

Supporting Information for the Manuscript:

Copper(II) Coordination Polymers: Tunable Structures and Different Activation Effect of Hydrogen Peroxide for the Degradation of Methyl Orange under Visible Light Irradiation

Lu Liu,^a Dongqing Wu,^{a,b} Bei Zhao,^a Xiao Han,^a Jie Wu,^{*a} Hongwei Hou^{*a} and Yaoting Fan^a

^aThe College of Chemistry and Molecular Engineering, Zhengzhou University, Zhengzhou 450052, P. R. China

^bState Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210093, China

Author for correspondence: Prof. Hongwei Hou, E-mail: houghw@zzu.edu.cn

Table S1. Crystal data and structure refinement details for polymers **1**, **2** and **3**.

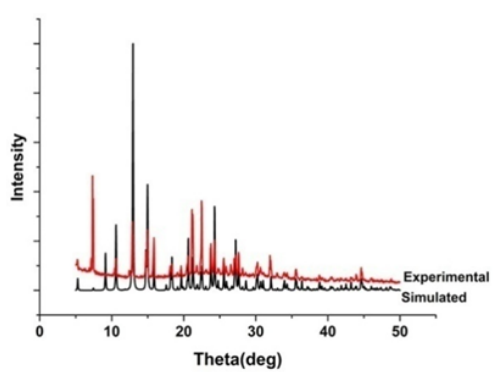
Complex	1	2	3
Formula	C ₃₂ H ₄₂ N ₁₄ O ₇ Cu	C ₃₂ H ₅₀ N ₁₂ O ₅ Cl ₂ Cu	C ₁₆ H ₂₀ N ₆ Cl ₂ Cu
Fw	798.34	817.28	430.82
Temp(K)	293(2)	293(2)	293(2)
Wavelength(Å)	0.71073	0.71073	0.71073
Crystal system	Orthorhombic	Triclinic	Monoclinic
Space group	<i>Ibam</i>	<i>P-1</i>	<i>P2(1)/c</i>
<i>a</i> (Å)	23.711(5)	7.9002(16)	13.329(3)
<i>b</i> (Å)	8.9025(18)	10.020(2)	14.147(3)
<i>c</i> (Å)	33.427(7)	13.153(3)	9.6681(19)
α (deg)	90	101.72(3)	90
β (deg)	90	93.69(3)	101.46(3)
γ (deg)	90	91.54(3)	90
<i>V</i> (Å ³)	7056(3)	1016.5(4)	1786.7(6)
<i>Z</i>	8	1	4
<i>D_c</i> (g·cm ⁻³)	1.503	1.335	1.602
μ (mm ⁻¹)	0.689	0.721	1.534
F(000)	3336	429	884
GOF on F ²	1.070	1.055	1.011
<i>R_I</i> [<i>I</i> >2 σ (<i>I</i>)] ^a	0.0741	0.0664	0.0772
<i>wR₂</i> (all data) ^b	0.1620	0.1679	0.1502

$$^a R_1 = [|\sum |F_o| - |\sum |F_c||] / \sum |F_o| \quad ^b wR_2 = [w(F_o^2 - F_c^2)^2] / [w(F_o^2)^2]^{1/2}$$

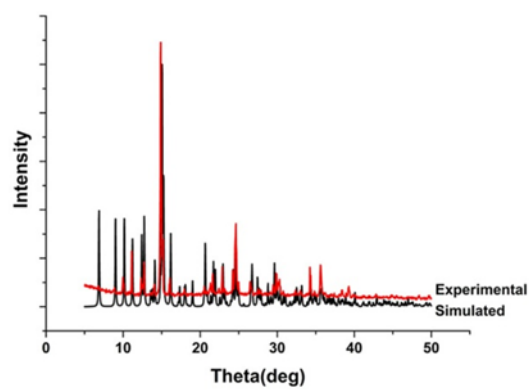
Table S2. Selected bond lengths / Å and angles /° for 1 and 2^a.

