Supplementary Information

Viologen-Derived Material Showing Photochromic, Visually Oxygen Responsive and Photomodulated Luminescent Behaviors

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Section 1. Additional Data and Figures

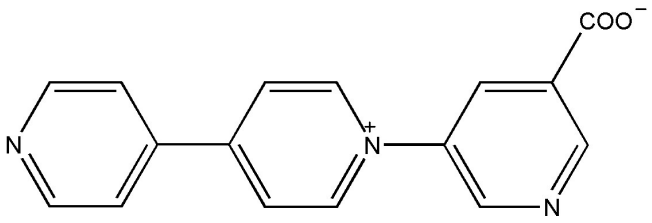
Table S1 Crystal data and structure refinements for **1**.

Compounds	**1**
Formula	$C_{22}H_{19}N_3O_9SZn$
M_r	610.80
Crystal system	Monoclinic
Space group	$P2_1/c$
a (Å)	7.6890(10)
b (Å)	19.055(3)
c (Å)	16.139(2)
a	90
β (°)	92.027(4)
γ	90
V (Å^3)	2363.0(6)
Z	4
ρ(g cm^{-3})	1.582
μ (mm^{-1})	1.186
F(000)	1144
GOF(F^2)	1.034
$R_1{}^a$ [I>2σ(I)]	0.0388
$wR_2{}^b$[I>2σ(I)]	0.0873

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

Compound **1**[a]					
Zn(1)−O(1)	1.941(2)	Zn(1)−O(4)#1	1.928(2)	Zn(1)−O(5)#2	2.375(3)
Zn(1)−O(6)#2	2.091(3)	Zn(1)−N(1)	2.111(2)		
O(5)#2− Zn(1)−N(1)	147.78(9)	N(1)−Zn(1)−O(1)	103.72(9)	O(1)−Zn(1)−O(5)#2	91.64(9)
O(1)−Zn(1)−O(6)#2	122.63(11)	O(4)#1−Zn(1)−N(1)	94.11(9)	O(4)#1−Zn(1)−O(1)	123.97(9)
O(4)#1−Zn(1)−O(5) #2	100.55(11)	O(4)#1−Zn(1)−O(6)#2	109.61(11)	O(6)#2−Zn(1)−N(1)	90.43(10)
O(6)#2−Zn(1)−O(5) #2	57.67(10)				

[a]Symmetry codes: #1 +X,1/2-Y,-1/2+Z; #2 -1+X,+Y,+Z.



Scheme 1s. Molecular structure of the N-(3-carboxypyridin-5-yl)-4,4'–bipyridinium.

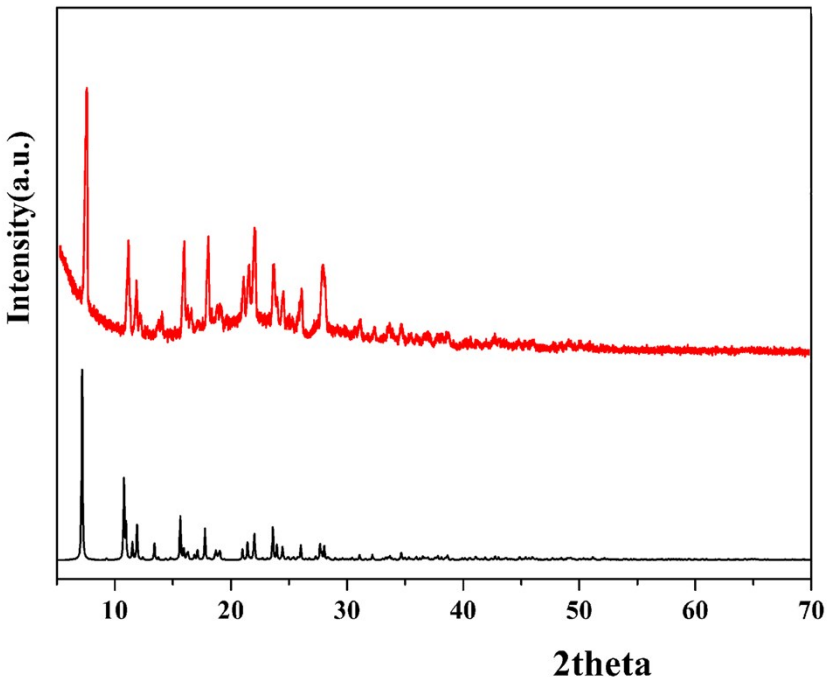


Fig.S1 PXRD patterns for **1**.

