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Template syntheses of diverse haloargentates with reversible photochromism behaviors and efficient photocatalytic properties

Zhen-Zhen Xue,[ab] A-Ni Wang,[a] Qi Wei,[a] Li Wei,[a] Song-De Han,[a] Jie Pan*,[a]

[a]College of Chemistry and Chemical Engineering, Qingdao University, Shandong 266071, China

[b]State Key Laboratory of Photocatalysis on Energy and Environment, Fuzhou University, Fuzhou, 350116, China

E-mail: tsingtaopj@163.com

Table S1 Selected bond lengths (Å) and angles (°) for **1-3**.

Compound **1**			
Ag(1)-I(2)#1	2.8509(7)	Ag(1)-I(2)	2.8509(7)
Ag(1)-I(1)#2	2.8741(7)	Ag(1)-I(1)	2.8741(7)
Ag(1)-Ag(1)#1	3.2796(17)	I(1)-Ag(1)#2	2.8741(8)
I(2)-Ag(1)#1	2.8509(7)	I(2)#1-Ag(1)-I(2)	109.77(3)
I(2)#1-Ag(1)-I(1)#2	115.193(19)	I(2)-Ag(1)-I(1)#2	108.359(18)
I(2)#1-Ag(1)-I(1)	108.359(18)	I(2)-Ag(1)-I(1)	115.193(19)
I(1)#2-Ag(1)-I(1)	99.85(3)	I(2)#1-Ag(1)-Ag(1)#1	54.887(16)
I(2)-Ag(1)-Ag(1)#1	54.887(16)	I(1)#2-Ag(1)-Ag(1)#1	130.077(15)
I(1)-Ag(1)-Ag(1)#1	130.077(15)	Ag(1)#2-I(1)-Ag(1)	80.15(3)
Ag(1)#1-I(2)-Ag(1)	70.23(3)		
Compound **2**			
Ag(1)-I(3)	2.7429(10)	Ag(1)-I(2)	2.7630(10)
Ag(1)-Ag(1)#1	2.9553(15)	Ag(1)-I(1)#1	2.9741(11)
Ag(1)-I(1)	2.9927(11)	I(1)-Ag(1)#1	2.9741(11)
I(1)-Ag(1)#3	2.9741(11)	I(1)-Ag(1)#4	2.9927(11)
I(2)-Ag(1)#2	2.7630(10)	I(3)-Ag(1)#4	2.7429(10)
I(3)-Ag(1)-I(2)	123.68(3)	I(3)-Ag(1)-Ag(1)#1	112.35(4)
I(2)-Ag(1)-Ag(1)#1	123.89(4)	I(3)-Ag(1)-I(1)#1	103.01(3)
I(2)-Ag(1)-I(1)#1	106.16(3)	Ag(1)#1-Ag(1)-I(1)#1	60.62(3)
I(3)-Ag(1)-I(1)	98.73(3)	I(2)-Ag(1)-I(1)	105.90(3)
Ag(1)#1-Ag(1)-I(1)	60.00(3)	I(1)#1-Ag(1)-I(1)	120.62(3)
Ag(1)#1-I(1)-Ag(1)#3	70.62(4)	Ag(1)#1-I(1)-Ag(1)	59.38(3)
Ag(1)#3-I(1)-Ag(1)	102.12(3)	Ag(1)#1-I(1)-Ag(1)#4	102.12(3)
Ag(1)#3-I(1)-Ag(1)#4	59.38(3)	Ag(1)-I(1)-Ag(1)#4	76.96(4)
Ag(1)#2-I(2)-Ag(1)	76.95(4)	Ag(1)#4-I(3)-Ag(1)	85.51(4)
Compound **3**			
Ag(1)-Br(2)	2.6124(13)	Ag(1)-Br(1)	2.6145(15)
Ag(1)-Br(3)	2.8381(16)	Ag(1)-Br(3)#1	2.8494(16)
Ag(1)-Ag(1)#1	2.9634(19)	Ag(1)-Ag(1)#2	3.306(2)
Br(1)-Ag(1)#3	2.6145(15)	Br(2)-Ag(1)#2	2.6124(13)
Br(3)-Ag(1)#3	2.8381(16)	Br(3)-Ag(1)#4	2.8494(16)
Br(3)-Ag(1)#1	2.8494(16)	Br(2)-Ag(1)-Br(1)	123.15(6)

