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Tuning the architectures of polyoxometalate-templated complexes by changing the spacer lengths of bis-pyridyl-bis-amide ligands (L): From 1D chain to 2D networks based on different $(CuL)_n$ loops†

Xiuli Wang,* Chuang Xu, Hongyan Lin, Guocheng Liu, Song Yang, Qiang Gao and Aixiang Tian

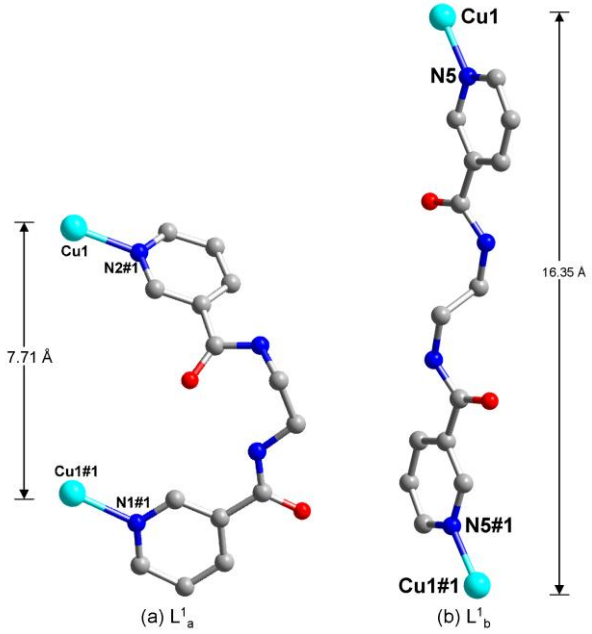

Fig. S1 Two types of configurations of L^1 in **1**. Symmetry code: #1 $-x + 1, -y + 1, -z + 3$.

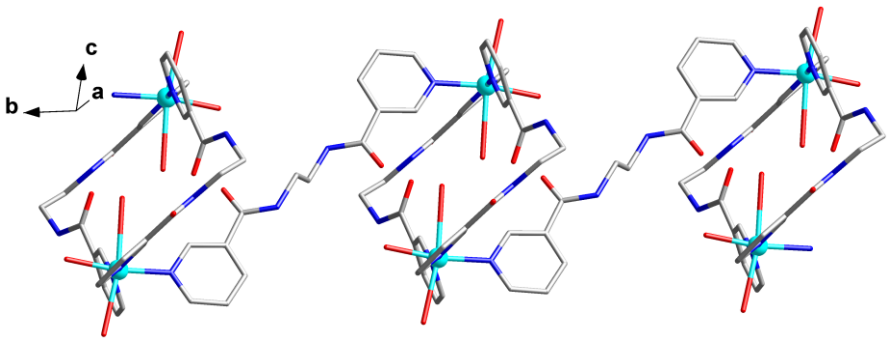

Fig. S2 The 1D chain based on the quadrate $Cu_2(L^1_a)_2$ loop and L^1_b in **1**.

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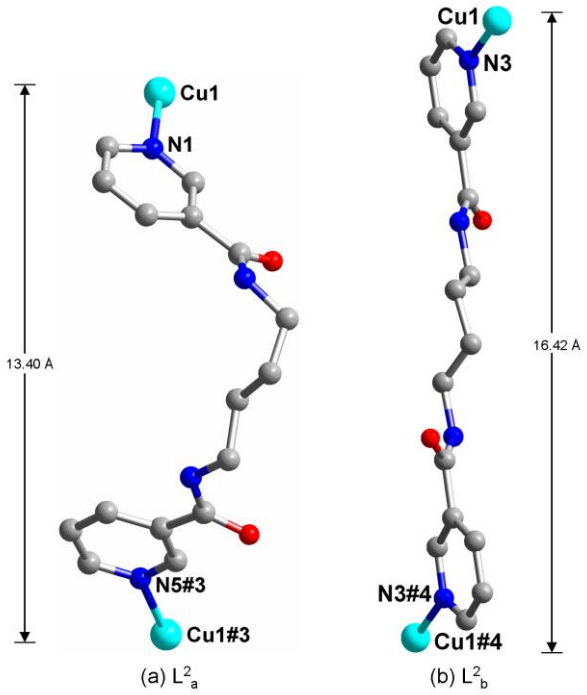

Fig. S3 Two types of configurations of L^2 in **2**. Symmetry code: #3 $-x + 1/2, -y - 1/2, -z + 1$; #4 $-x + 1/2, -y + 1/2, -z + 1$.

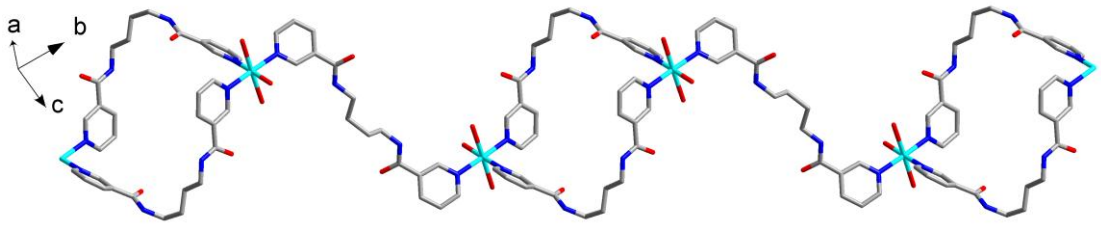

Fig. S4 The 1D chain based on the square $Cu_2(L^2_a)_2$ loop and L^2_b in **2**.

