Electronic Supplementary Material (ESI) for Dalton Transactions

Novel inorganic-organic hybrids constructed from multinuclear copper cluster and Keggin polyanions: from 1D wave-like chain to 2D network †

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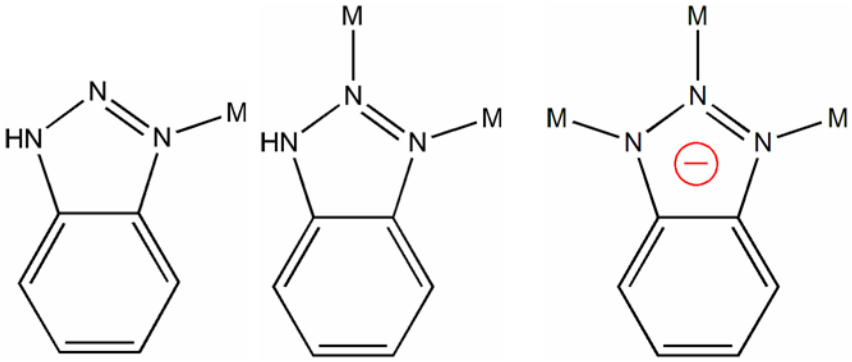

Fig. S1 Coordination modes of HBTA ligand in this report.

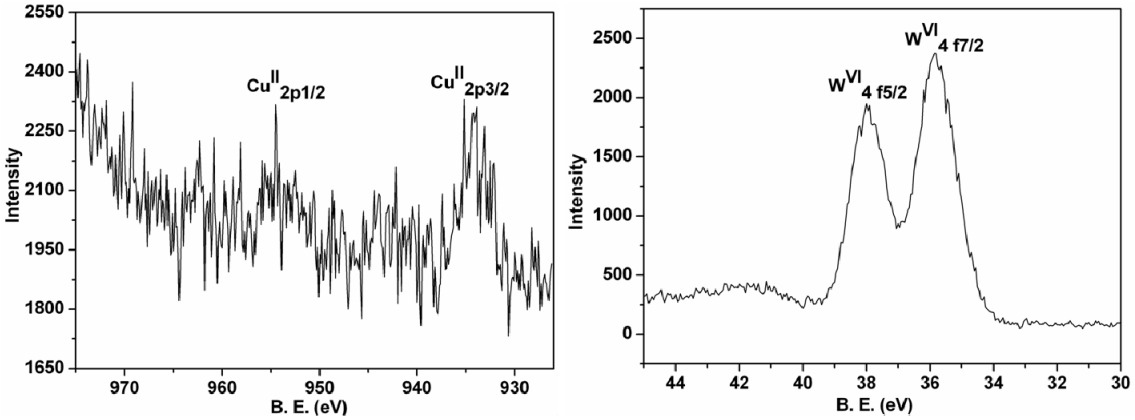

Fig. S2 The XPS spectrum of Cu and W in compound **2**.

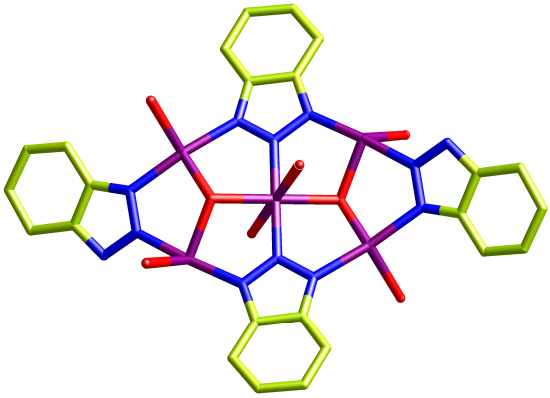

Fig. S3 View of the "porphyrin-like" cluster in **2**.

