Electronic Supplementary Information (ESI†)

Reversible single-crystal to single-crystal photoreaction between a coordination comb and a ladder displays photo-switchable fluorescence

Ni-Ya Li,[a] Xin-Yu Wang,[a] Pei-Xuan Zhang,[a] Ning-Ning Zou,[a] Wen Qiu,[a] Yu-Fei Xing,[a] Yun-Jian Wang,*[b] Xiao-Yan Tang*[c] and Dong Liu*[a]

[a.] *Jiangsu Key Laboratory for Chemistry of Low-Dimensional Materials, School of Chemistry and Chemical Engineering, Huaiyin Normal University, Huaian 223300, Jiangsu, P. R. China. E-mail: dongliu@hytc.edu.cn*

[b.] *Key Laboratory of Green and Precise Synthetic Chemistry and Applications, Ministry of Education; School of Chemistry and Materials Science, Huaibei Normal University, Huaibei 235000, P.R. China. E-mail: wangyunjianmail@163.com*

[c.] *School of Materials Engineering, Changshu Insititute of Technology, Changshu 215500, Jiangsu, PR China. E-mail: tangxy@cslg.edu.cn*

Table of Contents

Table S1 Selected Bond Lengths (Å) and Angles (º) for **1** and **1a**

Compound **1**			
Zn(1)-O(1)	1.9581(15)	Zn(1)-O(4A)	1.9719(15)
Zn(1)-O(5)	1.9993(18)	Zn(1)-N(1)	2.0256(17)
O(1)-Zn(1)-O(4A)	103.40(6)	O(1)-Zn(1)-O(5)	108.20(8)
O(4A)-Zn(1)-O(5)	105.11(8)	O(1)-Zn(1)-N(1)	118.43(7)
O(4A)-Zn(1)-N(1)	110.48(7)	O(5)-Zn(1)-N(1)	110.26(8)
Compound **1a**			
Zn(1)-O(4A)	1.971(2)	Zn(1)-O(1)	1.974(2)
Zn(1)-O(5)	2.011(2)	Zn(1)-N(1)	2.023(2)
O(4A)-Zn(1)-O(1)	102.43(9)	O(4A)-Zn(1)-O(5)	112.45(10)
O(1)-Zn(1)-O(5)	104.37(10)	O(4A)-Zn(1)-N(1)	120.03(10)
O(1)-Zn(1)-N(1)	107.37(9)	O(5)-Zn(1)-N(1)	108.73(10)

Symmetry codes: for **1**: (A) *x*, *y* - 1, *z*. for **1a**: (A) *x*, *y* - 1, *z*.

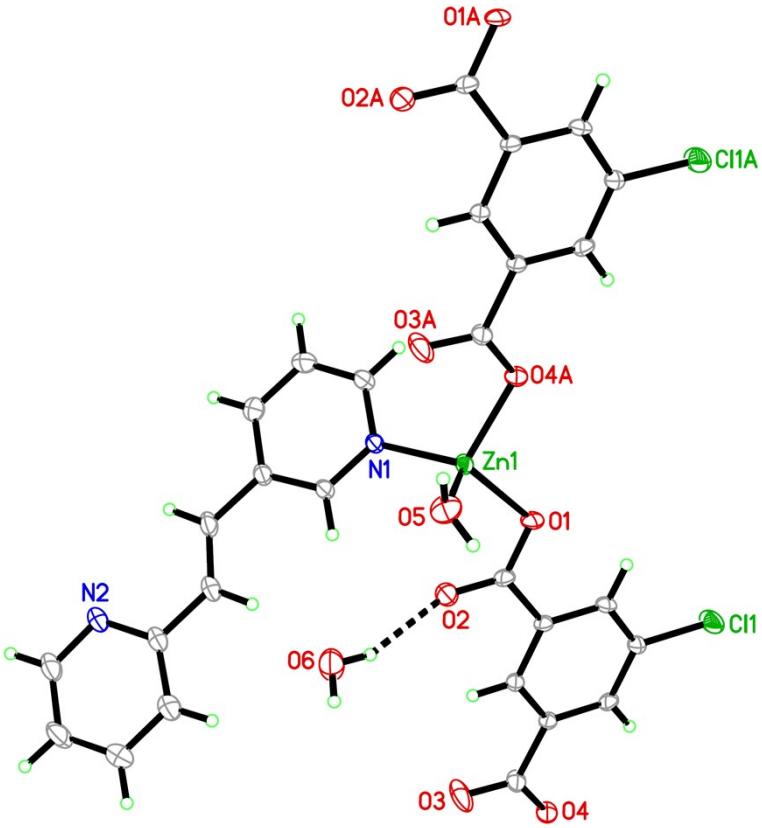
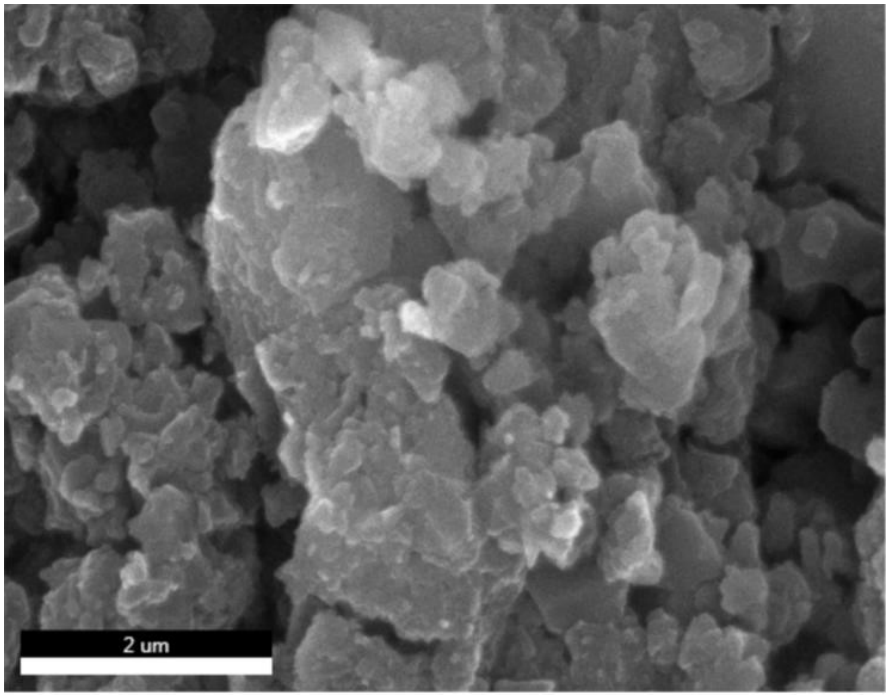


Fig. S1. View of the coordination environment of Zn1 in **1** with labeling scheme. Symmetry codes: (A) *x*, *y* - 1, *z*.

