

Supplementary Information

Building Metal-functionalized Porous Carbons from Microporous Organic Polymers for CO₂ Capture and Conversion under Ambient Conditions

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1. Character

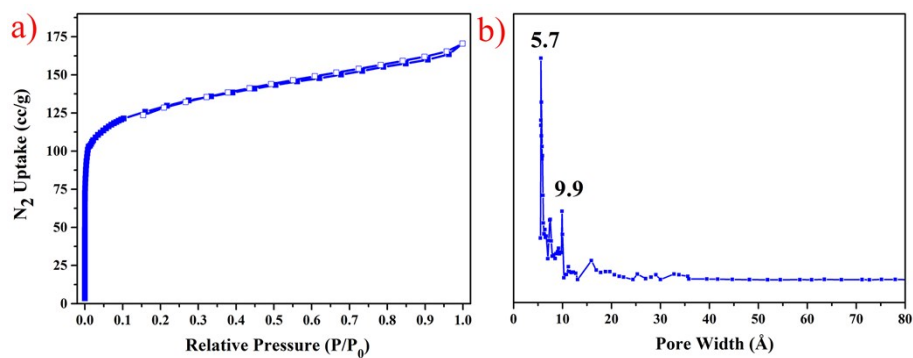


Figure S1. (a) N_2 adsorption (solid symbols)/desorption (open symbols) isotherms at 77K and (b) NLDFT pore size distribution of the precursor.

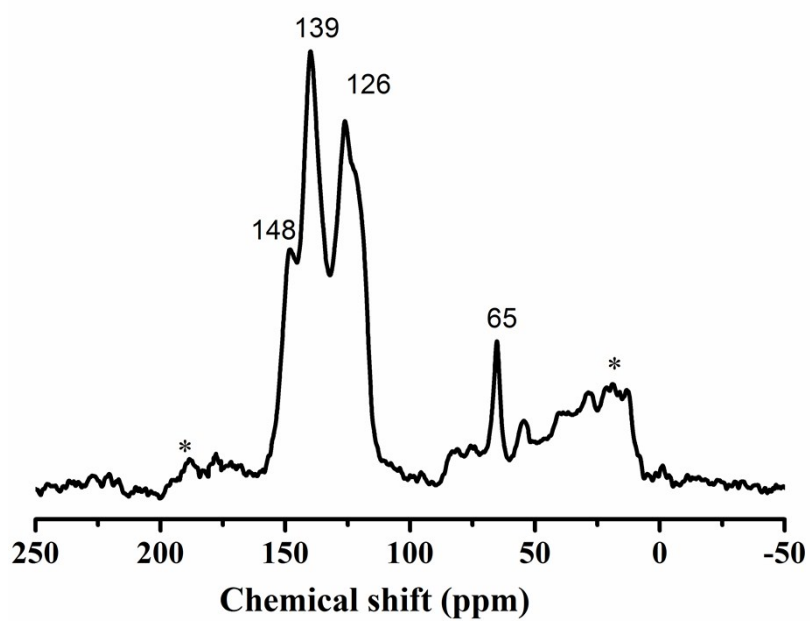


Figure S2. ^{13}C CP-MAS NMR spectrum of the precursor.

2. Powder X-Ray Diffraction

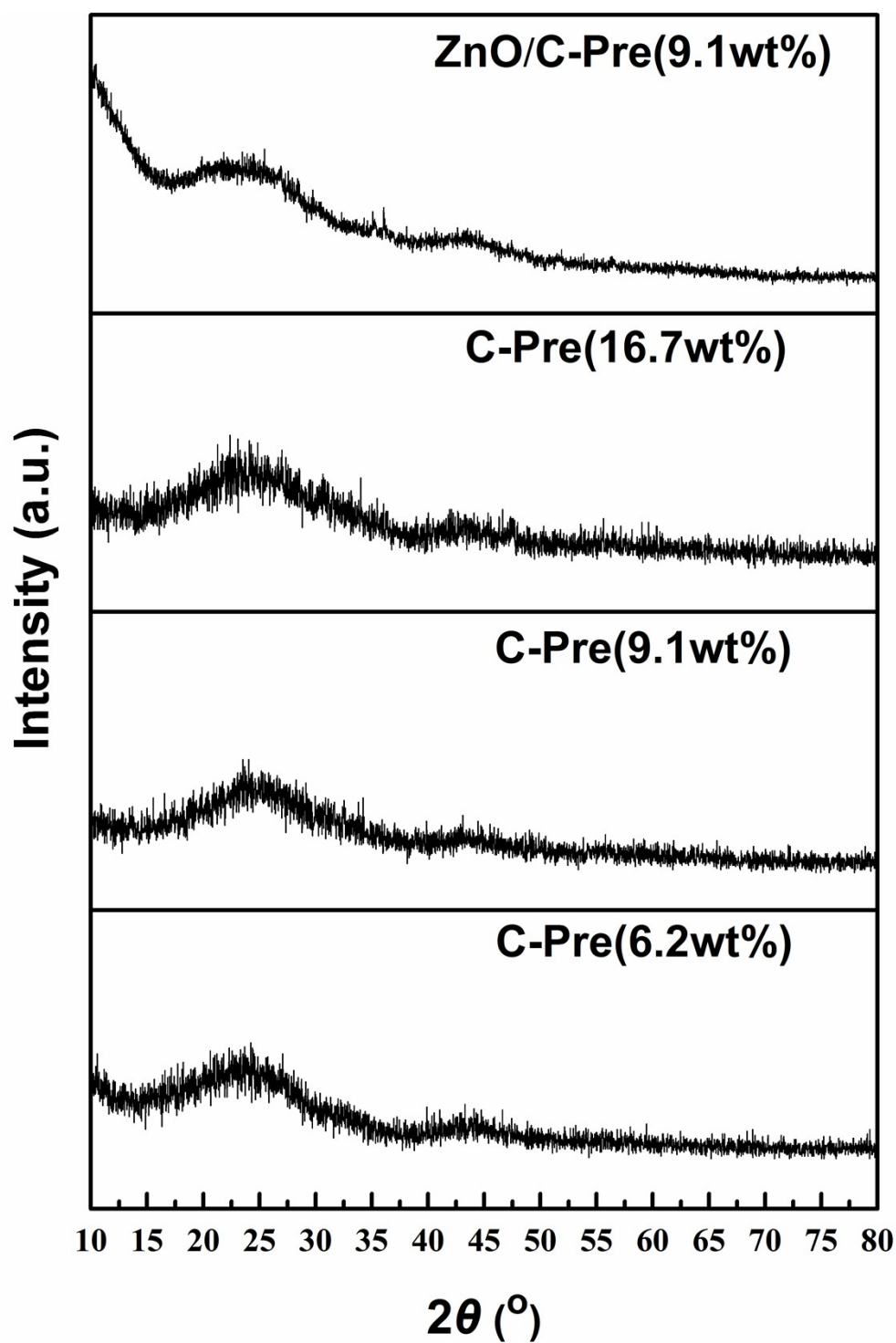


Figure S3. Powder X-Ray Diffraction of porous carbons.

3. Morphology analysis by SEM

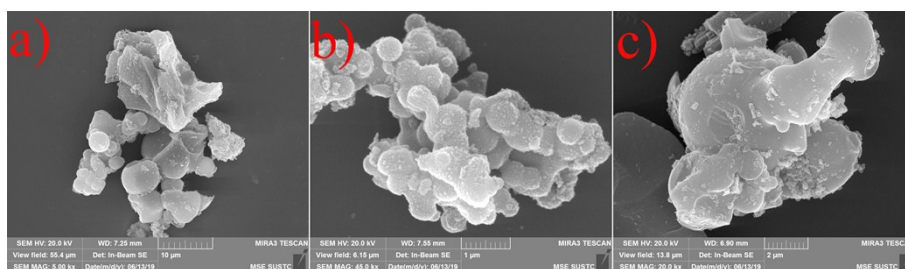


Figure S4. SEM images of (a) ZnO/C-Pre(9.1wt%), (b) C-Pre(9.1wt%) and (c) ZnO/C-Pre(9.1wt%)/PBM.

