Electronic Supporting Information

Design and synthesis of three new copper coordination polymers: efficient degradation of organic dye at alkaline pH

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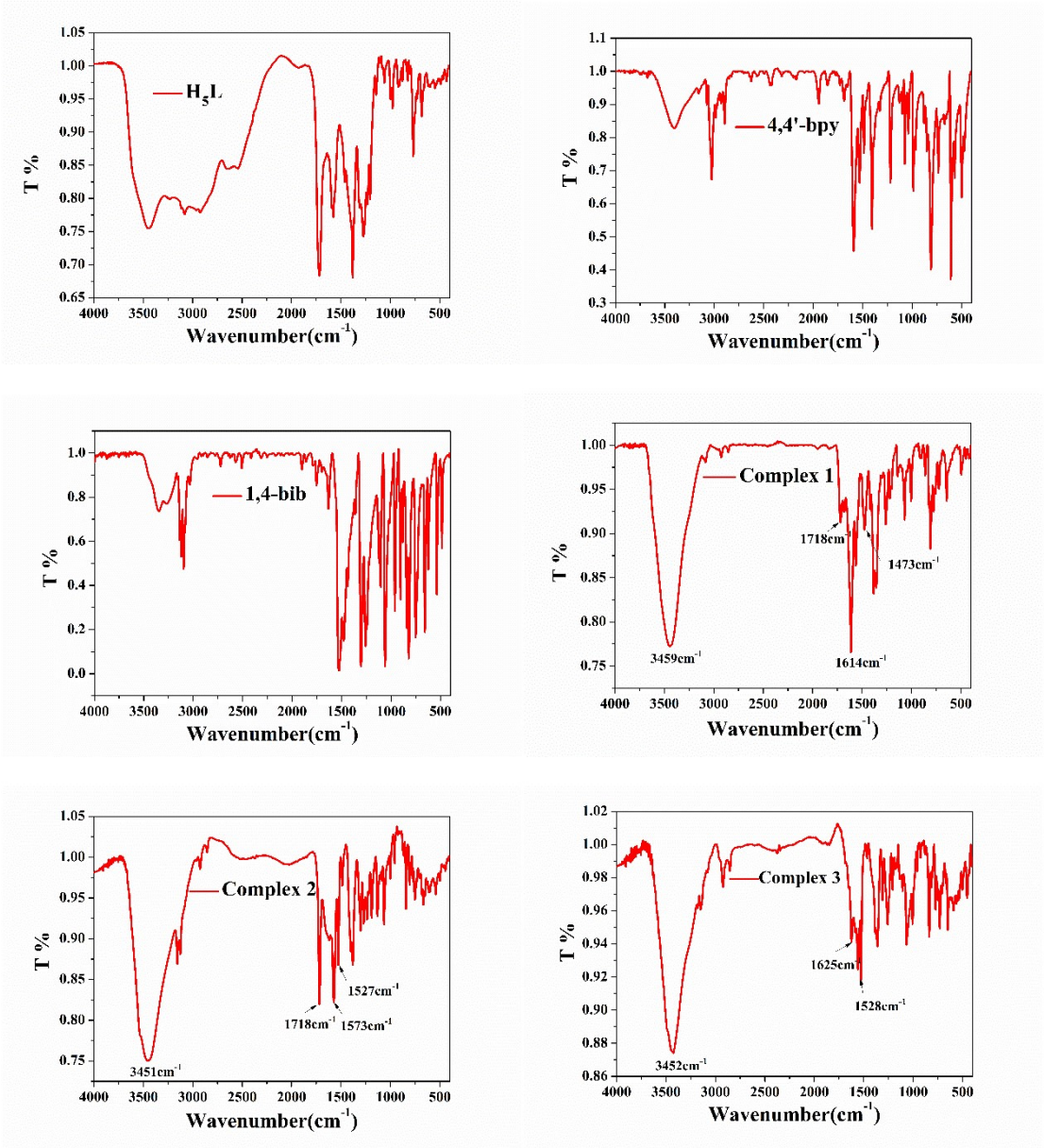

Fig. S1 IR spectra of ligand and compounds **1–3** (KBr, cm^{-1}).

