

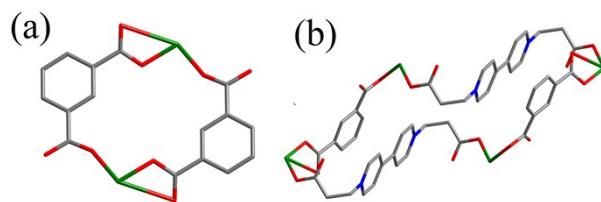
## Supporting Information

### A novel photochromic metal-organic framework with good anions and amines sensing

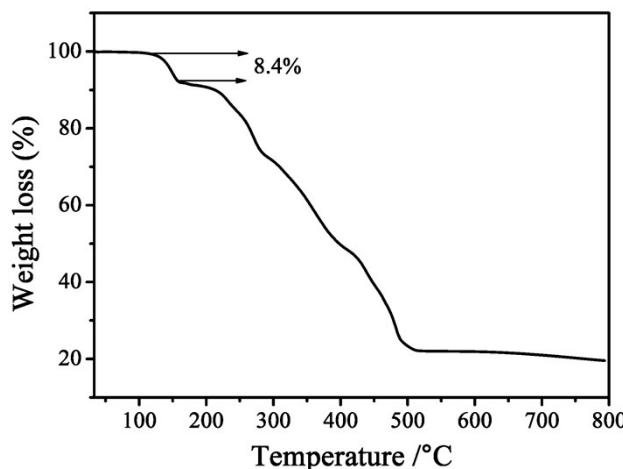
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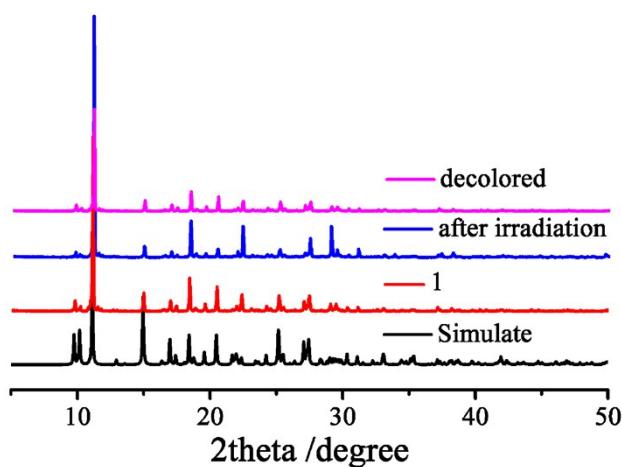
Fax: +86-0431-85098827; Tel: +86-0431-85099372; E-mail: hope 20130122@163. com, zhangh@nenu. edu. cn



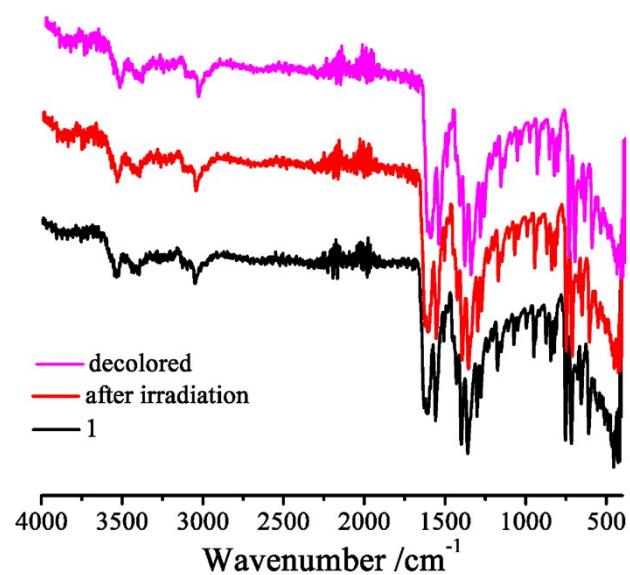
**Figure S1.** (a) The binuclear ring in **1**. (b) The tetrameric ring in **1**.



