Supplementary Information

Table of Contents

Table S1 Selected bond lengths [Å] and angles [°] for complexes **1**-**4.**

1

Cu(1)-O(6)D	1.949(2)	Cu(2)-O(1)A	1.944(2)
Cu(1)-O(3)C	1.955(2)	Cu(2)-O(4)C	1.957(2)
Cu(1)-O(2)	1.959(2)	Cu(2)-O(2)	1.984(2)
Cu(1)-N(7)	2.001(3)	Cu(2)-O(2)B	2.014(2)
Cu(1)-O(7)B	2.128(3)	Cu(2)-O(8)	2.135(2)
O(6)D-Cu(1)-O(3)C	157.85(13)	O(1)A-Cu(2)-O(4)C	84.38(10)
O(6)D-Cu(1)-O(2)	92.50(10)	O(1)A-Cu(2)-O(2)	175.13(11)
O(3)C-Cu(1)-O(2)	94.40(10)	O(4)C-Cu(2)-O(2)	95.80(10)
O(6)D-Cu(1)-N(7)	84.37(11)	O(1)A-Cu(2)-O(2)B	97.10(10)
O(3)C-Cu(1)-N(7)	85.96(11)	O(4)C-Cu(2)-O(2)B	159.18(11)
O(2)-Cu(1)-N(7)	172.00(11)	O(2)-Cu(2)-O(2)B	81.01(10)
O(6)D-Cu(1)-O(7)B	101.09(14)	O(1)A-Cu(2)-O(8)	99.63(11)
O(3)C-Cu(1)-O(7)B	99.48(14)	O(4)C-Cu(2)-O(8)	102.03(11)
O(2)-Cu(1)-O(7)B	93.37(11)	O(2)-Cu(2)-O(8)	85.11(10)
N(7)-Cu(1)-O(7)B	94.45(12)	O(2)C-Cu(2)-O(8)	98.20(10)
		2	
Cu(1)-N(1)	1.993(2)	Cu(2)-O(6)E	1.906(2)
Cu(1)-O(7)	1.995(2)	Cu(2)-O(6)	1.906(2)
Cu(1)-O(5)D	2.020(2)	Cu(2)-O(1)B	1.943(3)
Cu(1)-N(2)A	2.036(3)	Cu(2)-O(1)C	1.943(3)
Cu(1)-O(2)B	2.252(2)		
N(1)-Cu(1)-O(7)	91.55(9)	O(5)D-Cu(1)-O(2)B	97.16(9)
N(1)-Cu(1)-O(5)D	88.09(9)	N(2)A-Cu(1)-O(2)B	89.38(10)
O(7)-Cu(1)-O(5)D	153.92(9)	O(6)E-Cu(2)-O(6)	180.00(19)
N(1)-Cu(1)-N(2)A	178.32(10)	O(6)E-Cu(2)-O(1)B	90.16(13)
O(7)-Cu(1)-N(2)A	90.13(10)	O(6)-Cu(2)-O(1)B	89.84(13)
O(5)D-Cu(1)-N(2)A	90.41(9)	O(6)E-Cu(2)-O(1)C	89.84(13)
N(1)-Cu(1)-O(2)B	90.04(10)	O(6)-Cu(2)-O(1)C	90.16(13)
O(7)-Cu(1)-O(2)B	108.92(9)	O(1)B-Cu(2)-O(1)C	180.00(16)
		3	
Ni(1)-O(8)	1.9828(17)	Ni(2)-O(8)	2.0222(17)
Ni(1)-O(2)A	2.0482(18)	Ni(2)-O(7)	2.0496(18)
Ni(1)-N(2)	2.074(2)	Ni(2)-O(1)A	2.0561(18)
Ni(1)-O(4)C	2.0801(18)	Ni(2)-O(8)D	2.0571(17)
Ni(1)-O(6)	2.0817(18)	Ni(2)-O(3)B	2.0790(18)
Ni(1)-N(1)	2.121(2)	Ni(2)-O(9)	2.1415(19)
O(8)-Ni(1)-O(2)A	97.15(7)	O(8)-Ni(2)-O(7)	96.62(7)
O(8)-Ni(1)-N(2)	170.45(8)	O(8)-Ni(2)-O(1)A	97.02(8)
O(2)A-Ni(1)-N(2)	90.23(8)	O(7)-Ni(2)-O(1)A	89.34(8)
O(8)-Ni(1)-O(4)C	90.99(7)	O(8)-Ni(2)-O(8)D	80.72(7)
O(2)A-Ni(1)-O(4)C	171.01(8)	O(7)-Ni(2)-O(8)D	90.88(8)

