Electronic Supplementary Information

Photochromism and single-component white light emission from a metalloviologen complex based on 1,5-naphthyridine

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Additional graphics

Table S1. Crystal data and structural refinements for compound **1**.

	Compound 1
CCDC	2307757
Formula	$CdCl_2C_8H_6N_2$
Mr	313.45
Crystal size (mm^3)	0.42*0.17*0.1
Crystal system	monoclinic
Space group	C2/m
***a* (Å)**	15.1638(14)
***b* (Å)**	3.8071(4)
***c* (Å)**	8.2899(7)
α (deg)	90
β (deg)	103.338(5)
γ (deg)	90
***V* ($Å^3$)**	465.67(8)
D_{calcd} (g/cm^3)	2.236
Z	2
F(000)	300
Abs coeff (mm^{-1})	2.865
R_1[a]	0.0331(478)
ωR_2[b]	0.0903(480)
GOF on F^2	1.177

$$^{a}R_1 = \sum||F_o|-|F_c||/\sum|F_o|;$$

$$^{b}\omega R_2 = \{\sum\omega[(F_o)^2-(F_c)^2]^2/\sum\omega[(F_o)_2]^2\}^{1/2}.$$

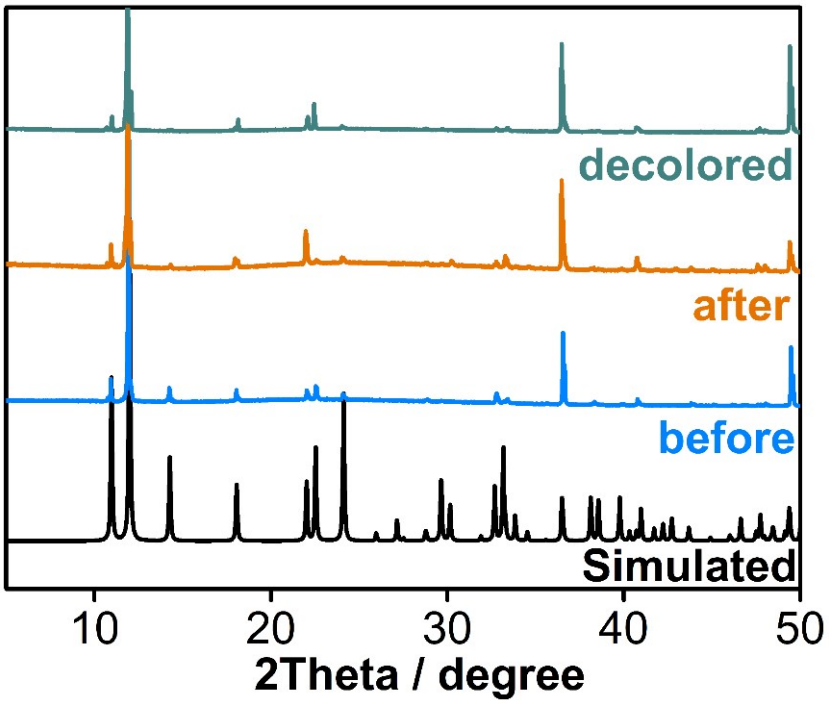

Fig. S1 PXRD patterns of compound **1**: **simulated**, simulated data using single-crystal data; **before**, measured data for as-synthesized samples; **after**, measured data for colored samples; **decolored**, measured data for its heated sample at 200 °C for 1 day.

