Supporting Information

An electron-transfer photochromic crystalline MOF accompanying photoswitchable luminescence in a host–guest system

Yu-Shuang Liu,[a] Yu-Hui Luo,[ab] Li Li,[a] and Hong Zhang*[a]

[a]*Institute of Polyoxometalate Chemistry, Department of Chemistry, Northeast Normal University, Changchun, Jilin 130024, PR China.*

E-mail: zhangh@nenu.edu.cn

[b]*Department of Chemical Engineering, Huaihai Institute of Technology, Lianyungang 222005, jiangsu, PR China*

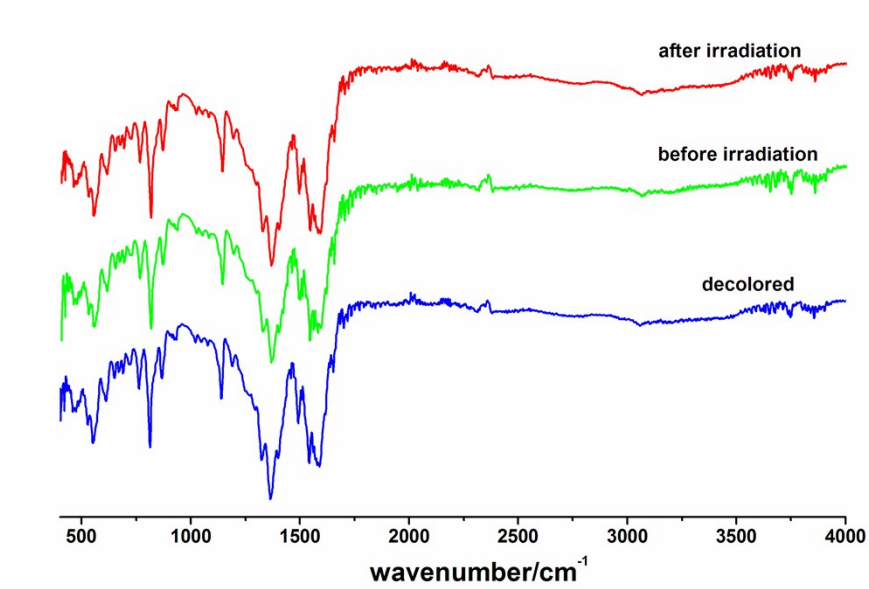

Figure S1. FTIR spectra of complex **1** before (green) , after (red) light irradiation and after thermal bleaching (blue).

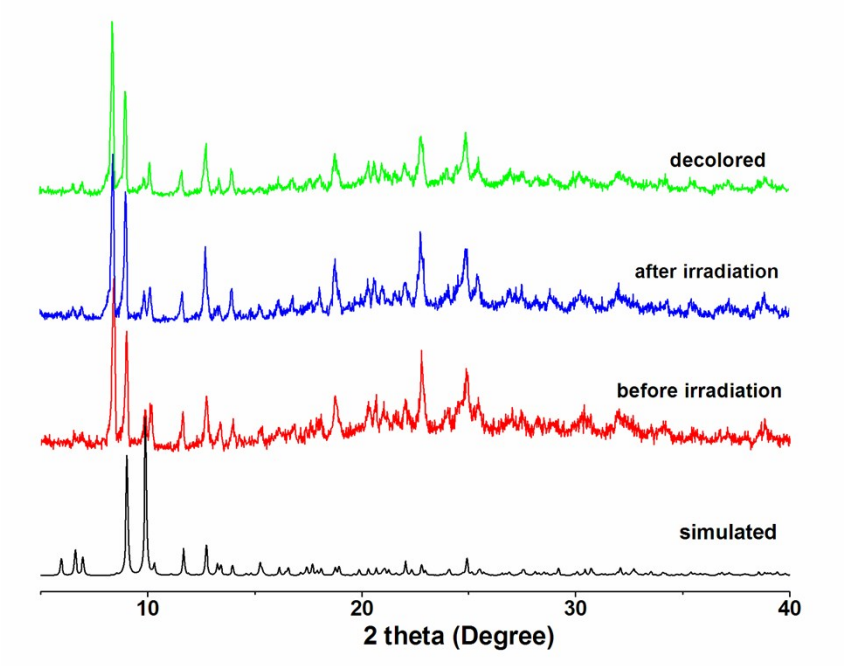

Figure S2. PXRD patterns of complex **1** before (red), after (blue) light irradiation and after thermal bleaching (green). The black line is simulated curve.

