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Supplementary Information

Integration of polypyridyl-based ionic liquids into MIL-101 for promoting CO_2 conversion into cyclic carbonates under cocatalyst-free and solventless conditions

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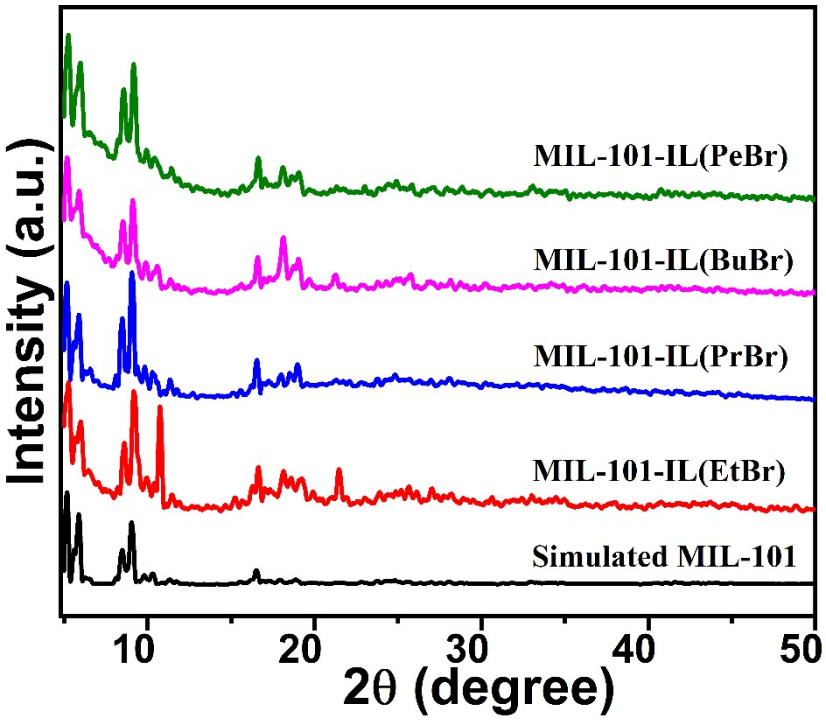

Fig. S1 PXRD patterns of MIL-101-IL(RBr).

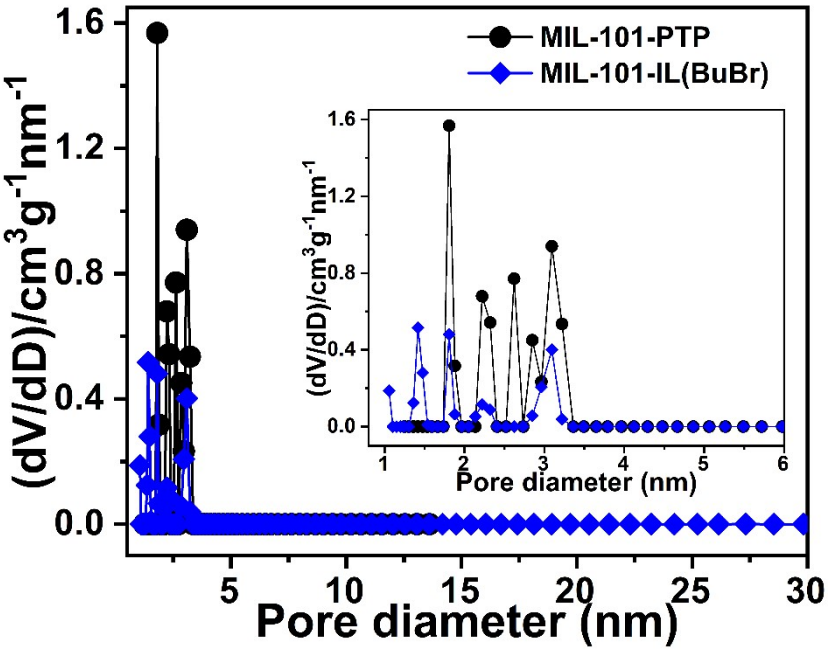

Fig. S2 NLDFT pore size distributions of MIL-101-PTP and MIL-101-IL(BuBr).

