Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Synthesis, structure, fluorescence and electrochemical properties of a new Zn(II)-organic framework constructed by tricarboxylic acid ligand

X-ray Crystallography

Single-crystal X-ray diffraction data for **1** were recorded on an Oxford Gemini R Ultra diffractometer with graphite-monochromated Mo-Kα radiation (λ = 0.71073 Å) at 293 K. All the structures were solved by Direct Method of SHELXS-2018 and refined by full-matrix least-squares techniques using the SHELXL-2018 program within WINGX.[1] Non-hydrogen atoms were refined with anisotropic temperature parameters. The disordered atoms Zn3, O15 and O4W were splited over two sites with a total occupancy of 1 for each pair of disordered atoms. All hydrogen atoms on carbon atoms were generated geometrically and refined using a riding model with d(C–H) = 0.93 Å, U_{iso} = 1.2U_{eq}(C) for aromatic. The detailed crystallographic data and structure refinement parameters of all compounds are summarized in Table 1. Selected bond distances and angles are given in the Table S1.

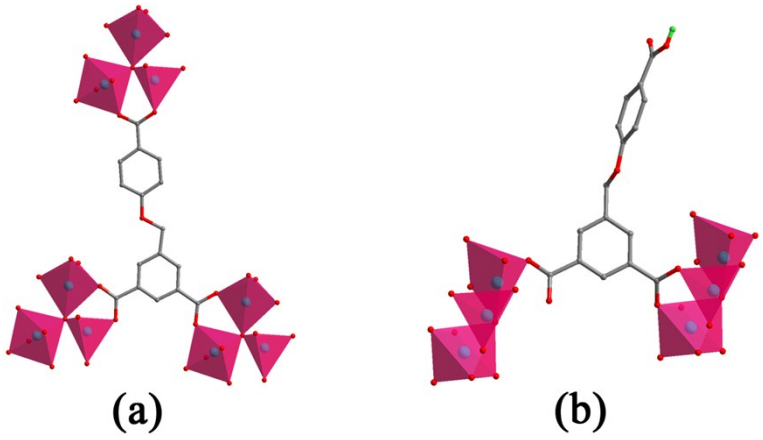


Fig. S1 Diverse coordination modes of Zn(Ⅱ) ion.

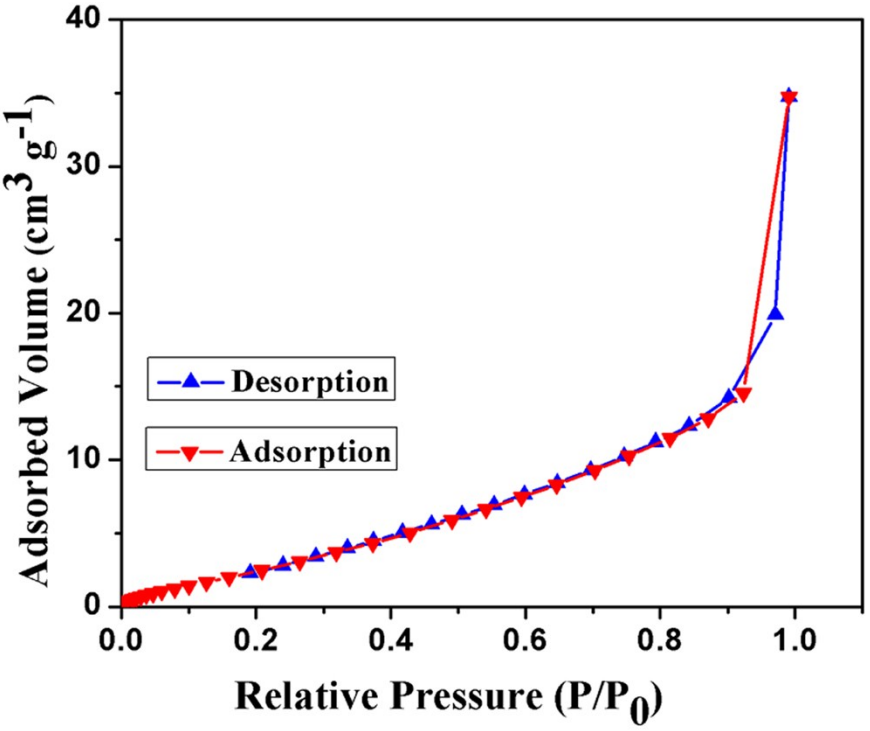


Fig. S2 N_2 adsorption/desorption isotherms of compound **1**.