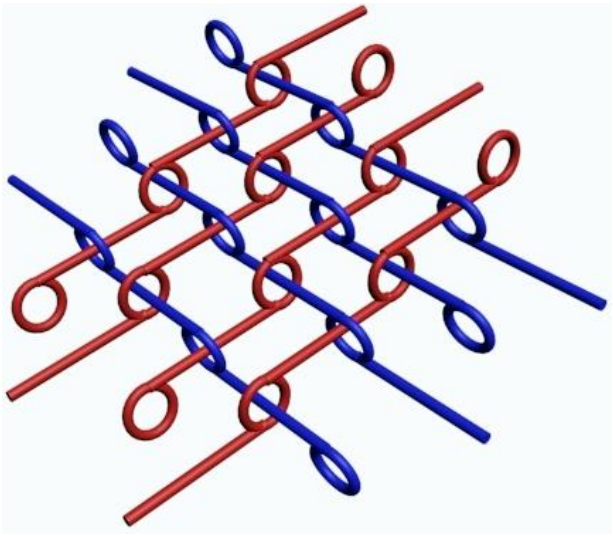

Fig. S5 Schematic illustration of the 1D→2D poly-rotaxane network in **2**.

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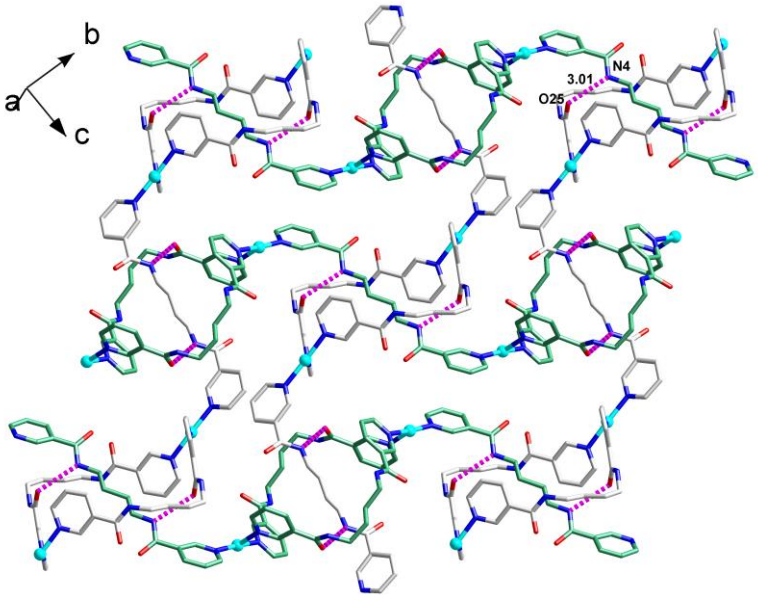

Fig. S6 The supramolecular interaction in compound **2**.

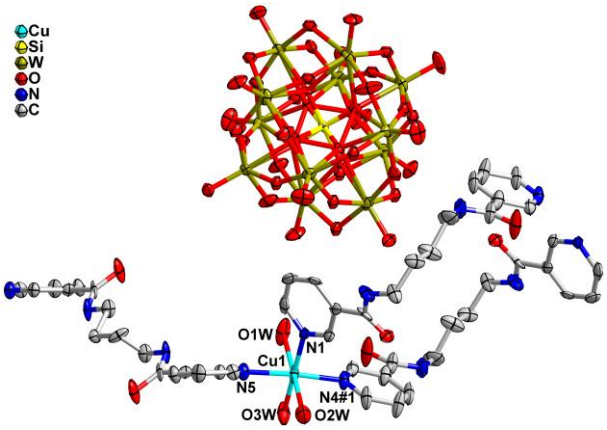

Fig. S7 The coordination environment of the Cu^{II} ion in **3**. All H atoms and lattice water molecules are omitted for clarity. Symmetry code: #1 $-x + 1/2, -y + 1/2, -z + 1$.

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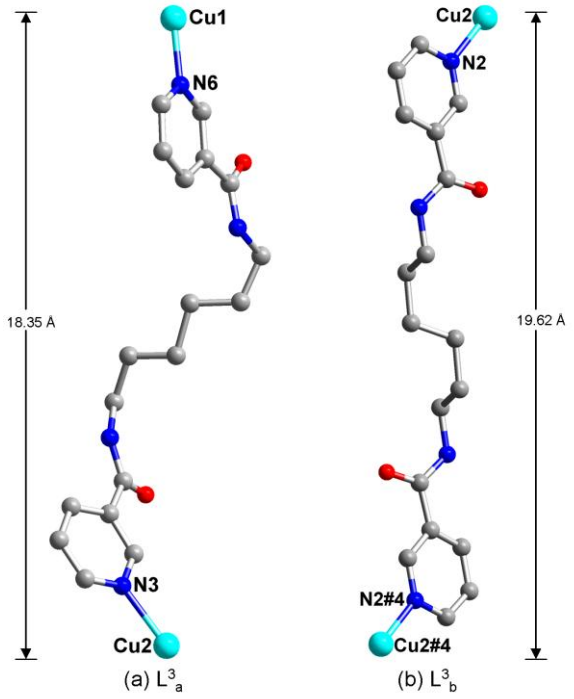

Fig. S8 Two types of configurations of L^3 in **4**. Symmetry code: #4 $-x-3, -y, -z-1$.

