Two magnesium based metal-organic frameworks (Mg-MOFs): Structures, photochromism, and fluorescence sensing to Fe^{3+} ions and cysteine molecules

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Table S1 Crystallographic data and structural refinement details

Compounds	**1**	**2**
Empirical formula	$C_{36}H_{36.11}Mg_2N_2O_{15.05}$	$C_{34}H_{34.5}Mg_2N_4O_{15.25}$
CCDC number	2527599	2527600
Formula weight	786.23	791.77
Crystal system	monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$
T/K	100(2)	100(2)
a/ Å	14.7942(4)	14.9938(4)
b/ Å	17.2223(4)	16.9392(5)
c/ Å	14.5709(4)	14.4824(4)
α/°	90	90
β/º	90.156(2)	90.481(2)
γ/°	90	90
V/ Å^3	3712.51(17)	3678.15(18)
Z	4	4
ρ_{calc} g/cm^3	1.407	1.430
μ/mm^{-1}	0.140	0.143
F(000)	1642	1650
R_{int}	0.0271	0.0256
GOF	1.052	1.046
$^aR_1$, $^bwR_2$ [$I > 2\sigma(I)$]	0.0419, 0.1037	0.0471, 0.1326
$^aR_1$, $^bwR_2$ (all data)	0.0561, 0.1101	0.0581, 0.1393

$^aR_1 = \sum \| F_o | - | F_c \| / \sum | F_o |$. $^bwR_2 = [\sum w(F_o^2 F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$

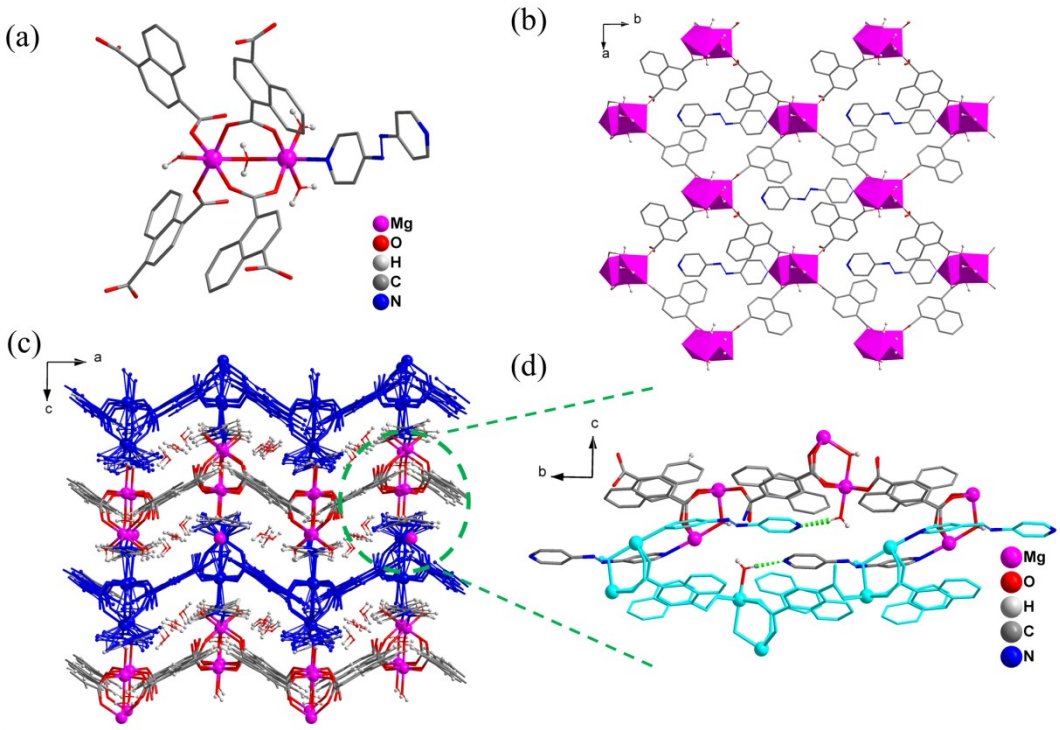

Figure 1. (a) The coordination environment of Mg^{2+} in compound **2**. (b) The 2D plane formed by Mg^{2+} and 1,4-NDC^{2-}. (c) The 3D super framework formed by stacking the layers. (d) The H-bonding between the terminal water and L2 ligand from two layers in compound **2**.