Br(2)-Ag(1)-Br(3)	111.85(5)	Br(1)-Ag(1)-Br(3)	97.91(4)
Br(2)-Ag(1)-Br(3)#1	105.07(4)	Br(1)-Ag(1)-Br(3)#1	102.10(5)
Br(3)-Ag(1)-Br(3)#1	117.20(4)	Br(2)-Ag(1)-Ag(1)#1	127.33(6)
Br(1)-Ag(1)-Ag(1)#1	109.47(6)	Br(3)-Ag(1)-Ag(1)#1	58.78(4)
Br(3)#1-Ag(1)-Ag(1)#1	58.41(4)	Br(2)-Ag(1)-Ag(1)#2	50.75(3)
Br(1)-Ag(1)-Ag(1)#2	132.84(3)	Br(3)-Ag(1)-Ag(1)#2	128.79(3)
Br(3)#1-Ag(1)-Ag(1)#2	54.54(2)	Ag(1)#1-Ag(1)-Ag(1)#2	92.41(4)
Ag(1)-Br(1)-Ag(1)#3	85.69(6)	Ag(1)-Br(2)-Ag(1)#2	78.51(6)
Ag(1)#3-Br(3)-Ag(1)	77.57(5)	Ag(1)#3-Br(3)-Ag(1)#4	62.80(4)
Ag(1)-Br(3)-Ag(1)#4	105.65(5)	Ag(1)#3-Br(3)-Ag(1)#1	105.65(5)
Ag(1)-Br(3)-Ag(1)#1	62.80(4)	Ag(1)#4-Br(3)-Ag(1)#1	70.92(5)

Symmetry codes for **1**: (#1) -x+2, -y, -z+1; (#2) -x+2, -y+1, -z+1. **2**: (#1) -x+1, -y+2, -z+1; (#2) x, -y+5/2, z; (#3) -x+1, y-1/2, -z+1; (#4) x, -y+3/2, z. **3**: (#1) -x, -y, -z+1; (#2) x, -y-1/2, z; (#3) x, -y+1/2, z; (#4) -x, y+1/2, -z+1.

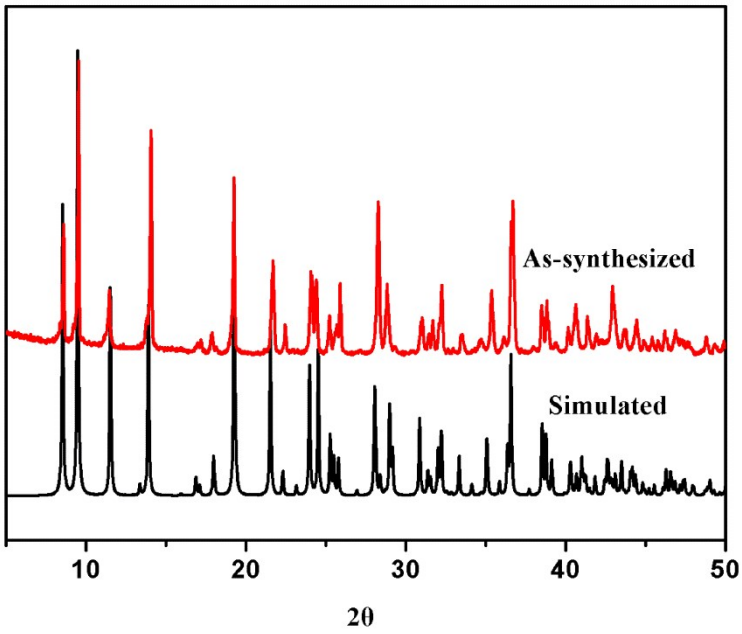

Figure S1 PXRD patterns of simulated from the single-crystal data of compound **1** (black); as-synthesized (red).