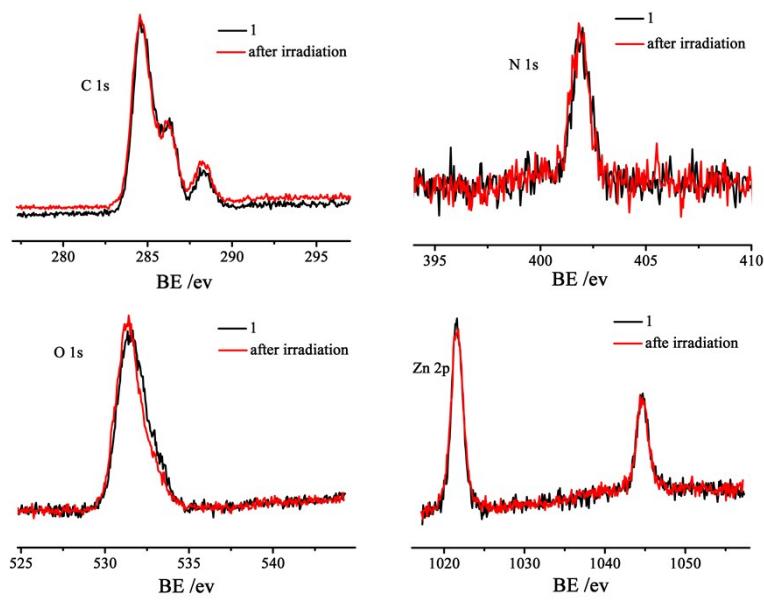
**Figure S2.** TGA curve of compound **1** was investigated using powder samples under N<sub>2</sub>. The weight loss of **1** is 8.4 % from 117 to 165 °C corresponding to the loss of two free water molecules in channels and the framework was collapsed until 524 °C.



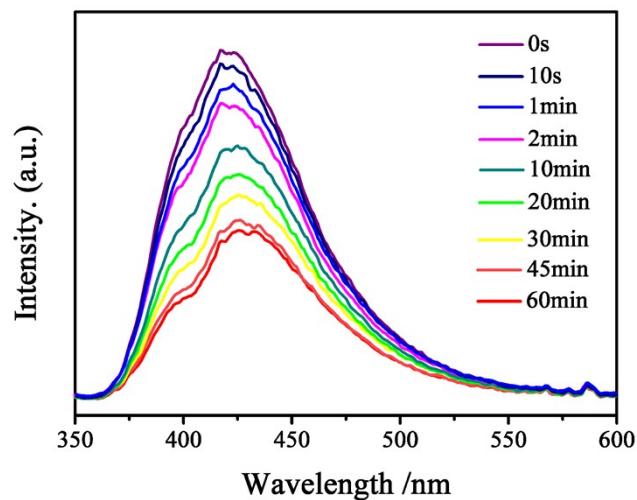
**Figure S3.** Simulated and experimental powder X-ray diffraction of **1** in the color-decoloration process.



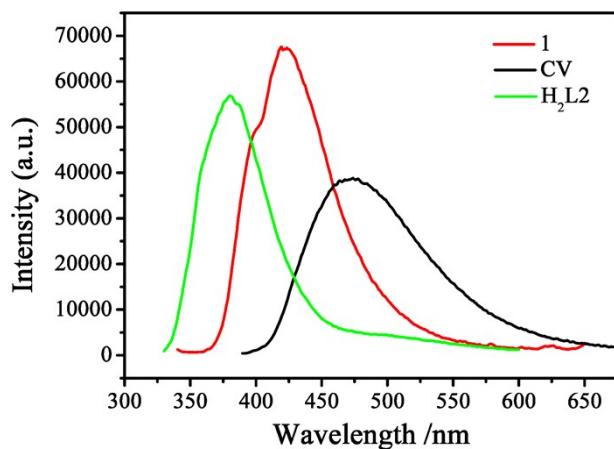
**Figure S4.** The IR spectrum of **1** in the color-decoloration process.