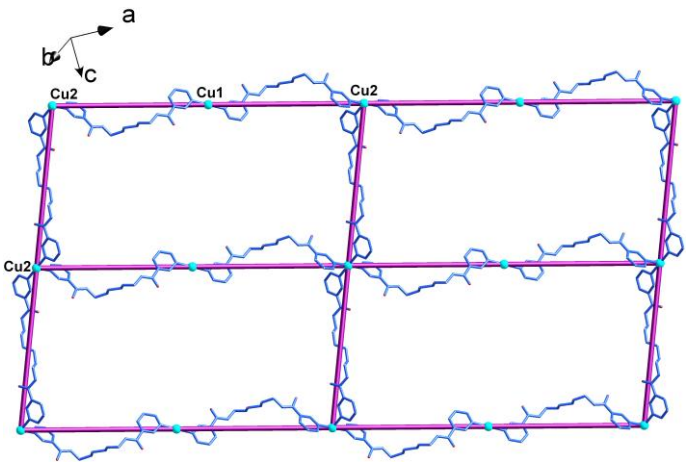

Fig. S9 The 2D network of **4**.

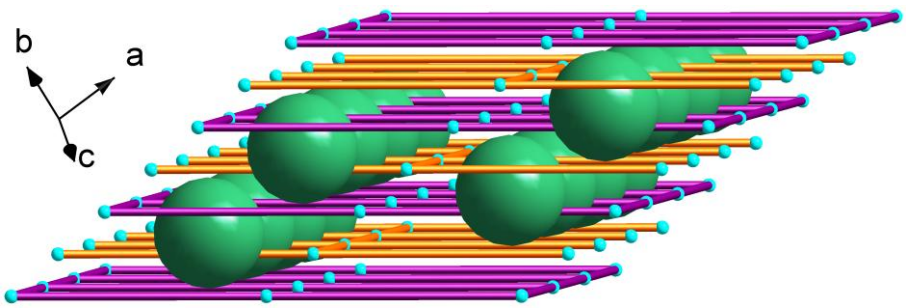

Fig. S10 The schematic view of $SiMo_{12}$ anions sandwiched by adjacent stagger-packed 2D layers in **4**.

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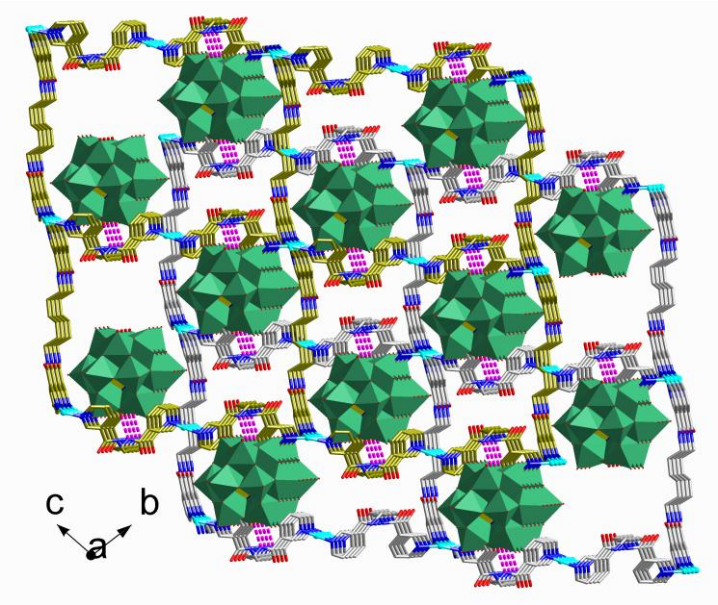

Fig. S11 The supramolecular interaction in compound **4**.

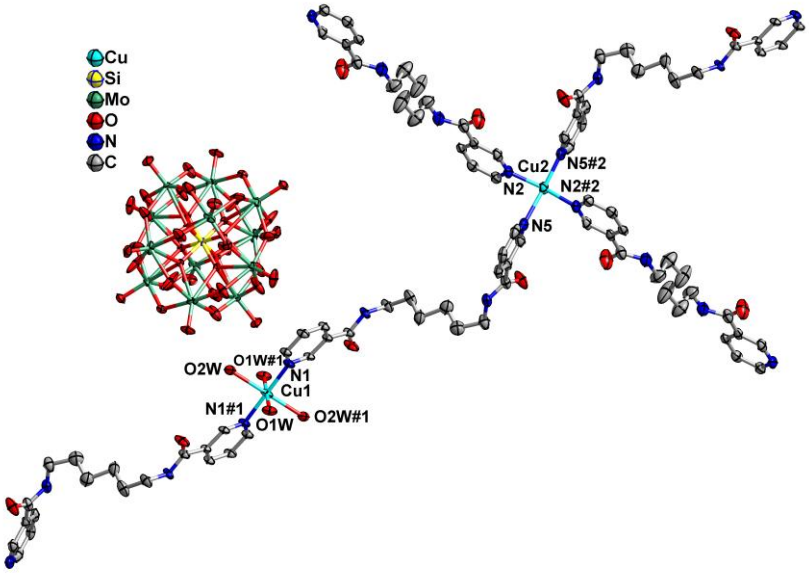

Fig. S12 The coordination environment of the Cu^{II} ions in **5**. All H atoms and lattice water molecules are omitted for clarity. Symmetry code: #1 $-x-1, -y+1, -z$; #2 $-x+2, -y, -z+1$