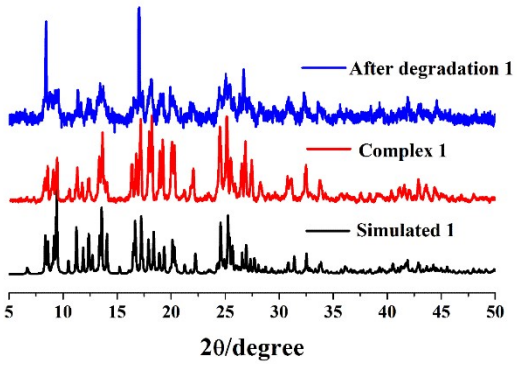

Fig. S2 PXRD patterns (simulation based on the single crystal structure, experimental, experimental after degradation) for complex **1** in the 2θ range of 5 to 50°.

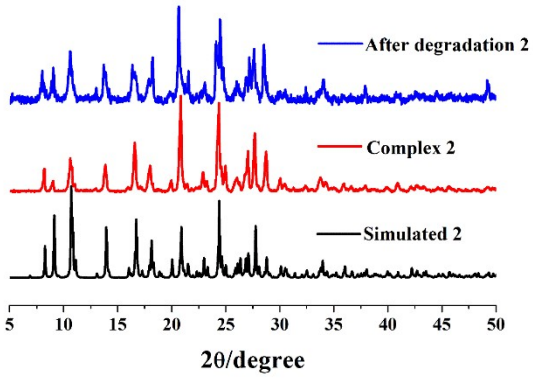

Fig. S3 PXRD patterns (simulation based on the single crystal structure, experimental, experimental after degradation) for complex **2** in the 2θ range of 5 to 50°.

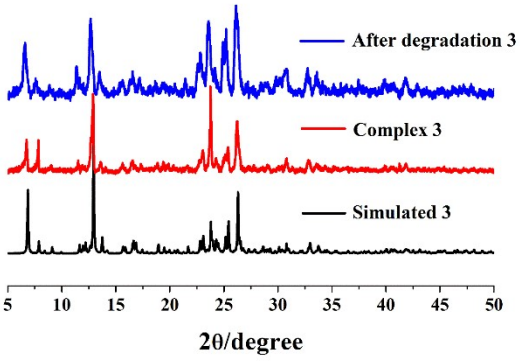

Fig. S4 PXRD patterns (simulation based on the single crystal structure, experimental, experimental after degradation) for complex **3** in the 2θ range of 5 to 50°.

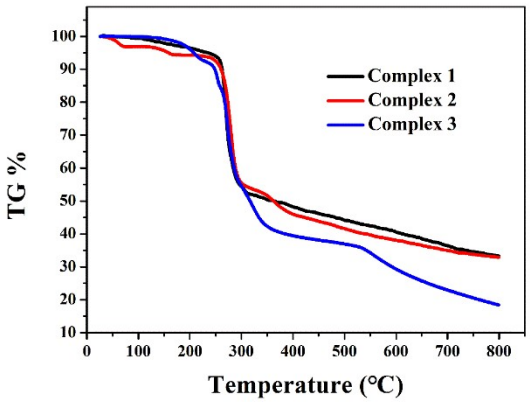

Fig. S5 TGA curves for compounds **1**-**3** collected under N_2 atmosphere.

