Electronic Supplementary Information

A novel multifunction photochromic metal-organic framework for rapid ultraviolet light detection, amine-selective sensing and inkless and erasable prints

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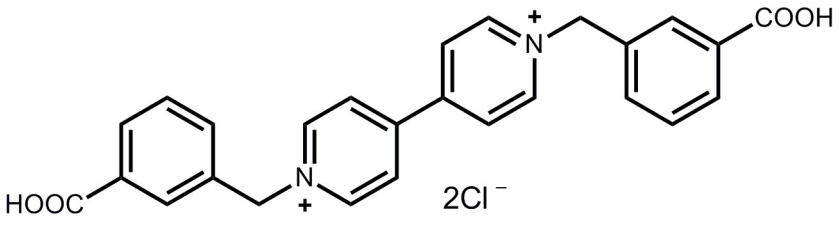

Scheme 1. The molecular structure of H_2bcbpy·2Cl.

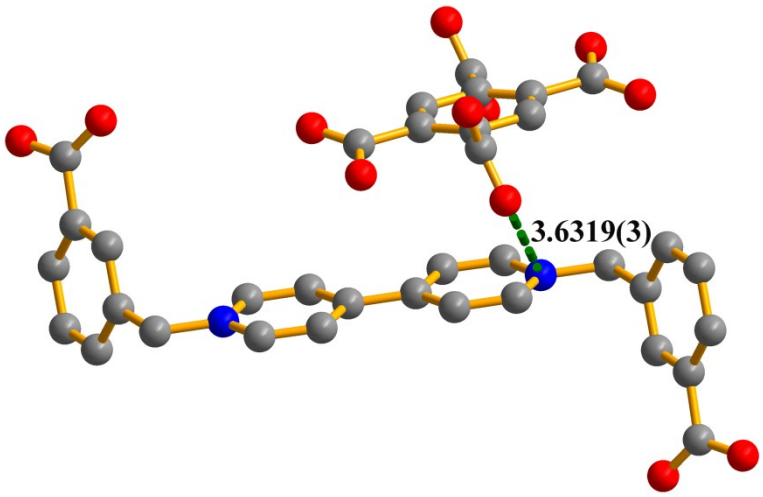

Fig. S1 The distance between the electron donor and acceptor.

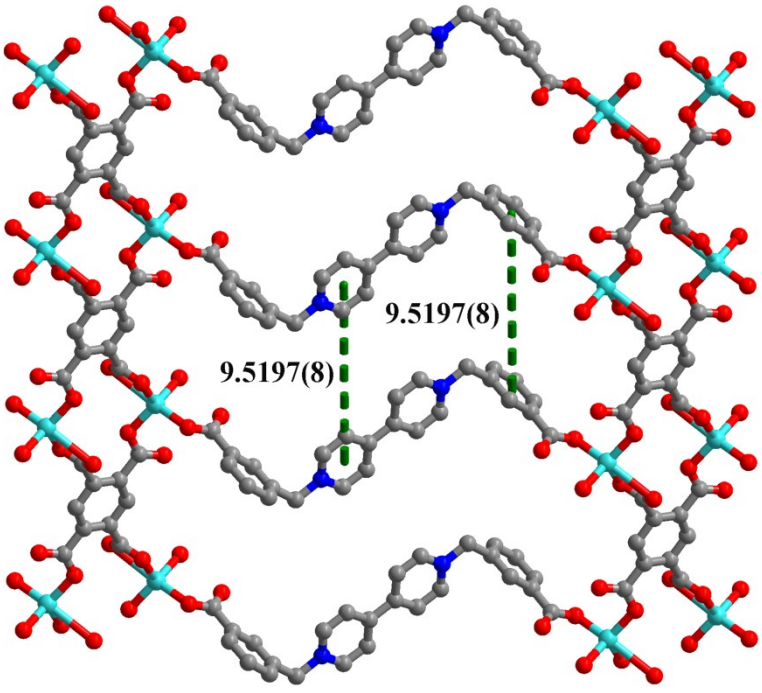

Fig. S2 π···π stacking interactions in compound **1**. All distances for H bonds are labelled in angstrom.

