

## Supplementary Information

### Viologen-Based Ln-MOFs Material with Photochromic and Photoluminescence for Anticounterfeiting

Wen-Bo Cui, Li Huang, Yuan Shen, Xiao-Yang Yu, Zi-Yi Li and Hong Zhang\*

Key Laboratory of Polyoxometalate Science of Ministry of Education, Department of  
Chemistry, Northeast Normal University, Changchun, Jilin 130024, P.R. China

\*Corresponding author.

E-mail address: [zhangh@nenu.edu.cn](mailto:zhangh@nenu.edu.cn); [hope20130122@163.com](mailto:hope20130122@163.com)

Table S1 Crystallographic data for **1** and **2**

Empirical formula	C <sub>40</sub> H <sub>28</sub> ClEu <sub>2</sub> N <sub>4</sub> O <sub>23</sub>	C <sub>40</sub> H <sub>30</sub> ClN <sub>4</sub> O <sub>24</sub> Tb <sub>2</sub>
Formula weight	1272.03	1303.97
Temperature/K	298.15	298.15
Crystal system	monoclinic	monoclinic
Space group	<i>C2/c</i>	<i>C2/c</i>
<i>a</i> /Å	36.492(3)	36.461(3)
<i>b</i> /Å	12.6245(10)	12.5228(9)
<i>c</i> /Å	20.7562(16)	20.6904(14)
$\alpha$ /°	90	90
$\beta$ /°	101.443(3)	101.468(3)
$\gamma$ /°	90	90
Volume/Å <sup>3</sup>	9372.2(12)	9258.5(12)
<i>Z</i>	8	8
$\rho_{\text{calc}}$ /cm <sup>3</sup>	1.803	1.871
$\mu$ /mm <sup>-1</sup>	2.798	3.181
F(000)	4984	5096
Radiation	Mo- <i>K</i> $\alpha$ ( $\lambda$ = 0.71073)	Mo- <i>K</i> $\alpha$ ( $\lambda$ = 0.71073)
2 $\theta$ range for data collection/°	4.836 to 50.128	4.72 to 50.228
Reflections collected	47815	39508
Independent reflections	8256 [R <sub>int</sub> = 0.0476, R <sub>sigma</sub> = 0.0307]	8184 [R <sub>int</sub> = 0.1685, R <sub>sigma</sub> = 0.0978]
Data/restraints/parameters	8256/240/632	8184/0/649
Goodness-of-fit on F <sup>2</sup>	1.073	1.048
Final R indexes [I >= 2 $\sigma$ (I)]	R <sub>1</sub> = 0.0449 wR <sub>2</sub> = 0.1295	R <sub>1</sub> = 0.0584 wR <sub>2</sub> = 0.1490
Final R indexes [all data]	R <sub>1</sub> = 0.0529 wR <sub>2</sub> = 0.1353	R <sub>1</sub> = 0.0795 wR <sub>2</sub> = 0.1613

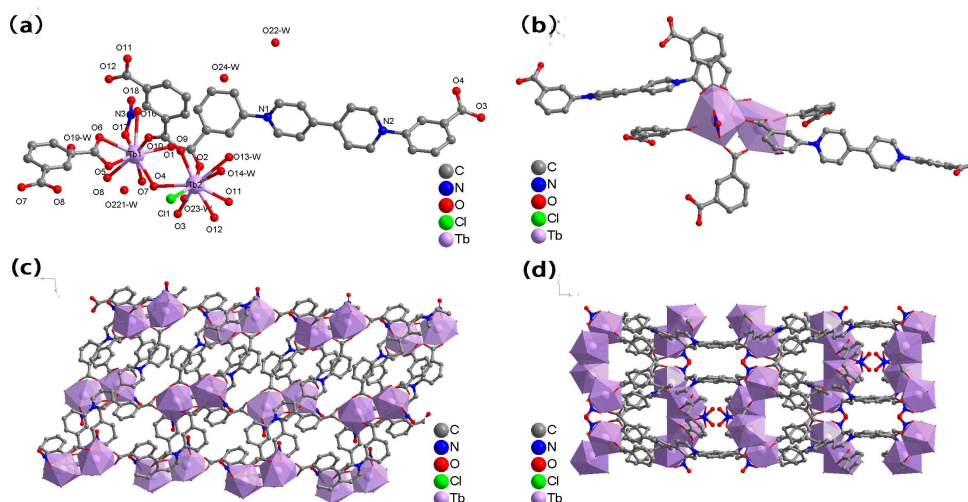


Figure S1. (a) Metal coordination environments of compound 2. (b) Metal coordination environments of compound 2. (c-d) 3D network stacking structure of 2 in the *b,c* direction.

