

A Two-fold Interpenetrated Zinc-Organic Framework: Luminescent Detection of $\text{CrO}_4^{2-}/\text{Cr}_2\text{O}_7^{2-}$ and Chemical Conversion of CO_2

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Table S1. Crystal data and structure refinement for compound **1**.

Identification code	1
Empirical formula	$\text{C}_{23}\text{H}_{21.4}\text{N}_3\text{O}_{8.2}\text{Zn}$
Formula weight	536.44
Temperature/K	120.00(10)
Crystal system	triclinic
Space group	<i>P-1</i>
<i>a</i> /Å	10.1188(7)
<i>b</i> /Å	10.9420(11)
<i>c</i> /Å	11.7024(10)
$\alpha/^\circ$	63.853(9)
$\beta/^\circ$	82.358(6)
$\gamma/^\circ$	72.588(7)
Volume/Å ³	1109.81(18)
<i>Z</i>	2
$\rho_{\text{calc}}/\text{cm}^3$	1.579
μ/mm^{-1}	1.164
F(000)	535.0
Radiation	MoK α ($\lambda = 0.71073$)
2 Θ range for data collection/°	5.728 to 50.016
Index ranges	-11 ≤ <i>h</i> ≤ 12, -12 ≤ <i>k</i> ≤ 13, -7 ≤ <i>l</i> ≤ 13
Independent reflections	3894 [$R_{\text{int}} = 0.0469$, $R_{\text{sigma}} = 0.0784$]
Goodness-of-fit on F^2	0.941
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0544$, $wR_2 = 0.1313$
Final R indexes [all data]	$R_1 = 0.0761$, $wR_2 = 0.1459$

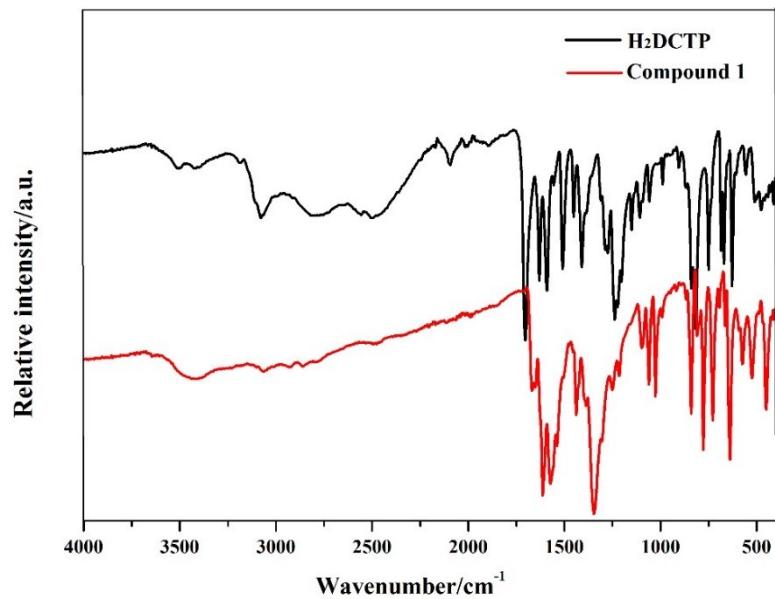


Figure S1. The FT-IR spectra of the ligand (black) and the compound 1 (red).

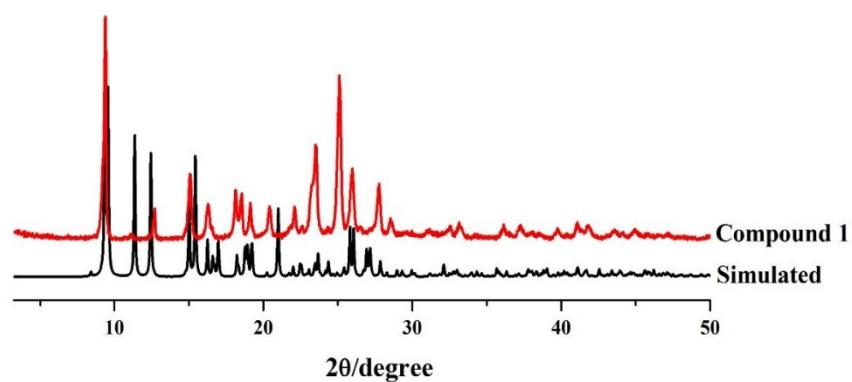


Figure S2. The PXRD patterns of **1**, synthesized compounds (red) and simulated from the single-crystal data (black).