(a)



(b)

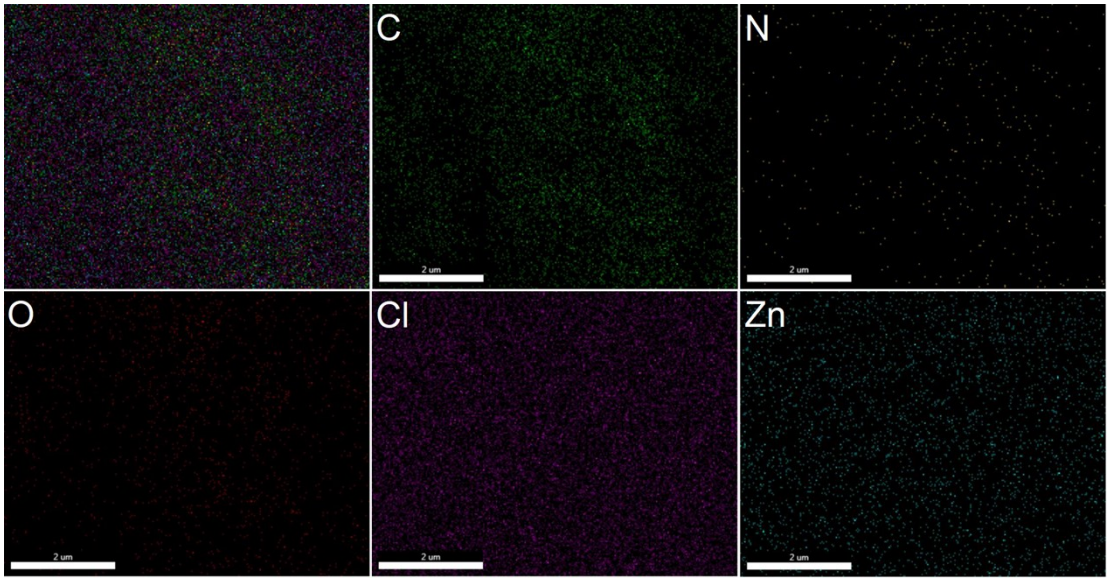


Fig. S2. (a) SEM image of **1** at 2 µm scale. (b) Element mapping images of **1**.

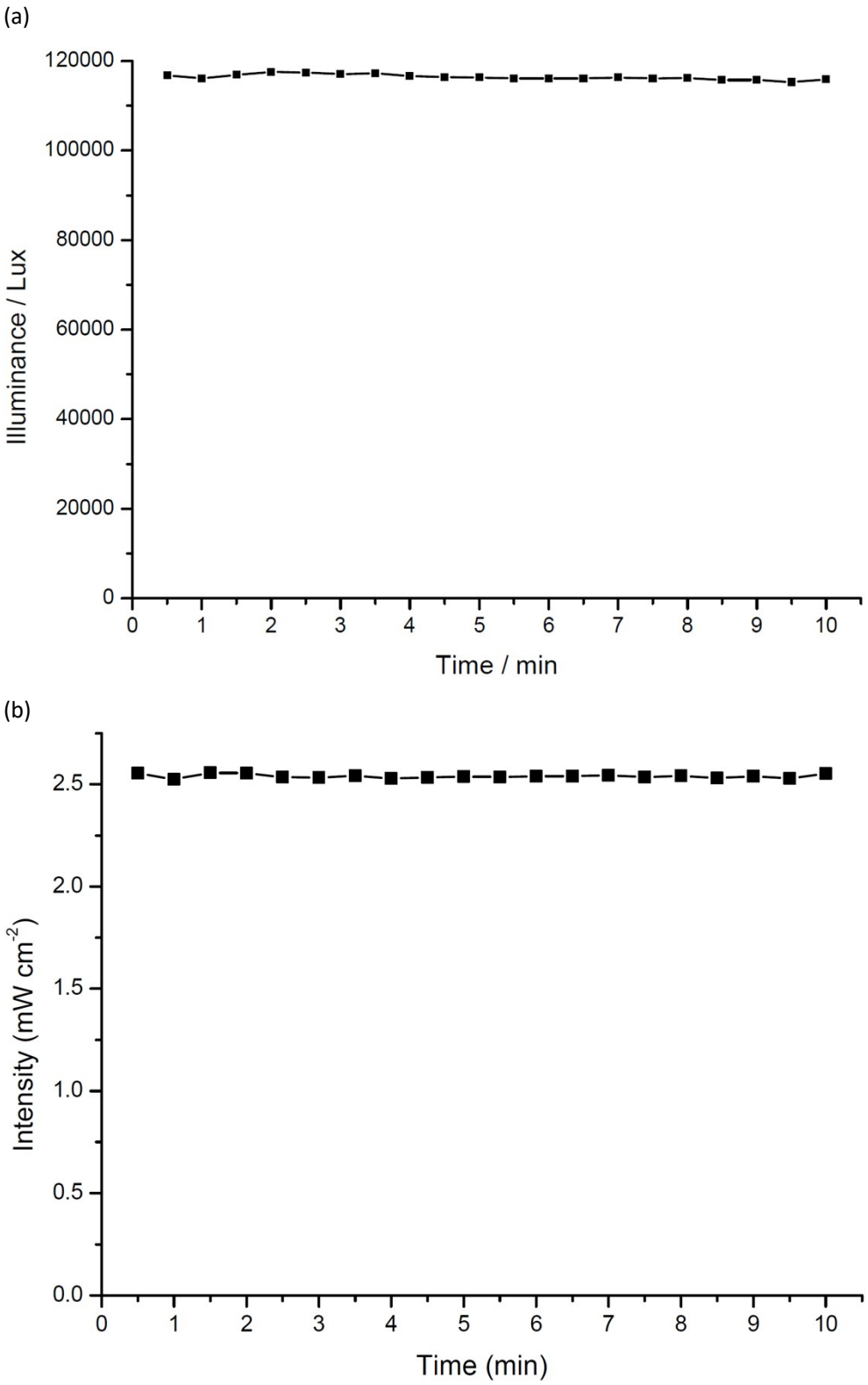
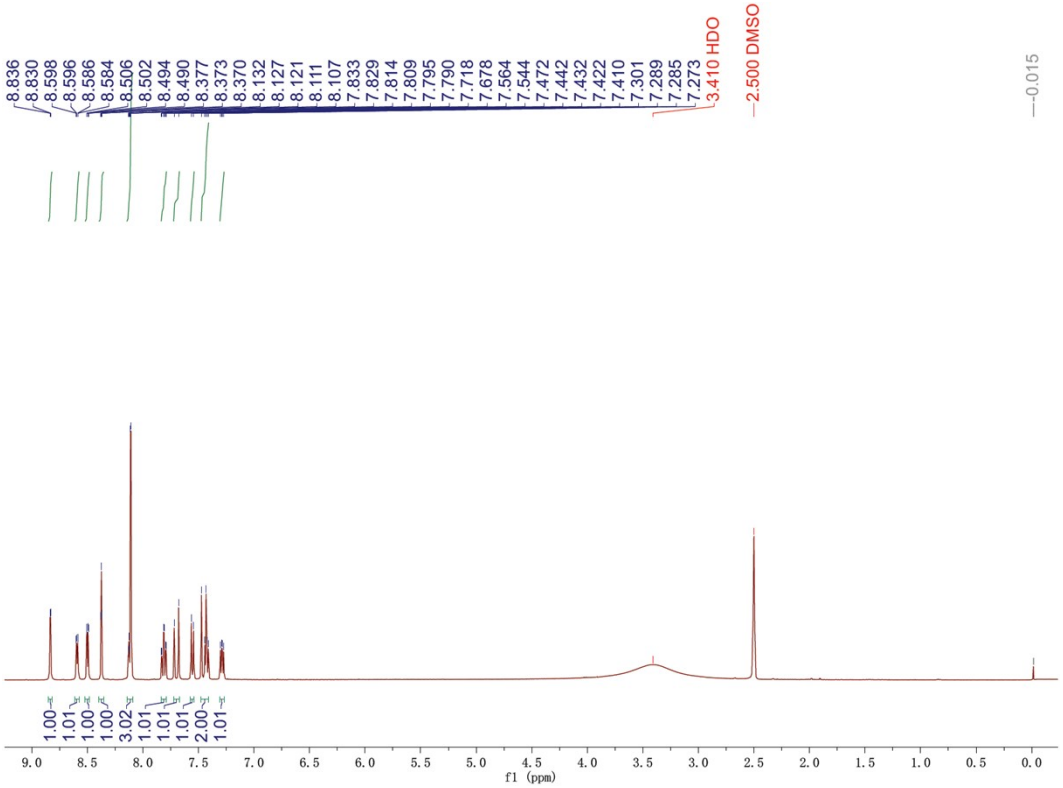


Fig. S3. (a) Illumination intensity of sunlight every 30 s within 10 min during the sunlight-induced [2+2] cycloaddition reaction of **1**. (b) Irradiation intensity of UV light in the range of 290-390 nm every 30 s within 10 min during the sunlight-induced [2+2] cycloaddition reaction of **1**.

