Fluorescence Detection of Aromatic Amines and Photocatalytic Degradation of Rhodamine B under UV light irradiation by Luminescent Metal-Organic Frameworks

Fengqin Wang*[a], Caifu Dong [a], Chengmiao Wang [a], Zongchao Yu [a], Shukun Guo [b], Zechuan Wang [a], Yongnan Zhao [b], Guodong Li [c]

[a]College of Environmental and Chemical Engineering & Key Lab of Hollow Fiber Membrane Materials & Membrane Process, Tianjin Polytechnic University, Tianjin 300387, China
[b]School of Materials Science and Engineering & Tianjin Key Lab of Fiber Modification and Functional Fiber, Tianjin Polytechnic University, Tianjin 300387, China
[c]The State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, Jilin University,130023, China
E-mail: wangfengqin@tjpu.edu.cn Tel: (+86)-22-83955457

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Supplementary

Table S1 Crystal data and structure refinement for **1** and **2**

Compound	**1**	**2**
Chemical formula	$C_8H_7NO_5Zn$	$C_8H_{11}CdNO_7$
Formula weight	262.51	345.58
Temperature [K]	293(2)	113(2)
Wavelength[Å]	0.71073	0.71073
Crystal system	Monoclinic	Triclinic
Space group	P2(1)/n	P-1
a[Å]	9.0342(18)	7.7683(16)
b[Å]	8.2698(17)	8.6089(17)
c[Å]	11.623(2)	8.6695(17)
α/[°]	90	84.04(3)
β/[°]	100.90(3)	76.23(3)
γ/[°]	90	66.04(3)
Volume [$Å^3$]	852.7(3)	514.56(18)
Z, Calculated density[Mg/m^3]	4, 2.045	2, 2.230
Absorption coefficient[mm^{-1}]	2.880	2.148
Theta range for data collection (deg)	2.63 to 27.89	2.42 to 27.87
Limiting indices	$-11 \le h \le 11$, $-10 \le k \le 10$, $-13 \le l \le 15$	$-8 \le h \le 10$, $-11 \le k \le 11$, $-11 \le l \le 10$
F(000)	528	340
Reflections collected/unique	8135 / 2027 [*R(int*) = 0.0291]	5113 / 2395 [*R(int)* = 0.0256]
Data / restraints / parameters	2027 / 6 / 148	2395 / 12 / 178
Goodness-of-fit on F^2	1.085	1.059
Final *R* indices[$I>2\sigma(I)$]	*R1* = 0.0270, *wR2* = 0.0730	*R1* = 0.0222, *wR2* = 0.0581
R indices (all data)	*R1* = 0.0321, *wR2* = 0.0747	*R1*= 0.0239, *wR2* = 0.0584
Largest diff. peak and hole[$e.Å^{-3}$]	0.399 and -0.627	0.501 and -0.985

Table S2. Selected bond lengths and angles for **1** and **2**(Å, º)

1			
Zn(1)-O(2)#1	1.9570(16)	Zn(1)-O(5)	1.9636(18)
Zn(1)-O(4)#2	1.9756(15)	Zn(1)-N(1)	2.0363(18)
O(2)#1-Zn(1)-O(5)	109.50(7)	O(2)#1-Zn(1)-O(4)#2	94.77(6)
O(5)-Zn(1)-O(4)#2	110.23(7)	O(2)#1-Zn(1)-N(1)	104.85(7)
O(5)-Zn(1)-N(1)	118.10(7)	O(4)#2-Zn(1)-N(1)	116.38(7)
2			
Cd(1)-O(1)	2.239(2)	Cd(1)-O(5)	2.2614(18)
Cd(1)-O(2)#1	2.287(2)	Cd(1)-O(4)#2	2.3339(18)
Cd(1)-N(1)#3	2.417(2)	Cd(1)-O(3)#2	2.452(2)
O(1)-Cd(1)-O(5)	132.84(7)	O(1)-Cd(1)-O(2)#1	100.66(7)
O(5)-Cd(1)-O(2)#1	87.94(7)	O(1)-Cd(1)-O(4)#2	84.99(7)
O(5)-Cd(1)-O(4)#2	142.00(7)	O(2)#1-Cd(1)-O(4)#2	87.82(7)
O(1)-Cd(1)-N(1)#3	86.46(8)	O(5)-Cd(1)-N(1)#3	85.27(7)
O(2)#1-Cd(1)-N(1)#3	172.41(6)	O(4)#2-Cd(1)-N(1)#3	95.46(7)
O(1)-Cd(1)-O(3)#2	137.78(7)	O(5)-Cd(1)-O(3)#2	87.61(7)
O(2)#1-Cd(1)-O(3)#2	90.82(7)	O(4)#2-Cd(1)-O(3)#2	54.72(6)
N(1)#3-Cd(1)-O(3)#2	85.54(7)		