4. Morphology analysis by TEM

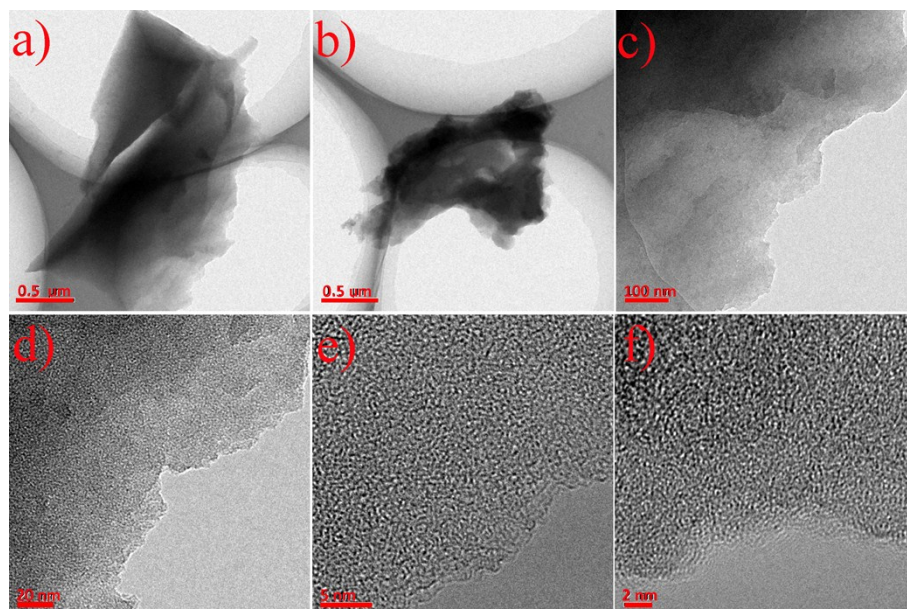


Figure S5. TEM images of precursor.

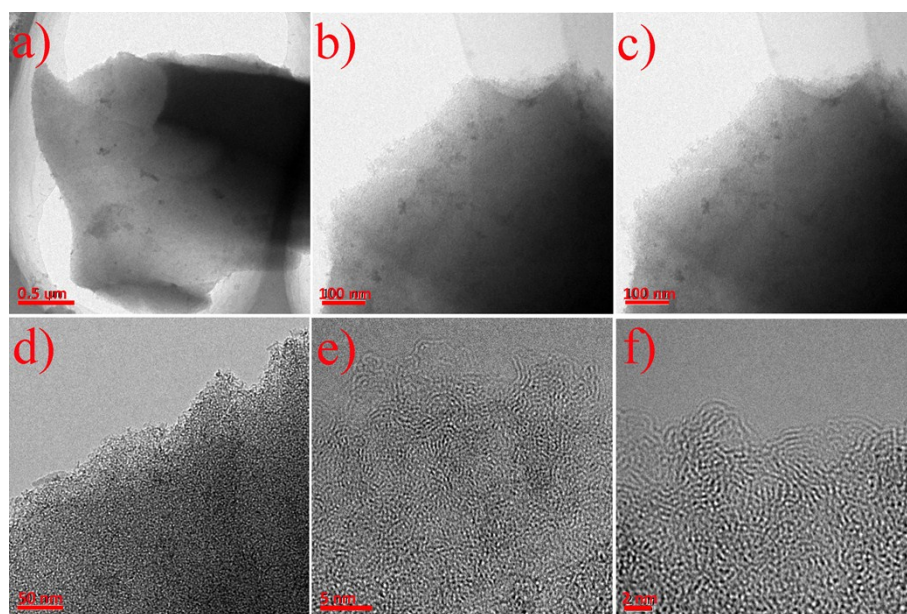


Figure S6. TEM images of C-Pre(9.1wt%).

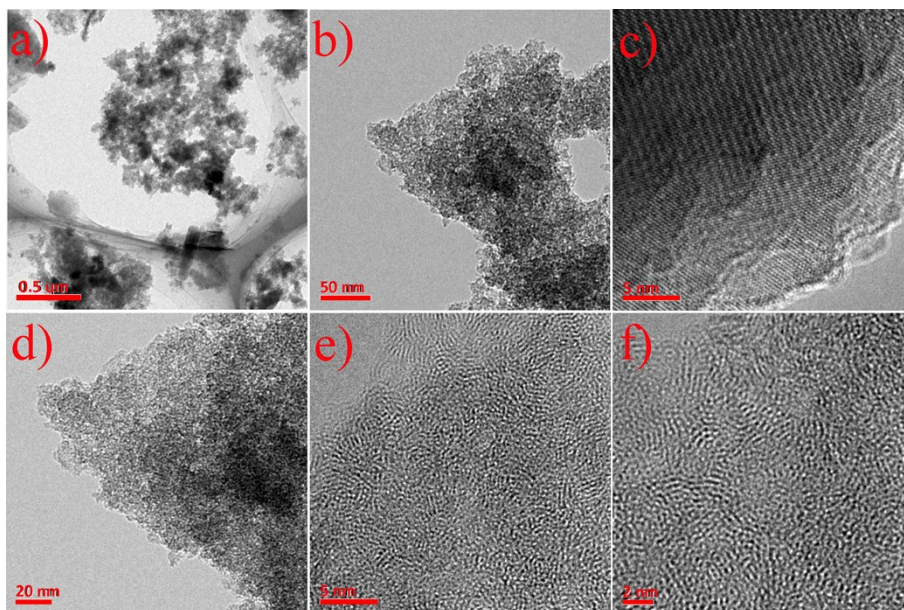


Figure S7. TEM images of ZnO/C-Pre(9.1wt%).

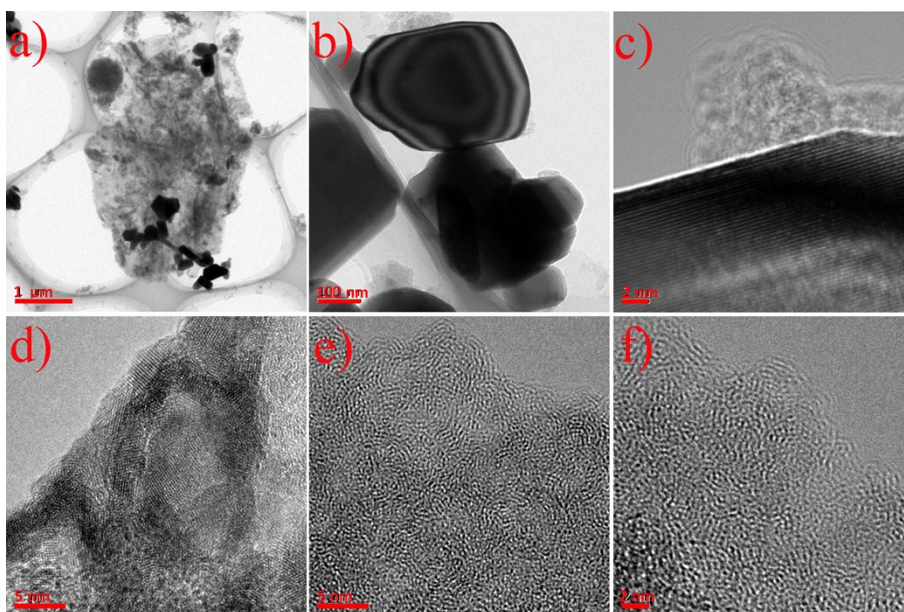


Figure S8. TEM images of ZnO/C-Pre(9.1wt%)/PBM.