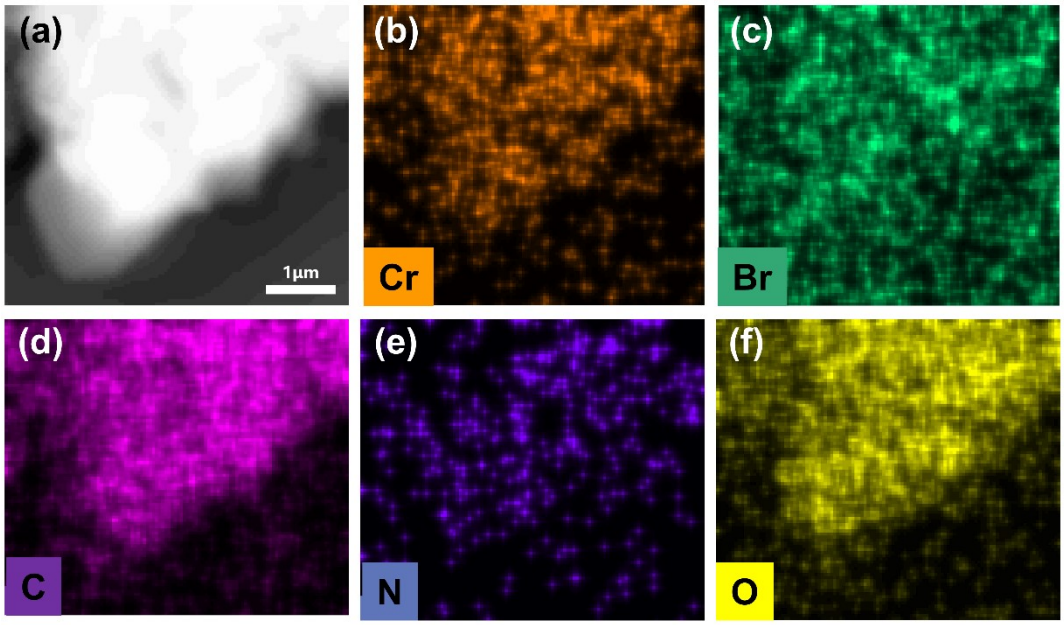

Fig. S3 SEM image and the elemental mapping of MIL-101-IL(BuBr).

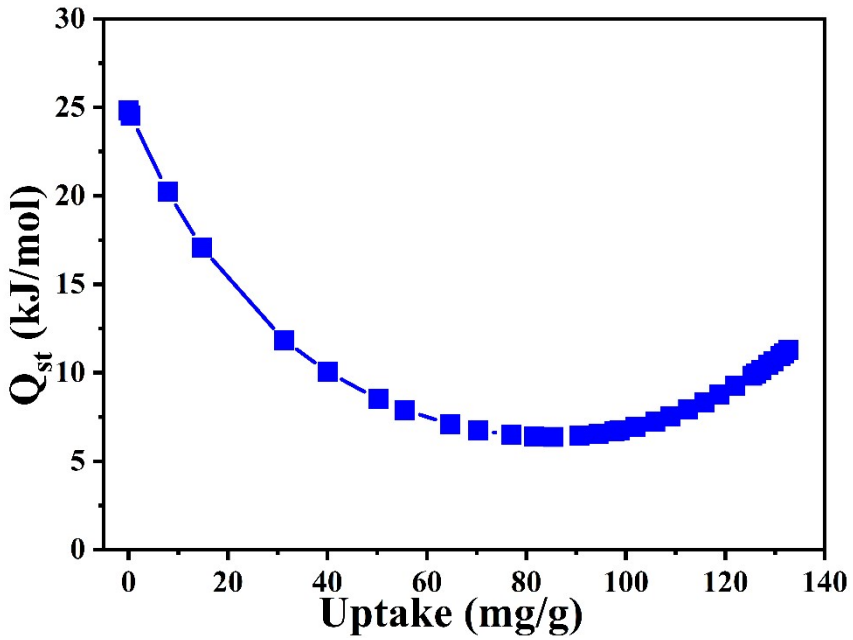

Fig. S4 Isosteric heat of CO_2 adsorption for of MIL-101-IL(BuBr) by Clausius–Clapeyron equation.

