

*Electronic supplementary information*

**A unique zinc-organic framework constructed through *in situ* ligand synthesis for conversion of CO<sub>2</sub> under mild conditions and as a luminescent sensor for Cr<sub>2</sub>O<sub>7</sub><sup>2-</sup>/CrO<sub>4</sub><sup>2-</sup>**

Tian-Qun Song,<sup>a</sup> Jie Dong,<sup>b</sup> Hong-Ling Gao,<sup>a</sup> Jian-Zhong Cui,<sup>\*a</sup> Bin Zhao<sup>\*b</sup>

*a. Department of Chemistry, National Demonstration Center for Experimental Chemistry & Chemical engineering Education, National Virtual Simulation Experimental Teaching Center for Chemistry & Chemical engineering Education, Tianjin University, Tianjin 300072, P. R. China*

*b. Department of Chemistry, Nankai University, Tianjin 300071, P. R. China*

E-mail: cuijianzhong@tju.edu.cn and zhaobin@nankai.edu.cn

**List of Contents**

**Supplementary Experimental Section**

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

**Table S2.** Hydrogen bonding data for **1**.

**Figure S1.** The FT-IR spectra of compound **1** and after catalytic recyclings.

**Figure S2.** The PXRD patterns for the simulated and as-synthesized samples for **1** (a); The PXRD patterns for **1** immersing in common organic solvents (b); The PXRD patterns for **1** in various pH values solutions from 1.0 to 14.0 (c).

**Figure S3.** TG curve for compound **1**.

**Figure S4.** The PXRD patterns of **1** after six catalytic recyclings and simulated one from **1**.

**Figure S5.** CO<sub>2</sub> isotherm of **1** at 273 K.

**Figure S6.** The possible mechanism for the cycloaddition reaction with epoxides and CO<sub>2</sub>.

**Figure S7.** The emission spectrum of **1** ( $\lambda_{\text{excited}} = 270 \text{ nm}$ ).

**Figure S8.** The luminescence intensity of **1**-Cr<sub>2</sub>O<sub>7</sub><sup>2-</sup> (a) and **1**-CrO<sub>4</sub><sup>2-</sup> (b) under mixed anions.

**Figure S9.** The PXRD patterns of **1** after luminescent recycling and simulated one from **1**.

**Figure S10.** The UV-vis spectra of the K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> and K<sub>2</sub>CrO<sub>4</sub> solutions.

**Table S3.** The ICP results of **1** after catalytic recyclings (filter liquor) and luminescent recyclings (soild sample), respectively.

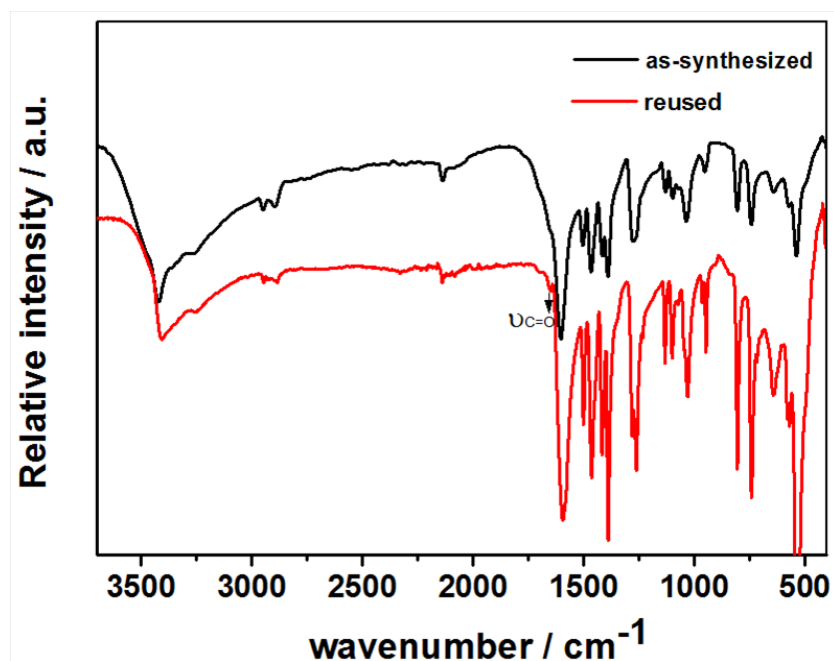
**Table S1.** Selected bond lengths (Å) and bond angles (°) for compound **1**.

