Supporting Information

Bifunctional Imidazolium-Based Ionic Liquid Decorated UiO-67 Type MOF for Selective CO_2 Adsorption and Catalytic Property for CO_2 Cycloaddition with Epoxides

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Content

1. Calculation of Q_{st} and by the Virial Method[1]

Heat of adsorption. To calculate heats of adsorptions, the corresponding adsorption isotherms at two different temperatures (273 K / 293 K for CO_2) were simultaneously fitted using the virial type, Equation 1:

$$\ln P = \ln N + \frac{1}{T}\sum_{i=0}^{m} a_i N^i + \sum_{i=0}^{n} b_i N^i \quad (1)$$

The heat of adsorption at zero coverage was calculated from Equation 2, where as a function of surface coverage, from Equation 3:

$$Q_{st} = -Ra_0 \quad (2)$$

$$Q_{st}(N) = -R\sum_{i=0}^{m} a_i N^i \quad (3)$$

2. Characterization of Ligand L

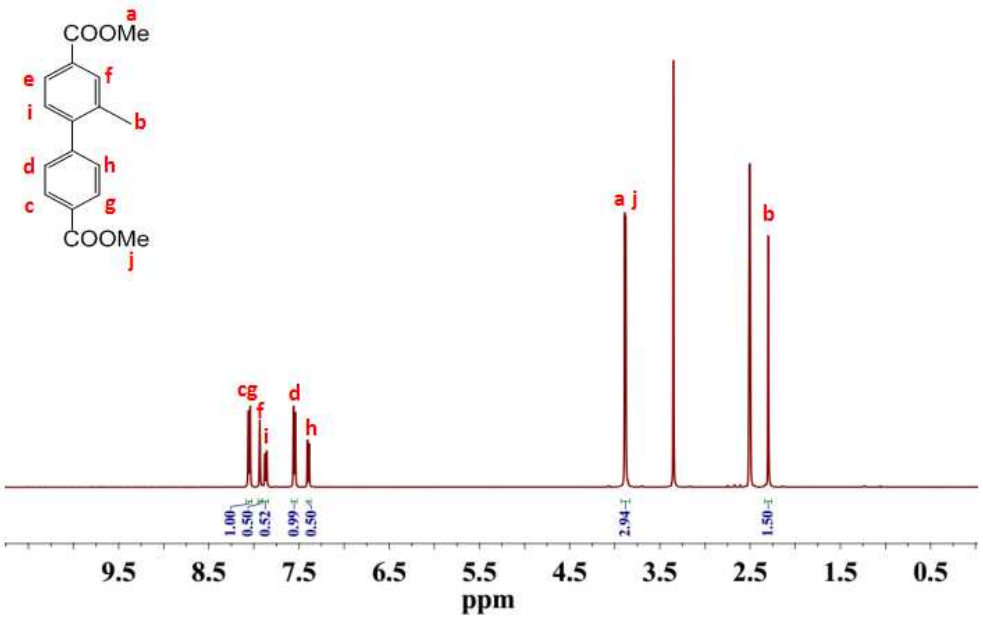

Figure S1. The ^{1}H-NMR spectrum of intermediate **A**.

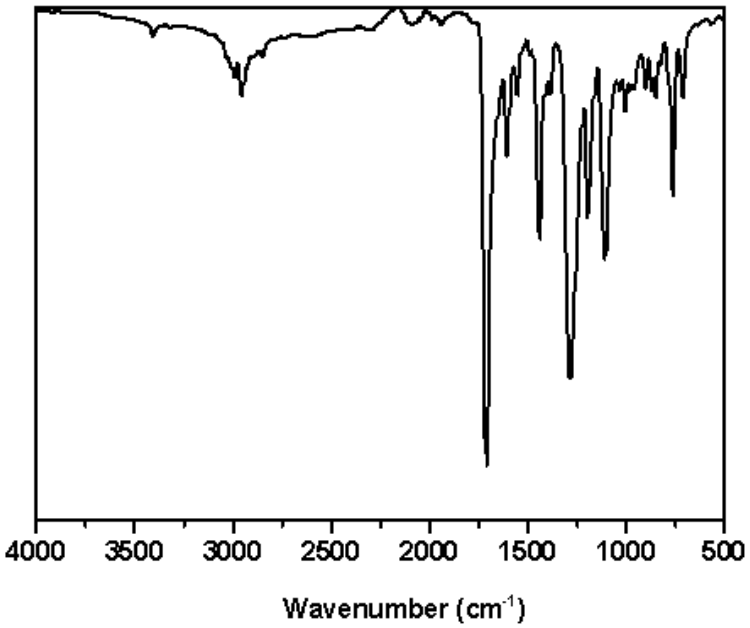

Figure S2. FTIR spectrum for intermediate **A**.