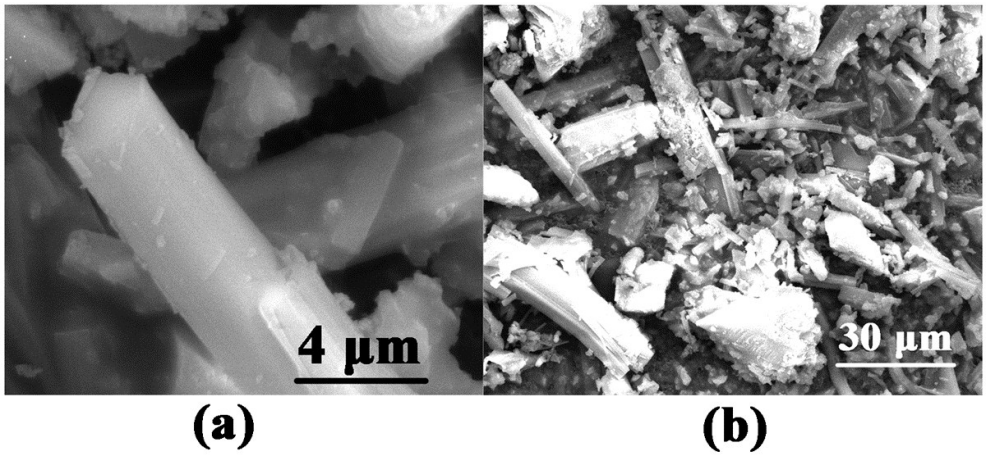
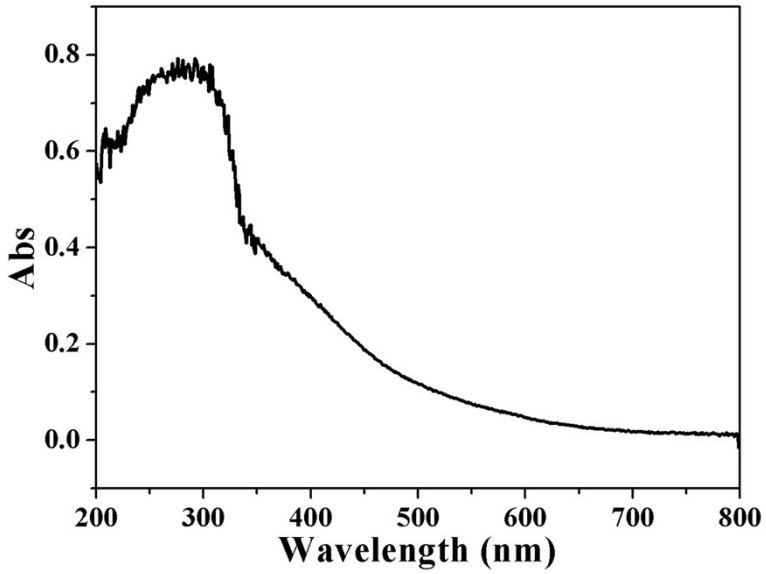
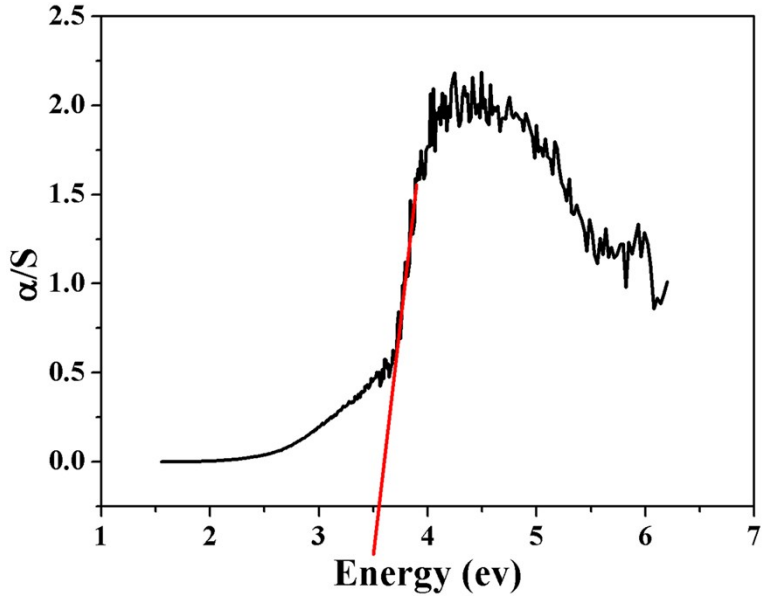


Fig. S3 SEM images of compound **1**.