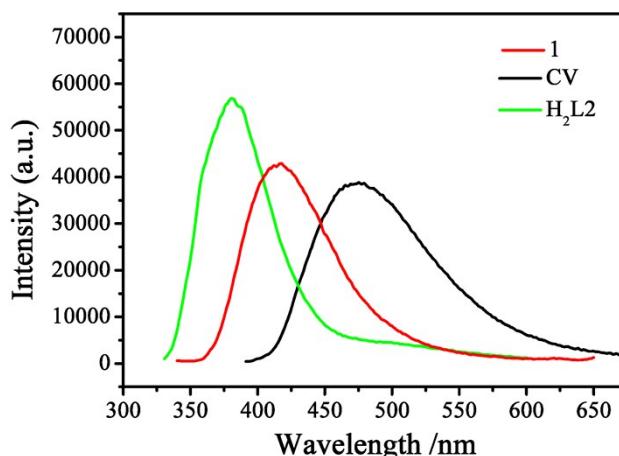
**Figure S5.** XPS (Al-K $\alpha$ ) core-level spectra of 1 before and after photoirradiation



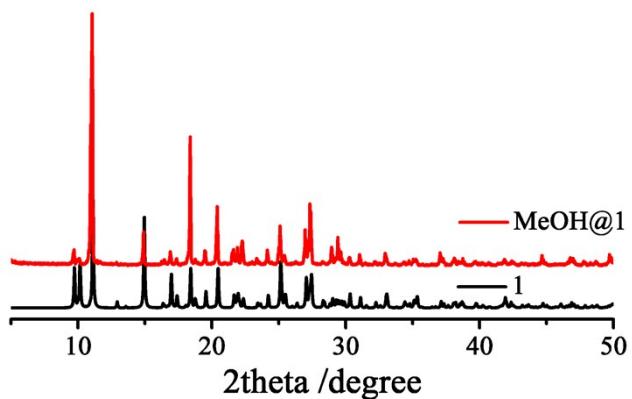
**Figure S6.** Time-dependent solid fluorescent spectra of 1.



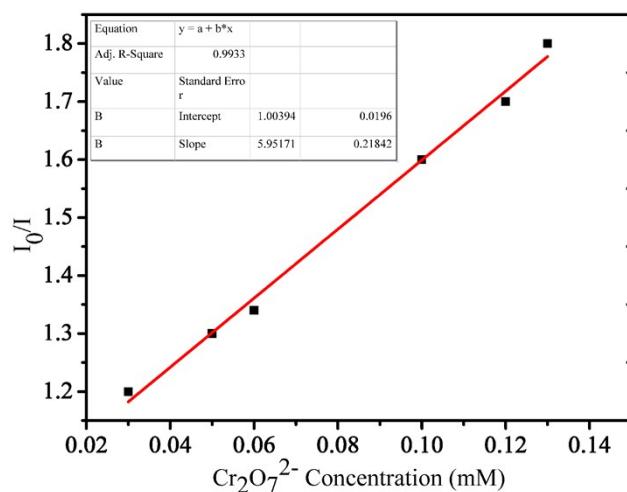
**Figure S7.** Solid-state emission spectra of CV, H<sub>2</sub>L2 ligands and compound 1 at room temperature



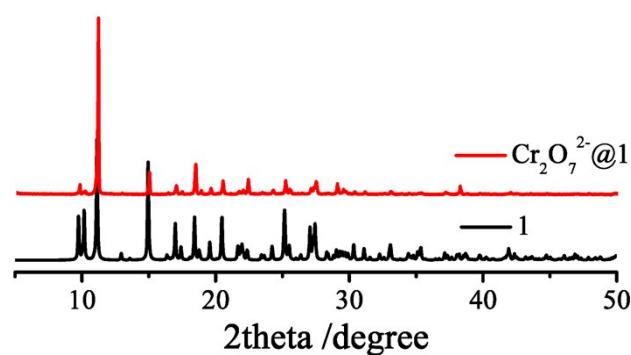
**Figure S8.** Emission spectra of CV and H<sub>2</sub>L2 ligands and compound 1 in MeOH/H<sub>2</sub>O (4:1) solution at room temperature.