Table S2. Hydrogen bonds in compound **1**.

D-H...A	D (D-H)/Å	D (H...A)/Å	D (D...A)/Å
O(9)-H(9C)...O(7)#1	0.852(8)	1.761(10)	2.5848(14)
O(10)-H(10B)...O(8)#3	0.826(9)	1.992(9)	2.8175(13)
O(10)-H(10C)...O(3W)	0.837(9)	1.917(10)	2.7447(16)
O(11)-H(11B)...O(3)#6	0.834(9)	1.836(10)	2.6541(13)
O(11)-H(11C)...O(1W)	0.848(9)	1.984(10)	2.8072(16)
O(12)-H(12B)...N(2)#7	0.842(8)	1.880(9)	2.7192(15)
O(12)-H(12C)...O(11)#8	0.825(9)	2.216(11)	2.9335(14)
C(1)-H(1A)...O(4W)	0.95	2.37	3.04(3)
C(9)-H(9A)...O(2W)#3	0.95	2.62	3.524(2)
O(1W)-H(1B)...O(4)#2	0.840(9)	1.896(10)	2.7232(17)
O(2W)-H(2B)...O(7)#1	0.847(9)	1.935(11)	2.7671(17)
O(2W)-H(2C)...O(12)#9	0.852(9)	2.478(17)	3.1579(16)
O(3W)-H(3B)...O(2W)	0.840(9)	1.977(10)	2.8035(18)
O(4W)-H(4B)...O(3W)#3	0.820(10)	2.02(19)	2.78(3)

Symmetry transformations used to generate equivalent atoms:
#1 -x,y-1/2,-z+1/2; #2 -x+1,y-1/2,-z+1/2; #3 -x,-y+1,-z+1; #4 -x+1,y+1/2,-z+1/2; #5 -x,y+1/2,-z+1/2; #6 -x+1,-y+1,-z+1; #7 x,-y+3/2,z-1/2; #8 x,-y+1/2,z-1/2; #9 x,-y+1/2,z+1/2.

Table S3. Hydrogen bonds in compound **2**.

D-H...A	D (D-H)/Å	D (H...A)/Å	D (D...A)/Å
O(9)-H(9A)...O(7)#2	0.839(9)	2.59(2)	2.9835(15)
O(9)-H(9A)...O(8)#2	0.839(9)	1.792(11)	2.6135(17)
O(10)-H(10A)...N(2)#5	0.824(9)	1.932(9)	2.753(2)
O(10)-H(10B)...O(11)#6	0.816(9)	2.274(12)	2.9683(17)
O(11)-H(11A)...O(7)#7	0.831(9)	1.845(11)	2.6571(16)
O(11)-H(11B)...O(3W)#7	0.847(9)	1.963(11)	2.795(2)
O(12)-H(12A)...O(2W)	0.841(9)	1.854(10)	2.693(2)
O(12)-H(12B)...O(4)#8	0.829(9)	1.956(9)	2.7842(16)
C(36)-H(36A)...O(1W)#3	0.95	2.53	3.450(3)
O(1W)-H(1A)...O(10)	0.872(10)	2.52(3)	3.208(2)
O(1W)-H(1B)...O(3^a)#9	0.869(10)	1.893(14)	2.748(4)
O(1W)-H(1B)...O(3B^b)#9	0.869(10)	1.90(2)	2.698(8)
O(2W)-H(2B)...O(3B^b)#1	0.836(10)	2.64(3)	3.051(9)
O(2W)-H(2B)...O(1W)#10	0.836(10)	2.038(14)	2.848(3)
O(3W)-H(3C)...O(8)#11	0.827(10)	1.980(13)	2.788(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y+1/2,-z+1/2; #2 -x,y+1/2,-z+1/2; #3 -x+1,y-1/2,-z+1/2; #4 -x,y-1/2,-z+1/2; #5 x,-y+1/2,z-1/2; #6 x,-y+3/2,z-1/2; #7 -x,-y+1,-z+1; #8 -x+1,-y+1,-z+1; #9 -x+1,-y+1,-z; #10 x,-y+3/2,z+1/2; #11 x,-y+1/2,z+1/2.