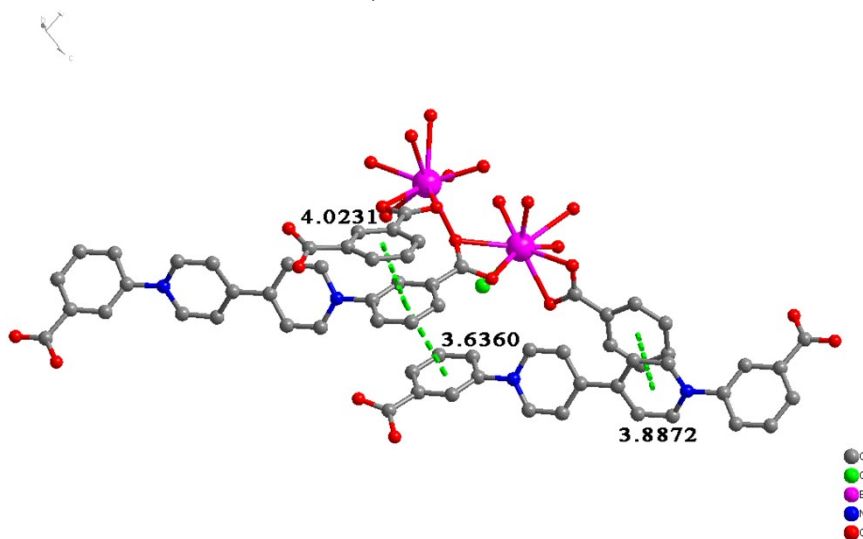


Figure S2. Structures of compound 1 by  $\pi \cdots \pi$  interactions.

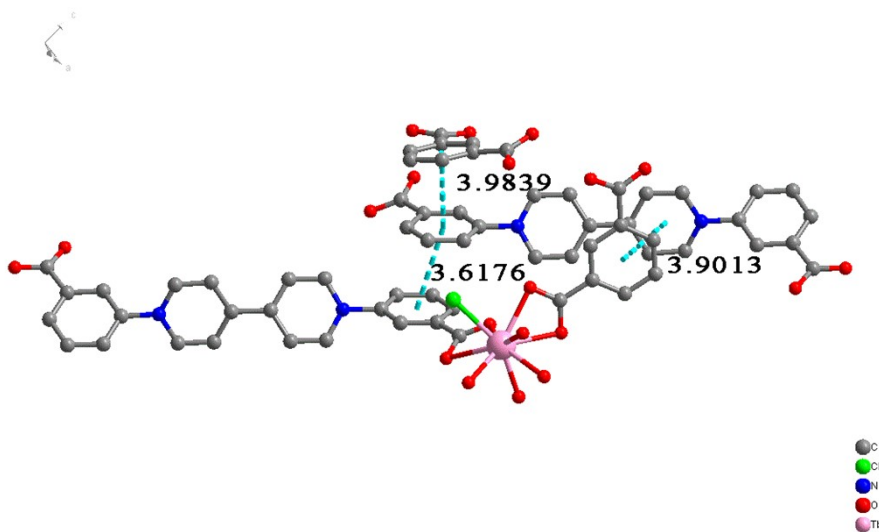


Figure S3. Structures of compound 2 by  $\pi \cdots \pi$  interactions.

