Supporting Information

Temperature/Water Triggered Reversible Emission Transition in a One-Dimensional Mn(II)-Based Metal Halide

Yue Wu,[*a] *Xin Zhang,*[a] *Bo Zhang*[a], *Liu-Di Xin*[a], *Xiao-Meng Zhen*[*a] *and Liang-Jin Xu*[*bc]

E-mail: xuliangjin@fjirsm.ac.cn; ywu_lcu@163.com; 1337498078@qq.com

a College of Chemistry and Chemical Engineering, Shandong Provincial Key Laboratory/Collaborative Innovation Center of Chemical Energy Storage and Novel Cell Technology, Liaocheng University, Liaocheng 252059, China

b State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou 350002, China

c Fujian Science & Technology Innovation Laboratory for Optoelectronic Information of China, Fuzhou 350108, China

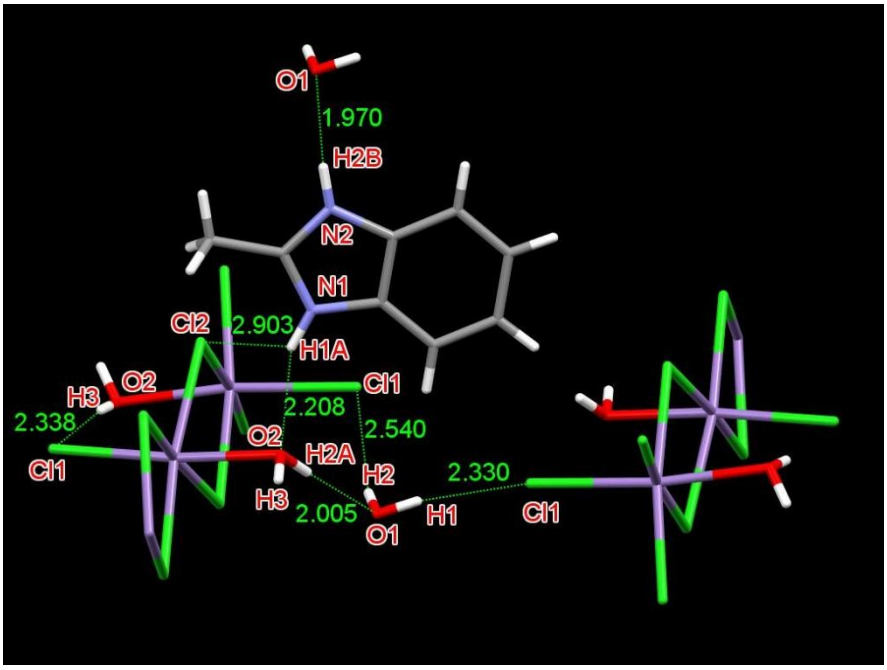


Figure S1. The view of 1D structural diagram of compound **1**, illustrating intermolecular hydrogen bonding such as O-H···O, O-H···Cl, N-H···O and N-H···Cl with short bond lengths.

