Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

In-situ cleavage and rearrangement synthesis of an easy-obtained and high stable Cu(II)-based MOF for efficient heterogeneous catalysis of carbon dioxide conversion

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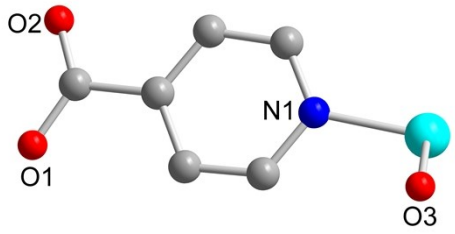


Figure S1 Asymmetric unit of **1**. Selective bond distance (Å) and angle (°) in **1**. Cu(1)-O(1) 1.940(4), Cu(1)-O(2) 1.945(4), Cu(1)-O(3) 2.296(5), Cu(1)-N(1) 2.018(5), O(1)-Cu(1)-O(2) 175.36(19), O(1)-Cu(1)-N(1) 92.1(2), O(2)-Cu(1)-N(1) 90.3(2), O(1)-Cu(1)-O3(1) 91.28(17), O(2)-Cu(1)-O(3) 84.56(17).

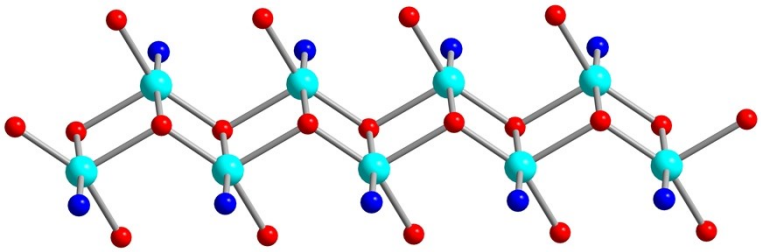


Figure S2 The coordination environment and connected mode of Cu chains.

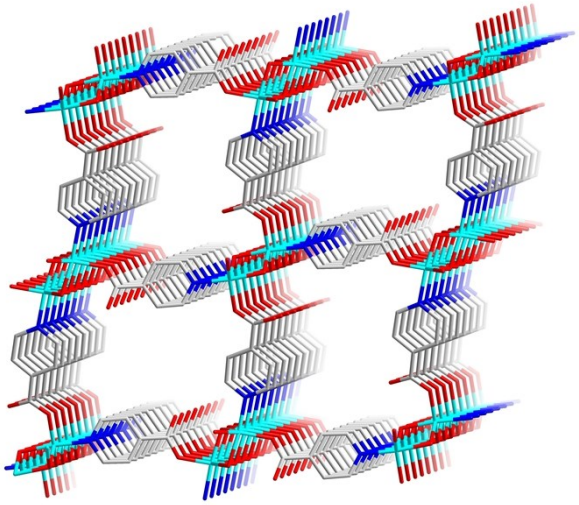


Figure S3 Structure of **1** showing the three-dimensional frameworks with one-dimensional channels.

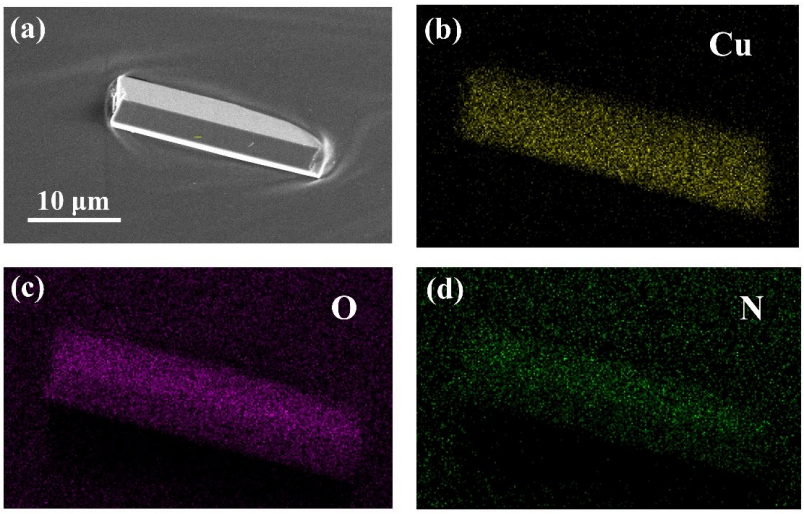


Figure S4 (*a*) The SEM image of **1**; (*b-d*) the element mapping image of **1** for Cu, O, and N, respectively.