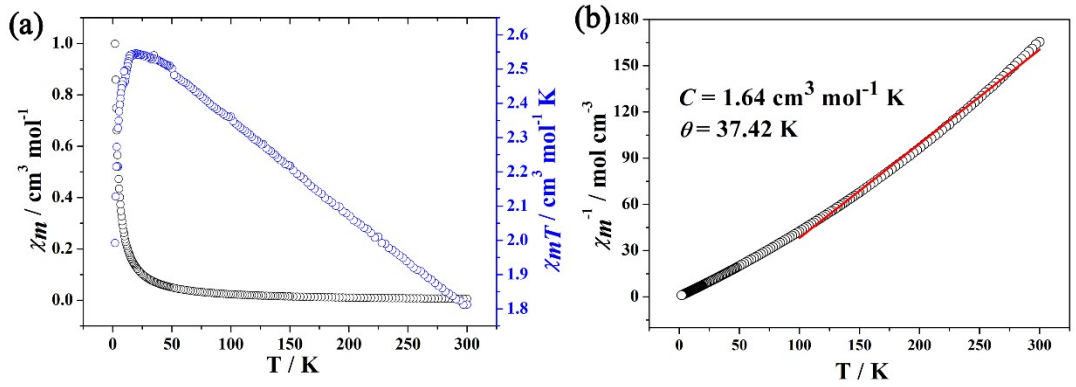

Fig.S6 (a) χ_M and $\chi_M T$ vs T plots for complex **1**; (b) χ_M^{-1} vs T plot for **1**. The solid line represents the best fits.

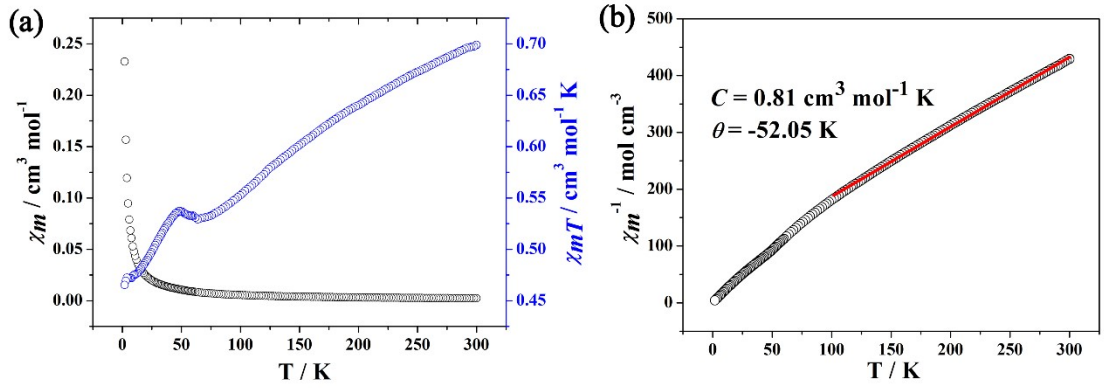

Fig.S7 (a) χ_M and $\chi_M T$ vs T plots for complex **2**; (b) χ_M^{-1} vs T plot for **2**. The solid line represents the best fits.

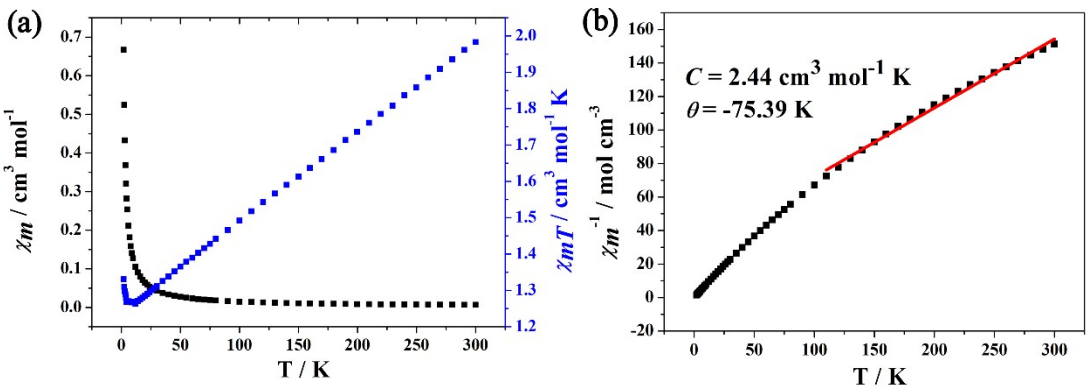

Fig.S8 (a) χ_M and $\chi_M T$ vs T plots for complex **3**; (b) χ_M^{-1} vs T plot for **3**. The solid line represents the best fits.

