pH-Dependent Assembly of Three Novel Inorganic-Organic Hybrids Based on Different Isopolymolybdates and $Cu^{I/II}(bbx)_n$ Units

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Table S1. Selected bond lengths (Å) and angles (°) of the compounds **1–3**.

		Compound 1	
Cu(1)-N(4)#1	1.909(8)	Cu(1)-N(1)	1.944(8)
Cu(1)-O(9)	1.993(6)	Cu(1)-O(14)	2.045(7)
Mo(1)-O(6)	1.688(6)	Mo(1)-O(7)	1.719(6)
Mo(1)-O(5)	1.938(6)	Mo(1)-O(4)	1.959(6)
Mo(1)-O(13)	2.158(6)	Mo(1)-O(13)#2	2.336(6)
Mo(2)-O(12)	1.685(7)	Mo(2)-O(9)	1.713(6)
Mo(2)-O(1)	1.886(7)	Mo(2)-O(10)	1.912(7)
Mo(2)-O(7)#2	2.275(7)	Mo(2)-O(13)	2.357(6)
Mo(3)-O(11)	1.707(6)	Mo(3)-O(2)	1.712(7)
Mo(3)-O(10)	1.876(6)	Mo(3)-O(4)	1.975(6)
Mo(3)-O(5)#2	2.313(6)	Mo(3)-O(13)	2.343(6)
Mo(4)-O(8)	1.680(7)	Mo(4)-O(3)	1.717(7)
Mo(4)-O(1)	1.898(7)	Mo(4)-O(5)	1.989(6)
Mo(4)-O(4)#2	2.328(6)	Mo(4)-O(13)	2.355(6)
O(4)-Mo(4)#2	2.328(6)	O(5)-Mo(3)#2	2.313(6)
O(7)-Mo(2)#2	2.275(7)	O(13)-Mo(1)#2	2.336(6)
N(4)-Cu(1)#3	1.909(8)	N(4)#1-Cu(1)-O(9)	89.4(3)
N(4)#1-Cu(1)-N(1)	172.5(4)	N(4)#1-Cu(1)-O(14)	90.1(3)
N(1)-Cu(1)-O(9)	85.4(3)	O(9)-Cu(1)-O(14)	163.3(3)
N(1)-Cu(1)-O(14)	96.4(3)		
		Compound 2	
N(8)-Cu(1)#1	2.003(5)	N(4)-Cu(1)#2	1.969(5)
Mo(1)-O(6)	1.729(4)	Mo(1)-O(13)	1.700(4)
Mo(1)-O(7)	1.913(4)	Mo(1)-O(2)	1.880(4)
Mo(1)-O(7)#3	2.385(4)	Mo(1)-O(1)	2.293(4)
Mo(2)-O(4)	1.692(5)	Mo(2)-O(5)	1.689(4)
Mo(2)-O(1)	1.869(4)	Mo(2)-O(3)	1.822(4)
Mo(3)-O(12)	1.686(4)	Mo(2)-O(2)	2.413(4)

Mo(3)-O(10)	1.905(4)	Mo(3)-O(11)	1.707(4)
Mo(3)-O(2)#3	2.114(4)	Mo(3)-O(3)#3	2.008(4)
Mo(4)-O(9)	1.687(5)	Mo(3)-O(7)	2.519(4)
Mo(4)-O(10)	1.900(4)	Mo(4)-O(8)	1.692(5)
Mo(4)-O(7)	2.229(4)	Mo(4)-O(1)	2.017(4)
Cu(1)-N(4)#4	1.969(5)	Mo(4)-O(6)#3	2.364(4)
Cu(1)-N(5)	1.987(5)	Cu(1)-N(1)	1.983(5)
Cu(1)-O(11)	2.408(5)	Cu(1)-N(8)#5	2.003(5)
O(7)-Mo(1)#3	2.385(4)	N(4)#4-Cu(1)-N(1)	172.7(2)
N(4)#4-Cu(1)-N(5)	92.3(2)	N(1)-Cu(1)-N(5)	92.4(2)
N(4)#4-Cu(1)-N(8)#5	86.5(2)	N(1)-Cu(1)-N(8)#5	88.3(2)
N(5)-Cu(1)-N(8)#5	174.5(2)	N(4)#4-Cu(1)-O(11)	93.62(19)
N(1)-Cu(1)-O(11)	91.84(19)	N(5)-Cu(1)-O(11)	90.65(19)
Compound 3			
Cu(1)-N(1)#1	1.889(5)	N(1)#1-Cu(1)-O(1)	96.1(2)
Cu(1)-O(1)	2.269(6)	N(1)#1-Cu(1)-N(3)	165.0(3)
Mo(1)-O(2)	1.709(6)	N(3)-Cu(1)-O(1)	98.3(2)
Mo(1)-O(3)#2	1.850(15)	Cu(1)-N(3)	1.894(5)
O(3)-Mo(1)#2	1.850(15)	N(1)-Cu(1)#3	1.889(5)