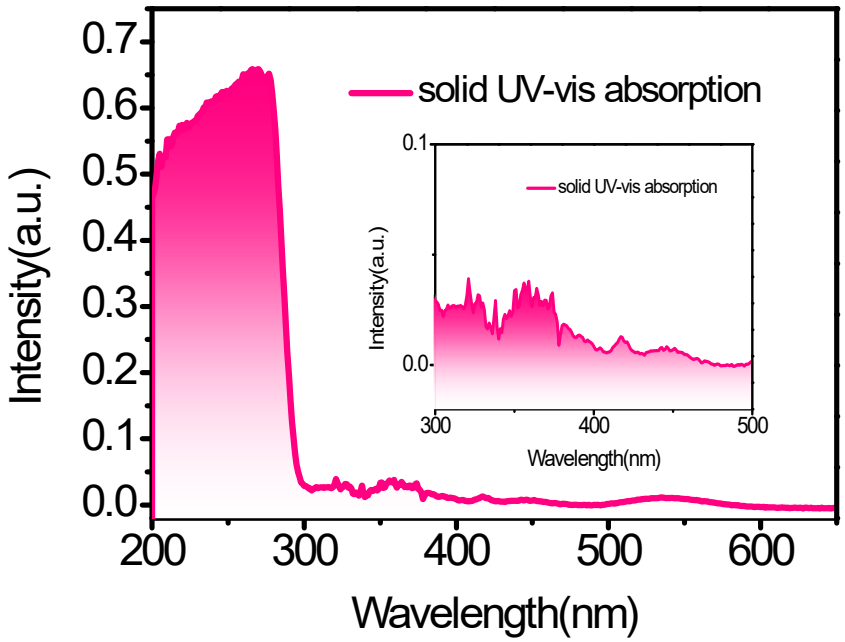


Figure S2. The solid UV-vis absorption spectrum of compound **1**. (Inset: the enlarged region of 300-500 nm)

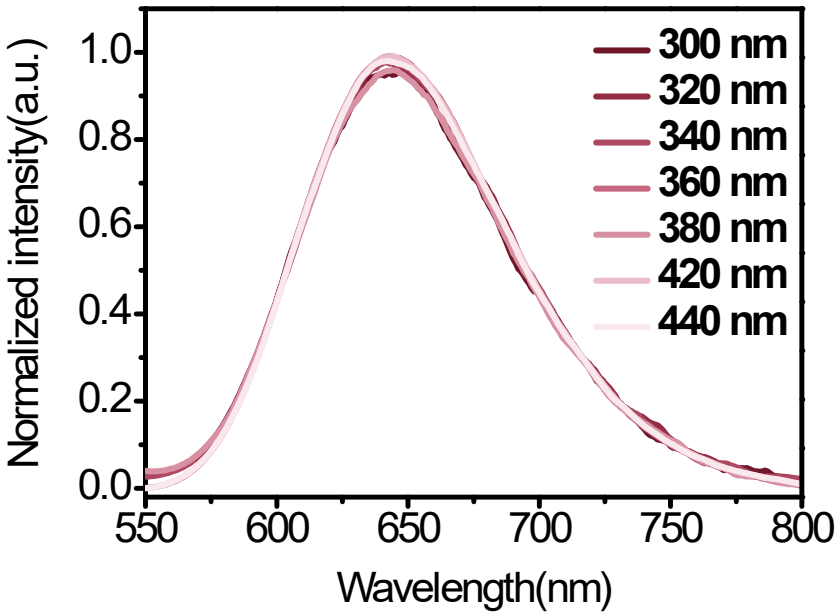


Figure S3. The excitation-dependent PL spectrum of compound **1**.

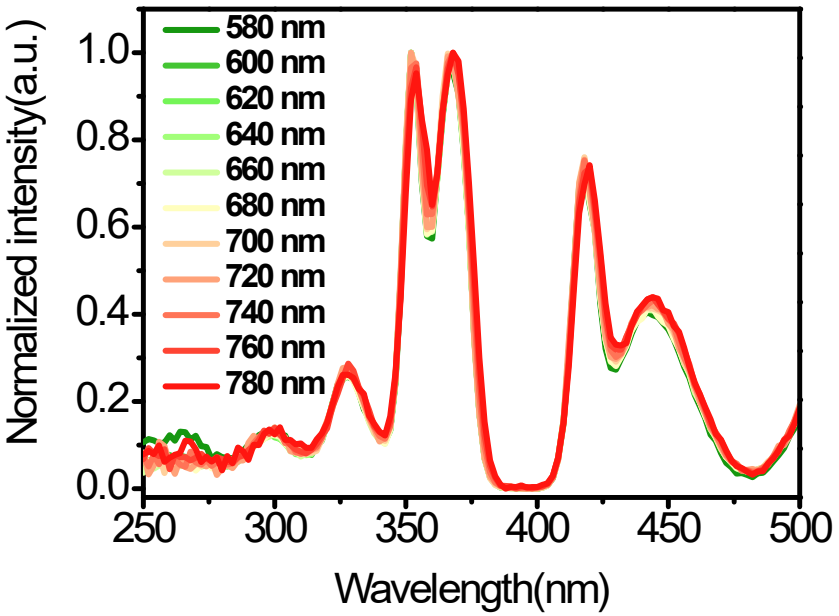


Figure S4. The emission-dependent PLE spectrum of compound **1**.

