Electronic Supplementary Material (ESI) for RSC Advances.

Two Luminescent Metal-Organic Frameworks with Multifunctional Properties for Nitroaromatic Compounds Sensing and Photocatalysis

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Supplementary Materials

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

Compound	**1**	**2**
Chemical formula	$C_{24}H_{20}N_3O_8Zn$	$C_{48}H_{40}Cd_2N_6O_{16}$
Formula weight	543.80	1181.66
Temperature [K]	113(2)	113(2)
Wavelength[Å]	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic
Space group	P2(1)/c	P2(1)/c
a[Å]	10.170(2)	10.275(2)
b[Å]	16.233(3)	16.704(3)
c[Å]	12.934(3)	13.021(3)
α/[°]	90	90
β/[°]	100.72(3)	102.80(3)
γ/[°]	90	90
Volume [$Å^3$]	2098.1(7)	2179.2(8)
Z, Calculated density [Mg/m^3]	4, 1.722	2, 1.801
Absorption coefficient[mm^{-1}]	1.233	1.062
Theta range for data collection (deg)	2.04 to 28.02	2.01 to 27.95
Limiting indices	-13<=h<=13, -17<=k<=21, -16<=l<=17	-13<=h<=13, -21<=k<=21, -17<=l<=16
F(000)	1116	1188
Reflections collected/unique	21070/5032[R(int) = 0.0448]	21709/5203 [R(int) = 0.0356]
Goodness-of-fit on F^2	0.999	1.085
Final R indices[$I>2\sigma(I)$]	R_1 = 0.0373, wR_2 = 0.0946	R1 = 0.0313, wR2 = 0.0638
R indices (all data)	R_1 = 0.0463, wR_2 = 0.0993	R1 = 0.0381, wR2 = 0.0667
Largest diff. peak and hole[$e.Å^{-3}$]	0.764 and -0.578	0.785 and -0.882

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

1			
Zn(1)-O(1)	2.0408(15)	Zn(1)-N(3)	2.1097(17)
Zn(1)-O(6)	2.1148(15)	Zn(1)-N(2)	2.1597(17)
Zn(1)-O(4)#1	2.1831(16)	Zn(1)-O(3)#1	2.3191(16)
O(1)-Zn(1)-N(3)	117.04(6)	O(1)-Zn(1)-O(6)	93.39(6)
N(3)-Zn(1)-O(6)	92.84(7)	N(3)-Zn(1)-N(2)	77.92(7)
O(6)-Zn(1)-N(2)	168.09(6)	O(4)#1-Zn(1)-O(3)#1	58.13(6)
O(1)-Zn(1)-O(4)#1	92.59(6)	N(3)-Zn(1)-O(4)#1	147.52(6)
O(6)-Zn(1)-O(4)#1	98.67(6)	N(2)-Zn(1)-O(4)#1	85.68(6)
O(1)-Zn(1)-O(3)#1	148.99(6)	N(3)-Zn(1)-O(3)#1	93.90(6)
O(6)-Zn(1)-O(3)#1	82.34(6)	N(2)-Zn(1)-O(3)#1	90.71(6)
O(4)#1-Zn(1)-O(3)#1	58.13(6)	O(1)-Zn(1)-C(8)#1	121.75(7)
2			

Cd(1)-O(4)#1	2.240(4)	Cd(1)-O(7)	2.289(4)
Cd(1)-N(3)	2.298(5)	Cd(1)-N(2)	2.335(4)
Cd(1)-O(1)	2.391(4)	Cd(1)-O(2)	2.441(4)
O(4)#1-Cd(1)-O(7)	98.66(14)	O(4)#1-Cd(1)-N(3)	123.85(16)
O(7)-Cd(1)-N(3)	91.28(15)	O(4)#1-Cd(1)-N(2)	97.25(15)
O(7)-Cd(1)-N(2)	161.70(14)	N(3)-Cd(1)-N(2)	72.29(16)
O(4)#1-Cd(1)-O(1)	85.77(14)	O(7)-Cd(1)-O(1)	106.79(14)
N(3)-Cd(1)-O(1)	143.02(14)	N(2)-Cd(1)-O(1)	83.32(15)
O(4)#1-Cd(1)-O(2)	137.04(14)	O(7)-Cd(1)-O(2)	80.74(14)
N(3)-Cd(1)-O(2)	99.06(15)	N(2)-Cd(1)-O(2)	93.68(15)
O(1)-Cd(1)-O(2)	54.41(13)	O(4)#1-Cd(1)-C(1)	112.40(15)