5. Elemental analysis

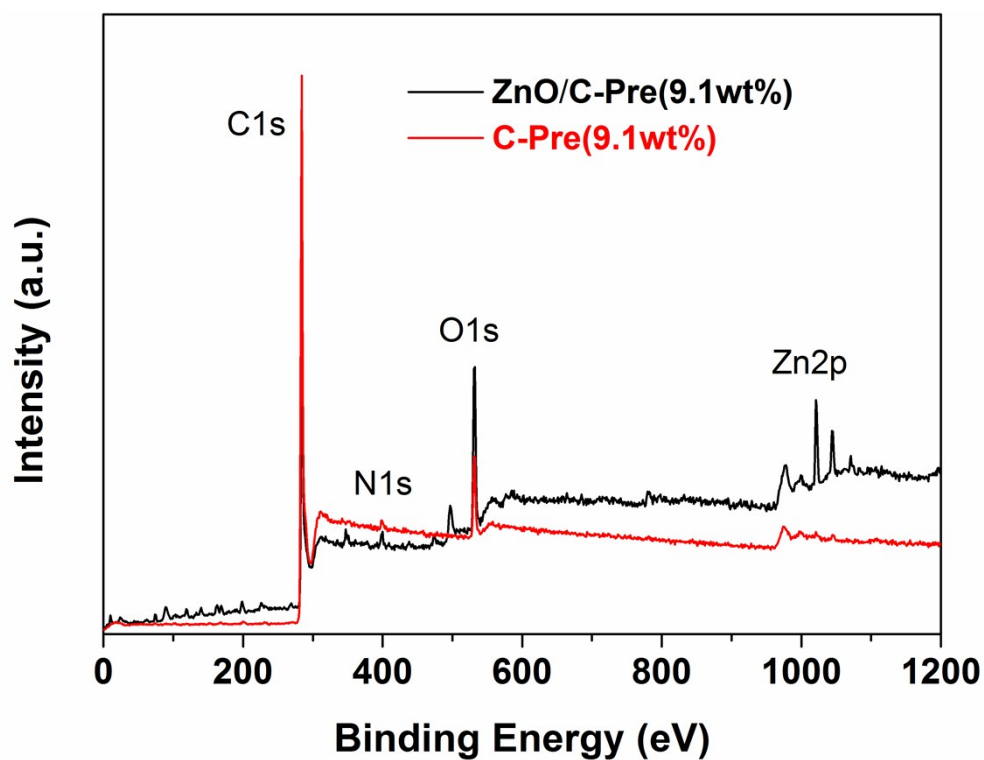


Figure S9. Wide XPS survey spectra of carbons.

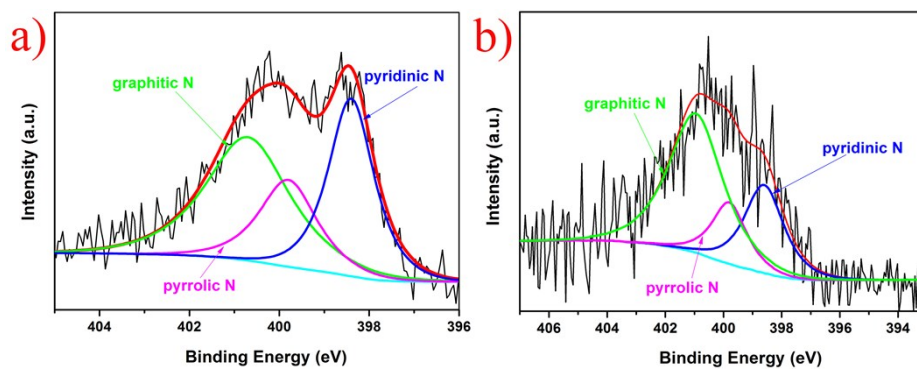


Figure S10. High-resolution N 1s XPS spectra of (a) ZnO/C-Pre(9.1wt%) and (b) C-Pre(9.1wt%).

6. Infrared spectroscopy

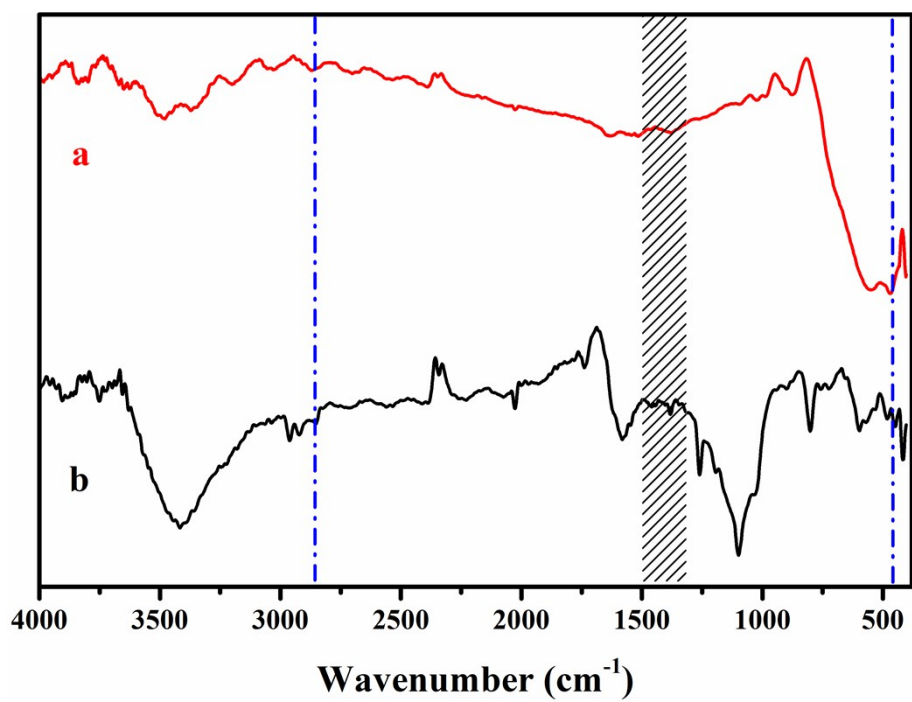


Figure S11 FTIR spectra of (a) ZnO and (b) ZnO/C-Pre(9.1wt%).

Table S1. XPS elemental data (at%) of carbon materials.

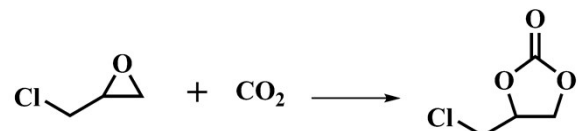
| Sample | C | O | N | Zn | Cl |
|-------------------|-------|-------|------|------|------|
| ZnO/C-Pre(9.1wt%) | 78.87 | 11.51 | 6.86 | 2.36 | - |
| C-Pre(9.1wt%) | 97.22 | ND | 2.14 | 0.35 | 0.29 |

Table S2. ICP-AES data (wt%) of carbon materials.

| Sample | Zn |
|-------------------|------|
| ZnO/C-Pre(9.1wt%) | 2.42 |
| C-Pre(16.7wt%) | 0.05 |
| C-Pre(9.1wt%) | 0.12 |
| C-Pre(6.2wt%) | 0.14 |

7. CO₂ cycloaddition reaction

Table S3. Catalytic cycloaddition of CO₂ with epichlorohydrin to form cyclic carbonates^a.



| Entry | Catalyst | Time (h) | Yield ^b (%) |
|-------|-----------------------|----------|------------------------|
| 1 | ZnO/C-Pre(9.1wt%) | 12 | 57 |
| 2 | ZnO/C-Pre(9.1wt%) | 24 | 75 |
| 3 | ZnO/C-Pre(9.1wt%) | 36 | 87 |
| 4 | ZnO/C-Pre(9.1wt%) | 48 | 91 |
| 5 | ZnO/C-Pre(9.1wt%) | 60 | 92 |
| 6 | C-Pre(16.7wt%) | 48 | 61 |
| 7 | C-Pre(9.1wt%) | 48 | 45 |
| 8 | C-Pre(6.2wt%) | 48 | 60 |
| 9 | MOP-8C | 48 | 69 |
| 10 | ZnO/C-Pre(9.1wt%)/PBM | 48 | 54 |

^a Reaction conditions: 10 mmol epoxide, 10 mg catalyst, 1 mmol TBAB, CO₂ (0.1 MPa), 25 °C. ^b

Products were characterized by ¹H NMR and the yields refer to isolated products.