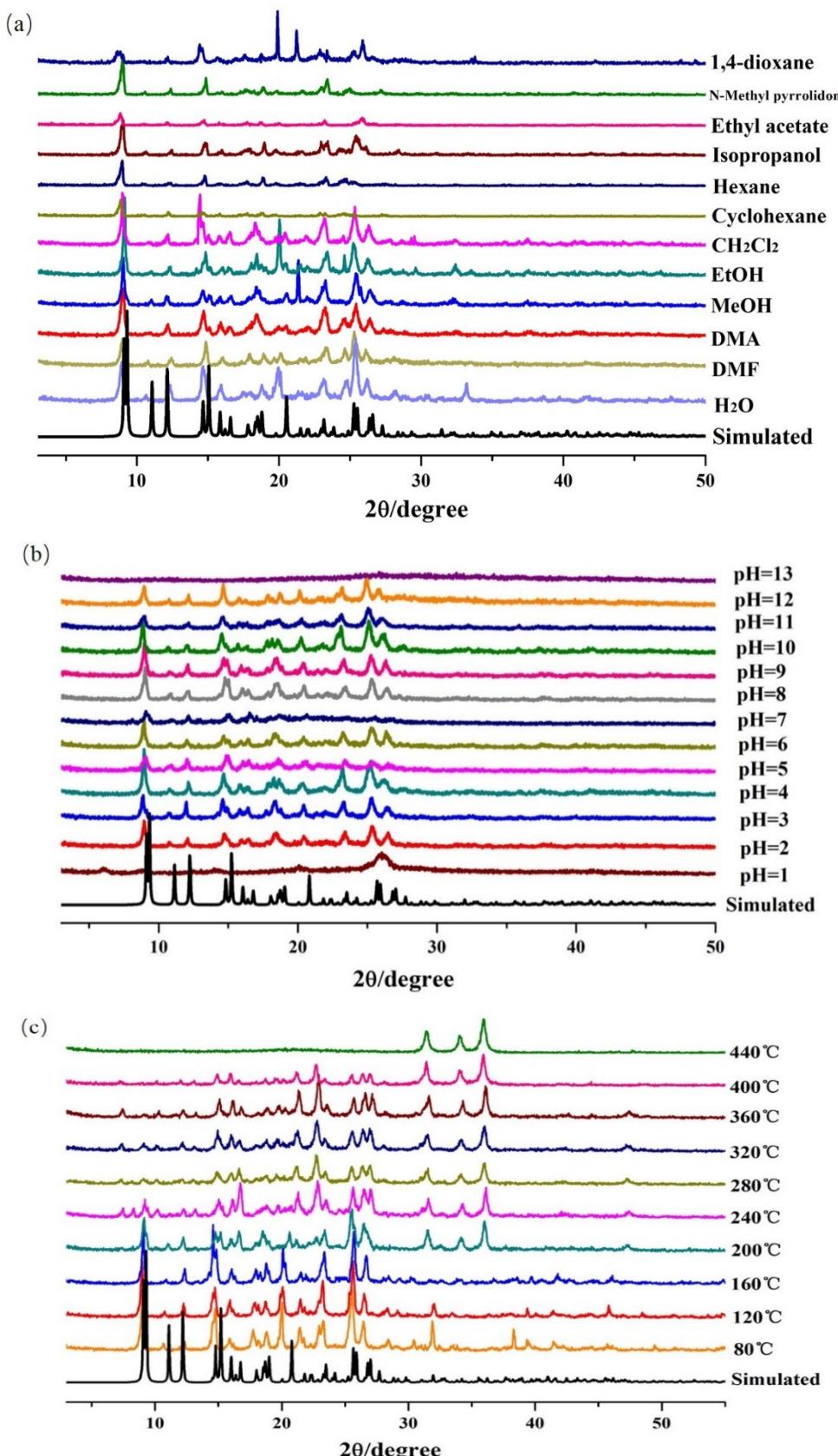


Figure S3. The PXRD patterns of compound **1** after immersing in various organic solvents (a) and different pH values from 1.0 to 13.0 (b); the PXRD patterns of compound **1** after heating at different temperatures (c).

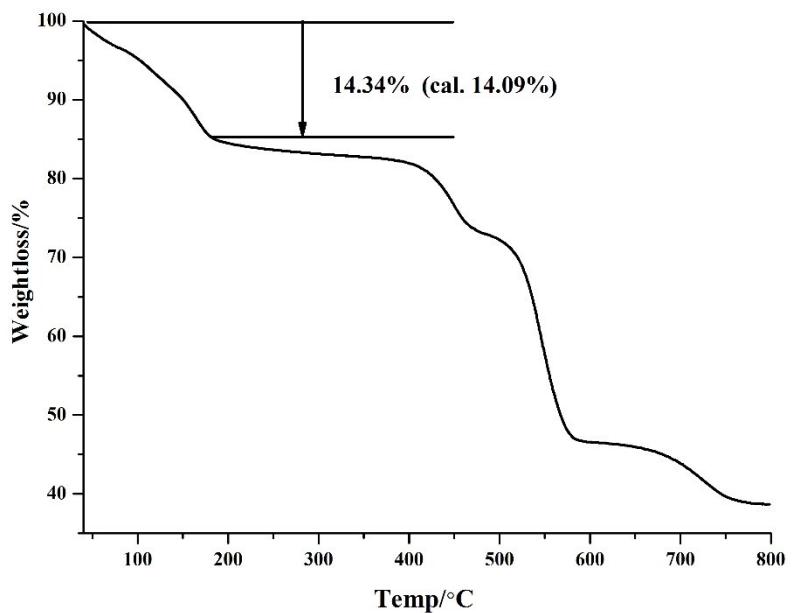
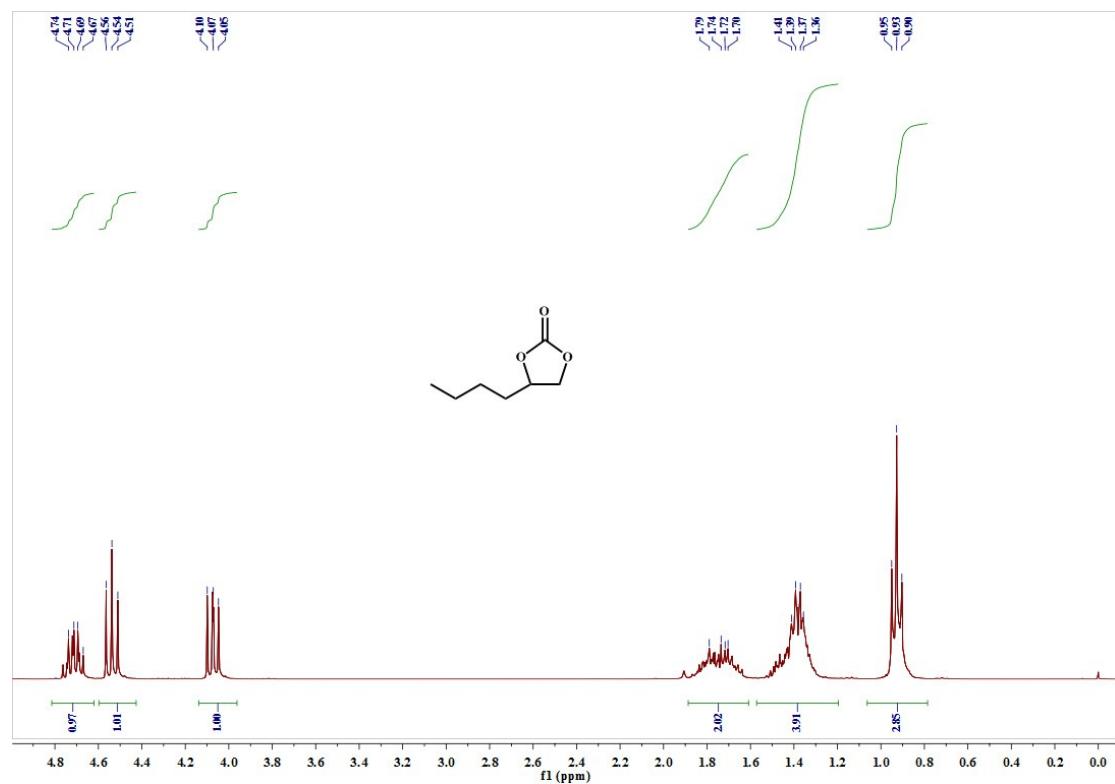