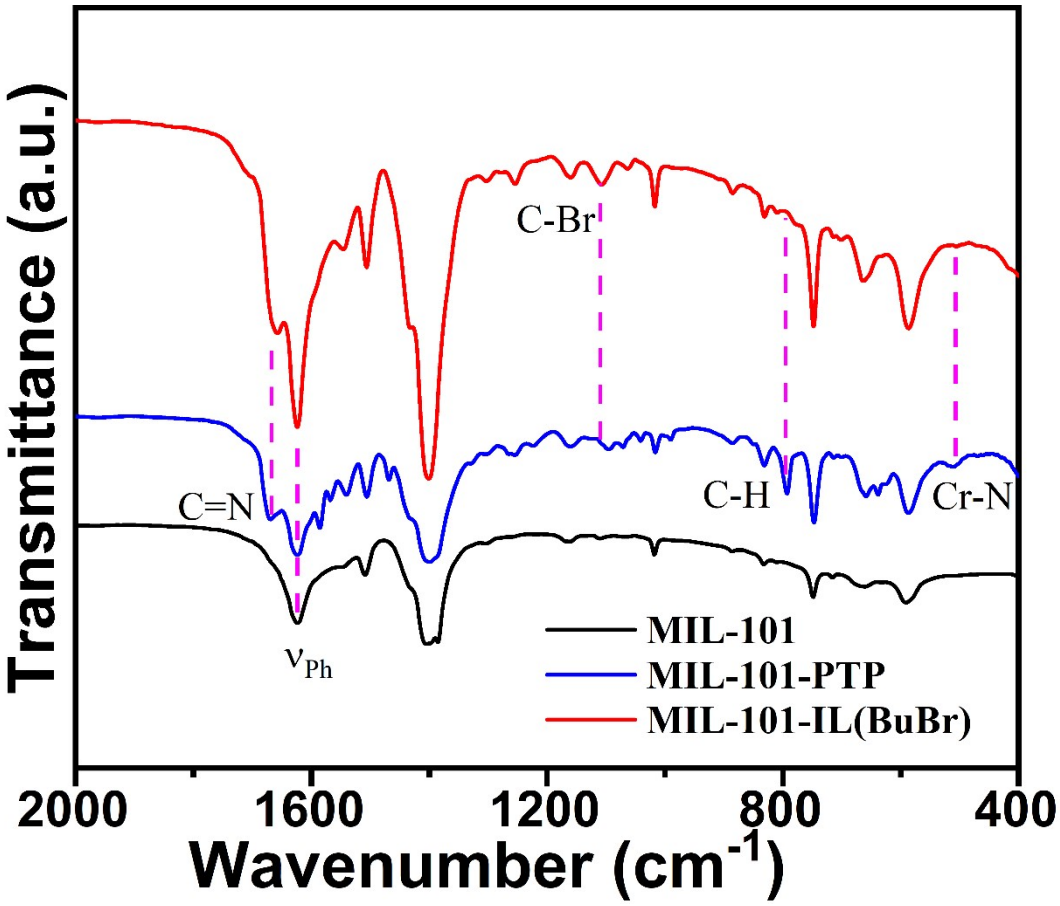

Fig. S5 FTIR spectra of MIL-101, MIL-101- PTP and MIL-101-IL(BuBr).