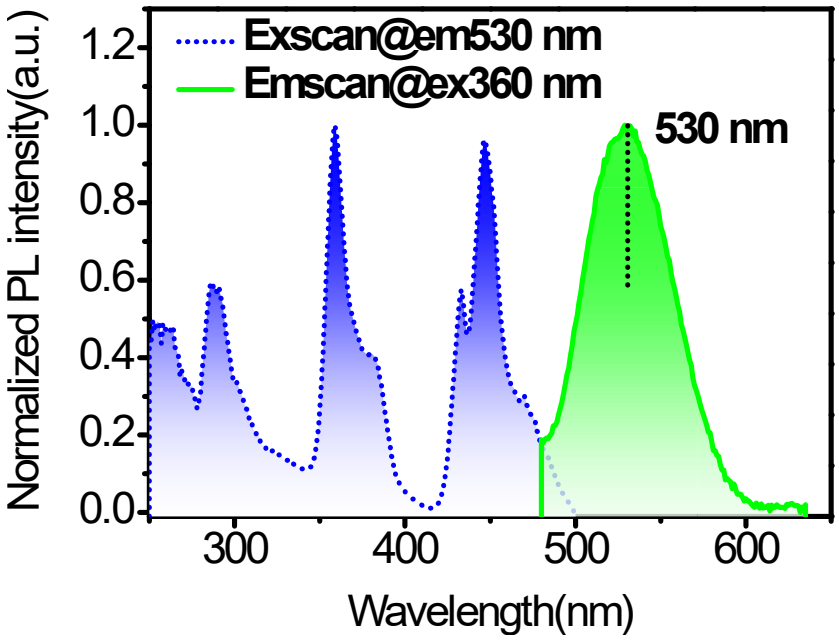
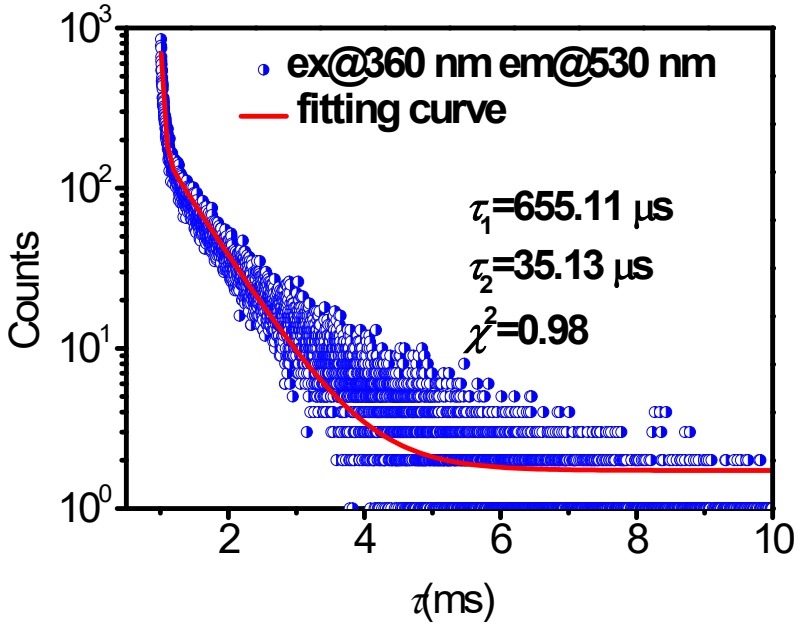
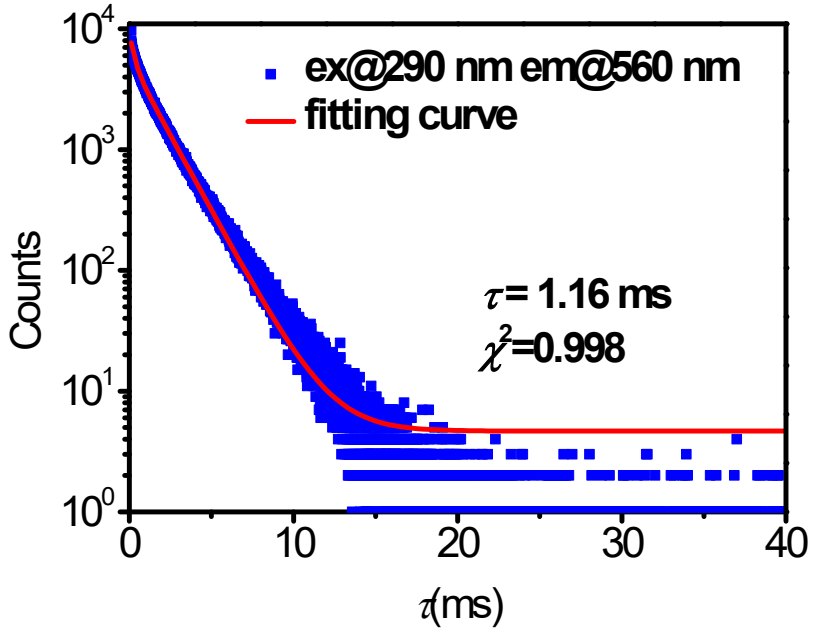