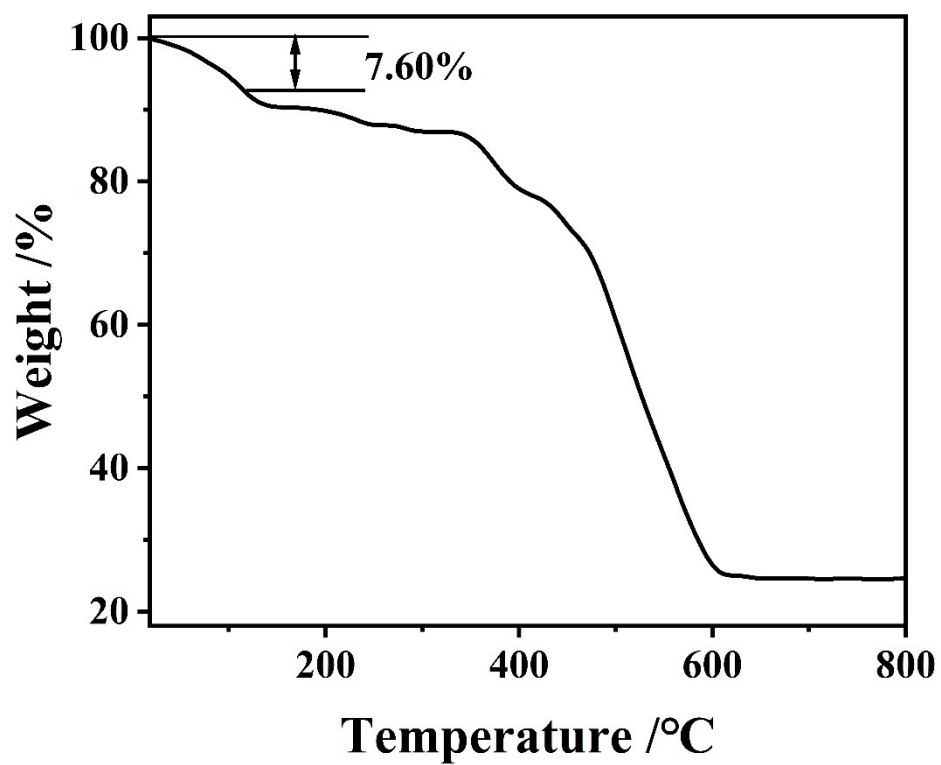


Figure S4. The TG plot for 1.

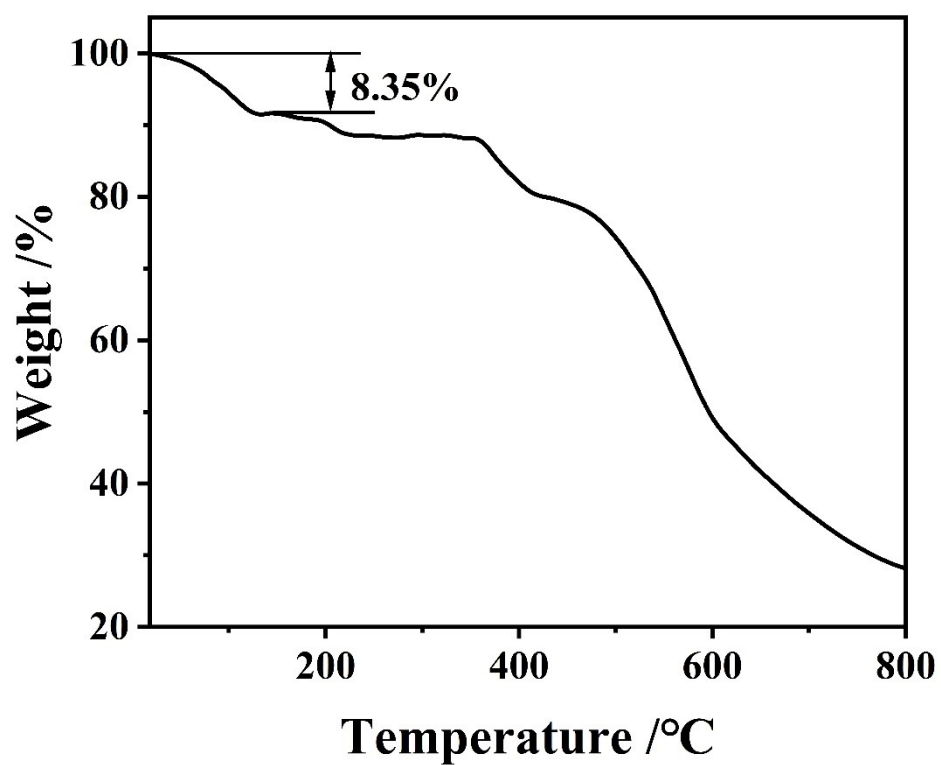


Figure S5. The TG plot for 2.