Complex 1					
Cu(1)-N(4)	2.047(4)	Cu(1)-O(1)	2.249(5)	Cu(1)-N(4)#1	2.047(4)
Cu(1)-N(1)	2.032(3)	Cu(1)-N(1)#1	2.032(3)	N(1)#1-Cu(1)-N(1)	173.3(2)
N(4)#1-Cu(1)-N(1)	91.05(14)	N(4)-Cu(1)-O(1)	103.49(11)	N(4)-Cu(1)-N(1)	90.51(14)
N(4)#1-Cu(1)-O(1)	103.50(11)	N(4)-Cu(1)-N(4)#1	153.0(2)	N(1)#1-Cu(1)-O(1)	86.67(10)
N(4)-Cu(1)-N(1)#1	91.05(14)	N(1)-Cu(1)-O(1)	86.67(10)	N(4)#1-Cu(1)-N(1)#1	90.51(14)
Complex 2					
Cu(1)-N(4)	2.021(2)	Cu(1)-N(1)#1	2.009(2)	Cu(1)-N(4)#1	2.021(2)
Cu(1)-N(1)	2.009(2)	N(4)-Cu(1)-N(1)#1	89.22(9)	N(4)-Cu(1)-N(1)	90.78(9)
N(4)#1-Cu(1)-N(1)#1	90.78(9)	N(4)#1-Cu(1)-N(1)	89.22(9)	N(4)-Cu(1)-N(4)#1	180.00(10)
N(1)#1-Cu(1)-N(1)	180.00(12)				
Complex 3					
Cu(1)-N(6)#1	2.023(5)	Cu(1)-N(3)	2.013(5)	Cu(1)-Cl(1)	2.3207(17)
Cu(1)-Cl(2)	2.2550(18)	N(6)#1-Cu(1)-Cl(1)	90.63(15)	N(3)-Cu(1)-Cl(1)	91.37(15)
N(6)#1-Cu(1)-Cl(2)	89.05(16)	N(3)-Cu(1)-Cl(2)	89.14(15)	N(6)-Cu(1)-N(3)	166.3(3)
Cl(1)-Cu(1)-Cl(2)	179.09(7)				

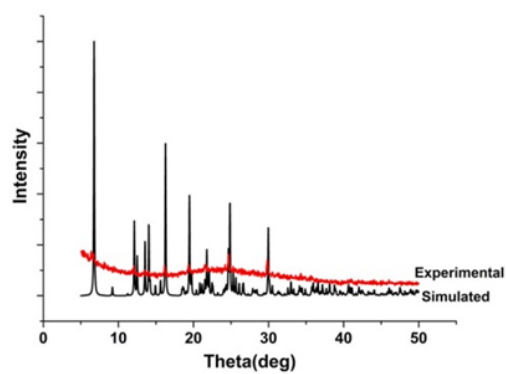
^a Symmetry transformations used to generate equivalent atoms in Complex 1: #1 1-x,1-y,z; Complex 2: #1 -x,-y+1,-z; Complex 3: #1 x+1,y,z+1.



(a) Complex 1

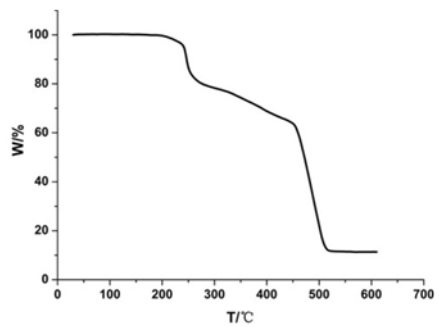


(b) Complex 2

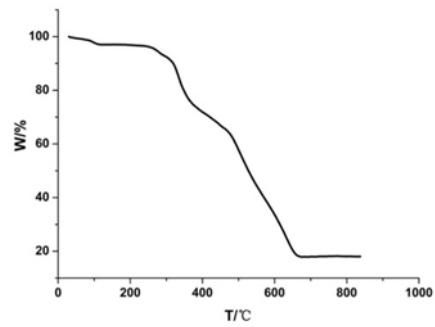


(c) Complex 3

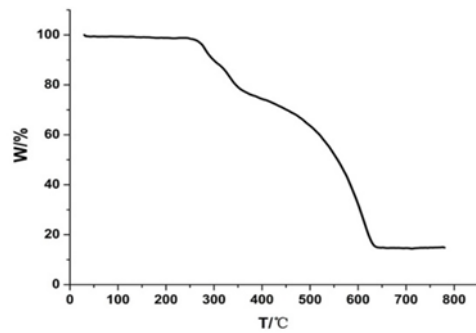
Fig. S1. Experimental (red) and simulated (black) PXRD patterns of complexes.