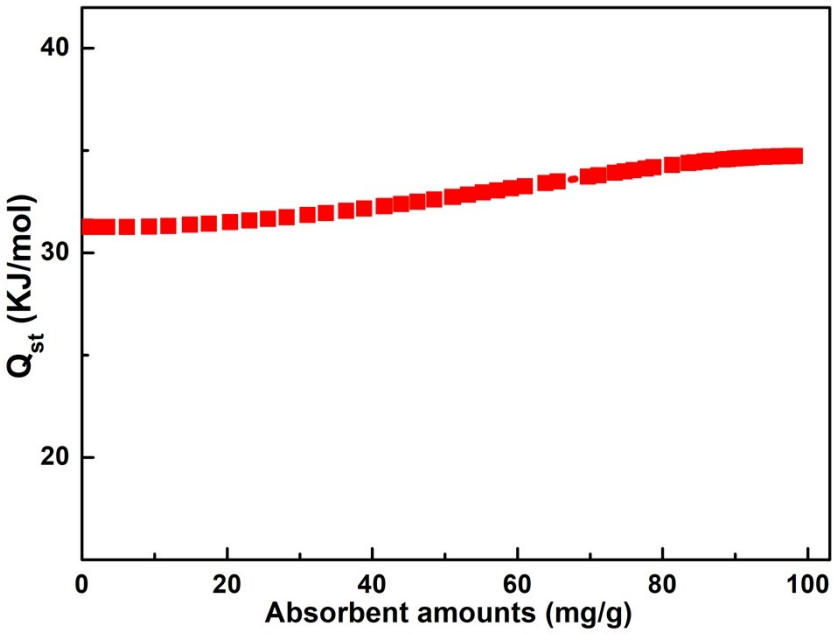


Figure S5 Isosteric adsorption enthalpy of CO_2 on **1**.

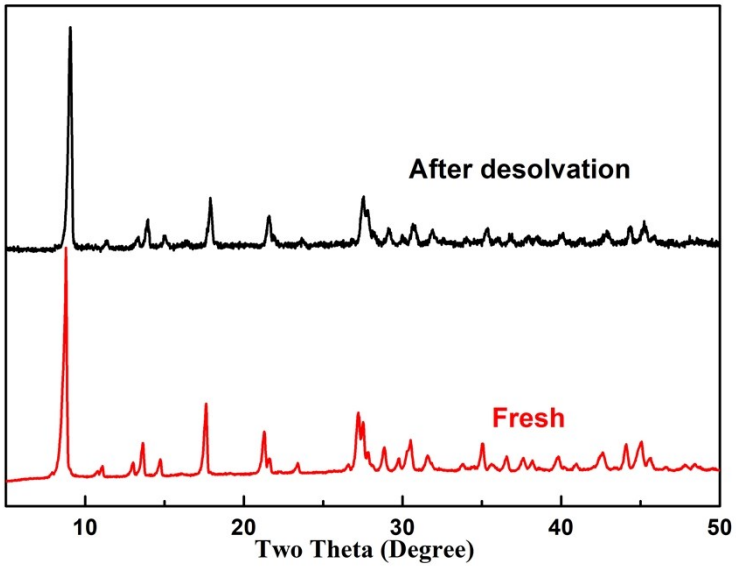


Figure S6 PXRD patterns of fresh **1** (red) and after desolvation (black).

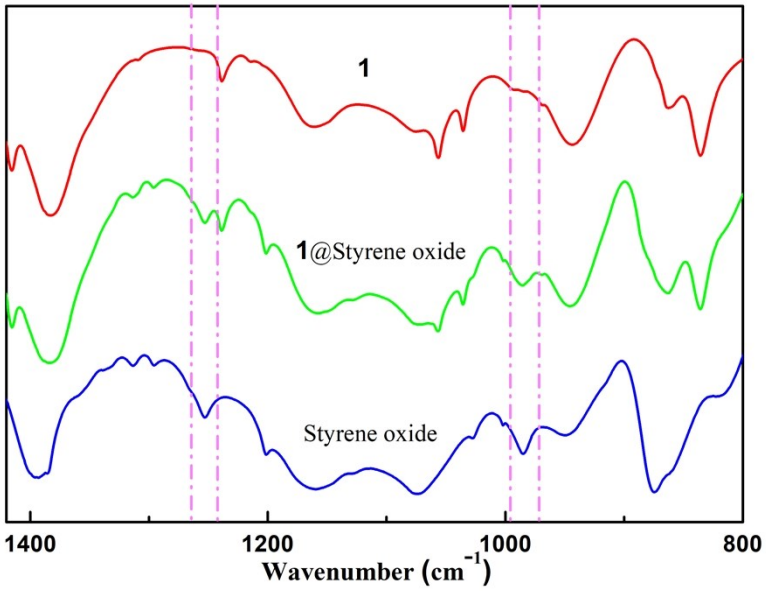
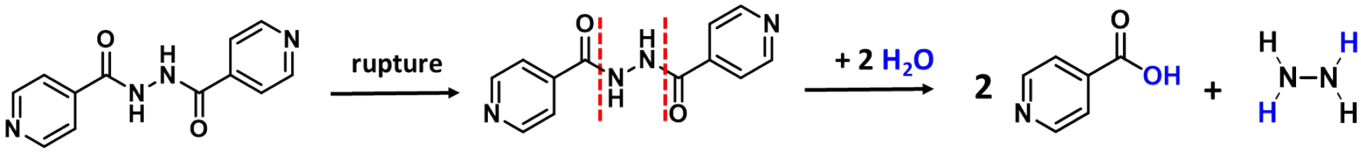


Figure S7. Comparisons of FT-IR spectra of **1**, **1** after immersed in styrene oxide and free styrene oxide.