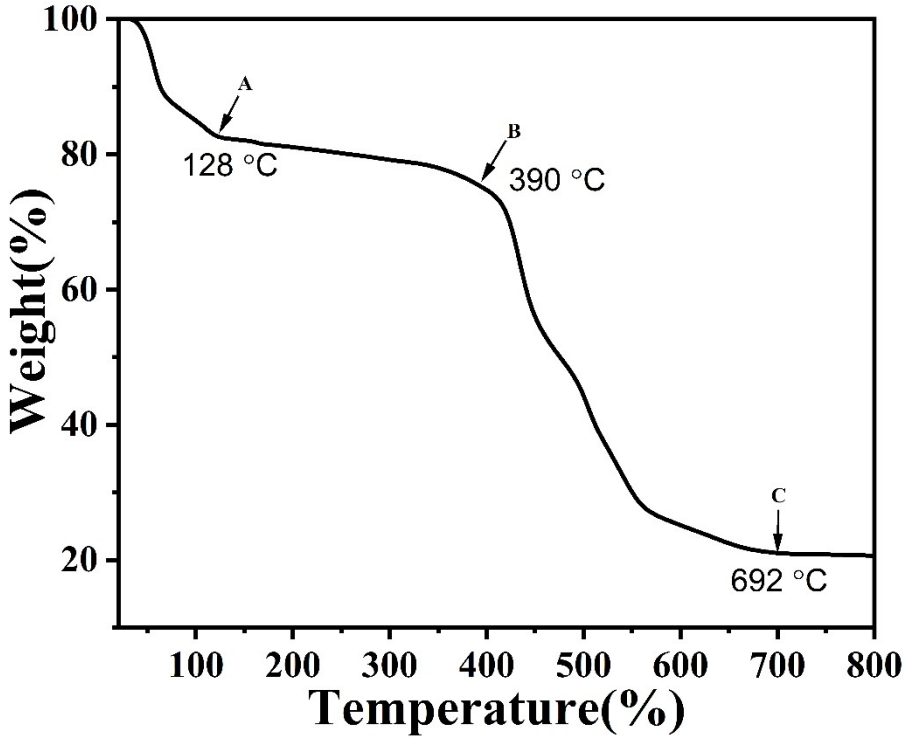

Fig. S6 TG curve of MIL-101-IL(BuBr).