(a) Complex 1



(b) Complex 2



(c) Complex 3

Fig. S2. TGA curves of complexes 1, 2, 3.

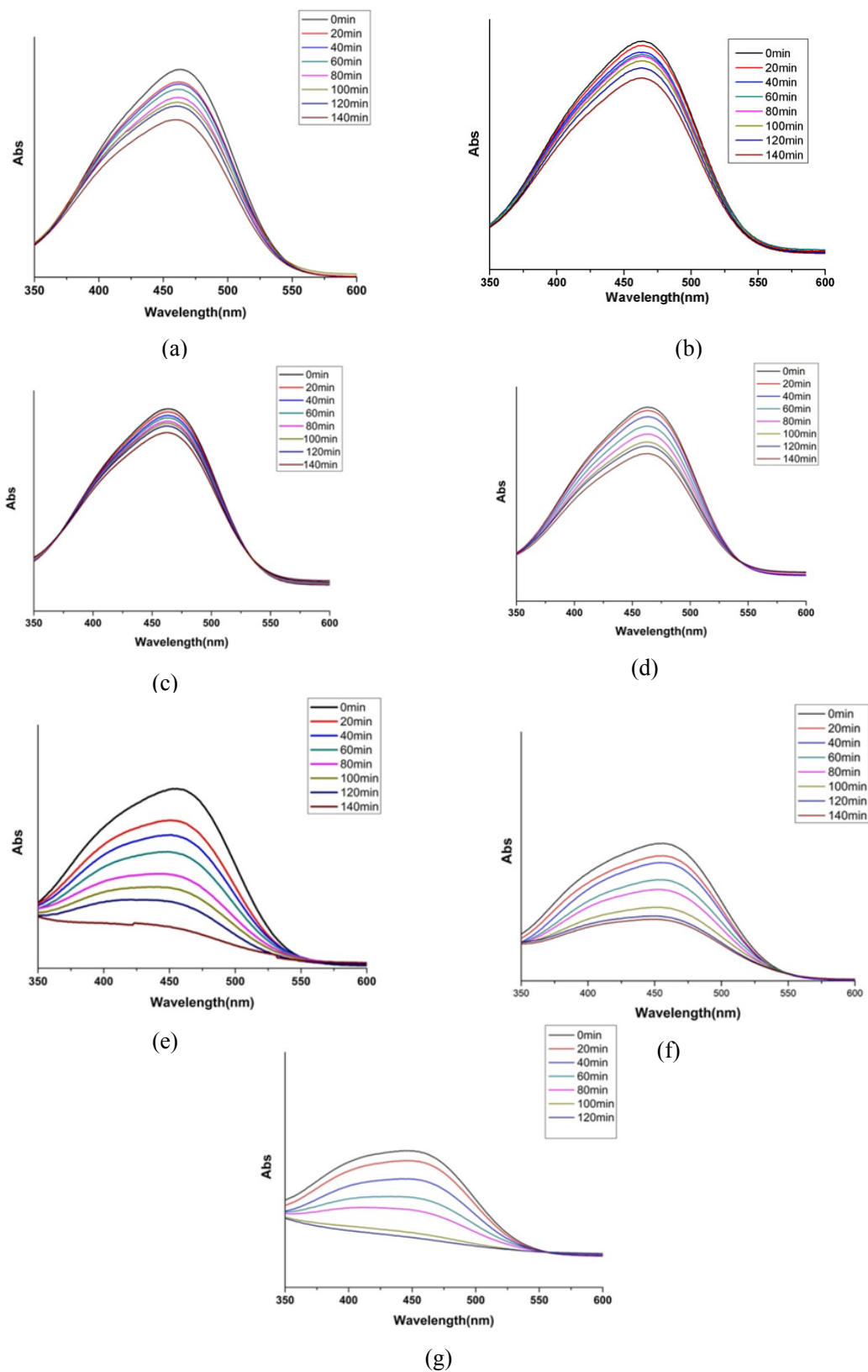


Fig.S3. UV-vis absorption of MO at different time intervals under Xe lamp irradiation: (a) with H_2O_2 ; (b) with complex 1; (c) with complex 2; (d) with complex 3; (e) with complex 1 and H_2O_2 ; (f) with complex 2 and H_2O_2 ; (g) with complex 3 and H_2O_2 .