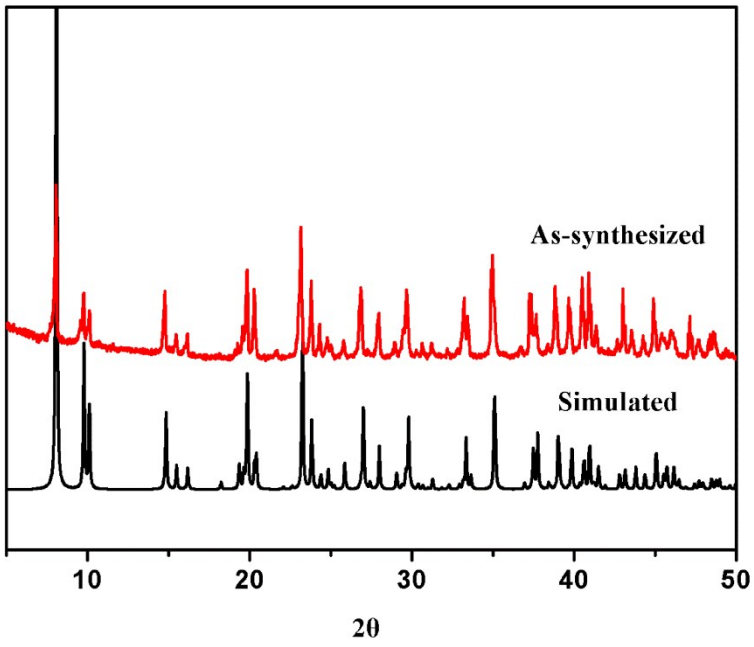

Figure S2 PXRD patterns of simulated from the single-crystal data of compound **2** (black); as-synthesized (red).

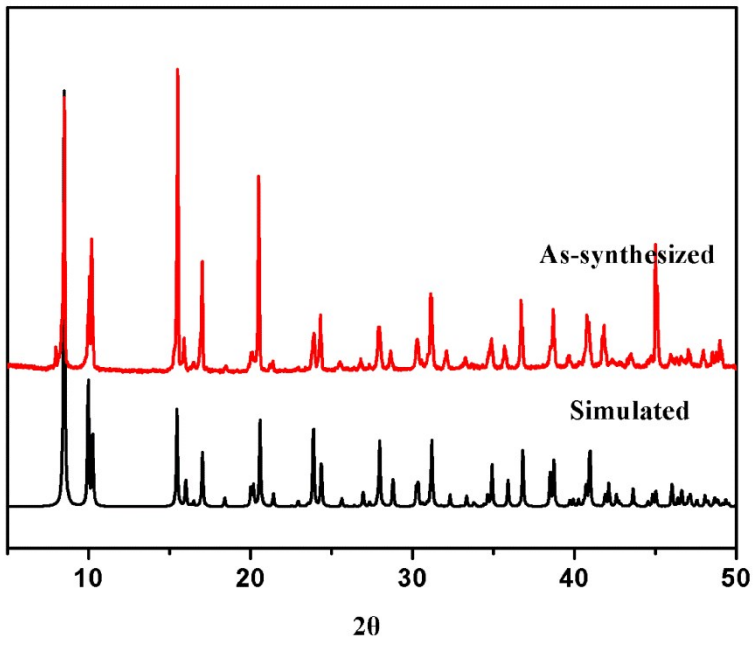

Figure S3 PXRD patterns of simulated from the single-crystal data of compound **3** (black); as-synthesized (red).

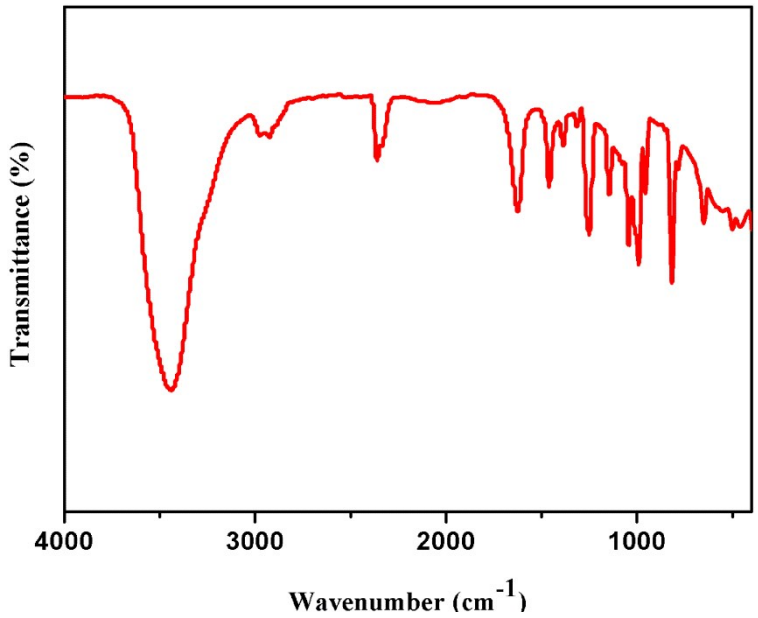

Figure S4 IR spectrum of compound **1**.