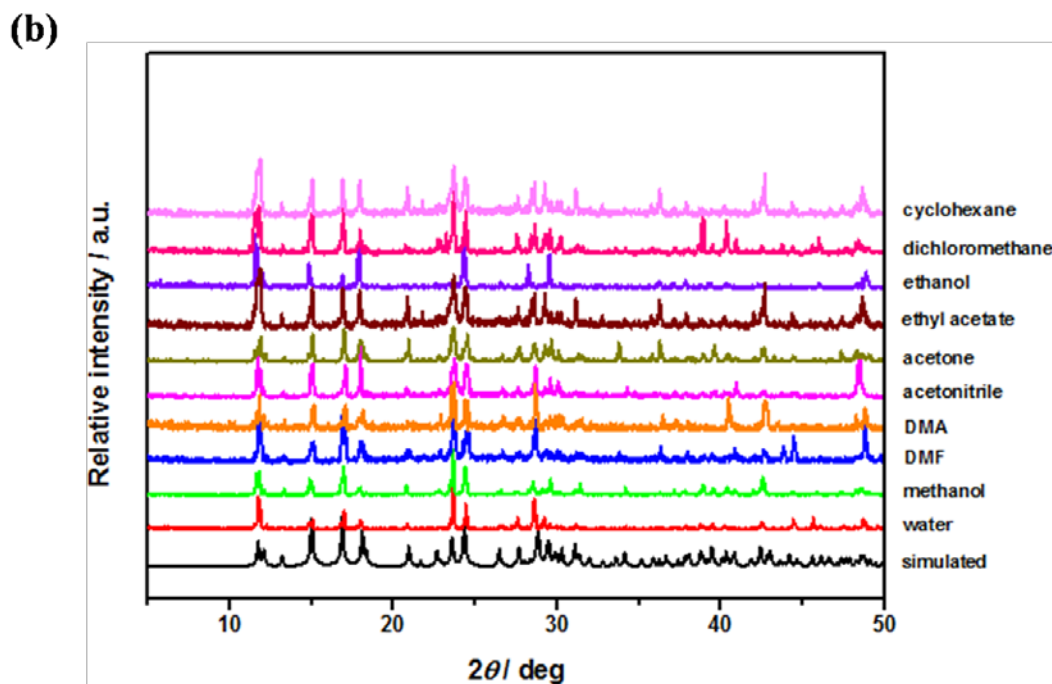
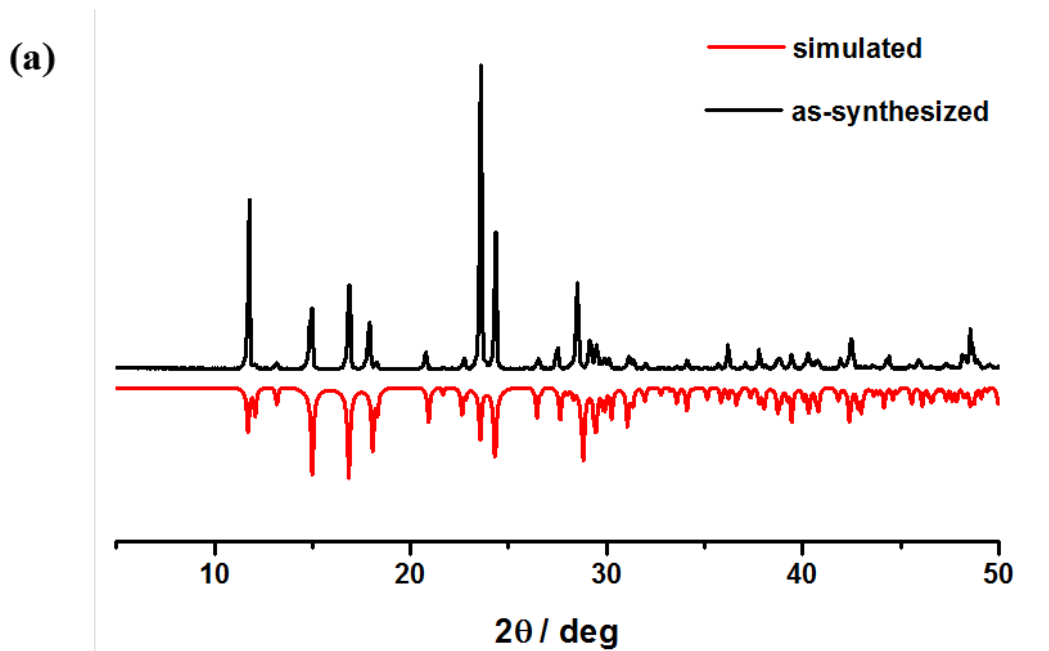
<i>Bond distances</i>			
Zn1-O4	2.071(5)	Zn2-N1	2.046 (7)
Zn1-O4#2	2.222(6)	Zn2-O3#1	1.915(6)
Zn1-O7#2	2.222(6)	Zn2-O3	1.922(5)
Zn1-O7	2.086(7)	Zn2#3-O3	1.915(5)
Zn1-N11	2.086(7)	Zn2-O5	1.997(6)
<i>Angles</i>			
O4#2-Zn1-O4	180.0(4)	O3#1-Zn2-N1	101.2(3)
O4#2-Zn1-O7#2	90.8(2)	O3-Zn2-N1	108.5(3)
O4-Zn1-O4#2	89.2(2)	O3-Zn2- O3#1	116.6(2)
O4-Zn1-N11	87.4(2)	O5-Zn2- O3#1	107.4(2)
O4-Zn1-N11#2	92.6(2)	O3-Zn2-O5	118.6(2)
O4#2-Zn1-N11#2	87.4(2)	O5-Zn2-N1	102.1(3)
O7-Zn1-O7#2	180.0(3)	N8-Zn1-N1	127.3(6)
N11-Zn1-O7#2	89.5(3)	C12-Zn2-N1	126.6(5)
N11-Zn1-O7	90.5(3)	Zn2-O3-Zn2#3	127.4(3)
C1-O4-Zn1	133.6(6)	C1-O5-Zn2	112.8(5)
N9-N11-Zn1	126.8(5)	N11-Zn1- C12#5	125.3(6)