Scheme S1. Proposed cleavage and rearrangement process of the ligand *N*,*N'*-bis(4-picolinoyl)hydrazine into isonicotinate moiety.

Table S1. Comparisons of CO_2 cycloaddition catalysis based on Cu-MOFs heterogeneous catalysts.

Entry	MOF	Amount MOF / TBABr	T / °C	P / atm	t / h	Yield / %	Ref.
1	Cu-NTTA	5 μmol / 1.5 mol%	100	10	8	56.3	39
2	Cu-MOF	2 μmol / 1.5 mol%	100	10	12	>99	40
3	JLU-Liu20	0.25 mol% / 5 mol%	80	1	48	72	41
4	Cu(TPA)	5 wt% / 5 mol%	70	1	10	93	42
5	Cu-MOF	0.4 mol% / 0.2 mol%	70	1	16	90	43
6	**1**	5 mol% / 0.5 mol%	100	5	12	>99	**This work**

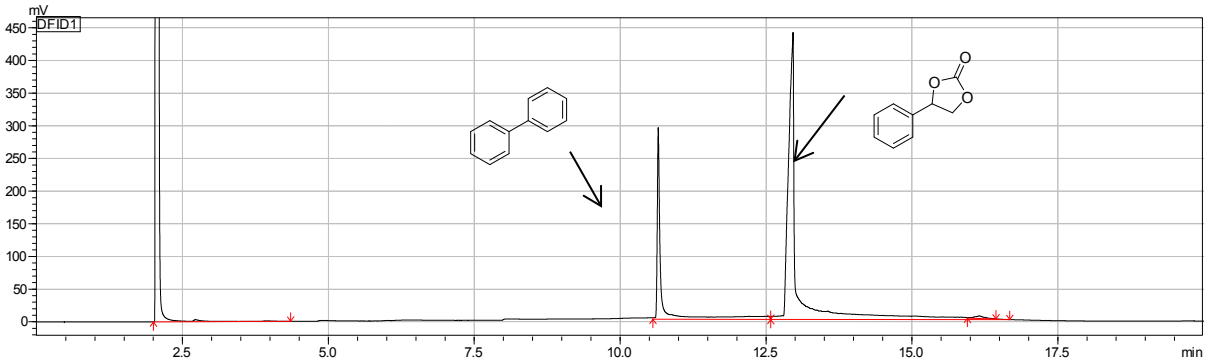


Figure S8 GC spectrum of cycloaddition product **1b**.

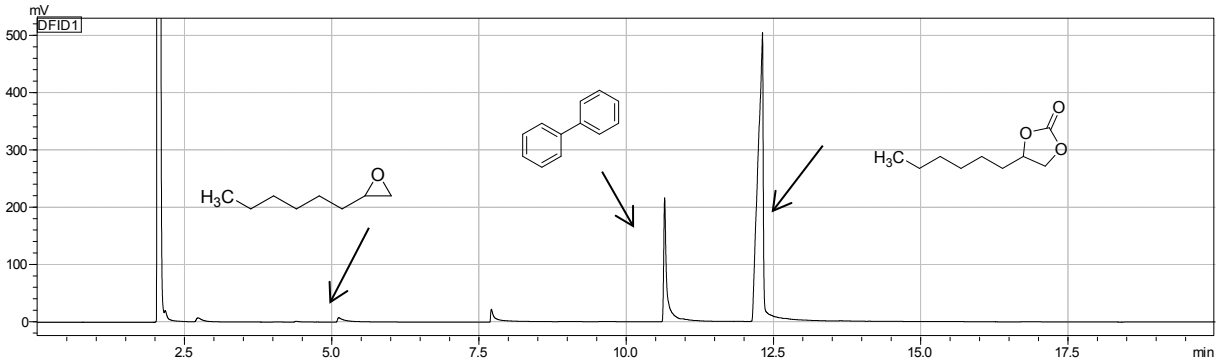


Figure S9 GC spectrum of cycloaddition product **2b**.

