Electronic Supplementary Information (ESI) for

Integration of Rigid and Flexible Organic Parts for the Construction of Homochiral Metal-Organic Framework with High Porosity

Zhong-Xuan Xu[1, 2], Yan-Xi Tan[1], Hong-Ru Fu[1], Yao Kang[1], Jian Zhang[1,*]

[1]*State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, the Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China.*

[2]*Department of Chemistry, Zunyi Normal College, Zunyi, Guizhou 563002, P. R. China*

E-mail: zhj@fjirsm.ac.cn .

General information: All of the reagents and solvents used in reactions were purchased commercially and used without purification, unless otherwise indicated. The enantiopure linkers (S)-H_3PIA and (R)-H_3PIA were synthesized from L-proline, D-proline and benzene-1,3,5-tricarboxylic acid by our group.[1] Elemental analyses was performed by the analysis center of our institute. FT-IR spectra were measured as KBr pellets on a Nicolet Magna 750 FT-IR spectrometer in the range of 400~4000cm^{-1}. All Powder X-ray diffraction (PXRD) analyses were recorded on a Rigaku Dmax2500 diffractometer with Cu Kα radiation (λ = 1.54056 Å). Thermal stability studies were carried out on a NETSCHZ STA-449C thermoanalyzer with a heating rate of 10°C/min under an N_2 atmosphere. Gas adsorption measurement was performed in the ASAP (Accelerated Surface Area and Porosimetry) 2020 System. SQUEEZE subroutine of the PLATON software suit was applied to remove the scattering from some highly disordered solvent molecules.

Measurements of solid CD spectra: The mixture of sample and 200 mg dry KCl powder was well grounded and then pressed into a disk for the CD measurement with a MOS-450 spectropolarimeter.

Enantioselective sorption experiments of 1-L and 1-D towards racemic alcohols: To exchange the guest molecules, 500 mg of 1-D (1-L) was soaked in dry methanol for two days at room temperature. After the methanol-exchanged and activated 1-D (1-L) was degassed at room temperature until no weight change prior to the measurements, about 100 mg of evacuated material 1-D (1-L) was soaked in the corresponding racemic alcohol three days at 0^oC and collected by filtration and flushed with CH_2Cl_2 for several times. Then the above sample was re-soaked in methanol (0.5 mL) for 48 hours to extract alcohol, and enantiomeric excess was measured by chiral GC.

Chiral GC analysis: The GC measurements were performed with FULI GC9790-2 gas chromatograph. The conditions were listed as follows. Column: Supelco Beta DEX 120 capillary column. Injection port temperature: 200 ^oC; column temperature: 100 ^oC (methyl lactate) or 140 ^oC (1-phenethylalcohol); flame ionization detector: 210 ^oC. Carrier gas: N_2: 0.1Mpa, H_2: 0.15Mpa. Injection volume: 0.2μL. [2]

Reference:

[1] Z. X. Xu, Y. X. Tan, H. R. Fu, J. Liu and J. Zhang, *Inorg. Chem.*, 2014, 53, 12199-12204.

[2] L. Lin, R. M. Yu, X. Y. Wu, W. B. Yang, J. Zhang, X. G. Guo, Z. J. Lin and C. Z. Lu., *Inorg.*

Chem., 2014, 53, 4794−4796.

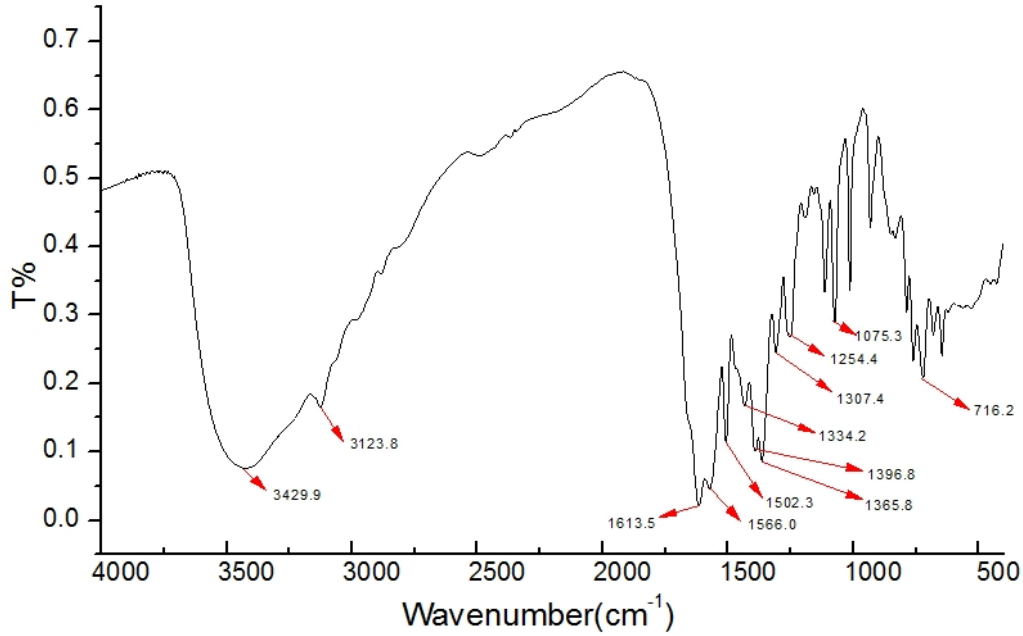

Figure S1. The IR spectra of **1-D**.

