

## Supporting Information

# A Two-Dimensional Metal-Organic Framework Assembled from Scandium-based Cages for the Selective Capture of Sulfur Hexafluoride

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# 1. Materials and general procedures

## Materials

1,10-phenanthroline monohydrate, 1,3-dibromopropane, chlorobenzene, *tert*-butanol, potassium *tert*-butoxide, sodium hydroxide, potassium phosphate tribasic (K<sub>3</sub>PO<sub>4</sub>), ScCl<sub>3</sub>·6H<sub>2</sub>O, *N,N*-dimethylformamide (DMF) were purchased from *Bidepharm*. Phosphoryl chloride, phosphorus pentachloride, Pd SPhos Gen III catalyst and chlorobenzene (MCB) were purchased from *Energy chemical*. 1,4-dioxane, ethyl alcohol, ether, dichloromethane (DCM), trichloromethane (CHCl<sub>3</sub>), and sodium sulfate were purchased from *Sinopharm*. Unless otherwise noted, all commercial chemicals were used without further purification.

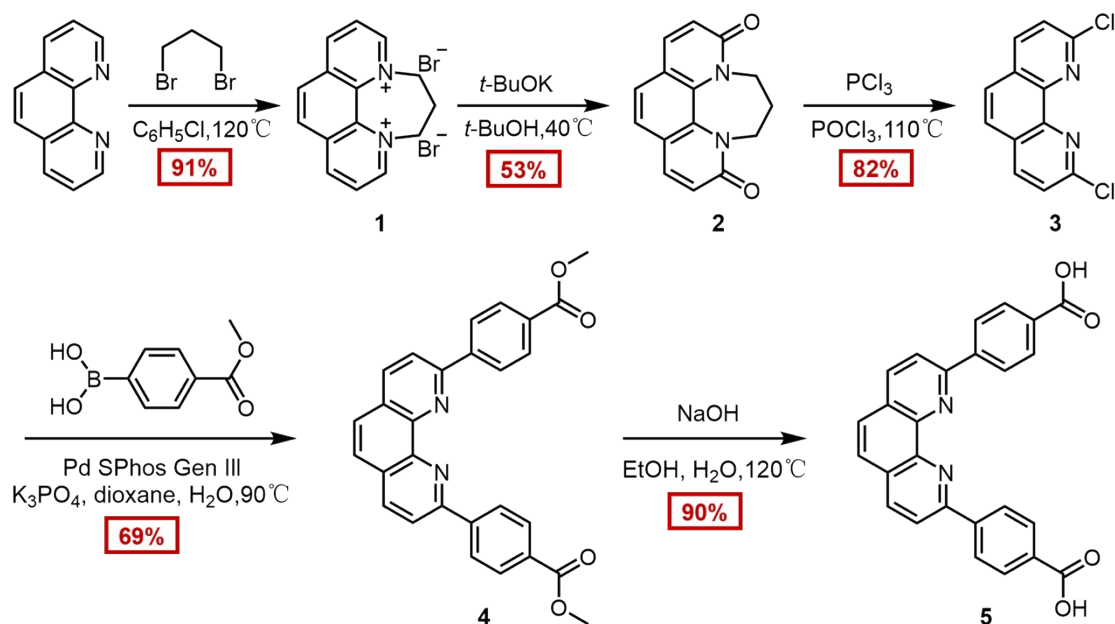
## Characterization

Fourier transform infrared (FT-IR) spectra were collected using a ThermoFisher iS50 FT-IR spectrometer. Nitrogen sorption isotherms at 77 K were measured using a Micromeritics 3Flex volumetric gas sorption instrument equipped with liquid nitrogen containers. <sup>1</sup>H NMR spectra were recorded on a Bruker Avance DMX-500 (500 MHz for <sup>1</sup>H NMR). The deuterated solvents used are indicated in the experimental part, chemical shifts are given in ppm from TMS with residual solvent resonances as internal standards. Powder X-ray diffraction (PXRD) of MOFs were measured on a Rigaku smartlab X-ray diffractometer operating at 40 kV/30 mA using the Cu K $\alpha$  line ( $\lambda = 1.5418\text{\AA}$ ). Data were measured over the range of 3-30° in 13°/min steps over two minutes.

**Crystal Structure Determination.** Single crystal data of Sc-cage-MOF was collected using a Bruker D8 Venture diffractometer equipped with a curved TRIUMPH focusing monochromator of Ga K $\alpha$  ( $\lambda = 1.34139\text{\AA}$ ) radiation, and a highly sensitive CPAD Photon II detector, coupled with a CryoStream 800 Plus (Oxford Cryosystems) temperature controller. Data reduction and cell parameter refinement were performed using Apex software with included SAINT and SADABS programs. Intensities of reflections for the sample absorption were corrected using multi-scan method. Structures were solved by intrinsic phasing method and refined anisotropically with weighted full-matrix least squares on  $F^2$  using SHELXT 6 and SHELXL 7 programs with Olex 2 graphic interface. All non-hydrogen atoms were refined anisotropically with restraints (DFIX, ISOR, SIMU and DELU) on DMF molecules and partially phenyl groups. Hydrogen atoms within structures were placed in idealized positions and refined using riding coordinate model. A solvent mask procedure was further performed due to highly disordered interstitial solvent molecules. Crystal data and structure refinement parameters are summarized in **Table S1**. Crystal structures are deposited in CCDC data base. The deposition number is 2295390.

## 2. Synthesis of ligands

### Synthetic protocols for 4,4'-(1,10-phenanthroline-2,9-diyl) dibenzoic acid



**Scheme S1.** Synthesis route of 4,4'-(1,10-phenanthroline-2,9-diyl) dibenzoic acid.

#### 6,7-dihydro-5H-[1,4]diazepino[1,2,3,4-lmn][1,10]phenanthroline-4,8-diium dibromide (1):

The compound was synthesized according to the reported procedure with slight modifications<sup>1</sup>. In a 250 mL round-bottom flask, 1,10-phenanthroline (10.0 g, 55.5 mmol) was added into a mixture of 80 mL chlorobenzene and 1,3-dibromopropane (29 mL, 285.8 mmol) under constant stirring. The resulting mixture was heated to  $120\text{ }^\circ\text{C}$  for 20 h. The crude product was collected by filtration, washed with  $CH_2Cl_2$  and further dried in vacuum at  $50\text{ }^\circ\text{C}$  overnight to obtain yellow powder (19.3 g, 91%).  $^1H$  NMR (500 MHz,  $DMSO-d_6$ )  $\delta$  9.85 (d,  $J = 5.6$  Hz, 2H), 9.56 (d,  $J = 8.3$  Hz, 2H), 8.73 – 8.65 (m, 4H), 5.13 (t,  $J = 6.8$  Hz, 4H), 3.23 (q,  $J = 6.8$  Hz, 2H) ppm.