Symmetry transformations used to generate equivalent atoms:

For **1** #1 x+1/2, -y+1/2, z-1/2 #2 x, y-1, z

For **2** #1 -x+1, -y+1, -z #2 x+1, y, z-1 #3 -x, -y+2, -z

Table S3 Hydrogen bonds geometries (nm, °) for **1** and **2**

1					
D-H...A	d(D-H)	d(H...A)	(D... A)	∠DHA	Symmetry code
N(1)-H(1A)...O(2)#5	0.895(9)	2.155(14)	2.981(3)	153.1(19)	-x+1/2, y-1/2, -z+3/2
N(1)-H(1B)...O(4)#6	0.892(9)	2.387(18)	2.998(2)	125.8(15)	-x+1, -y+1, -z+1
N(1)-H(1B)...O(1)#1	0.892(9)	2.476(16)	3.134(2)	131.0(17)	x+1/2, -y+1/2, z-1/2
O(5)-H(5A)...O(1)#7	0.844(9)	1.829(11)	2.660(2)	168(2)	-x, -y, -z+1
O(5)-H(5B)...O(3)#8	0.840(9)	1.804(10)	2.641(2)	175(2)	-x, -y+1, -z+1
2					
O(6)-H(6A)...O(2)	0.847(10)	2.11(2)	2.860(3)	148(3)	-x+1, -y+1, -z
N(1)-H(1A)...O(6)#5	0.900(9)	2.108(10)	2.992(3)	167(2)	x, y+1, z
N(1)-H(1B)...O(3)#5	0.893(9)	2.60(2)	3.224(3)	128(2)	x, y+1, z
O(5)-H(5A)...O(3)#6	0.855(9)	1.848(10)	2.701(3)	174(3)	-x, -y+1, -z
O(6)-H(6A)...O(6)#6	0.847(10)	2.45(4)	2.907(6)	114(3)	-x, -y+1, -z
O(5)-H(5B)...O(7)#7	0.853(10)	1.911(14)	2.732(3)	161(2)	x, y, z-1
O(6)-H(6B)...O(7)#7	0.848(10)	2.029(16)	2.846(4)	161(3)	x, y, z-1
O(7)-H(7A)...O(7)#8	0.838(10)	2.13(2)	2.805(5)	137(3)	-x+1, -y, -z+2
O(7)-H(7B)...O(1)#9	0.839(10)	2.339(19)	3.116(3)	154(3)	x, y-1, z+1