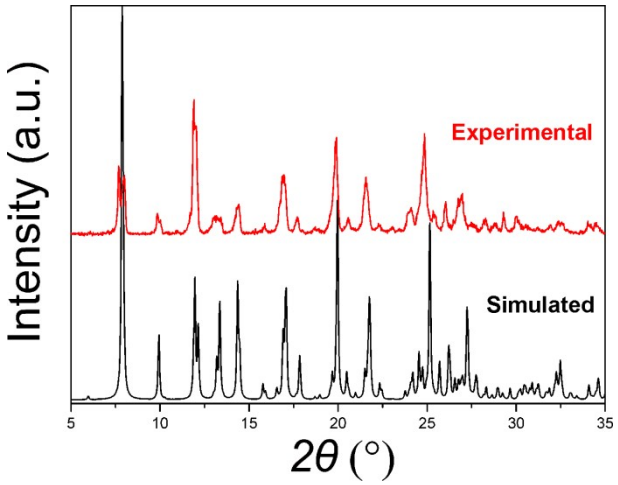

Figure S2. The PXRD of the as-made compound **1**.

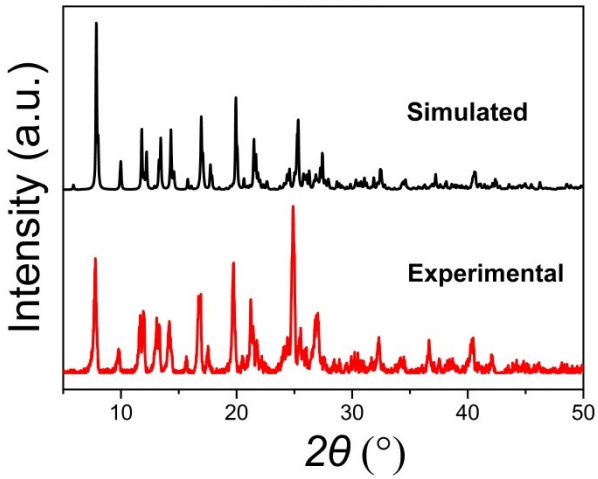

Figure S3. The PXRD of the as-made compound **2**.

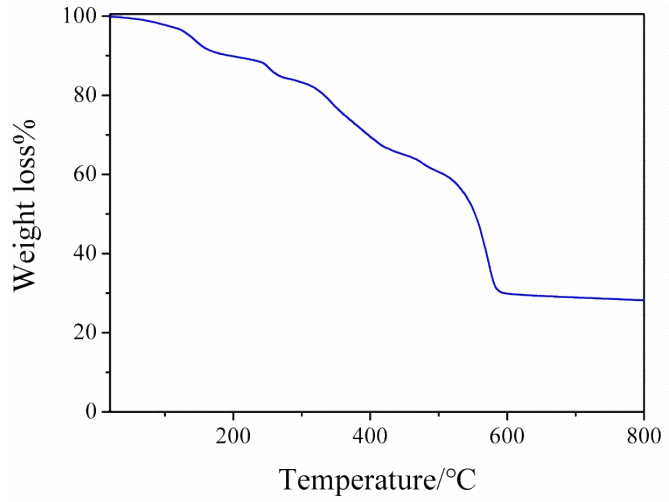

Figure S4. The TG curve for the as-made compound **1**.