#### 6,7-dihydro-5H [1,4] diazepino[1,2,3,4-lmn] [1,10] phenanthroline-3,9-dione (2):

In a 500 mL round-bottom flask, compound 1 (18.0 g, 46.0 mmol) was suspended in *tert*-butanol (250 mL) and the mixture was heated to  $40\text{ }^\circ\text{C}$ . Then followed with potassium *tert*-butoxide (17.5 g, 156.0 mmol), exposure to air and stirred at  $40\text{ }^\circ\text{C}$  overnight. After the reaction is completed, the mixture was allowed to cool to room temperature and the precipitate was collected by filtration and washed with ethanol, then the precipitate dissolved in chloroform and washed with water, the combined organic layers were washed with brine, dried over sodium sulfate, and chloroform was removed under reduced pressure to give yellow solid (6.2 g, 53%).  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  7.72 (d,  $J = 9.5$  Hz, 2H), 7.36 (s, 2H), 6.80 (d,  $J = 9.4$  Hz, 2H), 4.32 (s, 4H), 2.46 (m,  $J = 6.5$  Hz, 2H) ppm.

**2,9-dichloro-1,10-phenanthroline (3):** Compound **2** (6.50 g, 25.8 mmol) was mixed with phosphoryl chloride (78 mL, 834 mmol) in a round-bottom flask containing a magnetic stir bar. Phosphorus pentachloride (10.72 g, 51.5 mmol) was added, and the mixture was heated to reflux and stirred overnight under a nitrogen atmosphere. After the reaction is completed, the phosphoryl chloride was distilled off and the residue was quenched with iced water and basified to pH = 14 with 30% aqueous sodium hydroxide. The precipitate was filtered, washed copiously with water and then with diethyl ether (3 x 10 mL) to yield the product as a yellow solid (5.29 g, 82%). <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.22 (d, *J* = 8.4 Hz, 1H), 7.83 (s, 1H), 7.66 (d, *J* = 8.4 Hz, 1H) ppm.

**Dimethyl 4,4'-(1,10-phenanthroline-2,9-diyl) dibenzoate (4).** 2,9-dichloro-1,10-phenanthroline (0.43 g, 1.7 mmol) and 4-methoxycarbonylphenylboronic acid (0.81 g, 4.5 mmol) were suspended in 30 mL of dioxane and degassed by bubbling N<sub>2</sub> for 30 min. Then Pd SPhos Gen III catalyst (0.22 g, 0.28 mmol) and K<sub>3</sub>PO<sub>4</sub> (1.10 g) were added under a nitrogen atmosphere, the resulting mixture was heated to 90 °C and stirred overnight. After cooling to room temperature, the solvent was removed under reduced pressure. Then the crude product was dissolved in 70 mL dichloromethane and washed with 100 mL DI water. The organic layer was separated and dried with Na<sub>2</sub>SO<sub>4</sub>. Dichloromethane was removed under reduced pressure after filtered by diatomite, yielding off-white solid (0.53 g, 69% yield). <sup>1</sup>H NMR (500 MHz, DMSO-*d*<sub>6</sub>) δ 8.71 (d, *J* = 8.2 Hz, 4H), 8.66 (d, *J* = 8.4 Hz, 2H), 8.53 (d, *J* = 8.4 Hz, 2H), 8.24 (d, *J* = 8.2 Hz, 4H), 8.07 (s, 2H), 3.94 (s, 6H) ppm.

**4,4'-(1,10-phenanthroline-2,9-diyl) dibenzoic acid (5).** Compound **4** (0.17 g, 0.38 mmol) was suspended in 10 mL EtOH in a 50 mL round-bottom flask, followed by dropwise addition of 10 mL of 6 M NaOH (aq.). After the mixture was refluxed overnight, 1 M HCl (aq.) was slowly added until the pH was below 7. The precipitate was collected by filtration and washed with water, dried under vacuum to obtain pure product as a white solid (0.144 g, 90% yield) <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>) δ 13.15 (s, 4H), 8.67 (dd, *J* = 8.4, 4.4 Hz, 6H), 8.53 (d, *J* = 8.5 Hz, 2H), 8.22 (d, *J* = 8.4 Hz, 4H), 8.08 (s, 2H) ppm.

## 2.4. NMR spectroscopy

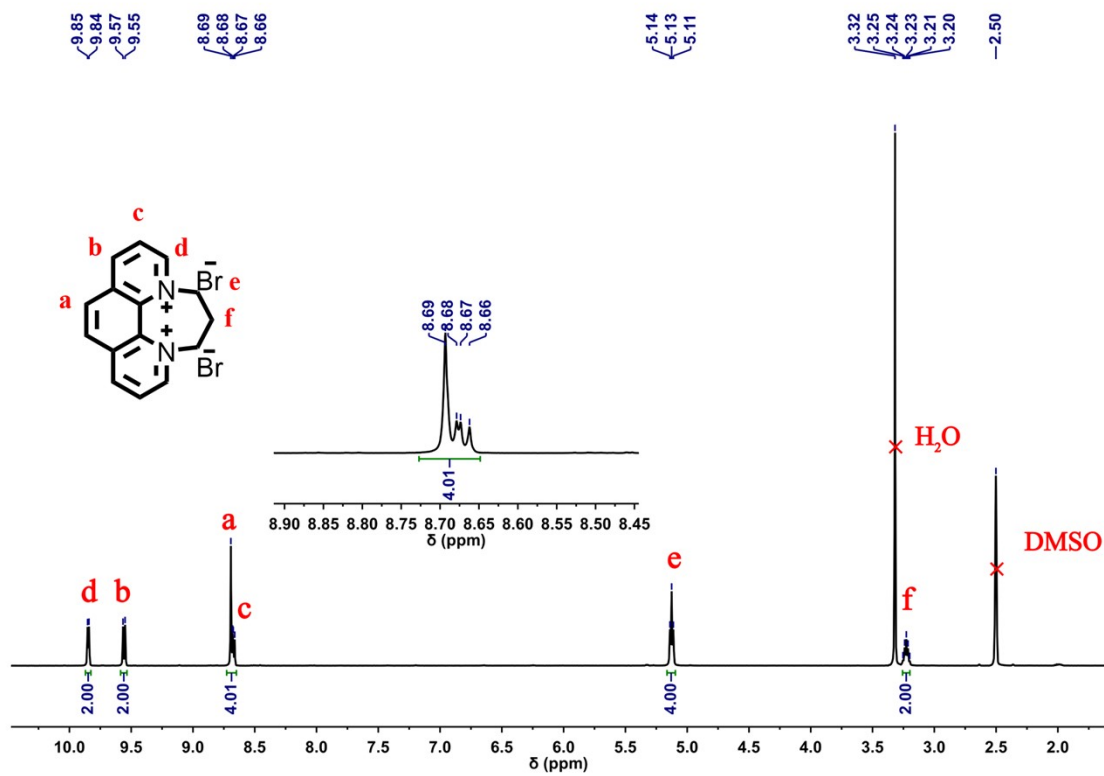


Figure S1.  $^1\text{H}$  NMR spectrum of compound 1.