Symmetry transformations used to generate equivalent atoms:

Compound 1: #1 x-1/2, -y+3/2, z+1/2; #2 -x+1, -y+2, -z+2; #3 x+1/2, -y+3/2, z-1/2.

Compound 2: #1 -x+3/2, y-1/2, -z+1/2; #2 x+1, y, z; #3 -x+2, -y, -z+1; #4 x-1, y, z; #5 -x+3/2, y+1/2, -z+1/2.

Compound 3: #1 x, y-1, z; #2 -x+3/2, -y+3/2,-z; #3 x, y+1, z.

Magnetism measurements were performed on a Quantum Design MPMS SQUID magnetometer. The experimental susceptibilities were corrected for the diamagnetism of the constituent atoms (Pascal's tables).

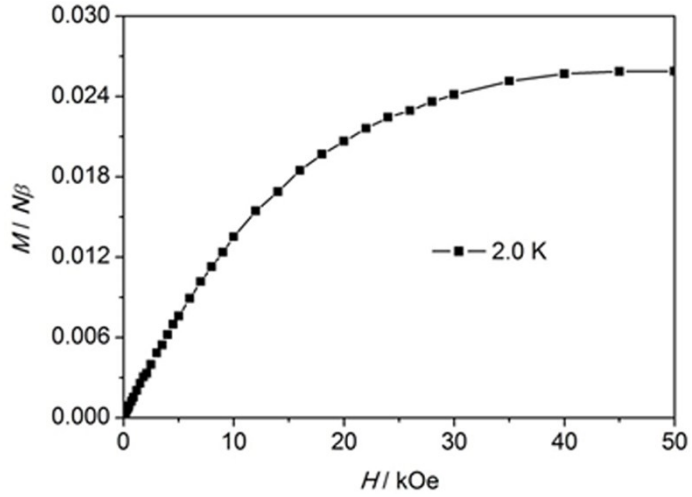

Fig. S1. M(H) data for polycrystalline samples of compound **3** at 2.0 K.

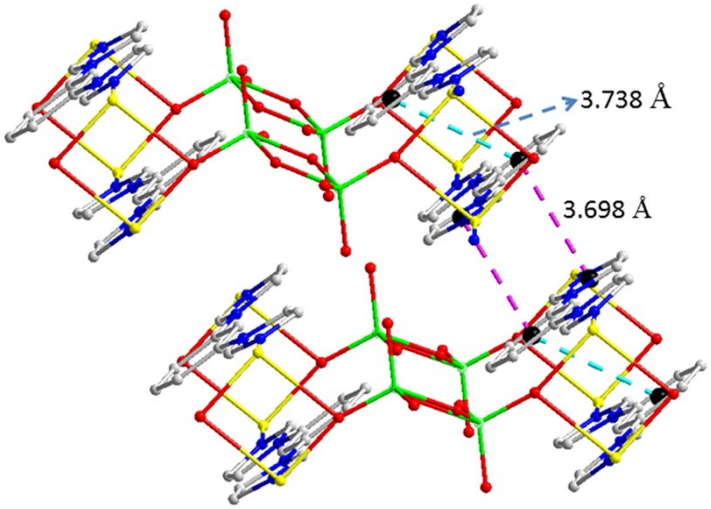

Fig. S2. The detail of π-π interactions in **3**.