Figure S5. The PLE and PL spectrum of the yellow-emitting sample from compound **1** with water release.



(a)



(b)

Figure S6. The emission decay time curves of yellow-emitting sample from compound **1** monitored at (a) 530 nm excited by 360 nm and (b) 560 nm excited by 290 nm at room temperature.

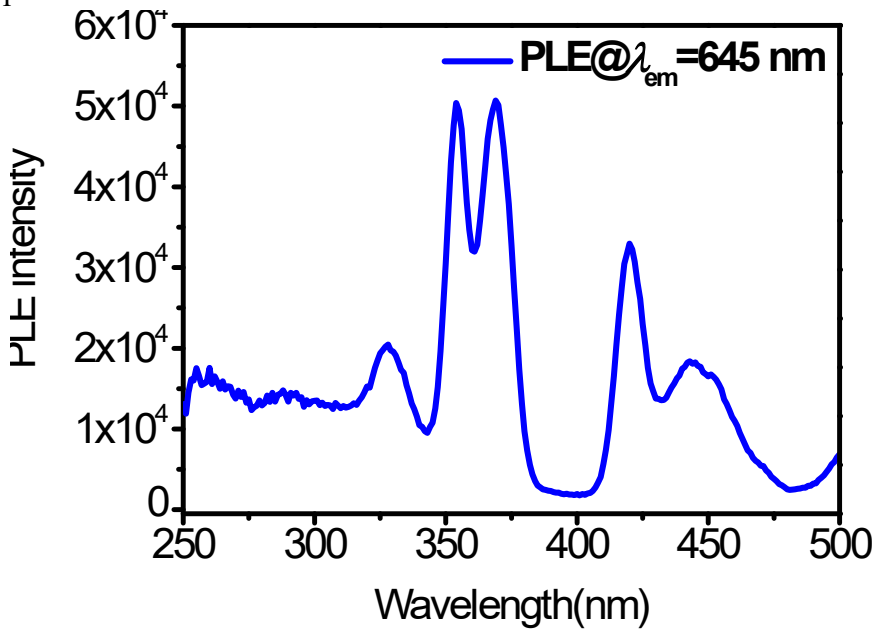


Figure S7. The PLE spectrum of yellow-emitting sample with water absorption.