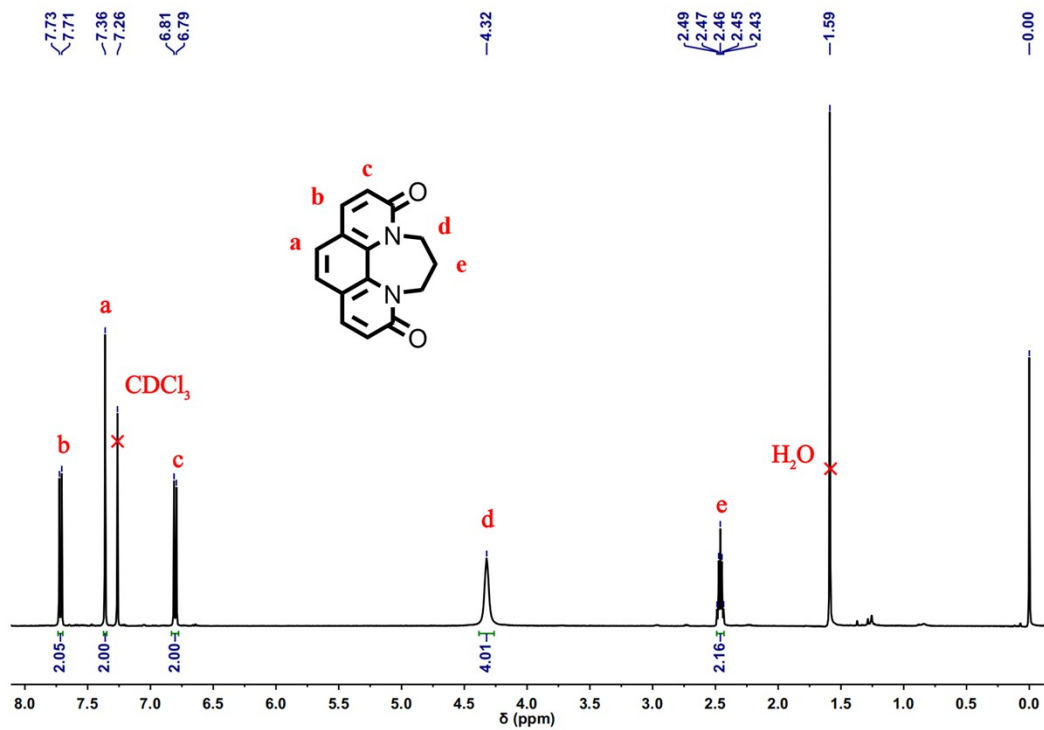


Figure S2. <sup>1</sup>H NMR spectrum of compound 2.

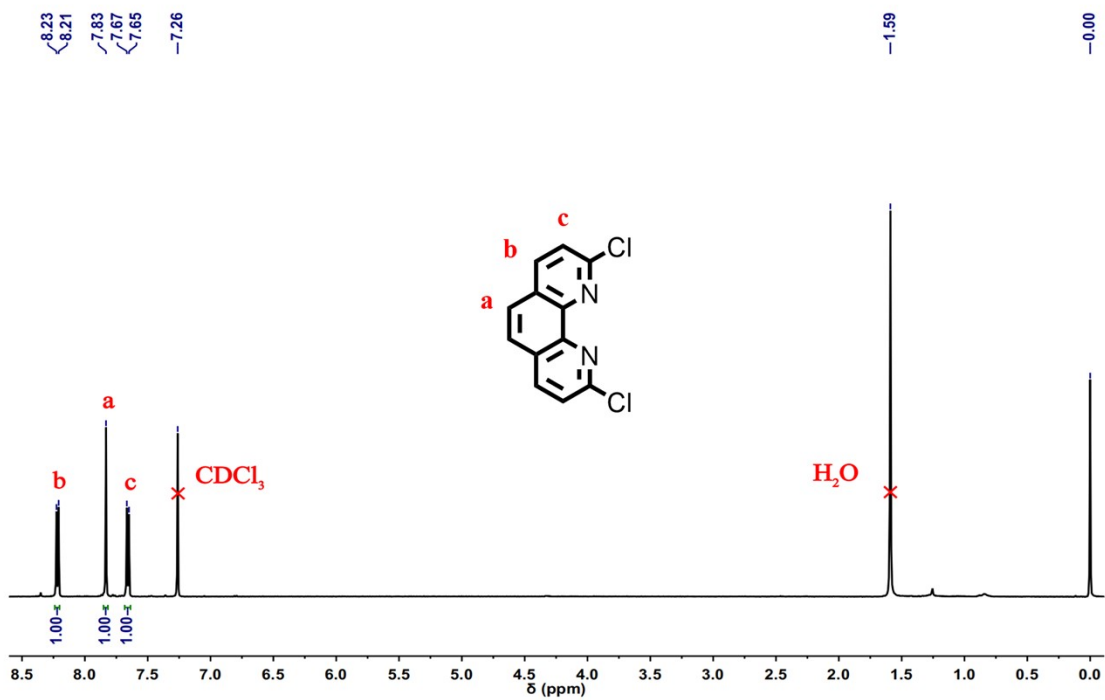


Figure S3. <sup>1</sup>H NMR spectrum of compound 3.

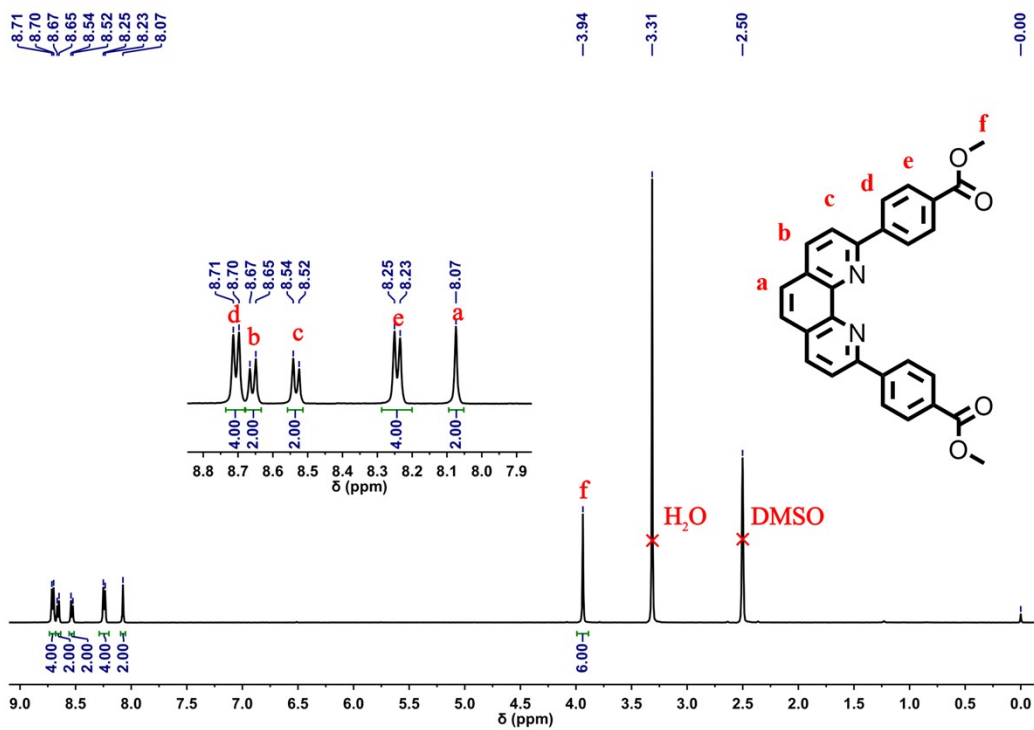


Figure S4. <sup>1</sup>H NMR spectrum of compound 4.