N(2)-Ni(1)-O(4)C	82.10(8)	O(1)A-Ni(2)-O(8)D	177.74(7)
O(8)-Ni(1)-O(6)	94.03(7)	O(8)-Ni(2)-O(3)B	171.93(7)
O(2)A-Ni(1)-O(6)	87.93(8)	O(7)-Ni(2)-O(3)B	89.64(7)
N(2)-Ni(1)-O(6)	92.28(8)	O(1)A-Ni(2)-O(3)B	88.11(8)
O(4)C-Ni(1)-O(6)	87.70(8)	O(8)D-Ni(2)-O(3)B	94.14(7)
O(8)-Ni(1)-N(1)	94.23(8)	O(8)-Ni(2)-O(9)	84.21(7)
O(2)A-Ni(1)-N(1)	95.84(9)	O(7)-Ni(2)-O(9)	175.53(8)
N(2)-Ni(1)-N(1)	78.93(9)	O(1)A-Ni(2)-O(9)	86.20(8)
O(4)C-Ni(1)-N(1)	87.32(9)	O(8)D-Ni(2)-O(9)	93.59(7)
O(6)-Ni(1)-N(1)	170.42(9)	O(3)B-Ni(2)-O(9)	89.94(8)

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Ni(1)-O(2)B	1.997(3)	Ni(2)-O(4)C	2.048(3)
Ni(1)-O(1)A	2.001(3)	Ni(2)-O(4)	2.048(3)
Ni(1)-N(1)	2.012(3)	Ni(2)-N(3)C	2.070(4)
Ni(1)-O(6)D	2.019(3)	Ni(2)-N(3)	2.070(4)
Ni(1)-O(7)	2.019(3)	Ni(2)-O(8)	2.084(3)
		Ni(2)-O(8)C	2.084(3)
O(2)B-Ni(1)-O(1)A	166.76(12)	O(4)C-Ni(2)-O(4)	180.000(1)
O(2)B-Ni(1)-N(1)	96.60(14)	O(4)C-Ni(2)-N(3)C	90.35(13)
O(1)A-Ni(1)-N(1)	96.64(14)	O(4)-Ni(2)-N(3)C	89.65(13)
O(2)B-Ni(1)-O(6)D	88.04(14)	O(4)C-Ni(2)-N(3)	89.65(13)
O(1)A-Ni(1)-O(6)D	89.95(13)	O(4)-Ni(2)-N(3)	90.35(13)
N(1)-Ni(1)-O(6)D	99.51(14)	N(3)C-Ni(2)-N(3)	180.0(2)
O(2)B-Ni(1)-O(7)	89.68(14)	O(4)C-Ni(2)-O(8)	89.40(12)
O(1)A-Ni(1)-O(7)	89.43(14)	O(4)-Ni(2)-O(8)	90.60(12)
N(1)-Ni(1)-O(7)	93.10(14)	N(3)C-Ni(2)-O(8)	91.29(14)
O(6)D-Ni(1)-O(7)	167.36(12)	N(3)-Ni(2)-O(8)	88.71(14)
O(2)B-Ni(1)-Ni(1)D	82.53(9)	O(4)C-Ni(2)-O(8)C	90.60(12)
O(1)A-Ni(1)-Ni(1)D	84.34(9)	O(4)-Ni(2)-O(8)C	89.40(12)
N(1)-Ni(1)-Ni(1)D	171.79(11)	N(3)C-Ni(2)-O(8)C	88.71(14)
O(6)D-Ni(1)-Ni(1)D	88.63(9)	N(3)-Ni(2)-O(8)C	91.29(14)
O(7)-Ni(1)-Ni(1)D	78.75(9)	O(8)-Ni(2)-O(8)C	180.00(13)