(a)



(b)

Fig. S4 (a) UV-vis absorption spectrum in solid state. (b) Kubelka−Munk-tranformed diffuse reflectance spectrum of compound **1**.

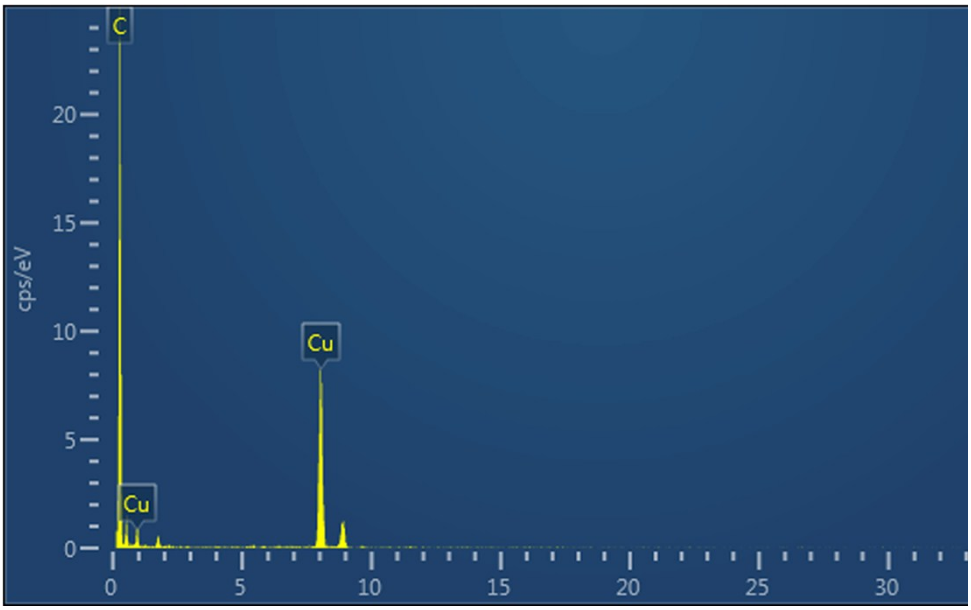


Fig. S5 Energy dispersive X-ray spectrometer of R-C@800.

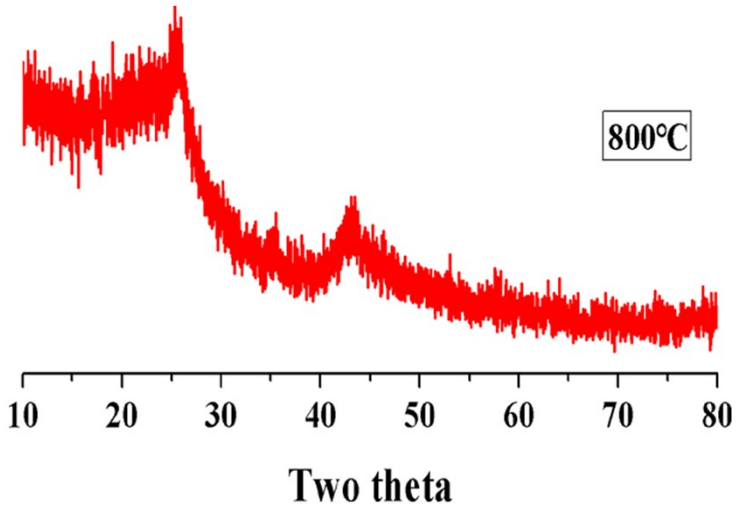


Fig. S6 PXRD pattern of R-C@800.

Table S1 Selected bond distances (Å) and angles (°) for **1**.