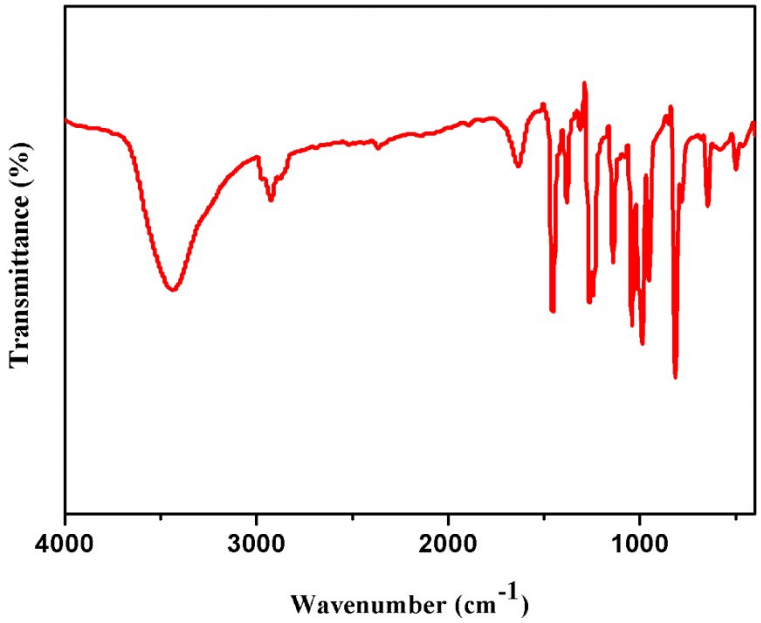

Figure S5 IR spectrum of compound **2**.

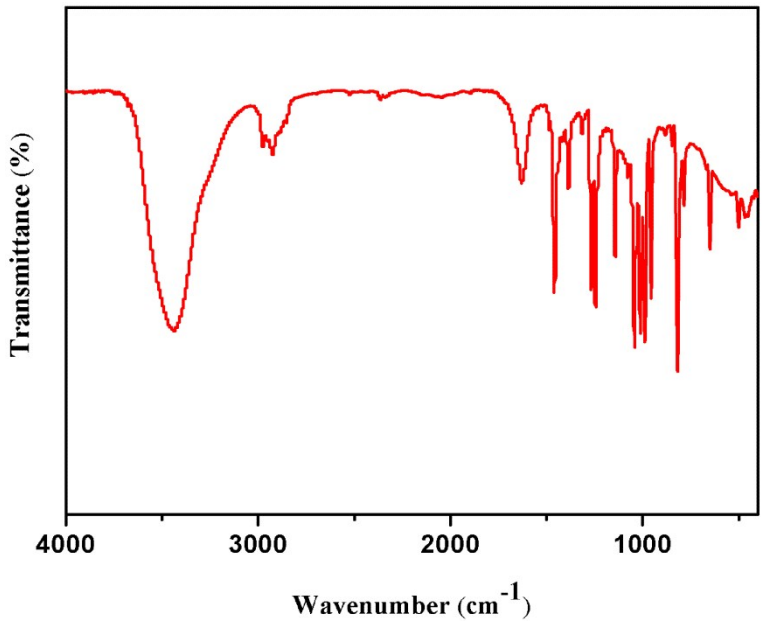

Figure S6 IR spectrum of compound **3**.