Symmetry transformations used to generate equivalent atoms:

For **1**：A: x,y+1,z; B: -x+1,-y,-z; C: -x+2,-y,-z; D: -x+1,-y-1,-z

For **2**：A: x,y,z+1; B: x-1,y+1,z; C: -x+2,-y,-z; D: x-1,y,z; E:-x+1,-y+1,-z

For **3**：A: -x+2,-y,-z+1; B: x,y,z+1; C: -x+1,-y,-z+1; D:-x+1,-y,-z+2

For **4**：A: -x,-y,-z+1; B: x,y+1,z; C: -x,-y,-z+2; D: -x,-y+1,-z+1

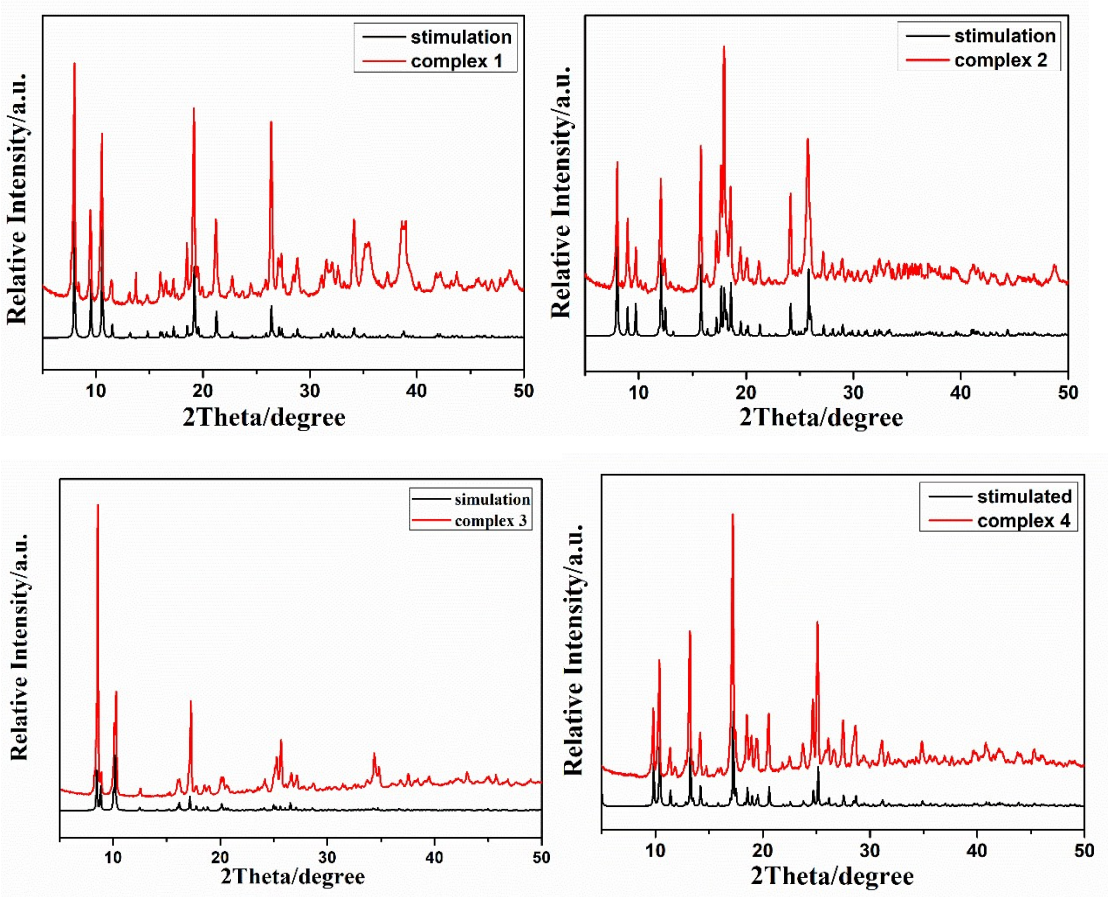

Fig. S1. The PXRD patterns of complexes **1-4**.