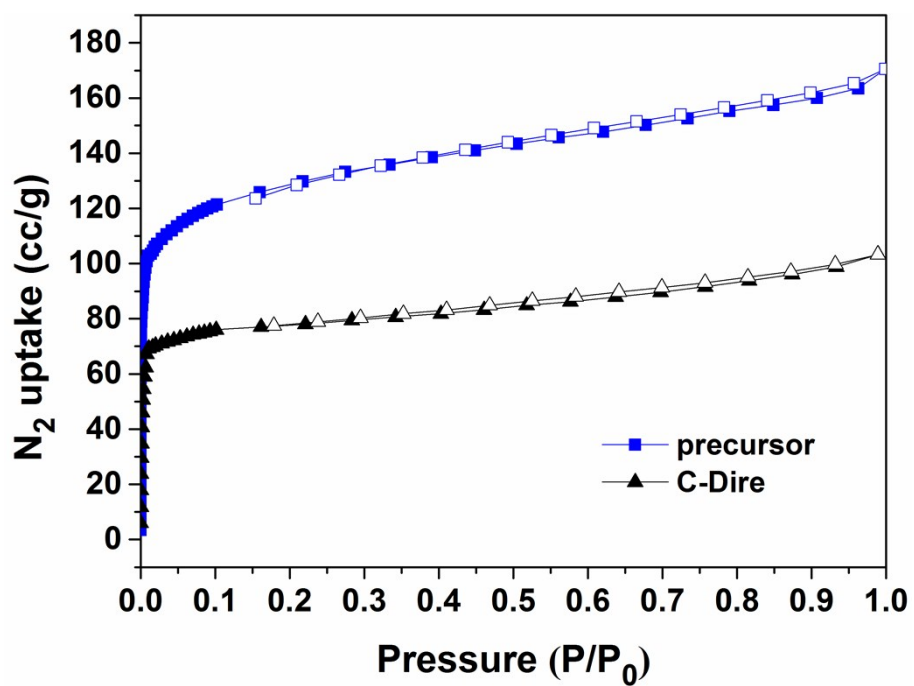


Figure S12. N₂ adsorption (solid symbols)/desorption (open symbols) isotherms of the precursor and the C-Dire (the carbon material pyrolysed without ZnCl₂ molten salt) at 77K.

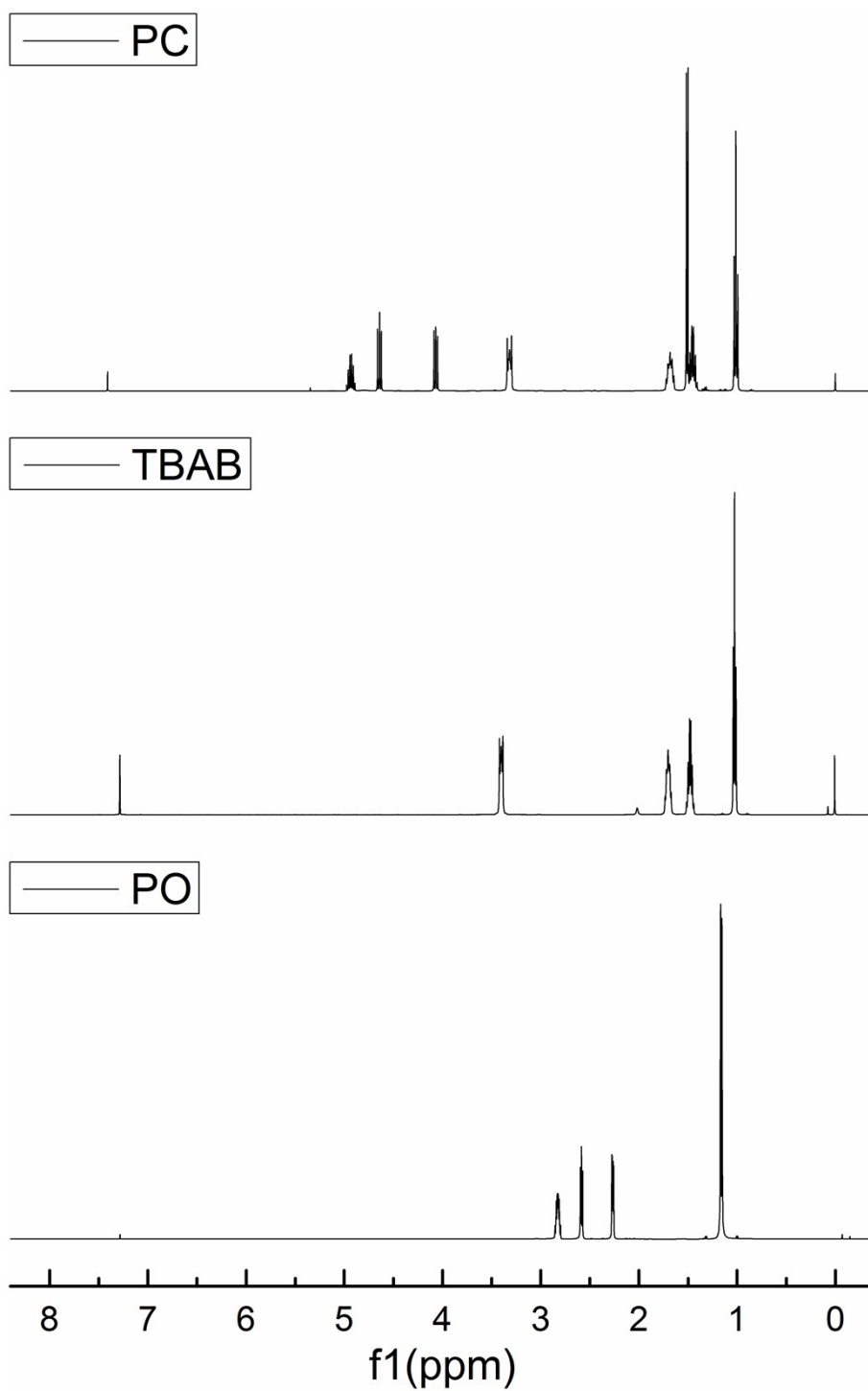


Figure S13. ^1H NMR (400 MHz, CDCl_3 , 298 K) spectra of (\pm)-propylene oxide and its corresponding cyclic carbonate (^1H NMR spectrum was obtained from the crude sample).