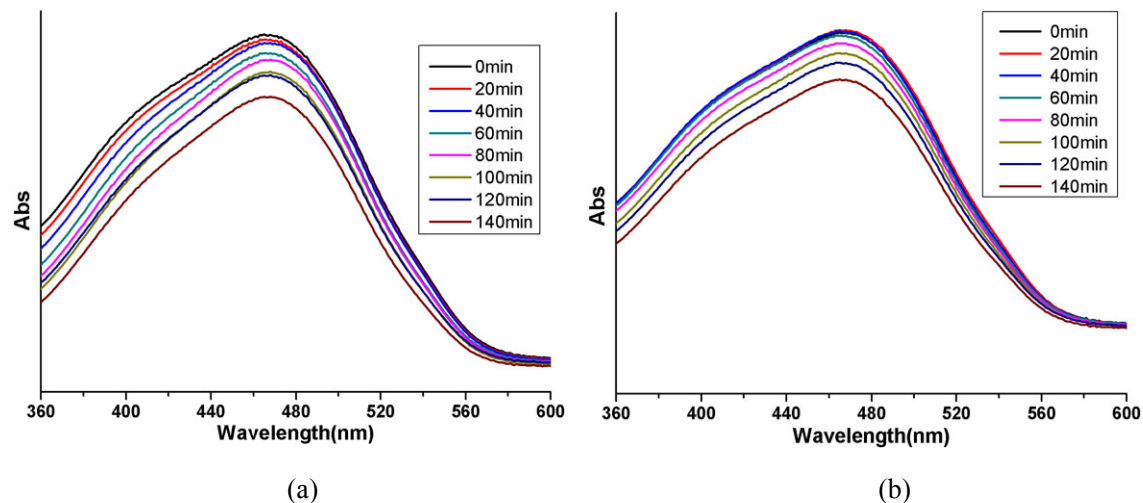


Fig.S4. UV-vis absorption of MO at different time intervals under Xe lamp irradiation: (a) with $\text{Cu}(\text{NO}_3)_2$ and H_2O_2 ; (b) with CuCl_2 and H_2O_2 .

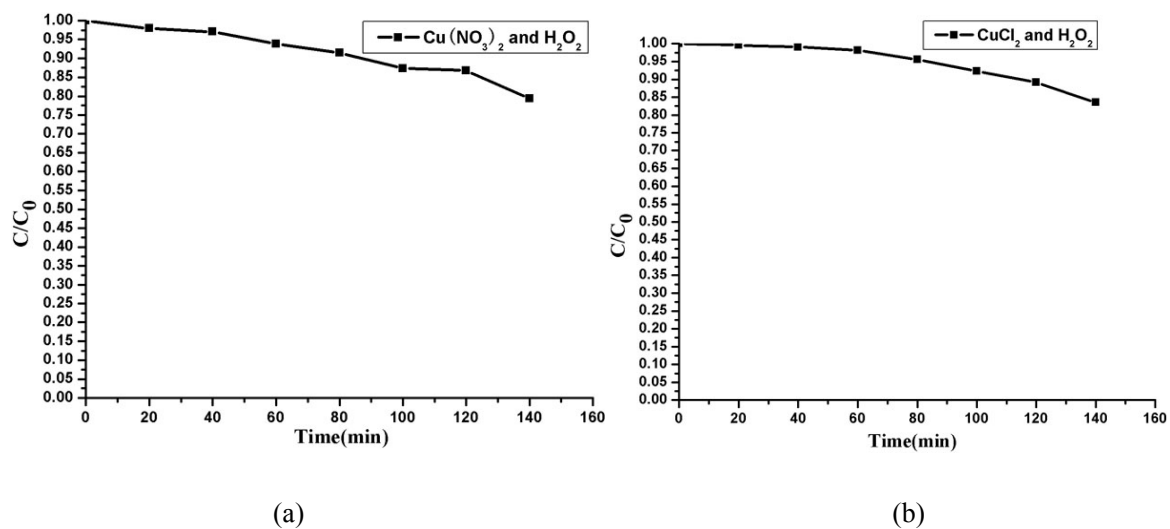


Fig.S5. Concentration changes of MO at different time intervals under Xe lamp irradiation: (a) For $\text{Cu}(\text{NO}_3)_2$ and H_2O_2 ; (b) For CuCl_2 and H_2O_2 .