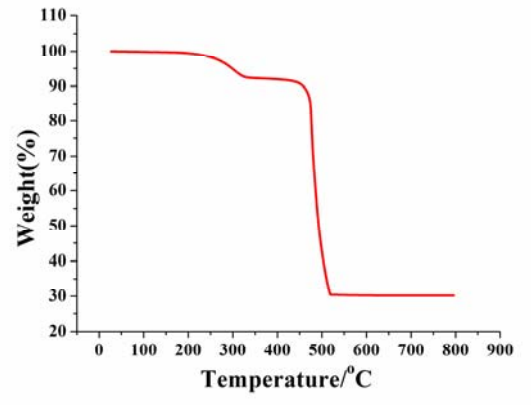

Fig. S1 TG curve of **1**

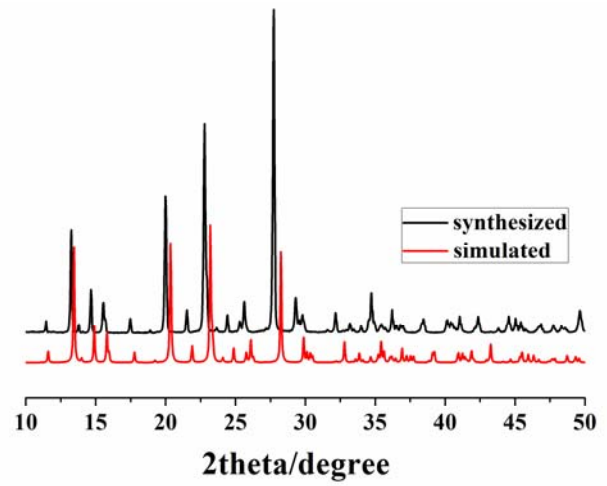

Fig. S2 PXRD pattern of **1**

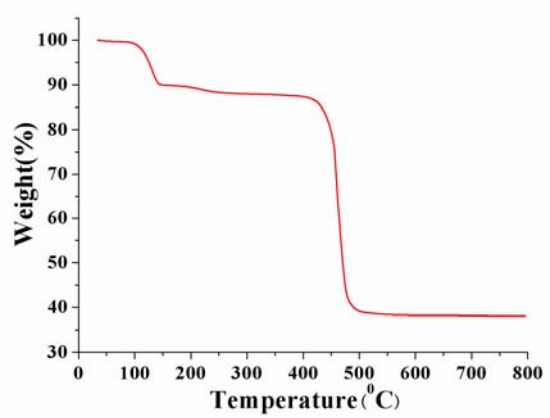

Fig. S3 TG curve of **2**

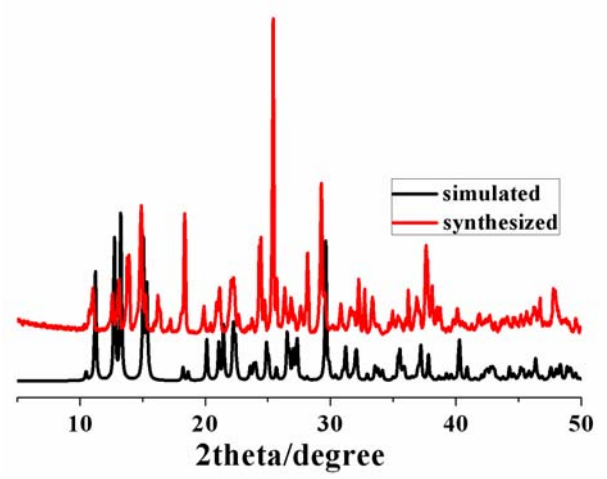

Fig. S4 PXRD pattern of **2**

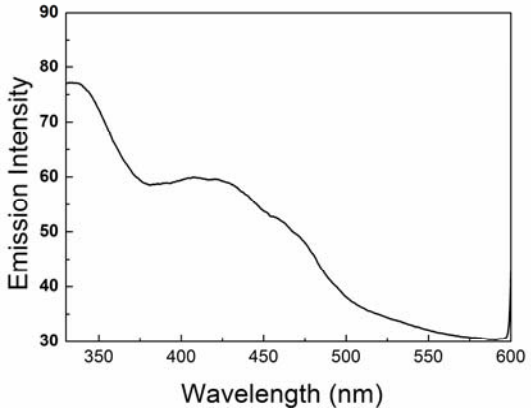

Fig. S5 The fluorescence spectra of **1** (λ_{ex} = 310 nm) at the solid state at room temperature