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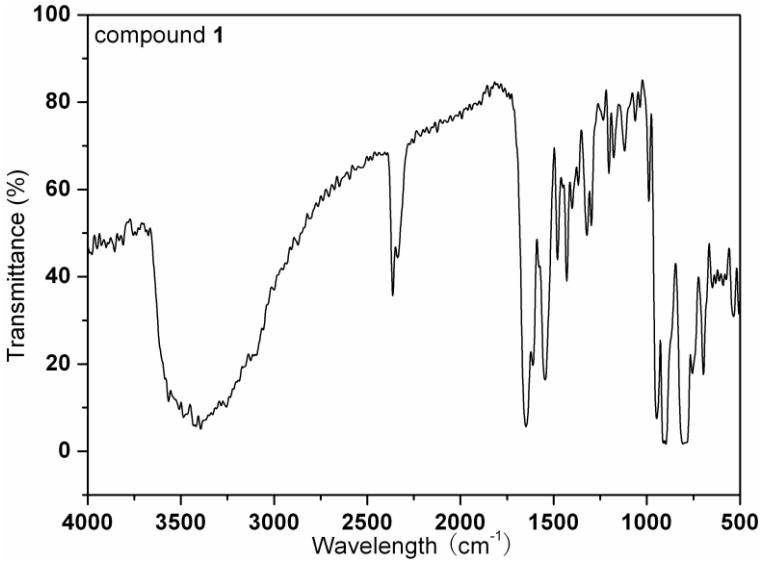