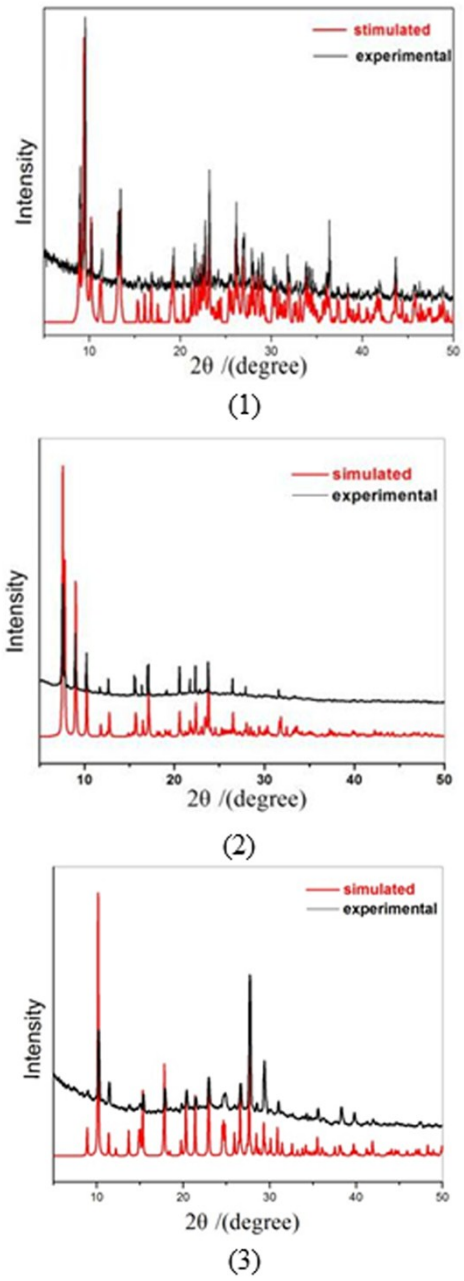

Fig. S3. PXRD patterns for simulated and experimental samples **1-3**.

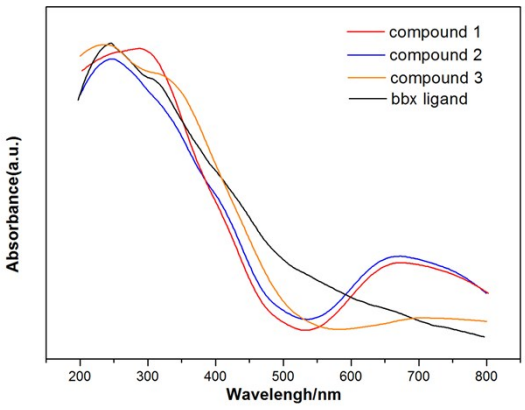

Fig. S4. UV−vis absorption spectra for compounds 1-3.

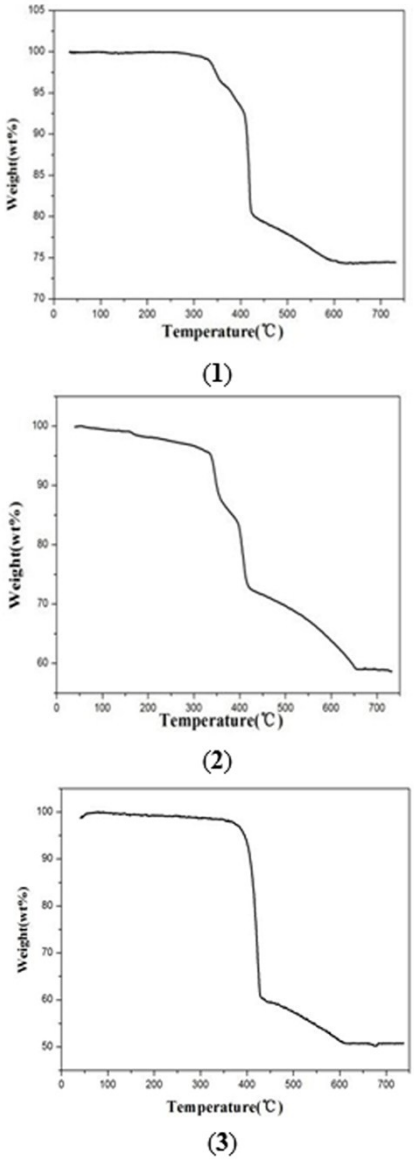

Fig. S5. TG curve of compounds **1-3**.