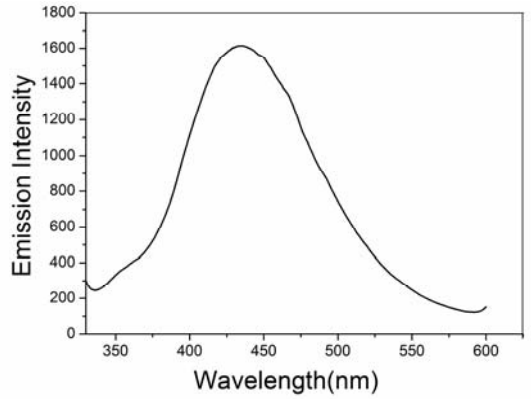

Fig. S6 The fluorescence spectra of **2** (λ_{ex}=310 nm) at the solid state at room temperature

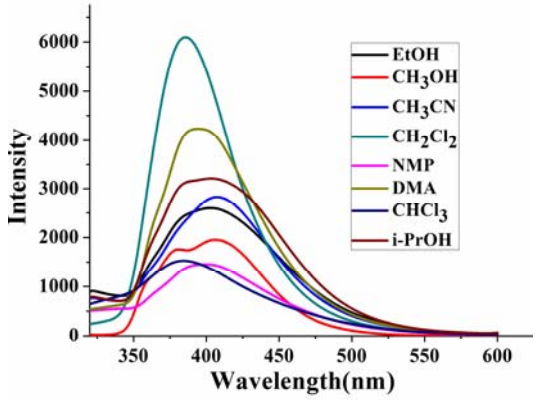

Fig. S7 Emission spectra of **1** in different organic solvent at room temperature.

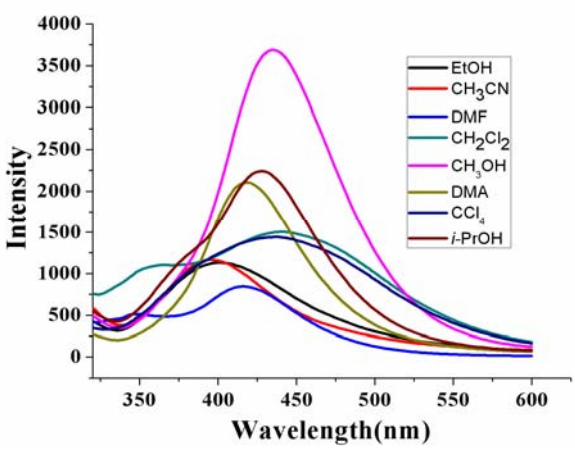

Fig. S8 Emission spectra of **2** in different organic solvent at room temperature