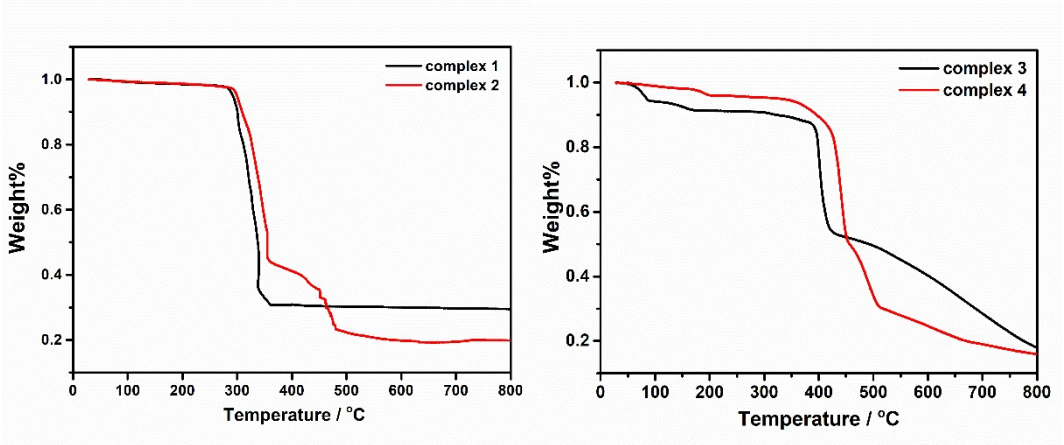

Fig. S2. TG curves of **1-4**.

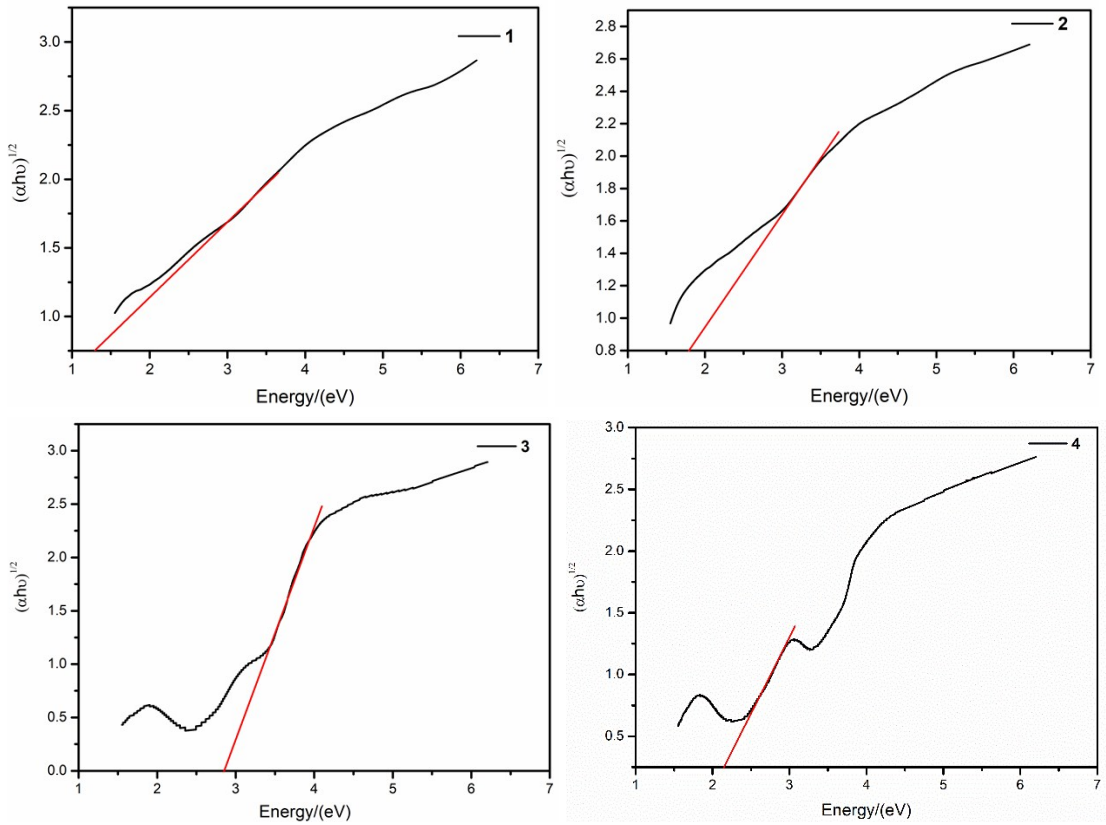

Fig. S3. Diffuse reflectance spectra of $(\alpha h\upsilon)^{1/2}$ versus energy (eV) of complexes **1**-**4**.