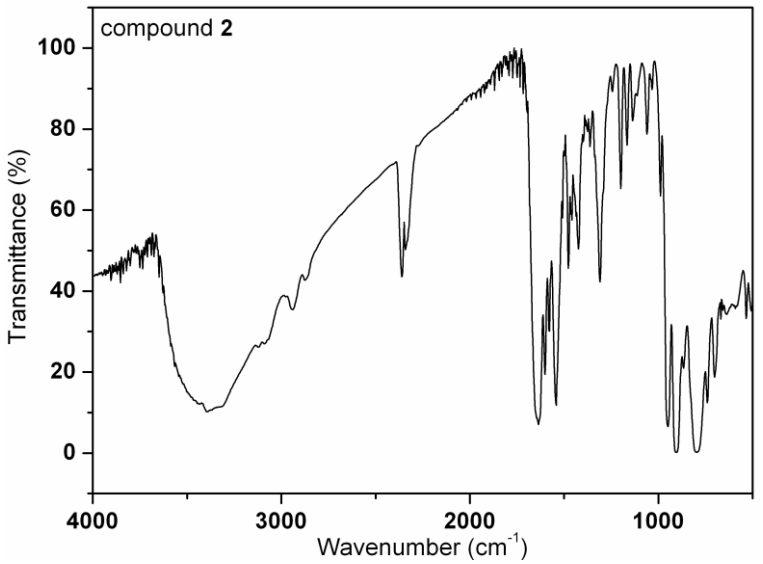

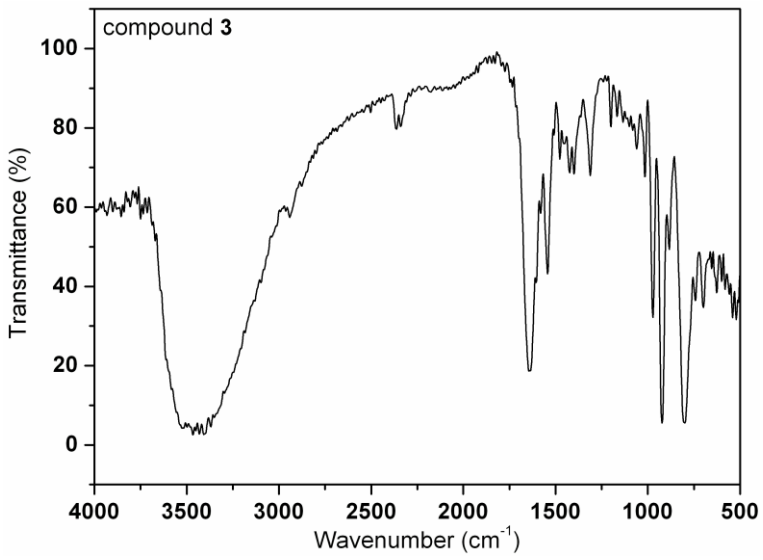

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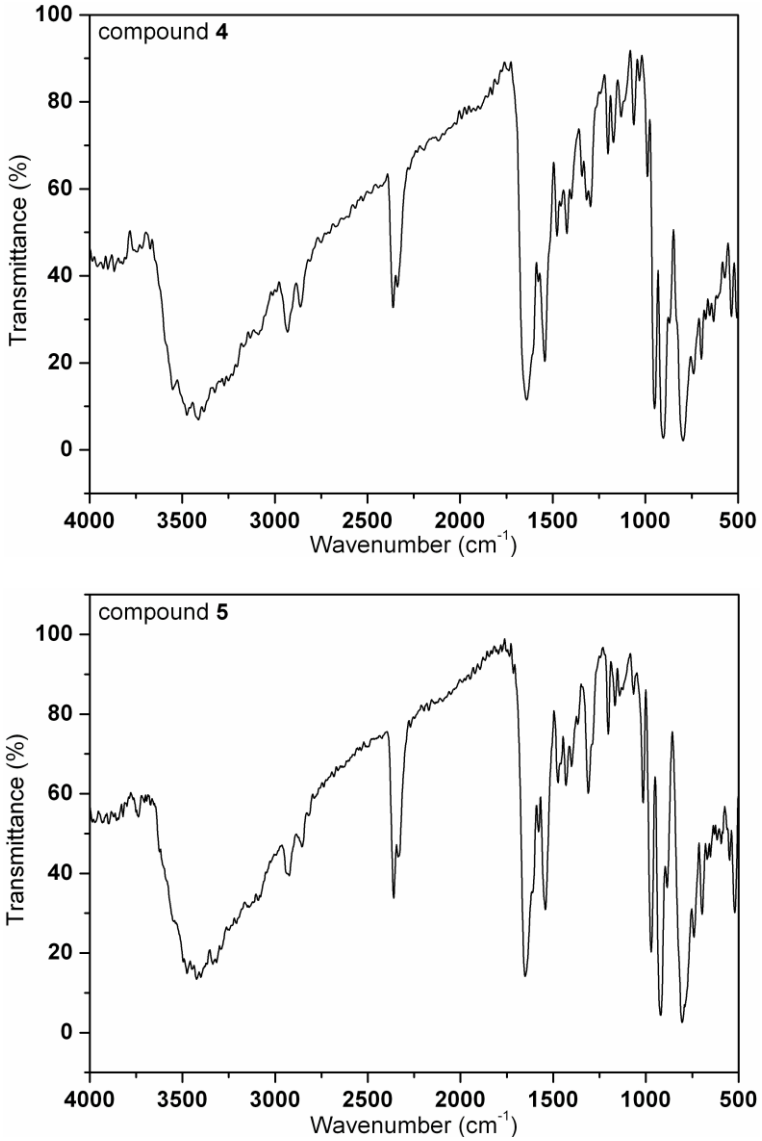

Fig. S13 The IR spectra of compounds **1**–**5**.

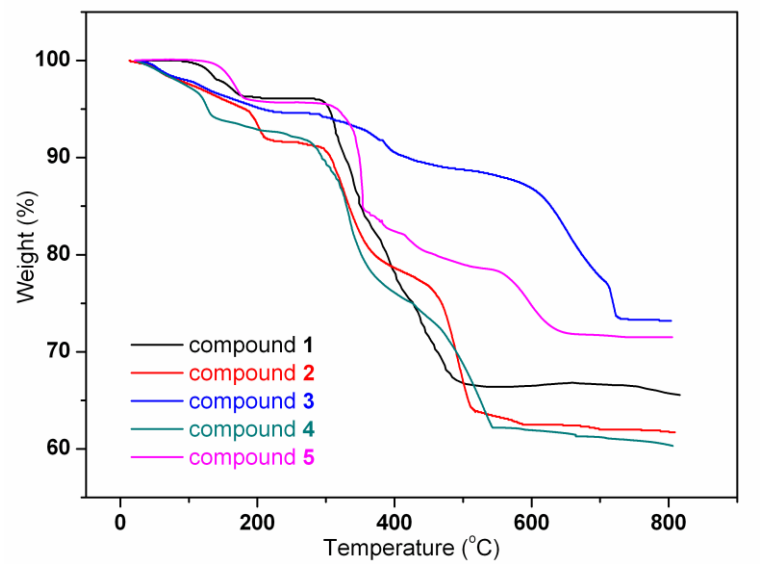

Fig. S14 The TG curves of compounds **1**–**5**.