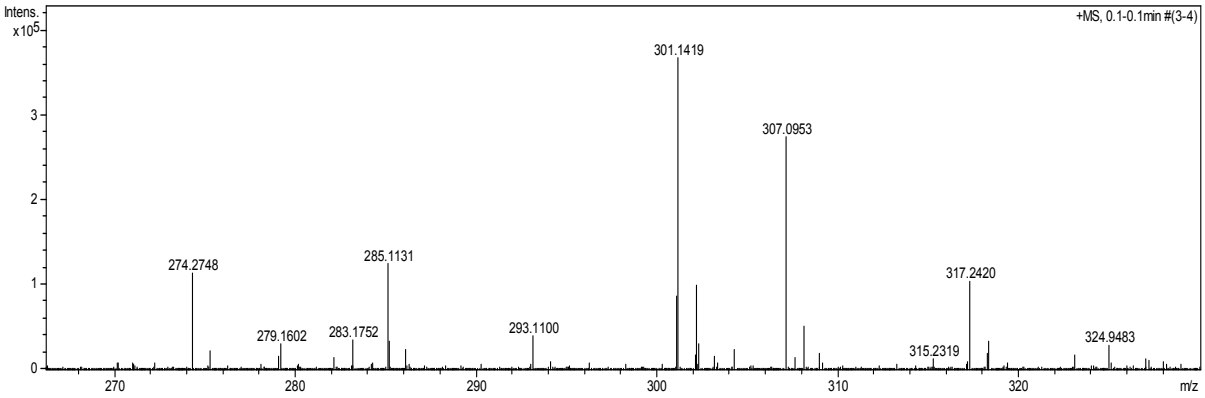

Figure S3. The mass spectrum (MS) of intermediate **A**.

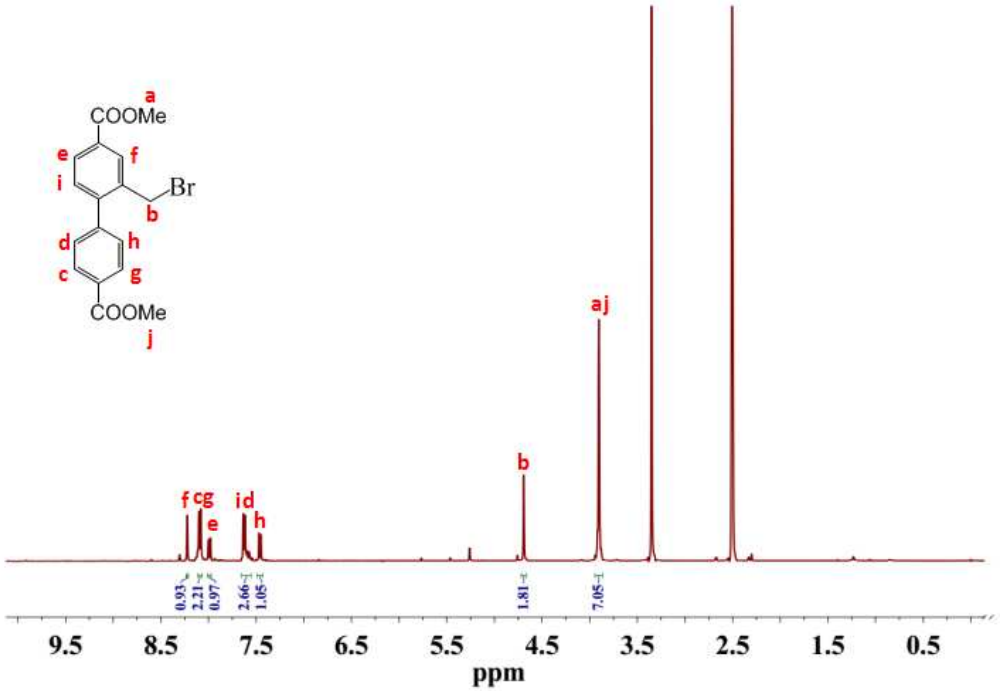

Figure S4. The ^{1}H-NMR spectrum of intermediate **B**.