Figure S4. The thermogravimetric analyses curve of compound **1**, the weight loss of 14.34% is similar to the calculated value (14.09%).

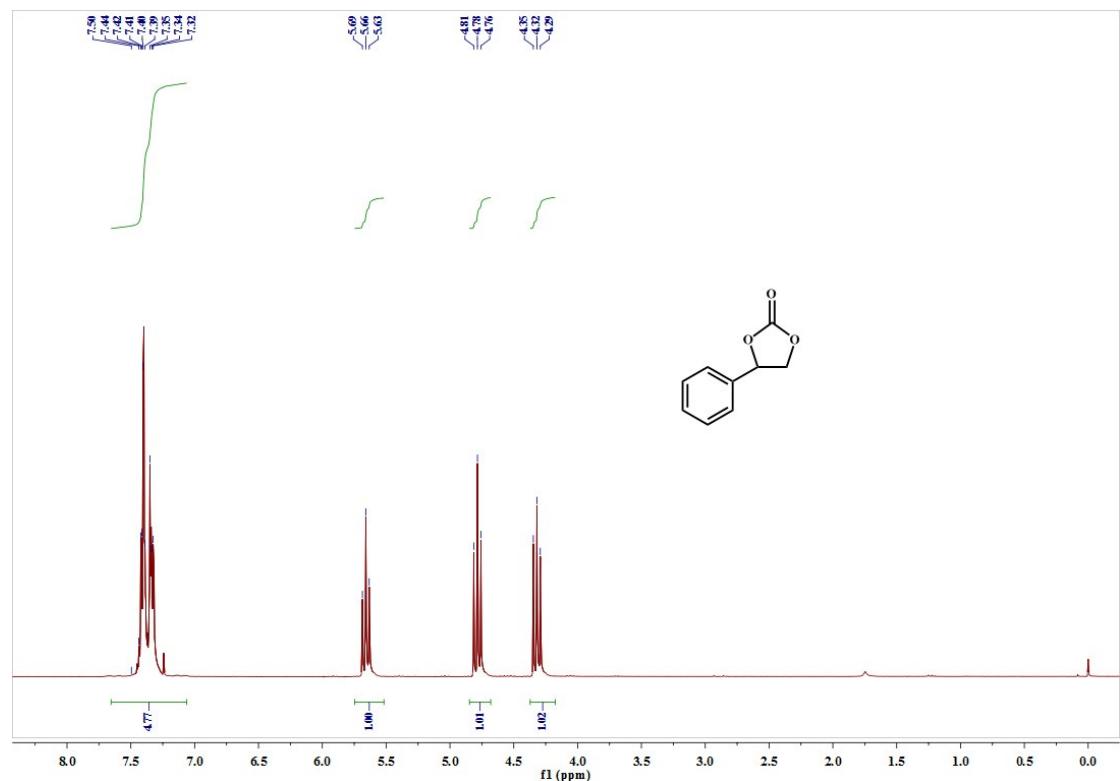
4-Butyl-1,3-dioxolan-2-one

^1H NMR (300 MHz, CDCl_3)