(a)



(b)

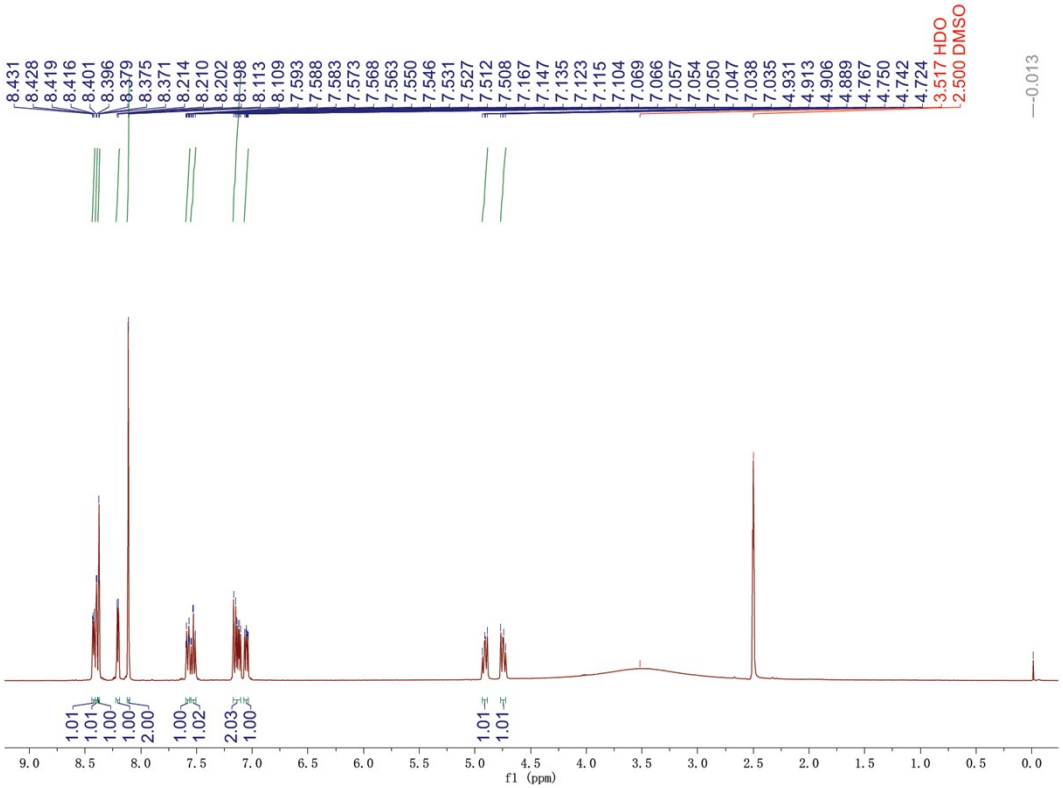
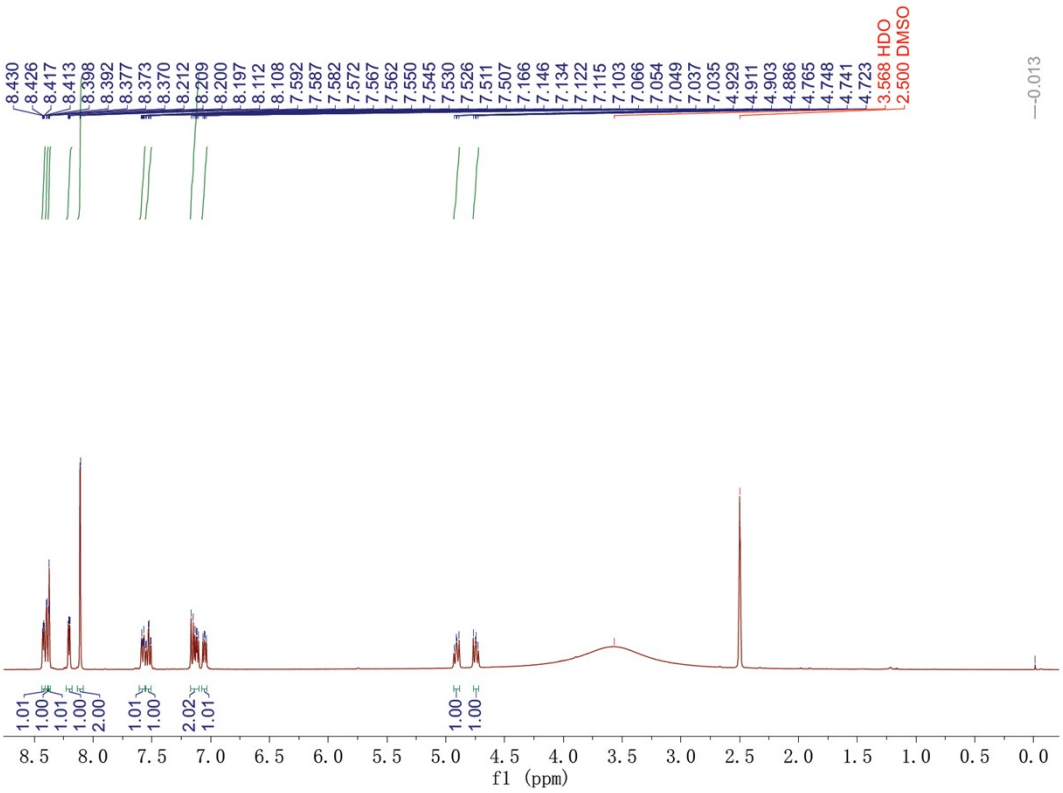
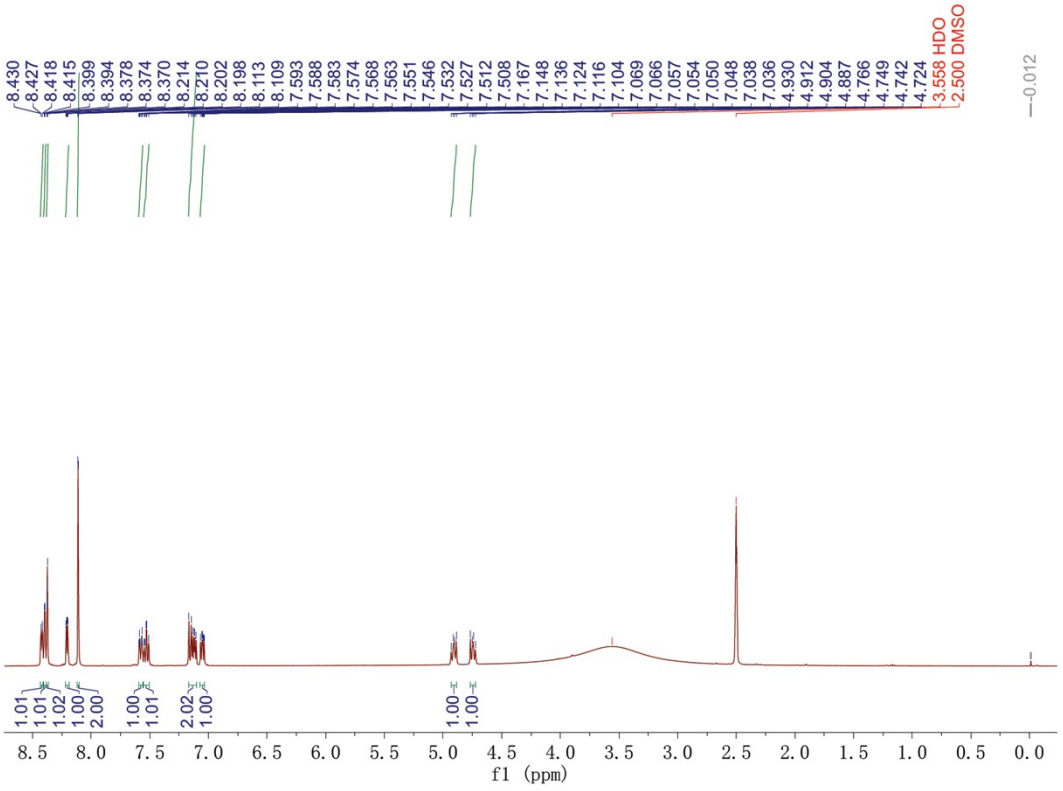