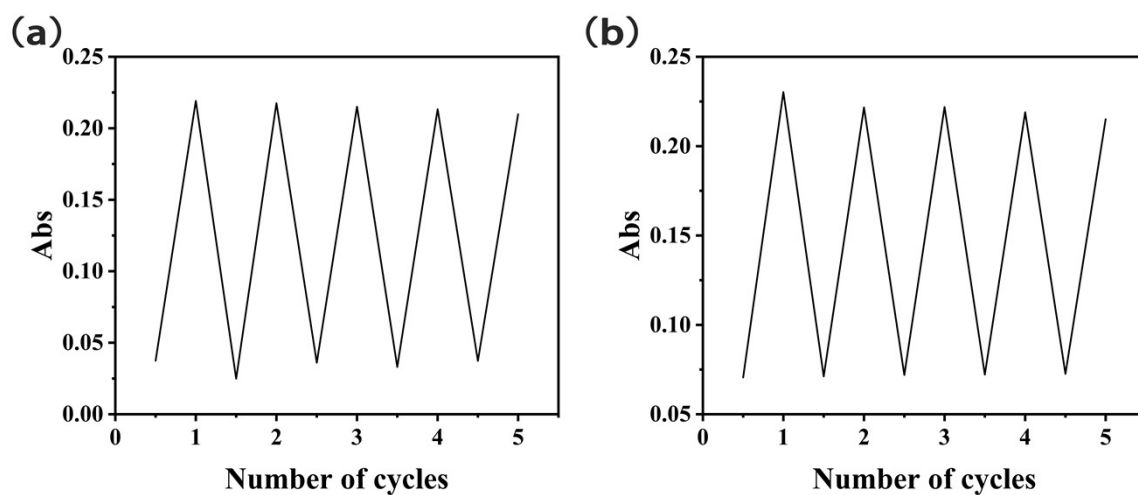


Figure S6. Stability of compounds 1 and 2

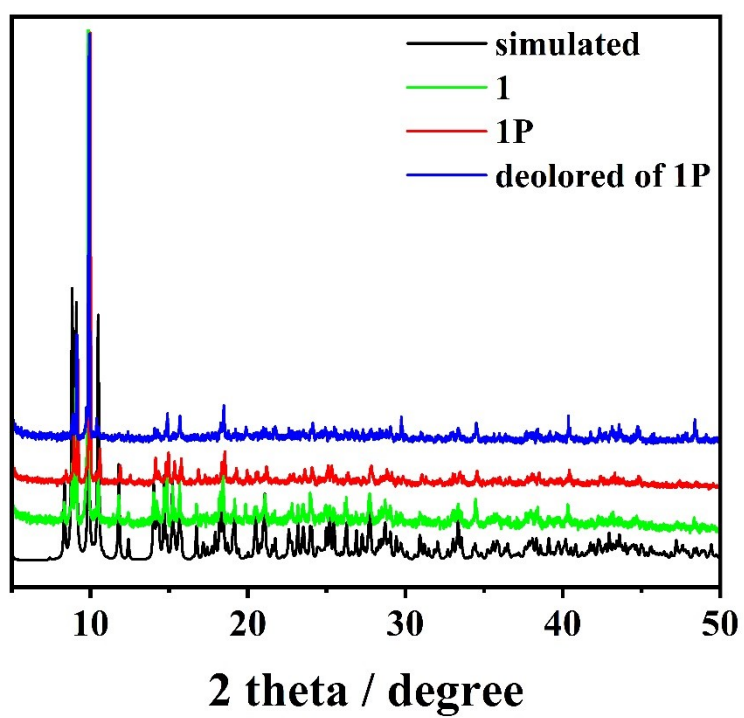


Figure S7. PXRD of simulated, 1, 1P, decolored of 1P.