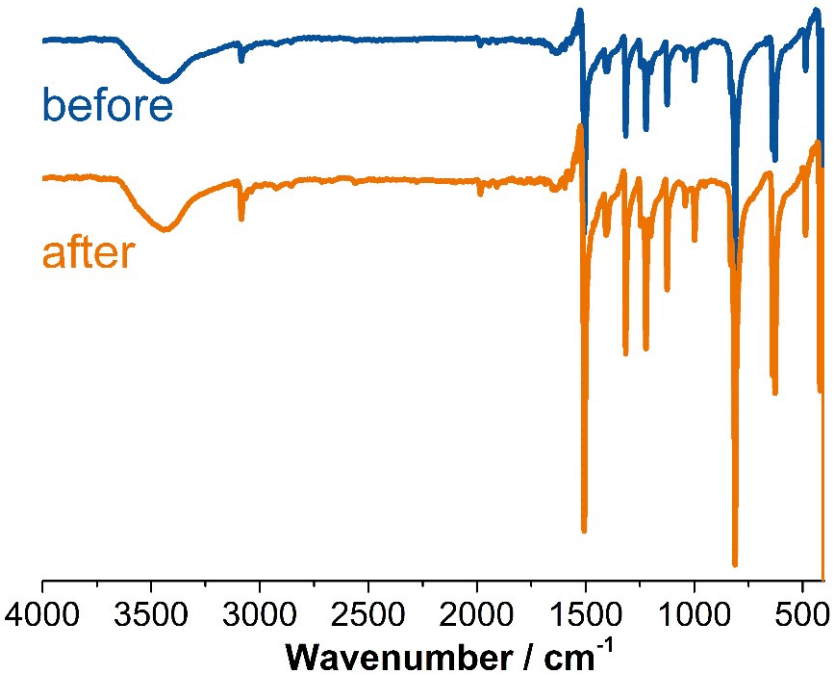

Fig. S2 IR spectra of compound **1**: **before**, measured data for as-synthesized samples; **after**, measured data for colored samples.

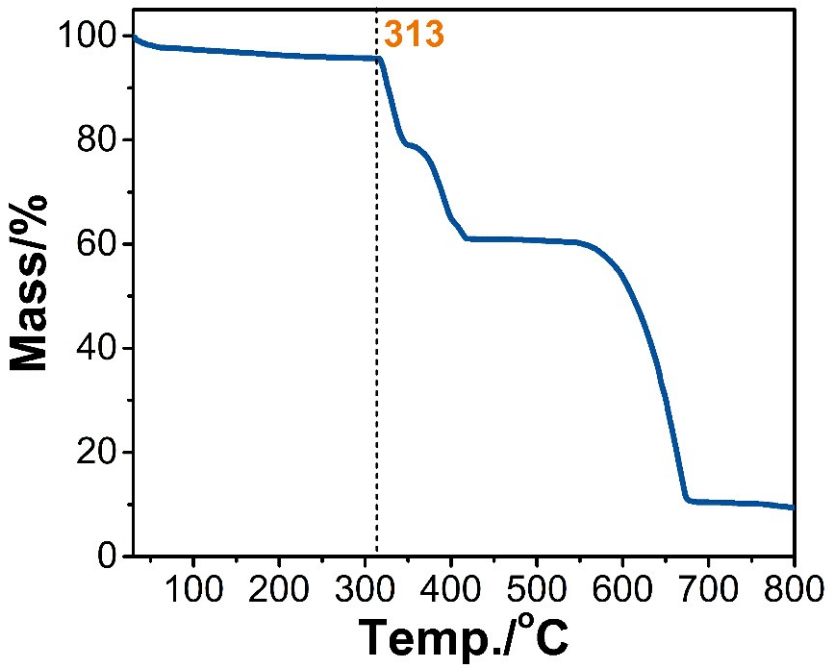

Fig. S3 Thermogravimetric curve of compound **1** under N_2 with heating rate of 10 °C/min.

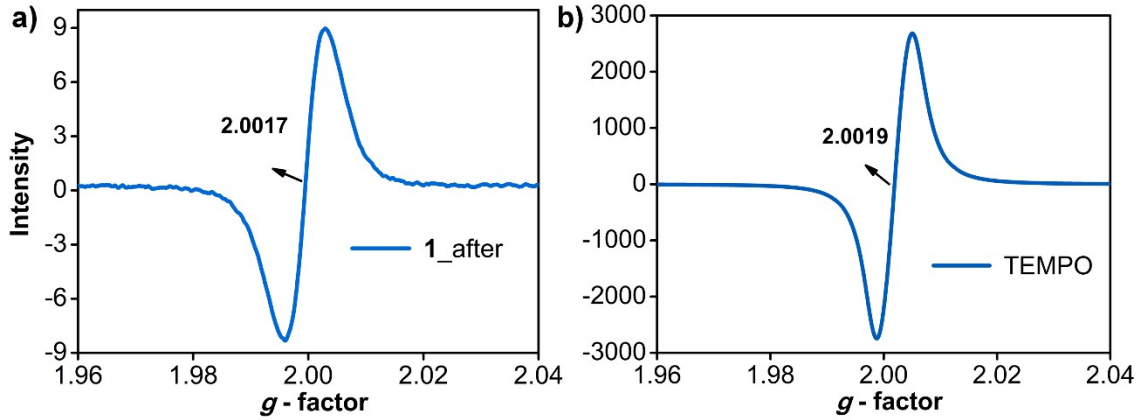

Fig. S4 ESR spectra of irradiated **1** (26 mg, a) and **TEMPO** (0.3 mg, b) in the solid state under the same test conditions.