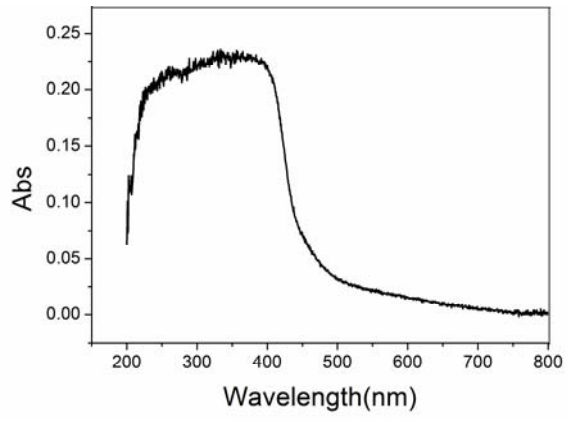

Fig. S9 UV−vis diffuse-reflectance spectra of **1** with $BaSO_4$ as background

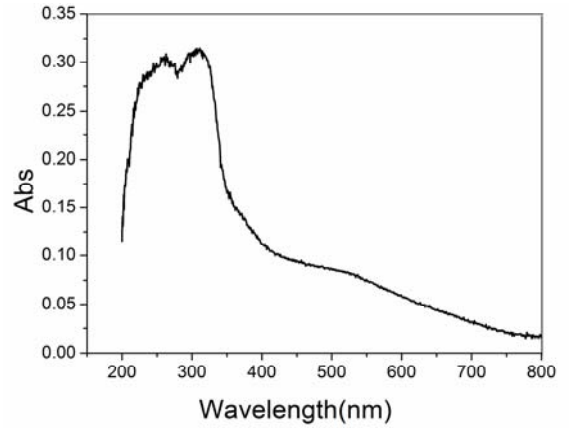

Fig. S10 UV−vis diffuse-reflectance spectra of **2** with $BaSO_4$ as background

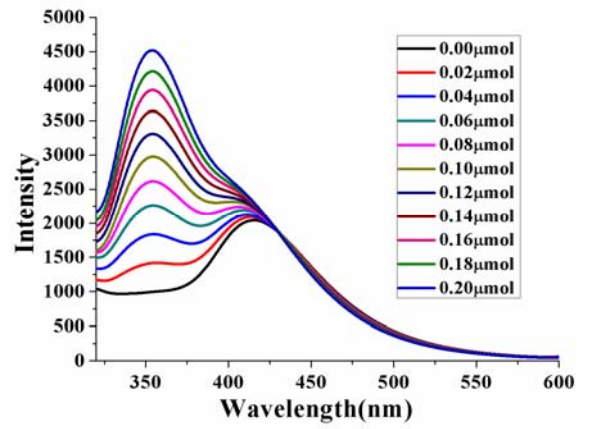

Fig. S11 Fluorescence titration of **1** dispersed in acetonitrile with the addition of different volume of 10^{-3} M acetonitrile solution of *p*-toluidine. The excitation wavelength was 310 nm and fluorescence emission was monitored from 320 nm to 600 nm. The slit width for both excitation and emission were 5 nm.

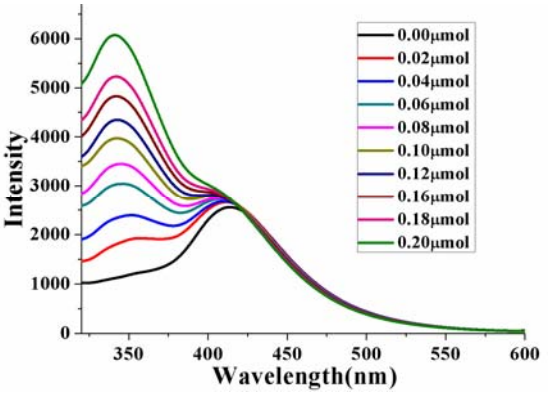

Fig. S12 Fluorescence titration of **1** dispersed in acetonitrile with the addition of different volume of 10^{-3} M acetonitrile solution of aniline. The excitation wavelength was 310 nm and fluorescence emission was monitored from 320 nm to 600 nm. The slit width for both excitation and emission were 5 nm.

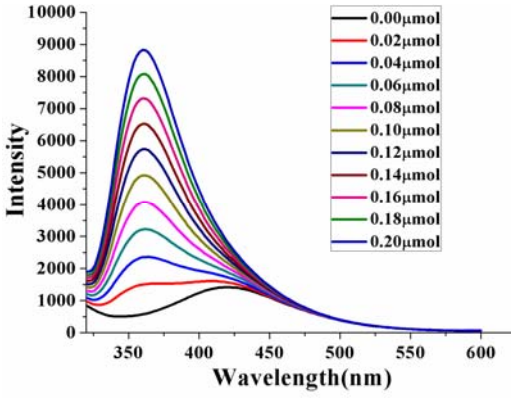

Fig. S13 Fluorescence titration of **2** dispersed in methanol with the addition of different volume of 10^{-3} M methanol solution of *p*-toluidine. The excitation wavelength was 310 nm and fluorescence emission was monitored from 320 nm to 600 nm. The slit width for both excitation and emission were 5 nm.

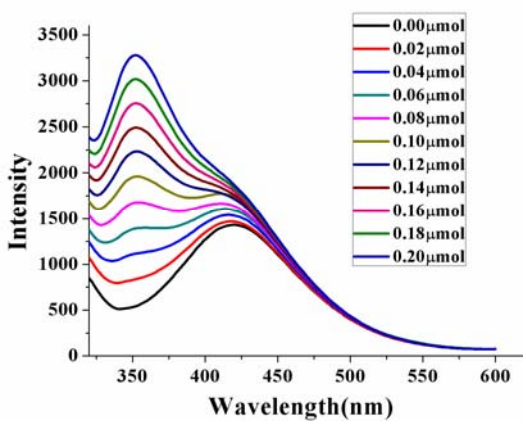

Fig. S14 Fluorescence titration of **2** dispersed in methanol with the addition of different volume of 10^{-3} M methanol solution of aniline. The excitation wavelength was 310 nm and fluorescence emission was monitored from 320 nm to 600 nm. The slit width for both excitation and emission were 5 nm.