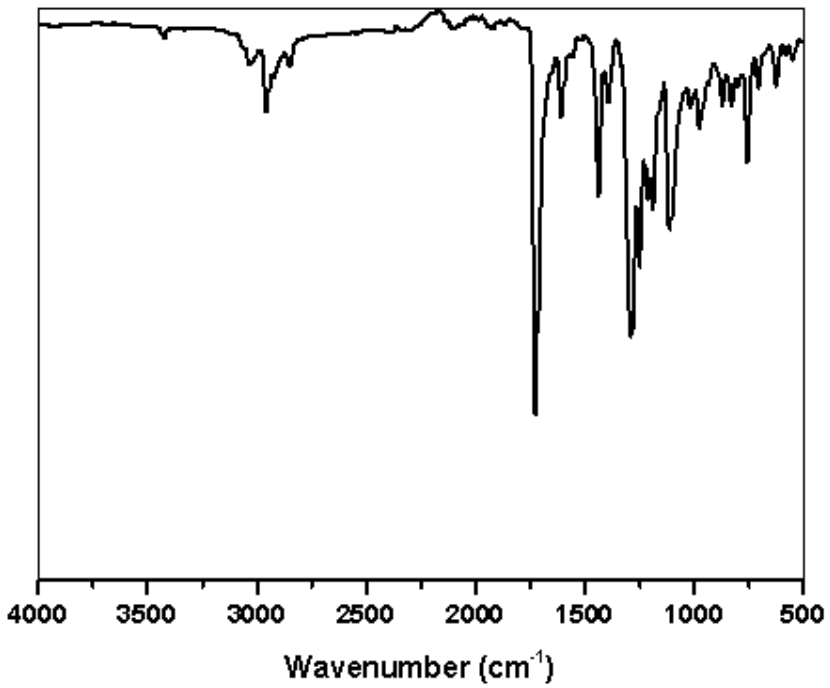

Figure S5. FTIR spectrum for intermediate **B**.

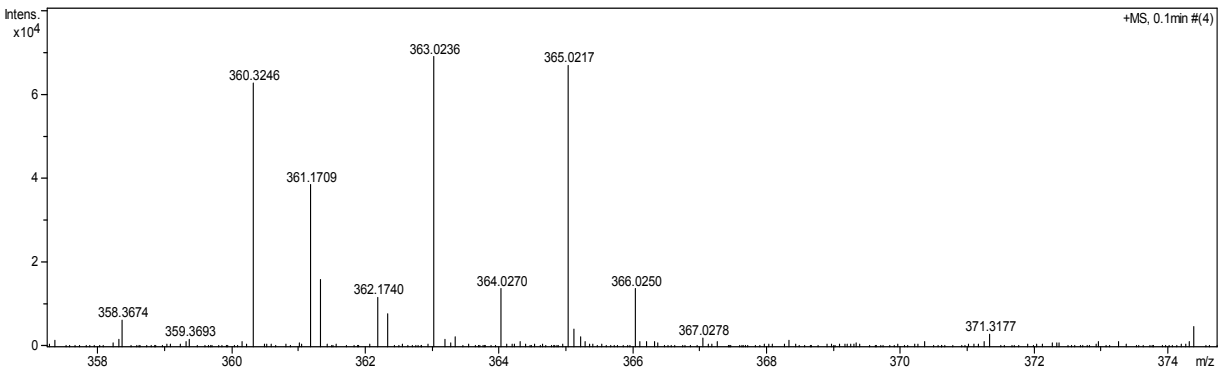

Figure S6. The mass spectrum (MS) of intermediate **B**.