Zn(1)-O(6)#1	1.910(4)	Zn(1)-O(2)	1.950(4)
Zn(1)-O(8)	1.969(5)	Zn(1)-O(15)	1.981(14)
Zn(1)-O(15A)	1.981(14)	Zn(2)-O(3)#2	2.011(4)
Zn(2)-O(15A)	2.049(18)	Zn(2)-O(1W)	2.049(4)
Zn(2)-O(5)#1	2.067(4)	Zn(2)-O(2W)	2.142(5)
Zn(2)-O(15)	2.163(17)	Zn(2)-O(9)	2.207(4)

Zn(3A)-O(4)#2	1.819(5)	Zn(3A)-O(1)	1.986(5)
Zn(3A)-O(15)	2.011(13)	Zn(3A)-O(4WA)	2.085(11)
Zn(3A)-O(11)#3	2.110(5)	Zn(3B)-O(11)#3	1.936(5)
Zn(3B)-O(15A)	1.997(14)	Zn(3B)-O(4)#2	2.109(6)
Zn(3B)-O(1)	2.175(5)	Zn(3B)-O(10)#3	2.255(6)
O(6)#1-Zn(1)-O(2)	112.42(18)	O(6)#1-Zn(1)-O(8)	113.0(2)
O(2)-Zn(1)-O(8)	107.99(17)	O(6)#1-Zn(1)-O(15)	120.3(4)
O(2)-Zn(1)-O(15)	107.1(5)	O(8)-Zn(1)-O(15)	94.3(5)
O(6)#1-Zn(1)-O(15A)	108.1(4)	O(2)-Zn(1)-O(15A)	109.5(5)
O(8)-Zn(1)-O(15A)	105.6(5)	O(3)#2-Zn(2)-O(15A)	97.7(4)
O(3)#2-Zn(2)-O(1W)	86.58(17)	O(15A)-Zn(2)-O(1W)	173.8(4)
O(3)#2-Zn(2)-O(5)#1	173.10(16)	O(1W)-Zn(2)-O(5)#1	87.28(18)
O(3)#2-Zn(2)-O(2W)	87.5(2)	O(15A)-Zn(2)-O(2W)	83.7(5)
O(1W)-Zn(2)-O(2W)	92.0(2)	O(5)#1-Zn(2)-O(2W)	89.58(19)
O(3)#2-Zn(2)-O(15)	88.7(4)	O(1W)-Zn(2)-O(15)	173.9(4)
O(5)#1-Zn(2)-O(15)	97.6(4)	O(2W)-Zn(2)-O(15)	91.8(5)
O(3)#2-Zn(2)-O(9)	93.92(19)	O(15A)-Zn(2)-O(9)	97.4(4)
O(1W)-Zn(2)-O(9)	86.77(18)	O(5)#1-Zn(2)-O(9)	88.88(17)
O(2W)-Zn(2)-O(9)	178.05(16)	O(15)-Zn(2)-O(9)	89.6(4)
O(4)#2-Zn(3A)-O(1)	164.7(3)	O(4)#2-Zn(3A)-O(15)	95.7(5)
O(1)-Zn(3A)-O(15)	91.6(5)	O(4)#2-Zn(3A)-O(4WA)	84.7(3)
O(1)-Zn(3A)-O(4WA)	81.4(3)	O(15)-Zn(3A)-O(4WA)	142.7(6)
O(4)#2-Zn(3A)-O(11)#3	102.8(2)	O(1)-Zn(3A)-O(11)#3	85.81(19)
O(15)-Zn(3A)-O(11)#3	116.5(6)	O(4WA)-Zn(3A)-O(11)#3	99.6(4)
O(11)#3-Zn(3B)-O(15A)	149.3(6)	O(11)#3-Zn(3B)-O(4)#2	98.9(2)

O(11)#3-Zn(3B)-O(1)	85.26(19)	O(15A)-Zn(3B)-O(1)	99.8(4)
O(4)#2-Zn(3B)-O(1)	123.3(2)	O(11)#3-Zn(3B)-O(10)#3	62.5(2)
O(4)#2-Zn(3B)-O(10)#3	131.3(2)	O(1)-Zn(3B)-O(10)#3	100.8(2)

Symmetry transformations used to generate equivalent atoms: [#1] x, y+1, z-1; [#2] *x+1, y, z;* [#3] x, y-1, z.

References

1 L. J. Farrugia, *J. Appl. Cryst.*, 2012, **45**, 849-854.