Supporting Information

A Microporous Indium-Organic Framework with High Capacity and Selectivity for CO₂ or Organosulfurs

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Powder X-ray Diffraction.

The synthesized products of **1** have been characterized by powder X-ray diffraction (PXRD) (Figure S2). The experimental PXRD patterns correspond well with the results simulated from the single crystal data, indicating the high purity of the synthesized samples. The difference in reflection intensities between the simulated and experimental patterns was due to the variation in preferred orientation of the powder samples during the collection of the experimental PXRD data.

Thermal Stability Analysis.

To study the thermal stabilities of **1**, thermogravimetric analyses (TGA) in N_2 atmosphere with a heating rate of 10 °C/min were performed on polycrystalline samples to determine their thermal stabilities from 30 to 600 °C (Figure S3).



Figure S1. (a) ACS-type 6 -connected topology in **1**. (b) Two acs-type frameworks are mutually interpenetrated in **1**;



Figure S2. The Powder XRD pattern of **1** (a, red); The Powder XRD pattern of **1** soaked in MeCN (b, blue); The Powder XRD pattern of **1** after adsorption (c, dark cyan); The Powder XRD pattern of **1** after desulphurize experiments (d, magenta).



Figure S3. The TGA diagrams of 1 (a, black); The TGA diagrams of 1 soaked in MeCN (b, red).



Figure S4. Pore size distribution based on Horvath–Kawazoe (H–K) model.



Figure S5. H₂ adsorption isotherms for 1 fitting by virial method.



Figure S6. The isosteric heat of H₂ adsorption for 1 estimated by the virial equation.



Figure S7. The concentrations of BT dissolved in n-hexane with 110mg 1 during repeated desulphurize experiments.



Figure S8. The concentrations of DBT dissolved in n-hexane with 110mg 1 during repeated desulphurize experiments.



Figure S9. The IR spectra of **1** (a, black); The IR spectra of **1** soaked in MeCN (b, red); The IR spectra of **1** after desulphurize experiments (c, blue).