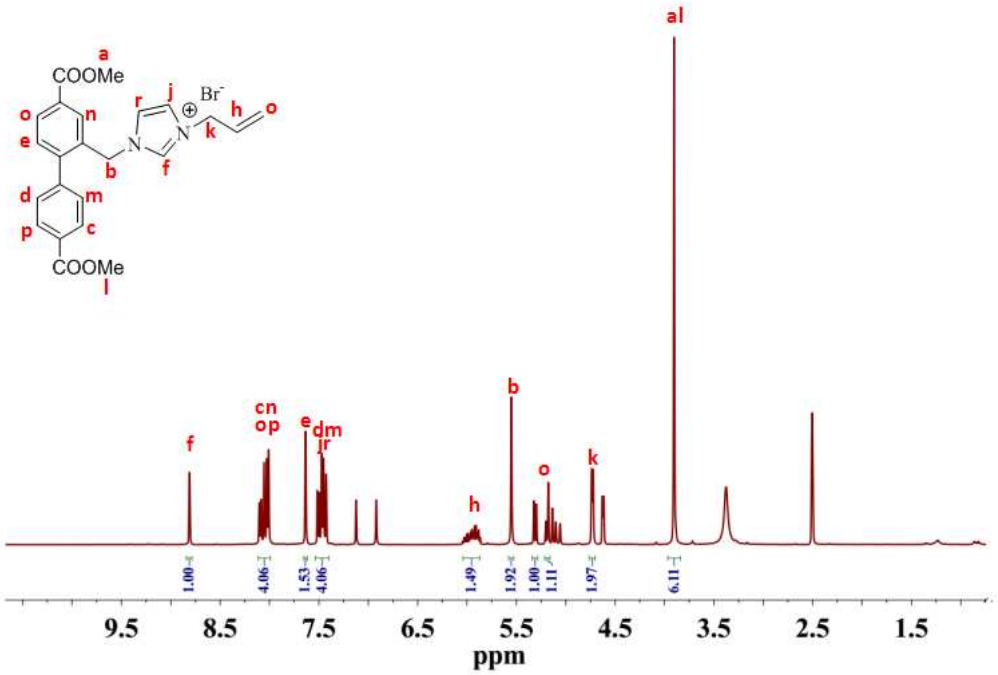

Figure S7. The ^{1}H-NMR spectrum of intermediate **C**.

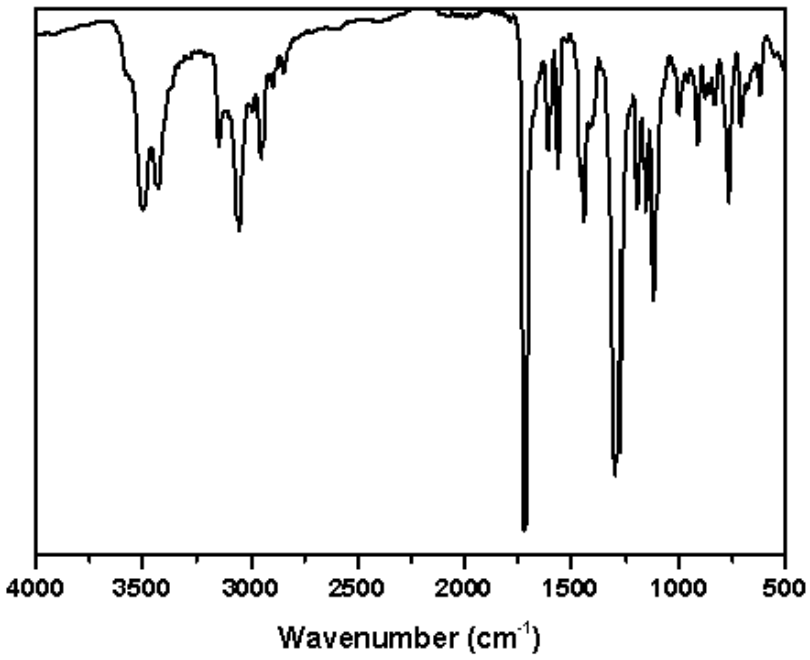

Figure S8. IR spectrum for intermediate **C**.