Fig. S4. The ^{1}H NMR spectra of **1** (a) and **1a** (b).

(a)


8.430
8.426
8.417
8.413
8.398
8.392
8.377
8.373
8.370
8.212
8.209
8.200
8.197
8.112
8.108
7.592
7.587
7.582
7.572
7.567
7.562
7.550
7.545
7.530
7.526
7.511
7.507
7.166
7.146
7.134
7.122
7.115
7.103
7.066
7.054
7.049
7.037
7.035
4.929
4.911
4.903
4.886
4.765
4.748
4.741
4.723
3.568 HDO
2.500 DMSO
-0.013
1.01
1.00
1.01
1.00
2.00
1.01
1.00
2.02
1.01
1.00
1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

(b)


8.430
8.427
8.418
8.415
8.399
8.394
8.378
8.374
8.370
8.214
8.210
8.202
8.198
8.113
8.109
7.593
7.588
7.583
7.574
7.568
7.563
7.551
7.546
7.532
7.527
7.512
7.508
7.167
7.148
7.136
7.124
7.116
7.104
7.069
7.066
7.057
7.054
7.050
7.048
7.038
7.036
4.930
4.912
4.904
4.887
4.766
4.749
4.742
4.724
3.558 HDO
2.500 DMSO
-0.012
1.01
1.01
1.02
1.00
2.00
1.00
1.01
2.02
1.00
1.00
1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

(c)

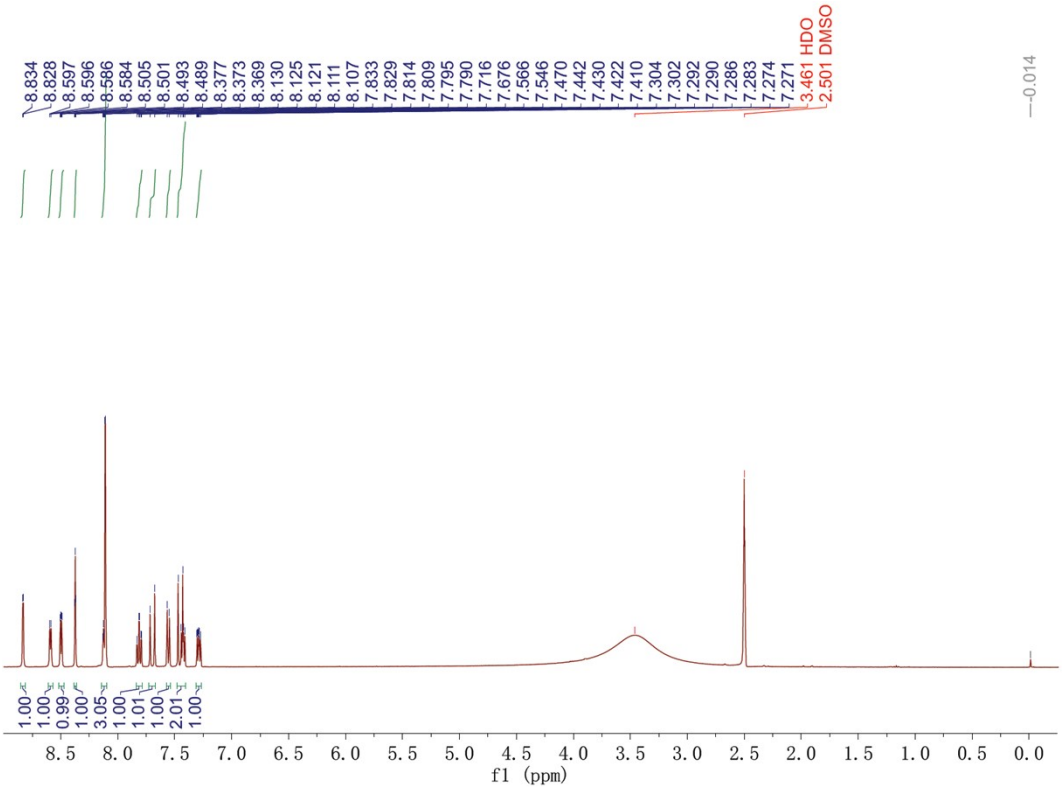


Fig. S5. (a) The ^{1}H NMR spectrum of the sample of **1** upon irradiation of 365 nm UV light in 5min. (b) The ^{1}H NMR spectrum of the sample of **1** upon irradiation of 320 nm UV light in 3 min. (c) The ^{1}H NMR spectrum of the sample of **1** upon irradiation of 254 nm UV light in 5min.

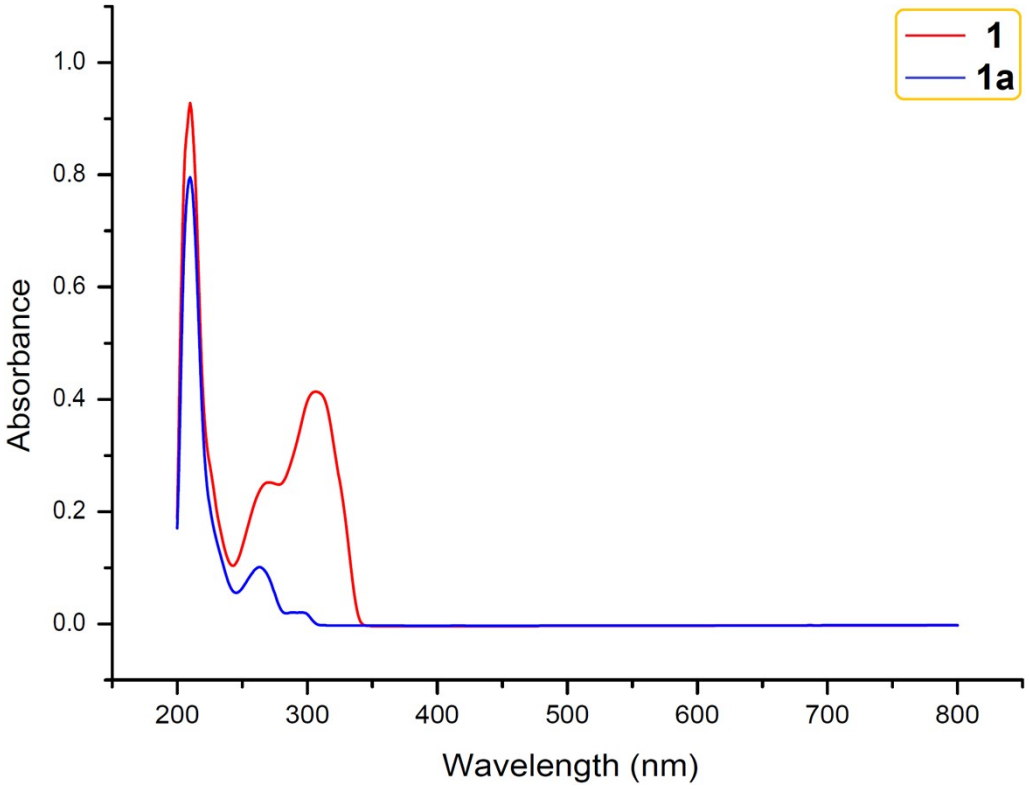


Fig. S6. The UV-vis absorption spectra of **1** and **1a** in ethanol.