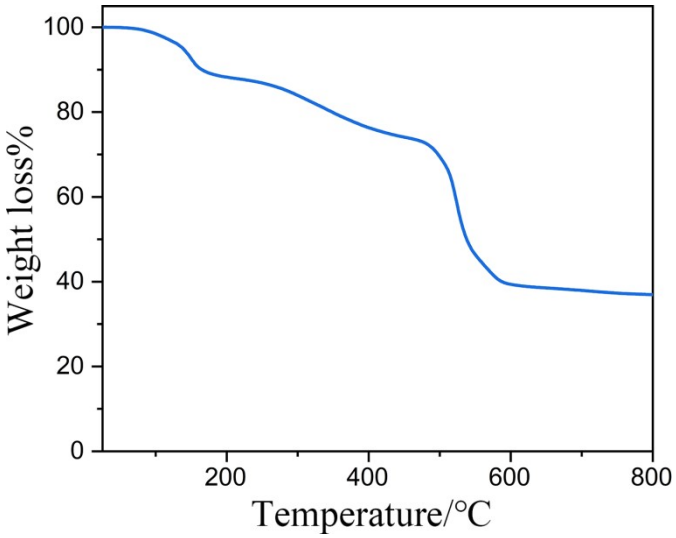

Figure S5. The TG curve for the as-made compound **2**.

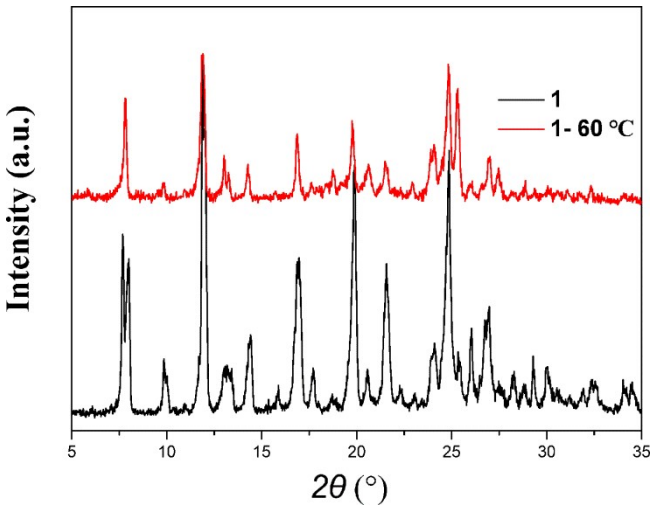

Figure S6. The PXRD of the as-made **1** and photochromic sample after 60 ℃ heating.

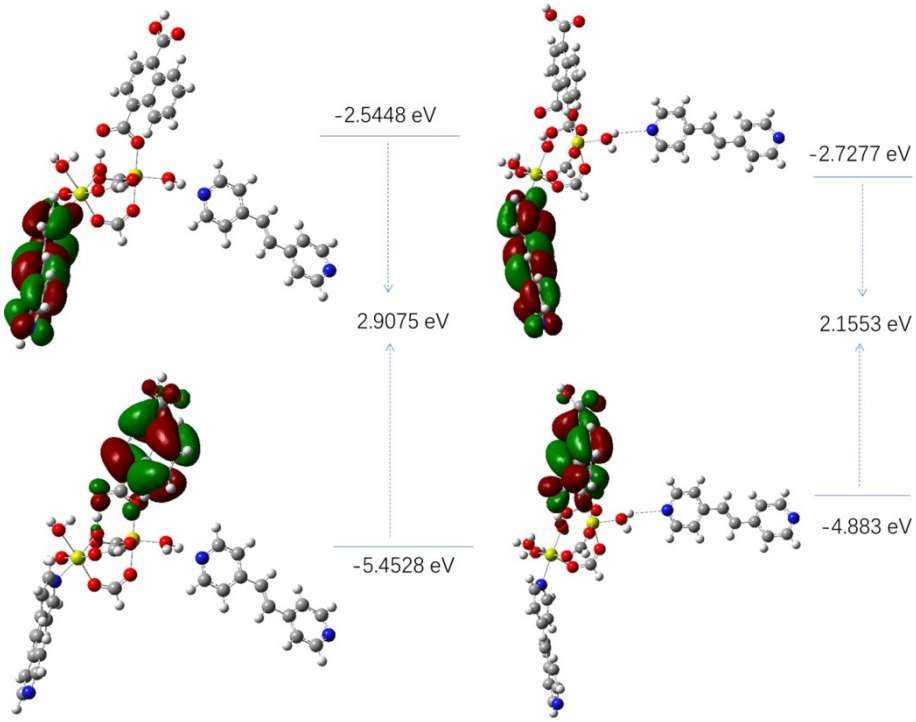

Fig. S7. DFT calculation of the selected structural fragment of compound **1** before and after hydrogen migration.