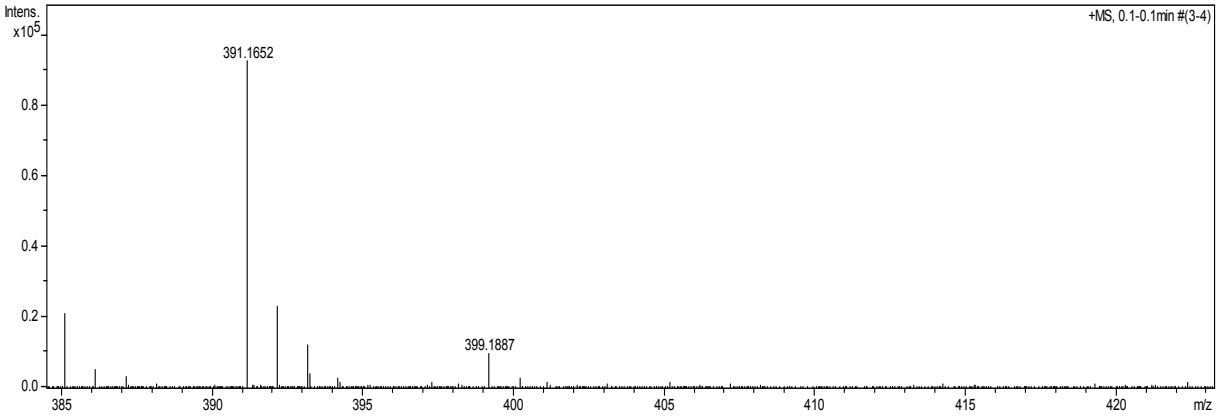

Figure S9. The mass spectrum (MS) of intermediate **C**.

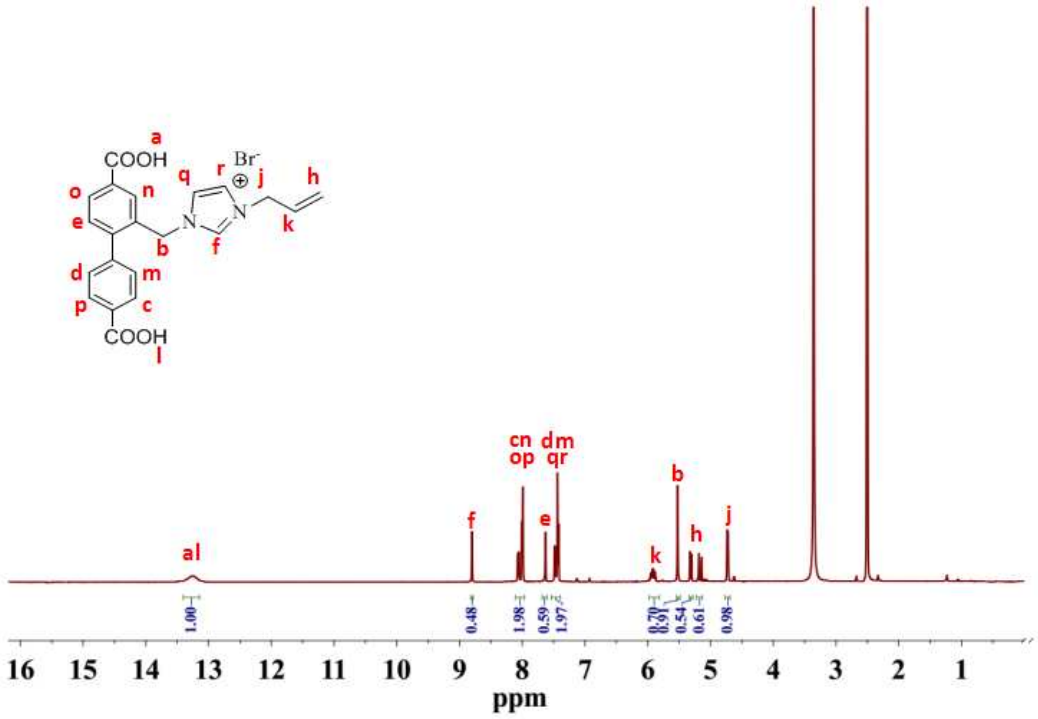

Figure S10. The ^{1}H-NMR spectrum of the imidazolium-based ligand **L**.