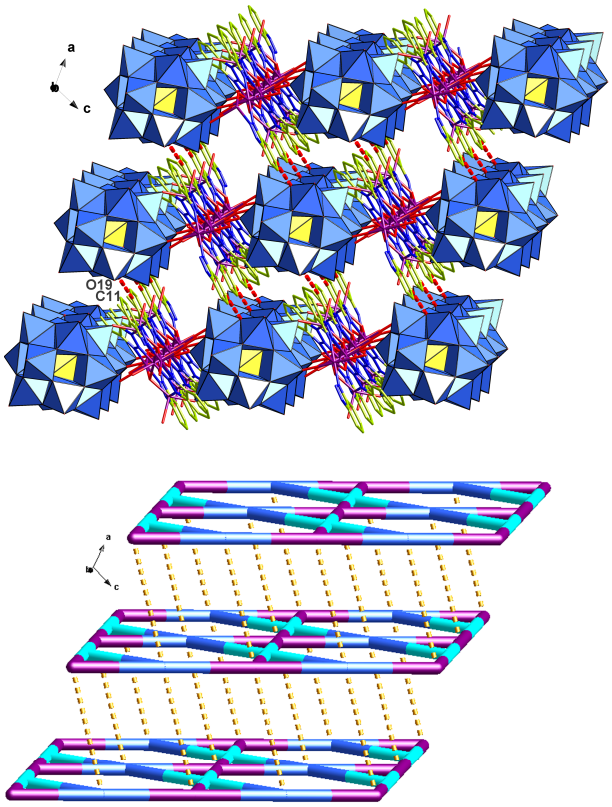

Fig. S4 (up) Polyhedral and stick represents 3D hydrogen-bonding supramolecular framework of compound **2**. (down) 3D supramolecular network of **2**.

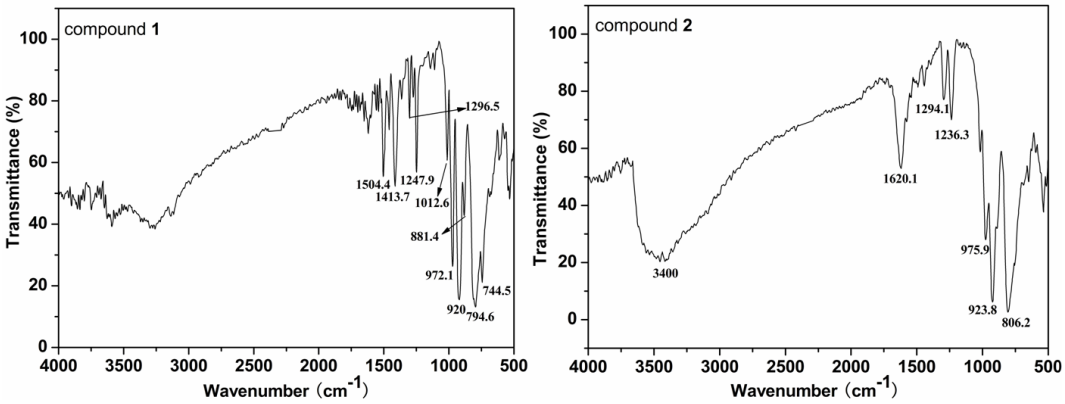

Fig. S5 The IR spectra of compounds **1** and **2**.

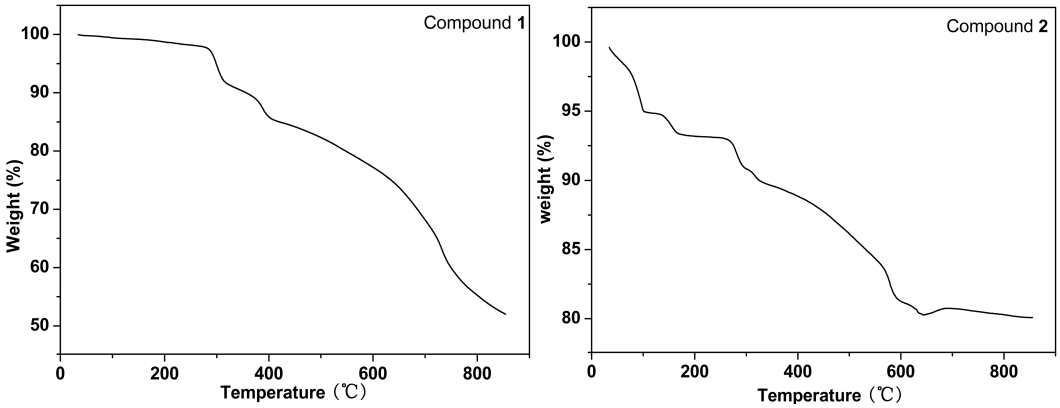

Fig. S6 The TG curves of compounds **1** and **2**.

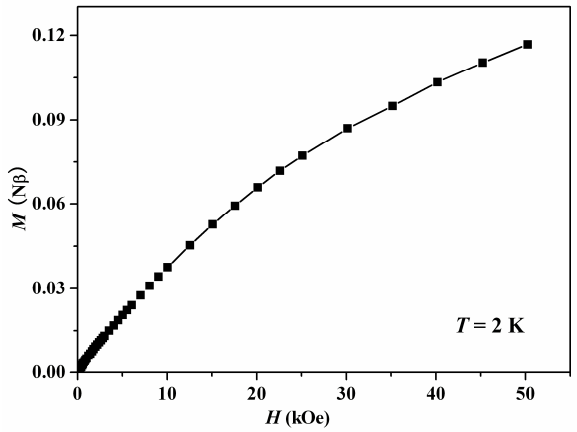

Fig. S7 *M* versus *H* plot for **2** at 2 K.