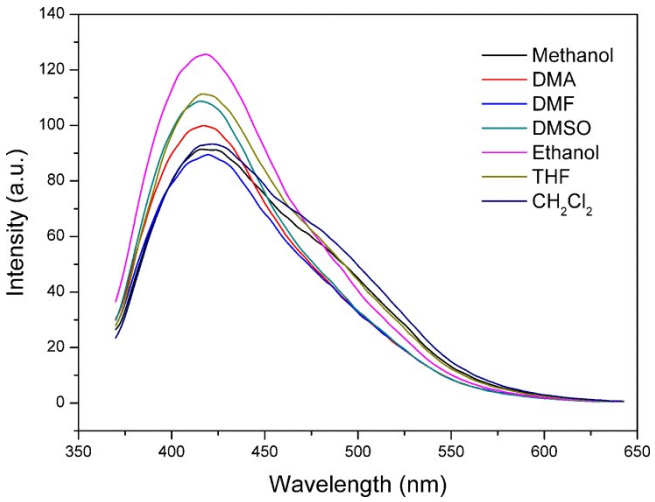

Figure S8. The fluorescence spectra for the powdered compound **1** dispersed in varied solvents.

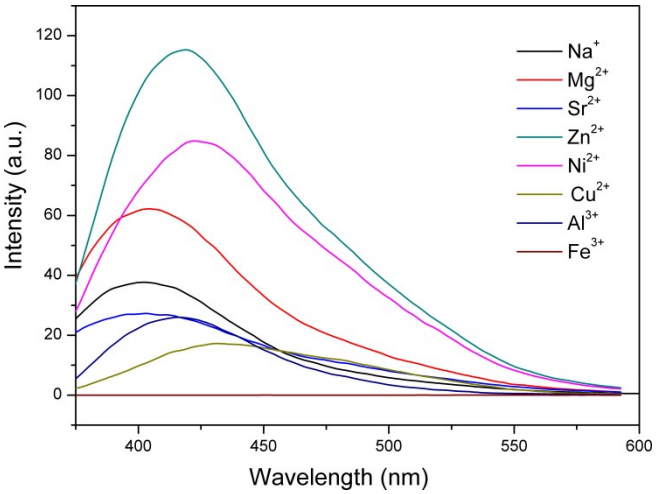

Figure S9. The fluorescence spectra for the powdered compound **1** dispersed in varied ethanol solution of 10^{-2} M metal ions.

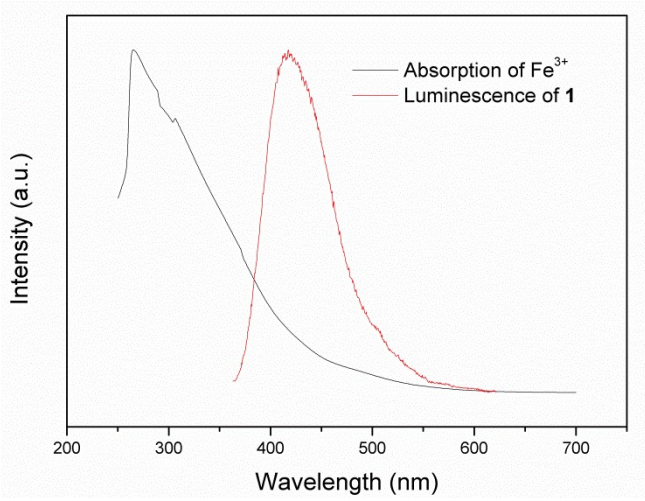

Figure S10. The absorption spectra of the Fe^{3+} solution and the luminescence of compound **1**.