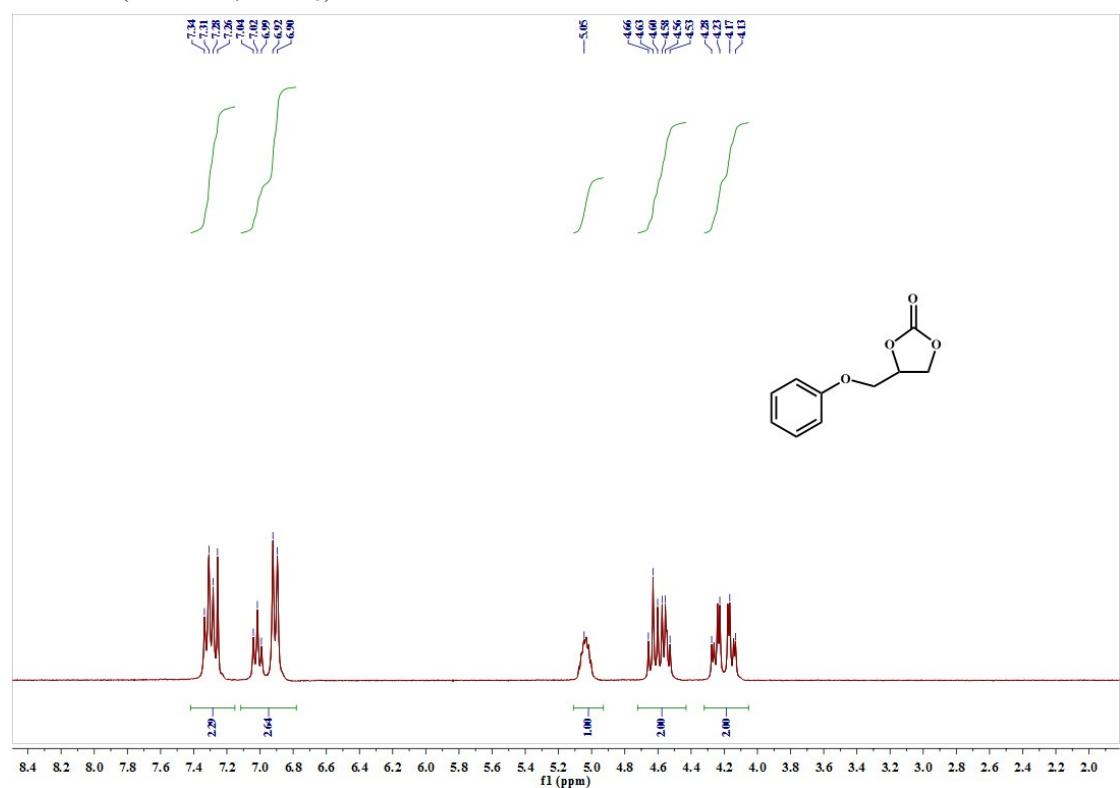
4-Phenyl-1,3-dioxolan-2-one

^1H NMR (300 MHz, CDCl_3)



4-(Phenoxy)methyl-1,3-dioxolan-2-one

^1H NMR (300 MHz, CDCl_3)



4-(Chloromethyl)-1,3-dioxolan-2-one

¹H NMR (300 MHz, CDCl₃)

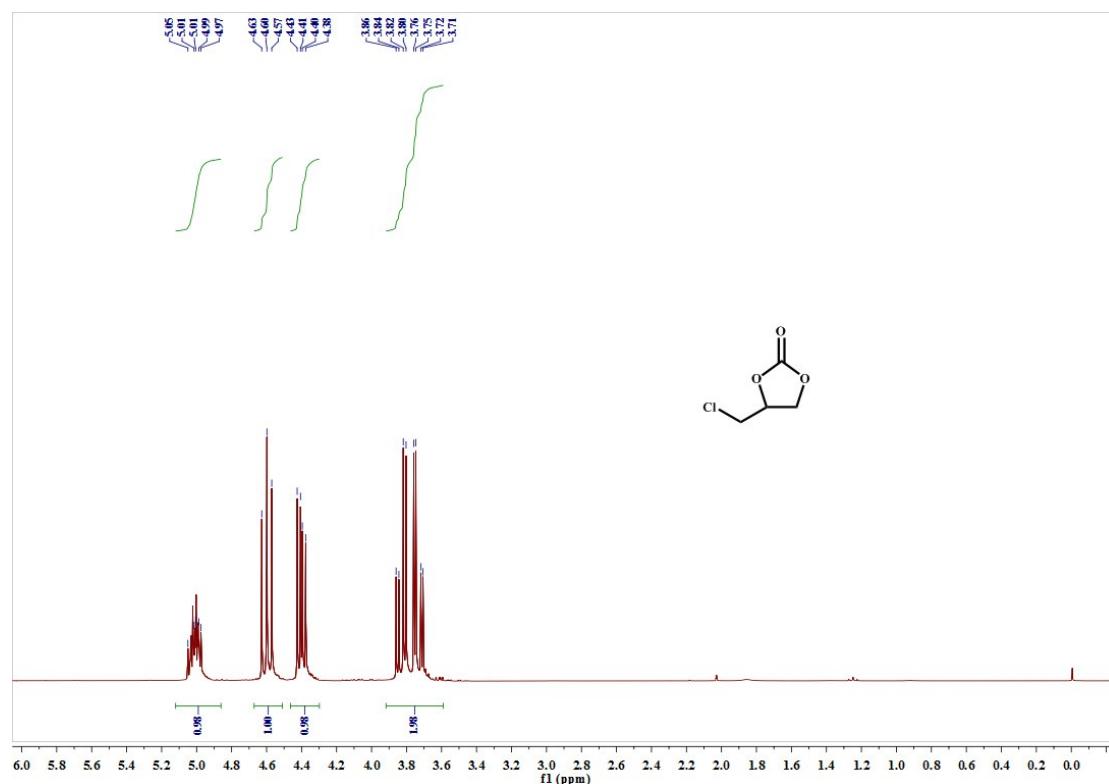


Figure S5. The ¹H NMR plots of the products converting from the cycloaddition reaction of CO₂ with epoxides.