**Figure S9.** PXRD pattern of MeOH@1 compared with **1**.



**Figure S10.** The Stern-Volmer plot of  $I_0/I$  versus the concentration of  $\text{Cr}_2\text{O}_7^{2-}$  for compound **1** at low concentration.



**Figure S11.** PXRD pattern of  $\text{Cr}_2\text{O}_7^{2-}@\mathbf{1}$  compared with **1**.

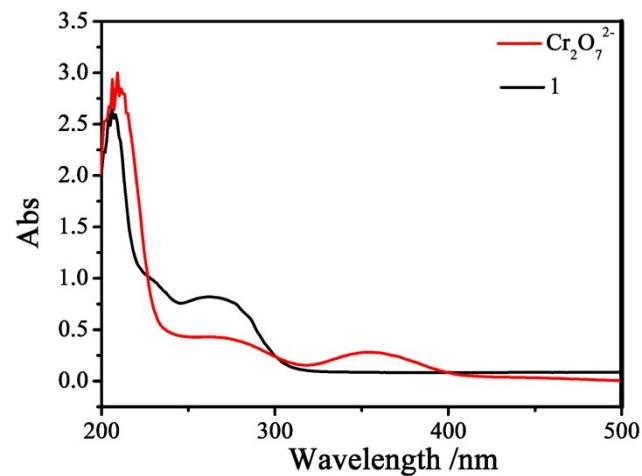
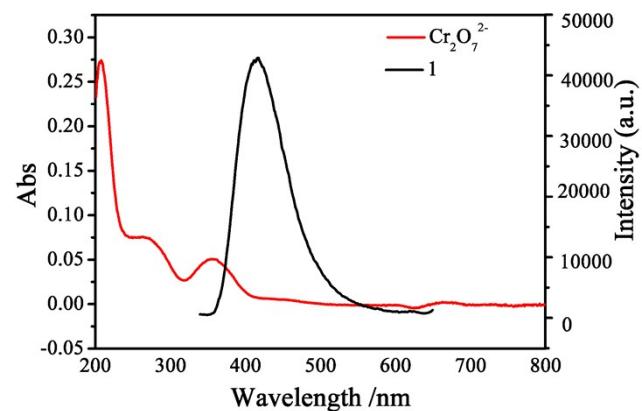
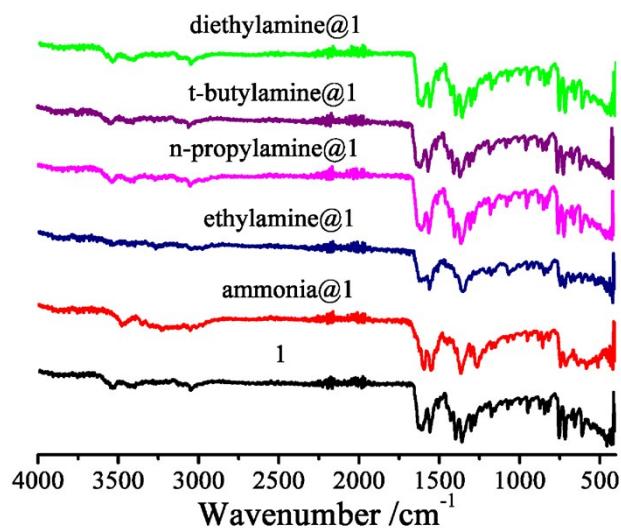