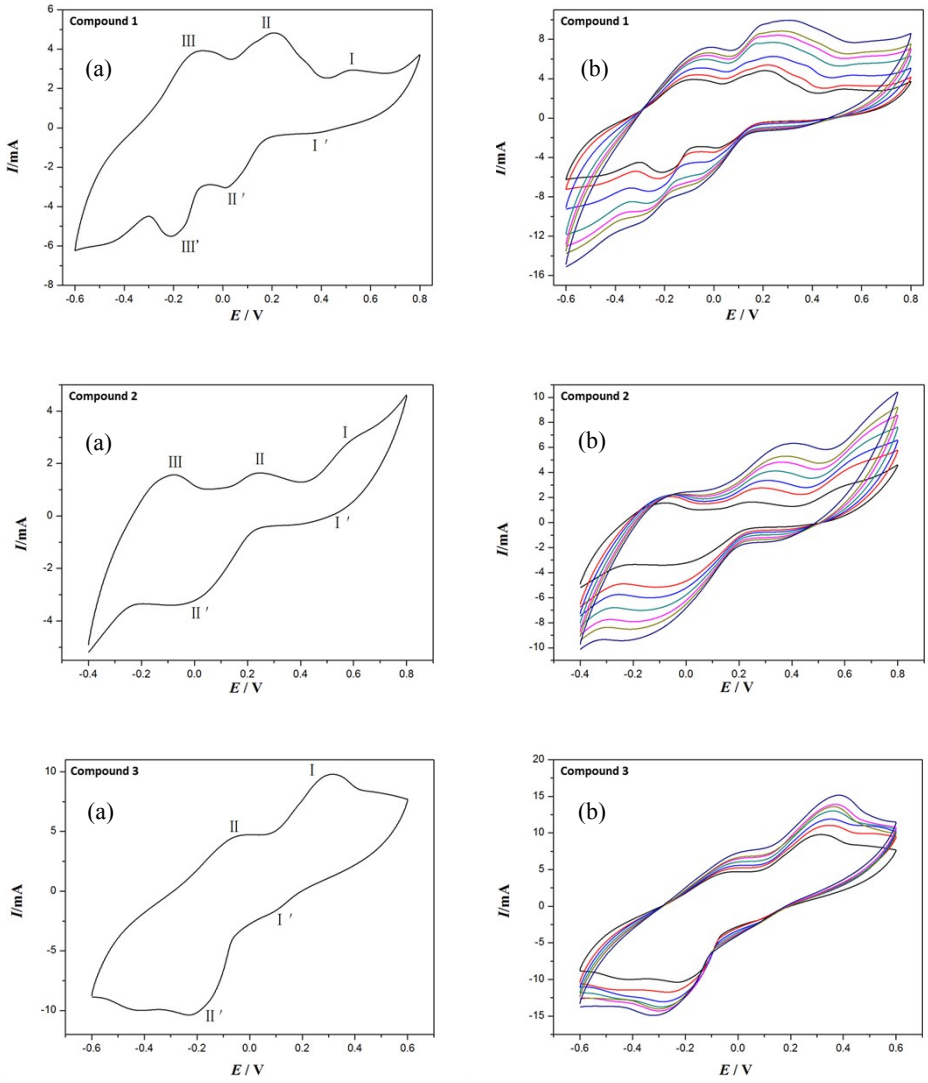

Fig. S6. (a) Cyclic voltammograms of Compounds **1-3** in 1 M H_2SO_4 at scan rates of 60mV/s. (b) Cyclic voltammograms of Compounds **1-3** in 1 M H_2SO_4 at different scan rates (from inner to outer: 60, 80, 100, 120, 140, 160, 200mV/s).

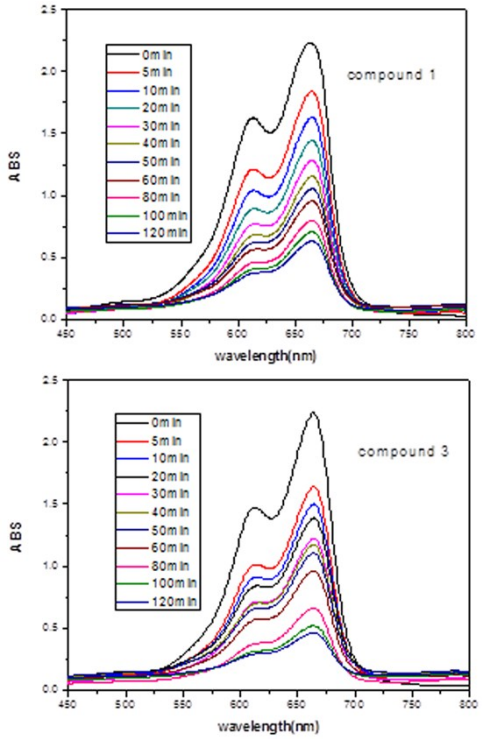

Fig. S7. Absorption spectra of the MB solution during the decomposition reaction use of PMS as compounds **1** and **3**.