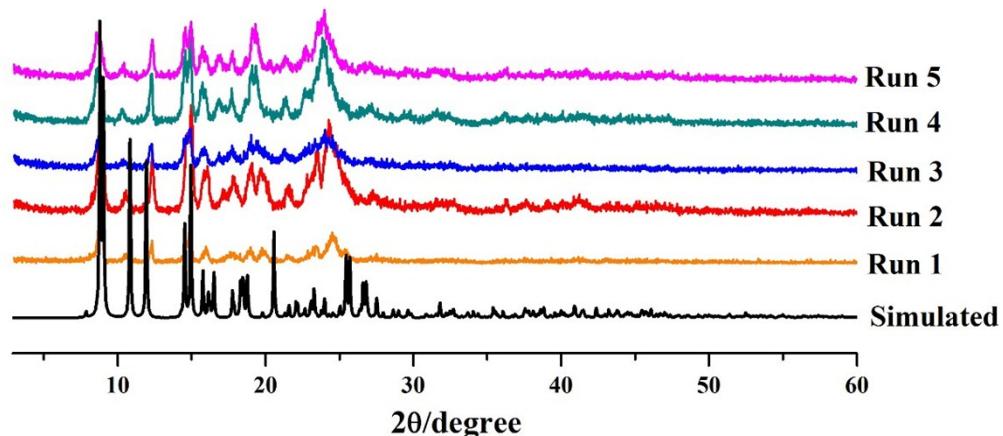


Figure S6. The PXRD patterns of **1** after five catalytic recyclings and the simulated one from **1**.

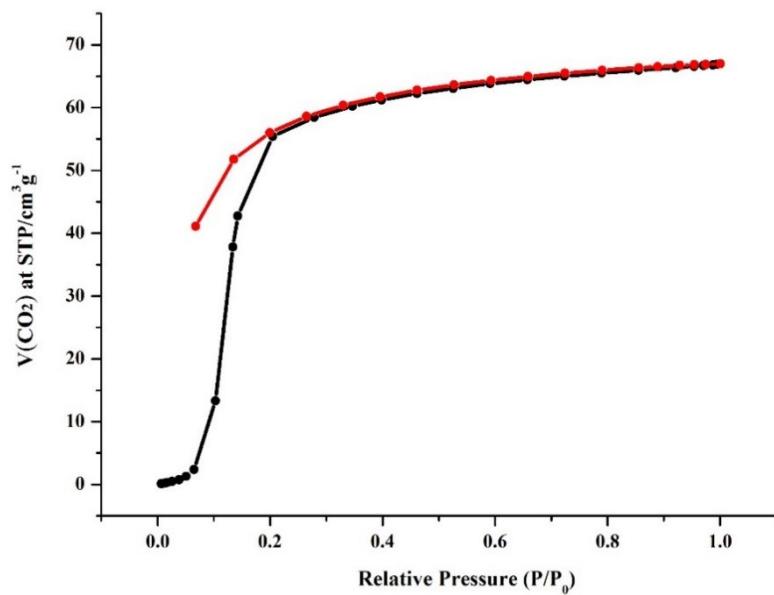


Figure S7. The CO_2 adsorption/desorption of **1** at 273 K.

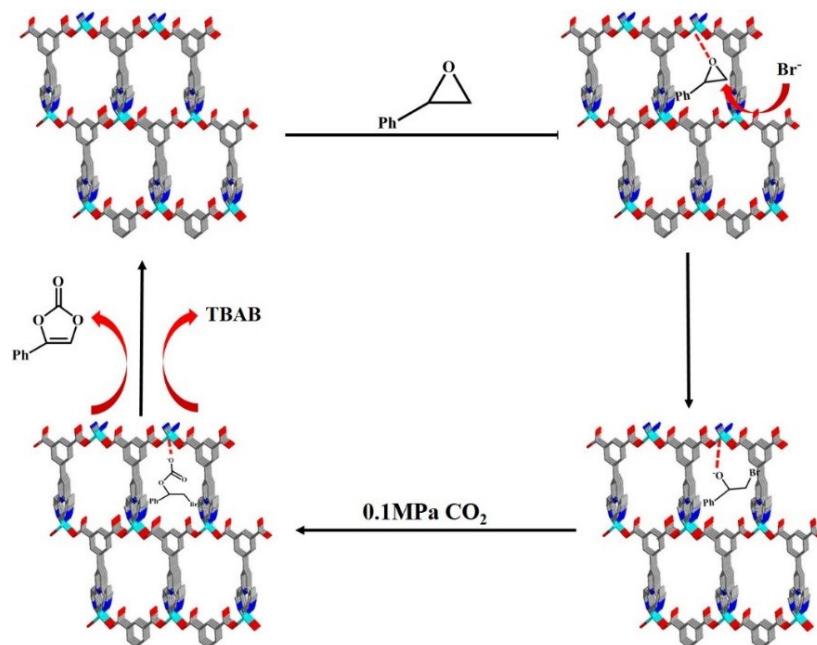


Figure S8. The possible mechanism for the reaction of epoxidation.