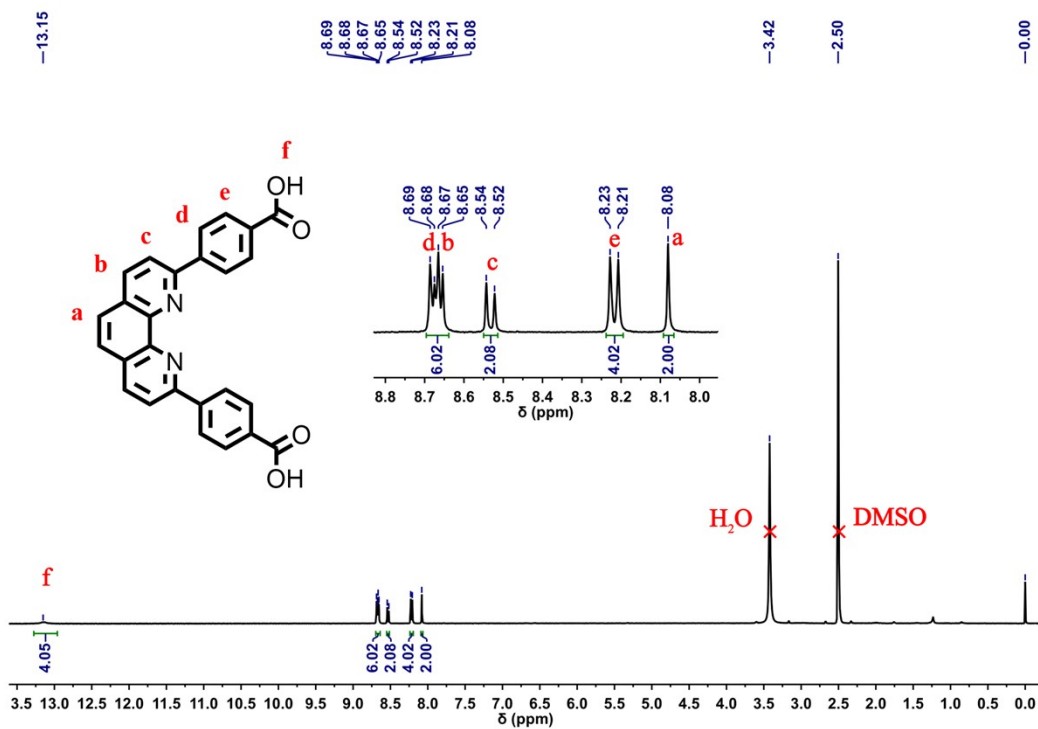
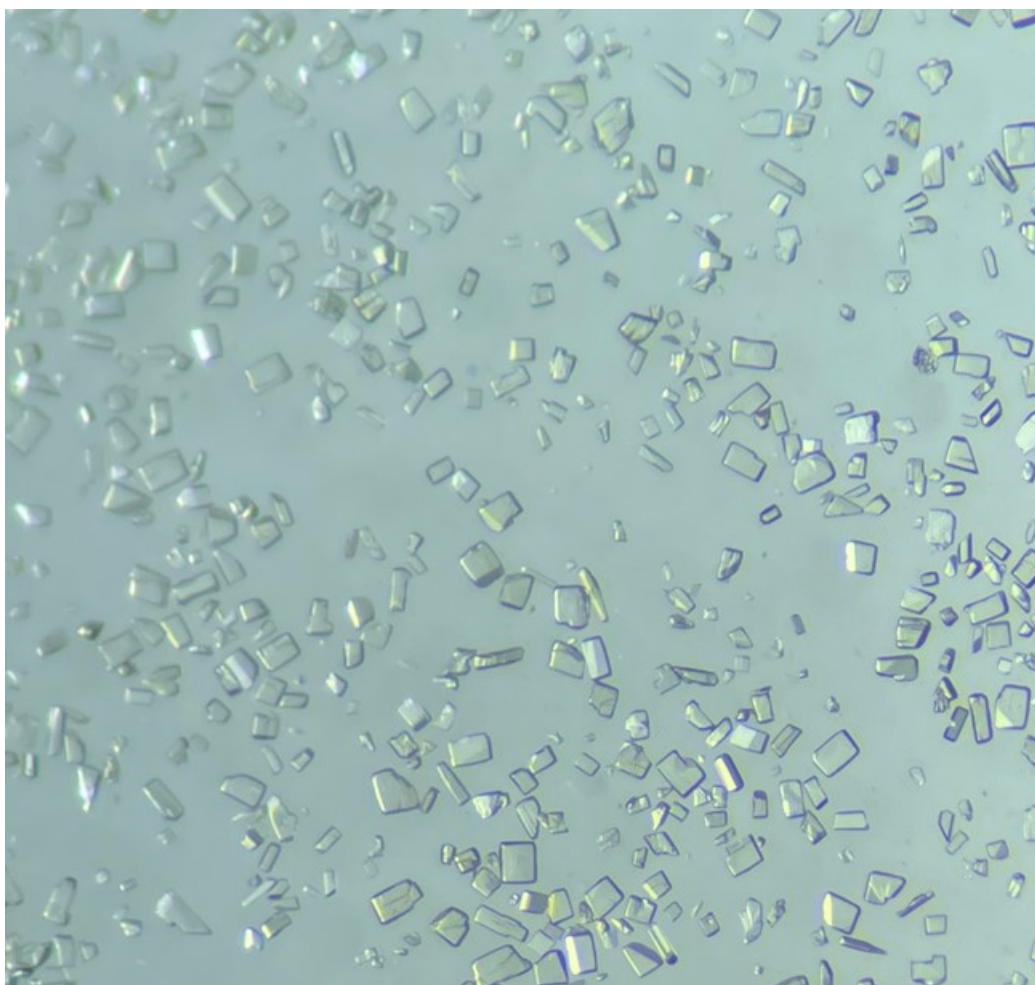


Figure S5. <sup>1</sup>H NMR spectrum of compound 5.