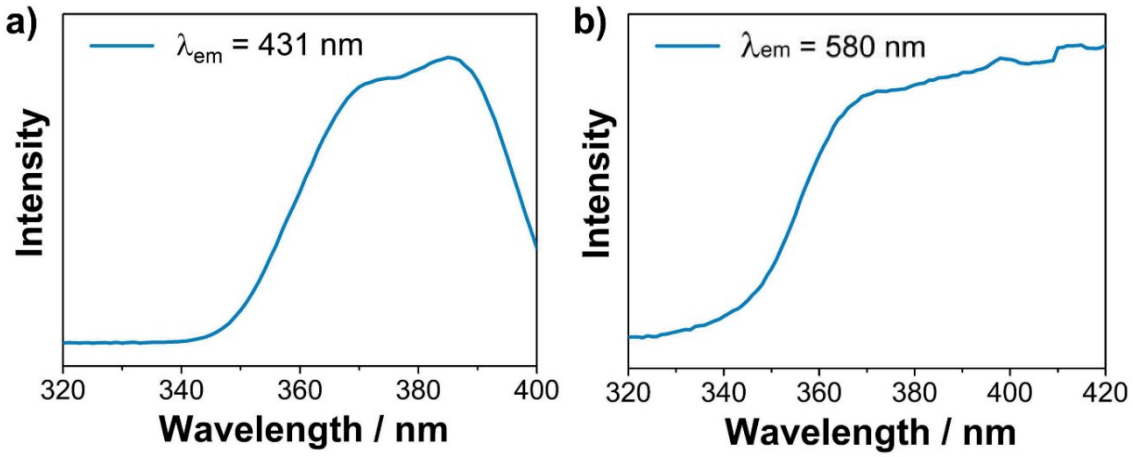

Fig. S5 The excitation spectra of fresh solid-state sample **1** monitored at 431 nm (a) and 580 nm (b), respectively.

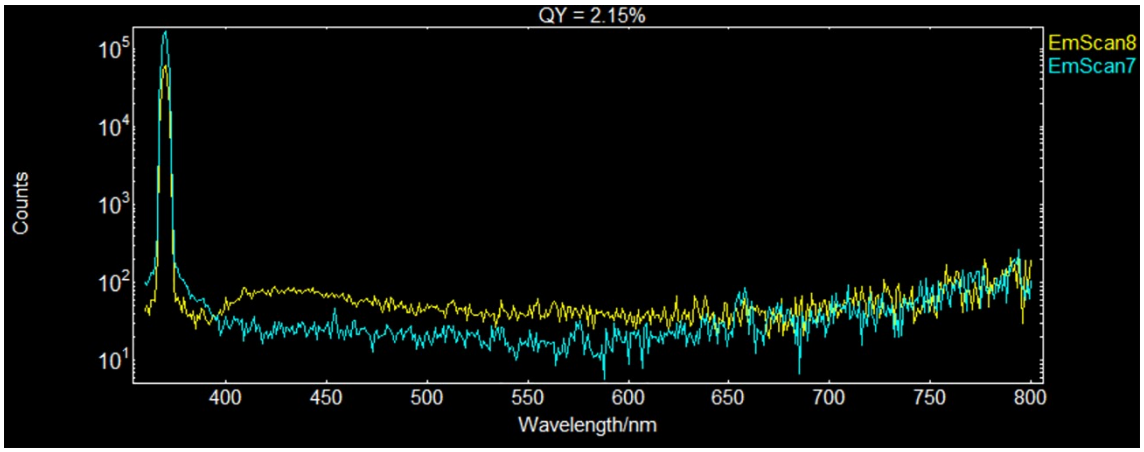

Fig. S6 Spectral diagram of quantum yield test of **1** at λ_{ex} = 370 nm.

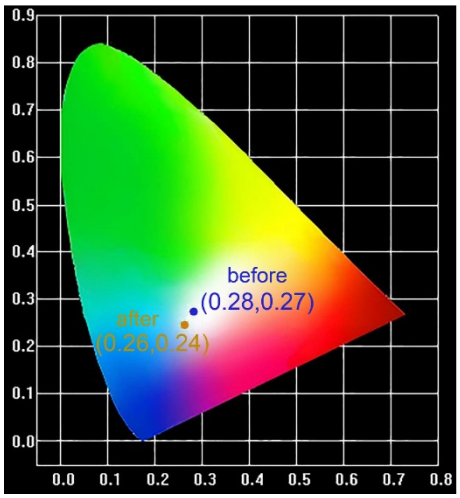

Fig. S7 The CIE maps of **1** before and after irradiation at excitation wavelength of 365 nm.