Possible catalytic pathway

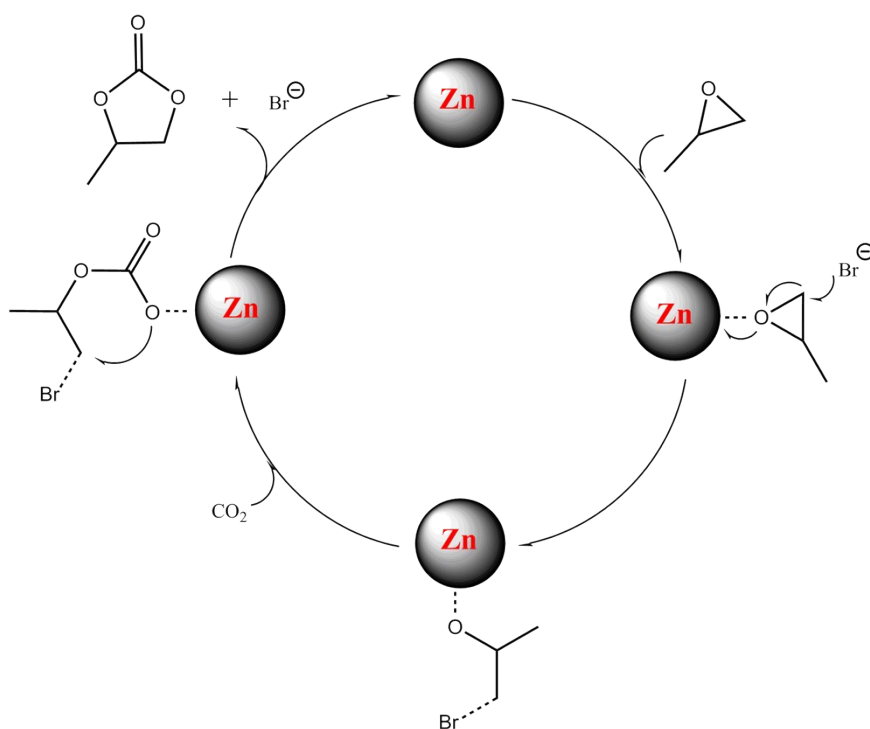


Figure S14. Scheme of possible catalytic mechanism for the reaction of epoxide and CO_2 into cyclic carbonate catalyzed by $\text{ZnO/C-Pre}(9.1\text{wt}\%)$.

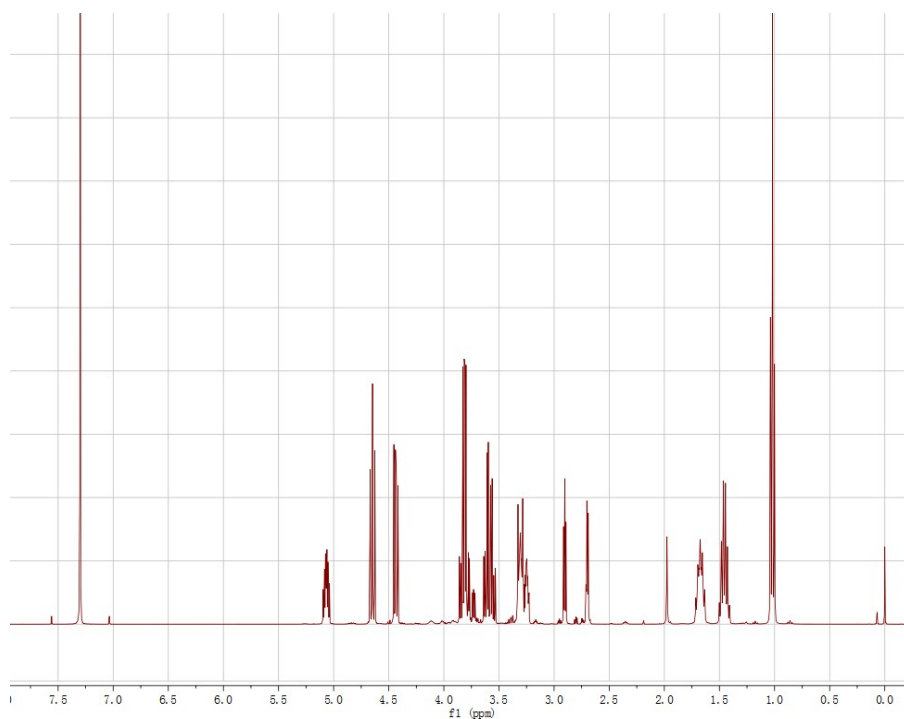


Figure S15. ^1H NMR (400 MHz, CDCl_3 , 298 K) spectra of epichlorohydrin and its corresponding cyclic carbonate at 12 h (^1H NMR spectrum was obtained from the crude sample).

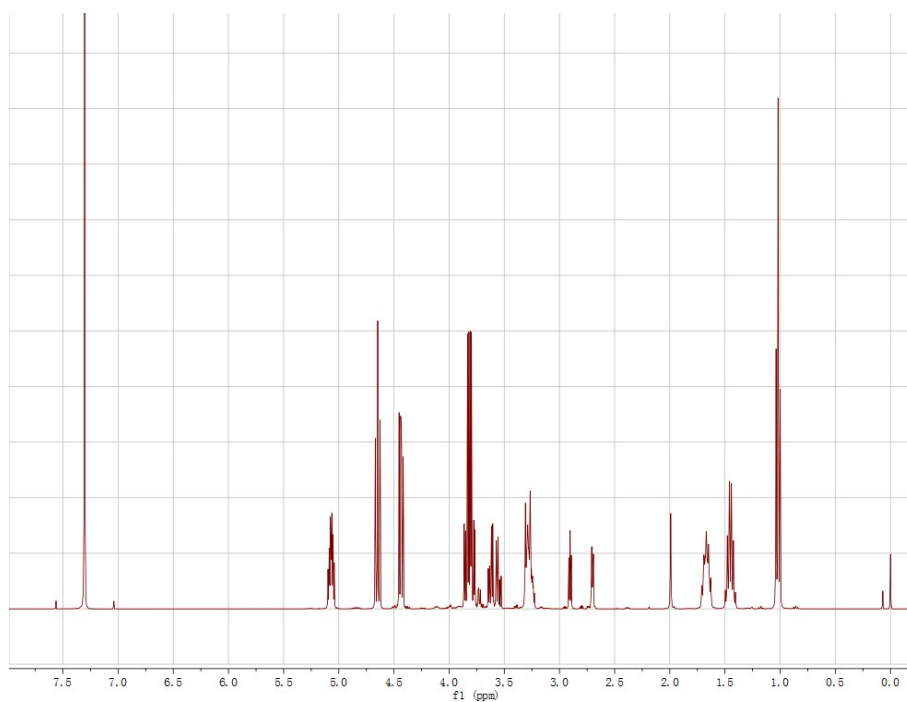


Figure S16. ¹H NMR (400 MHz, CDCl₃, 298 K) spectra of epichlorohydrin and its corresponding cyclic carbonate at 24 h (¹H NMR spectrum was obtained from the crude sample).

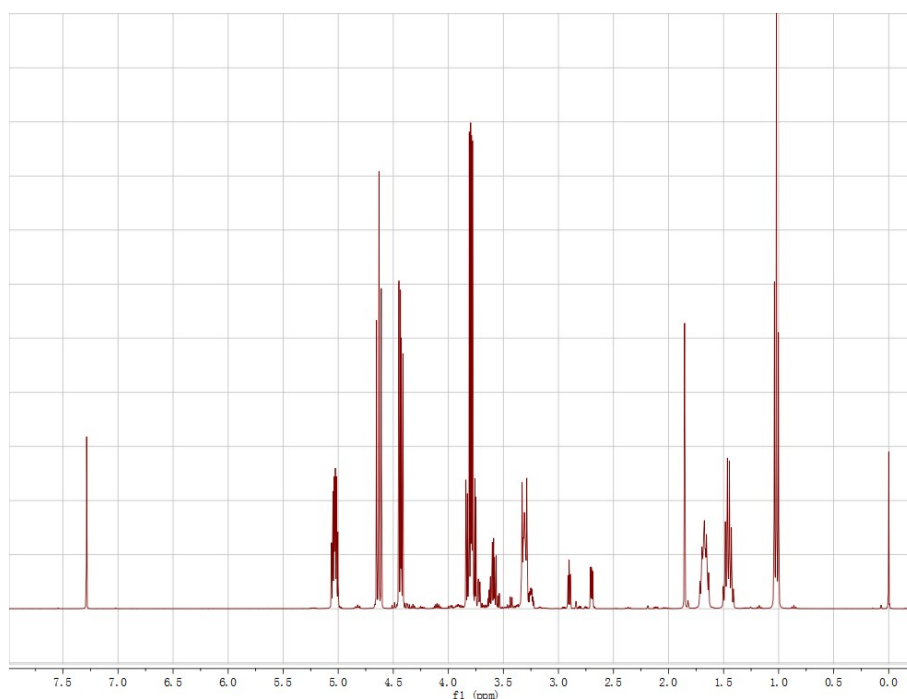


Figure S17. ¹H NMR (400 MHz, CDCl₃, 298 K) spectra of epichlorohydrin and its corresponding cyclic carbonate at 36 h (¹H NMR spectrum was obtained from the crude sample).

