Electronic Supplementary Information (ESI) for

Enantiopure anion templated synthesis of zeolitic metal−organic framework

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Experimental Section

General information: In this paper, all the chemical reagents were purchased from Energy-Chemical and used without further purification. The chiral compound (*R*)-H_3CIA ((*S*)-H_3CIA) was synthesized from L-(–)-lactic acid methyl ester (D-(–)-lactic acid methyl ester) and dimethyl 5-hydroxyisophthalate by our group. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra were recorded in deuterated trifluoroacetic acid (TFA-D, δ 11.50) solutions using a Burker AVANCE 400 spectrometer. Chemical shifts are reported as δ values in parts per million (ppm) relative to tetramethylsilane (TMS) for all recorded NMR spectra. Elemental analysis was carried out by the analysis center of our institute. FT-IR spectrum was measured as KBr pellets on a Nicolet Magna 750 FT-IR spectrometer in the range of 400~ 4000cm^{-1}. The powder X-ray diffraction (PXRD) analysis was recorded on a Rigaku Dmax2500 diffractometer with Cu Kα radiation (λ =1.54056Å) from 5.00−50.00°. Thermal stability study was performed on a NETSCHZ STA-449C thermoanalyzer with a heating rate of 10°C/min in a range of 30−800℃ under nitrogen and atmosphere. Luminescence spectra were recorded on a Shimadzu RF-5301 spectrophotometer.

Measurements of solid CD spectra: The mixture of sample and 100 mg dry KCl powder was well grounded and then pressed into a disk for the CD measurement with a MOS-450 spectropolarimeter.

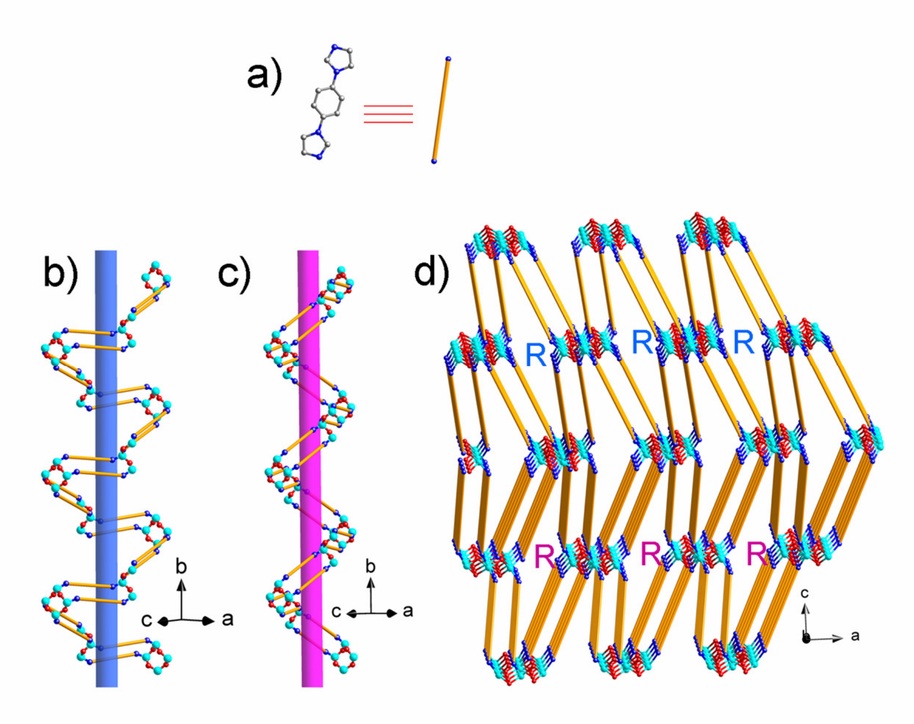

Figure S1. Schematic illustrations of complex **1-D**: a) the 1.4-DIB linand is simplified as a line; b) the right-handed helical A-chain in complex **1-D;** c) the right-handed helical B-chain in complex **1-D;** d) the 3D framework of **1-D** consisting of two types of right-handed helical chains along b-axe.

Absolute helicity often goes with chirality in some compounds, such as proteins, nucleic acids, carbohelicenes and so on, which is a special form of one-dimensional chirality. Such a phenomenon also exists in complex **1-D** and one of prominent structural features is the presence of two types of helical chains: right-handed helical A-chain and right-handed helical B-chain (Figure S1), dictated by the chirality of induction agent. As depicted in Figure 2b-c, two types of helical chains were all built from $Zn_4(\mu_2\text{-}OH)_4$ units and parallel 1.4-DIB ligands running along the b-axis. These helixes are generated around the crystallographic 4_3 screw axis and contain four $Zn_4(\mu_2\text{-}OH)_4$ units and four pairs of 1.4-DIB ligands per turn, respectively. As a result, these helical chains formed a 3D cationic homochiral framwork at a ratio of 1:1.

