Electronic Supplementary Information (ESI) for

A pair of homochiral porous metal−organic frameworks with helical metal-carboxylate layer

Zhong-Xuan Xu[1, 2], Liyang Liu[1] and 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 .

Experimental Section

General information: All reagents and solvents employed in reactions were purchased from Energy-Chemical and directly used without further purification. The corresponding chiral ligands, (*S*)-H_3PIA and (*R*)-H_3PIA, were prepared from L-proline, D-proline and benzene-1,3,5-tricarboxylic acid. Elemental analyses were performed by the analysis center of our institute. To verify the phase purity of **1-D** and **1-L**, the powder X-ray diffraction (XRD) data were collected using a Miniflex(Ⅱ) diffractometer with Cu-Kα radiation (λ = 1.54056 Å) in a range of 5.00−50.00°. Thermal stability studies of **1-D** and **1-L** were performed on a NETSCHZ STA-449C thermoanalyzer with a heating rate of 10°C/min under an N_2 atmosphere from 30 to 800°C. Luminescence spectra were recorded on a Shimadzu RF-5301 spectrophotometer.

X-ray single-crystal measurement: Intensity data collections of complexes **1-D** and **1-L** were performed on a SuperNova Oxford diffractometer with graphite-monochromated Cu Kα radiation (λ = 1.54184 Å) and graphite-monochromated Mo Kα radiation (λ = 0.71073 Å) at room temperature, respectively.

Measurements of solid CD spectra: The solid circular dichroism (CD) spectra were measured on a MOS-450 spectropolarimeter using KCl pellets at room temperature.

Gas adsorption measurement: A freshly prepared sample of **1-D** was soaked in methanol at 5-10℃ for a week to exchange guest molecules. Subsequently, the sample was degassed under dynamic vacuum at 40℃ for 10 h to activate the sample. Finally, gas adsorption measurements was carried out on the ASAP (Accelerated Surface Area and Porosimetry) 2020 System.

Table S1. Summary of Crystal Data and Refinement Results

Compound reference	**1-D**	**1-L**
Chemical formula	$C_{29}H_{22}Cd_{1.5}N_4O_7$	$C_{29}H_{22}Cd_{1.5}N_4O_7$
Formula Mass	707.10	707.10
Crystal system	Orthorhombic	Orthorhombic
a/Å	15.7377(5)	15.6969(6)
b/Å	21.1254(8)	20.9233(7)
c/Å	11.7487(3)	11.7168(4)
α/°	90	90
β/°	90	90
γ/°	90	90
Unit cell volume/Å^3	3906.0(2)	3848.2(2)
Temperature/K	293(2)	293(2)
Space group	*P*21212	*P*21212
No. of formula units per unit cell, *Z*	4	4
Radiation type	CuKα	MoKα
Absorption coefficient, μ/mm^{-1}	6.932	0.876
No. of reflections measured	10122	18514
No. of independent reflections	6524	6750
R_{int}	0.0358	0.0426
Final R_1 values ($I > 2\sigma(I)$)	0.0413	0.0387
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.1113	0.0993
Final R_1 values (all data)	0.0456	0.0427
Final $wR(F^2)$ values (all data)	0.1143	0.1018
Goodness of fit on F^2	1.043	1.090
Flack parameter	-0.003(8)	-0.022(18)
CCDC number	1420035	1420036