Symmetry transformations used to generate equivalent atoms:

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

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

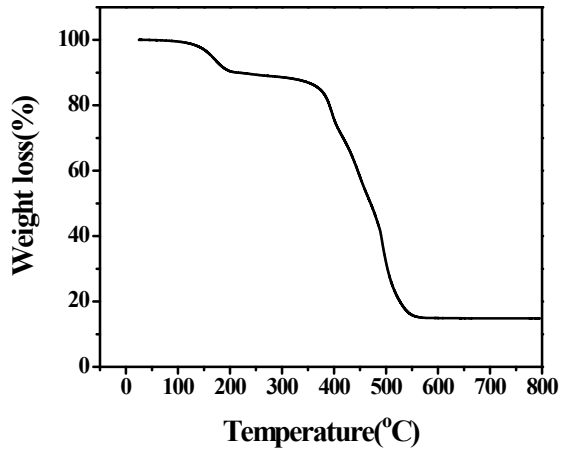

Fig. S1 TG curve of **1**.

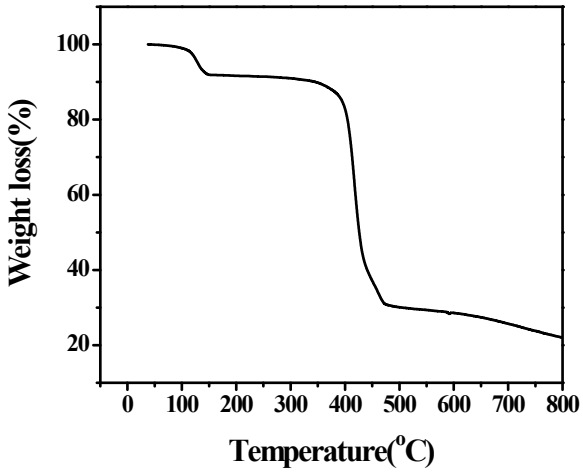

Fig. S2 TG curve of **2.**

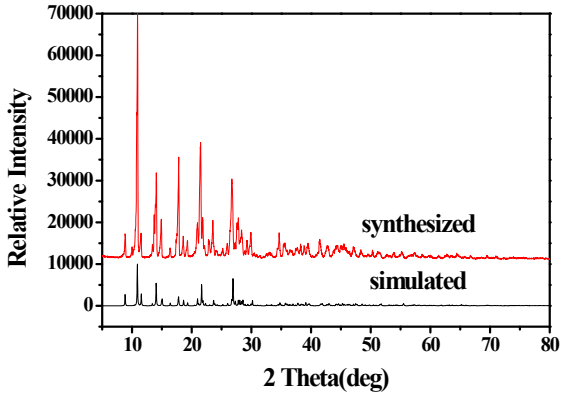

Fig. S3 PXRD pattern of **1**

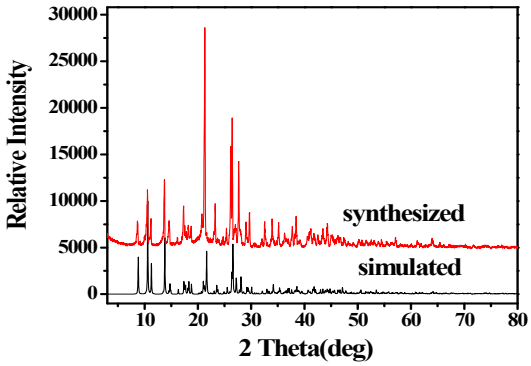

Fig. S4 PXRD pattern of **2**

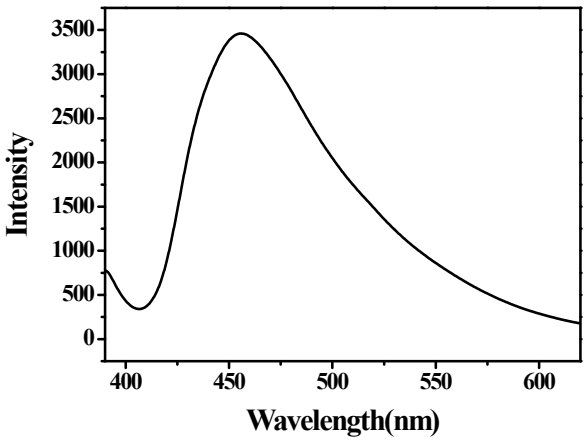