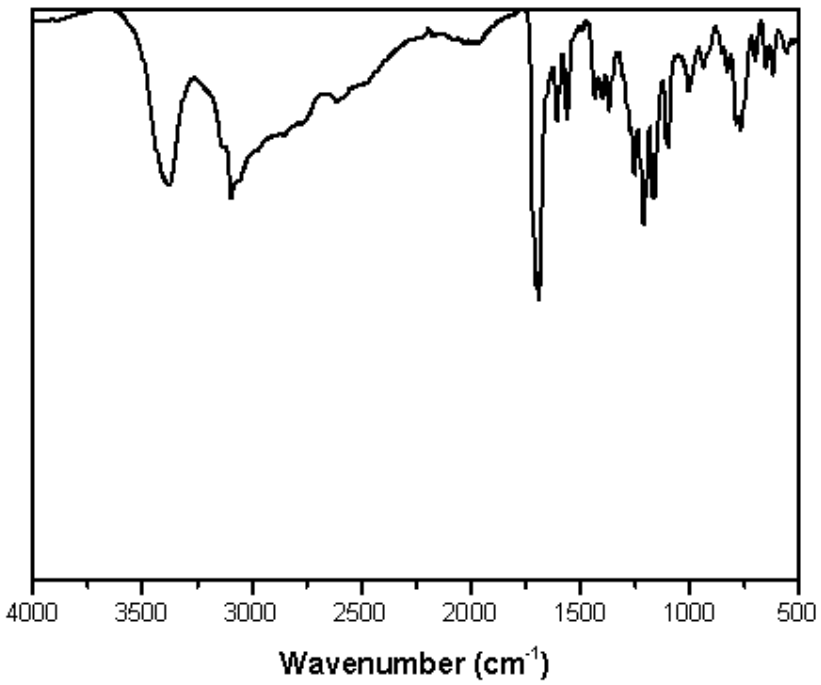

Figure S11. FTIR spectrum for the imidazolium-based ligand **L**.

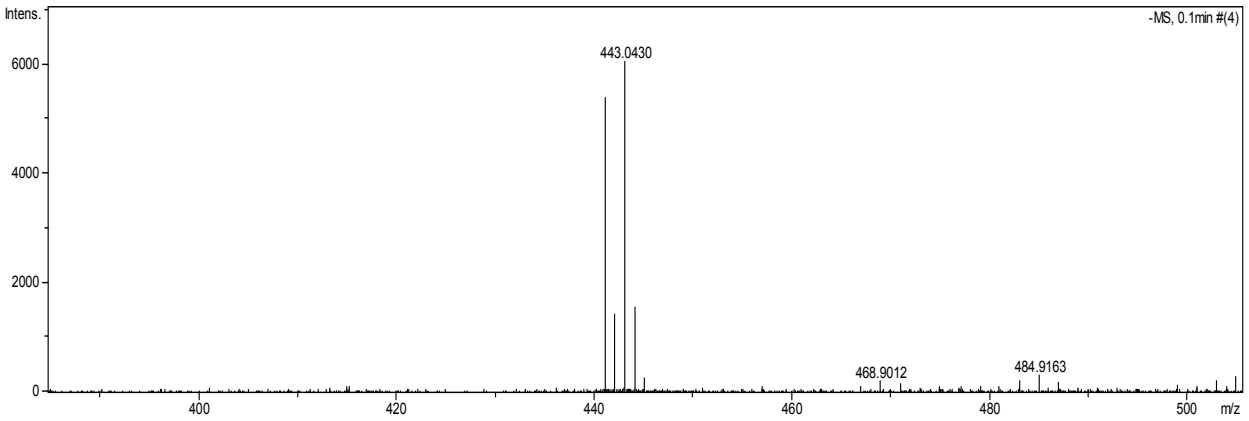

Figure S12. The mass spectrum (MS) of the imidazolium-based ligand **L**.

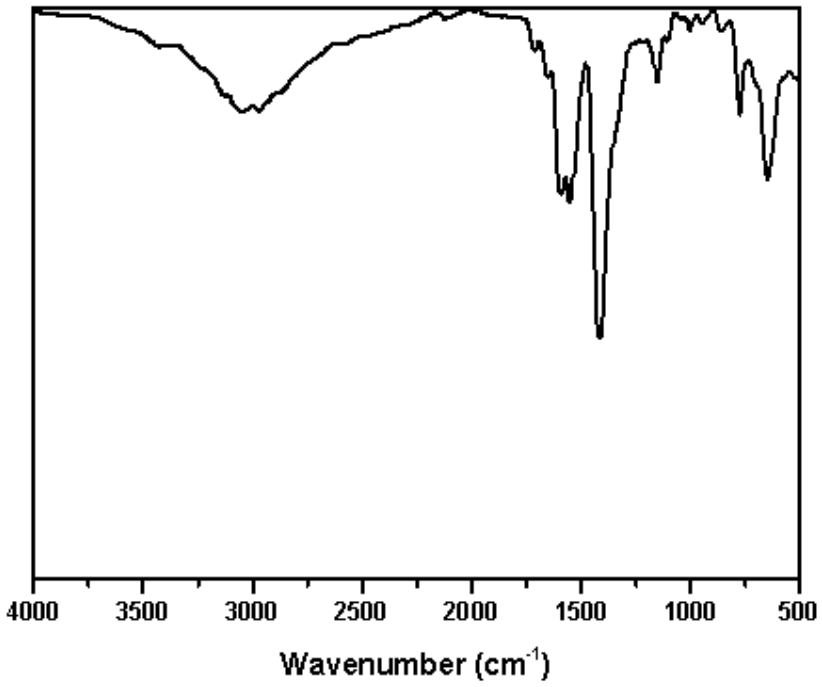

Figure S13. FTIR spectrum for UiO-67-IL, **1**.

