

Construction of 3D Metal-Organic Frameworks Bearing Heteropolyoxometalates Units and Multi-azole Molecules and Exploration of Their Photocatalytic Activities

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Table S1 Selected bond lengths and angles for compounds **1** and **2**.

Compound 1			
Cu1–N1	2.108(3)	Cu2–O3W	2.267(3)
Cu1–N14	1.998(3)	Cu2–O3W#5	1.915(3)
Cu1–O1	2.307(3)	Cu3–N4	2.137(3)
Cu2–Cu2#5	3.0364(10)	Cu3–N7	1.969(3)
Cu2–N3	1.955(3)	Cu3–N8	2.113(3)
Cu2–N9	2.039(4)	Cu3–O3W	1.919(3)
Cu2–O1W	2.230(3)	Cu3–O4W	2.214(4)
Cu2–O2W	2.305(10)		
N1–Cu1–O1#1	96.74(11)	N9#5–Cu2–Cu2#5	103.41(9)
N1–Cu1–O1	83.26(11)	N9#5–Cu2–O3W	109.60(12)
N14#2–Cu1–O1	90.37(11)	N9#5–Cu2–O1W	160.33(14)
N14#3–Cu1–O1	89.63(11)	N9#5–Cu2–O2W	86.0(3)
N14#3–Cu1–N1	88.97(11)	O1W–Cu2–Cu2#5	90.83(9)
N14#2–Cu1–N1	91.03(11)	O1W–Cu2–O3W	90.02(12)
N3–Cu2–Cu2#5	122.51(9)	O1W–Cu2–O2W	74.3(3)
N3–Cu2–O3W	83.47(11)	O2W–Cu2–Cu2#5	138.8(2)
N3–Cu–2N9#5	97.93(13)	O3W–Cu3–N4	86.41(10)
N3–Cu2–O1W	85.35(12)	O3W–Cu3–O4W	91.57(12)
N3–Cu2–O2W	94.9(3)	O3W–Cu3–N7	172.00(12)
O3W–Cu2–Cu2#5	39.11(6)	O3W–Cu3–N8	87.98(11)
O3W#5–Cu2–Cu2#5	48.15(8)	N4–Cu3–O4W	94.81(13)
O3W#5–Cu2–N3	170.13(11)	N7–Cu3–N4	91.20(12)
O3W#5–Cu2–O3W	87.25(10)	N7–Cu3–O4W	96.24(13)
O3W#5–Cu2–N9#5	88.35(11)	N7–Cu3–N8	92.23(12)
O3W#5–Cu2–O1W	91.29(10)	N8–Cu3–N4	163.49(12)
O3W–Cu2–O2W	164.4(3)	N8–Cu3–O4W	100.86(13)

O3W#5–Cu2–O2W		93.1(2)	
Symmetry codes : #1 1–x, 2–y, –z; #2 1–x, 1–y, 1–z; #3 1–x, 1–y, –z; #5 2–x, 2–y, 1–z.			
Compound 2			
Cu1–N8	1.99(2)	Cu2–O2W	1.95(3)
Cu1–N10	2.00(2)	Cu2–N12	1.96(2)
Cu1–N2	2.06(2)	Cu2–N5	2.00(2)
Cu1–N9	2.10(2)	Cu2–O4W	2.05(3)
Cu1–O1W	2.367(18)	Cu2–O3W	2.19(3)
N8–Cu1–N10	176.6(9)	O2W–Cu2–N12	171.5(11)
N8–Cu1–N2	93.9(9)	O2W–Cu2–N5	90.5(11)
N10–Cu1–N2	89.3(9)	N12–Cu2–N5	96.2(9)
N8–Cu1–N9	88.0(9)	O2W–Cu2–O4W	87.0(12)
N10–Cu1–N9	88.7(9)	N12–Cu2–O4W	84.7(10)
N2–Cu1–N9	172.6(9)	N5–Cu2–O4W	153.2(11)
N8–Cu1–O1W	87.1(8)	O2W–Cu2–O3W	87.5(12)
N10–Cu1–O1W	93.7(8)	N12–Cu2–O3W	94.8(10)
N2–Cu1–O1W	97.6(8)	N5–Cu2–O3W	112.3(10)
N9–Cu1–O1W	89.6(8)	O4W–Cu2–O3W	94.3(10)