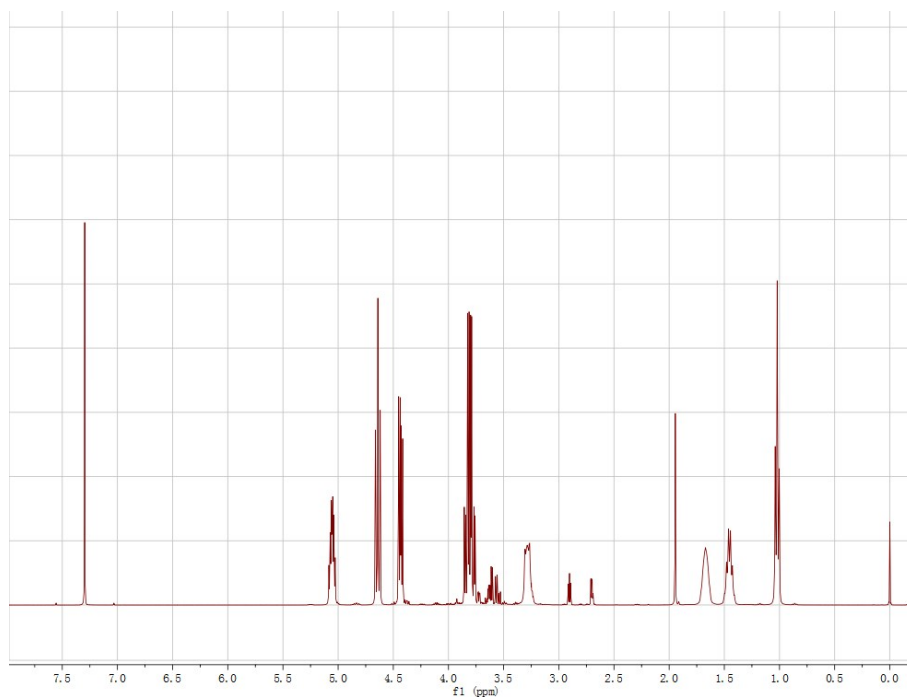


Figure S18. ¹H NMR (400 MHz, CDCl₃, 298 K) spectra of epichlorohydrin and its corresponding cyclic carbonate at 48 h (¹H NMR spectrum was obtained from the crude sample).

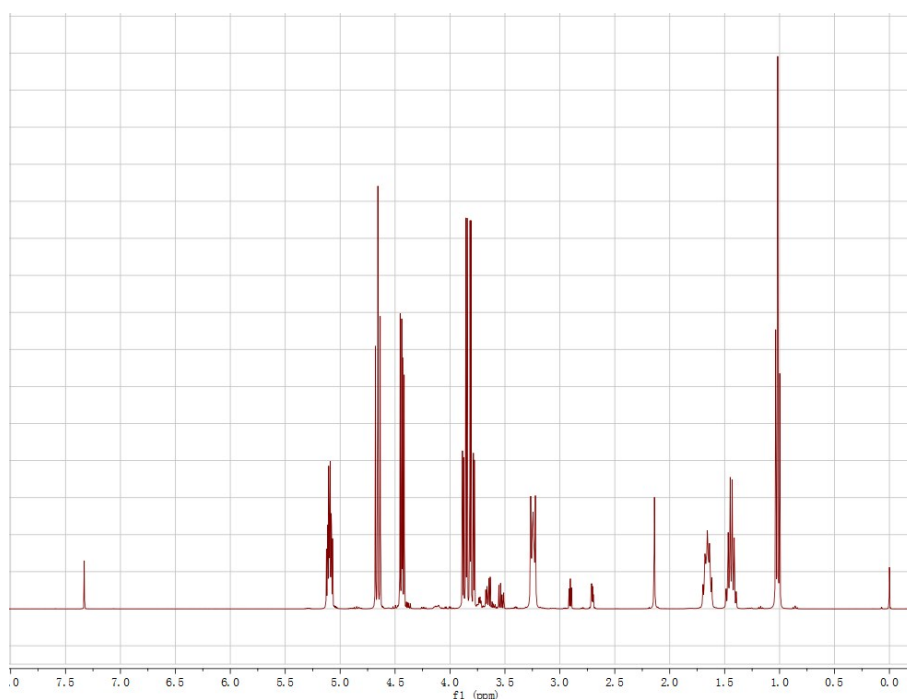


Figure S19. ¹H NMR (400 MHz, CDCl₃, 298 K) spectra of epichlorohydrin and its corresponding cyclic carbonate at 60 h (¹H NMR spectrum was obtained from the crude sample).

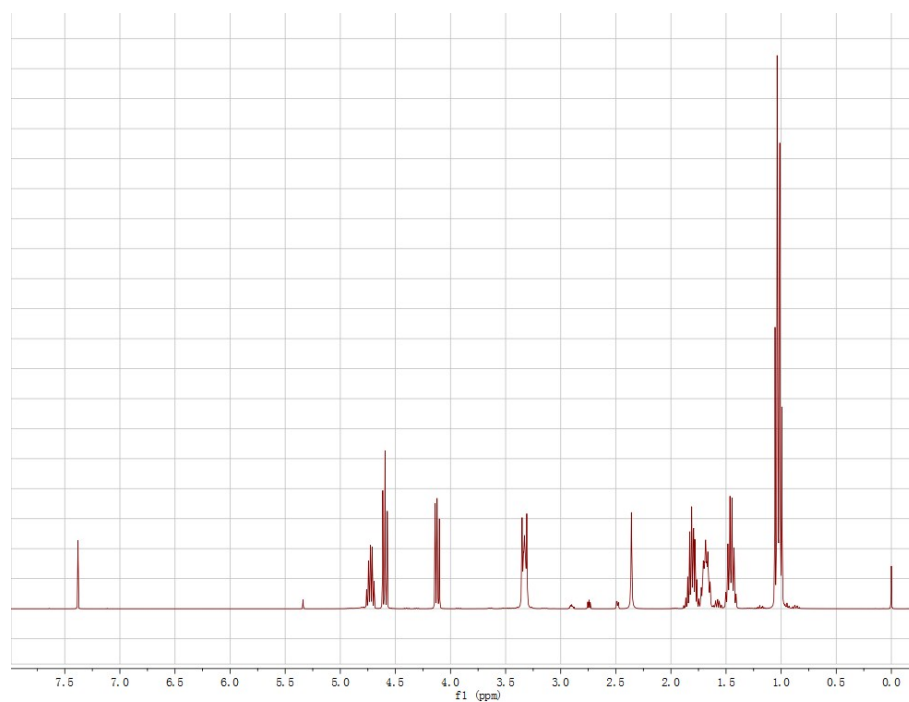


Figure S20. ¹H NMR (400 MHz, CDCl₃, 298 K) spectra of 1,2-epoxybutane and its corresponding cyclic carbonate (¹H NMR spectrum was obtained from the crude sample).