Fig. S5 The fluorescence spectra of **1** (λ_{ex} = 330 nm) at the solid state at room temperature

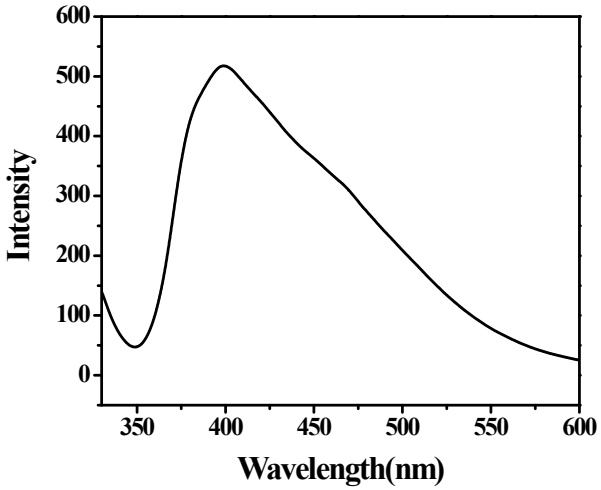

Fig. S6 The fluorescence spectra of **2** (λ_{ex} = 318 nm) at the solid state at room temperature

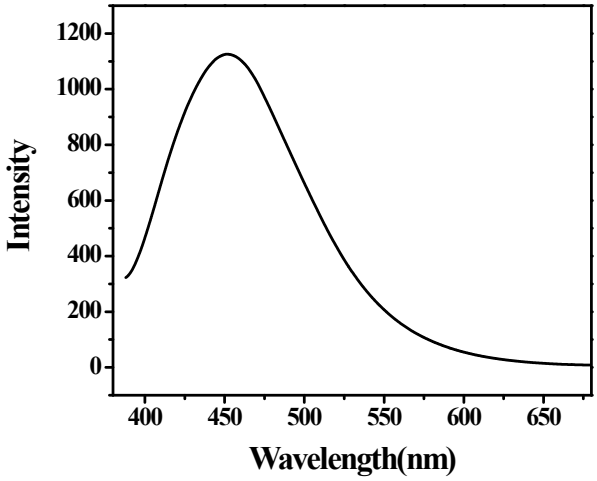

Fig. S7 The fluorescence spectra of **L** ligand (λ_{ex} = 357 nm) at the solid state at room temperature

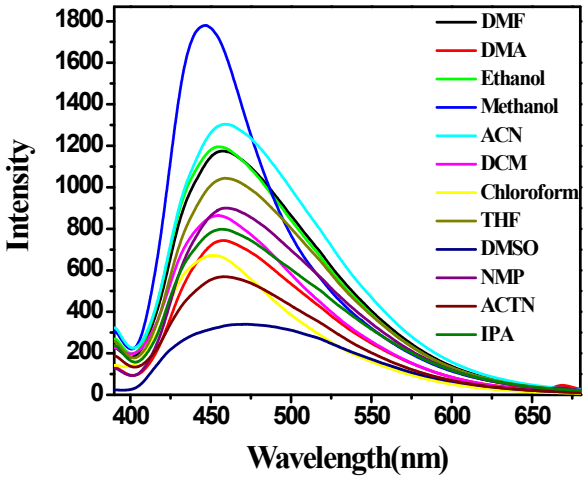

Fig. S8 Fluorescence emission spectra of **1** in different organic solvent at room temperature.