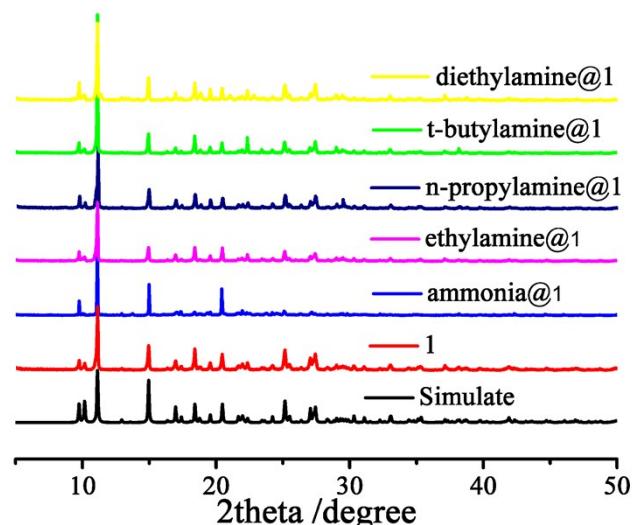
Figure S12. Liquid UV-vis spectra of  $\text{Cr}_2\text{O}_7^{2-}$  and **1** in MeOH/H<sub>2</sub>O (4:1) solution .



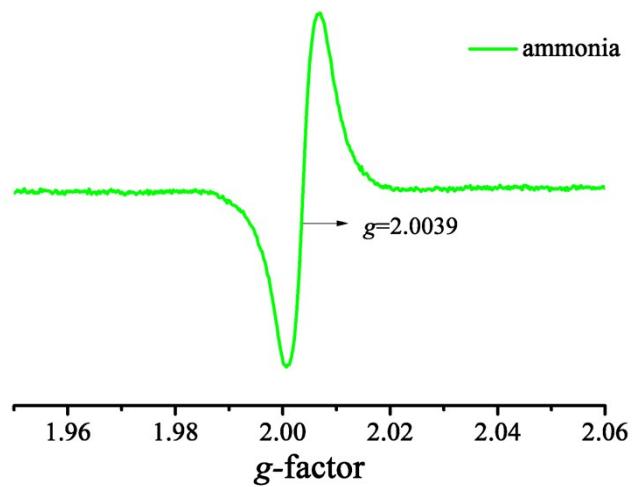
**Figure S13.** Spectra overlap between the absorption spectra of  $\text{Cr}_2\text{O}_7^{2-}$  anions and the excitation spectrum of **1** in MeOH/H<sub>2</sub>O (4:1) solution.



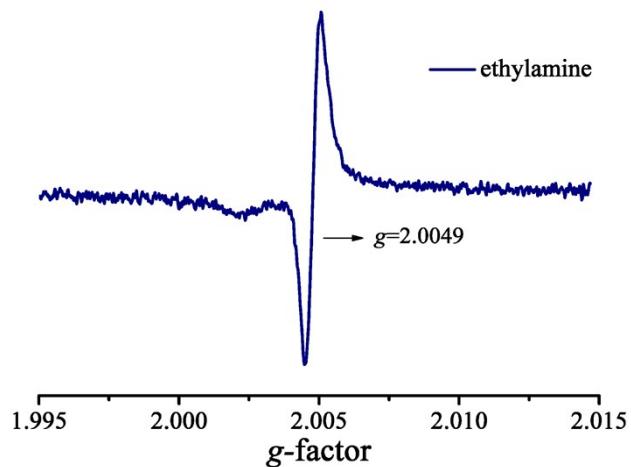
**Figure S14.** The FT-IR spectra of **1** and amine@**1**.



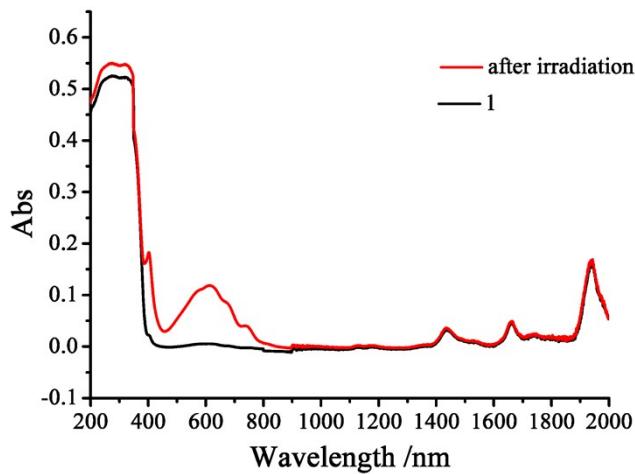
**Figure S15.** PXRD pattern of amine@**1** compared with the simulated pattern of **1**.