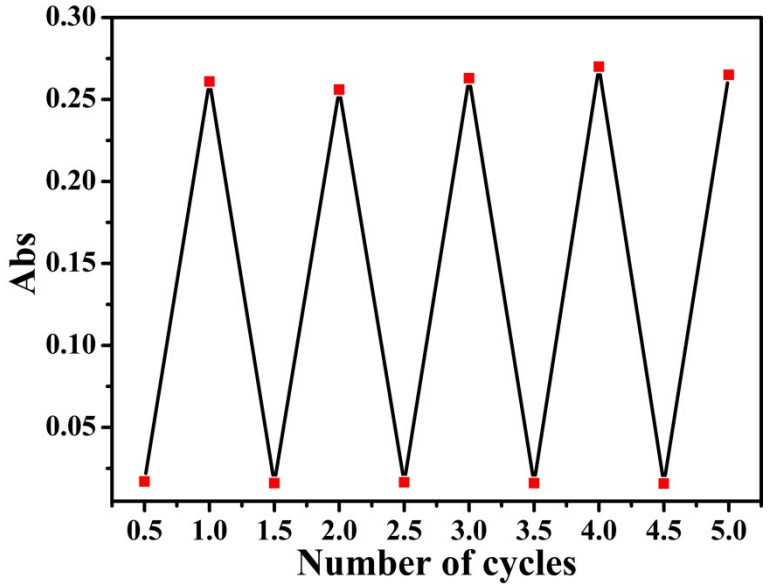

Fig. S3 Variation of the absorbance at λ = 616 nm in the repeated response cycles to ultraviolet light.

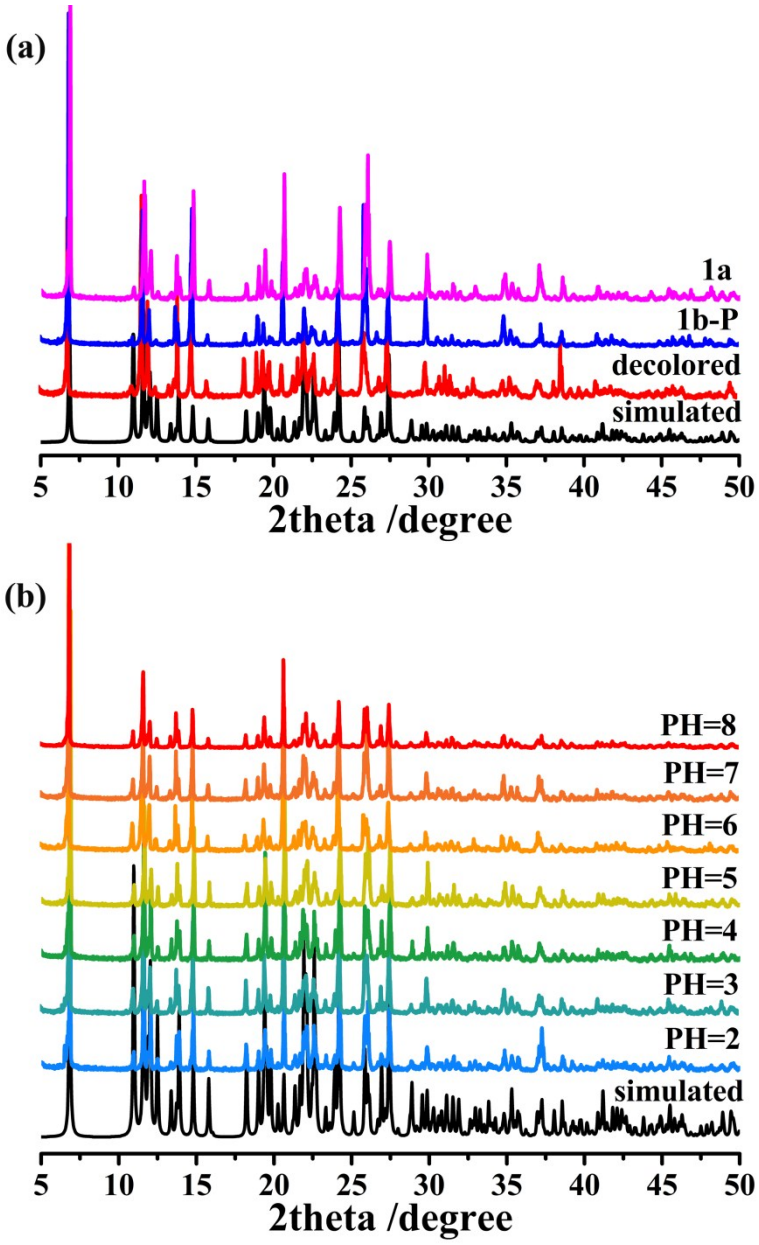

Fig. S4 (a) Simulated and experimental PXRD patterns of **1**. (b) PXRD patterns of samples soaking in pH = 2–8 water solution for 24 h. Labels: **1a**: before irradiation; **1b-P**: after photo irradiation; decolored: heating in 50 °C for 20 min.