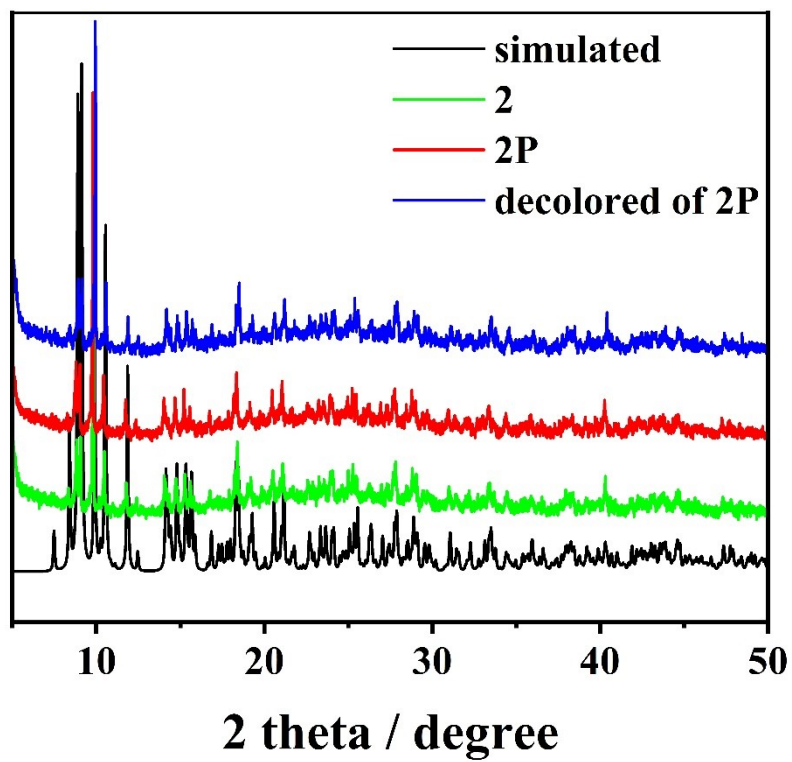


Figure S8. PXRD of simulated, 2, 2P, decolored of 2P.

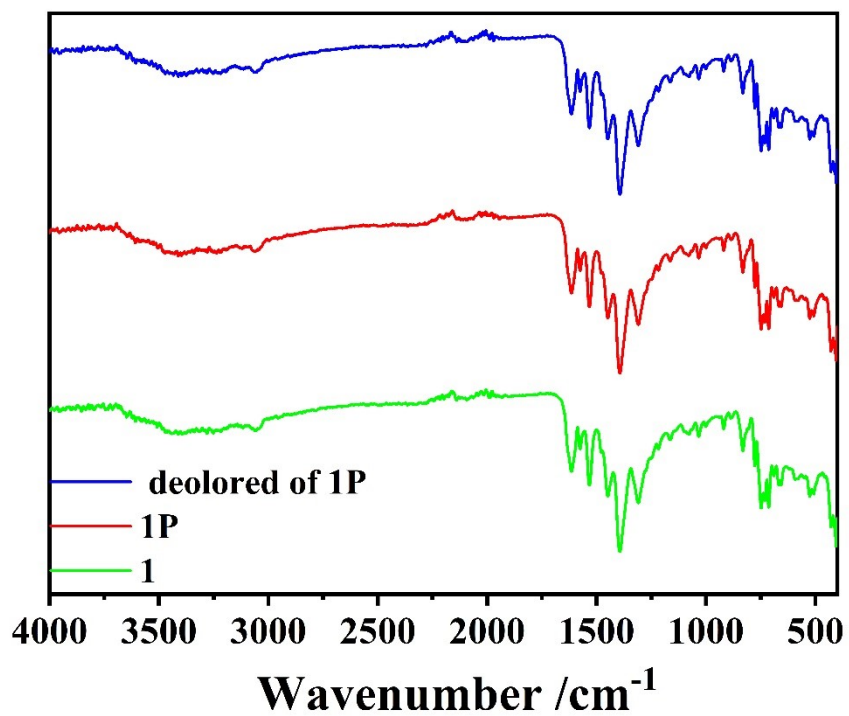


Figure S9. FT-IR spectra of 1, 1P, decolored of 1P.