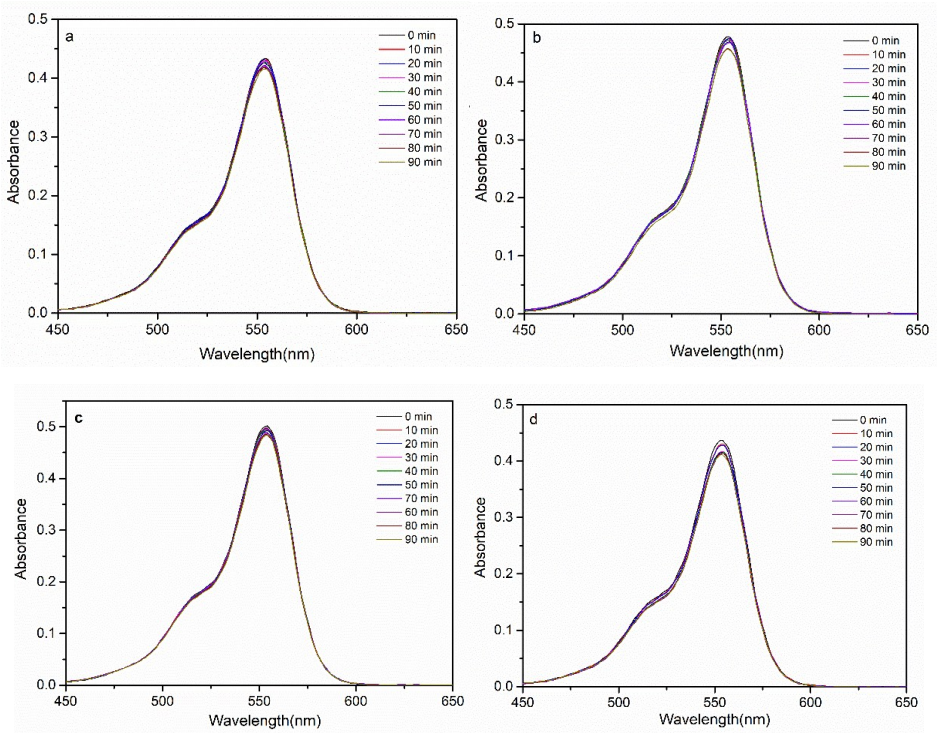

Fig. S4. Absorption spectra of RhB degraded with complex (**1** (a), **2** (b), **3** (c) and **4** (d)) under visible light illumination.

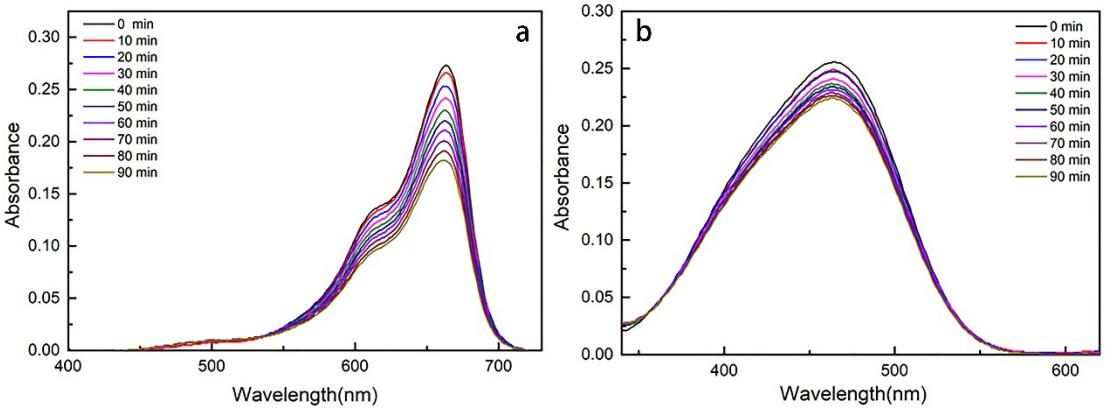

Fig. S5. Change of absorption spectra of the solution (MB(a) and MO(b)) with H_2O_2 under visible light irradiation at room temperature.