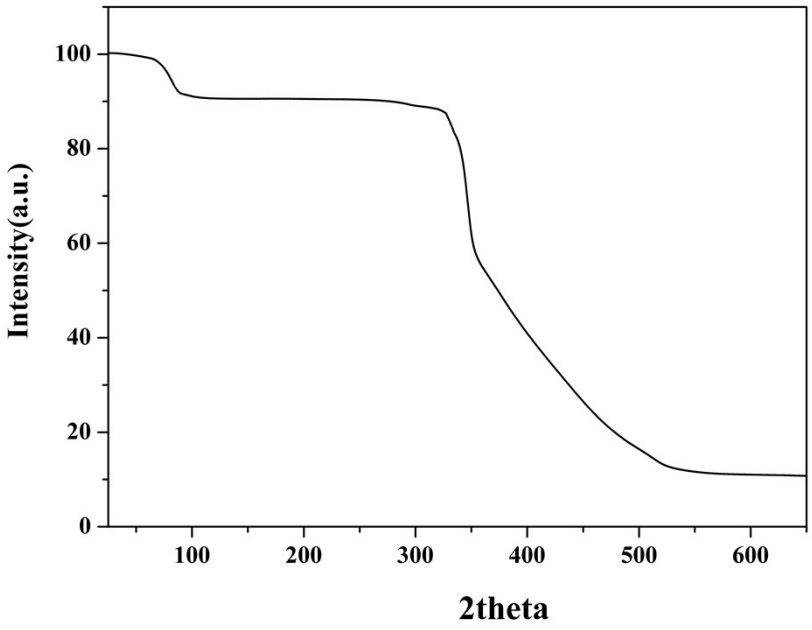


Fig.S2 TGA curve for **1**.

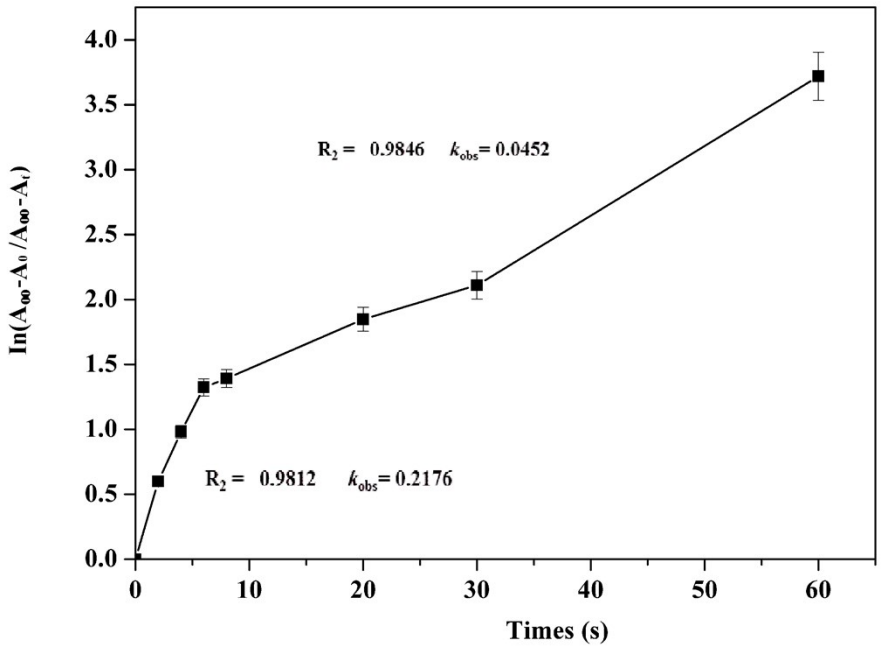


Fig.S3 Solid state kinetic trace of **1**, light coloration based on UV absorption at 653 nm.