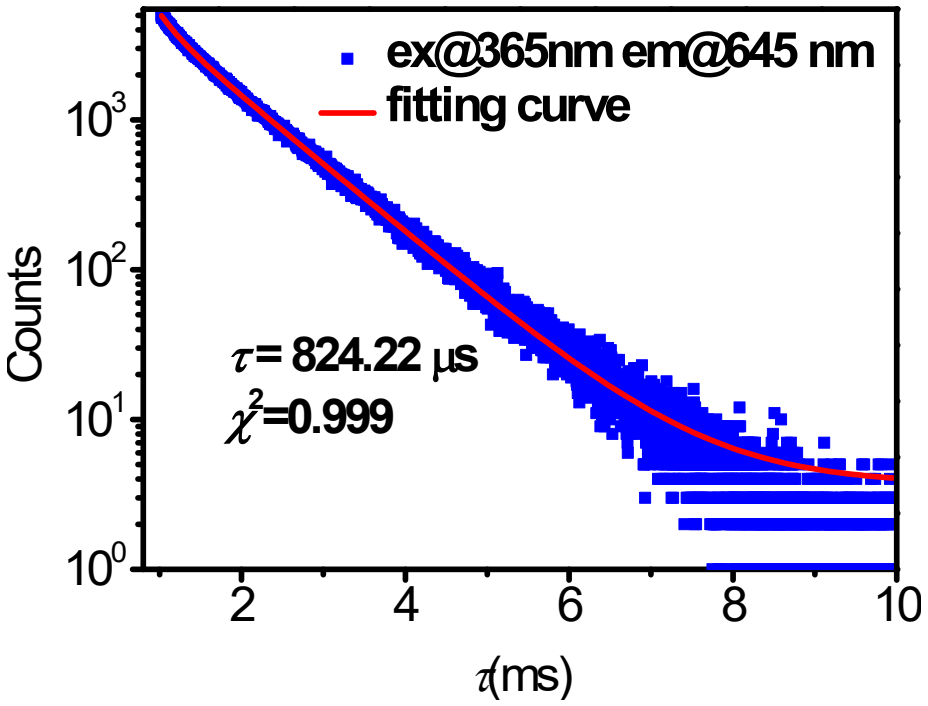


Figure S8. The emission decay time curves of yellow-emitting sample with water absorption monitored at 645 nm when excited at 365 nm at room temperature.

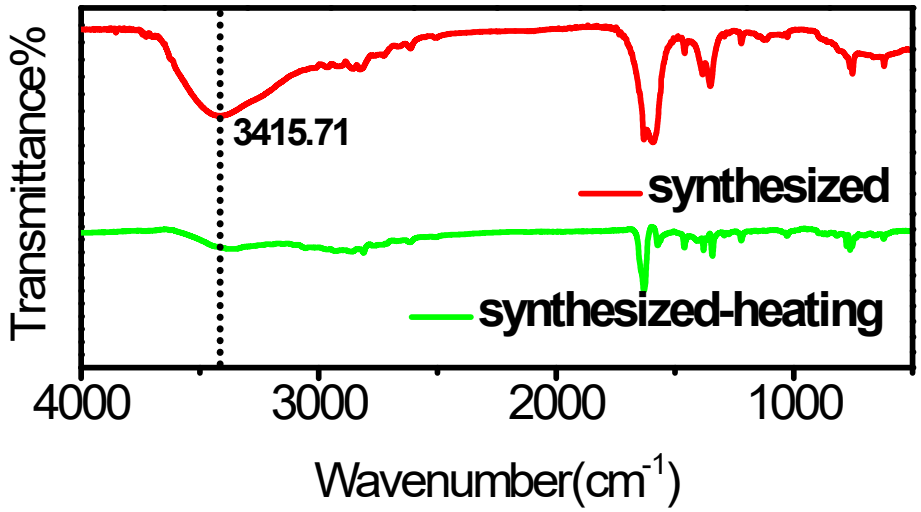


Figure S9. The Fourier transform infrared spectrum of compound **1** and yellow-emitting sample from compound **1** with a heating treatment.