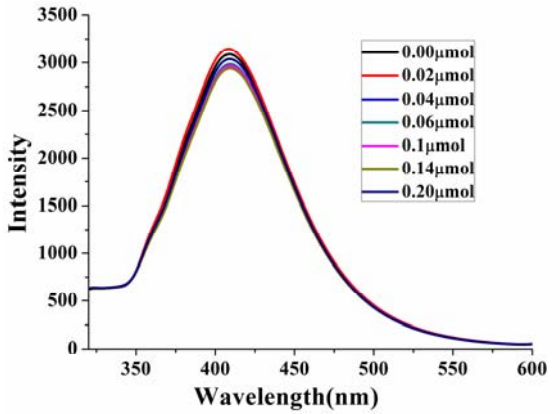

Fig. S15 Fluorescence titration of **1** dispersed in acetonitrile with the addition of different volume of 10^{-3} M acetonitrile solution of triethylamine. The excitation wavelength was 310 nm and fluorescence emission was monitored from 320 nm to 600 nm. The slit width for both excitation and emission were 5 nm.

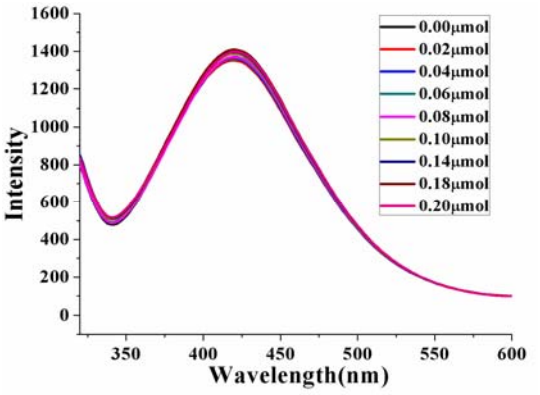

Fig. S16 Fluorescence titration of **2** dispersed in methanol with the addition of different volume of 10^{-3} M methanol solution of triethylamine. The excitation wavelength was 310 nm and fluorescence emission was monitored from 320 nm to 600 nm. The slit width for both excitation and emission were 5 nm.

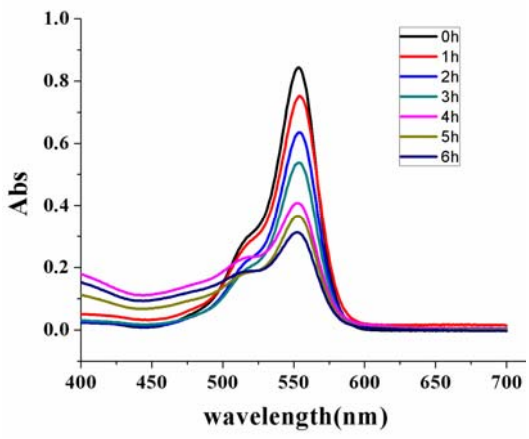

Fig. S17 UV-Vis absorption spectra of RhB solution degraded by **1** in 6h under UV light irradiation.

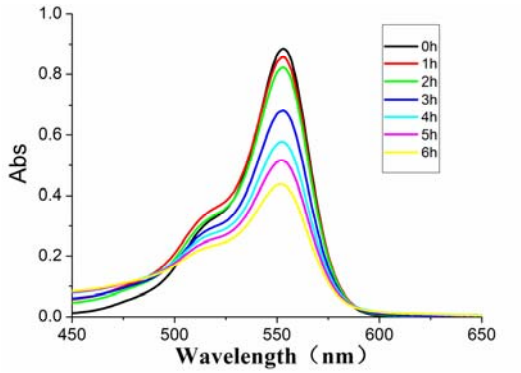

Fig. S18 UV-Vis absorption spectra of RhB solution degraded by **2** in 6h under UV light irradiation.