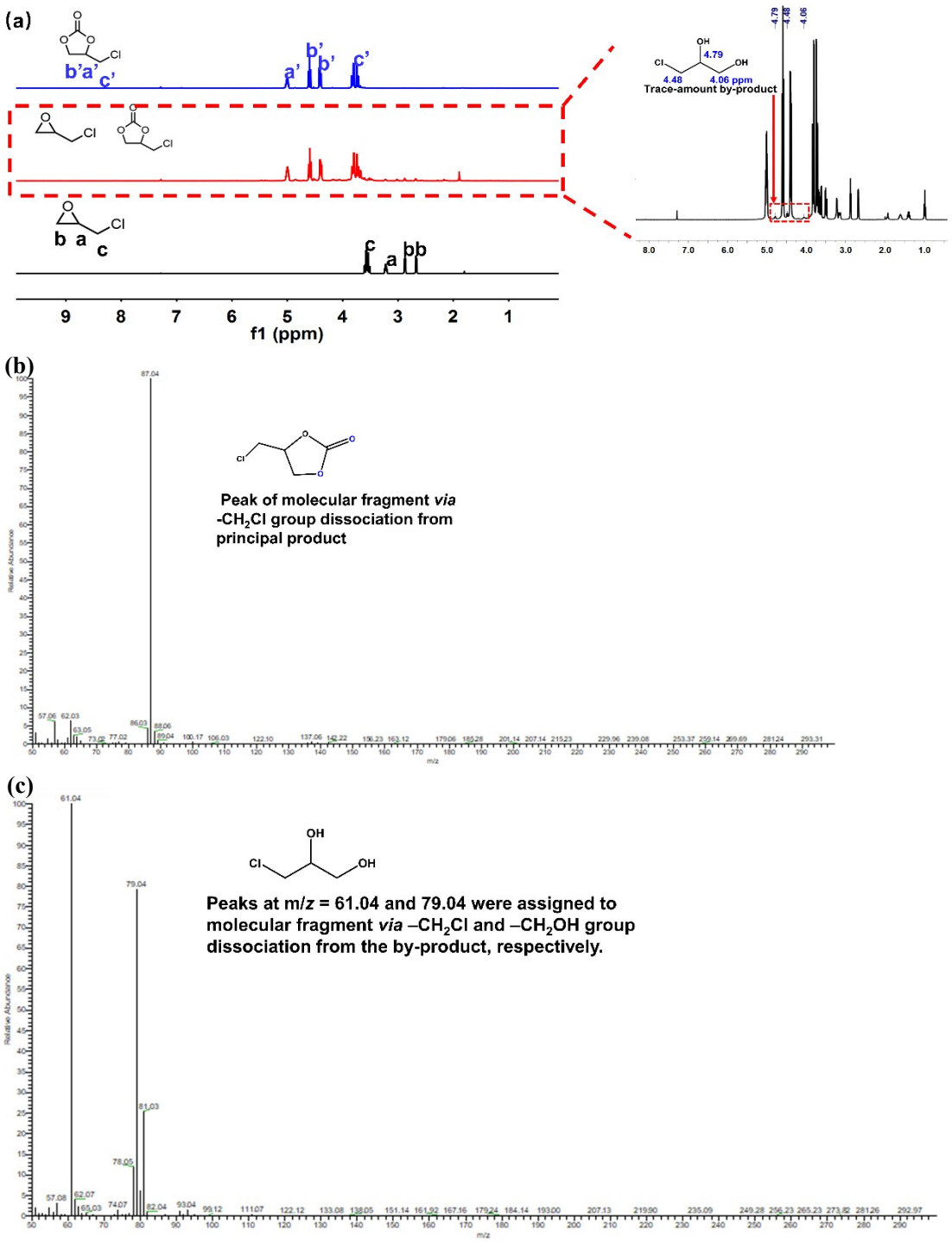

Fig. S7 (a) ^{1}H-NMR (a) spectra ($CDCl_3$) for ECH cycloaddition with CO_2 using MIL-101-IL(BuBr) catalyst. Black line: the substrate; Red line: the reaction solution after centrifugation (conditions: 100 mg catalyst, 1.0 MPa CO_2 and 110 ˚C for 6 h); Blue line: the isolated product; (b) mass spectra of the principal product; (c) mass spectra of the by-product.

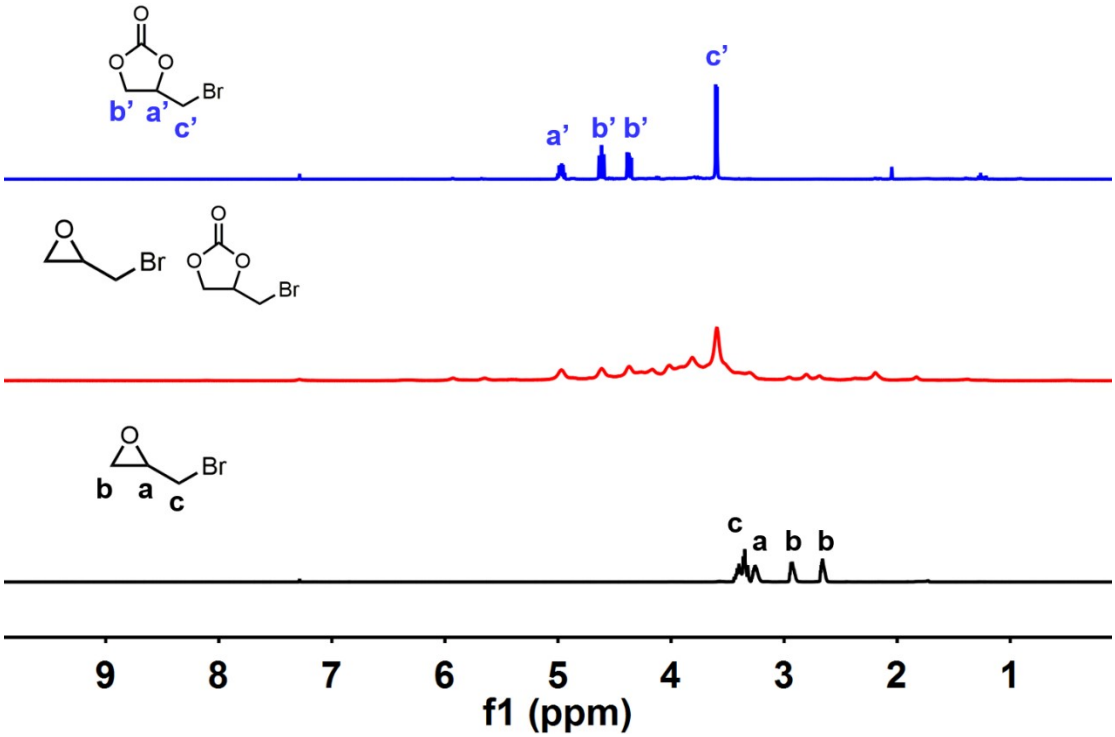

Fig. S8 ^{1}H-NMR spectra ($CDCl_3$) for CO_2 cycloaddition with epibromohydrin using MIL-101-IL(BuBr) catalyst. Black line: the substrate; Red line: the reaction solution after centrifugation (conditions: 100 mg catalyst, 1.0 MPa CO_2 and 110 ˚C for 6 h); Blue line: the isolated product.