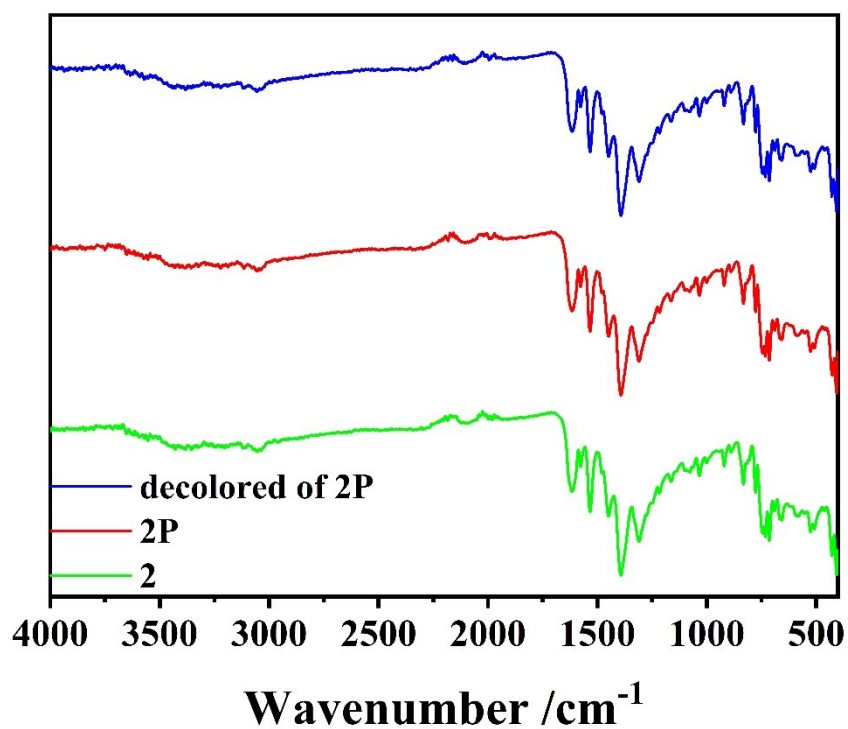


Figure S10. FT-IR spectra of 2, 2P, decolored of 2P.

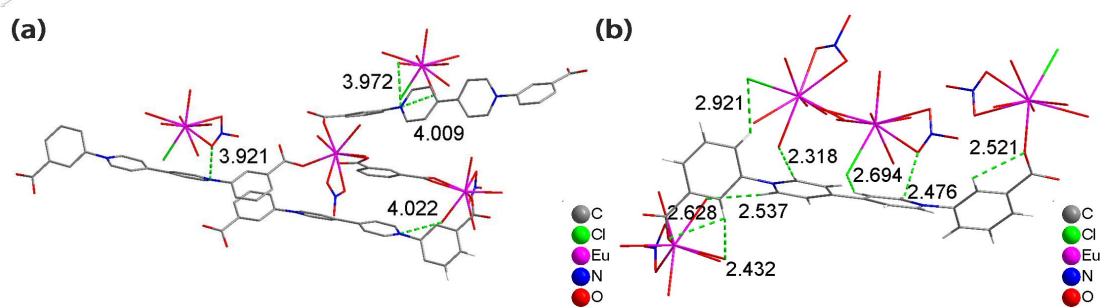


Figure S11. Electron transfer path of compound 1 : (a) N-O; (b)  $\alpha/\beta$  C-H...O/Cl.

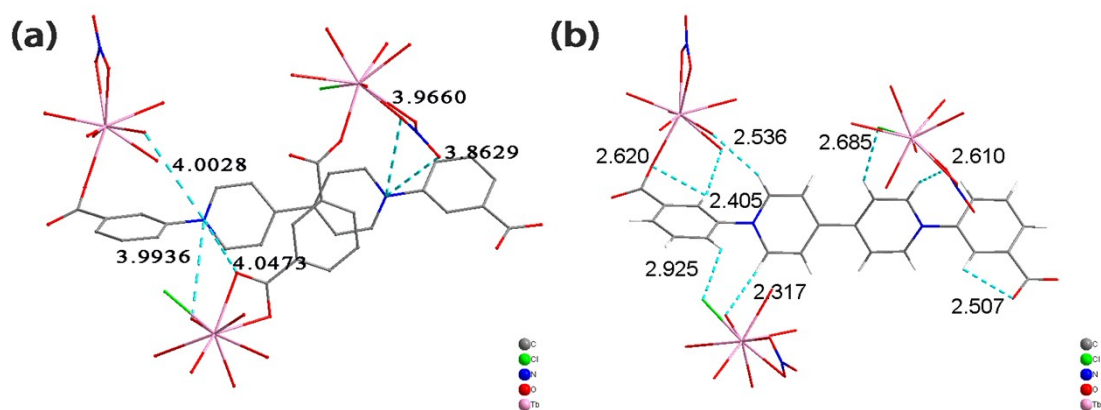


Figure S12. Electron transfer path of compound 2 : (a) N-O; (b)  $\alpha/\beta$  C-H...O/Cl.