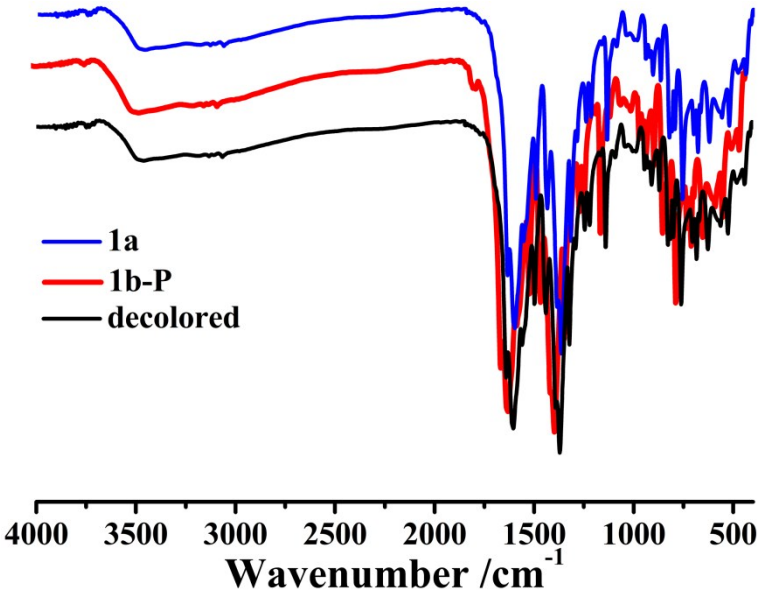

Fig. S5 FT-IR spectra of **1**. Labels: **1a**: before irradiation; **1b-P**: after photo irradiation; **decolored**: heating in 50 °C for 20 min.

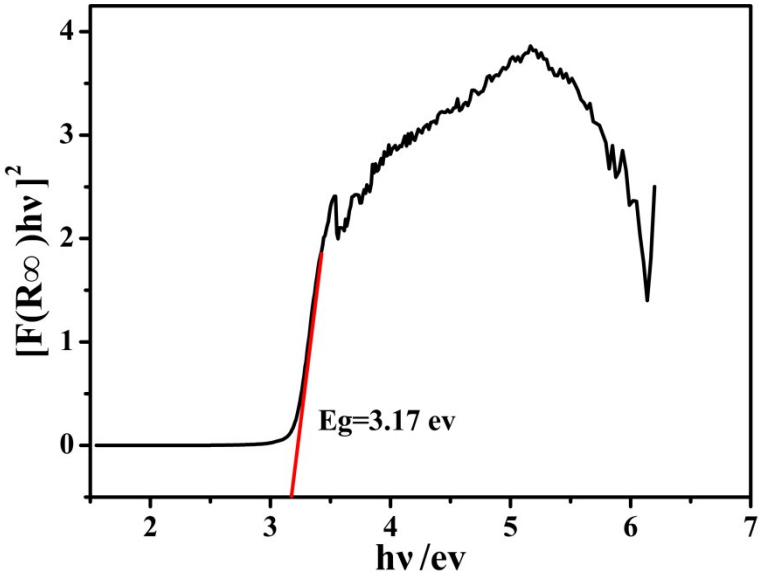

Fig. S6 Optical band gap energy of compound **1**.