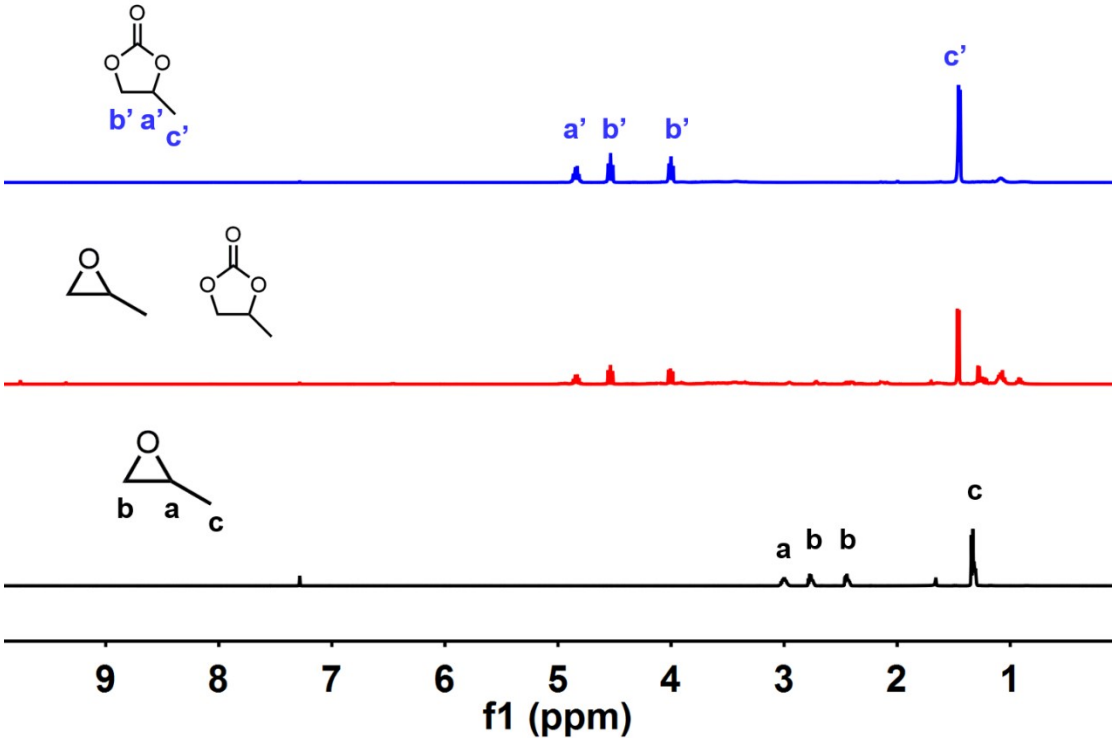

Fig. S9 ^{1}H-NMR spectra ($CDCl_3$) for CO_2 cycloaddition with propylene oxide using MIL-101-IL(BuBr) catalyst. Black line: the substrate; Red line: the reaction solution after centrifugation (conditions: 100 mg catalyst, 1.0 MPa CO_2 and 110 ˚C for 6 h); Blue line: the isolated product.