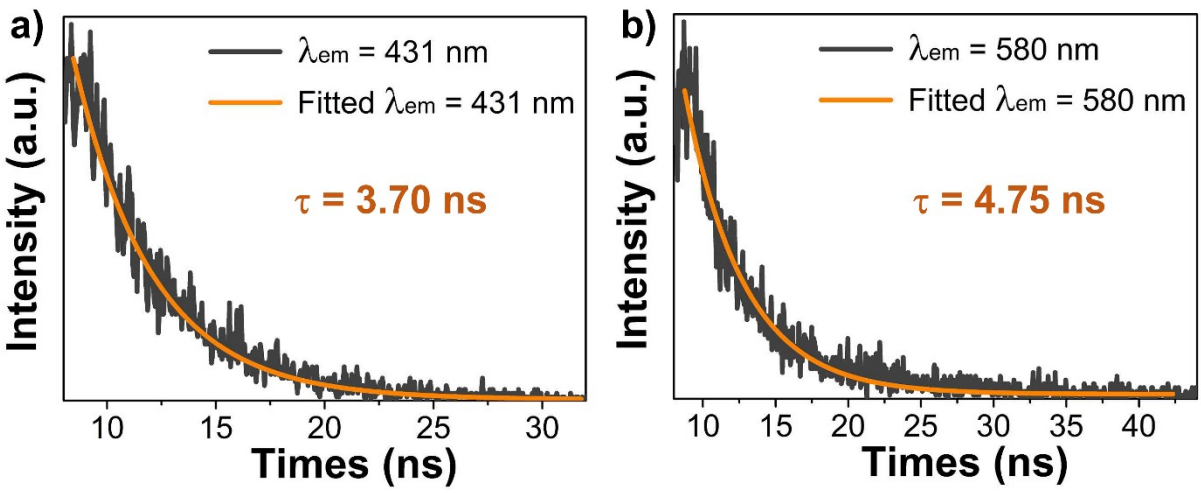

Fig. S8 Lifetime curves of **1** monitored at 431 nm (a) and 580 nm (b), respectively.

Table S2. The CIE coordinates, Color Temperature (CT) and Color-rendering Index (CRI) of fresh solid-state sample **1** at different excitation wavelength from 340 to 370 nm.

λ_{ex} of Complex 1	CIE	CT (T/K)	CRI
340 nm	(0.401, 0.393)	3615	82.54
350 nm	(0.371, 0.366)	4191	87.08
360 nm	(0.300, 0.293)	7981.	**94.04**
365 nm_before	(0.283, 0.272)	10640	**92.94**
365 nm_after	(0.262, 0.244)	19603	**92.49**
370 nm	(0.269, 0.252)	15718	**92.00**

Table 3. Typical part single-component white light emitting compounds and CRI values at specific excitation wavelengths (λ_{ex}).

Compounds[ref]	CRI values	λ_{ex} (nm)
$(H_2DABCO)(Pb_2Cl_6)$[1]	96	300
$Ba_2[Sn(OH)_6][B(OH)_4]_2$[2]	94.1	283
Compound 1 [this work]	**94.04**	**360**
$[Mg_3(OH)_2(1,4\text{-}NDC)_2(dppe)(H_2O)]$[3]	93.12	380
$\{[Zn(bpdo)(fum)(H_2O)_2]\}_n$[4]	92.1	370
(C6H5C2H4NH3)2PbBr2Cl2[5]	91	385

$(C_5H_{14}N_2)PbBr_4$[6]	90	330
$(C_7H_{16}N)PbBr_3$[6]	89	330
$(C_6H_{14}N)PbBr_3$[6]	88	330
1-(4-carboxyphenyl)-1,2,3-triazole[7]	88	370
$(C_5H_{14}N_2)_2Pb_3Br_{10}$[6]	86	330
2-MOP[8]	86	383
$[H_2DABCO][Ag_2Br_4(DABCO)]$[9]	85	376
(3APr)PbCl4[10]	85	330
$(C_6H_{16}N_2)PbBr_4$[6]	84	330
$(2meptH_2)PbCl_4$[11]	84	330
1-(4-acetylphenyl)-1,2,3-triazole[7]	83	376
(3APr)PbBr4[10]	83	330
$[DMEDA]PbCl_4$[12]	78	365
$(C_6H_{16}N_2)_3Pb_2Br_{10}$[6]	77	330
(3APr)PbI4[10]	77	330
$(C_6H_{16}N_2)PbBr_4$[6]	76	330
$[DMPDA]PbCl_4$[12]	75	377

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