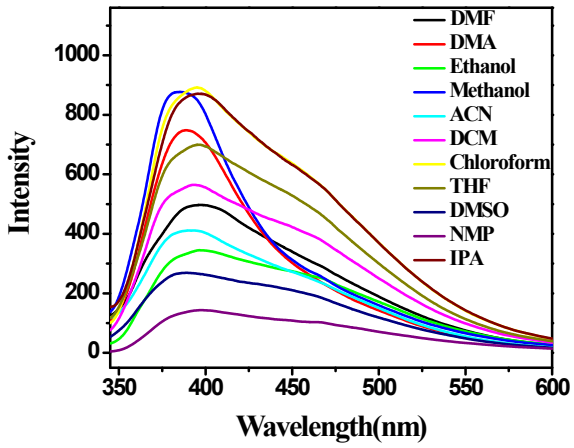

Fig. S9 Fluorescence emission spectra of **2** in different organic solvent at room temperature

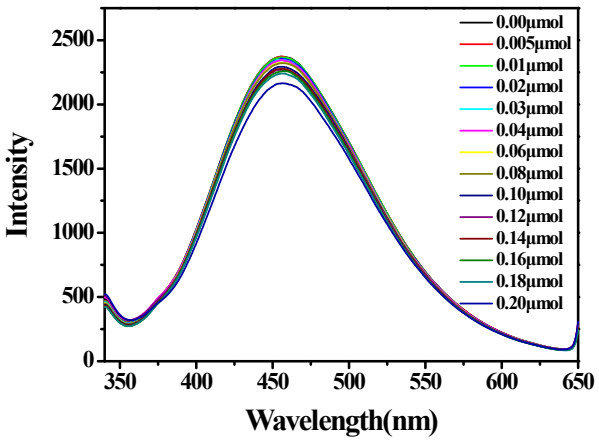

Fig. S10 Fluorescence titration of **1** dispersed in DMA with the addition of different volume of 10^{-3} M DMA solution of *p*-nitrotoluene. The excitation wavelength was 330 nm and fluorescence emission was monitored from 340 to 650 nm. The slit width for both excitation and emission were 5 nm.

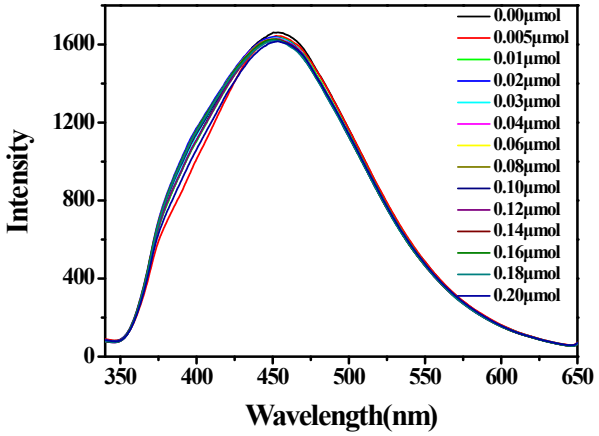

Fig. S11 Fluorescence titration of **1** dispersed in DMA with the addition of different volume of 10^{-3} M DMA solution of nitrobenzene. The excitation wavelength was 330 nm and fluorescence emission was monitored from 340 to 650 nm. The slit width for both excitation and emission were 5 nm.