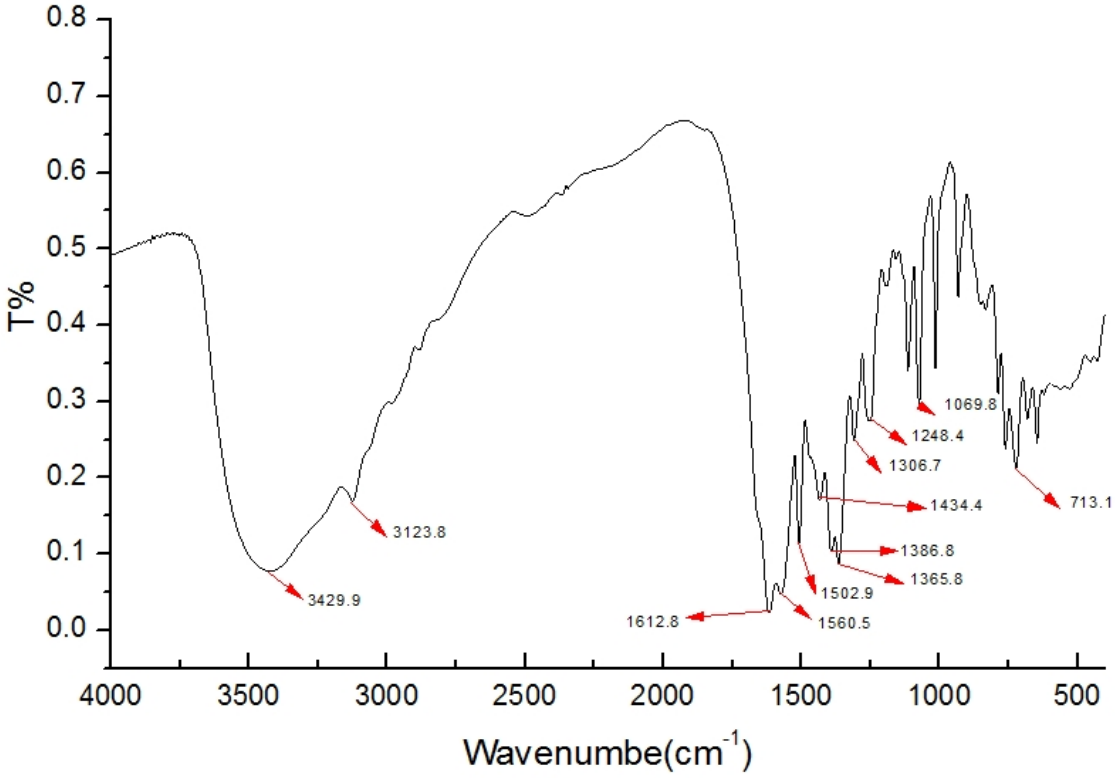

Figure S2. The IR spectra of **1-L**.