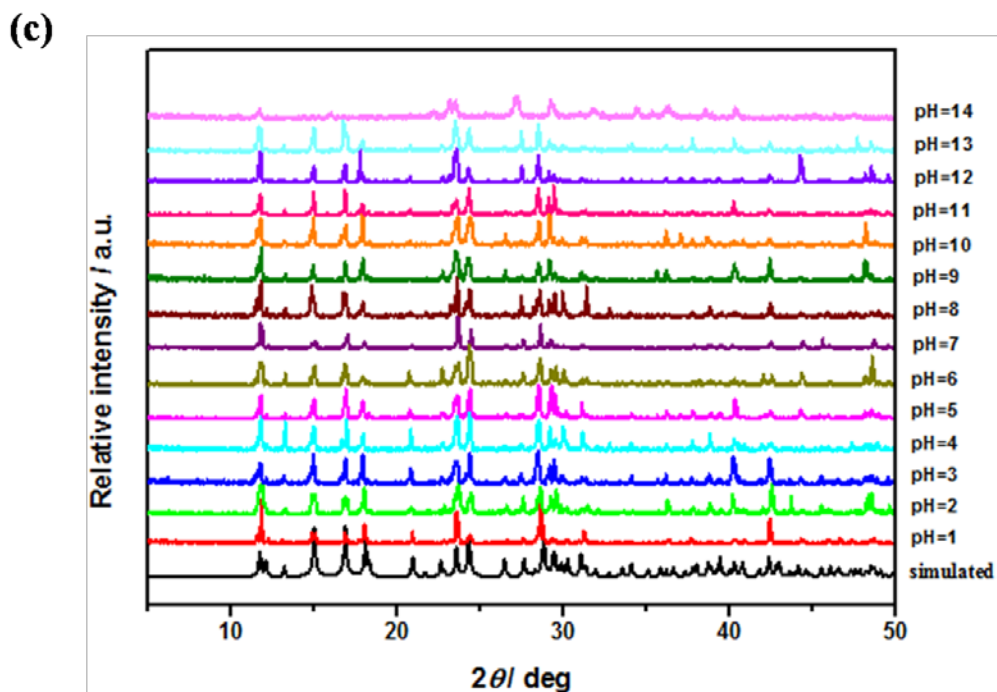
#1 +X, 1/2-Y, 1/2+Z; #2 -X, -Y, -Z, #3 +X, 1/2-Y, -1/2+Z; #4 1-X, 1/2+Y, 1/2-Z; #5 1-X, -1/2+Y, 1/2-Z