(a) (b)

Fig. S7. Optical micrographs of single crystals of **1** before (a) and after (b) photoreaction.

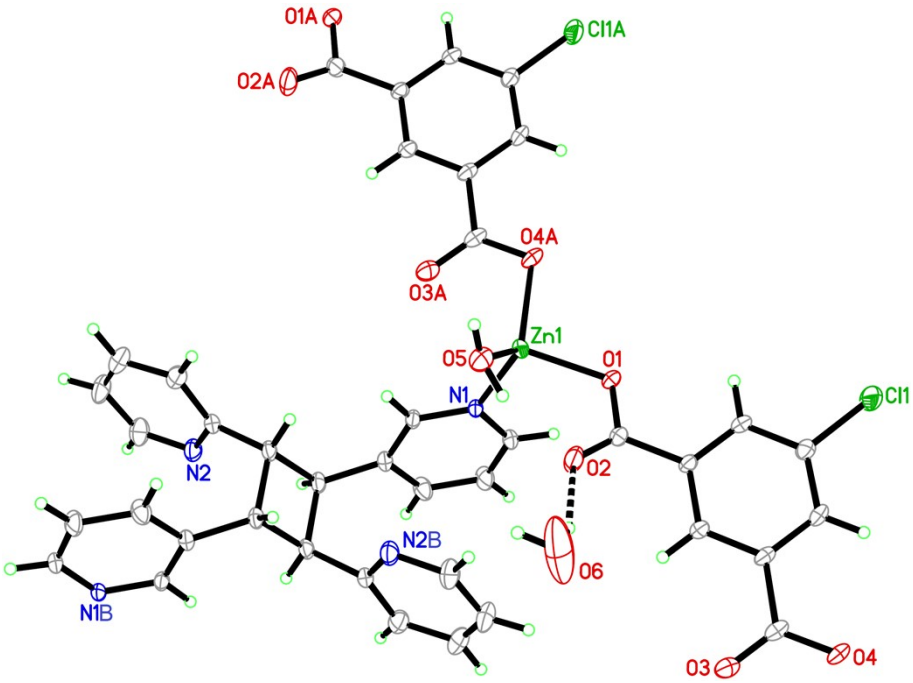


Fig. S8. View of the coordination environment of Zn1 in **1a** with labeling scheme. Symmetry codes: (A) *x*, *y* - 1, *z*.

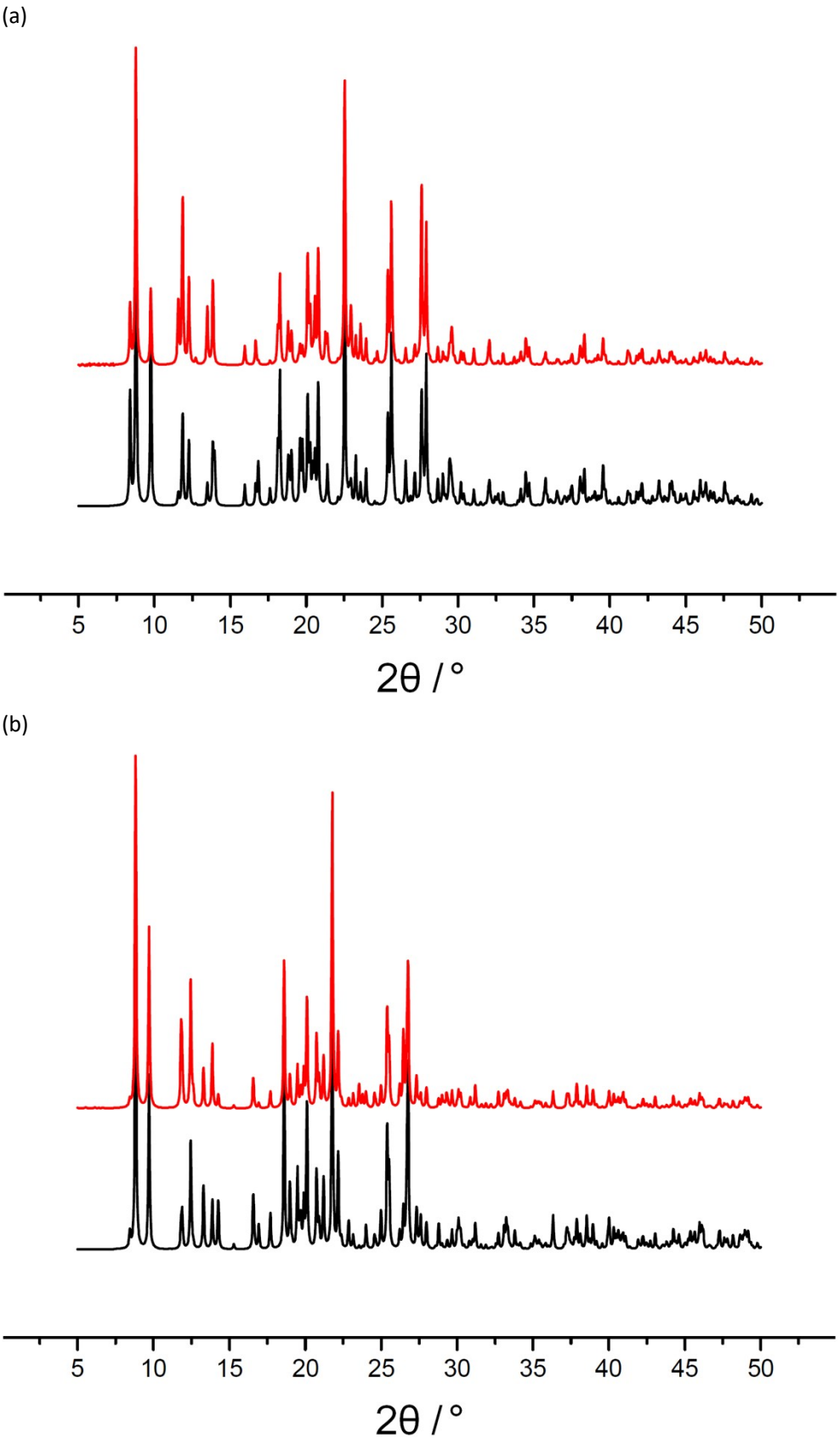


Fig. S9. PXRD patterns of **1** (a) and **1a** (b). Simulated patterns from single crystal: black; experimental patterns from grinding crystals: red.