**Figure S16.** ESR spectrum of ammonia@1 in the solid state.



**Figure S17.** ESR spectrum of ethylamine@1 in the solid state.



**Figure S18.** The UV-vis diffuse-reflectance spectra of **1**from 200 to 2000nm.

**Table S1.** Comparison among varous MOF sensors for  $\text{Cr}_2\text{O}_7^{2-}$  detection.

Fluorescent Materials	analyte	Quenching Constant ( $K_{sv}$ , M <sup>-1</sup> )	Detection Limits(μM)	Ref
$[\text{Eu}(\text{L})(\text{HCOO})(\text{H}_2\text{O})]_n$	$\text{Cr}_2\text{O}_7^{2-}$	2762.6	1.0	S1
$[\text{Tb}(\text{L})(\text{HCOO})(\text{H}_2\text{O})]_n$	$\text{Cr}_2\text{O}_7^{2-}$	2133.5	2.1	S1
$[\text{Zn}_2(\text{ttz})\text{H}_2\text{O}]_n$	$\text{Cr}_2\text{O}_7^{2-}$	$2.19 \times 10^3$	20	S2
$\{\text{[Cd}(\text{L})(\text{SDBA})(\text{H}_2\text{O})]\cdot 0.5\text{H}_2\text{O}\}_n$	$\text{Cr}_2\text{O}_7^{2-}$	$4.97 \times 10^3$	48.6	S3
$[\text{Zn}(\text{IPA})(\text{L})]_n$	$\text{Cr}_2\text{O}_7^{2-}$	$1.37 \times 10^3$	12.02	S4
$[\text{Cd}(\text{IPA})(\text{L})]_n$	$\text{Cr}_2\text{O}_7^{2-}$	$2.91 \times 10^3$	2.26	S4
$[\text{Eu}_7(\text{mtb})_5(\text{H}_2\text{O})_{16}] \cdot \text{NO}_3 \cdot 8\text{DMA} \cdot 18\text{H}_2\text{O}$	$\text{Cr}_2\text{O}_7^{2-}$	$3.3 \times 10^4$	0.011	S5
$[\text{Zn}(\text{btz})]_n$	$\text{Cr}_2\text{O}_7^{2-}$	$4.23 \times 10^3$	2	S2
$[\text{Zn}(\text{CV})(\text{L}2)] \cdot 2\text{H}_2\text{O}$	$\text{Cr}_2\text{O}_7^{2-}$	$5.95 \times 10^3$	2.49	This work

**Table S2.** The crystal data and structure refinement of compound **1**.

Empirical formula	$\text{C}_{16}\text{H}_{16}\text{NO}_8\text{Zn}$
Formula weight	415.70
Temperature/K	300.01
Crystal system	triclinic
Space group	$P\bar{1}$
a/Å	9.5023(4)
b/Å	9.5077(5)
c/Å	10.6017(6)

$\alpha/\circ$	68.918(2)
$\beta/\circ$	66.791(2)
$\gamma/\circ$	86.570(2)
Volume/ $\text{\AA}^3$	817.62(7)
$\rho_{\text{calcd}}/\text{cm}^3$	1.6884
$\mu/\text{mm}^{-1}$	1.550
F(000)	426.9
Goodness-of-fit on $F^2$	1.084
Final R indexes [ $ I >=2\sigma(I)$ ]	$R_1 = 0.0274, wR_2 = 0.0682$
Final R indexes [all data]	$R_1 = 0.0344, wR_2 = 0.0744$

<sup>a</sup> $R_1 = \sum ||F_0| - |F_c|| / \sum |F_0|$ . <sup>b</sup> $wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)]^{1/2}$