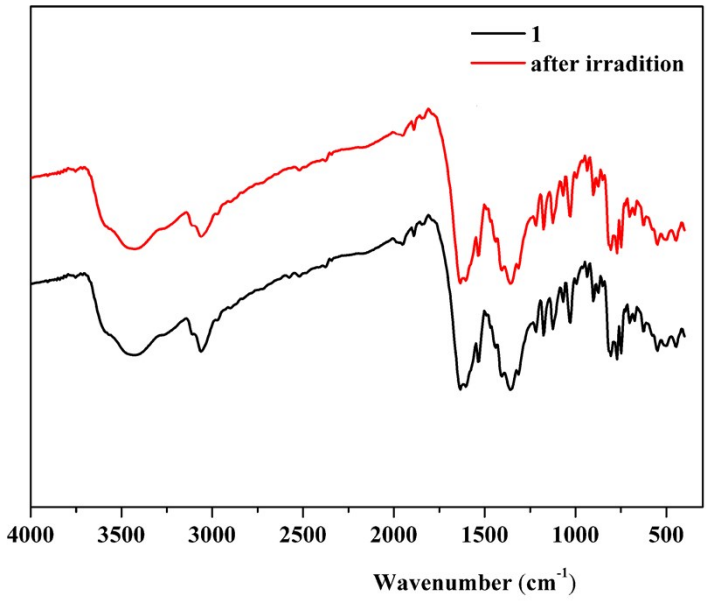


Fig.S4. The IR spectrum of compound **1** and **1** after irradiation.

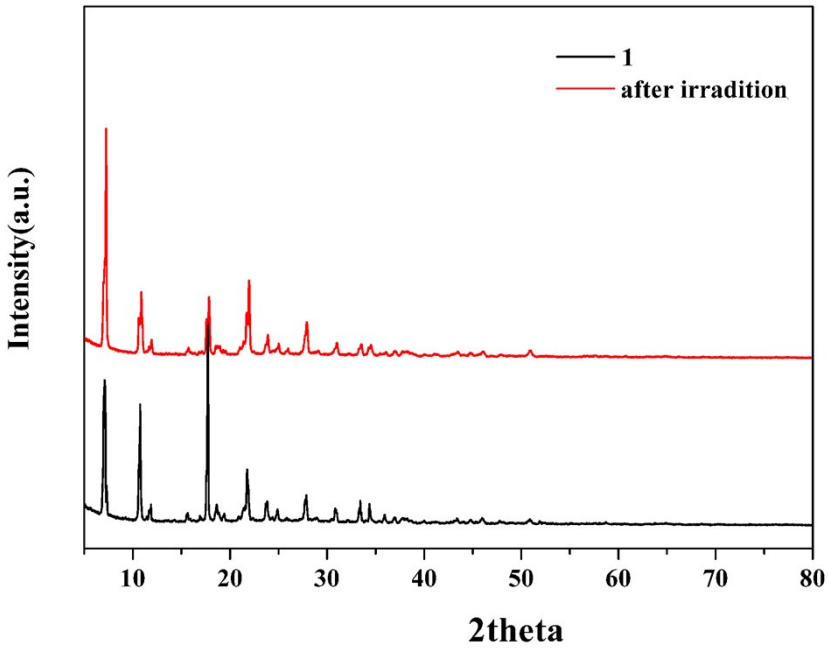


Fig. S5. PXRD patterns of compound **1** and **1** after irradiation.