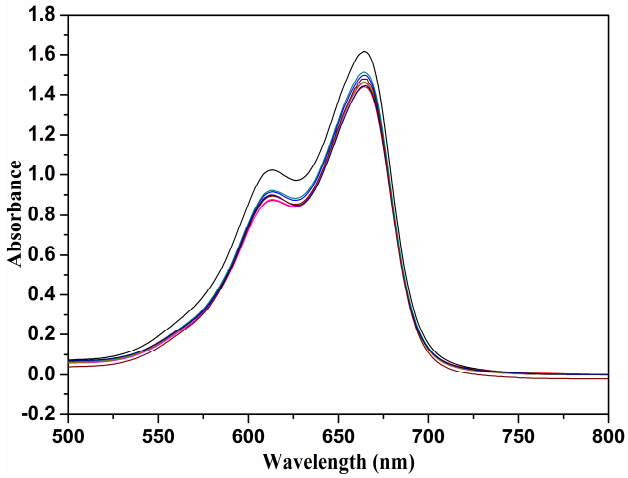

Fig. S8 Absorption spectra of the MB solution during the decomposition reaction under UV light irradiation without title compounds.

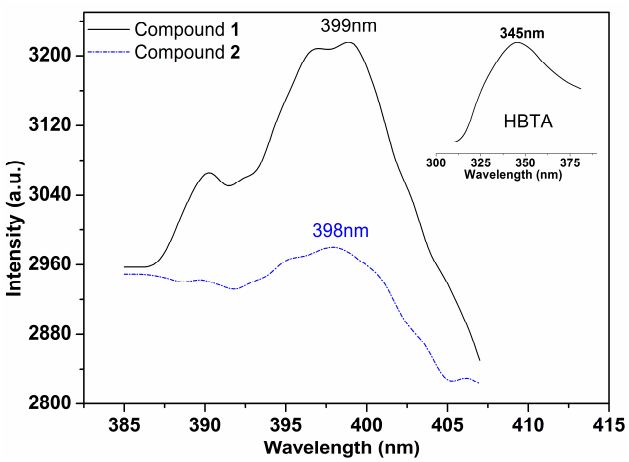

Fig. S9 Emission spectra of compounds **1** and **2** (Insert: Emission spectrum of HBTA).

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

Compound **1**			
N(3)–Cu(1)	2.040(7)	N(11)–Cu(1)#2	2.003(7)
N(5)–Cu(1)	2.169(7)	N(12)–Cu(4)	1.917(7)
N(6)–Cu(2)#2	1.946(6)	N(13)–Cu(3)	1.868(7)
N(7)–Cu(1)	2.025(8)	N(14)–Cu(4)	2.002(8)
N(8)–Cu(2)	1.962(7)	N(11)–Cu(1)#2	2.003(7)
N(9)–Cu(3)	1.882(7)	N(16)–Cu(4)	1.953(8)
N(10)–Cu(2)#2	1.961(7)	O(13)–Cu(4)	2.494(6)
N(11)#2–Cu(1)–N(7)	111.9(3)	N(9)–Cu(3)–Cu(4)	119.6(2)
N(11)#2–Cu(1)–N(3)	112.7(3)	N(13)–Cu(3)–Cu(2)	112.0(2)
N(7)–Cu(1)–N(3)	115.2(3)	N(9)–Cu(3)–Cu(2)	58.3(2)
N(11)#2–Cu(1)–N(5)	122.6(3)	Cu(4)–Cu(3)–Cu(2)	115.71(5)
N(7)–Cu(1)–N(5)	94.2(3)	N(12)–Cu(4)–N(16)	129.5(3)
N(3)–Cu(1)–N(5)	98.8(3)	N(12)–Cu(4)–N(14)	120.6(3)
N(11)#2–Cu(1) –Cu(4)#2	55.8(2)	N(16)–Cu(4)–N(14)	106.3(3)
N(7)–Cu(1)–Cu(4)#2	167.7(2)	N(12)–Cu(4)–O(13)	105.1(3)
N(3)–Cu(1)–Cu(4)#2	72.8(2)	N(16)–Cu(4)–O(13)	91.0(3)
N(5)–Cu(1)–Cu(4)#2	93.7(2)	N(14)–Cu(4)–O(13)	91.0(3)
N(11)#2–Cu(1)–Cu(2)	55.6(2)	N(12)–Cu(4)–Cu(3)	66.8(2)
N(7)–Cu(1)–Cu(2)	56.4(2)	N(16)–Cu(4)–Cu(3)	162.1(3)
N(3)–Cu(1)–Cu(2)	139.4(2)	N(14)–Cu(4)–Cu(3)	55.9(2)
N(5)–Cu(1)–Cu(2)	120.52(19)	O(13)–Cu(4)–Cu(3)	91.06(14)
Cu(4)#2–Cu(1)–Cu(2)	111.32(4)	N(12)–Cu(4)–Cu(1)#2	58.4(2)
N(6)#2–Cu(2)–N(10)#2	122.7(3)	N(16)–Cu(4)–Cu(1)#2	112.1(2)
N(6)#2–Cu(2)–N(8)	122.3(3)	N(14)–Cu(4)–Cu(1)#2	85.3(2)
N(10)#2–Cu(2)–N(8)	115.0(3)	O(13)–Cu(4)–Cu(1)#2	156.73(14)
N(6)#2–Cu(2)–Cu(3)	68.0(2)	Cu(3)–Cu(4)–Cu(1)#2	67.89(4)