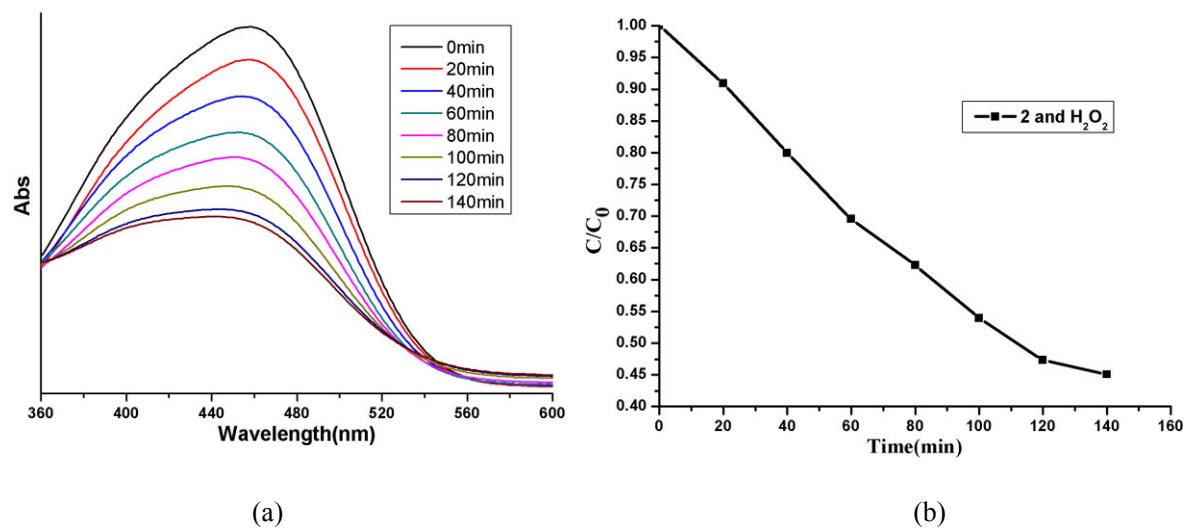
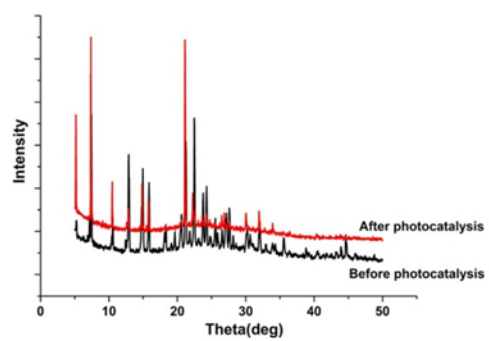
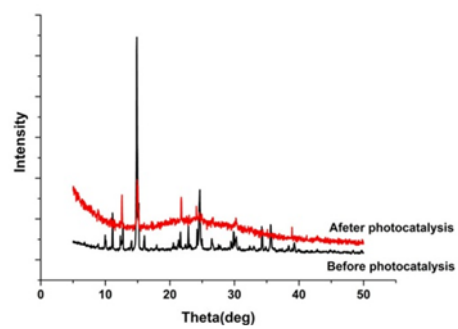


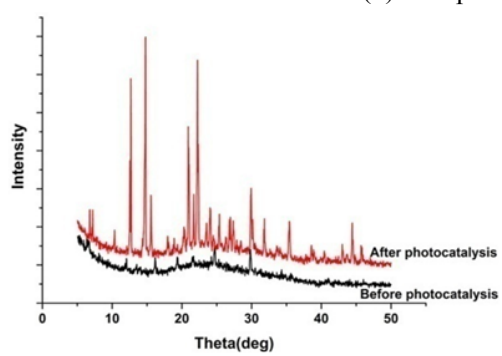
Fig.S6. (a) UV-vis absorption of MO at different time intervals under Xe lamp irradiation with complex **2**; (b) Concentration changes of MO at different time intervals under Xe lamp irradiation for **2** and H₂O₂.



(a) Complex 1



(b) Complex 2



(c) Complex 3

Fig. S7. PXRD patterns of complexes before and after catalysis.