–H···A	D–H	H···A	D···A	D–H···A
O(2W)–H(2WA)···O(15)#5	0.85	1.79	2.631(4)	170

Symmetry code for **1**: #1 $x-1, y, z$