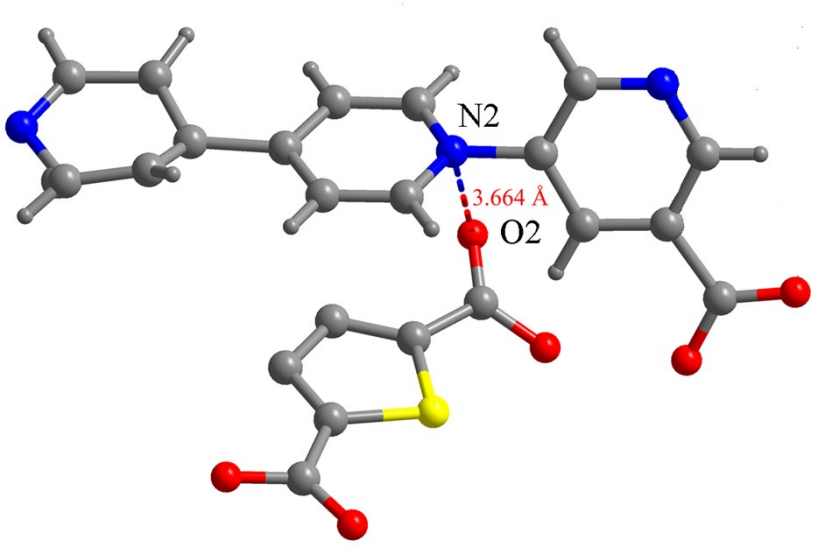


Fig. S6 detail of the structure of compound **1** showing short contacts involving the bipyridinium unit.

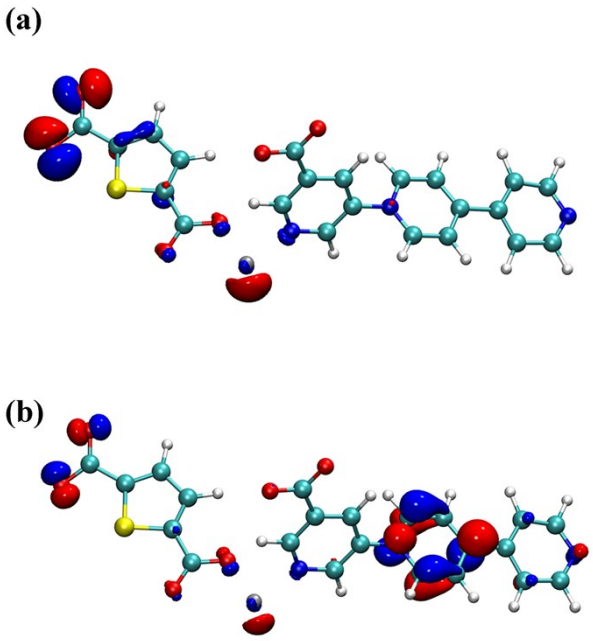


Fig. S7 The HOMO and LUMO sets for **1** possibly involving photoinduced electron transfer from the carboxy group to the pyridinum cation.