**Table S2.** Hydrogen bonding data for compound **1**.

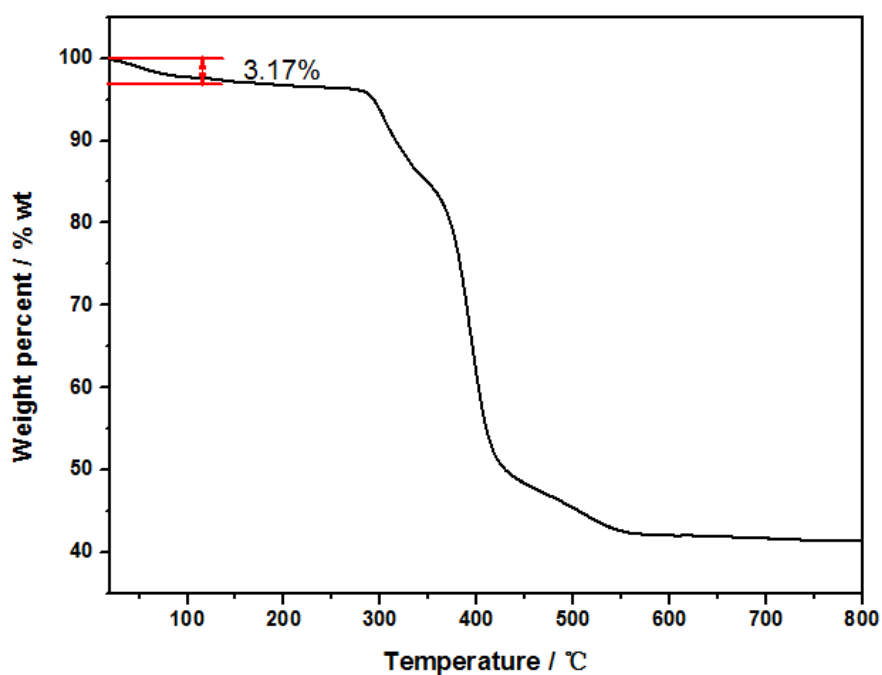
D-H...A	d(D-H) (Å)	d(H...A) (Å)	d(D...A) (Å)	D-H...A (°)
O(7)-H(7A)-O(5)	0.90	2.54	3.0759	118
O(7)-H(7B)-N(8)	0.85	2.04	2.8839	176
C(13)-H(13B)-O(5)	0.97	2.37	3.3380	176

**Figure S1.** The FT-IR spectra of compound **1** and after catalytic recyclings.





**Figure S2.** (a) The PXRD patterns for the simulated and as-synthesized samples for **1**; (b) The PXRD patterns for **1** immersing in common organic solvents; (c) The PXRD patterns for **1** in various pH values solutions from 1.0 to 14.0.