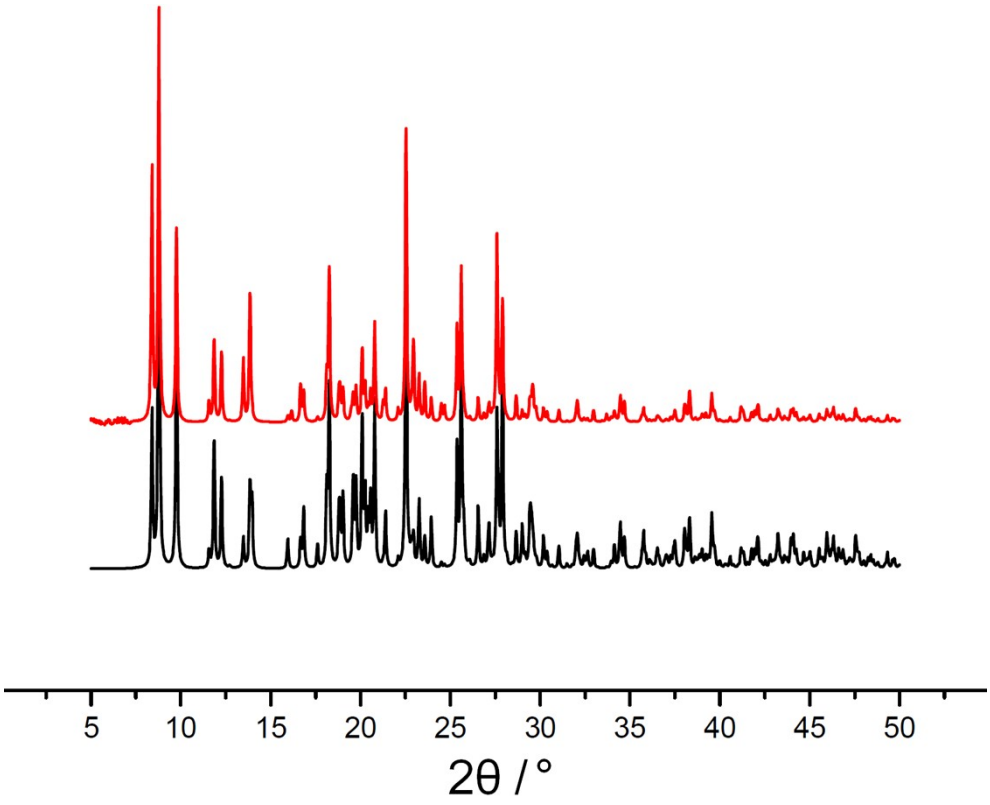


Fig. S10. PXRD pattern of regenerated **1** (simulated pattern from single crystal: black; experimental pattern from grinding crystals: red).

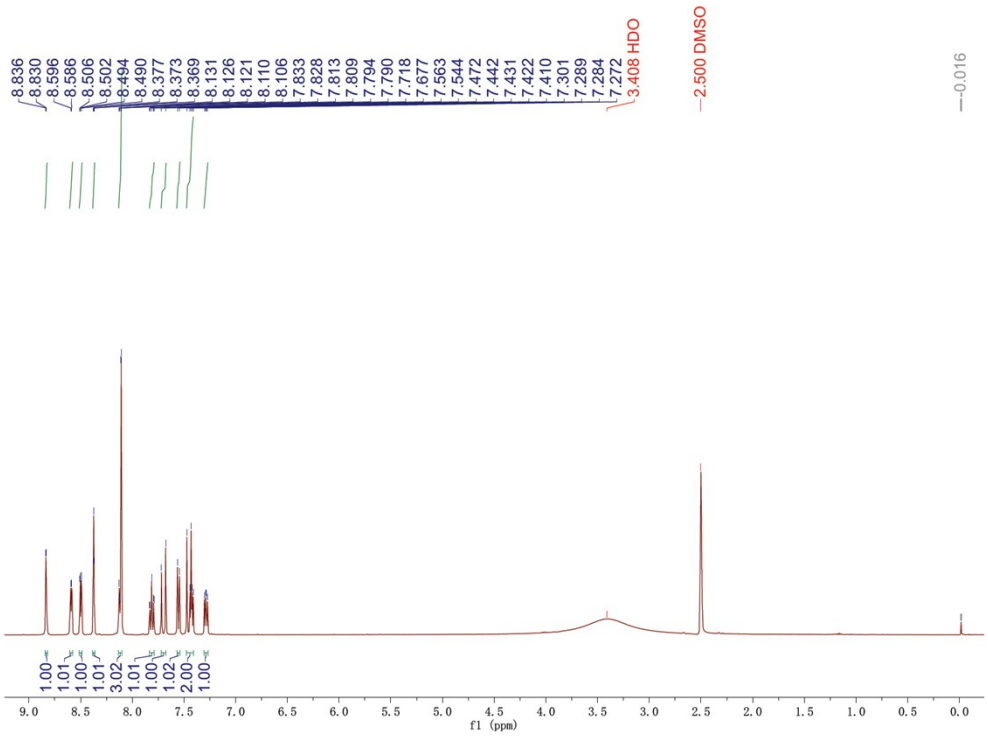


Fig. S11. The ^{1}H NMR spectrum of regenerated **1**.

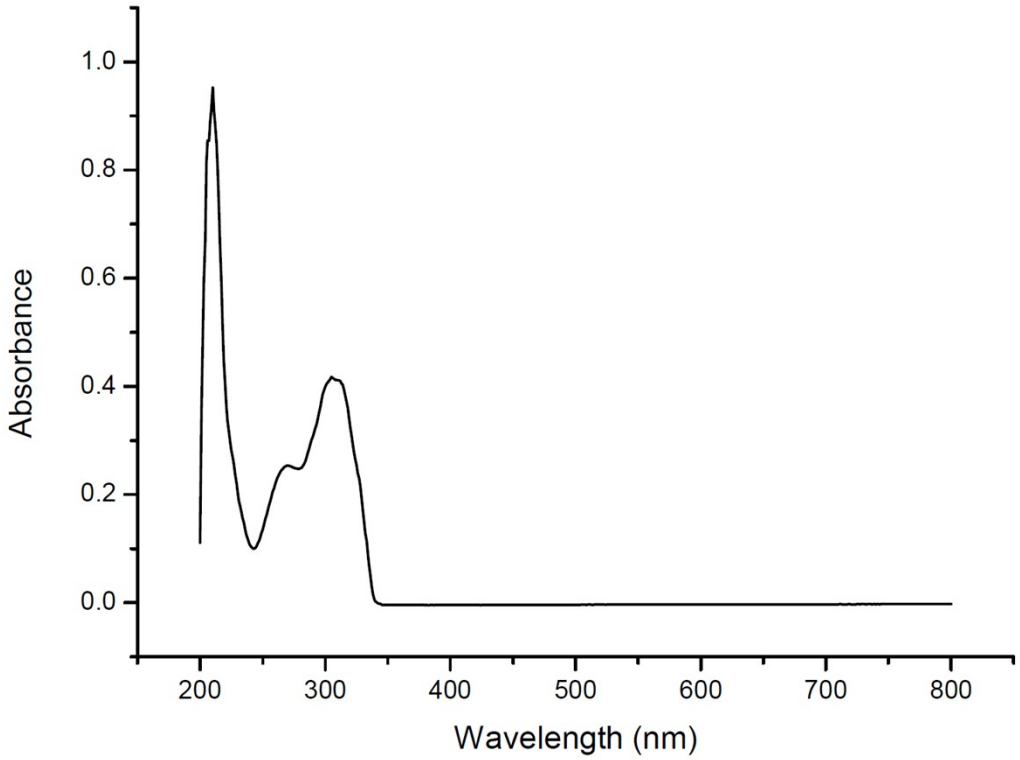


Fig. S12. The UV-vis absorption spectrum of regenerated **1** in ethanol.