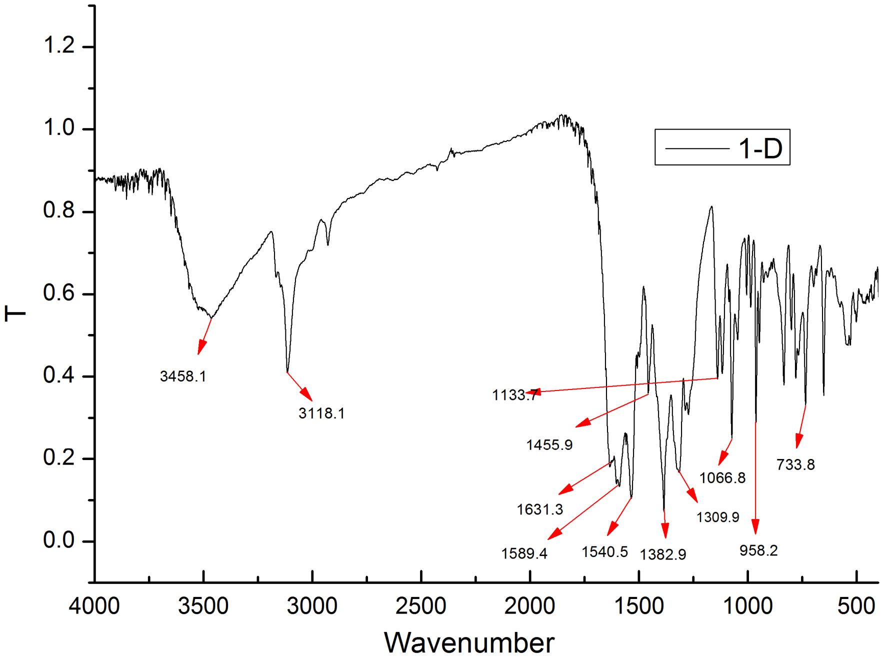

Figure S2. The IR spectra of **1-D**

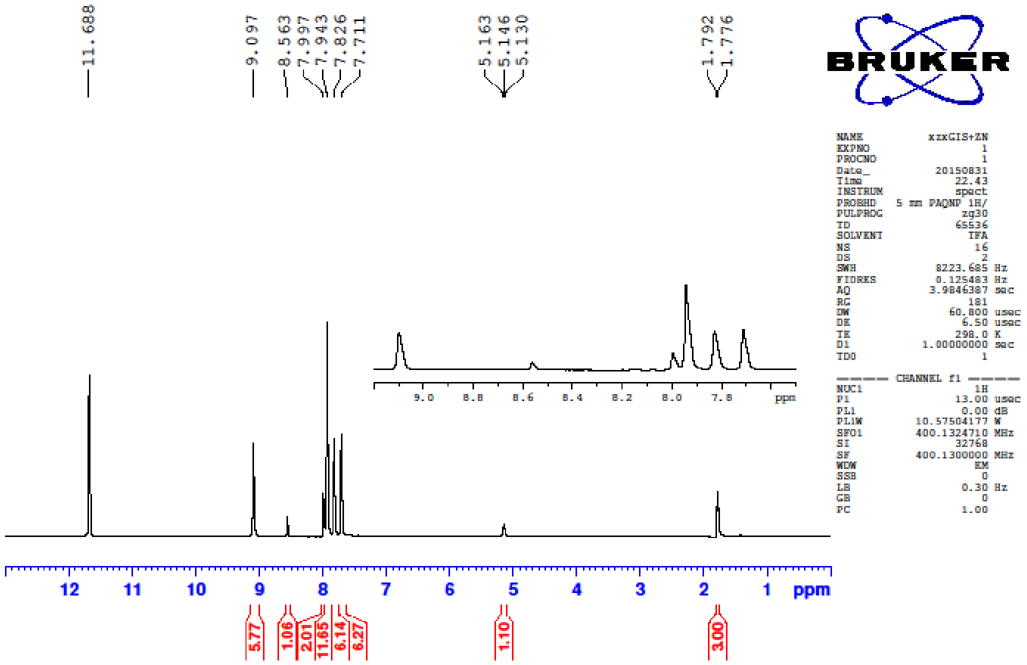

Figure S3. ^{1}H NMR spectra of **1-D** in TFA-D

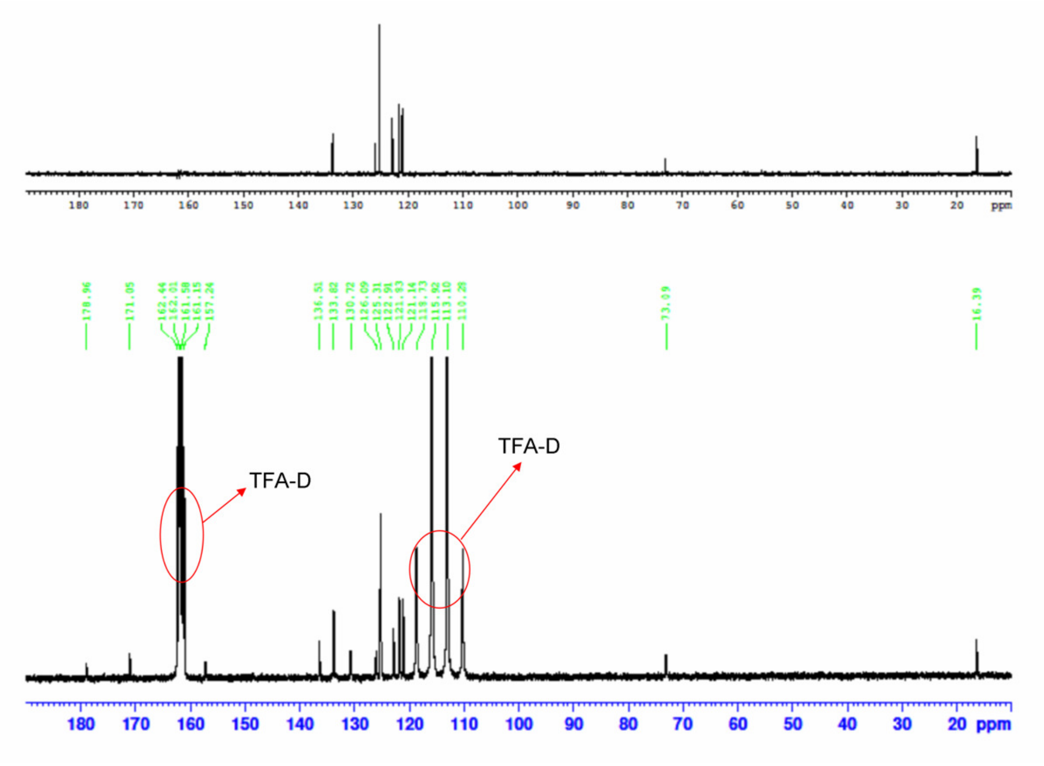

Figure. S4 ^{13}C NMR spectra of **1-D** in TFA-D

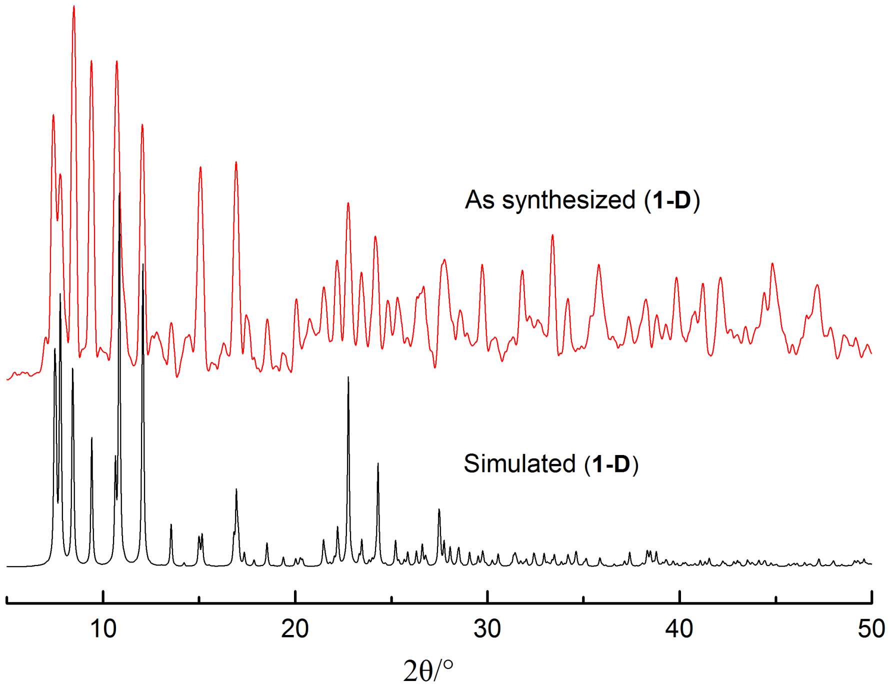

Figure S5. PXRD patterns of **1-D**

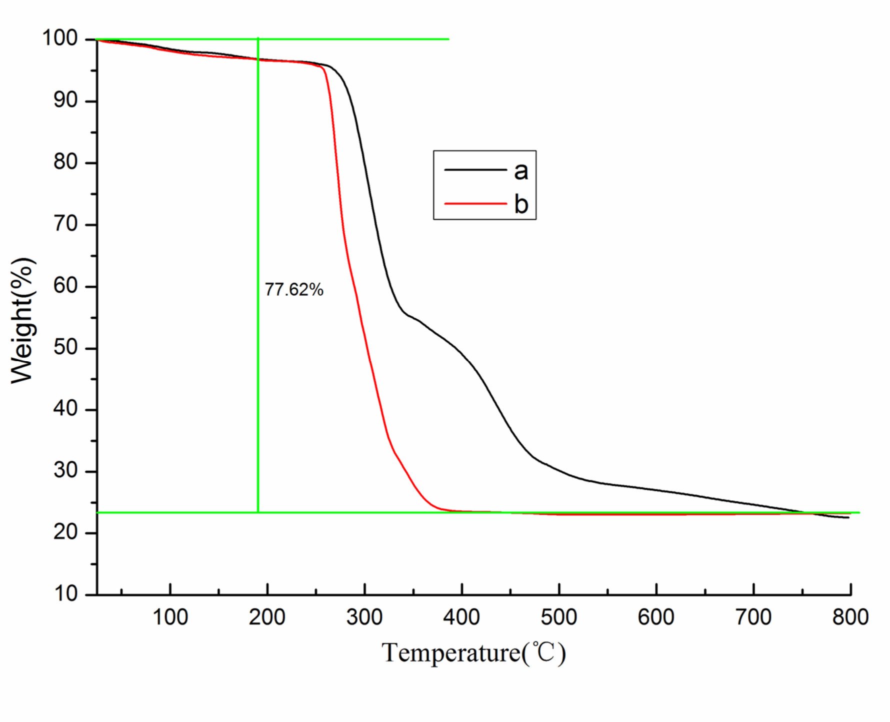

Figure S6. Thermogravimetric diagram of **1-D** under nitrogen (a) and atmosphere (b)