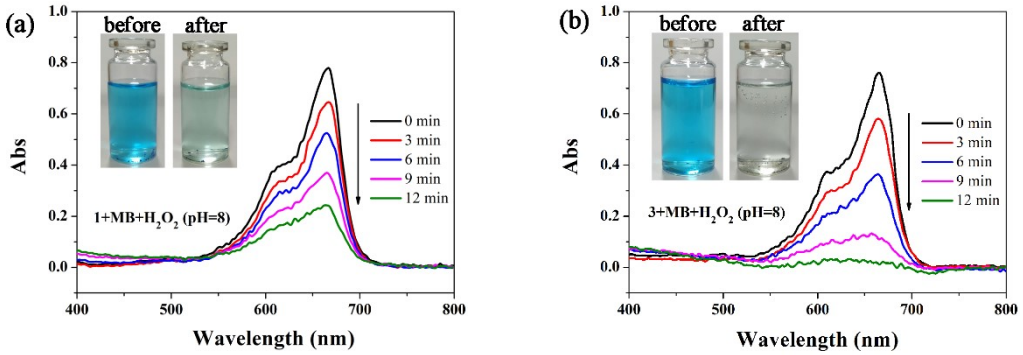

Fig. S9 UV-vis absorption spectra of MB (a) complex **1** (b) complex **3** ([MB] = 10 mg/L, $[H_2O_2]$ = 50 mM, complex = 5 mg, T = 25 °C, pH = 8). The illustrations are photographs before and after MB degradation.

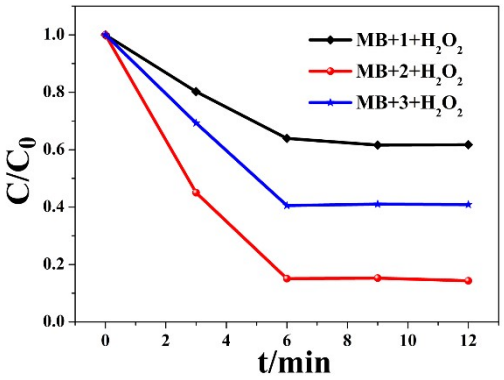

Fig. S10 Concentration of MB as a function of reaction time; catalysts were removed after 6 minutes. ([MB] = 10 mg/L, $[H_2O_2]$ = 50 mM, complex = 5 mg, T = 25 °C, pH = 8).

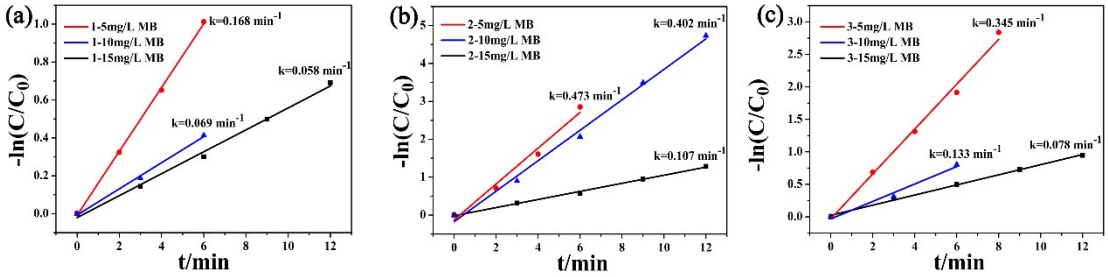

Fig. S11 Plot of -ln(C/C_0) vs. time for the pseudo-first-order kinetics curves of the photocatalytic degradation under different initial MB concentrations: (a) complex **1** (b) complex **2** (c) complex **3** ([H_2O_2] = 50 mM, complex = 5 mg, T = 25 °C, pH = 8).