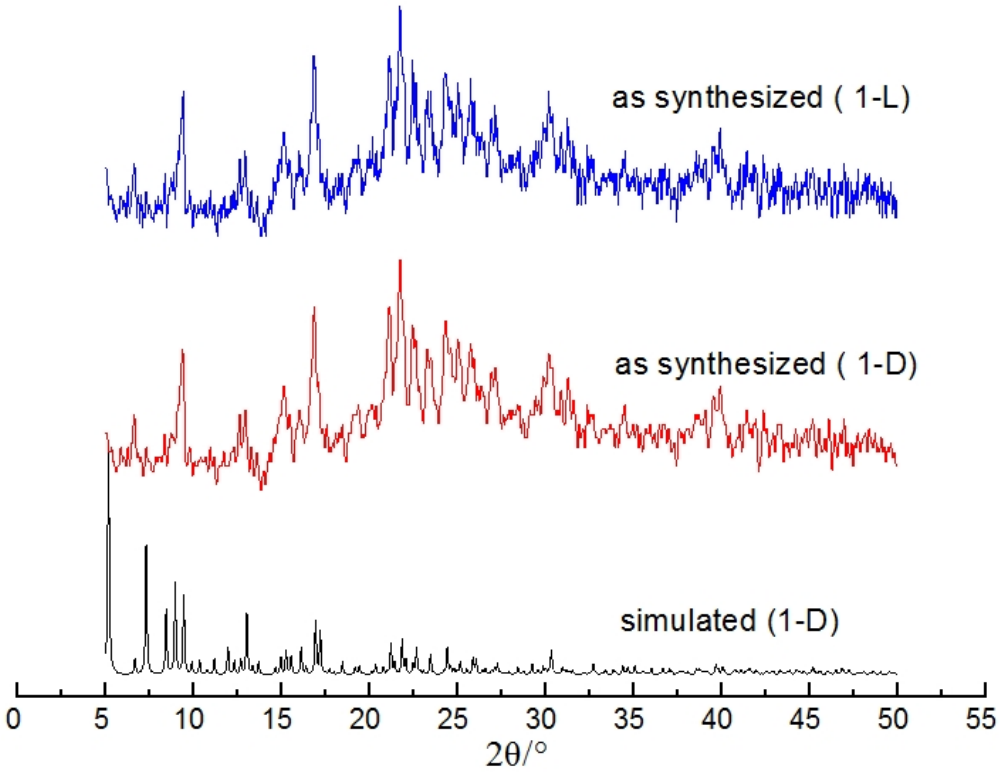

Figure S3. XRPD patterns of **1-D** and **1-L**.

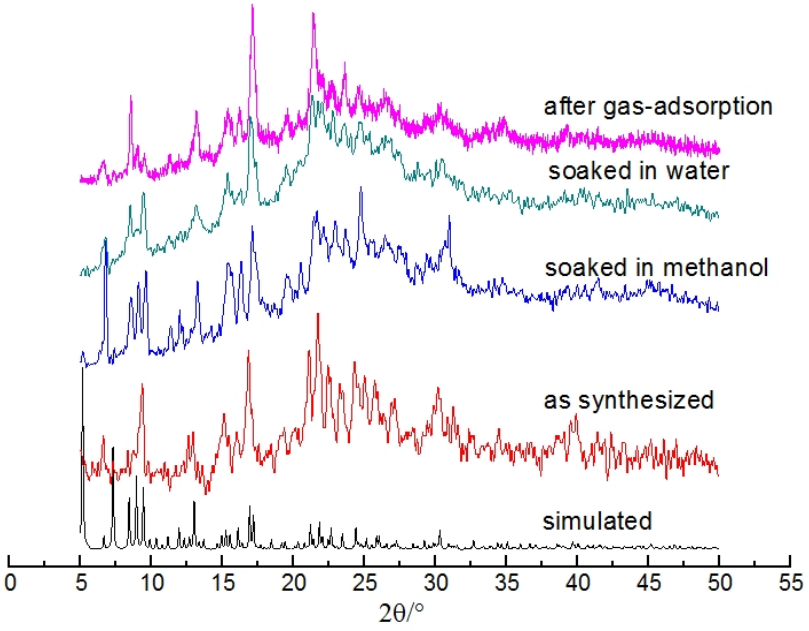

Figure S4. XRPD patterns of **1-D**.

To test the stabilities of **1-D** in different solvent systems, the crystal of **1-D** was respectively soaked in methanol and water for 5h. It is insoluble and stable in methanol, but some sensitive to water under room temperature.

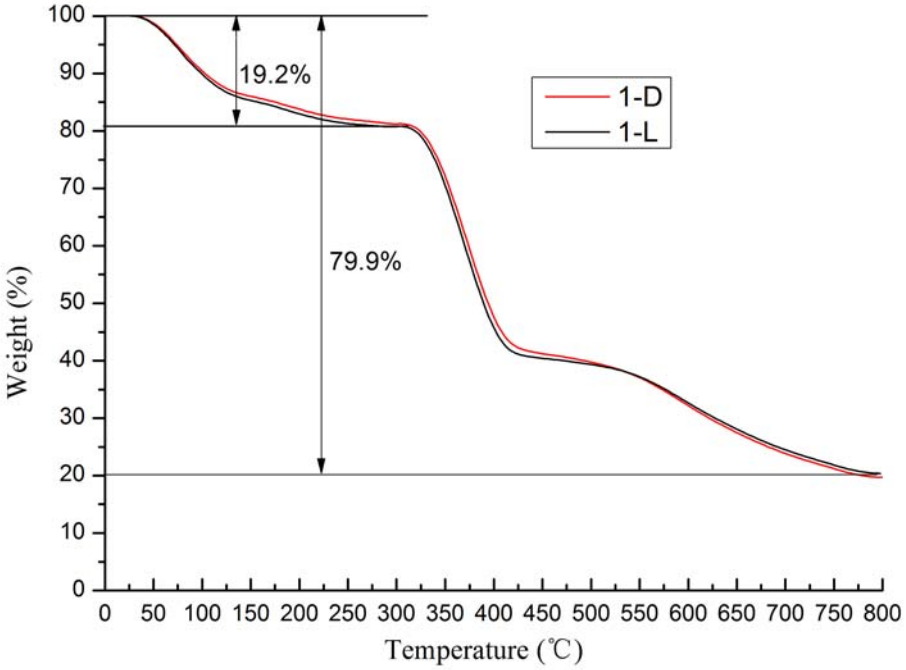

Figure S5. Thermogravimetric analyses of **1-D** and **1-L**.