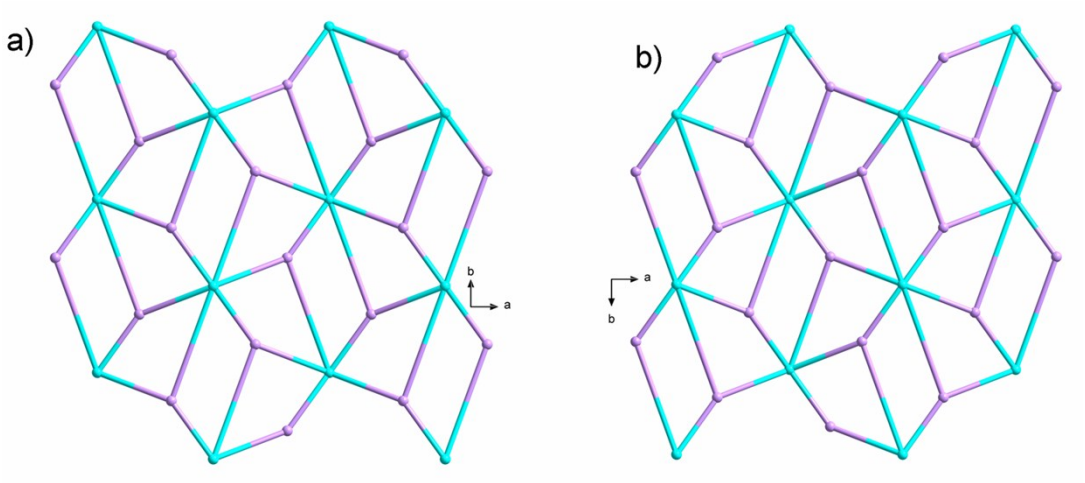

Figure S1. The ***kgd*** net in **1-D** (a) and **1-L** (b).

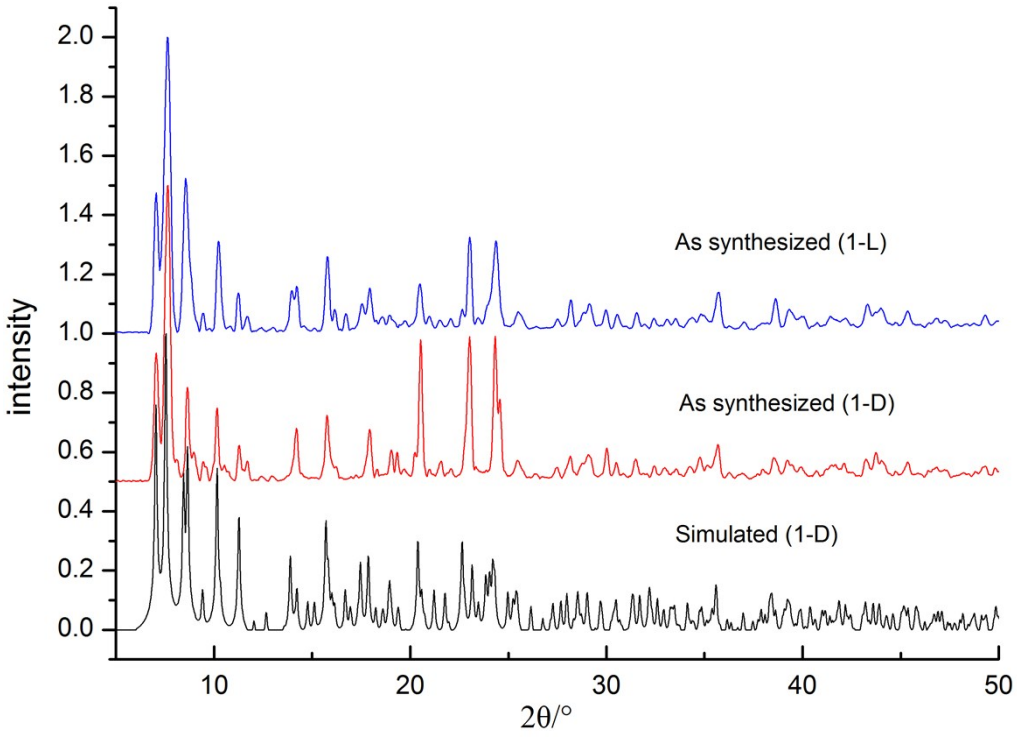

Figure S2. PXRD patterns of **1-D** and **1-L**.