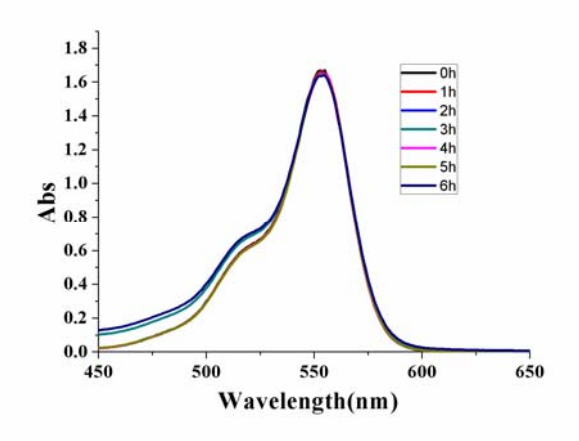

Fig. S19 UV-Vis absorption spectra of RhB solution degraded by **1** in 6h without illumination.

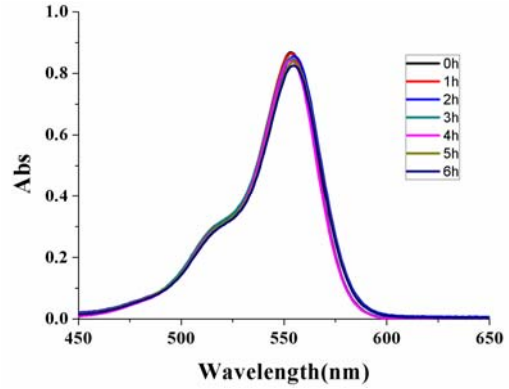

Fig. S20 UV-Vis absorption spectra of RhB solution degraded under UV light irradiation without photocatalysis.

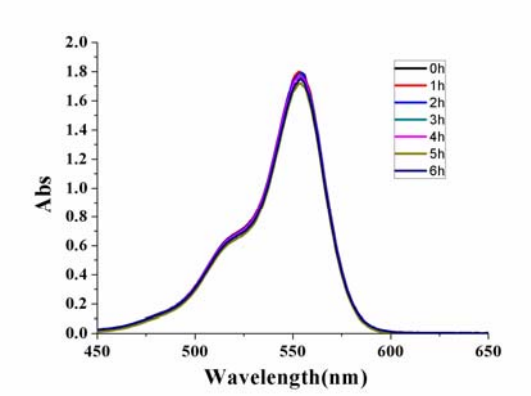

Fig. S21 UV-Vis absorption spectra of RhB solution degraded by **1** in 6h under natural light.

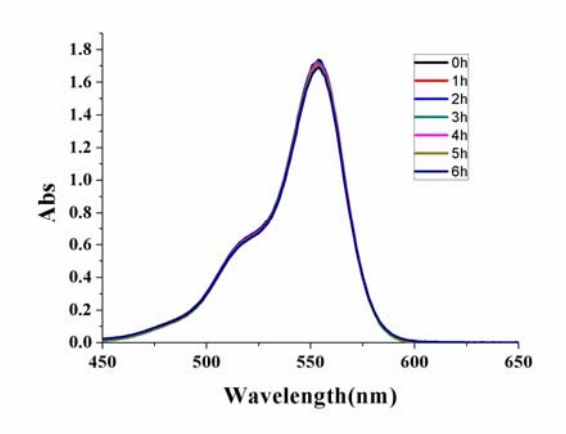

Fig. S22 UV-Vis absorption spectra of RhB solution degraded by **2** in 6h without illumination.