**Figure S3.** TG curve for compound **1**.

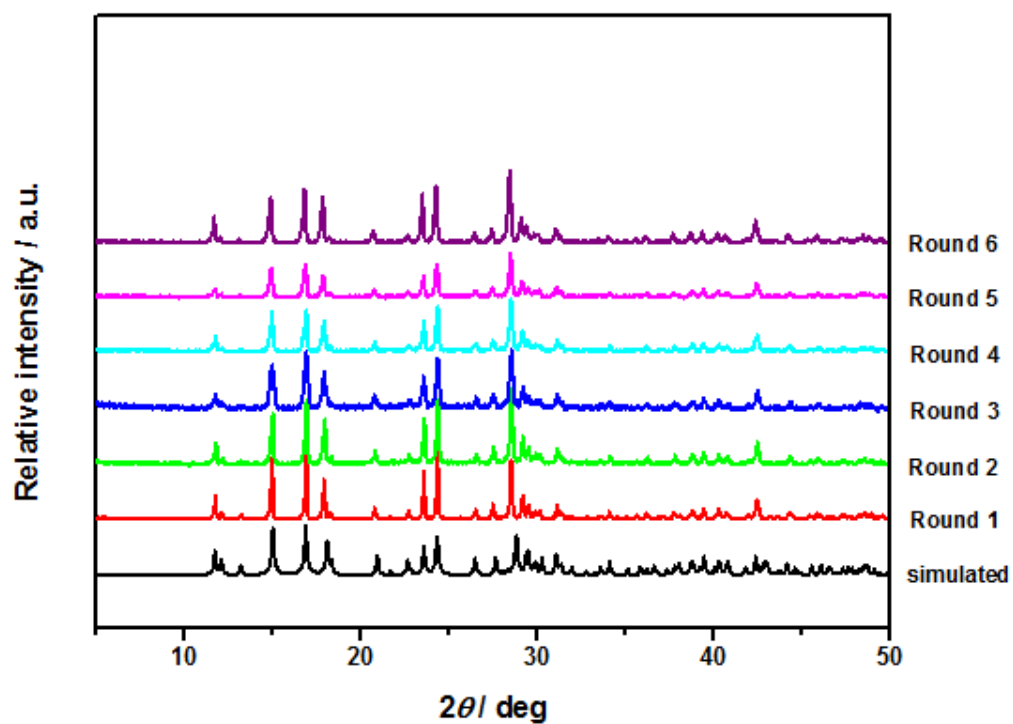


Figure S4. The PXRD patterns of **1** after catalytic recyclings and simulated one from **1**.