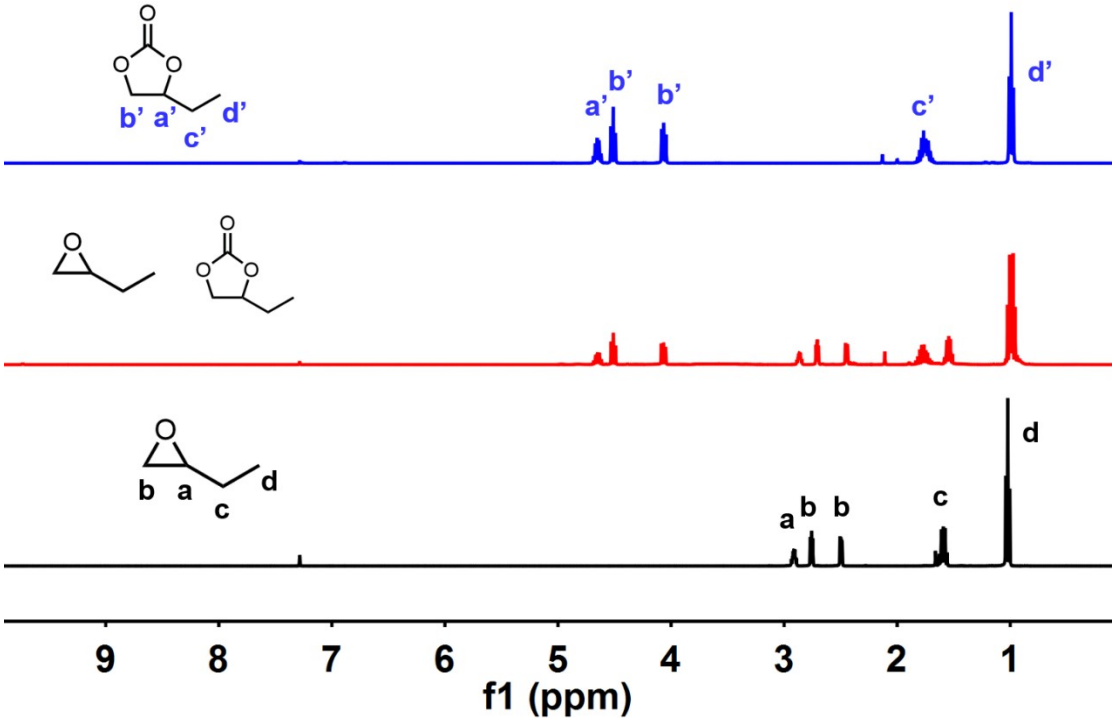

Fig. S10 ^{1}H-NMR spectra ($CDCl_3$) for CO_2 cycloaddition with 1,2-epoxybutane using MIL-101-IL(BuBr) catalyst. Black line: the substrate; Red line: the reaction solution after centrifugation (conditions: 100 mg catalyst, 1.0 MPa CO_2 and 110 ˚C for 6 h); Blue line: the isolated product.

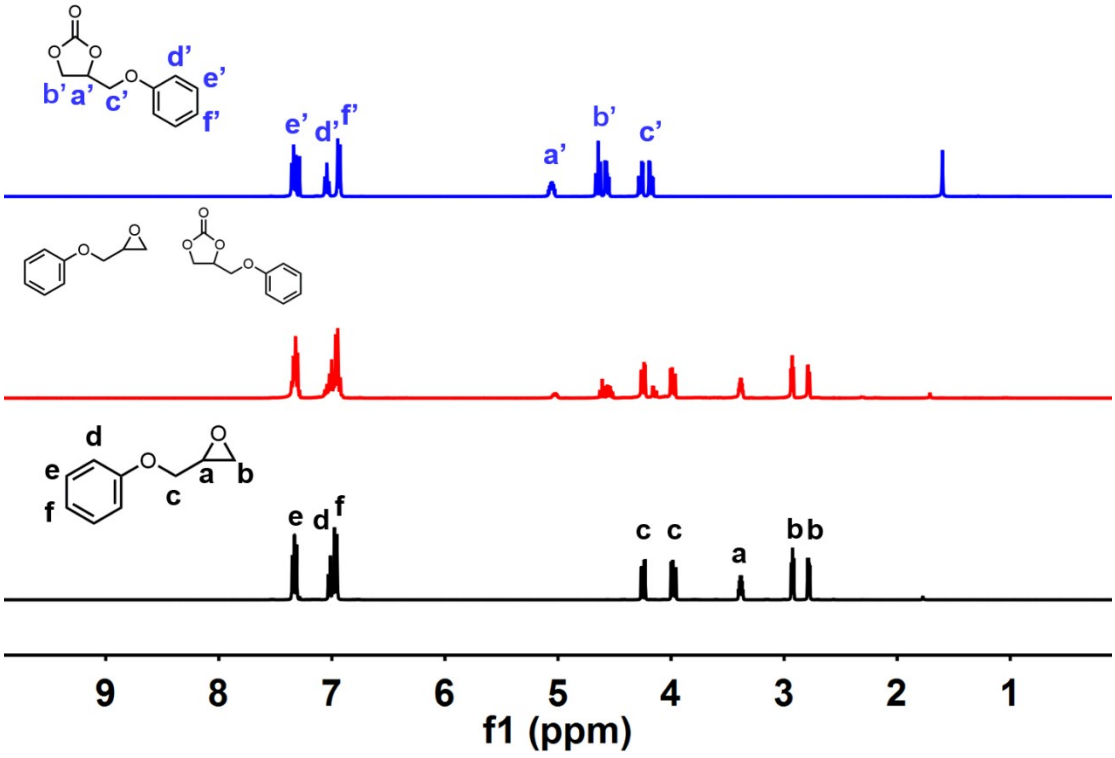

Fig. S11 ^{1}H-NMR spectra ($CDCl_3$) for CO_2 cycloaddition with epoxypropyl phenyl ether using MIL-101-IL(BuBr) catalyst. Black line: the substrate; Red line: the reaction solution after

centrifugation (conditions: 100 mg catalyst, 1.0 MPa CO_2 and 110 ˚C for 6 h); Blue line: the isolated product.