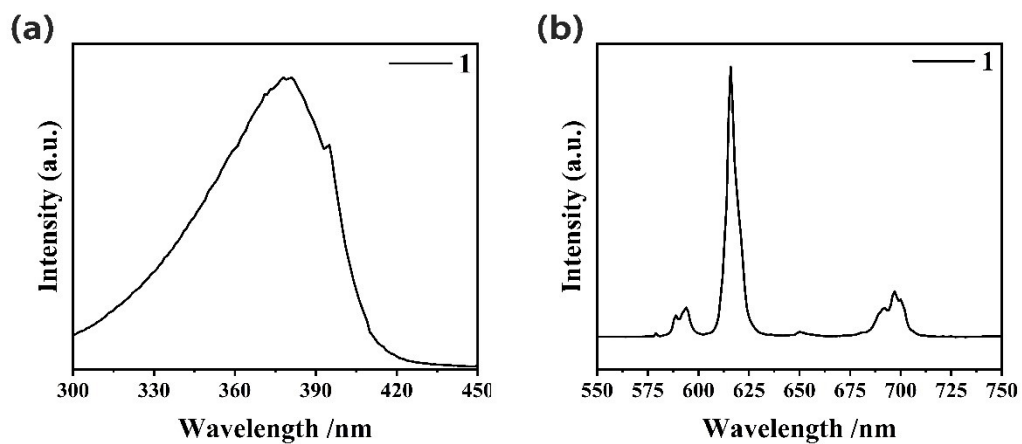


Figure S13. The solid-state excitation spectra (a) and emission spectra (b) of **1** at room temperature ( $\lambda_{\text{ex}} = 380$  nm)

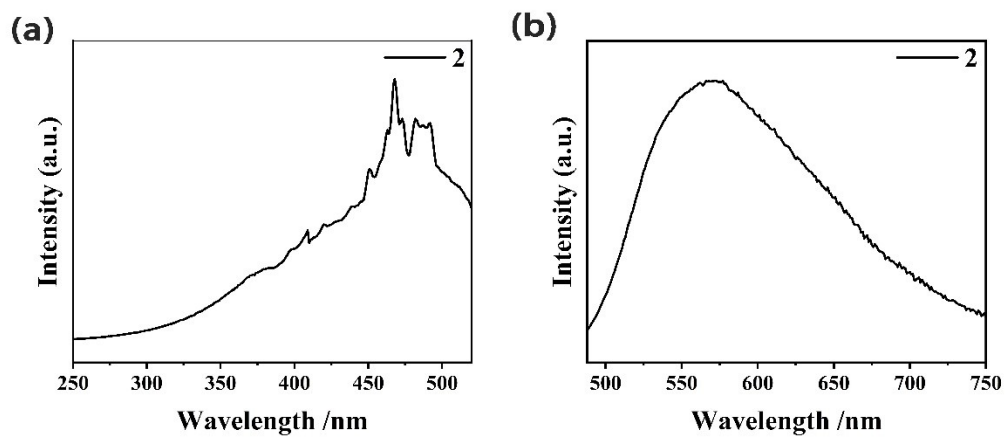


Figure S14. The solid-state excitation spectra (a) and emission spectra (b) of **2** at room temperature ( $\lambda_{\text{ex}} = 468$  nm)

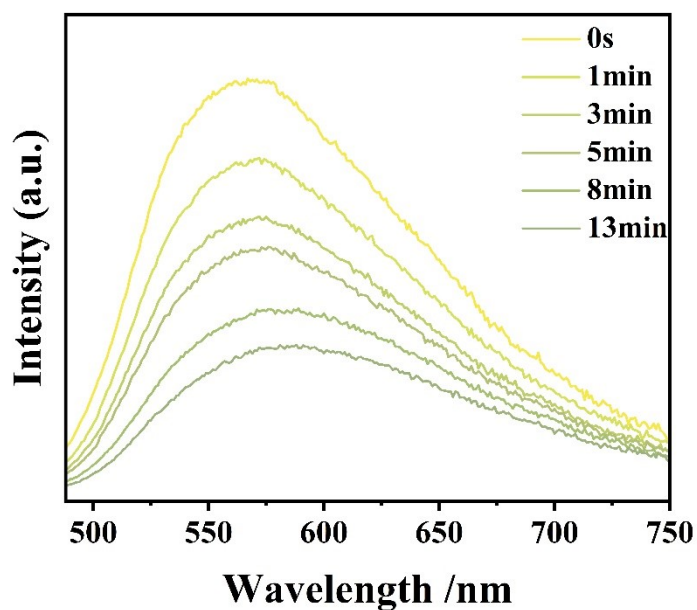


Figure S15. Photomodulated fluorescence spectra of **2**.