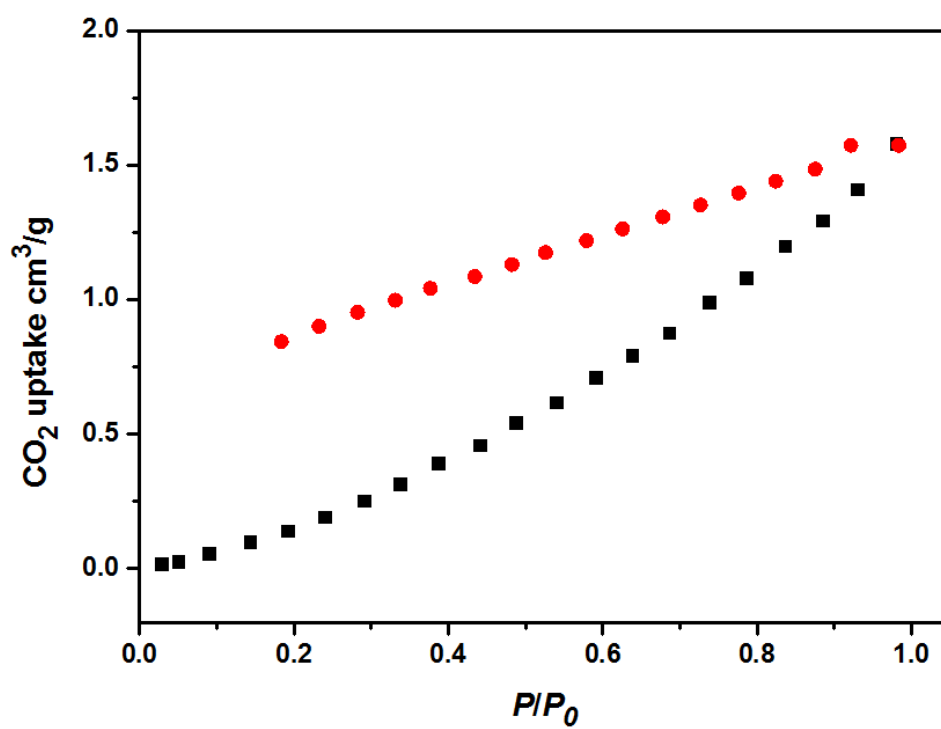
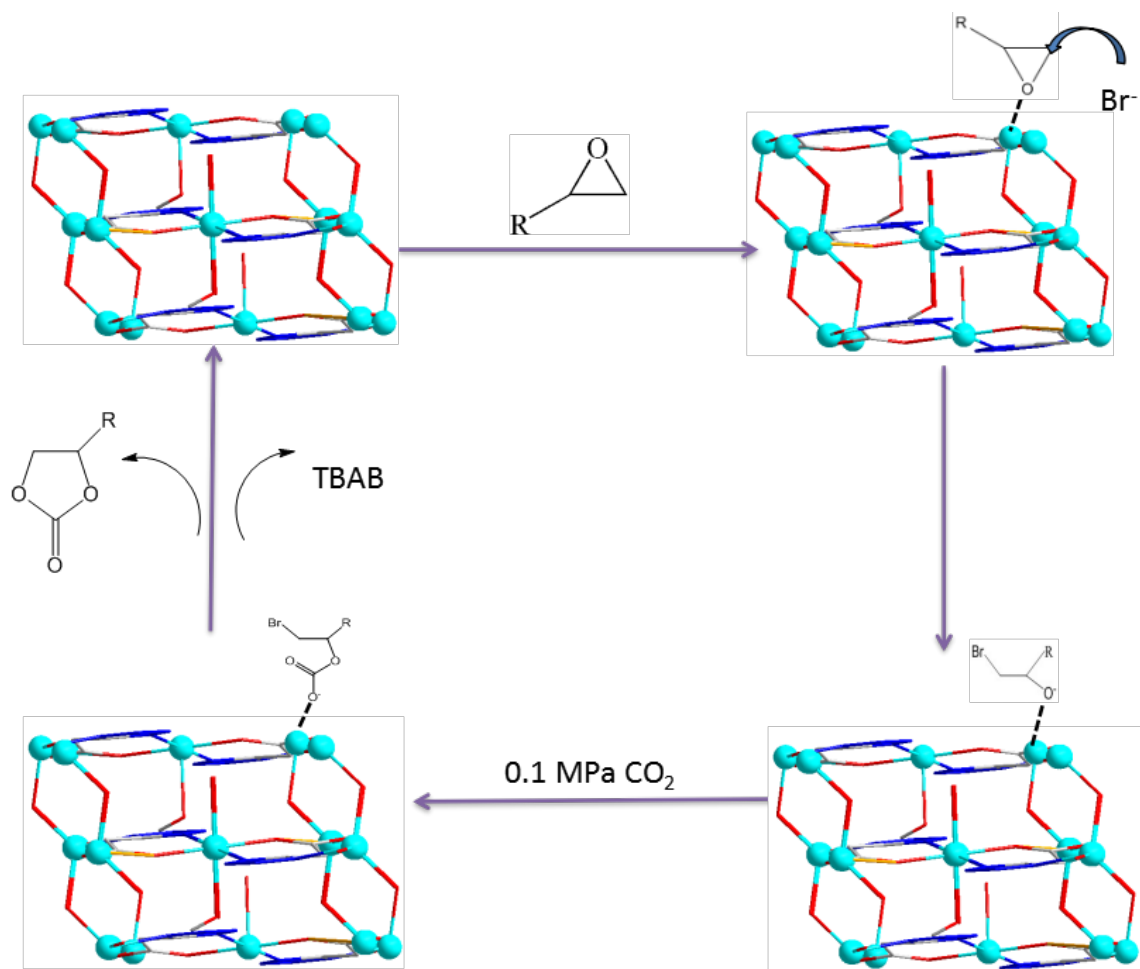
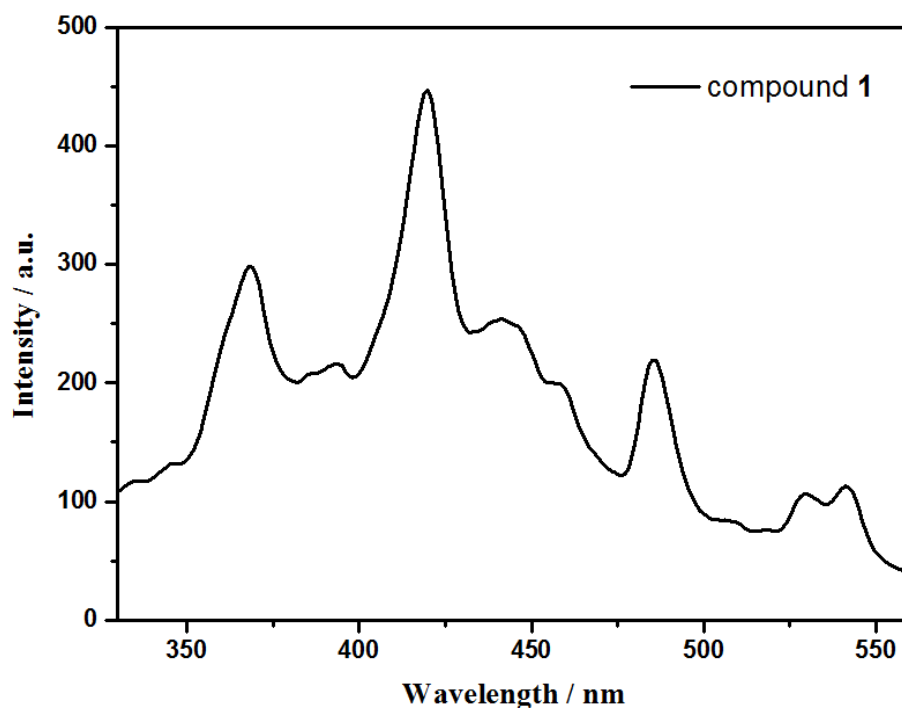