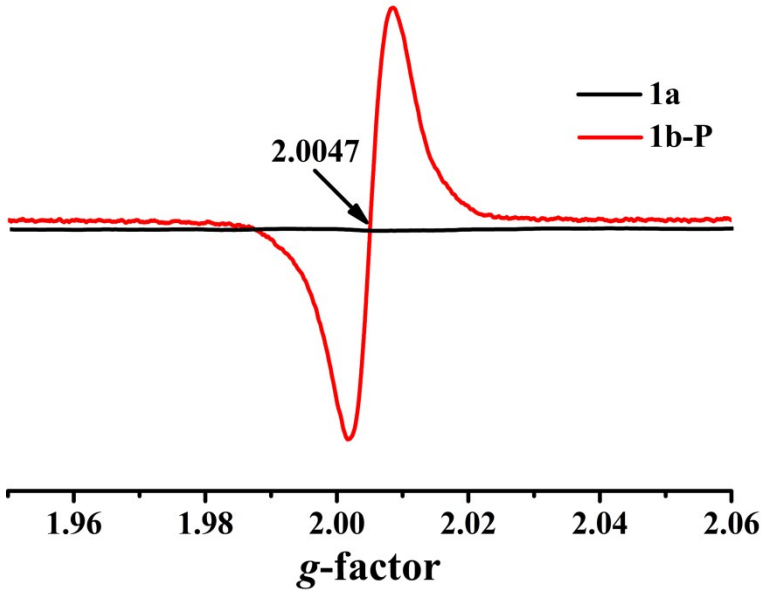

Fig. S7 ESR spectra of **1**. Labels: **1a**, before photo irradiation; **1b-P**, after photo irradiation.