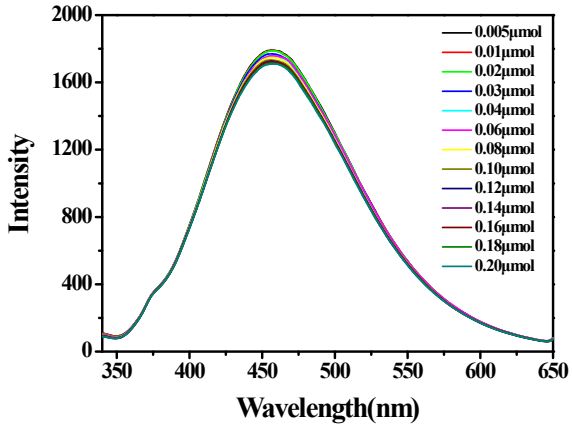

Fig. S12 Fluorescence titration of **1** dispersed in DMA with the addition of different volume of 10^{-3} M DMA solution of *m*-nitrotoluene. The excitation wavelength was 330 nm and fluorescence emission was monitored from 340 to 650 nm. The slit width for both excitation and emission were 5 nm.

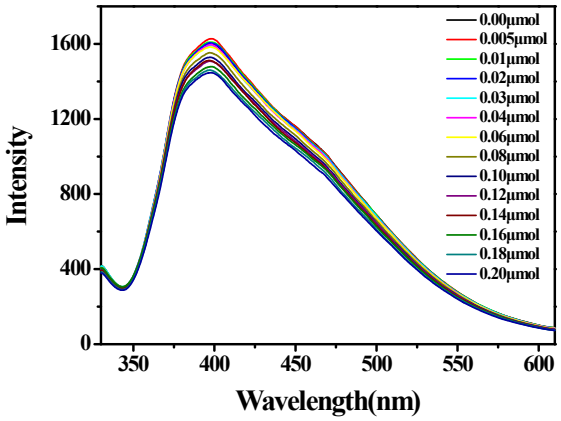

Fig. S13 Fluorescence titration of **2** dispersed in isopropanol with the addition of different volume of 10^{-3} M isopropanol solution of *p*-nitrotoluene. The excitation wavelength was 318 nm and fluorescence emission was monitored from 330 to 600 nm. The slit width for both excitation and emission were 5 nm.

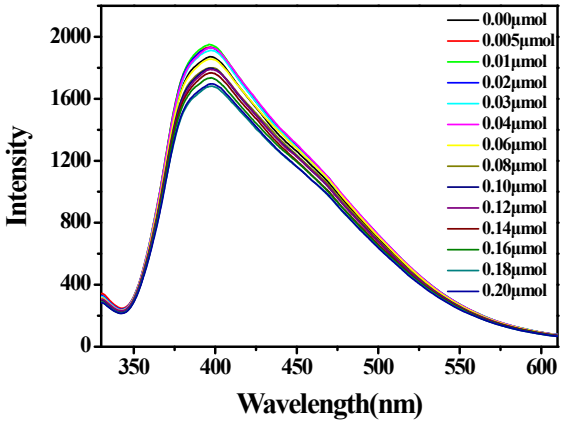

Fig. S14 Fluorescence titration of **2** dispersed in isopropanol with the addition of different volume of 10^{-3} M isopropanol solution of nitrobenzene. The excitation wavelength was 318 nm and fluorescence emission was monitored from 330 to 600 nm. The slit width for both excitation and

emission were 5 nm.

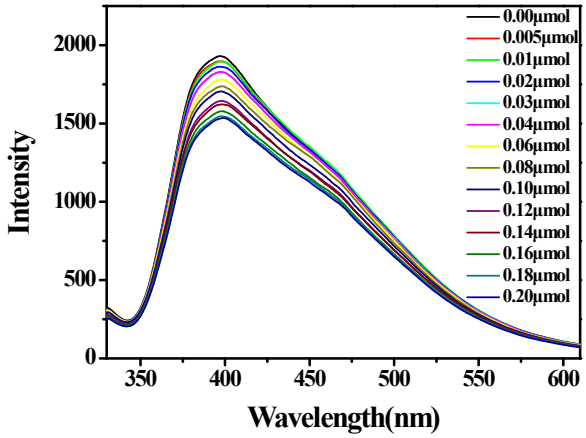

Fig. S15 Fluorescence titration of **2** dispersed in isopropanol with the addition of different volume of 10^{-3} M isopropanol solution of *m*-nitrotoluene. The excitation wavelength was 318 nm and fluorescence emission was monitored from 330 to 600 nm. The slit width for both excitation and emission were 5 nm.

