Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

A new strategy for constructing disulfide-functionalized ZIF-8 analogue using ligand-ligand covalent interaction as structure directing role

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Contents

Synthesis of CPM-8S

20 mg 1, 2, 4-triazole-3-thiol, 30 mg zinc chloride were added to a 23 mL glass vial and dissolved in 4 mL DMF. The vial was capped and placed in 120 °C oven. Pure colorless crystals were obtained after heating for 48 hours. The yiled was calculated to be ~ 60% based on ligand.

Single X-ray diffraction and structure determination

Data collection for CPM-8S was performed on Bruker APEXII diffractometer equipped with graphite monochromated Mo-*K*α radiation (λ = 0.71073 Å) by using the ω-scan and φ-scan mode at 298 K. The structure was solved by direct methods followed by successive difference Fourier methods. The structure was refined on F^2 by full-matrix least-squares using SHELXTL-2014 program package. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms of the organic ligands were generated theoretically. The sulfur atoms and their adjacent carbon and nitrogen atoms display disorder over two positions with equal occupancy. Disorder has been modeled as C1A-S1A-S2A-C3A and C1B-S2B-S3B-C3B. CCDC-1836214 contains the supplementary crystallographic data. Data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/-data_request/cif.

Powder X-ray diffraction

Powder X-ray diffraction (PXRD) data were collected on a Bruker D8 Advance powder diffractionmeter with Cu *K*α radiation (λ = 1.5418 Å) operating at 40 kV and 40 mA. The simulated powder pattern was calculated using single-crystal X-ray diffraction data and processed by the Mercury 2.3 program provided by the Cambridge Crystallographic Data Centre. The 2-theta angular collected ranges from 5 to 40°.

Thermal gravimetric measurement

The thermal gravimetric analysis (TGA) was carried out on TGA Q500 under nitrogen atmosphere. The samples were heated from 30 °C to 800 °C at a rate of 10 °C·min^{-1} with nitrogen flow rate being 60 milliliter per minute.

Sample activation

The as-synthesized crystalline samples were immersed in CH_2Cl_2 for 5 days, during which CH_2Cl_2 was refreshed every 24 h. The resulting CH_2Cl_2-exchanged samples were filtrated and then evacuated (10^{-3} torr) at 80 °C for 12 h to remove the remaining guests.

Gas sorption measurements

Gas sorption isotherms were measured on a Micromeritics ASAP 2020 Surface area and Porosity analyzer. The N_2 sorption measurement was performed at 77 K. The carbon dioxide, ethane, ethylene, acetylene and methane adsorption and desorption measurements were carried out at 273 and 298 K.

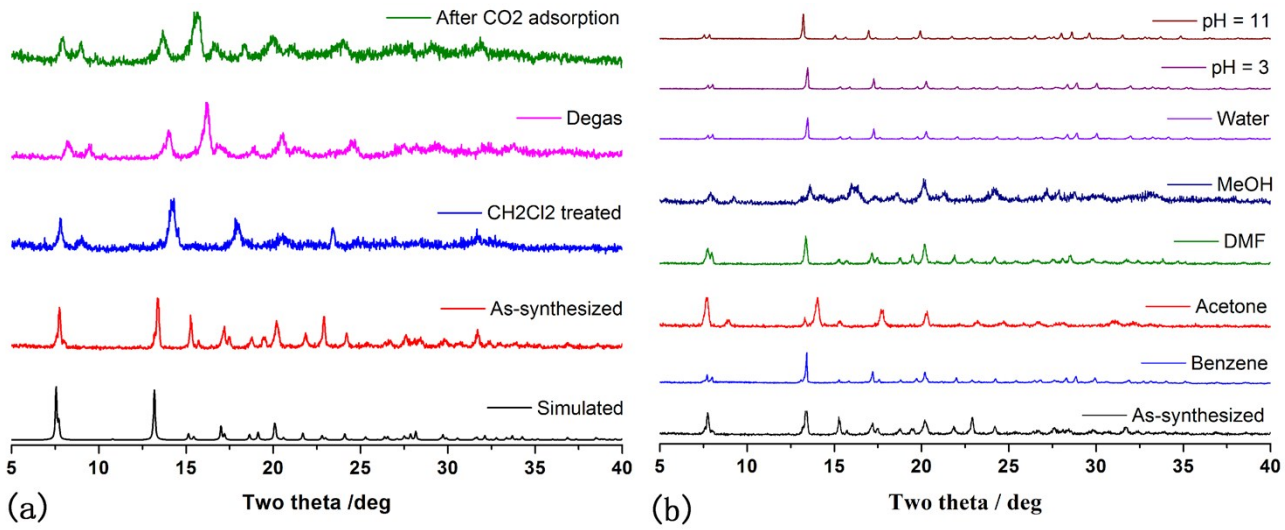

Fig. S1 (a) PXRD of the as-synthesized CPM-8S, as well as those after solvent exchange and degas; (b) PXRD patterns of CPM-8S after immersing in different solvent for one week at room temperature (the acid or base aqueous solution was prepared by adding HCl or NaOH to the deionized water).

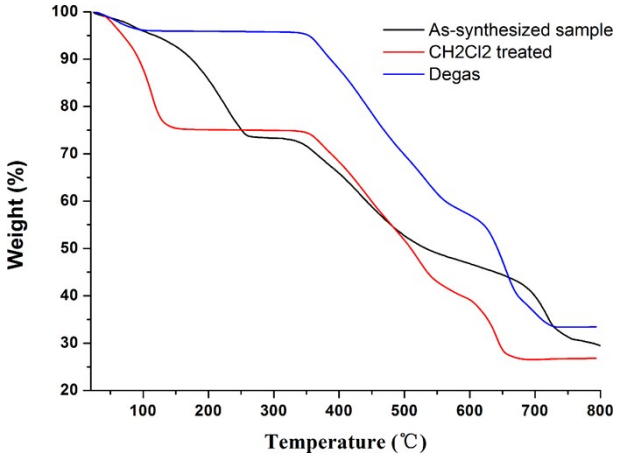

Fig. S2 TGA diagrams of as-synthesized CPM-8S, CH_2Cl_2 treated CPM-8S, and degas CPM-8S.

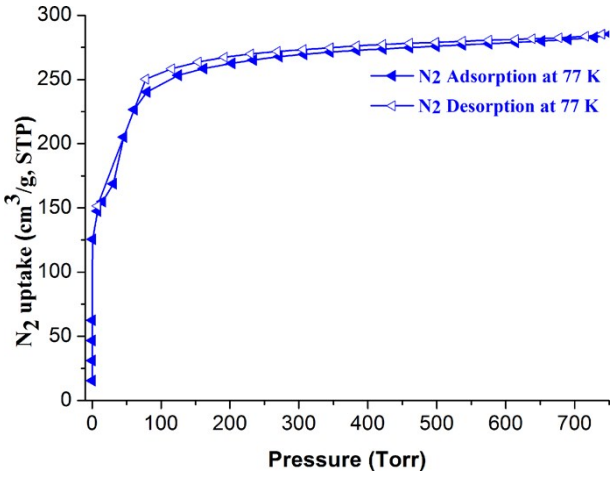

Fig. S3. The N_2 adsorption and desorption isotherms of CPM-8S at 77 K.