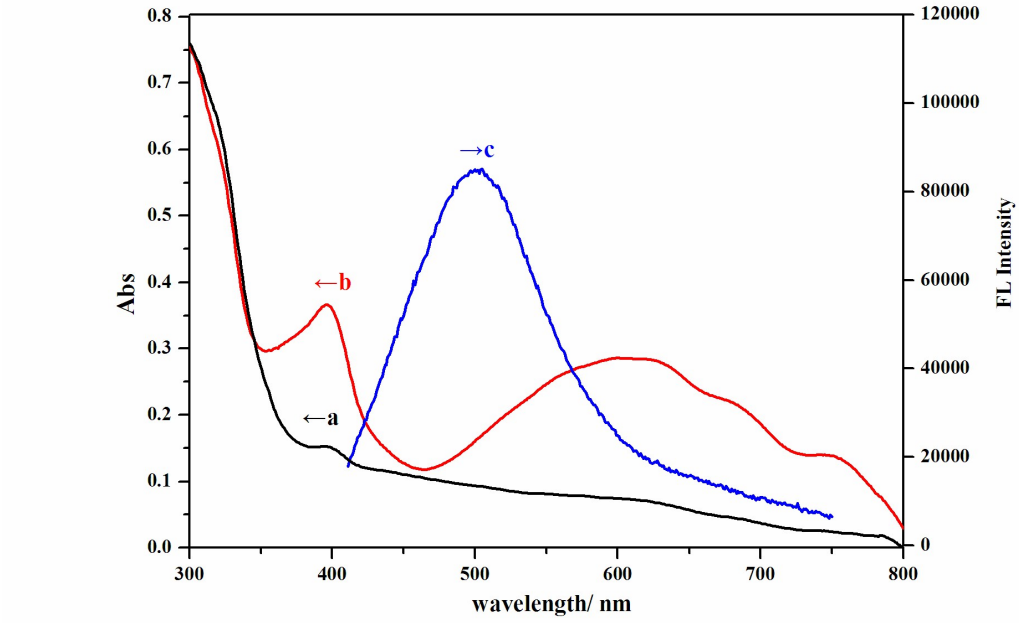

Figure S3. Absorption spectra of **1** before (a) and after light irradiation (b) and fluorescent spectrum of complex **1** (c).