### 3. Synthesis of MOFs

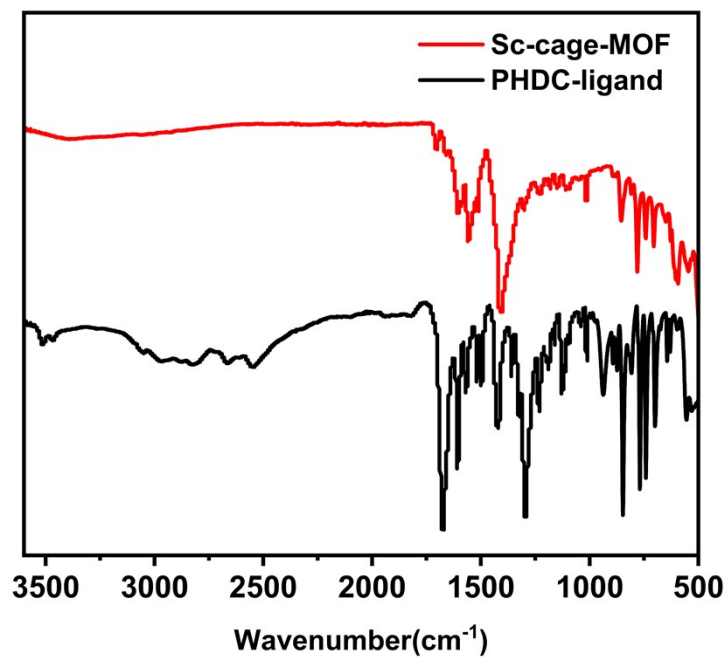
#### Synthesis of single crystals of Sc-cage-MOF

A 1 mL DMF solution of PHDC (5 mg) and a 1 mL DMF solution of  $\text{ScCl}_3 \cdot 6\text{H}_2\text{O}$  (10 mg) were combined in a 15 mL vial. Then, acetic acid (0.1 mL) was added. The mixture was sonicated for 2 min and sealed and heated to 120 °C for 3 days and cooled to room temperature. Single crystals were formed and used for single crystal X-ray diffraction measurements.