Table S2. Comparison of the catalytic activity of some reported interpenetrated-MOFs for the cycloaddition reaction of CO₂ with epoxides.

entry	catalyst	interpenetrated numbers	catalyst (mol %)	pressure (Mpa)	temp (°C)	time (h)	conversion (%)	ref
1 ^a	[{Ni(muco)(bpa)(2H ₂ O)}·2H ₂ O]	3-fold	0.5	0.8	80	12	81.3	1
2 ^a	[{Co(muco)(bpa)(2H ₂ O)}·2H ₂ O] _n	3-fold	0.5	0.8	80	12	>99	2
			0.5	0.1	80	12	85.6	
			0.5	0.1	100	15	94.2	
3 ^a	[Zn ₆ (TATAB) ₄ (DABCO) ₃ -(H ₂ O) ₃]·12DMF·9H ₂ O	3-fold	0.42	0.1	100	16	90	3
4 ^a	{[Zn(DCTP)]·3H ₂ O} _n	2-fold	2.8	0.1	70	12	88	this work
5 ^a	[Zn ₄ OL ₃] _n	2-fold	0.3	0.1	50	4	55	4
6 ^b	MMPF-18	4-fold	0.25	0.1	r.t.	48	96.97	5
7 ^b	[Cu(bpy) ₂ (EDS)] _n	2-fold	1.0	0.1	r.t.	48	>99	6
8 ^b	{Cu ₂ ((C ₅₇ H ₃₆ N ₁₂)(COO) ₄)-(H ₂ O) ₂ ·22(DMF)} _n	2-fold	0.4	0.1	r.t.	60	94	7
	{Cu ₂ ((C ₅₇ H ₃₆ N ₁₂)(COO) ₄)-(H ₂ O) ₂ ·7(DMF)} _n	4-fold	0.4	0.1	r.t.	60	49	

^a The epoxide is styrene oxide, ^b The epoxide is propylene oxide.

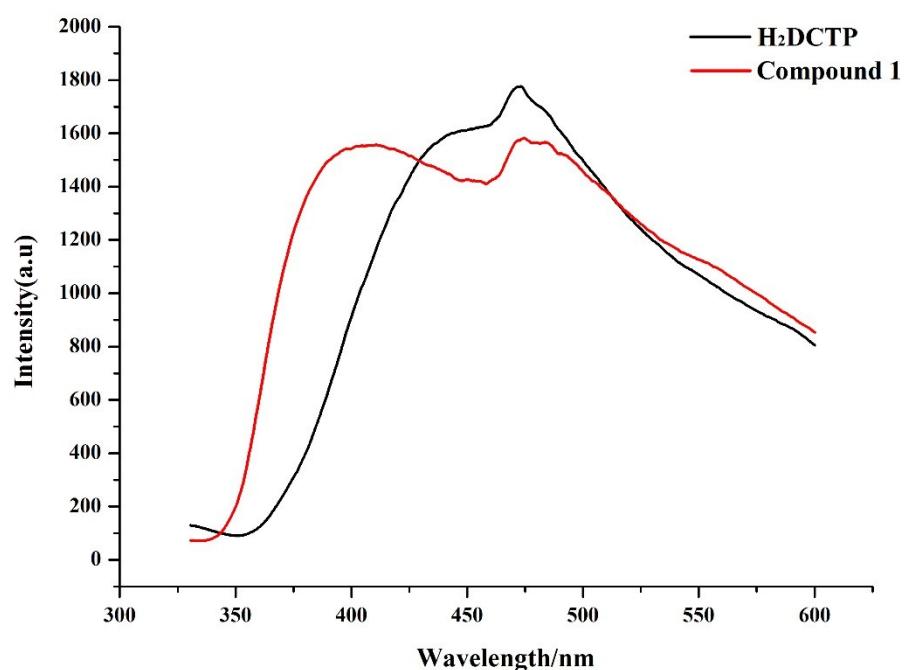


Figure S9. The solid-state photoluminescence spectra of H₂DCTP ($\lambda_{\text{excited}} = 320$ nm) and the emission spectra of compound 1 ($\lambda_{\text{excited}} = 320$ nm).