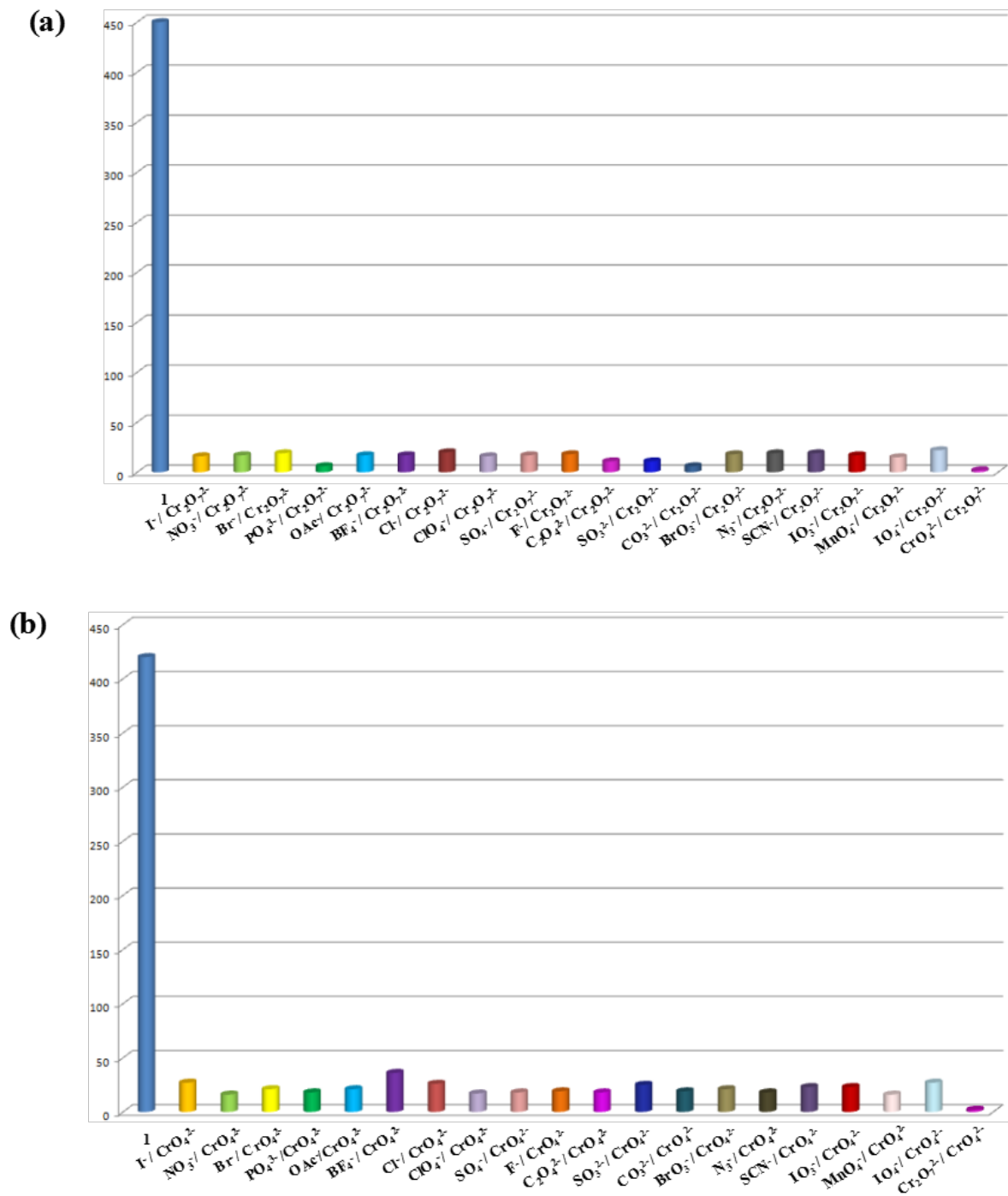
Figure S5. CO<sub>2</sub> isotherm of **1** at 273 K.