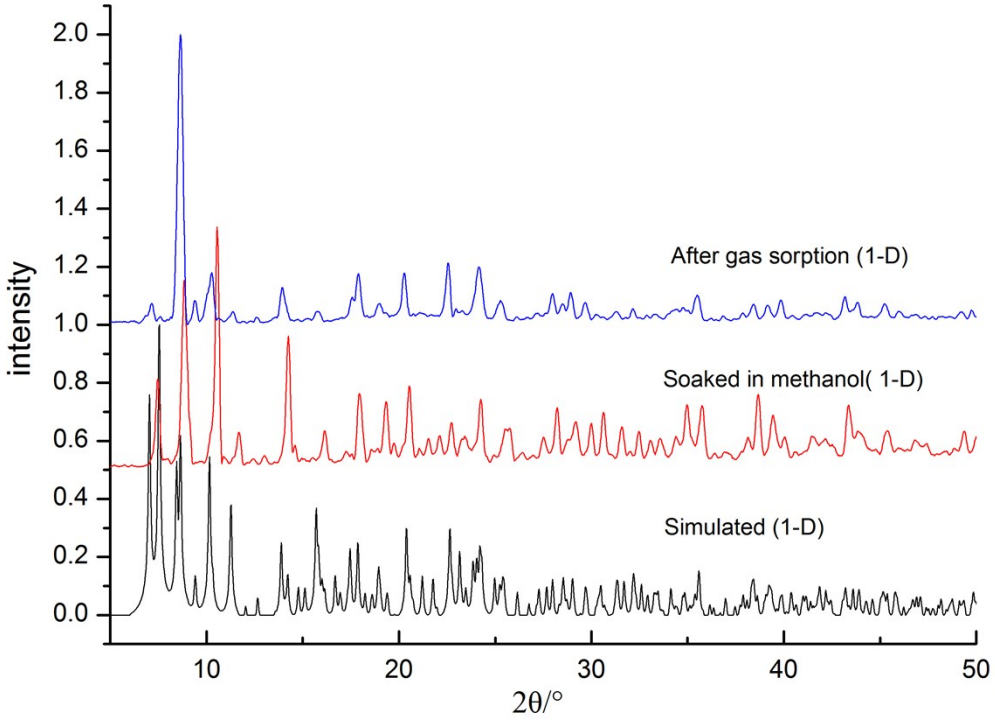

Figure S3. PXRD patterns of **1-D**.

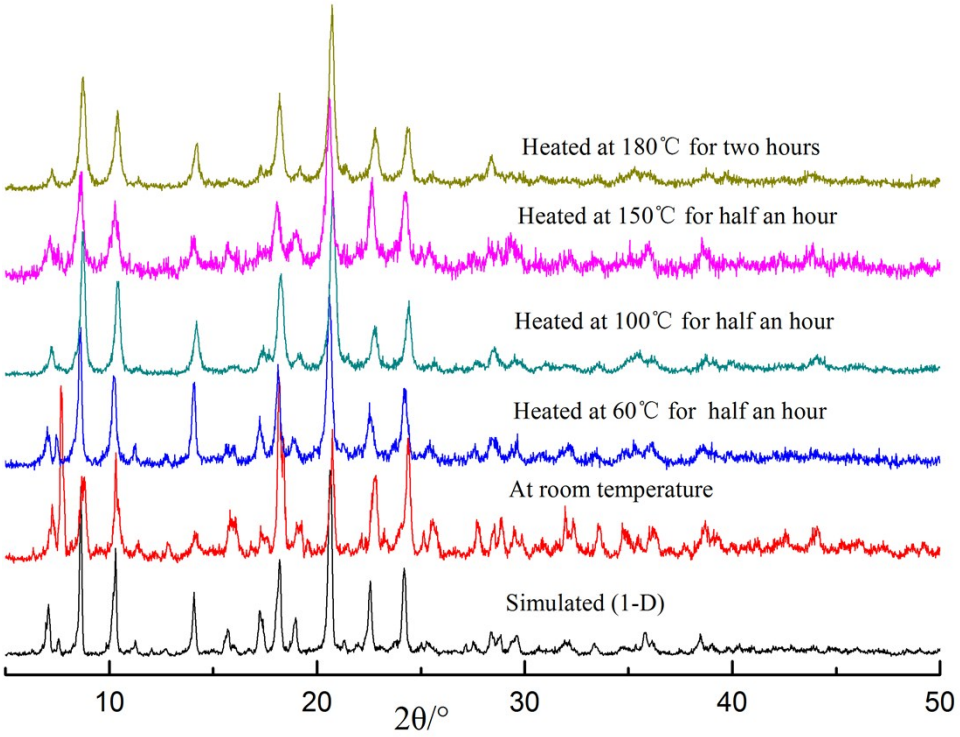

Figure S4. The PXRD patterns of **1-D** at different temperature. The figure shows that the framework of **1-D** is very stable at different temperature.