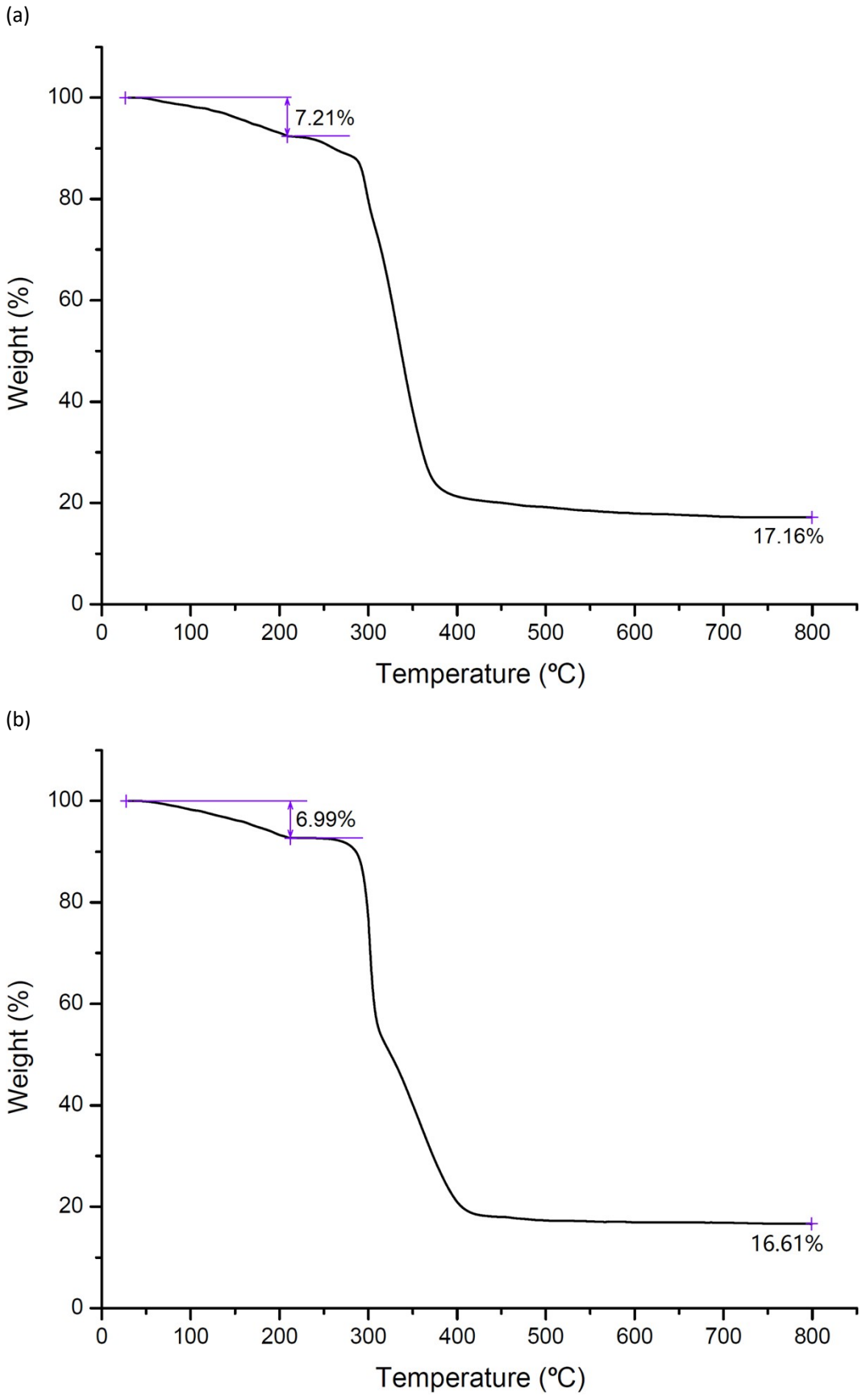
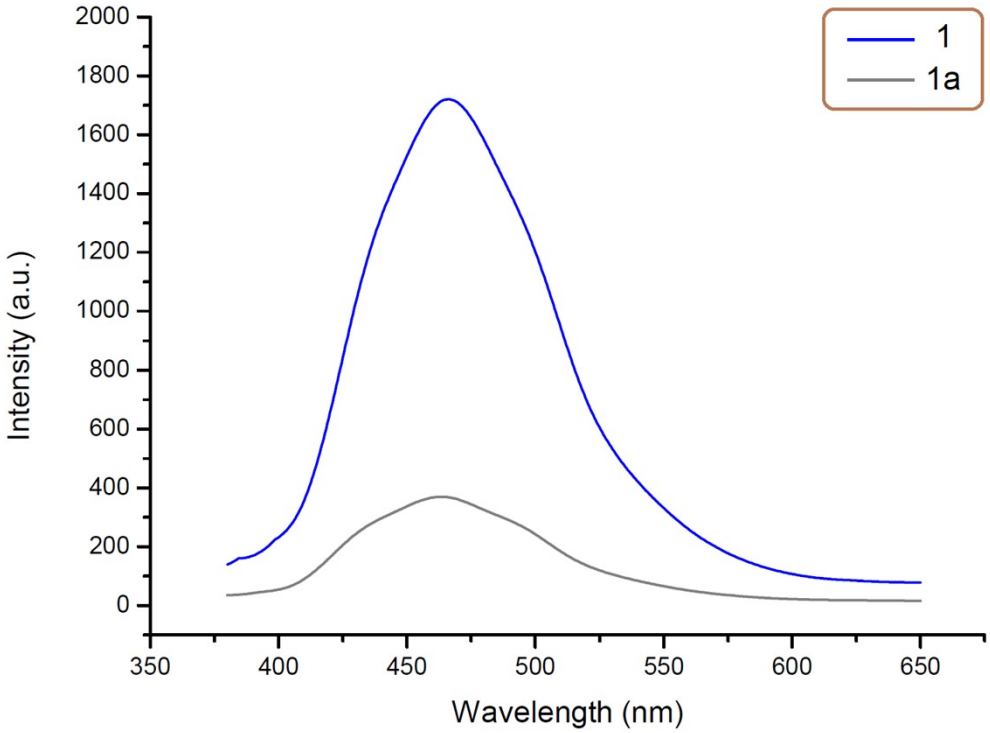


Fig. S13. The TGA curves for **1** (a) and **1a** (b).

(a)



(b)

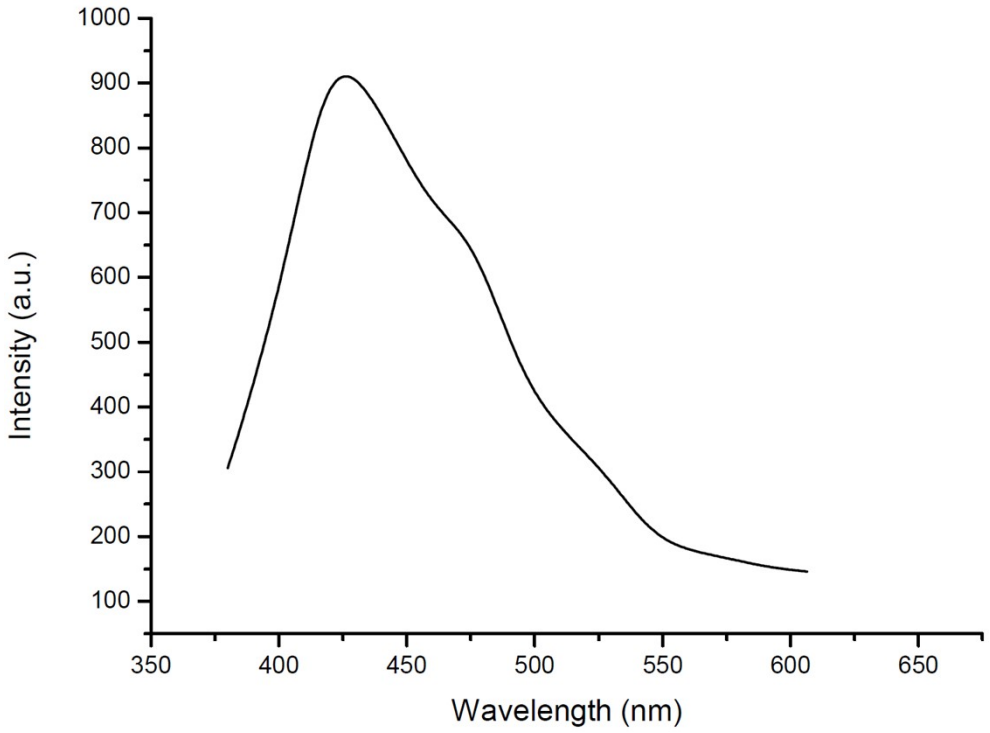


Fig. S14. (a) Solid state emission spectra of **1** and **1a** at room temperature. (b) Solid state emission spectrum of 2,3-ppe ligand at room temperature.