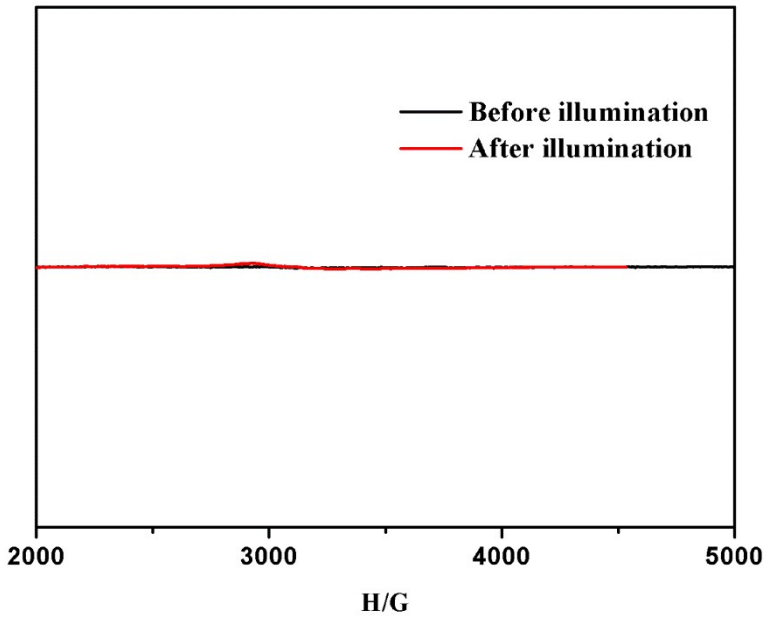

Figure S7 ESR spectra before and after light illumination for compound **1**.

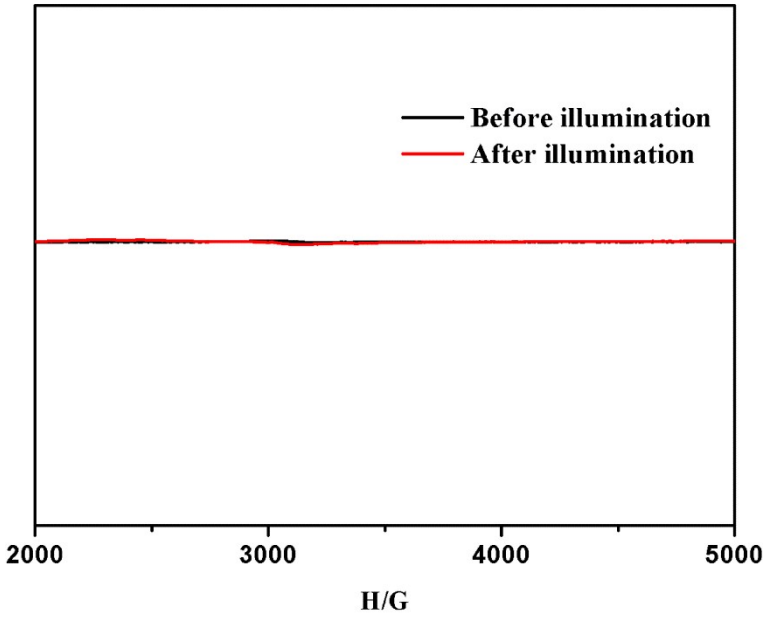

Figure S8 ESR spectra before and after light illumination for compound **2**.

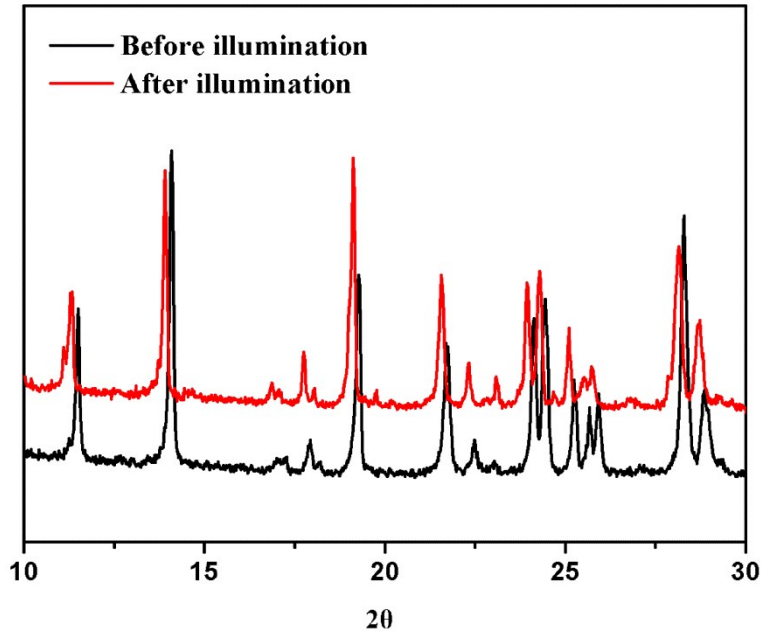

Figure S9 PXRD patterns of compound **1** before (black) and after (red) light illumination.