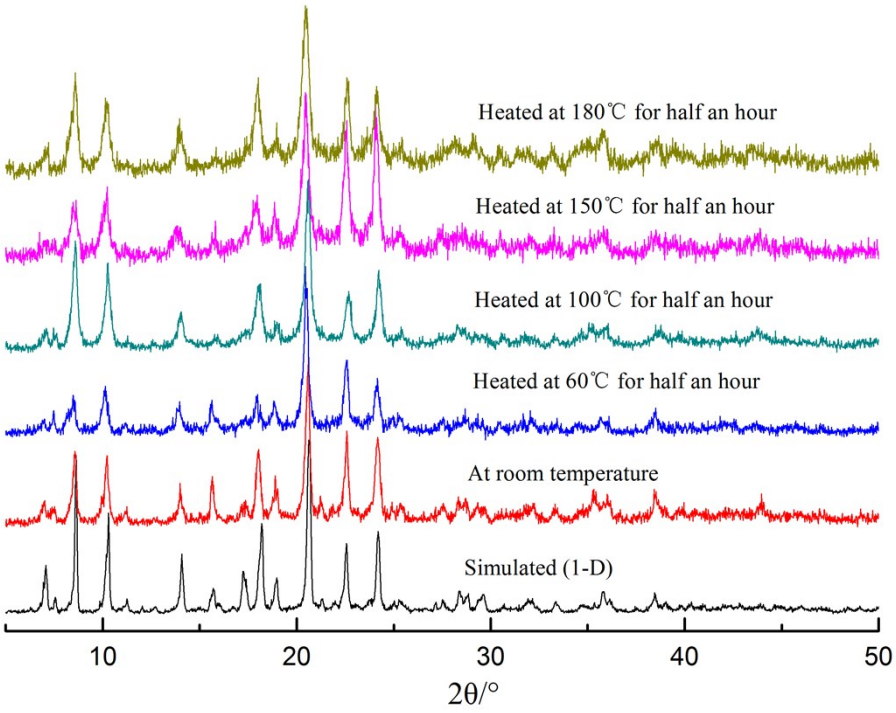

Figure S5. The PXRD patterns of **1-D** at different temperature after soaking in methanol for a week. It shows that the framework of **1-D** is still very stable at different temperature even if some guest molecules have been exchanged by soaking in methanol.

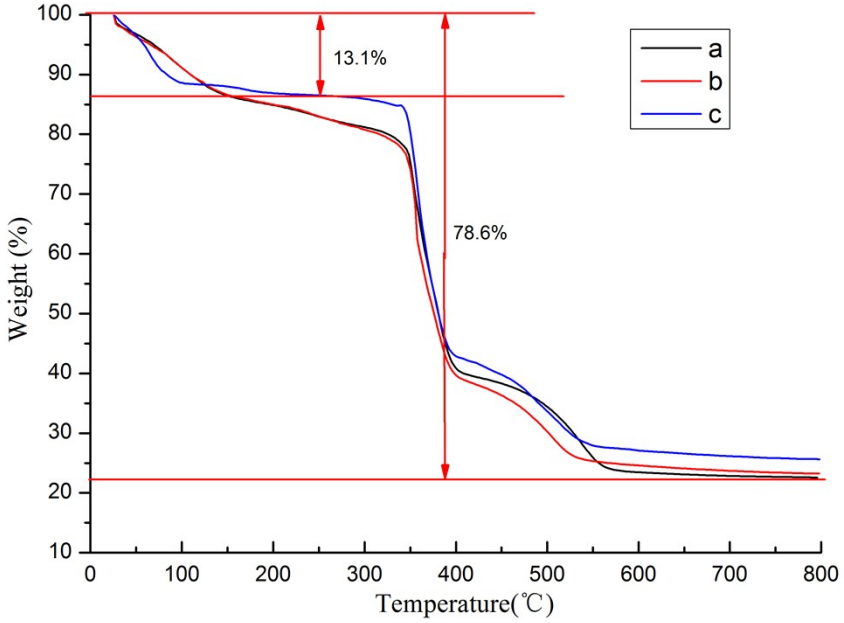

Figure S6. The TGA diagrams of **1-D** (a), the TGA diagrams of **1-L** (b) and the TGA diagrams of **1-D** soaked in methanol (c). The TG curves of **1-D** and **1-L** indicate that the frameworks of these two complexes are stable up to 250 °C. According to the gradual weight losses between 30 and 150 °C, a DMF molecule, a methanol molecule and a water molecule may be released from the frameworks as guest molecules(observed, 13.1%; calculated, 14.8%).