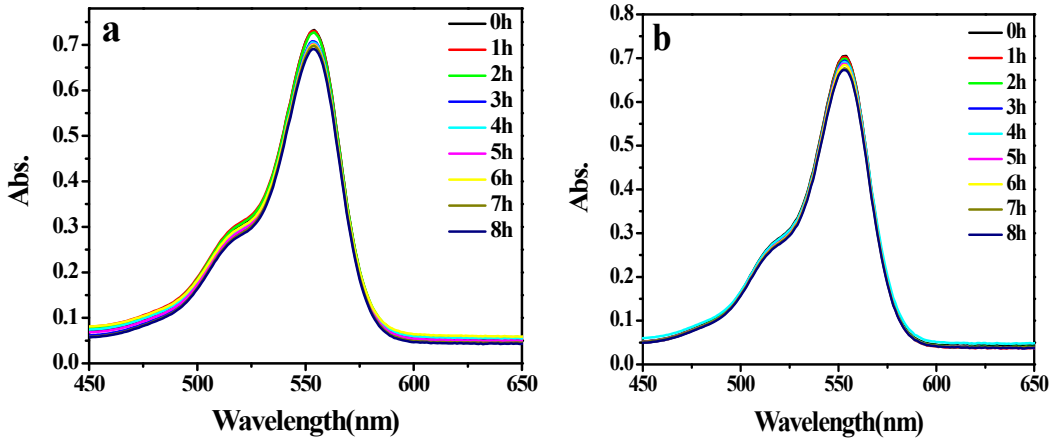

Fig. S16 Absorption spectra of RhB degraded by **1** (a) and **2** (b) under dark conditions.

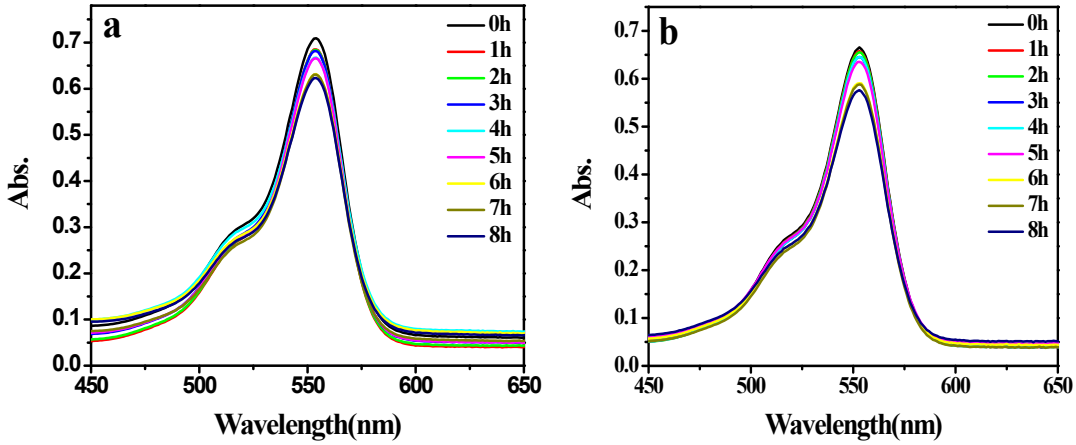

Fig. S17 Absorption spectra of RhB degraded by **1** (a) and **2** (b) under natural illumination.