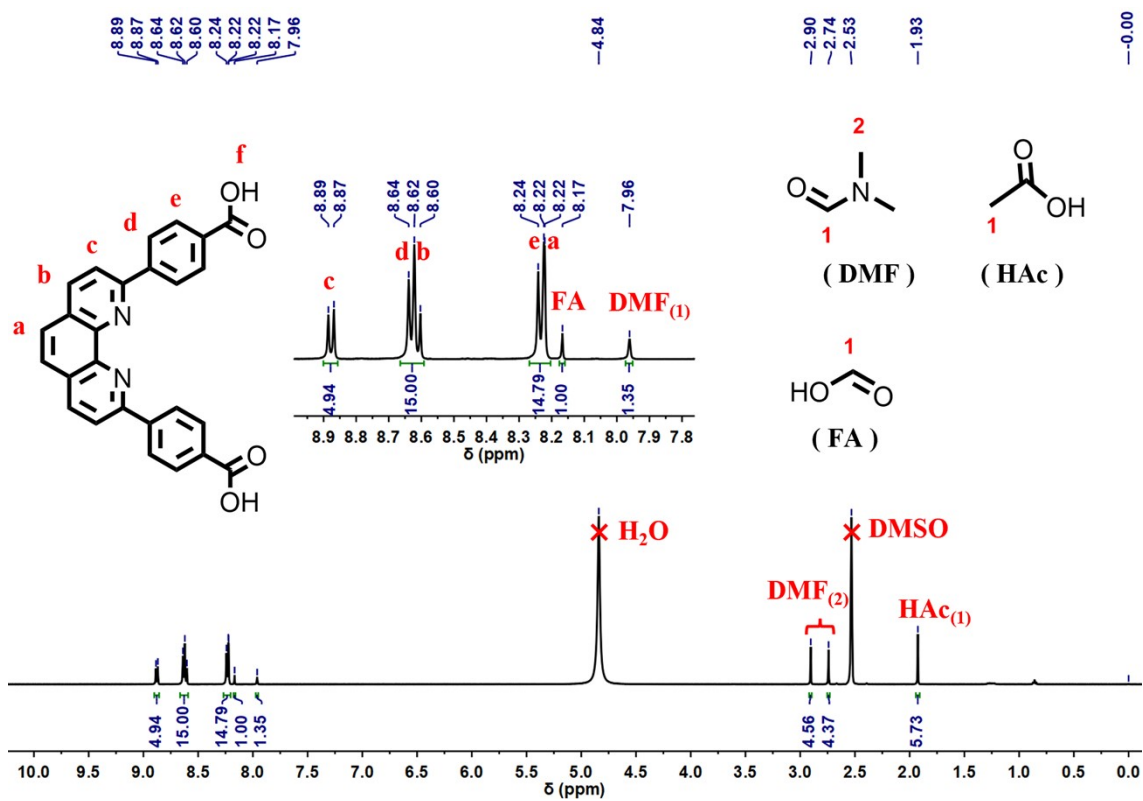


**Figure S6.** Optical images of the single crystals of Sc-cage-MOF.





**Figure S7.** FT-IR spectra of Sc-cage-MOF and PHDC ligand

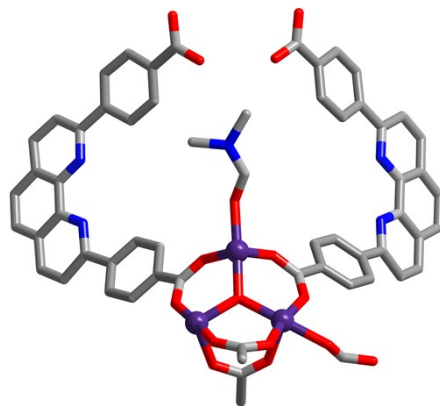


**Figure S8.**  $^1\text{H}$  NMR spectrum of the digested **Sc-cage-MOF** reveals the FA: HAc: DMF: PHDC = 1: 2 :1 :2.5

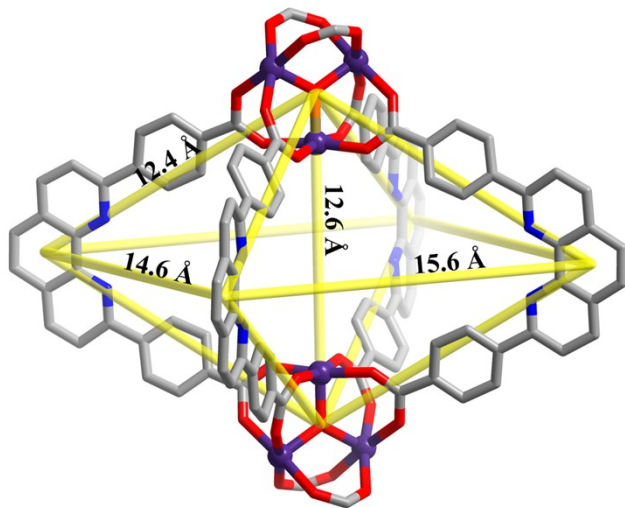
## 4. Single Crystal X-ray Data

**Table S1.** Crystallographic data of Sc-cage-MOF

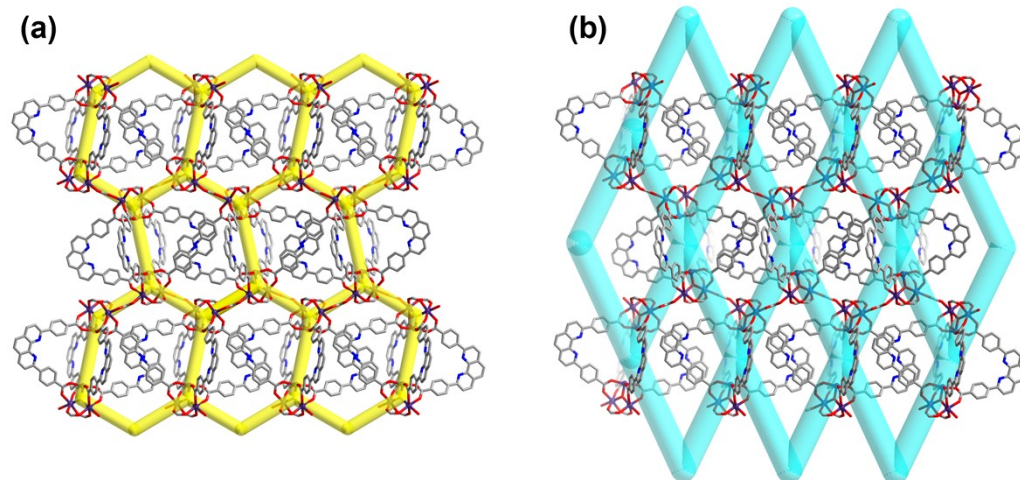
	Sc-Cage-MOF
Empirical formula	C <sub>84</sub> H <sub>98</sub> N <sub>13</sub> O <sub>24</sub> Sc <sub>3</sub>
Formula weight	1808.63
Temperature/K	170.00
Crystal system	monoclinic
Space group	<i>P</i> 2 <sub>1</sub> / <i>n</i>
<i>a</i> /Å	15.847(2)
<i>b</i> /Å	16.418(3)
<i>c</i> /Å	34.089(5)
$\alpha$ /°	90
$\beta$ /°	101.579(5)
$\gamma$ /°	90
Volume/Å <sup>3</sup>	8689(2)
<i>Z</i>	4
Calcd Density (g/cm <sup>3</sup> )	1.383
$\mu$ (mm <sup>-1</sup> )	1.771
<i>F</i> (000)	3792.0
Crystal size (mm <sup>3</sup> )	0.11×0.1×0.05
Radiation	GaK $\alpha$ ( $\lambda$ = 1.34139)
Total reflection	39396
<i>R</i> <sub>int</sub>	0.0901
Goodness-of-fit	1.061
<i>R</i> <sub>1</sub> [ <i>I</i> >2 $\sigma$ ( <i>I</i> )]	<i>R</i> <sub>1</sub> = 0.0863, w <i>R</i> <sub>2</sub> = 0.2510
w <i>R</i> <sub>2</sub> (all reflection)	<i>R</i> <sub>1</sub> = 0.1084, w <i>R</i> <sub>2</sub> = 0.2754
Largest diff. peak/hole	0.62/-0.39
CCDC-number	2295390



**Figure S9.** The asymmetric unit of **Sc-cage-MOF**. Atom color code: Sc (purple), O (red), N (blue), C (gray). Hydrogen atoms are omitted for clarity.



**Figure S10.** The illustration of the octahedron cage. Atom color code: Sc (purple), O (red), N (blue), C (gray), Hydrogen atoms are omitted for clarity.

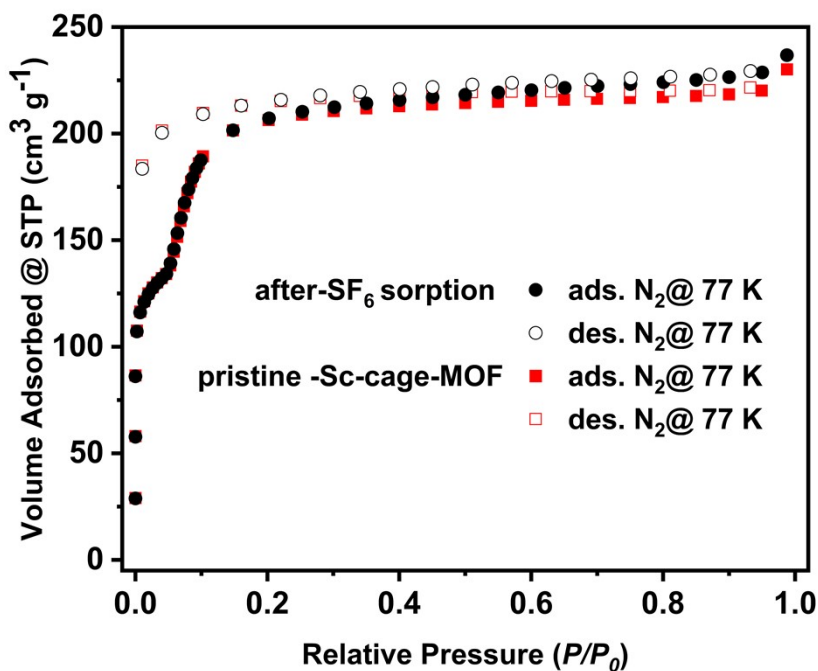


**Figure S11.** Two-dimensional layered structure of **Sc-cage-MOF** showing **hcb** net (a) and **sql** net (b).

## 5. N<sub>2</sub> and SF<sub>6</sub> Sorption

### 5.1 Sample activation and N<sub>2</sub> sorption isotherm

Prior to gas sorption, the as-synthesized samples (~ 40 mg) were washed 2 times with DMF and then sequentially immersed in acetone for 2 days, during which time the acetone was replaced three times. The solids were then activated at 60 °C under vacuum for 12 h.



**Figure S12.** The N<sub>2</sub> isotherms of Sc-cage-MOF at 77 K before and after SF<sub>6</sub> sorption.

## 6. IAST Calculations

### Prediction of multicomponent gas adsorption Ideal Adsorption Solution Theory (IAST)

The Ideal Adsorption Solution Theory (IAST) proposed by Mayer and Prausnitz (1965)<sup>2</sup> uses pure gas adsorption isotherms to predict the mixture adsorption equilibrium at the temperature of interest. For IAST application, the main condition to be fulfilled is the availability of (i) good quality single component adsorption data of different gases, and (ii) an excellent curve fitting model for such data (Chen and Sholl, 2007;<sup>3</sup> Bae et al., 2008<sup>4</sup>). In the current work, Dual-Site Langmuir-Freundlich model was used to fit the pure gas isotherms.