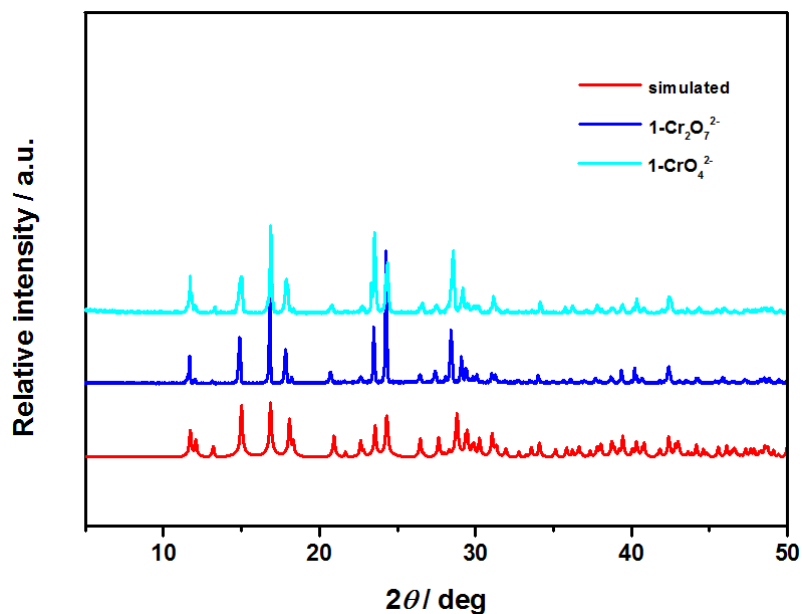
**Figure S6.** The possible mechanism for the cycloaddition reaction with epoxides and CO<sub>2</sub> into cyclic carbonates.



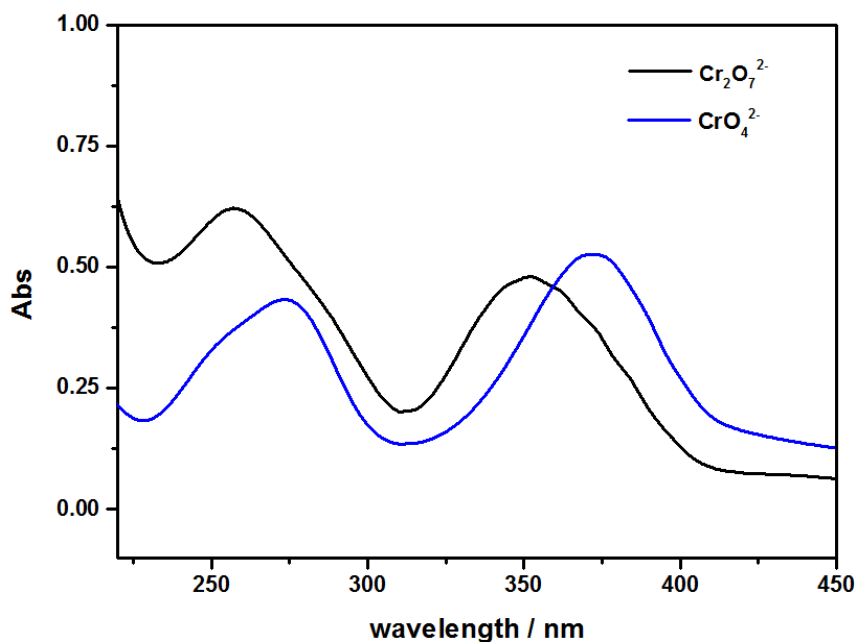
**Figure S7.** The emission spectrum of **1** ( $\lambda_{\text{excited}} = 270$  nm).



**Figure S8.** The luminescence intensity of **1**-Cr<sub>2</sub>O<sub>7</sub><sup>2-</sup> (a) and **1**-CrO<sub>4</sub><sup>2-</sup> (b) under mixed anions.



**Figure S9.** The PXRD patterns of **1** after luminescent recycling and simulated one from **1**.



**Figure S10.** The UV-vis spectra of the  $\text{K}_2\text{Cr}_2\text{O}_7$  and  $\text{K}_2\text{CrO}_4$  solutions.

**Table S3.** The ICP results of **1** after catalytic recyclings (filter liquor) and luminescent recyclings (soild sample), respectively.

	Compound <b>1</b>
<b>1</b> after catalytic recyclings ( $\text{Zn}^{2+}$ of filter liquor)	0.69 ppm
<b>1</b> as $\text{Cr}_2\text{O}_7^{2-}$ sensor after luminescent recyclings ( $\text{Cr}^{6+}$ of soild sample)	below detectable limit (0.0069 ppm)
<b>1</b> as $\text{CrO}_4^{2-}$ sensor after luminescent recyclings ( $\text{Cr}^{6+}$ of soild sample)	below detectable limit (0.0039 ppm)