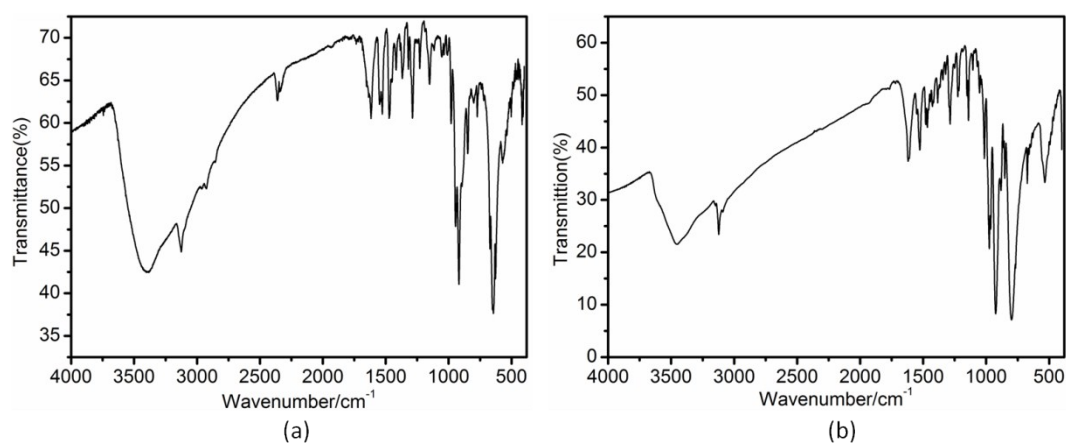


Fig. S1 The IR spectra of compounds **1** (a) and **2** (b).

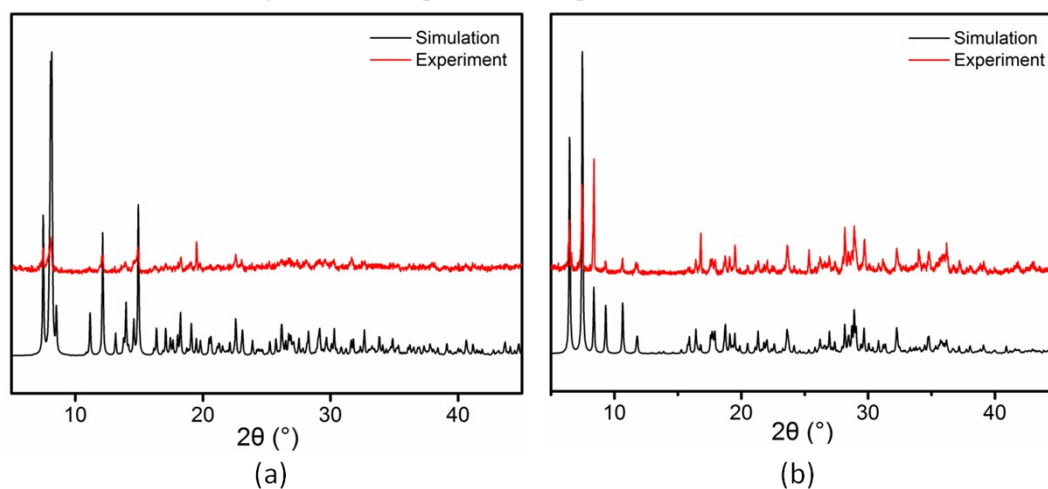


Fig. S2 The Powder X–ray diffraction of compounds **1** (a) and **2** (b)