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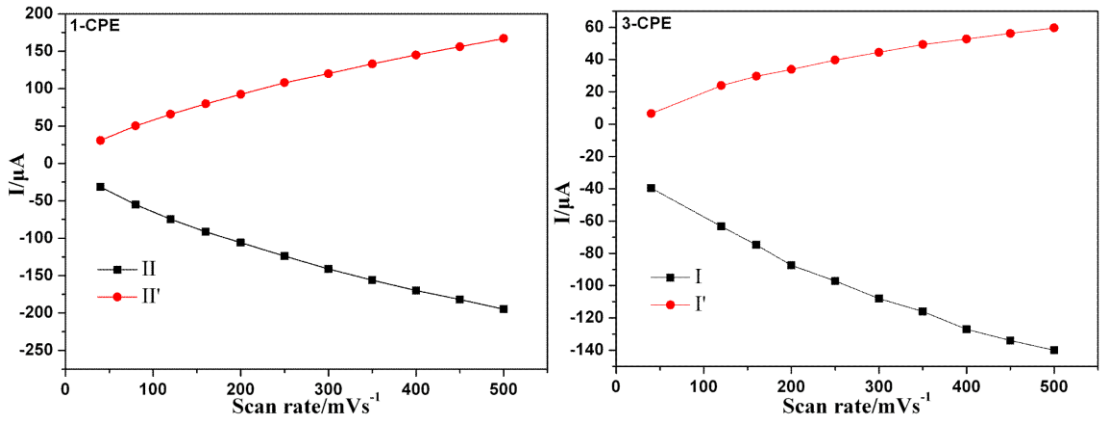
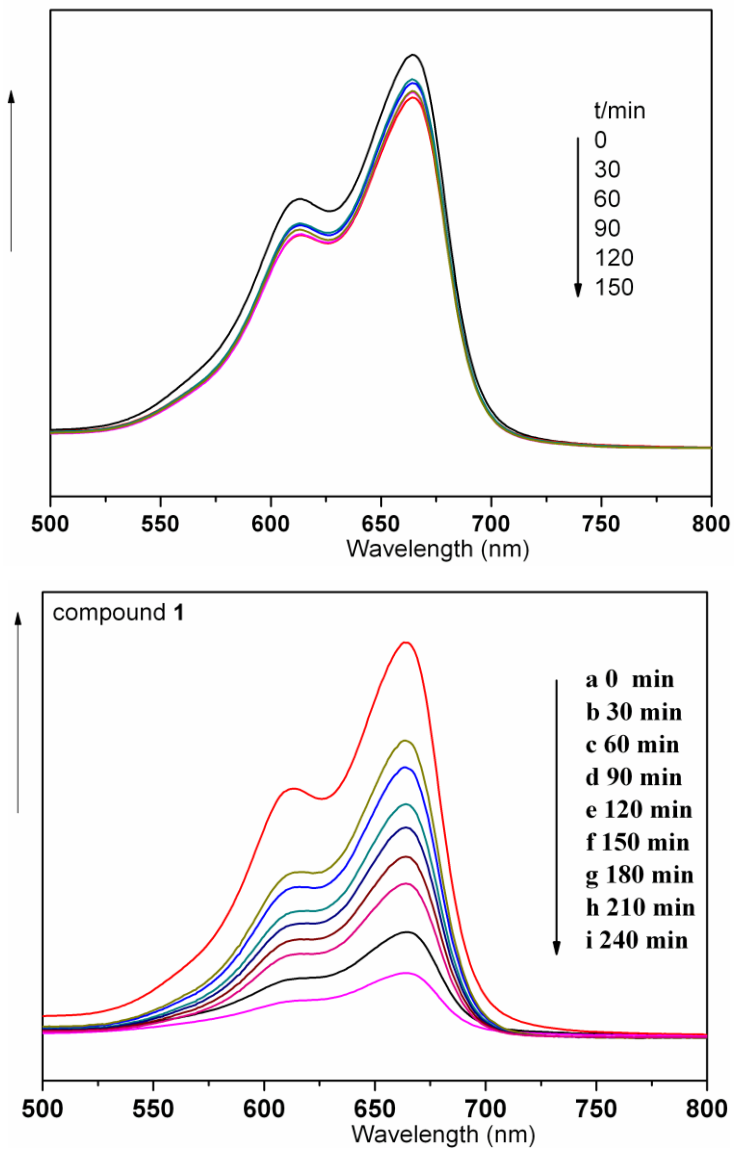


Fig. S15 The dependence of cathodic peak and anodic peak currents on scan rates of **1**–CPE and **3**–CPE.



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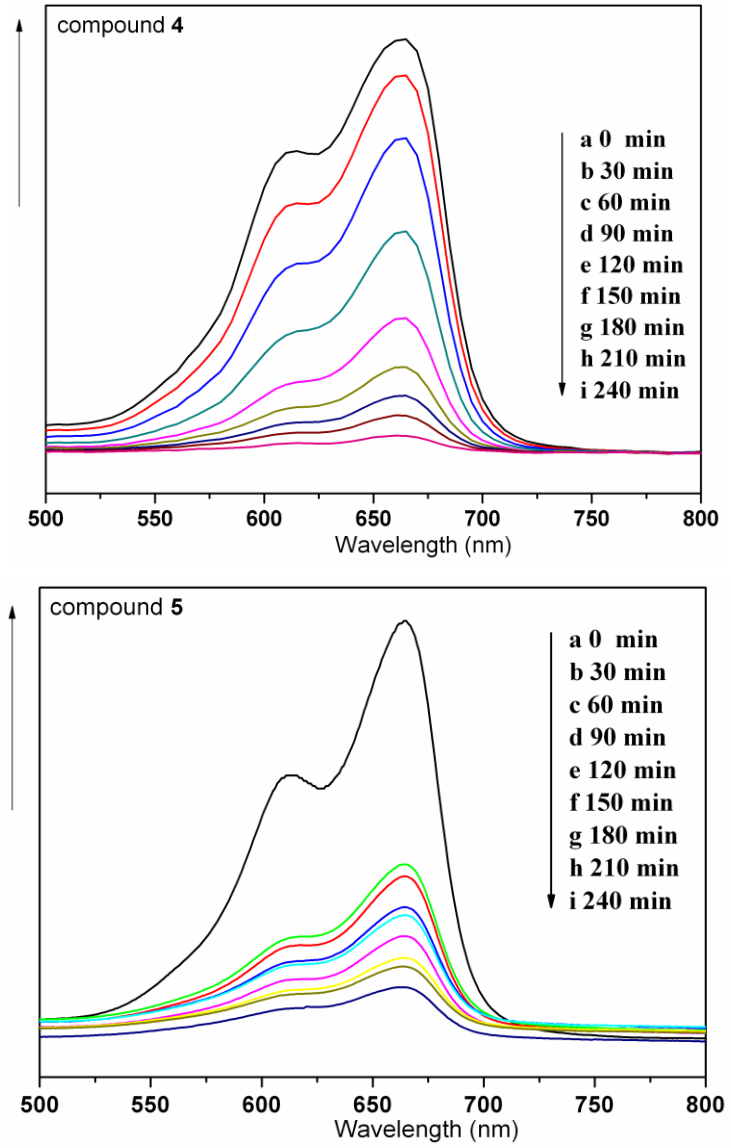