N(10)#2–Cu(2)–Cu(3)	169.2(2)	N(8)–Cu(2)–Cu(1)	57.7(2)
N(8)–Cu(2)–Cu(3)	54.4(2)	Cu(3)–Cu(2)–Cu(1)	111.88(4)
N(6)#2–Cu(2)–Cu(1)	172.8(2)	N(13)–Cu(3)–N(9)	169.7(3)
N(10)#2–Cu(2)–Cu(1)	57.8(2)	N(13)–Cu(3)–Cu(4)	59.7(2)

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

Compound **2**

Cu(1)–O(22)#1	1.90(2)	Cu(3)–O(21)#2	2.02(2)
Cu(1)–O(22)	1.90(2)	Cu(3)–O(20)	2.044(17)
Cu(1)–N(4)	2.03(2)	Cu(3)–O(2W)	2.135(19)
Cu(1)–N(4)#1	2.03(2)	Cu(4)–N(2)#2	1.91(2)
Cu(2)–O(22)#1	1.908(19)	Cu(4)–N(2)	1.91(2)
Cu(2)–N(1)	1.95(2)	Cu(4)–O(21)#2	1.98(2)
Cu(2)–N(5)	1.97(2)	Cu(4)–O(21)	1.98(2)
Cu(2)–O(21)	2.023(19)	O(1W)–Cu(2)#1	1.908(19)
Cu(3)–N(3)	1.96(2)	O(21)–Cu(3)#2	2.02(2)
Cu(3)–N(6)#2	1.99(2)	N(6)–Cu(3)#2	1.99(2)
O(22)#1–Cu(1)–O(22)	180	O(22)–Cu(1)–N(4)#1	87.5(8)
O(22)#1–Cu(1) –N(4)	87.5(8)	N(4)–Cu(1)–N(4)#1	180
O(22)–Cu(1)–N(4)	92.5(8)	O(22)#1–Cu(2)–N(1)	97.0(9)
O(22)#1–Cu(1)–N(4)#1	92.5(8)	O(22)#1–Cu(2)–N(5)	86.2(9)
N(1)–Cu(2)–N(5)	174.9(10)	N(3)–Cu(3)–O(2W)	93.3(9)
O(22)#1–Cu(2)–O(21)	168.3(9)	N(6)#2–Cu(3)–O(2W)	97.2(10)
N(1)–Cu(2)–O(21)	88.6(8)	O(21)#2–Cu(3)–O(2W)	116.2(8)
N(5)–Cu(2)–O(21)	87.5(9)	O(20)–Cu(3)–O(2W)	94.9(7)
N(3)–Cu(3)–N(6)#2	167.8(10)	N(2)#2–Cu(4)–N(2)	180
N(3)–Cu(3)–O(21)#2	91.1(9)	N(2)#2–Cu(4)–O(21)#2	89.2(9)
N(6)#2–Cu(3)–O(21)#2	89.8(9)	N(2)–Cu(4)–O(21)#2	90.8(9)
N(3)–Cu(3)–O(20)	87.6(8)	N(2)#2–Cu(4)–O(21)	90.8(9)
N(6)#2–Cu(3)–O(20)	85.4(9)	N(2)–Cu(4)–O(21)	89.2(9)
O(21)#2–Cu(3)–O(20)	148.9(8)	O(21)#2–Cu(4)–O(21)	180

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