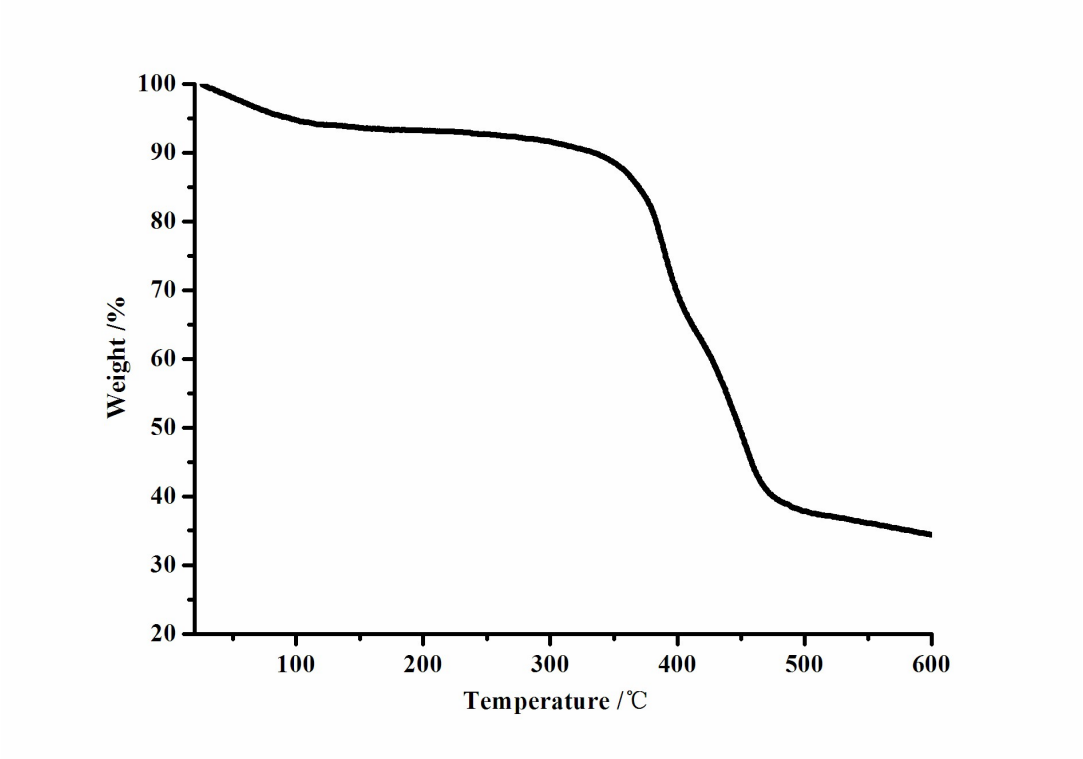

Fig S4. TGA curve of compound **1.**

Table S1. Crystal Data and Structure Refinements for compound **1**

Empirical formula	C_{24} H_{20} N_2 O_{16} Zn_3
Formula weight	788.59
Temperature	293
Crystal system	Orthorhombic
Space group	P n m a
a (Å)	14.3929(6)
b (Å)	17.8516(8)
c (Å)	26.7111(11)
α (deg)	90

β (deg)	90
γ (deg)	90
Volume	6863.1(5)
Z, Calculated density	8，1.526
Absorption coefficient	2.148
Goodness-of-fit on *F2*	1.024
Final *R* indices [*I>2sigma(I)*]	$R_1 = 0.0535$, $wR_2 = 0.1393$
R indices (all data)	$R_1 = 0.0819$, $wR_2 = 0.1558$

Table S2. Selected bond length (Å) and angle (º) for **1**

Zn(1)-O(1)	1.947(4)	Zn(1)-O(11)#1	1.974(3)
Zn(1)-O(13)	2.002(3)	Zn(1)-O(16)#2	2.010(3)
Zn(2)-O(3)	2.067(4)	Zn(2)-O(4)	1.968(3)
Zn(2)-O(10)#3	1.985(4)	Zn(2)-O(14)#4	1.986(3)
Zn(2)-O(15)#4	2.096(4)	Zn(3)-O(5)	1.949(4)
Zn(3)-O(6)	1.932(4)	Zn(3)-O(7)	1.922(3)
Zn(3)-O(9)#3	1.937(4)		
O(1)-Zn(1)-O(11)#1	105.78(17)	O(1)-Zn(1)-O(13)	113.95(15)
O(1)-Zn(1)-O(16)#2	105.77(17)	O(11)#1-Zn(1)-O(13)	113.43(15)
O(11)#1-Zn(1)-O(16)#2	125.97(15)	O(13)-Zn(1)-O(16)#2	91.70(14)
O(3)-Zn(2)-O(15)#4	177.77(15)	O(4)-Zn(2)-O(3)	94.77(17)
O(4)-Zn(2)-O(10)#3	132.05(16)	O(4)-Zn(2)-O(14)#4	106.45(15)
O(4)-Zn(2)-O(15)#4	86.00(15)	O(10)#3-Zn(2)-O(3)	90.57(16)
O(10)#3-Zn(2)-O(14)#4	121.32(15)	O(10)#3-Zn(2)-O(15)#4	90.46(16)
O(14)#4-Zn(2)-O(3)	88.58(14)	O(14)#4-Zn(2)-O(15)#4	89.19(14)
O(6)-Zn(3)-O(5)	116.9(2)	O(6)-Zn(3)-O(9)#3	107.8(2)
O(7)-Zn(3)-O(5)	100.84(17)	O(7)-Zn(3)-O(6)	102.33(17)
O(7)-Zn(3)-O(9)#3	122.43(17)	O(9)#3-Zn(3)-O(5)	107.14(18)

Symmetry codes: #1 -x+3/2,-y+1,z+1/2; #2 x+1/2,y,-z+3/2; #3 -x+2,-y+1,-z+1; #4 -x+1,-y+1,-z+1 ; #5 -x+3/2,-y+1,z-1/2; #6 x-1/2,y,-z+3/2; #7 x,-y+1/2,z

Table S3. N−H···O interactions Geometry (Å, °) for Compound **1**

D−H···A	d(D−H)	d(H···A)	d(D···A)	∠DHA
N(1)-H(1B)...O(8)	0.89	2.13	2.948(13)	153.3
N(1)-H(1B)...O(9)	0.89	2.52	3.019(10)	115.7
N(2)-H(2A)...O(2)	0.89	2.07	2.914(16)	158.3
N(2)-H(2B)...O(2)	0.89	2.07	2.914(16)	158.3