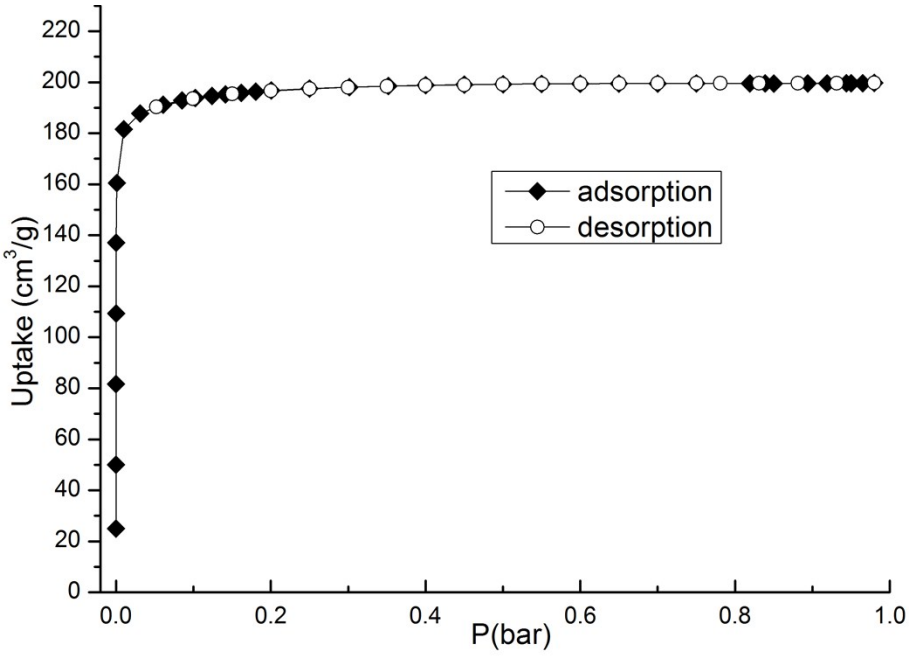

Figure S7. The N_2 sorption isothems of **1-D** at 77k.

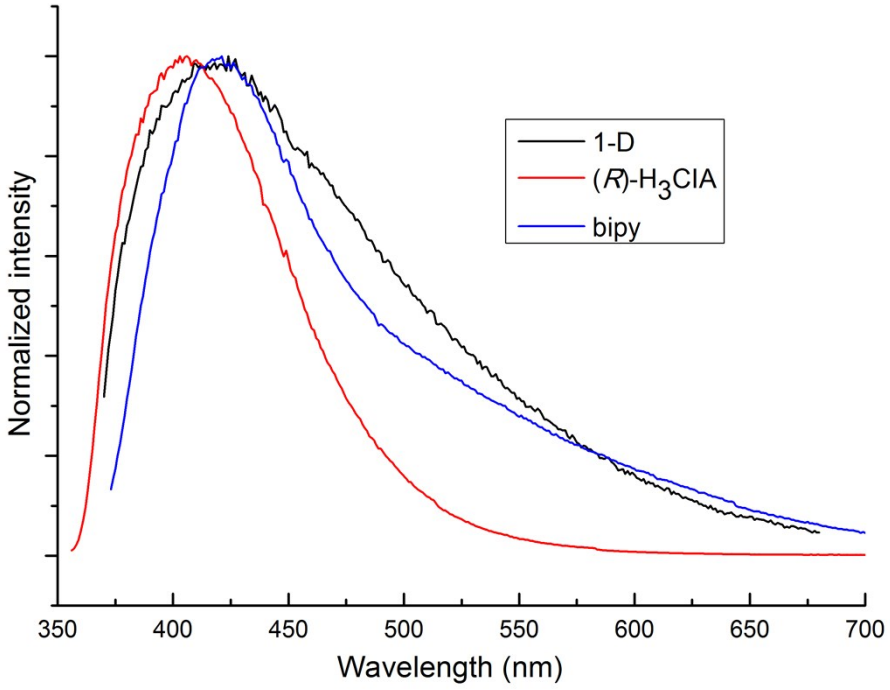

Figure S8. Fluorescent emission spectra of **1-D**, (*R*)-H_3CIA and bipy.