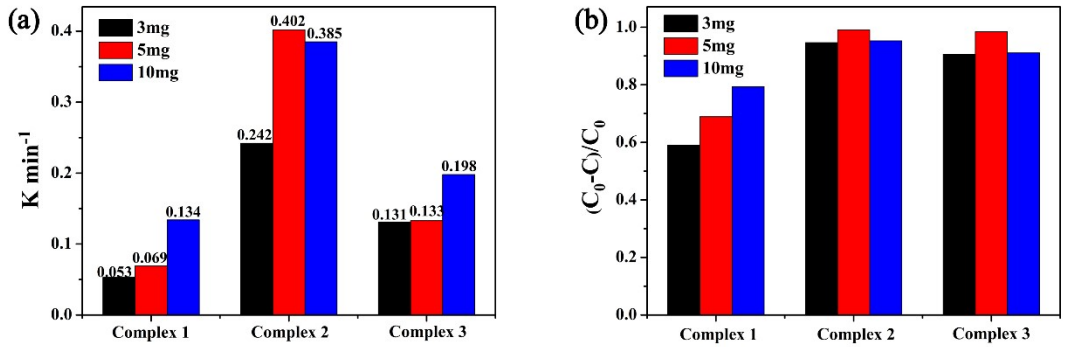

Fig. S12 The photocatalytic degradation rate constants (a) and removal efficiency (b)of complexes **1**-**3** under different catalyst dosages. ([MB] = 10 mg/L, [H_2O_2] = 50 mM, T = 25 °C, pH = 8).

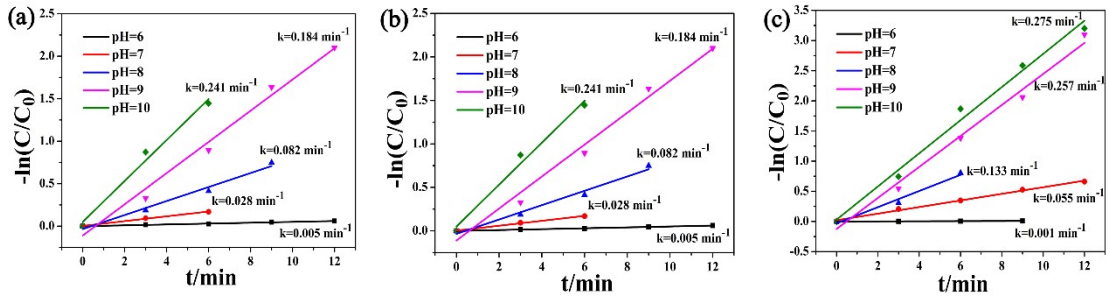

Fig. S13 Plot of -ln(C/C_0) vs. time for the pseudo-first-order kinetics curves of the photocatalytic degradation under different pH:(a) complex **1** (b) complex **2** (c) complex **3**. ([MB] = 10 mg/L, [H_2O_2] = 50 mM, complex = 5 mg, T = 25 °C).

Table S1 Selected Bond Angles (°) and Bond Lengths (Å) in **1**.

Bond distance (Å)		**Bond angle (°)**			
Cu1—O18^{ii}	1.975 (3)	O18^{ii}—Cu1—O1	170.78 (15)	N6—Cu2—O19^{iii}	89.84 (13)
Cu1—O1	1.976 (3)	O18^{ii}—Cu1—N1	88.92 (14)	O4—Cu3—O12	170.62 (14)
Cu1—O17^{ii}	2.769 (3)	O1—Cu1—N1	92.08 (14)	O4—Cu3—N3	91.76 (13)

Cu1—N1	2.016 (4)	O18^{ii}—Cu1—N2	91.36 (15)	O12—Cu3—N3	88.84 (13)
Cu1—N2	2.027 (4)	O1—Cu1—N2	90.37 (14)	O4—Cu3—N4^{vi}	88.63 (13)
Cu1—O23	2.249 (5)	N1—Cu1—N2	162.92 (17)	O12—Cu3—N4^{vi}	89.38 (14)
Cu2—O20^{v}	1.974 (3)	O18^{ii}—Cu1—O23	83.31 (19)	N3—Cu3—N4^{vi}	171.34 (15)
Cu2—O11	1.974 (3)	O1—Cu1—O23	87.47 (18)	O4—Cu3—O3^{iii}	102.95 (12)
Cu2—N5^{iv}	2.013 (3)	N1—Cu1—O23	97.1 (2)	O12—Cu3—O3^{iii}	86.26 (13)
Cu2—N6	2.015 (4)	N2—Cu1—O23	99.9 (2)	N3—Cu3—O3^{iii}	97.01 (13)
Cu2—O19^{iii}	2.314 (3)	O20^{v}—Cu2—O11	167.03 (13)	N4^{vi}—Cu3—O3^{iii}	91.33 (13)
Cu3—O4	1.951 (3)	O20^{v}—Cu2—N5^{iv}	92.09 (13)	O11—Cu2—N6	90.07 (13)
Cu3—O12	1.967 (3)	O11—Cu2—N5^{iv}	88.36 (13)	N5^{iv}—Cu2—N6	174.13 (15)
Cu3—N3	2.015 (4)	O20^{v}—Cu2—N6	88.18 (13)	O20^{v}—Cu2—O19^{iii}	109.88 (12)
Cu3—N4^{vi}	2.020 (4)	O11—Cu2—N6	90.07 (13)	O11—Cu2—O19^{iii}	82.96 (12)
Cu3—O3^{iii}	2.257 (3)	N5^{iv}—Cu2—N6	174.13 (15)	N5^{iv}—Cu2—O19^{iii}	95.57 (13)
		O20^{v}—Cu2—O19^{iii}	109.88 (12)	N6—Cu2—O19^{iii}	89.84 (13)
		O11—Cu2—O19^{iii}	82.96 (12)	O4—Cu3—O12	170.62 (14)
		N5^{iv}—Cu2—O19^{iii}	95.57 (13)	O4—Cu3—N3	91.76 (13)