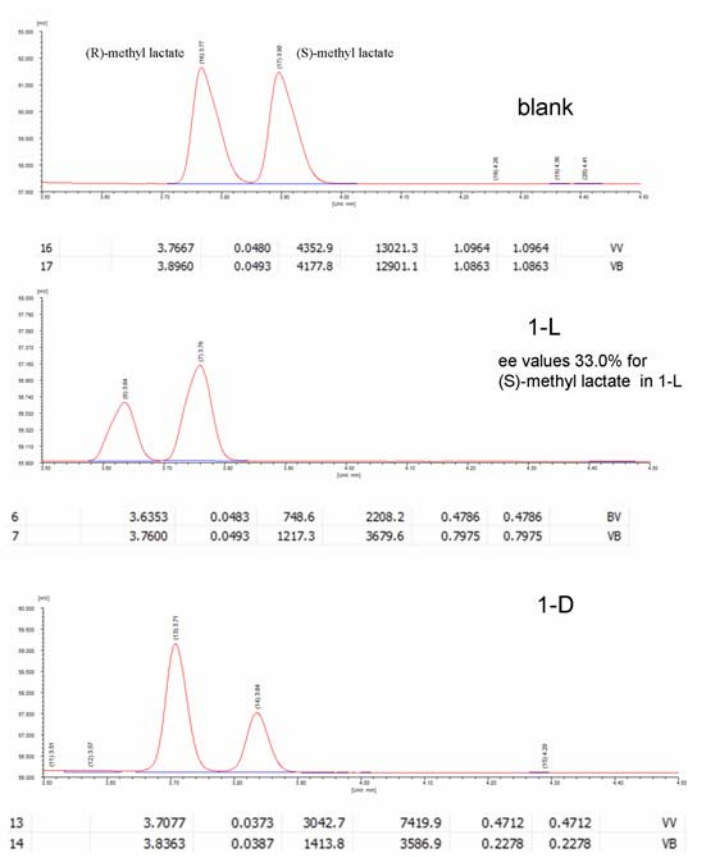

Figure S6. GC graphs for methyl lactate desorbed from **1-L** and **1-D**.

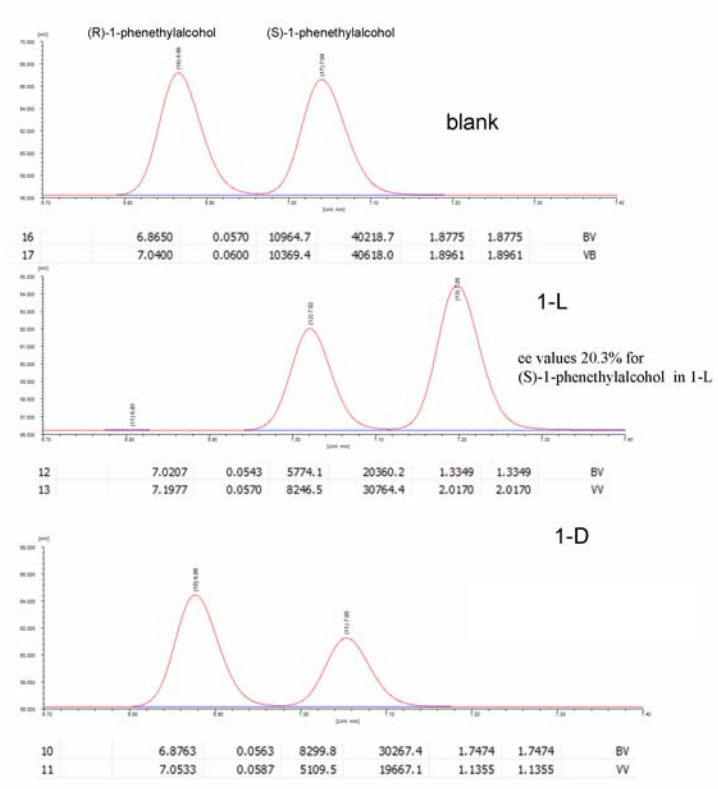

Figure S7. GC graphs for 1-phenethylalcohol desorbed from **1-L** and **1-D**.