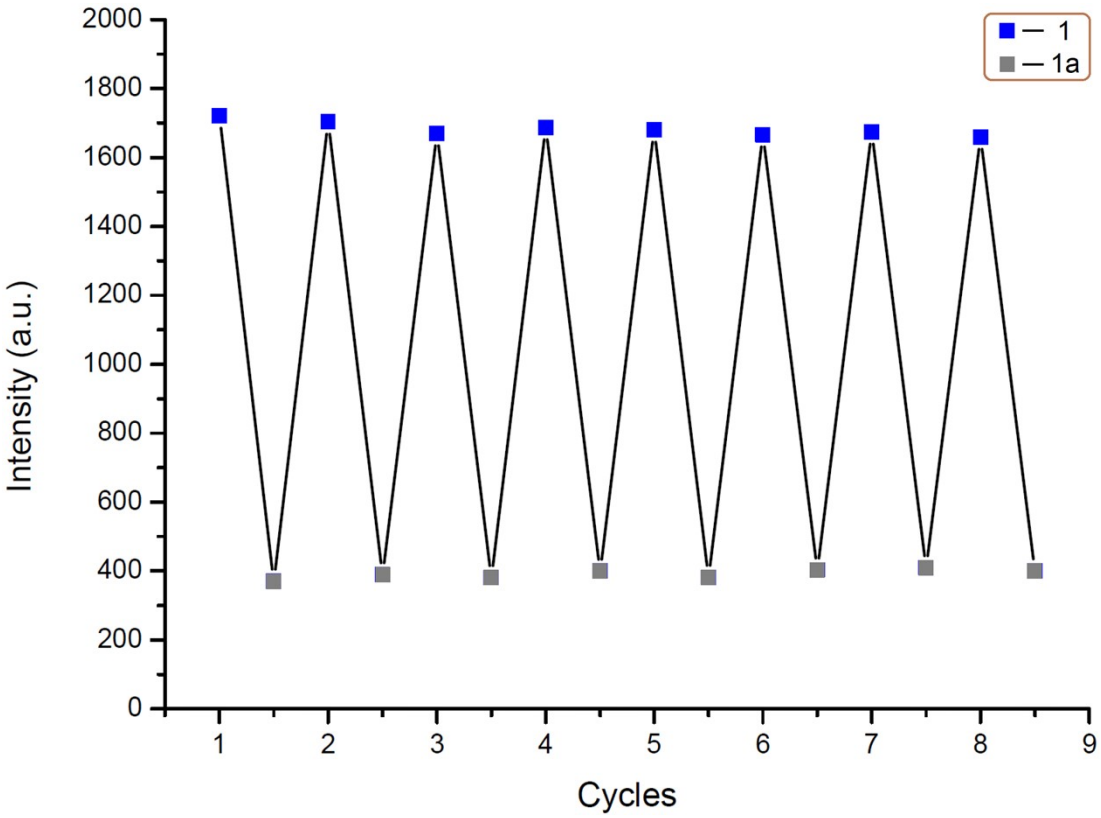


Fig. S15. The reaction reversibility for solid state emission spectra of **1**.

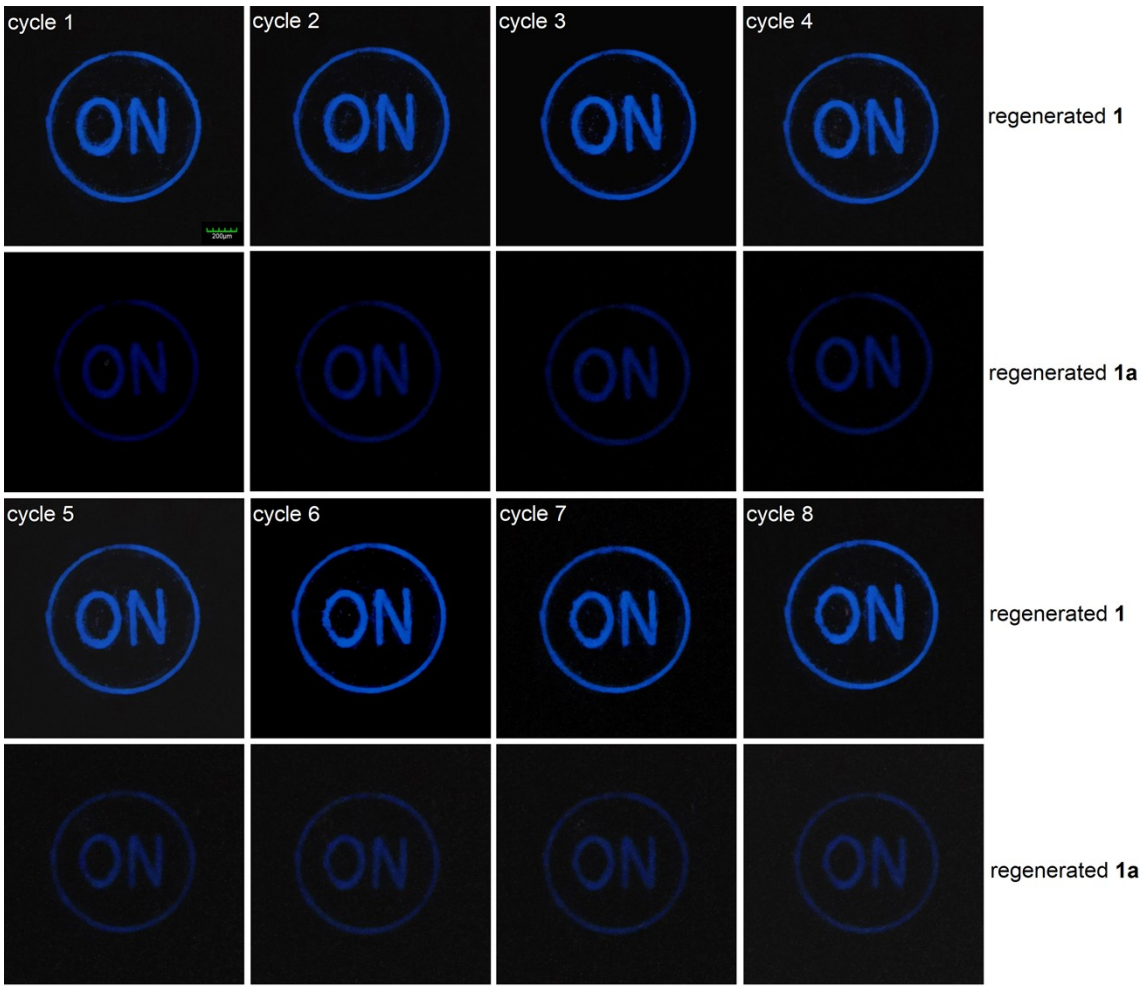


Fig. S16. LSCM fluorescence images of a carved pattern with powdered sample of regenerated **1** and **1a** during 8 cycles of reversible photoreaction. All samples were excited at 405 nm with a semiconductor laser.