Symmetry codes: (ii) -x, -y, -z; (iii) -x+1, -y, -z; (iv) x-1, y, z; (v) x, y-1, z+1; (vi) x+1, y, z

Table S2 Selected Bond Angles (°) and Bond Lengths (Å) in **2**.

Bond distance (Å)		**Bond angle (°)**			
Cu1—O8^{i}	1.943 (3)	O8^{i}—Cu1—N4^{ii}	93.49 (12)	N4^{ii}—Cu1—O1	93.05 (12)
Cu1—N4^{ii}	1.991 (3)	O8^{i}—Cu1—N1	97.45 (12)	N4^{ii}—Cu1—N1	153.66 (12)
Cu1—N1	1.996 (3)	O8^{i}—Cu1—O1	148.49 (11)	N1—Cu1—O1	90.03 (12)
Cu1—O1	2.066 (2)	O8^{i}—Cu1—O2	92.40 (11)	N1—Cu1—O2	98.81 (12)
Cu1—O2	2.551 (2)	N4^{ii}—Cu1—O2	104.60 (12)	O1—Cu1—O2	56.98 (11)

Symmetry codes: (i) x-1, y, z; (ii) x, y, z-1.

Table S3 Selected Bond Angles (°) and Bond Lengths (Å) in **3**.

Bond distance (Å)		**Bond angle (°)**			
Cu1—O5^{i}	1.965 (3)	O5^{i}—Cu1—O1	164.35 (15)	N1—Cu1—O6^{iii}	86.64 (15)
Cu1—O1	1.997 (3)	O5^{i}—Cu1—N1	87.53 (15)	N4^{ii}—Cu1—O6^{iii}	96.79 (15)
Cu1—N1	2.006 (4)	O1—Cu1—N1	88.72 (15)	O12^{iv}—Cu2—O12	180.0
Cu1—N4^{ii}	2.012 (4)	O5^{i}—Cu1—N4^{ii}	92.31 (15)	O12^{iv}—Cu2—N5	90.9 (2)
Cu1—O6^{iii}	2.317 (4)	O1—Cu1—N4^{ii}	90.50 (15)	O12—Cu2—N5	89.1 (2)

Cu2—O12^{iv}	1.933 (4)	N1—Cu1—N4^{ii}	176.45 (17)	O12^{iv}—Cu2—N5^{iv}	89.1 (2)
Cu2—O12	1.933 (4)	O5^{i}—Cu1—O6^{iii}	107.05 (14)	O12—Cu2—N5^{iv}	90.9 (2)
Cu2—N5	1.998 (5)	O1—Cu1—O6^{iii}	87.88 (14)	N5—Cu2—N5^{iv}	180.0
Cu2—N5^{iv}	1.999 (5)				

Symmetry codes: (i) x-1, y, z; (ii) x, y, z-1; (iii) -x+2, -y+2, -z+1; (iv) -x+2, -y+1, -z+1.

Table S4 Results of leached copper in solution after degradation

Catalyst	**Cu/mg·L^{-1}**
Complex 1	4.1
Complex 2	1.3
Complex 3	2.0