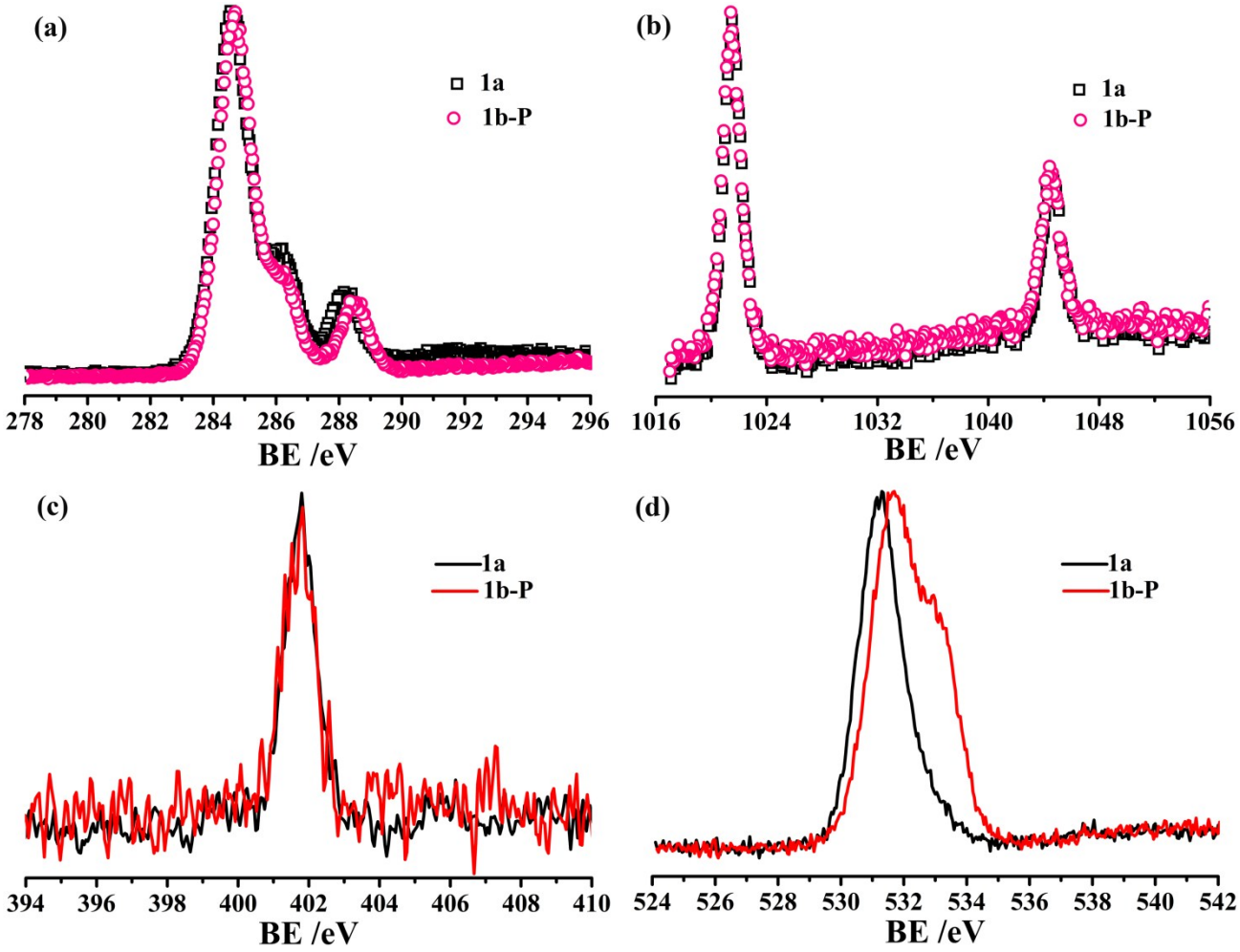

Fig. S8 XPS (Al-*Kα*) core-level spectra of compound **1** for C 1s (a), Zn 1s (b), N 1s (c) and O 1s (d) before and after photo irradiation in a vacuum. Labels: **1a**, before irradiation; **1b-P**, after photo irradiation; BE: Binding Energy.

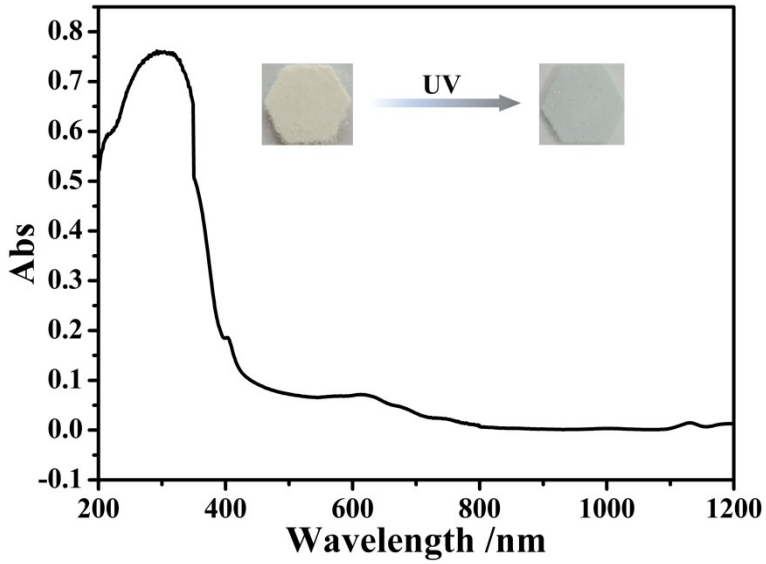

Fig. S9 UV–Vis diffuse reflectance spectra of the crystal samples upon UV light irradiation with intensity of 0.001 mW/cm^2. The colors change was shown in the inset before and after photo-irradiation.

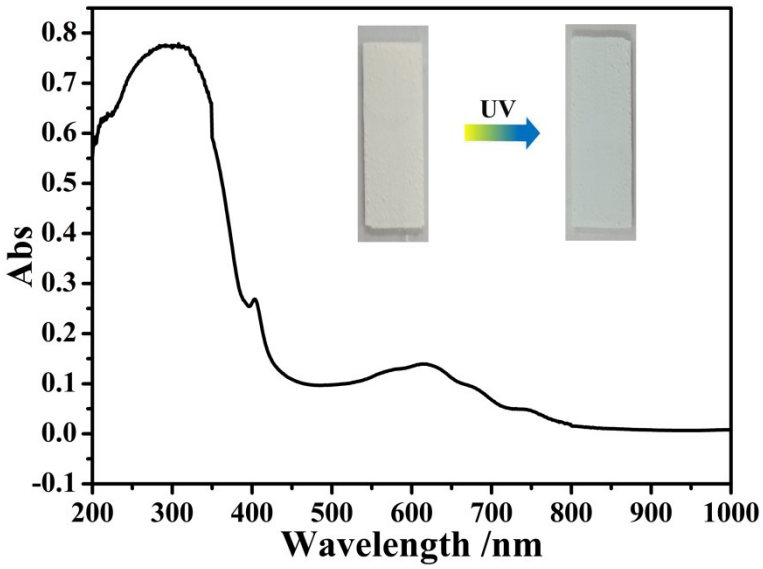

Fig. S10 The photos of the composite films exposed to sunlight. The exposure time was 3 min.