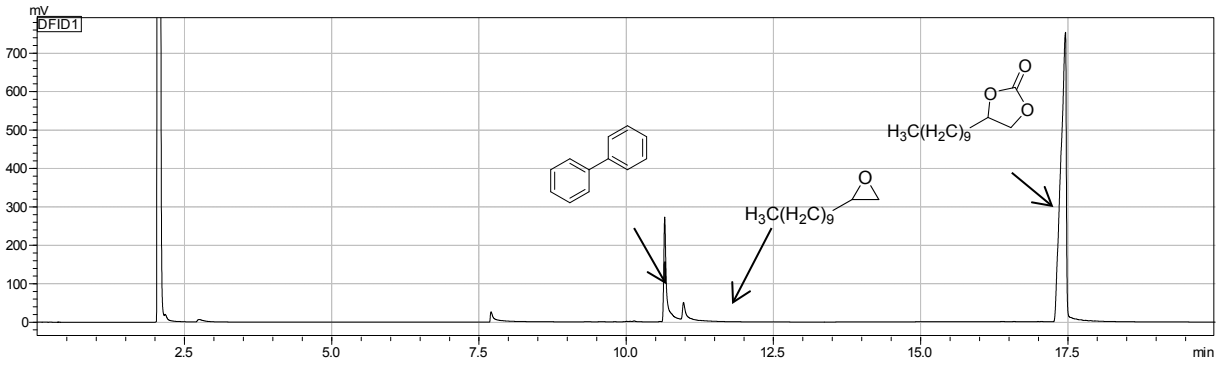


Figure S10 GC spectrum of cycloaddition product **3b**.

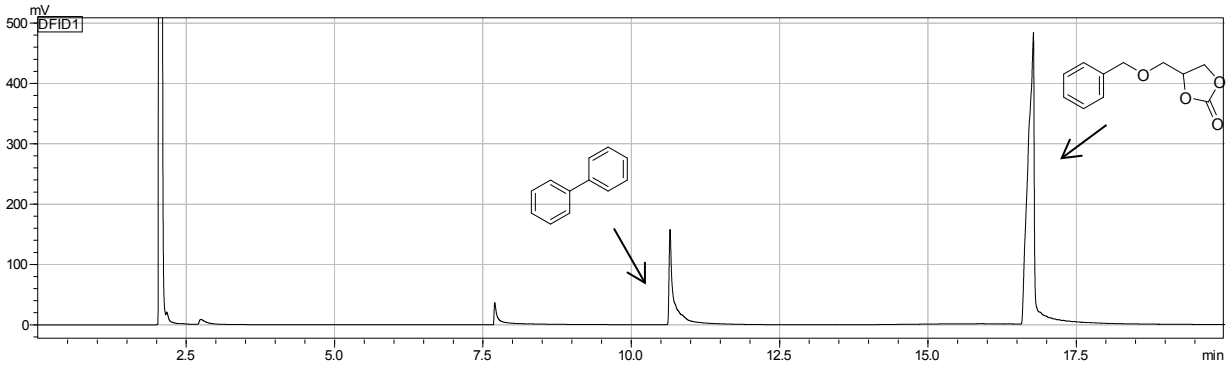


Figure S11 GC spectrum of cycloaddition product **4b**.

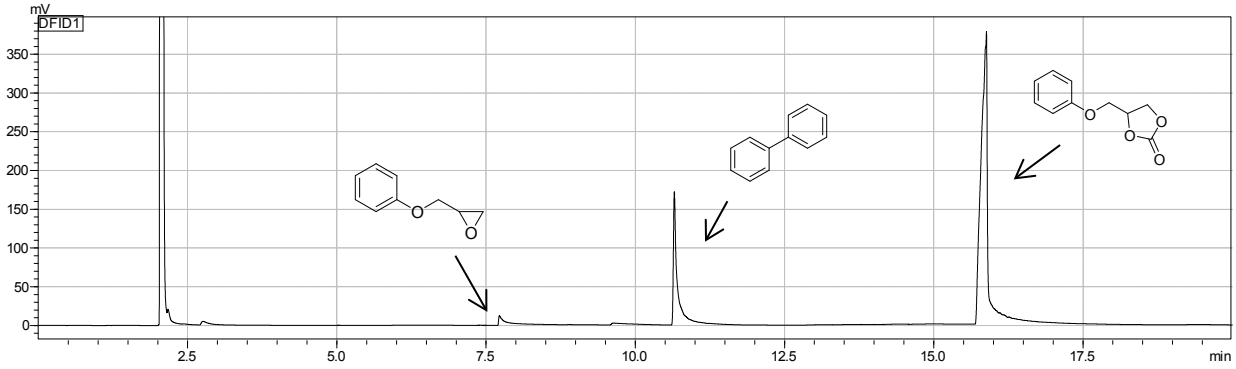


Figure S12 GC spectrum of cycloaddition product **5b**.