3. The ^{1}H NMR spectra for Catalytic CO_2 Cyclic Addition

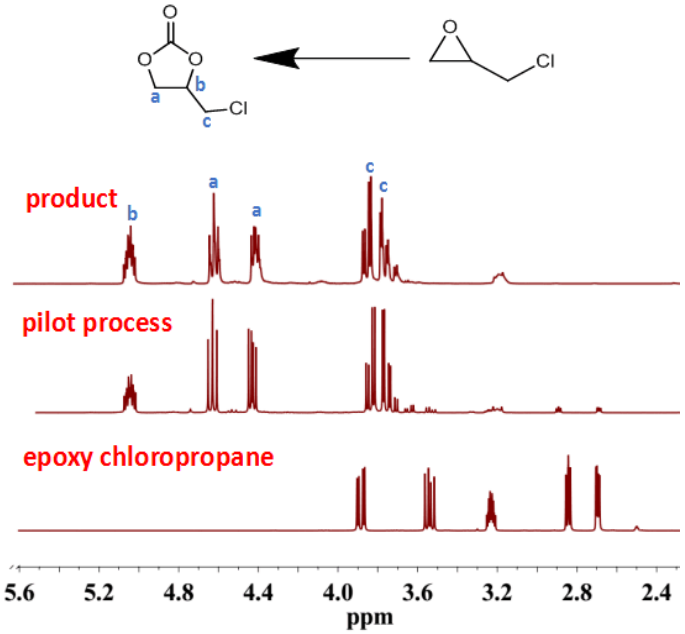

Figure S14. The ^{1}H-NMR spectrum of the epichlorohydrin and catalytic product.

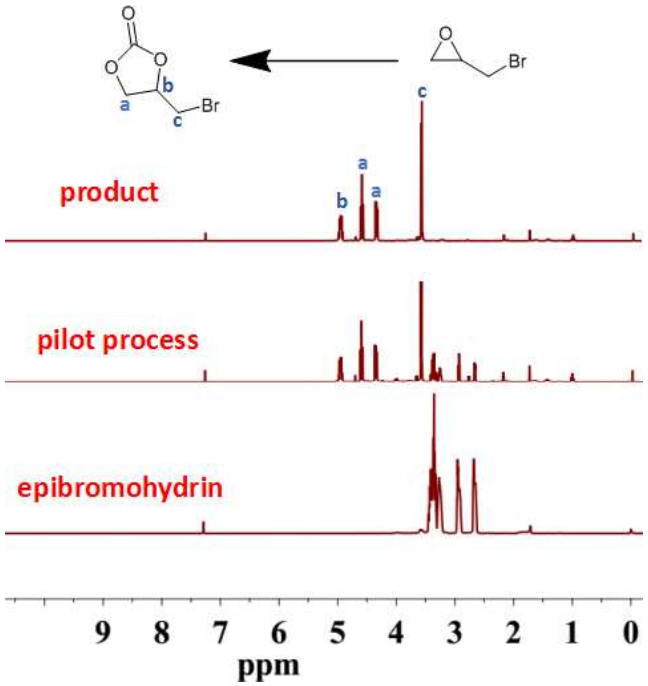

Figure S15. The ^{1}H-NMR spectrum of the epoxy bromopropane and catalytic product.