**Table S3.** Selected bond lengths for compound **1**.

Zn(1)-O(1)	1.9389(16)	C(5)-C(6)	1.391(3)
Zn(1)-O(2)#1	1.9679(16)	C(6)-C(15)	1.386(3)
O(1)-C(12)	1.285(3)	C(7)-C(16)	1.392(3)
O(2)-Zn(1)#1	1.9679(16)	C(7)-C(7)#4	1.482(5)
O(3)-C(1)	1.261(3)	C(8)-H(8)	0.9300
O(4)-C(3)	1.289(3)	C(9)-H(9)	0.9300
N(1)-C(14)	1.346(3)	C(10)-H(10)	0.9300
N(1)-C(11)	1.489(3)	C(11)-H(11B)	0.9700
C(1)-C(2)	1.493(3)	C(13)-H(13)	0.9300
C(2)-C(8)	1.391(3)	C(14)-H(14)	0.9300
C(3)-C(4)	1.514(3)	C(16)-H(16)	0.9300
C(4)-C(11)	1.520(4)	O(1W)-H(1WA)	0.844(10)

Symmetry transformations used to generate equivalent atoms: <sup>1</sup>1-X, -Y, 1-Z; <sup>2</sup>1+X, +Y, +Z; <sup>3</sup>1-X, 1-Y, -Z.

**Table S4.** Selected angles for **1**.

O(1)-Zn(1)-O(4)	117.67(8)	C(13)-C(7)-C(7)#4	121.7(3)
O(1)-Zn(1)-O(2)#1	99.58(7)	C(15)-C(9)-C(2)	120.1(2)
O(4)-Zn(1)-O(2)#1	116.58(8)	N(1)-C(10)-H(10)	119.7
O(1)-Zn(1)-O(3)#2	112.64(7)	N(1)-C(11)-C(4)	112.0(2)
O(4)-Zn(1)-O(3)#2	100.66(8)	O(6)-C(12)-O(1)	123.8(2)
O(2)#1-Zn(1)-O(3)#2	110.13(8)	C(14)-C(13)-C(7)	120.7(2)
C(12)-O(1)-Zn(1)	114.70(15)	C(7)-C(13)-H(13)	119.7
C(1)-O(2)-Zn(1)#1	137.16(16)	C(13)-C(14)-H(14)	119.8
C(1)-O(3)-Zn(1)#3	113.73(15)	C(9)-C(15)-C(6)	120.1(2)
C(3)-O(4)-Zn(1)	116.38(16)	C(10)-C(16)-H(16)	119.6
C(14)-N(1)-C(10)	120.7(2)	C(7)-C(16)-H(16)	119.6
O(2)-C(1)-O(3)	124.0(2)	H(1WA)-O(1W)-H(1WB)	104(2)

C(9)-C(2)-C(1)	121.20(19)	H(2WA)-O(2W)-H(2WB)	106(2)
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Symmetry transformations used to generate equivalent atoms:  $^{11}\text{-X, -Y, 1-Z; }^{21}\text{+X, +Y, +Z; }^{31}\text{-1+X, +Y, +Z.}$

**References:**

- S1:** Z. Sun, M. Yang, Y. Ma and L. Li. *Cryst. Growth Des.*, 2017, **17**, 4326-4335.
- S2:** C.-S. Cao, H.-C. Hu, H. Xu, W.-Z. Qiao and B. Zhao, *CrystEngComm.*, 2016, **18**, 4445-4451.
- S3:** S. Chen, Z. Shi, L. Qin, H. Jia and H. Zheng, *Cryst. Growth Des.*, 2017, **17**, 67-72.
- S4:** B. Parmar, Y. Rachuri, K. K. Bisht, R. Laiya and E. Suresh, *Inorg. Chem.*, 2017, **56**, 2627-2638.
- S5:** W. Liu, Y. Wang, Z. Bai, Y. Li, Y. Wang, L. Chen, L. Xu, J. Wu, Z. Chai and S. Wang, *ACS Appl. Mater. Interfaces*, 2017, **9**, 16448-16457.