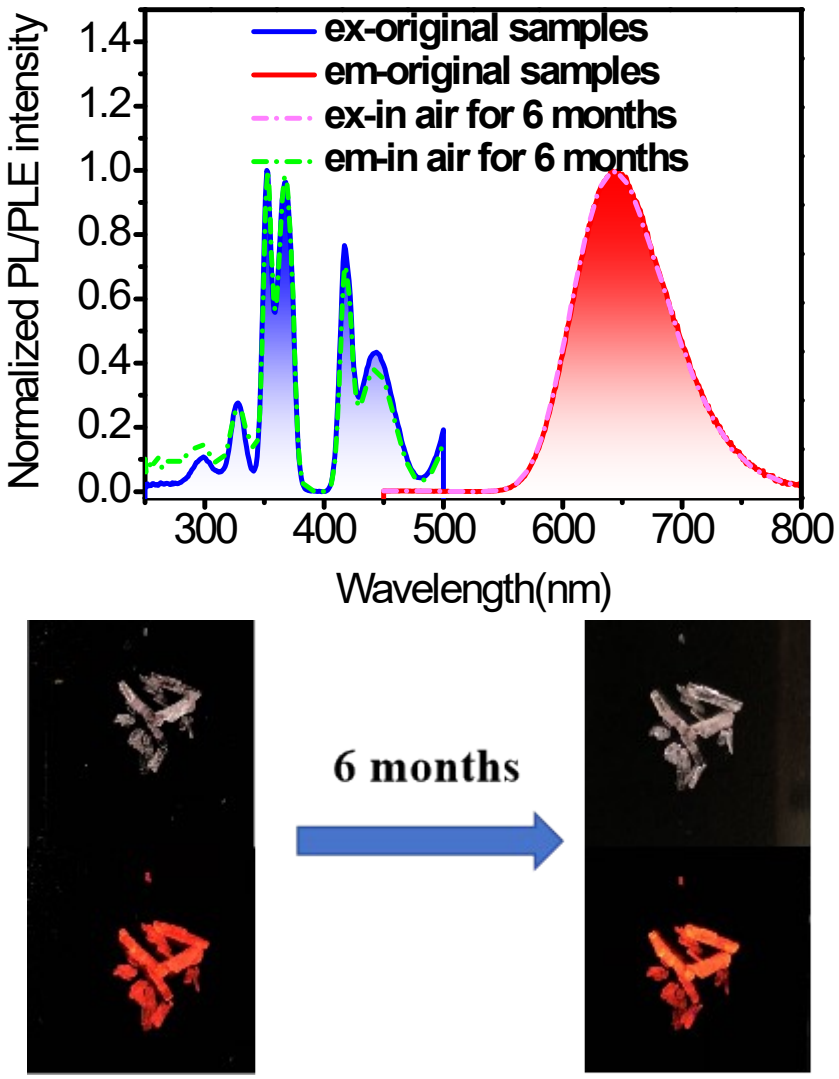


Figure S10. (a) The PL and PLE spectrum and (b) corresponding photographs of the original compound **1** and sample exposed to air conditions for 6 months.

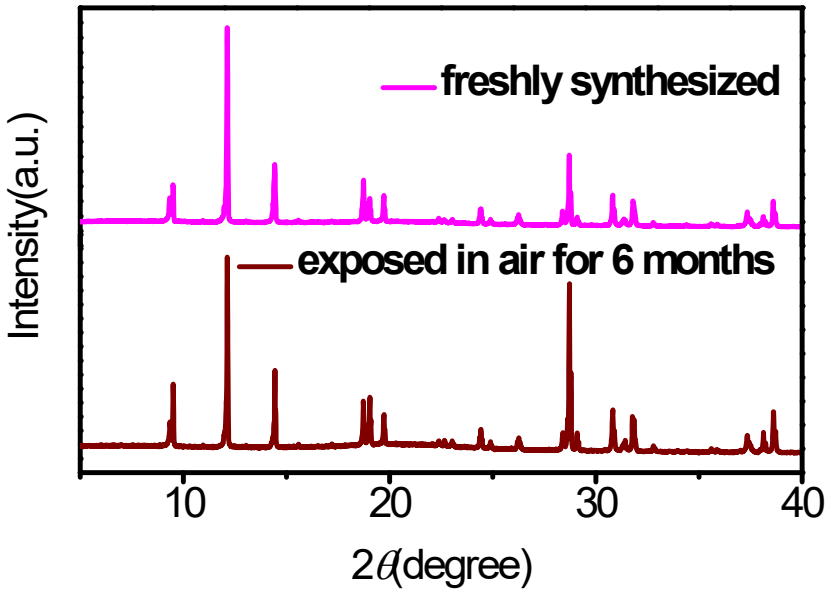


Figure S11. The PXRD patterns of compound **1** and corresponding sample exposed to air conditions for 6 months.