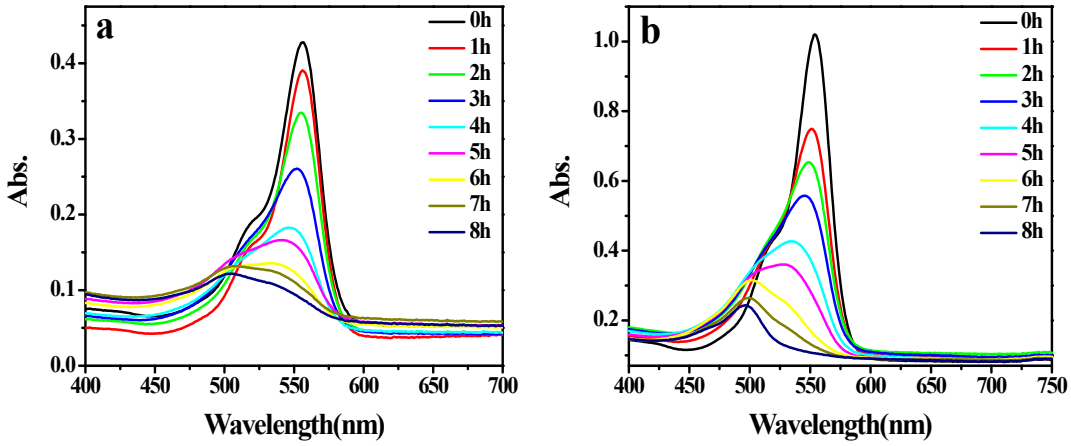

Fig. S18 Absorption spectra of RhB degraded by **1** (a) and **2** (b) under UV light.

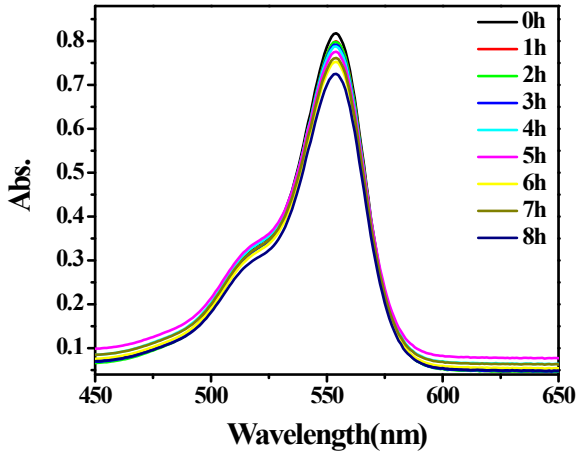

Fig. S19 Absorption spectra of RhB degraded without any catalyst under UV light.

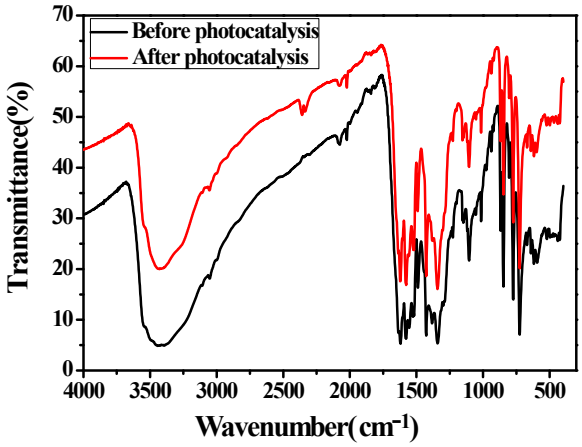

Fig. S20 The IR spectra of **1** before and after photocatalysis

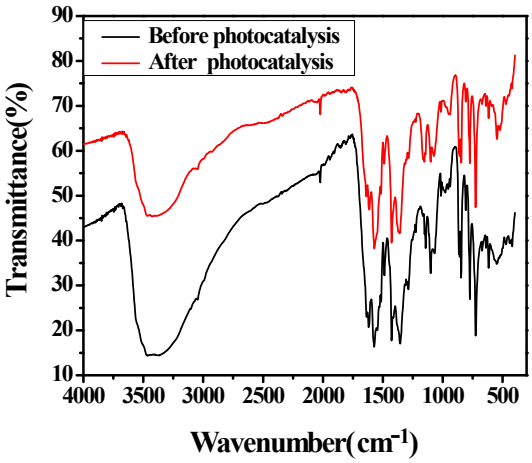

Fig. S21 The IR spectra of **2** before and after photocatalysis