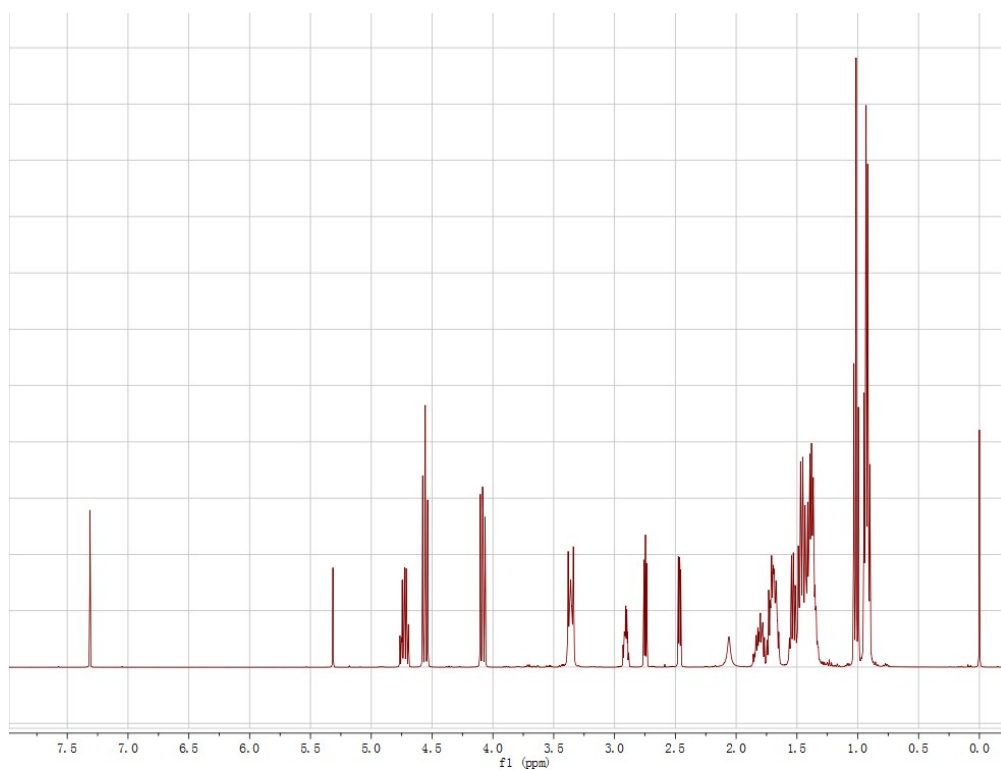


Figure S21. ¹H NMR (400 MHz, CDCl₃, 298 K) spectra of cyclohexane oxide and its corresponding cyclic carbonate (¹H NMR spectrum was obtained from the crude sample).

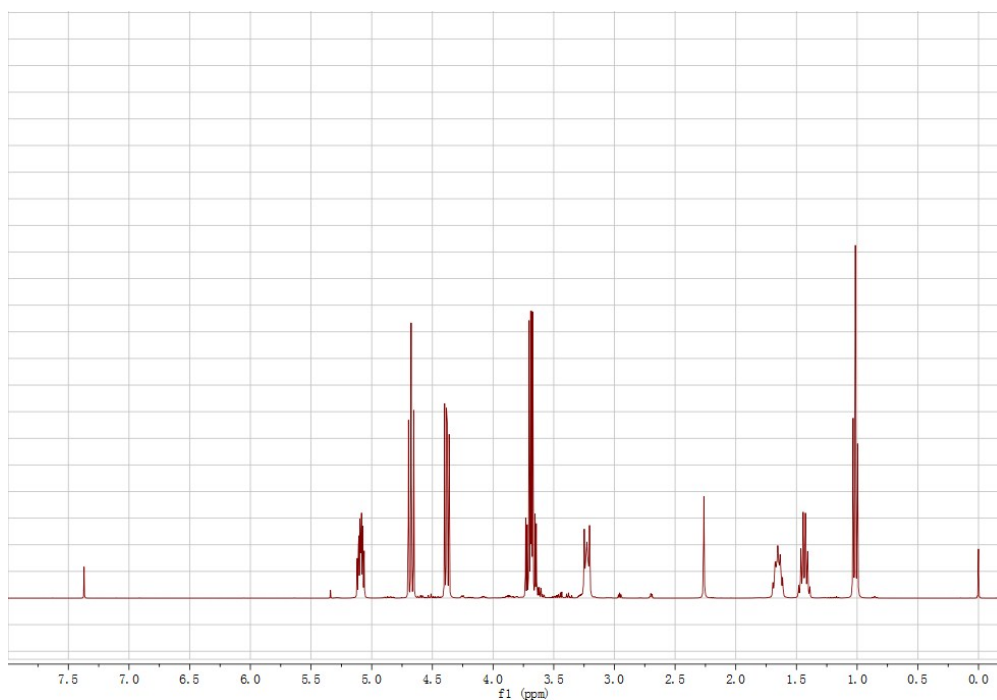


Figure S22. ^1H NMR (400 MHz, CDCl_3 , 298 K) spectra of epibromohydrin and its corresponding cyclic carbonate (^1H NMR spectrum was obtained from the crude sample).

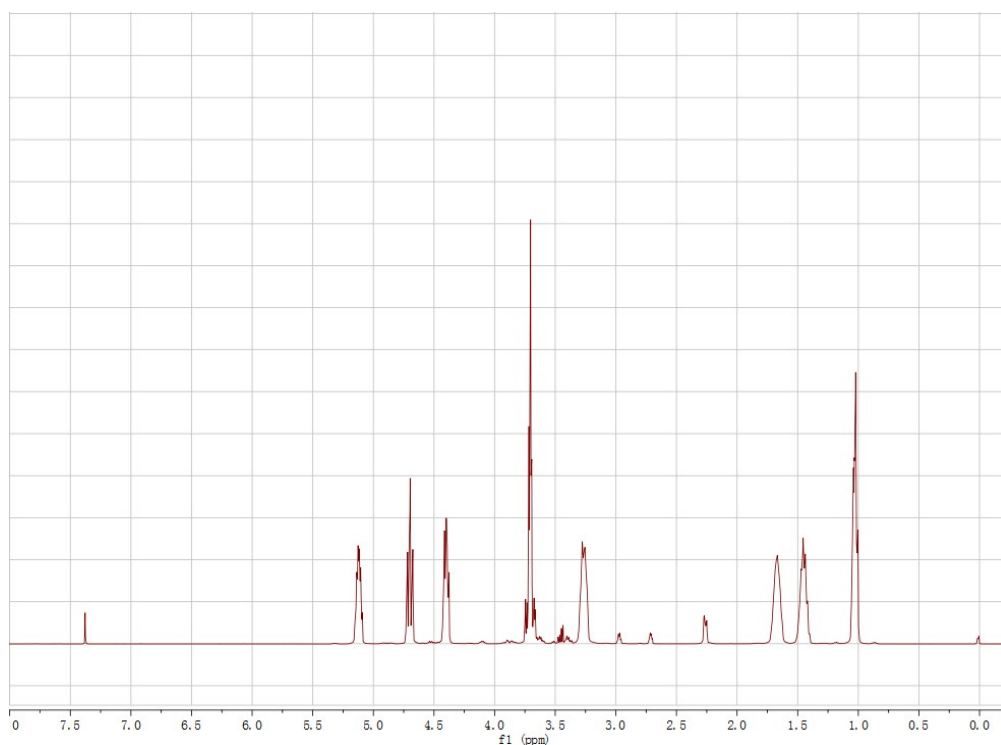


Figure S23. ^1H NMR spectra (in CDCl_3) of the reaction mixture (epibromohydrin) using $\text{ZnO/C-Pre}(9.1\text{wt}\%)$ as a catalyst in the 2nd cycle of recyclability test.