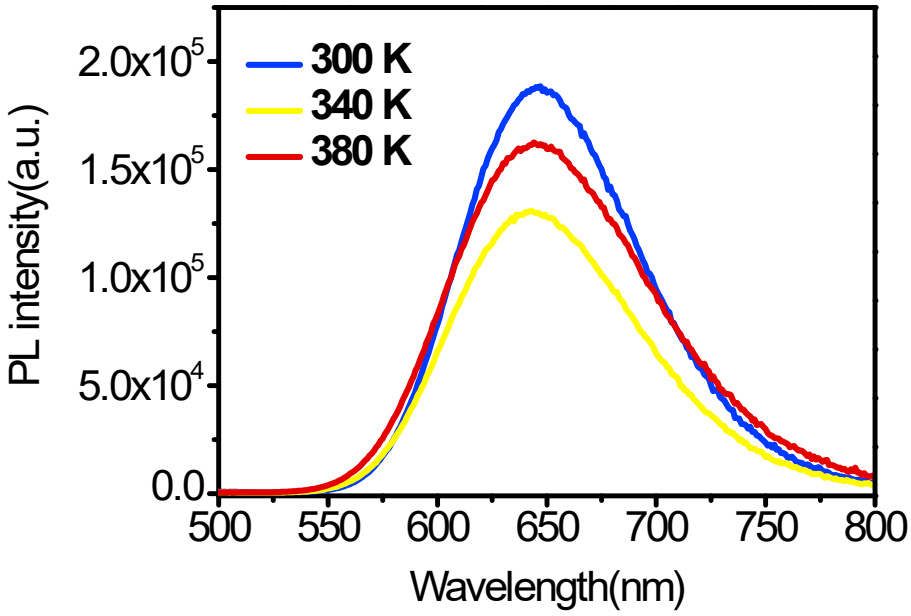


Figure S12. The PL spectrum of the original compound **1** under different heating treatments at various temperatures.

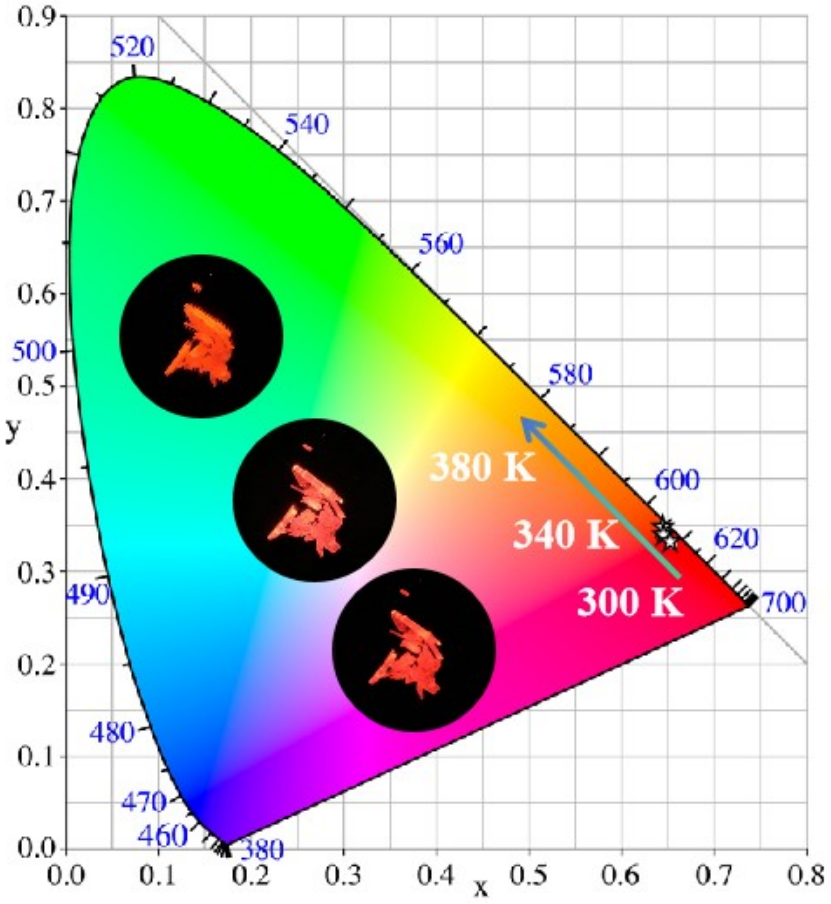


Figure S13. The CIE diagram of compound **1** at different temperatures (inset: photographs of compound **1** crystals).

Table S1. Single X-ray Diffraction Crystallographic Data of compound **1**.