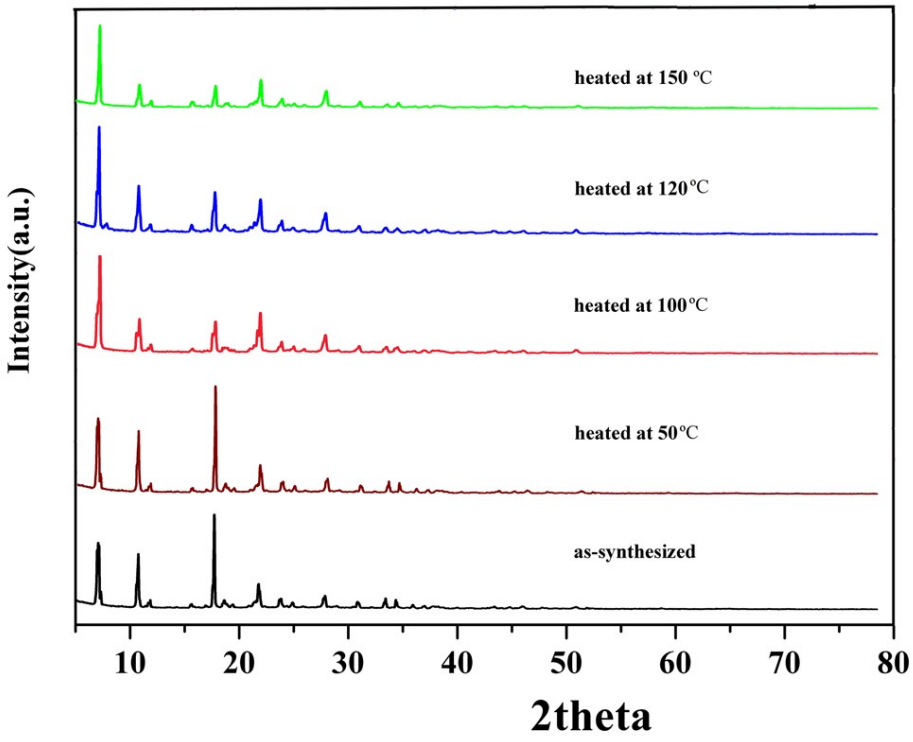


Fig. S8 PXRD patterns of compound **1** heated at different temperature.

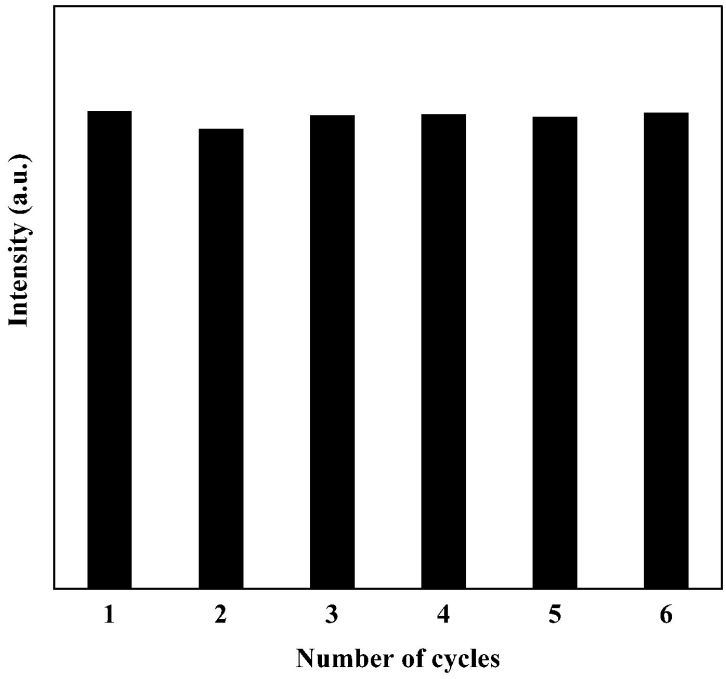


Fig. S9 Six cycle tests of the luminescence intensity of compound **1** in the repeated photochromism/decoloration processes.

Section 2. Kinetic rate calculations

After irradiation for 2 s, 4 s, 6 s ,8 s, 20 s, 40 s, 80 s, 120 s, UV-Vis diffuse reflectance and photoluminescence spectra were recorded and the calculations of kinetics of photoreaction kinetic rates were based on the intensity values of the wavelength at 653 nm,. The kinetic rate constants are determined by the following equation is used for data treatment [S1]: ′

$$ln\frac{A_\infty - A_0}{A_\infty - A_t} = kt$$

where k is the first-order rate constant and A_0, A_t, A_∞ refer to the observed absorption data at 653 nm at the beginning, versus time, and at the end of the reaction, respectively.

[S1] J. Sworakowski, K. Janus, S. Nešpůrek. *Adv. Colloid Interface Sci.* **2005**, 116, 97.