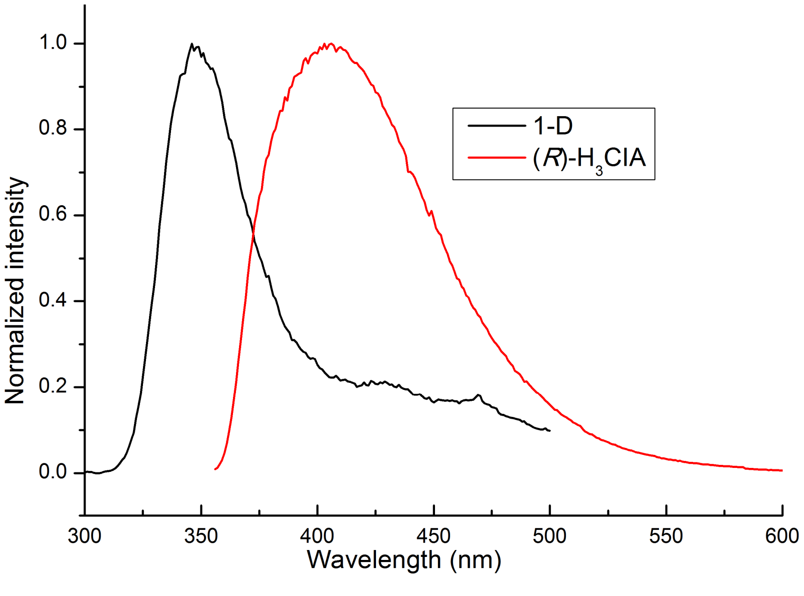

Figure S7. The fluorescent emission spectra of **1-D** and (*R*)-H_3CIA

At room temperature the photoluminescence properties of 1-D were studied in the solid state. Excitation of the microcrystalline sample of **1-D** at 270 nm produces the intense luminescence with the peak maxima at 349 nm. In order to understand the nature of above emission band better, the photoluminescent property of guest molecule (*S*)-H_3CIA is also tested. As shown in Figure S6, upon excitation at 336 nm, (*S*)-H_3CIA has similar emissions at 404 nm. In comparison to (*R*)-H_3CIA ligand, the emission maxima in **1-D** has changed and indicates blue shift, which may be attributed to a charge transfer transition between cationic frameworks and anionic guest molecules.[1]

References:

1. (a) Z. C. Hu, B. J. Deibert, J. Li, *Chem. Soc. Rev.*, 2014, **43**, 5815; (b) Y. J. Cui, Y. F. Yue, G. D. Qian, B. L. Cheng, *Chem. Rev.*, 2012, **112**, 1126.