Compounds	**$(C_8H_9N_2)_n\{(MnCl_3(H_2O)\cdot H_2O\}_n$**
Moiety formula	$C_8H_{13}O_2N_2Mn_2Cl_3$
chemical_formula_moiety	$(C_8H_9N_2)MnCl_3(H_2O)\cdot H_2O$
Formula weight / g.mol^{-1}	330.49
Temperature / K	298
Crystal system	Monoclinic
Space group	$P2_1/c$
***a* / Å**	9.6164(9)
***b* / Å**	7.2631(7)
***c* / Å**	18.8935(16)
***α* / deg**	90
***β* / deg**	99.858(2)
***γ* / deg**	90
volume / Å^3	1300.1(2)
Z	4
ρ_{calc} / g.cm^{-3}	1.688
***F*(000)**	668.0
Crystal size / mm^3	0.10 × 0.12 × 0.42
μ / mm^{-1}	1.618
Data completeness	0.997
Radiation	Mo Kα (λ = 0.71073 Å)
Final *R* indexes [all data]	R_1[a] =0.0483 wR_2[b]=0.1205
GOF	1.016
CCDC number	2360551

(a) $R_1 = \sum |F_o - F_c| / \sum F_o$

(b) $wR_2 = \sum \left[w(F_o^2 - F_c^2)^2 \right] / \sum \left[w(F_o)^2 \right]^{1/2}$

TableS2. Selected bond angle (°) of compound **1**.

	Bond	Bond angle(°)
1	Cl1-Mn1-Cl2	91.31(4)
2	Cl1-Mn1-Cl3	95.40(4)
3	Cl1-Mn1-Cl2^{a}	95.71(4)
4	Cl1-Mn1-Cl3^{a}	91.85(4)
5	Cl2^{a}-Mn1-Cl3	90.36(4)
6	Cl3^{a}-Mn1-Cl2^{a}	87.49(4)
7	Cl3^{a}-Mn1^{b}-Cl2^{a}	86.96(4)
8	Cl2-Mn1-Cl3^{a}	94.31(4)
9	O2-Mn1-Cl2^{a}	87.92(8)
10	O2-Mn1-Cl3^{a}	82.28(8)
11	O2-Mn1-Cl2	85.32(8)
12	O2-Mn1-Cl3	90.58(8)
13	Mn1-Cl2^{a}-Mn1^{b}	92.51(4)
14	Mn1-Cl3^{a}-Mn1^{b}	92.08(4)

Symmetry code: (a) -*x*+1, *y*-1/2, -*z*+1/2; (b) -*x*+1, *y*+1/2, -*z*+1/2.

TableS3. Selected bond length (Å) of compound **1**.

	Bond	Bond length(Å)
1	Mn1-O2	2.294(3)
2	Mn1-Cl1	2.542(1)
3	Mn1-Cl2	2.532(1)
4	Mn1-Cl3	2.536(1)
5	Mn1-Cl2^{a}	2.514(1)
6	Mn1-Cl3^{a}	2.528(1)
7	Mn1⋯Mn1^{b}	3.6454(9)

Symmetry code: (a) -*x*+1, *y*-1/2, -*z*+1/2; (b) -*x*+1, *y*+1/2, -*z*+1/2.

TableS4. List of hydrogen bonds in compound **1**.

D-H···A	d(D-H) (Å)	d(H···A) (Å)	d(D···A) (Å)	<(DHA) (°)
O1-H1···Cl1[a]	0.82(6)	2.35(6)	3.164(4)	172(5)
O1-H2···Cl1[b]	0.75(5)	2.55(5)	3.254(4)	157(5)
O2-H2A···O1[c]	0.82	2.01	2.823(4)	175.1
O2-H3···Cl1[d]	0.82(6)	2.36(6)	3.178(3)	171(6)
N1-H1A···Cl2[e]	0.86	2.90	3.385(4)	117.4
N1-H1A···O2[f]	0.86	2.21	3.016(4)	156.7
N2-H2B···O1[g]	0.86	1.97	2.820(4)	171.0

Symmetry code: (a) -*x*+1, -*y*+1, -*z*; (b) *x*, *y*-1, *z*; (c) -*x*+1, *y*+1/2, -*z*+1/2; (d) -*x*+1, *y*+1/2, -*z*+1/2; (e) *x*, *y*-1, *z*; (f) -*x*+1, *y*-1/2, -*z*+1/2; (g) *x*-1, *y*, *z*.