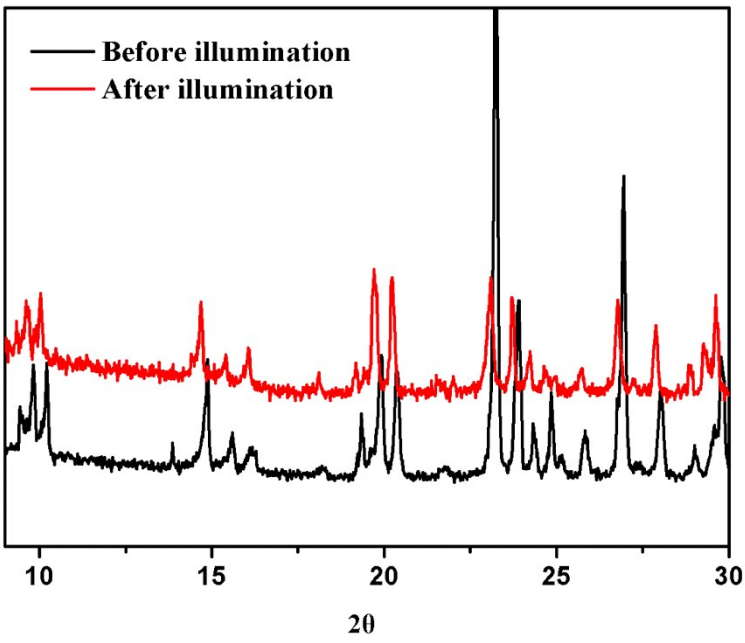

Figure S10 PXRD patterns of compound **2** before (black) and after (red) light illumination.

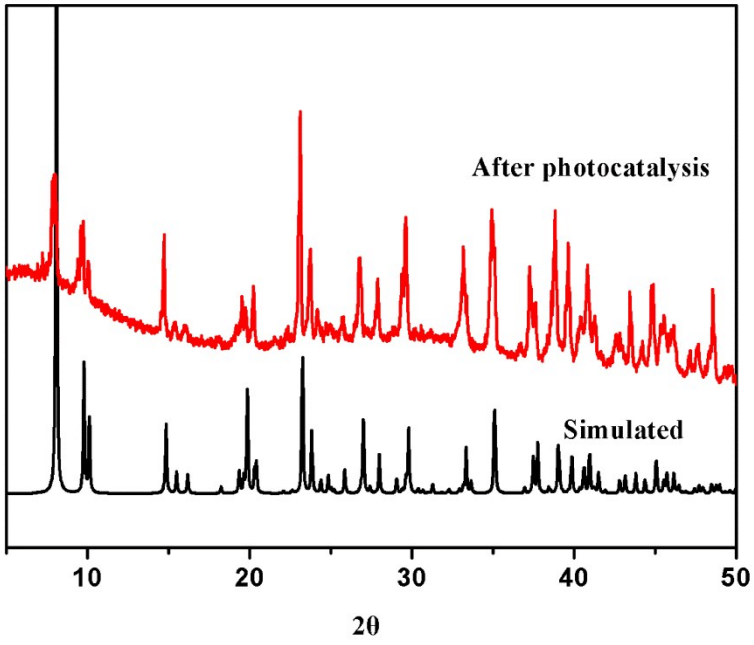

Figure S11 PXRD pattern of compound **2** after photocatalysis experiment.