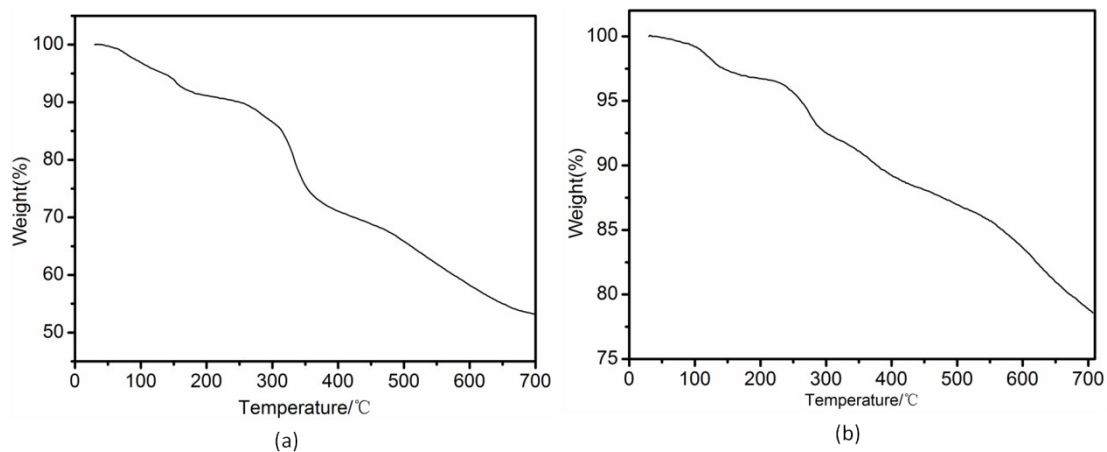


Fig. S3 The TG curves of compounds **1** (a) and **2** (b).