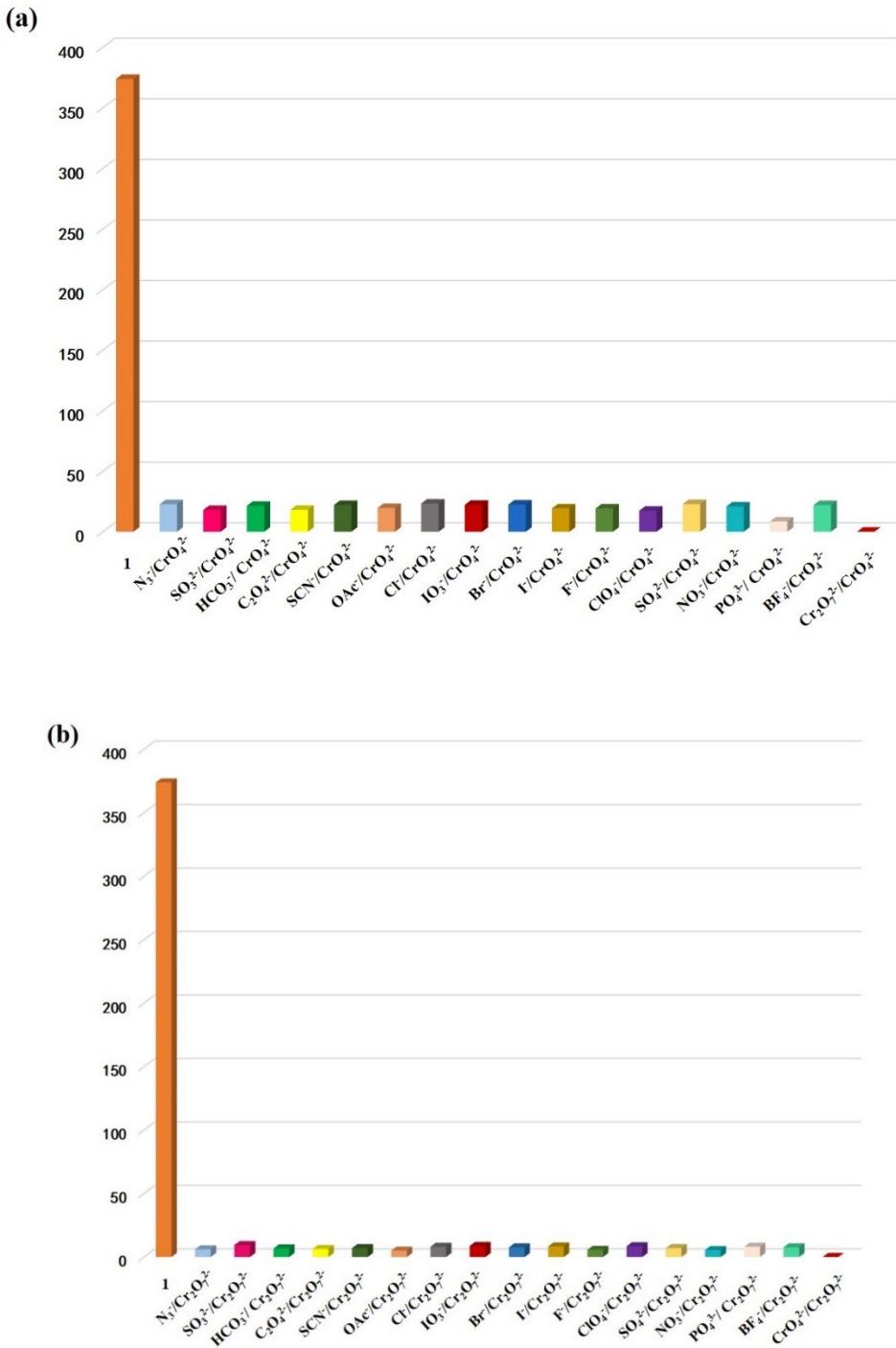


Figure S10. The luminescence intensity of **1**- CrO_4^{2-} (a) and **1**- $\text{Cr}_2\text{O}_7^{2-}$ (b) under mixed anions (5×10^{-3} M).

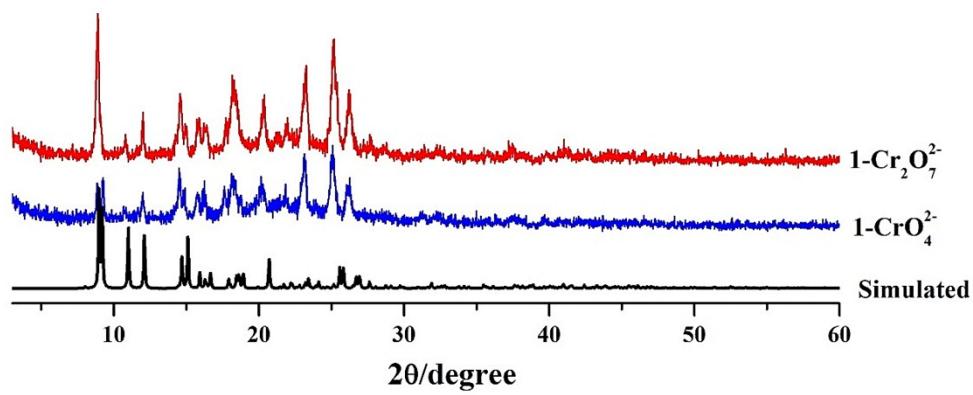


Figure S11. The PXRD patterns of **1** after five luminescent recyclings and the simulated one from compound **1**.