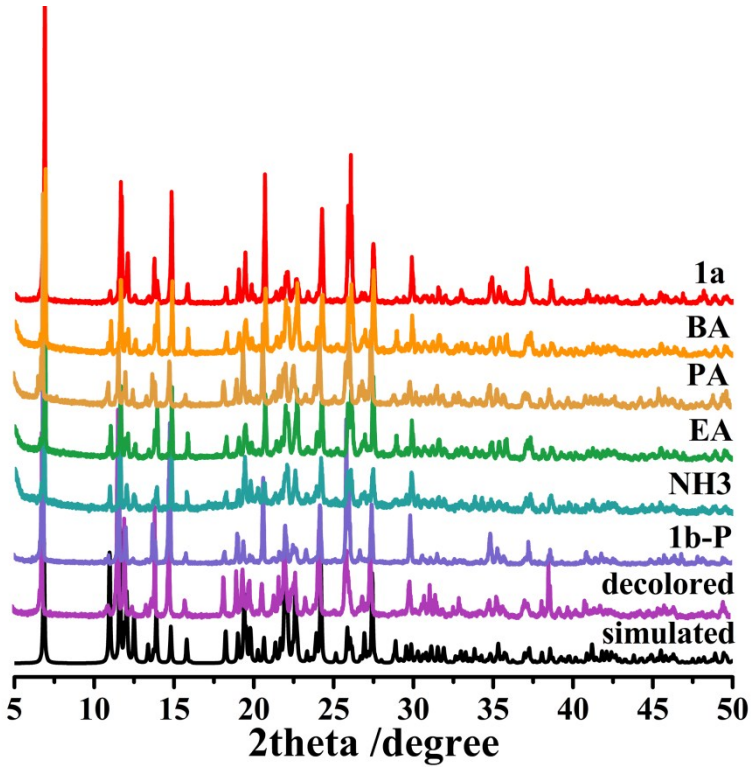

Fig. S11 PXRD patterns of **1**. Labels: **1a**, before irradiation; **1b-P**, after photo irradiation; EA, PA, BA, NH_3, **1a** exposed to ethamine, n-propylamine, n-butylamine, NH_3 vapor respectively in the solid state at room temperature; simulated, simulated patterns from single-crystal X-ray structure data; **decolored**, heating in 50 °C for 20 min.

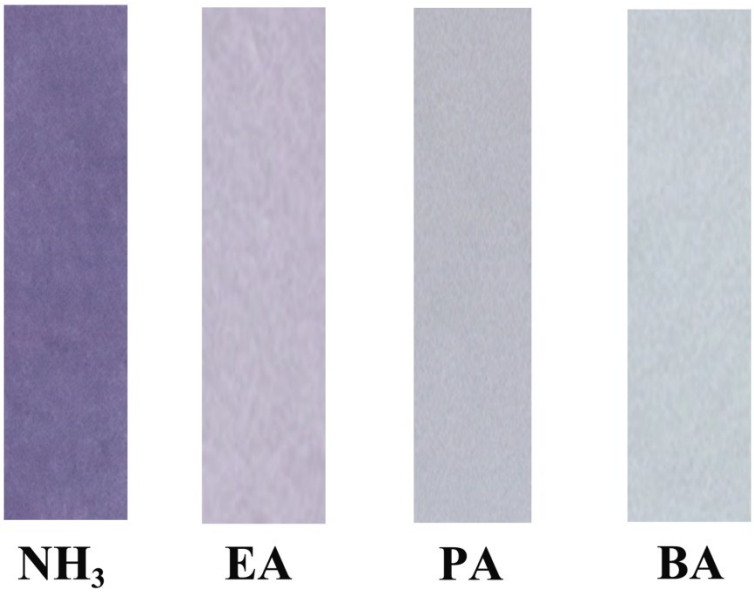

Fig. S12 Portable test strips for visual and differentiable detection of amines. Labels: EA, PA, BA, NH_3, **1a** exposed to ethamine, n-propylamine, n-butylamine, NH_3.

