

Supporting Information

Interpenetration-Enabled Photochromism and Fluorescence Photomodulation in a Metal-Organic Framework with the Thiazolothiazole Extended Viologen Fluorophore

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Physical Measurements. Fourier transform infrared (FT-IR) spectra were measured with KBr pellets using a Nicolet NEXUS 670 spectrophotometer. NMR spectroscopy was carried out with a Bruker Advance 400 MHz spectrometer. Carbon, hydrogen, and nitrogen (C H and N) analysis was performed on an Elementar Vario ELIII analyzer. Powder X-ray diffraction (PXRD) patterns were obtained at a scan speed of 10 °C/min using a Rigaku Ultima IV X-ray diffractometer (Cu-K α radiation, $\lambda = 1.54056 \text{ \AA}$). UV-vis spectra were determined on a SHIMADZU UV-2700 spectrometer using finely ground samples coated on BaSO₄ plates. Room-temperature X-band electron spin resonance (ESR) spectroscopy was performed using a Bruker Elexsys 580 spectrometer with a 100 kHz magnetic field.

Crystal structure determination. Data collection for **1** was performed at 293 K using a Bruker APEX-II Diffraction diffractometer (Cu-K α radiation, $\lambda = 1.54184 \text{ \AA}$) equipped with a graphite monochromator and a CCD area detector. Structure solution was carried out using the direct method, and full-matrix least-squares refinements were performed on F^2 with the SHELX-2014 program. Non-hydrogen atoms were all refined anisotropically. The H atoms attached to carbons were added geometrically and refined isotropically with the riding model. The H atoms of water molecules were assigned from the difference maps and refined isotropically.

Photochromic experiments. Photochromic tests were carried out using a 300W xenon lamp system (CEL-HXUV300, Ceaulight, China) equipped with an IR filter, and the samples was placed at 22 cm from the lamp. The solid-state UV-vis diffusive reflectance and fluorescence spectra were recorded using the same sample after irradiation for the given time.

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

1	
Empirical formula	C ₃₂ H ₂₄ N ₄ O ₁₃ S ₂ Cl ₂ Cd ₂
Formula weight	1036.40
Crystal system	monoclinic
Space group	<i>P2₁/c</i>
<i>a</i> , Å	12.979(3)
<i>b</i> , Å	17.0407(19)
<i>c</i> , Å	17.367(2)
β , deg	110.474(14)
<i>V</i> , Å ³	3598.6(10)
<i>Z</i>	4
ρ calcd, g cm ⁻³	1.913
μ , mm ⁻¹	12.823
θ range collected	3.64 to 68.36
<i>S</i> on <i>F</i> ²	1.121
R ₁ [<i>I</i> > 2 σ (<i>I</i>)]	0.0485
wR ₂ (all data)	0.1456

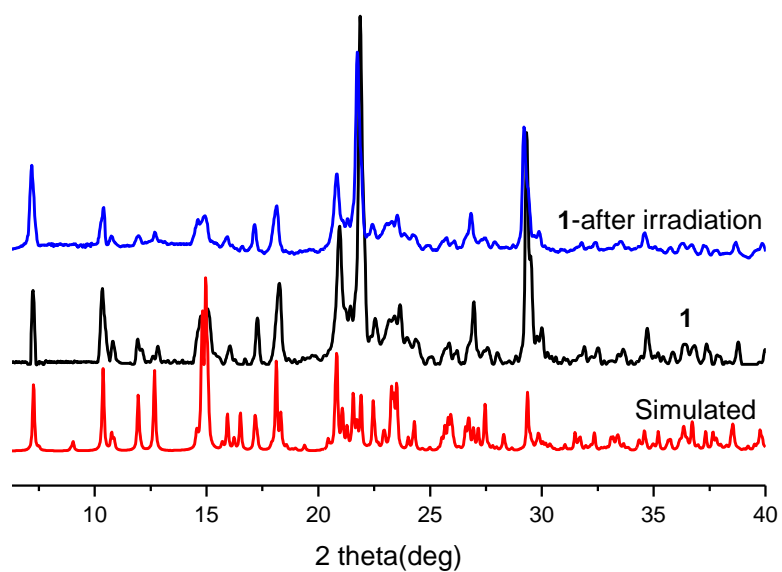


Figure S1. PXRD profiles of **1** before and after Xe light irradiation.