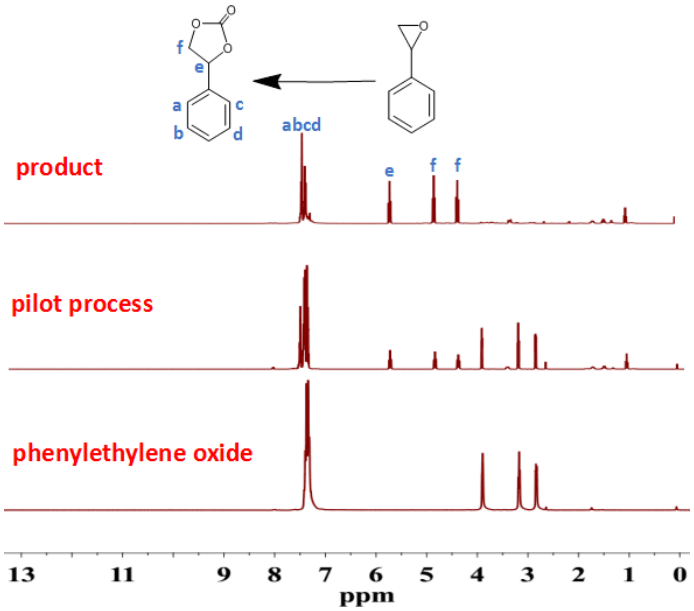

Figure S16. The ^{1}H-NMR spectrum of the epoxy styrene and catalytic product.

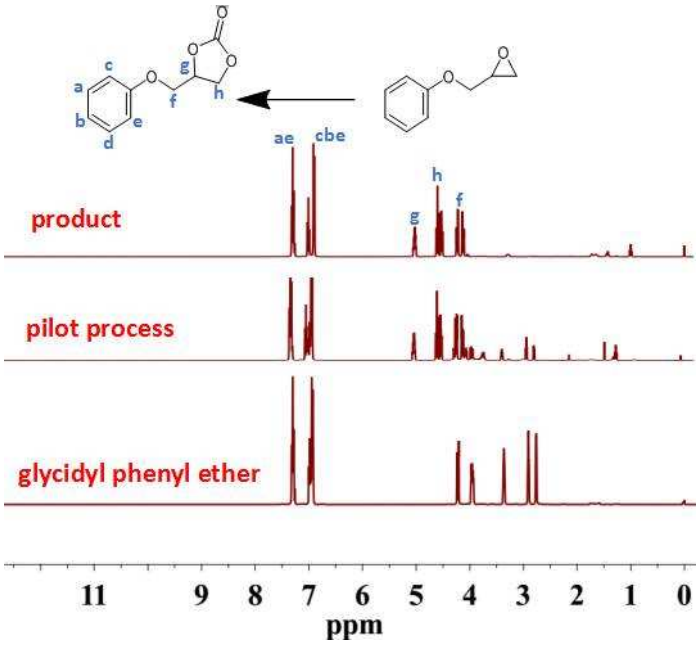

Figure S17. The ^{1}H-NMR spectrum of the phenyl glycidyl ether and catalytic product.

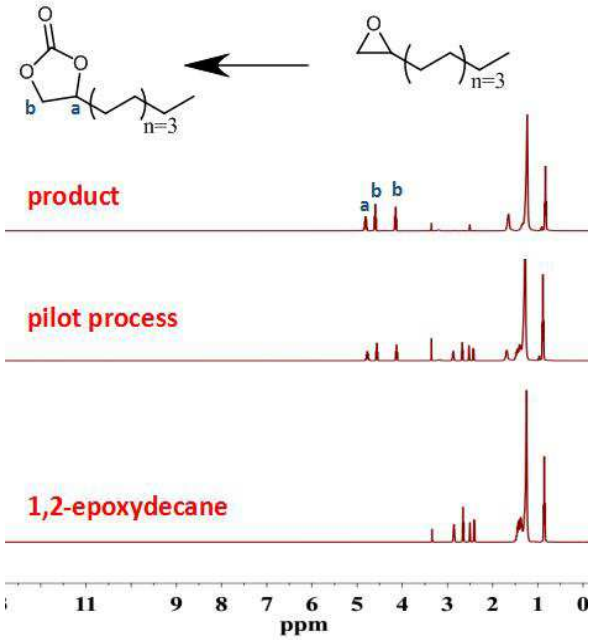

Figure S18. The ^{1}H-NMR spectrum of the 1,2-epoxydecane and catalytic product.

4. References

(1) Xydias, P.; Spanopoulos, I.; Klontzas, E.; Froudakis, G.E.; Trikalitis, P. N.; Drastic Enhancement of the CO_2 Adsorption Properties in Sulfone Functionalized Zr- and Hf-UiO-67 MOFs with Hierarchical Mesopores. *Inorg. Chem*. **2014**, *53*, 679–681.