Fig. S16 Absorption spectra of the MB solution during the decomposition reaction under UV light irradiation with the use of **1**, **4**, **5** and without catalyst.

Table S1 Selected bond distances (Å) and angles (°) for compounds **1–5**.

Compound **1**			
Cu(1)–O(1W)	2.004(10)	Cu(1)–N(5)	2.004(11)
Cu(1)–N(2)#1	2.024(11)	Cu(1)–N(1)	2.058(11)
Cu(1)–O(2W)#1	2.728(10)	Cu(1)–O(3W)#1	2.525(10)
O(1W)–Cu(1)–N(5)	171.2(4)	O(1W)–Cu(1)–N(2)#1	90.0(4)
N(5)–Cu(1)–N(2)#1	91.1(4)	O(1W)–Cu(1)–N(1)	87.8(4)
N(5)–Cu(1)–N(1)	91.7(4)	N(2)#1–Cu(1)–N(1)	175.6(4)
O(2W)#1–Cu(1)–N(5)	89.5(4)	O(2W)#1–Cu(1)–N(2)#1	94.5(4)
O(2W)#1–Cu(1)–O(3W)#1	169.5(4)	O(2W)#1–Cu(1)–O(1W)	81.6(4)
O(2W)#1–Cu(1)–N(1)	88.7(4)	O(3W)#1–Cu(1)–N(5)	100.1(4)
O(3W)#1–Cu(1)–N(2)#1	89.1(4)	O(3W)#1–Cu(1)–N(1)	87.1(4)
O(3W)#1–Cu(1)–O(1W)	88.6(4)		

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Symmetry code for **1**: #1 –*x* + 1, –*y* + 1, –*z* + 3

Compound **2**

N(1)–Cu(1)	2.028(9)	N(3)–Cu(1)	2.042(8)
N(5)–Cu(1)	2.043(9)	O(3W)–Cu(1)	2.019(8)
O(1W)–Cu(1)	2.502(9)	O(2W)–Cu(1)	2.551(8)
O(3W)–Cu(1)–N(1)	179.1(3)	O(3W)–Cu(1)–N(5)	86.6(3)
N(1)–Cu(1)–N(5)	94.3(3)	O(3W)–Cu(1)–N(3)	88.5(3)
N(1)–Cu(1)–N(3)	90.6(3)	N(5)–Cu(1)–N(3)	174.8(4)
O(3W)–Cu(1)–O(1W)	92.1(4)	N(1)–Cu(1)–O(1W)	87.9(4)
N(5)–Cu(1)–O(1W)	91.5(4)	N(3)–Cu(1)–O(1W)	90.5(3)
O(3W)–Cu(1)–O(2W)	89.4(4)	N(1)–Cu(1)–O(2W)	90.6(4)
N(5)–Cu(1)–O(2W)	89.9(4)	N(3)–Cu(1)–O(2W)	88.3(3)
O(1W)–Cu(1)–O(2W)	178.1(4)		

Compound **3**

Cu(1)–O(3W)	2.025(12)	Cu(1)–N(1)	2.028(12)
Cu(1)–N(5)	2.043(11)	Cu(1)–N(4)#1	2.053(12)
Cu(1)–O(2W)	2.431(15)	Cu(1)–O(1W)	2.522(15)
O(3W)–Cu(1)–N(1)	178.2(5)	O(3W)–Cu(1)–N(5)	89.7(5)
N(1)–Cu(1)–N(5)	90.5(5)	O(3W)–Cu(1)–N(4)#1	85.8(5)
N(1)–Cu(1)–N(4)#1	94.0(5)	N(5)–Cu(1)–N(4)#1	175.3(5)
O(3W)–Cu(1)–O(2W)	89.9(6)	N(1)–Cu(1)–O(2W)	91.9(5)
N(5)–Cu(1)–O(2W)	89.3(5)	N(4)#1–Cu(1)–O(2W)	89.2(5)
N(5)–Cu(1)–O(1W)	89.3(5)	N(1)–Cu(1)–O(1W)	87.7(5)
O(1W)–Cu(1)–O(2W)	178.6(5)	N(4)–Cu(1)–O(1W)	92.2(5)
O(3W)–Cu(1)–O(1W)	90.5(5)		