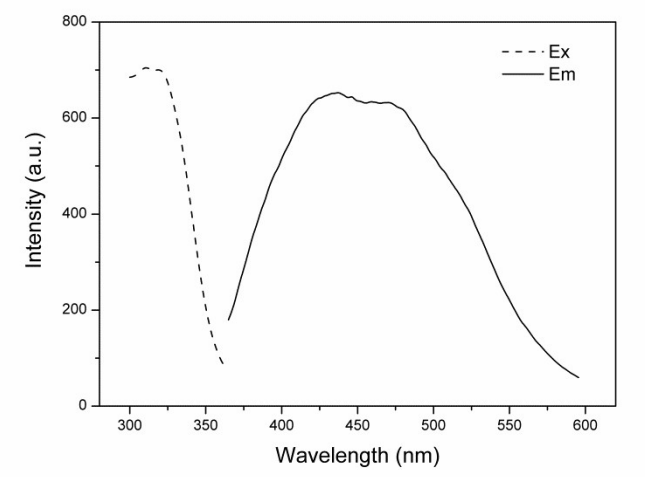

Figure S11. The solid state fluorescence spectra for the compound **1-CuI**.

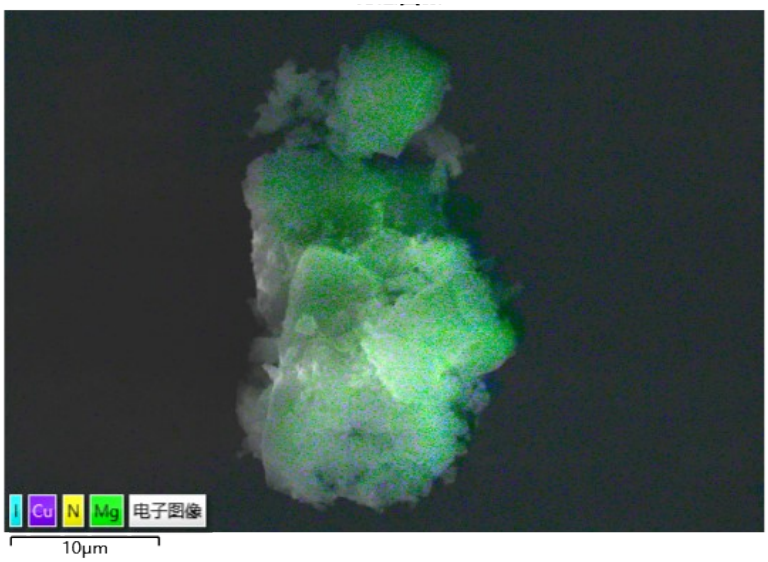

Figure S12. The SEM photograph for the sample **1-CuI**.

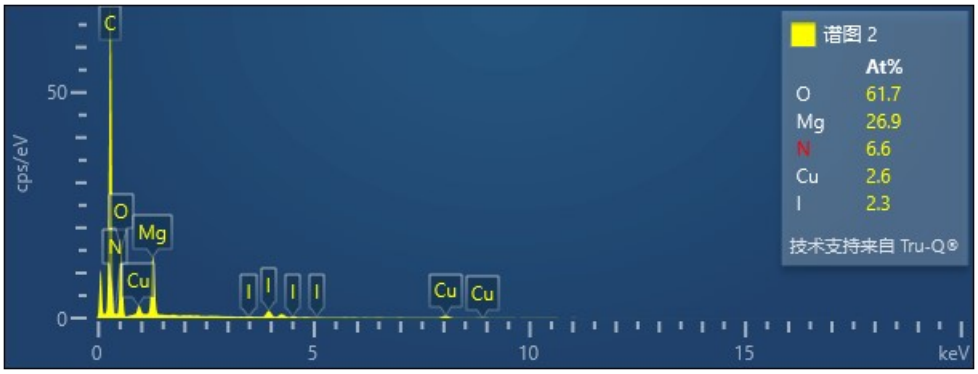

Figure S13. The EDS result of the sample **1-CuI**.