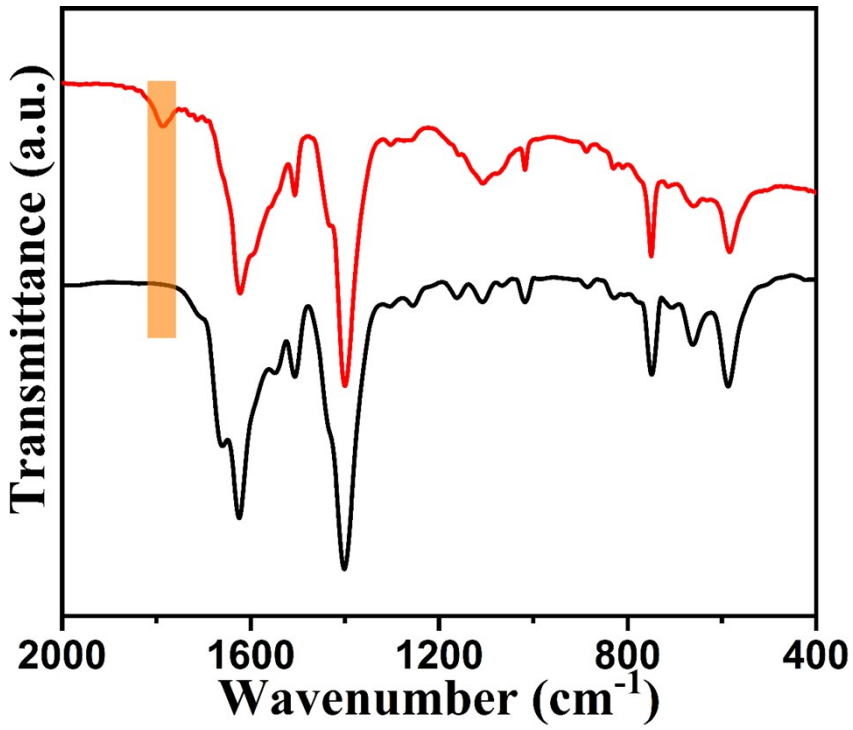

Fig. S12 FTIR spectra for the fresh (black line) and reused (red line) MIL-101-IL(BuBr).

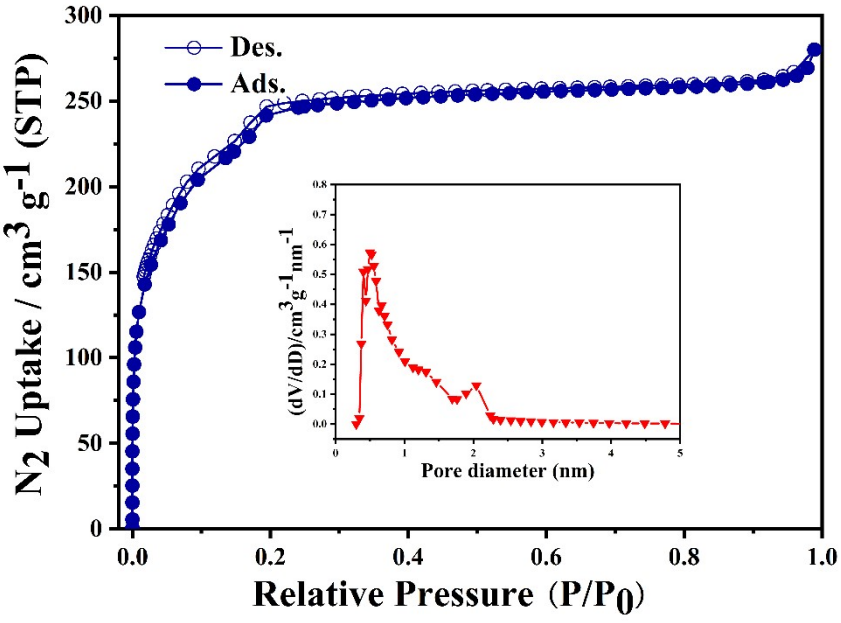

Fig. S13 N_2 adsorption and desorption isotherms at 77 K of the reused MIL-101-IL(BuBr). Inset: the NLDFT pore size distribution.

Table S1. Elemental analysis of the MIL-101 derivatives.

Element	C wt%	N wt%	H wt%
Theoretical MIL-101(Cr)	24.64	0	5.69
MIL-101-PTP	47.18	5.61	3.15
MIL-101-IL(BuBr)	32.38	0.81	2.81