The most important equations used in the IAST calculation are listed hereafter:

$$f_i = x_i f_i^0(\pi) \quad (1)$$

$$\frac{\pi A}{RT} = \int_0^{f_i^0} n_i d \ln f_i \quad (2)$$

$$\frac{1}{n_i} = \sum_i \frac{x_i}{n_i^0} \quad (3)$$

$$S_{SF_6-i} = \frac{x_{SF_6}/x_i}{y_{SF_6}/y_i} \quad (4)$$

where  $f_i$  is the fugacity of component  $i$  in the gas phase;  $f_i^0$  is the standard-state fugacity (i.e., the fugacity of pure component  $i$  at the equilibrium spreading pressure of the mixture,  $\pi$ );  $x_i$  and  $y_i$  are the mole fractions of component  $i$  in the adsorbed and gas phase, respectively;  $A$  is the surface area of the adsorbent;  $n_i$  is the number of moles adsorbed of pure component  $i$  (i.e., the pure-component isotherm); and  $n_i^0$  is the number of moles adsorbed of pure component  $i$  at the standard-state pressure.

Equation (1) is the central equation of IAST, specifying the equality of the chemical potential of component  $i$  in the gas and the adsorbed phase (which is assumed to be ideal in the sense of Raoult's law). Equation (2) allows the calculation of the spreading pressure from the pure component adsorption isotherm. The total amount adsorbed of the mixture,  $n_i$ , and the selectivity of SF<sub>6</sub> with respect to  $i$ ,  $S_{SF_6-i}$ , are given by equations (3) and (4), respectively. The selectivity  $S_{SF_6-i}$ , reflects the efficiency of SF<sub>6</sub> separation.

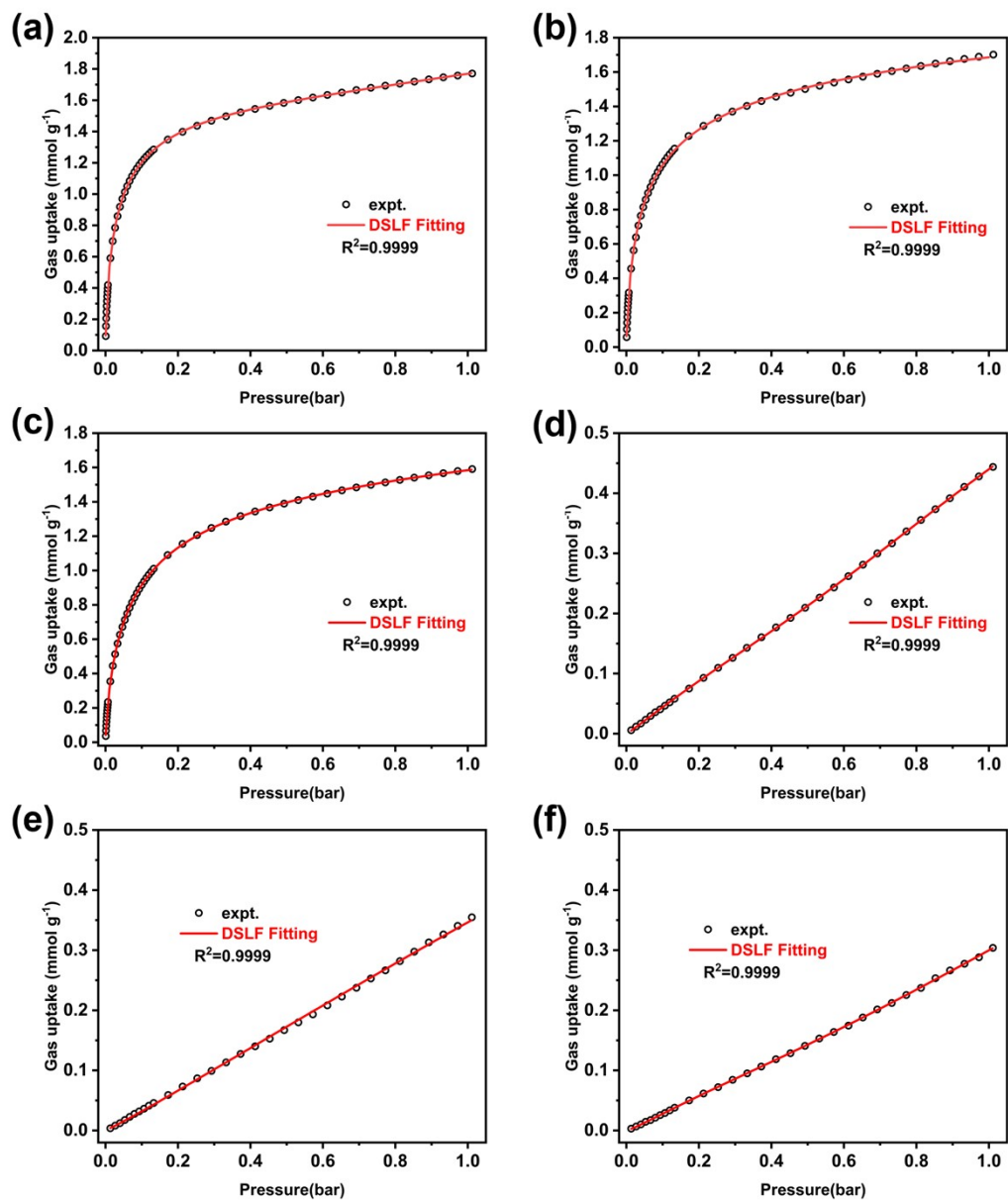
### Dual-Site Langmuir-Freundlich Model for single gas sorption fitting

In the current work, the Dual-Site Langmuir-Freundlich (DSLFL) model was used to fit the pure gas isotherms and its simple formulation as expressed by equation (5).

$$N_i = N_{i,A}^{max} \frac{b_{i,A} p^{V_{i,A}}}{1 + b_{i,A} p^{V_{i,A}}} + N_{i,B}^{max} \frac{b_{i,B} p^{V_{i,B}}}{1 + b_{i,B} p^{V_{i,B}}} \quad (5)$$

where  $N_i$  represents the loading (unit: mmol g<sup>-1</sup>) of species  $i$  adsorbed in the sample;  $p$  represents the pressure of the bulk gas at equilibrium with the adsorbed phase (unit: bar);  $N_{i,A}^{max}$  and  $N_{i,B}^{max}$  represent the maximum saturation capacities (unit: mmol g<sup>-1</sup>) at the two different sites (type A and B) respectively;  $b_{i,A}$  (unit: bar<sup>-V<sub>A</sub></sup>) and  $b_{i,B}$  (unit: bar<sup>-V<sub>B</sub></sup>) represent the affinities on sites A and B at the temperature of interest respectively;  $V_A$  (dimensionless) and  $V_B$  (dimensionless) represent the deviations from an ideal homogeneous surface.