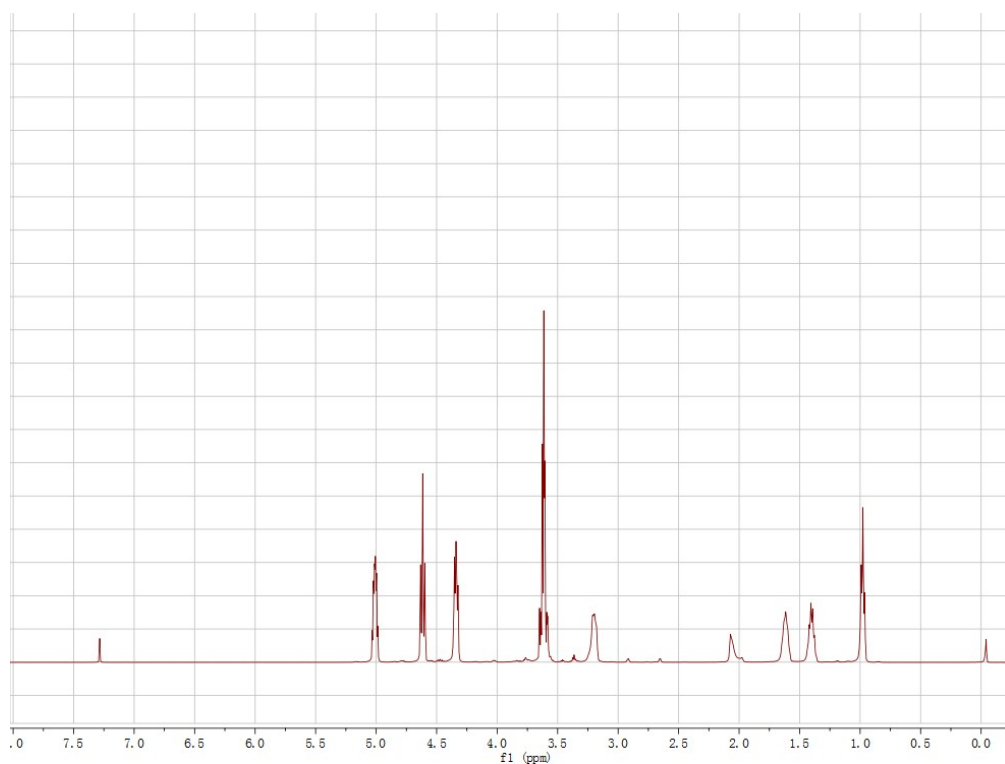


Figure S24. ¹H NMR spectra (in CDCl₃) of the reaction mixture (epibromohydrin) using ZnO/C-Pre(9.1wt%) as a catalyst in the 3rd cycle of recyclability test.

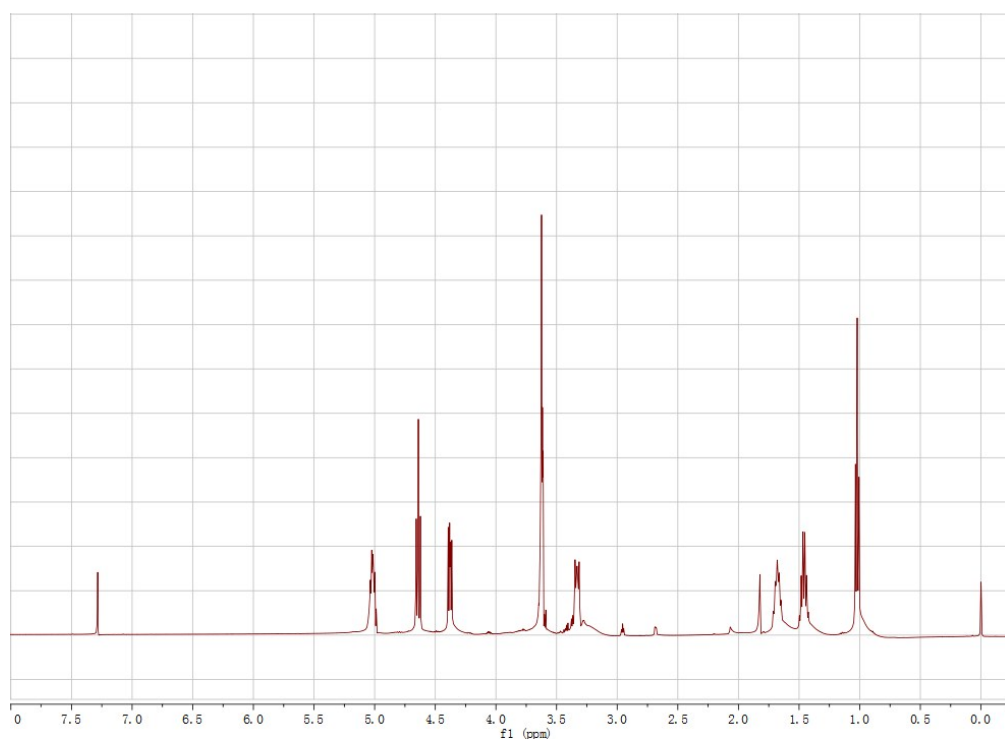


Figure S25. ¹H NMR spectra (in CDCl₃) of the reaction mixture (epibromohydrin) using ZnO/C-Pre(9.1wt%) as a catalyst in the 4th cycle of recyclability test.

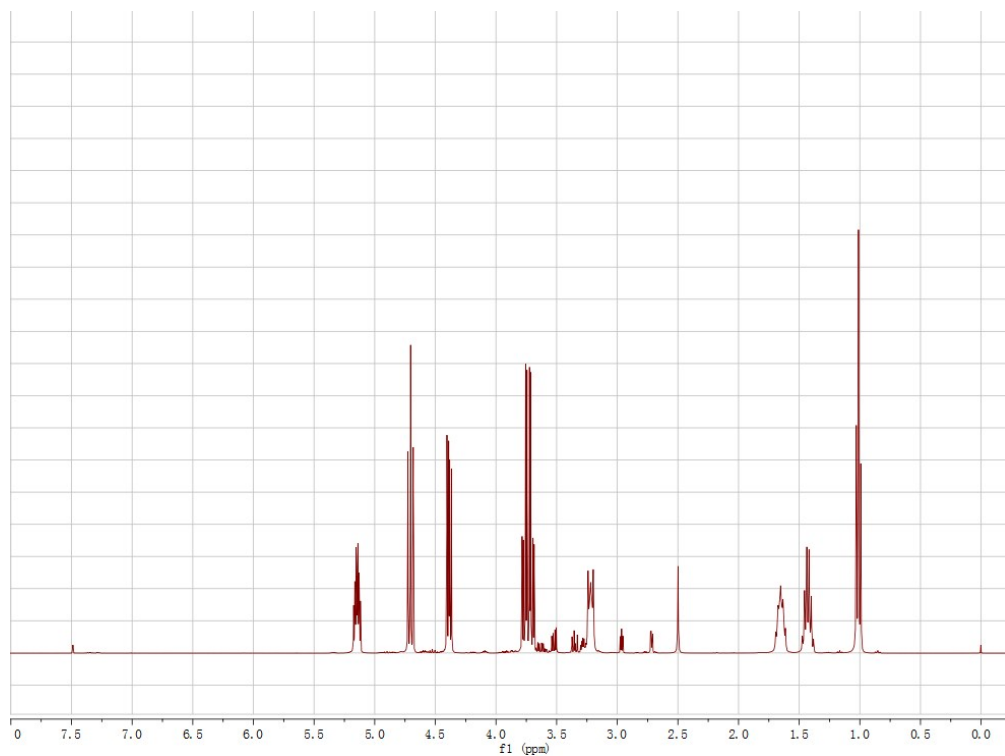


Figure S26. ¹H NMR spectra (in CDCl₃) of the reaction mixture (epibromohydrin) using ZnO/C-Pre(9.1wt%) as a catalyst in the 5th cycle of recyclability test.