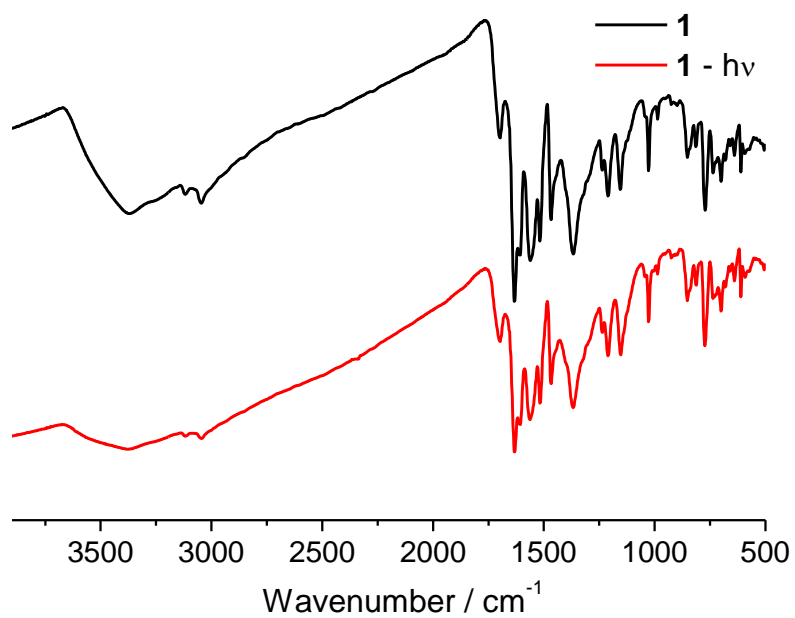


Figure S2. IR spectra of **1** before and after Xe light irradiation.

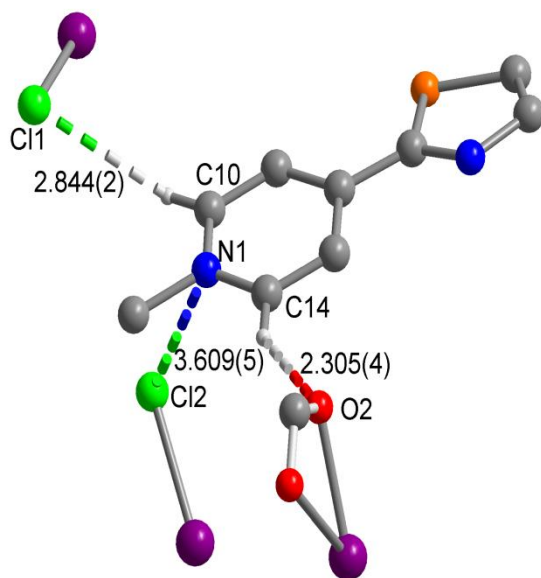
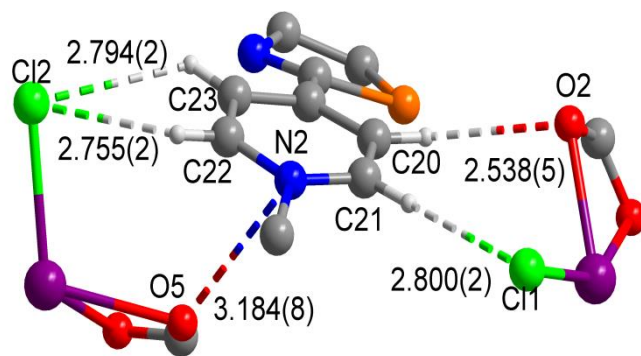


Figure S3. Hydrogen bonds and the $O_{\text{carboxylate}}/\text{Cl}\cdots\text{N}_{\text{pyridinium}}$ contacts between the interpenetrating frameworks. The distances are given in Å.

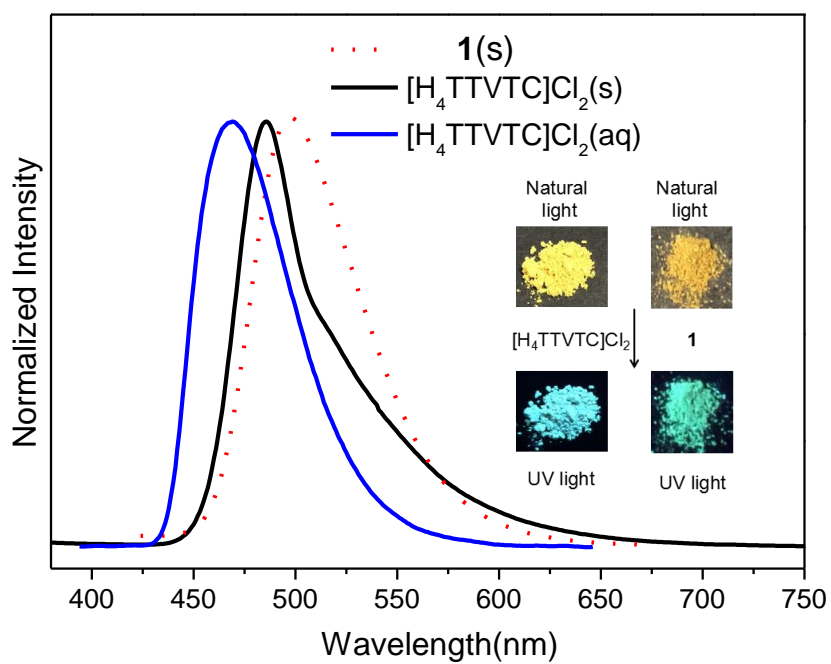


Figure S4. Emission spectra of **1** (solid, $\lambda_{ex} = 360$ nm) and $[H_4TTVTC]Cl_2$ (solid, $\lambda_{ex} = 370$ nm; aqueous solution, $\lambda_{ex} = 362$ nm). The inset shows the color of the solid samples under natural and UV light.