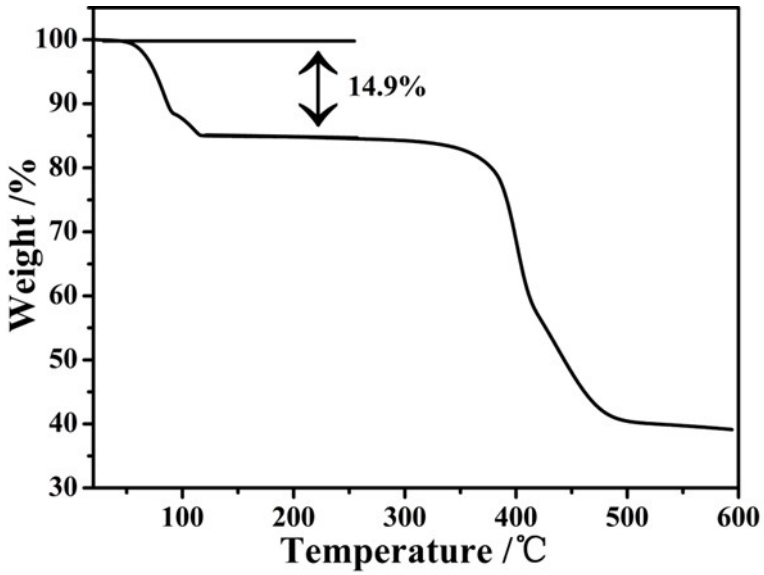

Fig. S13 TGA curve of **1** was investigated using powder samples under N_2. The weight loss is 14.9 % (calcd 15.1 %) up to 116 °C corresponding to the loss of three free H_2O and one coordinated H_2O.

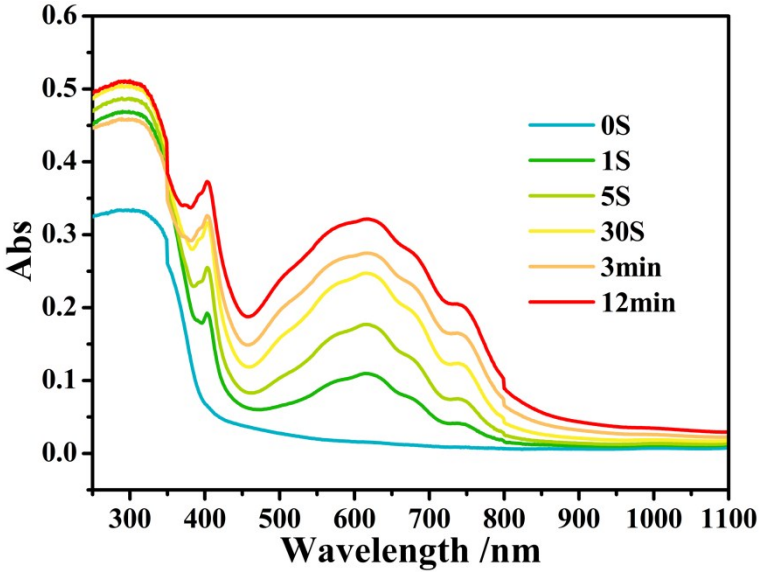

Fig. S14 Time-dependent UV–Vis diffuse reflectance spectra of **1** upon 300 W ultraviolet light irradiation at room temperature in air.

Tables.

Table S1. Crystal Data and Structure Refinements for **1**

Empirical formula	C_{18} H_{17} N O_{10} Zn **(1)**
Formula weight	472.7
Temperature /K	296
Crystal system	Triclinic
Space group	*P*–1
a /Å	9.1059(10)
b /Å	9.2243(10)
c /Å	13.2852(15)
α /deg	76.875(2)
β /deg	80.247(2)
γ /deg	62.573(2)
Volume /Å^3	961.88(18)
Z	2
D_c /g·cm^{-3}	1.632
Absorption coefficient /mm^{-1}	1.335
Goodness-of-fit on F^2	1.058
Final *R* indices [$I > 2\sigma(I)$]	R_1 = 0.0353, wR_2 = 0.1061
R indices (all data)	R_1 = 0.0385, wR_2 = 0.1082

[a]$R_1 = \sum||F_o|-|F_c||/\sum|F_o|$, [b]$wR_2 = \{\sum w[(F_o)^2-(F_c)^2]^2/\sum w[(F_o)_2]^2\}^{1/2}$.

Table S2. Selected bond lengths (Å) and angles (deg) for **1**

bond lengths (Å)		**angles (deg)**	
Zn(1)-O(3)	1.9212(17)	O(3)-Zn(1)-O(4)	125.33(8)
O(1)-C(7)	1.273(3)	O(4)-Zn(1)-O(1)	98.58(7)
O(3)-C(5)	1.274(3)	C(7)-O(1)-Zn(1)	121.56(16)
N(1)-C(12)	1.333(4)	C(12)-N(1)-C(15)	120.1(2)
C(1)-C(4)	1.392(3)	C(4)-C(1)-C(5)	123.1(2)
Zn(1)-O(1)	2.0116(18)	O(5)-C(7)-O(1)	125.1(2)
C(2)-C(4)	1.504(3)	C(6)-C(11)-N(1)	112.6(2)