Symmetry code for **3**: #1 –*x* + 1/2, –*y* + 1/2, –*z* + 1

Compound **4**

Cu(1)–N(6)#1	2.003(4)	Cu(1)–N(6)	2.003(4)
Cu(1)–O(2W)#1	2.041(4)	Cu(1)–O(3W)#1	2.346(4)
Cu(1)–O(3W)	2.346(4)	Cu(1)–O(2W)	2.041(4)
Cu(2)–N(3)#2	1.950(7)	Cu(2)–N(2)	1.995(6)
Cu(2)–N(2)#2	2.053(6)	Cu(2)–N(3)	2.176(7)
N(6)#1–Cu(1)–N(6)	179.998(1)	N(6)#1–Cu(1)–O(2W)#1	90.16(17)
N(6)–Cu(1)–O(2W)#1	89.84(17)	N(6)#1–Cu(1)–O(2W)	89.84(17)
N(6)–Cu(1)–O(2W)	90.16(17)	O(2W)#1–Cu(1)–O(2W)	180.0
N(6)#1–Cu(1)–O(3W)#1	88.62(17)	N(6)–Cu(1)–O(3W)#1	91.38(17)
O(2W)#1–Cu(1)–O(3W)#1	89.52(18)	O(2W)–Cu(1)–O(3W)#1	90.48(18)
N(6)#1–Cu(1)–O(3W)	91.39(17)	N(6)–Cu(1)–O(3W)	88.61(17)
O(2W)#1–Cu(1)–O(3W)	90.48(18)	O(2W)–Cu(1)–O(3W)	89.52(18)
O(3W)#1–Cu(1)–O(3W)	179.997(1)	N(3)#2-Cu(2)-N(2)	92.3(3)
N(3)#2–Cu(2)–N(2)#2	91.8(3)	N(2)–Cu(2)–N(2)#2	162.82(10)
N(2)#2–Cu(2)–N(3)	84.6(2)	N(3)#2–Cu(2)–N(3)	164.28(12)
N(2)–Cu(2)–N(3)	87.0(2)		

Symmetry code for **4**: #1 –*x*, –*y*, –*z* + 1; #2 –*x* – 3, –*y* + 1, –*z*

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Compound **5**			
N(1)–Cu(1)	1.992(10)	O(2W)–Cu(1)	2.348(10)
O(1W)–Cu(1)	2.054(9)	Cu(1)–N(1)#1	1.992(10)
Cu(1)–O(1W)#1	2.054(9)	Cu(1)–O(2W)#1	2.348(10)
Cu(2)–N(5)#2	2.007(12)	Cu(2)–N(2)#2	2.073(14)
N(2)–Cu(2)	2.073(14)	N(5)–Cu(2)	2.007(12)
N(1)–Cu(1)–N(1)#1	179.997(1)	N(1)–Cu(1)–O(1W)	90.2(4)
N(1)#1–Cu(1)–O(1W)	89.8(4)	N(1)–Cu(1)–O(1W)#1	89.8(4)
N(1)#1–Cu(1)–O(1W)#1	90.2(4)	O(1W)–Cu(1)–O(1W)#1	179.997(1)
N(1)–Cu(1)–O(2W)	89.3(4)	N(1)#1–Cu(1)–O(2W)	90.7(4)
O(1W)–Cu(1)–O(2W)	90.6(4)	O(1W)#1–Cu(1)–O(2W)	89.4(4)
N(1)–Cu(1)–O(2W)#1	90.7(4)	N(1)#1–Cu(1)–O(2W)#1	89.3(4)
O(1W)–Cu(1)–O(2W)#1	89.4(4)	O(1W)#1–Cu(1)–O(2W)#1	90.6(4)
O(2W)–Cu(1)–O(2W)#1	179.999(1)	N(5)#2–Cu(2)–N(5)	179.999(2)
N(5)#2–Cu(2)–N(2)	90.0(5)	N(5)–Cu(2)–N(2)	90.0(5)
N(5)#2–Cu(2)–N(2)#2	90.0(5)	N(5)–Cu(2)–N(2)#2	90.0(5)
N(2)–Cu(2)–N(2)#2	180.0(7)		
Symmetry code for **5**: #1 $-x-1, -y+1, -z$; #2 $-x+2, -y, -z+1$			

Table S2. Selected Hydrogen-Bonding Geometry (Å, °) for compound **1**

D–H···A	D–H	H···A	D···A	D–H···A
C(15)–H(15A)···O(16)	0.97	2.33	3.02	128

Table S3. Selected Hydrogen-Bonding Geometry (Å, °) for compound **2**

D–H···A	D–H	H···A	D···A	D–H···A
N(4)–H(4C)···O(25)	0.86	2.18	3.01	163

Table S4. Selected Hydrogen-Bonding Geometry (Å, °) for compound **4**

D–H···A	D–H	H···A	D···A	D–H···A
N(5)–H(5B)···O(19)	0.86	2.04	2.85	158