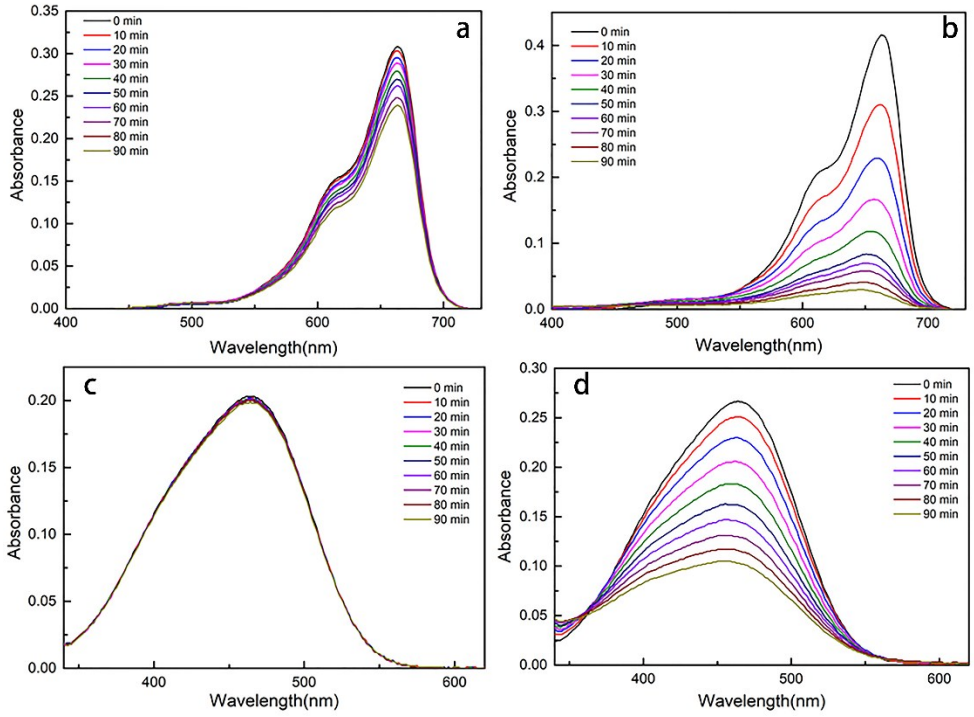

Fig. S6. Absorption spectra of solution degraded with complex **1** ((a) **1** + MB, (b) **1** + H_2O_2 and MB, (c) **1** + MO, (d) **1** + H_2O_2 and MO) under visible light illumination.