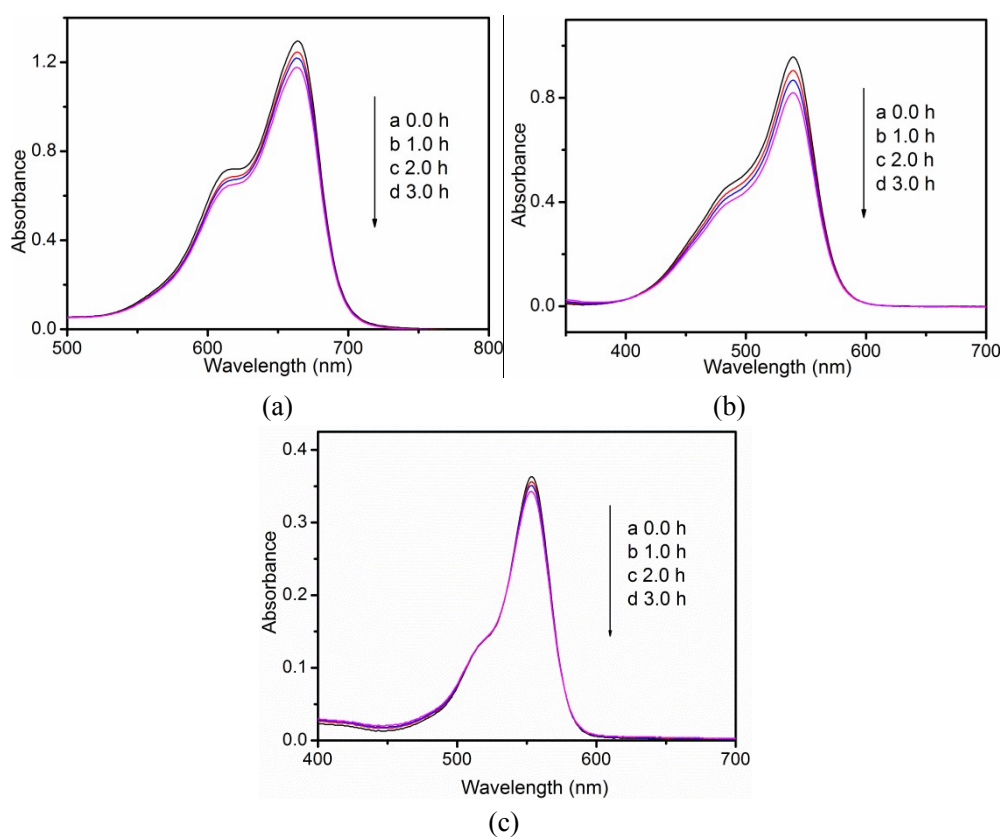


Fig. S4 The blank experiments for the photocatalytic degradation of MB (a), PH(b) and RhB (c) against irradiation time (h) in absence of **1** and **2**, respectively.

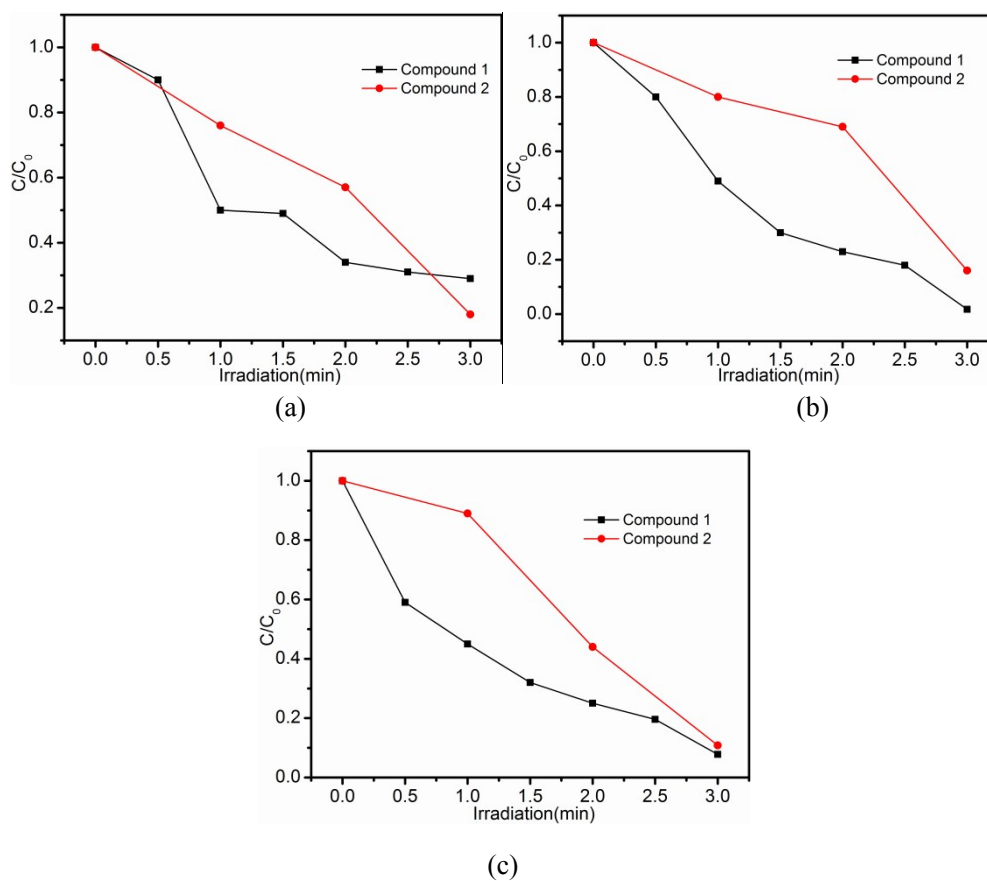


Fig. S5 Plots of the concentration ratios of MB (a), PH(b) and RhB (c) against irradiation time (h) in the presence of **1** and **2**, respectively.