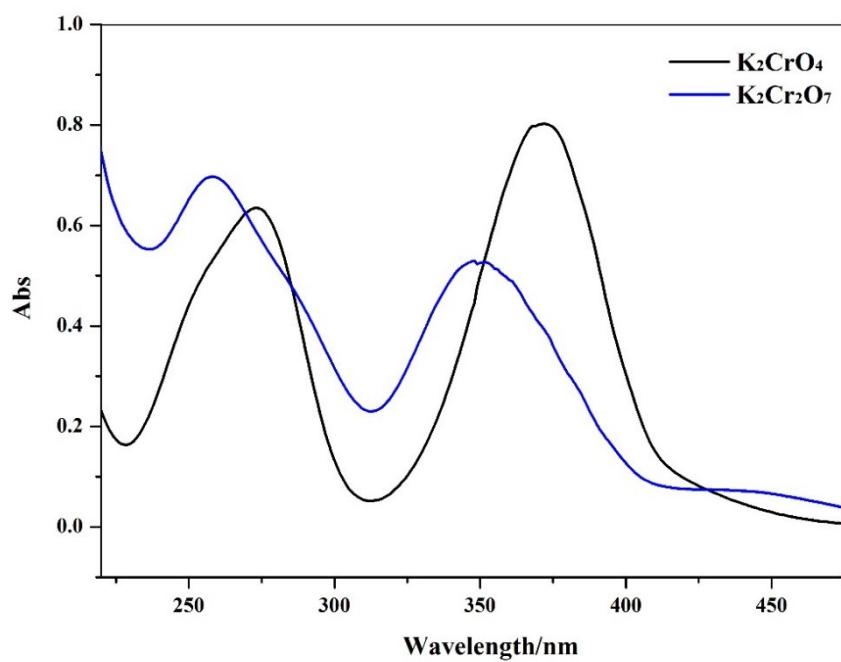


Figure S12. The UV-vis spectra of the K_2CrO_4 and $\text{K}_2\text{Cr}_2\text{O}_7$ solutions.

Table S3. Comparison of the detective limit in some reported $\text{CrO}_4^{2-}/\text{Cr}_2\text{O}_7^{2-}$ sensors.

entry	molecular formula	analyte($\text{CrO}_4^{2-}/\text{Cr}_2\text{O}_7^{2-}$)	LOD(mol/L)	ref
1	$[\text{Y}(\text{BTC})(\text{H}_2\text{O})_6]_n \cdot 0.1\text{Eu}$	$\text{CrO}_4^{2-}/\text{Cr}_2\text{O}_7^{2-}$	$3.0 \times 10^{-8}/4.0 \times 10^{-8}$	8
2	$\text{Eu}^{3+}@\text{MIL}-121$	$\text{Cr}_2\text{O}_7^{2-}$	5.4×10^{-8}	9
3	$\{\text{Tb}_4\text{Mn}-(\text{BPDC})_3(\mu_3-\text{H})_4-(\text{HCOO})_{1.5}(\text{H}_2\text{O})_4\} \cdot 2.5\text{OH} \cdot 8\text{H}_2\text{O}\}_n$	$\text{Cr}_2\text{O}_7^{2-}$	10^{-7}	10
4	$\{\text{[Zn}_3(\text{bpanth})(\text{oba})_3]\cdot 2\text{DMF}\}_n$	$\text{CrO}_4^{2-}/\text{Cr}_2\text{O}_7^{2-}$	$1.54 \times 10^{-6}/2.38 \times 10^{-6}$	11
5	$\{\text{[Zn}(\text{DCTP})]\cdot 2.5\text{H}_2\text{O}\}_n$	$\text{CrO}_4^{2-}/\text{Cr}_2\text{O}_7^{2-}$	$1.0 \times 10^{-6}/1.5 \times 10^{-6}$	this work
6	$[\text{Cd}(\text{IPA})(\text{L})]_n$	$\text{CrO}_4^{2-}/\text{Cr}_2\text{O}_7^{2-}$	$2.52 \times 10^{-6}/2.26 \times 10^{-6}$	12
	$[\text{Zn}(\text{IPA})(\text{L})]_n$	$\text{CrO}_4^{2-}/\text{Cr}_2\text{O}_7^{2-}$	$1.83 \times 10^{-5}/1.2 \times 10^{-5}$	
7	$\{\text{[Zn}_3(\text{tza})_2(\mu_2-\text{OH})_2(\text{H}_2\text{O})_2\} \cdot \text{H}_2\text{O}\}_n$	$\text{CrO}_4^{2-}/\text{Cr}_2\text{O}_7^{2-}$	$4.0 \times 10^{-6}/1.0 \times 10^{-6}$	13
8	$[\text{Zn}_2(\text{TPOM})(\text{NH}_2-\text{BDC})_2] \cdot 4\text{H}_2\text{O}$	$\text{CrO}_4^{2-}/\text{Cr}_2\text{O}_7^{2-}$	$4.8 \times 10^{-6}/3.9 \times 10^{-6}$	14
9	$\{\text{[Zn}(\text{btz})]\}_n$	$\text{CrO}_4^{2-}/\text{Cr}_2\text{O}_7^{2-}$	$1.0 \times 10^{-5}/2.0 \times 10^{-6}$	15
	$\{\text{[Zn}_2(\text{ttz})\text{H}_2\text{O}\}_n\}$	$\text{CrO}_4^{2-}/\text{Cr}_2\text{O}_7^{2-}$	$2.0 \times 10^{-5}/2.0 \times 10^{-5}$	
10	$\{\text{[Cd}(\text{L})(\text{BPDC})]\cdot 2\text{H}_2\text{O}\}_n$	$\text{Cr}_2\text{O}_7^{2-}$	3.76×10^{-5}	16
	$\{\text{[Cd}(\text{L})(\text{SDBA})(\text{H}_2\text{O})\} \cdot 0.5\text{H}_2\text{O}\}_n$	$\text{Cr}_2\text{O}_7^{2-}$	4.86×10^{-5}	

Table S4. The ICP results of compound **1** after catalytic recyclings (filter liquor) and luminescent recyclings (solid sample), respectively.

	Compound 1
Compound 1 after recyclings (Zn^{2+} of filter liquor)	0.68 ppm
Compound 1 as CrO_4^{2-} sensor after luminescent recyclings (Cr^{6+} of solid sample)	Below detection limit
Compound 1 as $\text{Cr}_2\text{O}_7^{2-}$ sensor after luminescent recyclings (Cr^{6+} of solid sample)	Below detection limit

References

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