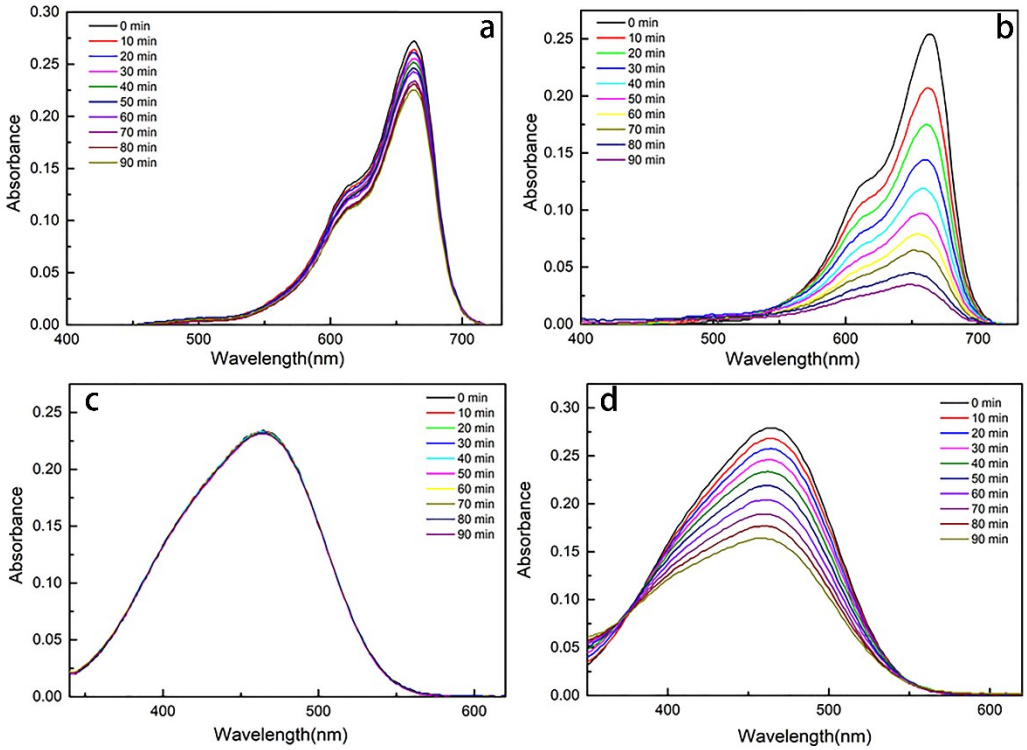

Fig. S7. Absorption spectra of solution degraded with complex **2** ((a) **2** + MB, (b) **2** + H_2O_2 and MB, (c) **2** + MO, (d) **2** + H_2O_2 and MO) under visible light illumination.

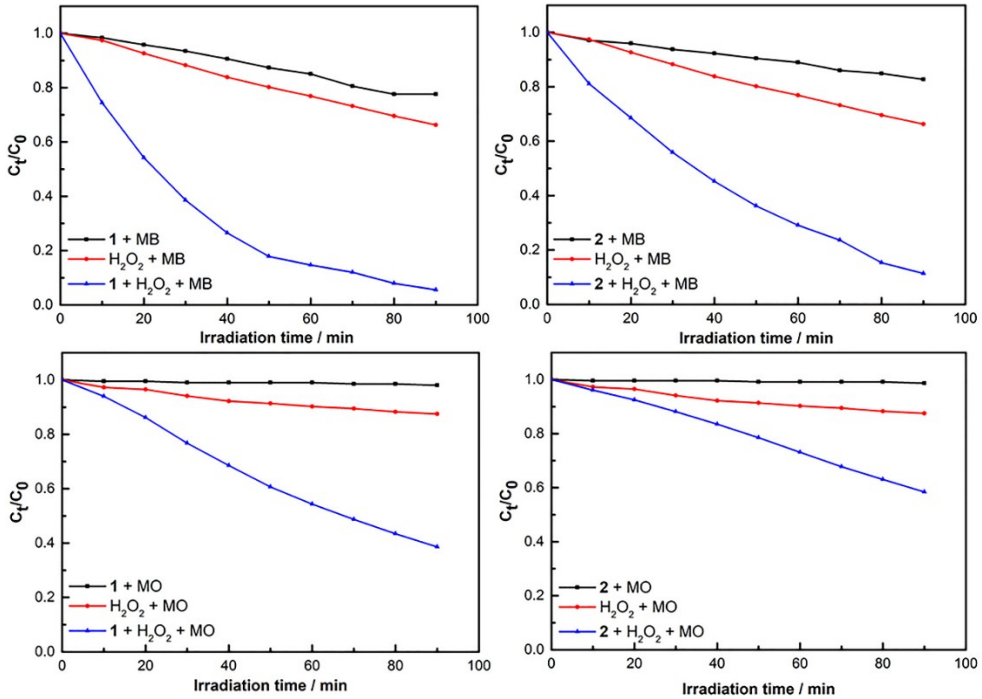

Fig. S8. Dyes degradation profile under different conditions: (black) visible light with the presence of MOFs, (red) visible light with the presence of H_2O_2, (blue) visible light with the presence of H_2O_2 and MOFs. C_t and C_0 stand for the dyes concentrations after and before irradiation.