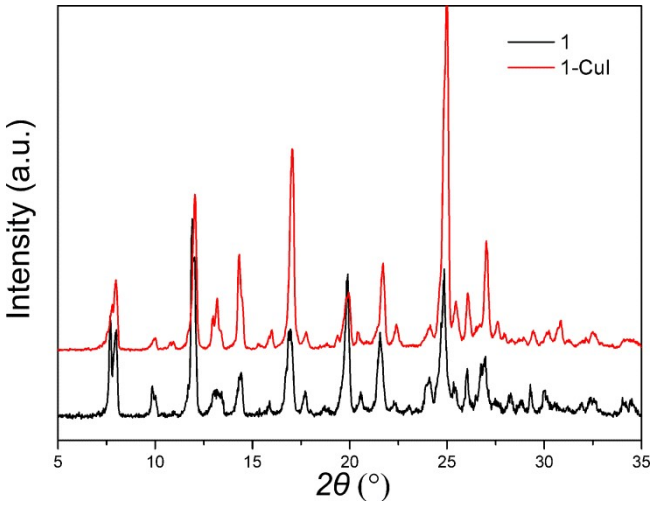

Figure S14. The PXRD of the as-made **1-CuI**. The experimental pattern for the pristine **1** was added for a comparative study.

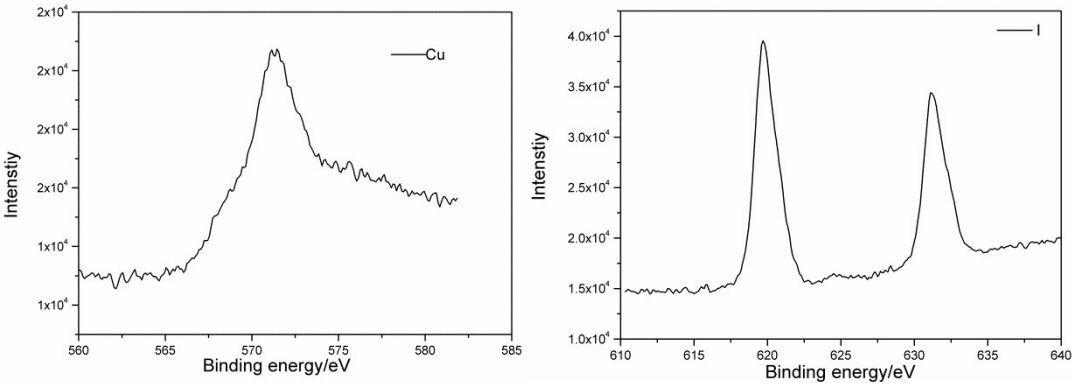

Figure S15. The core-level spectra of Cu and I in compound **1-CuI**.

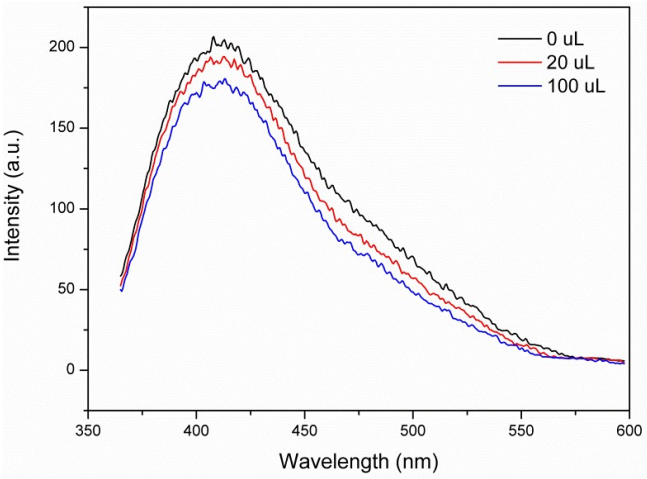

Figure S16. The fluorescence spectra for the ethanol suspension of compound **1** with the addition of varied concentration of Cys.