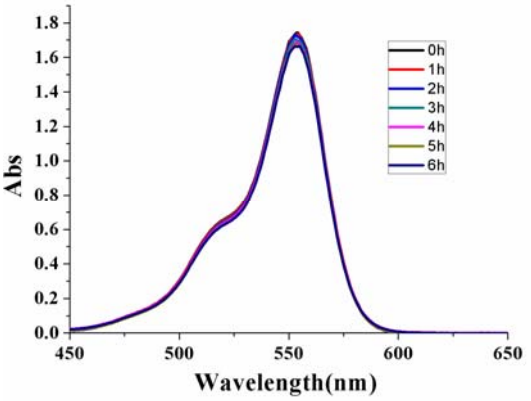

Fig. S23 UV-Vis absorption spectra of RhB solution degraded by **2** in 6h under natural light.

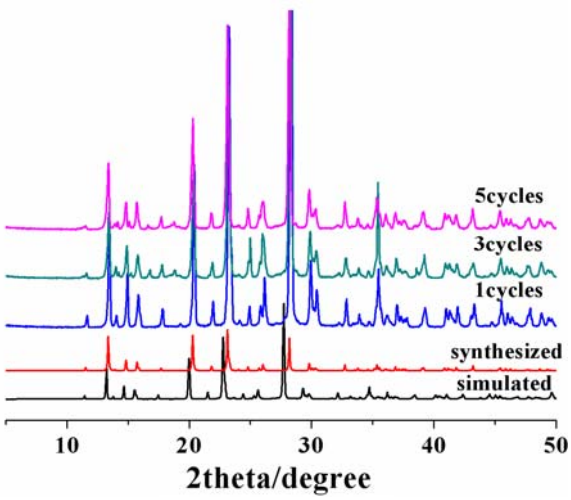

Fig. S24 PXRD patterns of **1** and recycled **1**.

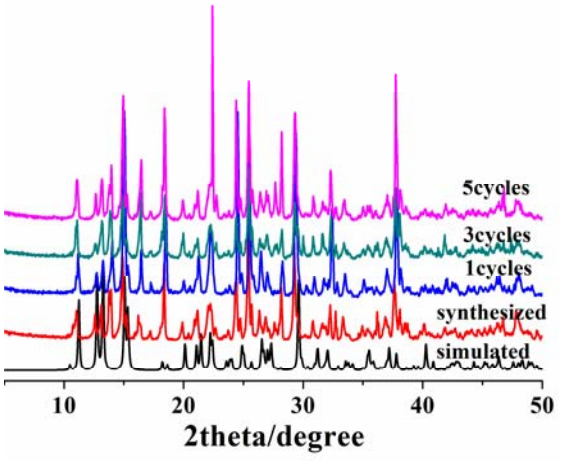

Fig. 25 PXRD patterns of **2** and recycled **2.**

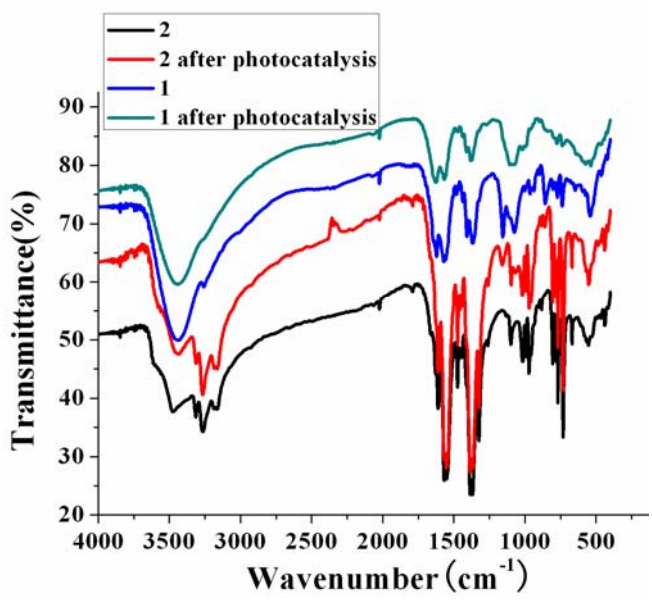

Fig. S26 IR spectra of **1** and **2** before and after photocatalytic reactions.