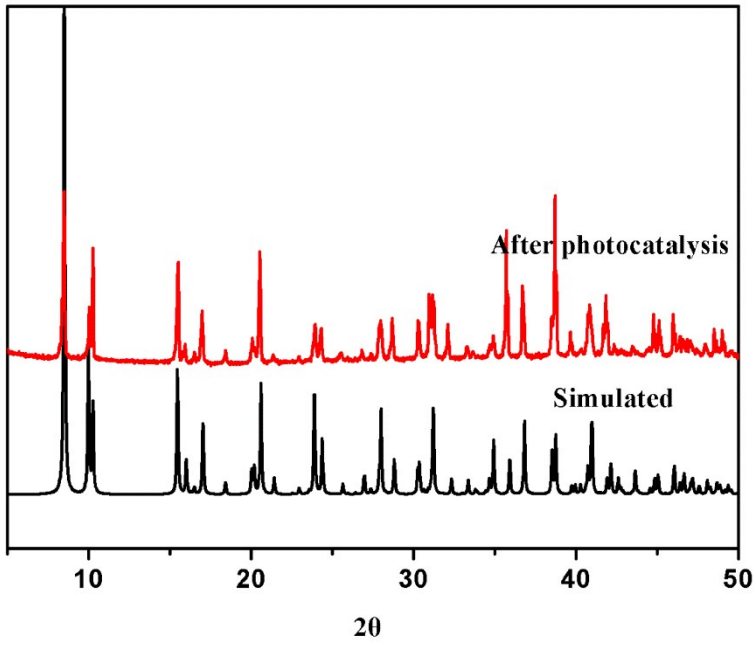

Figure S12 PXRD pattern of compound **3** after photocatalysis experiment.

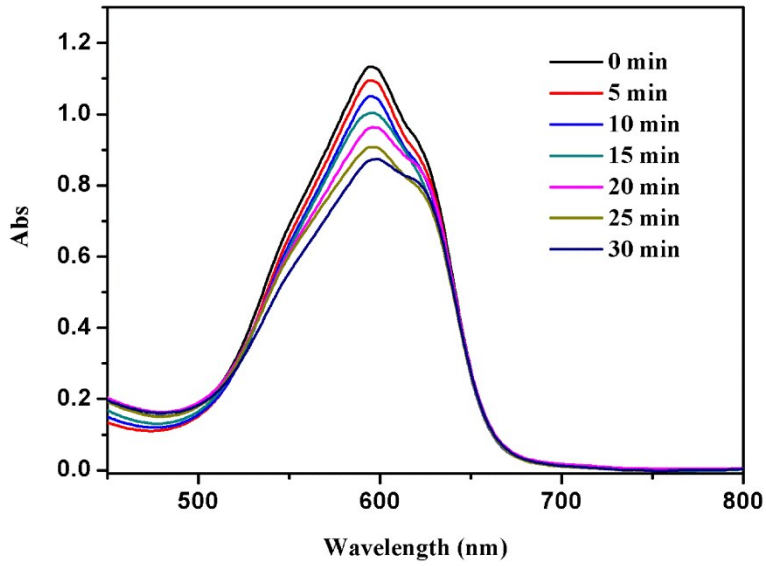

Figure S13 UV-vis spectra for MB in the presence of compound **2** and BQ under UV light.

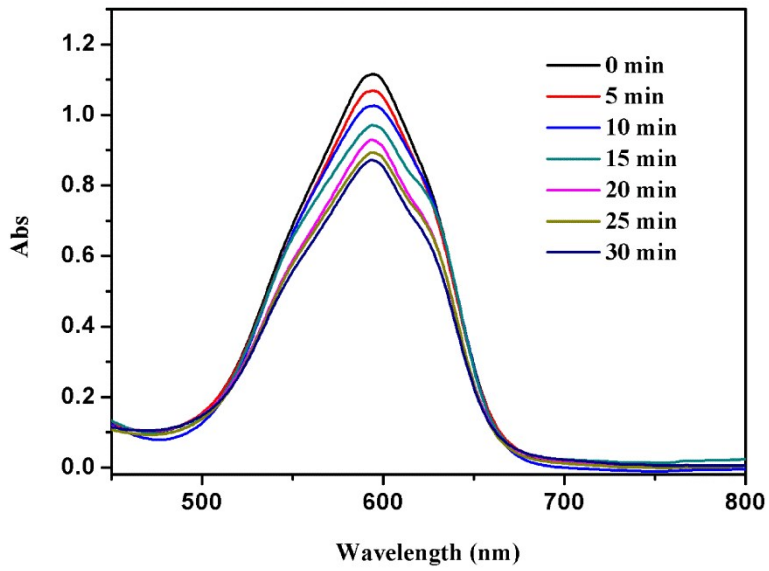

Figure S14 UV-vis spectra for MB in the presence of compound **3** and BQ under UV light.