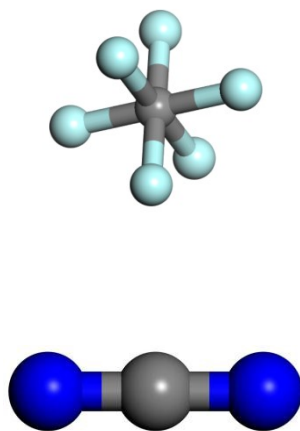
**Figure S13.** (a-c) The DSLF model for fitting SF<sub>6</sub> isotherms of **Sc-cage-MOF** at 278, 288 and 298 K. (d-f) The DSLF model for fitting N<sub>2</sub> isotherms of **Sc-cage-MOF** at 278, 288 and 298 K.

**Table S2.** The fitted parameters by using the DSLF model based on the single-component isotherms data of SF<sub>6</sub> and N<sub>2</sub> in **Sc-cage-MOF** at 278, 288 and 298 K.

	Gas	$N_A$	$b_A$	$V_A$	$N_B$	$b_B$	$V_B$
278K	SF <sub>6</sub>	1.8229	0.39355631	0.693083	1.26004	4.39948E-06	2.18703
	N <sub>2</sub>	0.452742	1.14191E-06	2.86626	0.480014	0.007987148	1.09833
288K	SF <sub>6</sub>	1.13108	0.011489957	0.724559	1.55661	0.325932317	0.734549
	N <sub>2</sub>	0.571439	4.89386E-06	2.4629	0.287536	0.00965036	1.13459
298K	SF <sub>6</sub>	1.20707	0.003333129	0.881176	1.58323	0.226083689	0.750247
	N <sub>2</sub>	0.945909	1.26944E-05	2.10852	0.193273	0.010378047	1.1807

## 7. Molecular Simulation

The molecular model and parameters of SF<sub>6</sub> and N<sub>2</sub> adopted the rigid molecular model proposed by Koukaras et al.<sup>5</sup>. The schematic diagram of the molecular model is shown in Figure S14, and the relevant parameters are listed in Table S3.



**Figure S14.** Molecular structures of SF<sub>6</sub> and N<sub>2</sub>

**Table S3.** Molecular parameters of SF<sub>6</sub> and N<sub>2</sub>

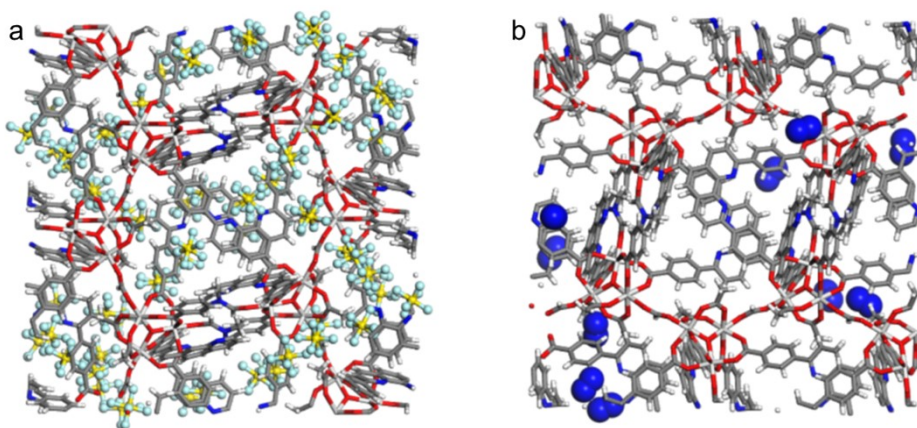
Gas molecules	Correlated atom	$\varepsilon/k_B$ [K]	$\sigma$ [Å]	$Q$ [e]
SF <sub>6</sub>	S_SF <sub>6</sub>	165.14	3.228	0.66
	F_SF <sub>6</sub>	27.02	2.947	-0.11
N <sub>2</sub>	N_N <sub>2</sub>	36	3.31	-0.482
	COM_N <sub>2</sub>	0	0	0.964

Note: SF<sub>6</sub> molecular bond length is 1.564 Å; The bond length of N<sub>2</sub> molecule is 1.1 Å.

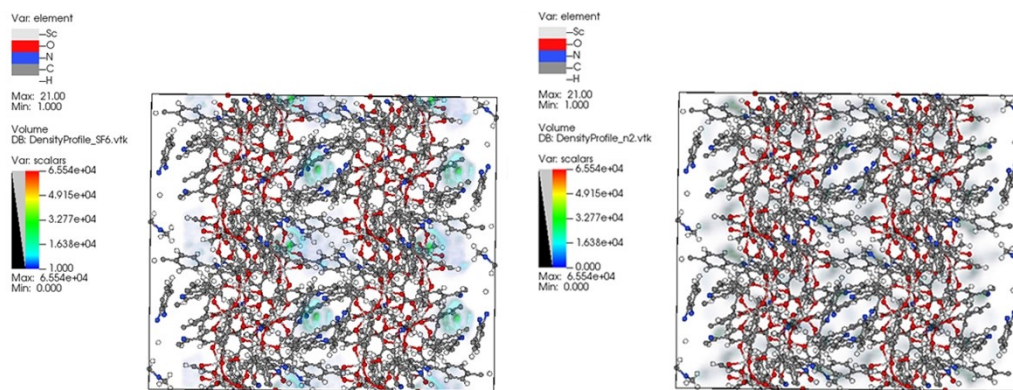
The GCMC in RASPA<sup>6</sup> software package was used to simulate the adsorption behavior of pure SF<sub>6</sub> gas molecules, pure N<sub>2</sub> gas molecules and 1:1 SF<sub>6</sub>/N<sub>2</sub> mixture in the SC-Caged metal-organic framework (MOF) at 298 K and 1.0 bar, respectively. During the simulation, the potential energies of SF<sub>6</sub> and N<sub>2</sub> molecules themselves and their interactions with the MOF were calculated, the atoms in MOFs are evaluated using electrostatic and Lennard-Jones (LJ) potential energy functions, as follows:

$$u_{LJ+elec}(\mathbf{r}) = \sum 4\epsilon_{ij} \left[ \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] + \sum \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}}$$

Where  $i$  and  $j$  represent two atoms interacting in a force field;  $u_{LJ+elec}(r)$  is the interaction energy between two atoms; the minimum distance at which two atoms collide is denoted by  $\sigma_{ij}$ ,  $\epsilon_{ij}$  and  $r_{ij}$  indicate the depth of the well and the true distance between the atoms, respectively. permittivity of vacuum is  $\epsilon_0 = 8.8542 \times 10^{-12} \text{ C}^2\text{N}^{-1}\text{m}^{-2}$ ; The number of charges carried by the two atoms  $i$  and  $j$  are represented by  $q_i$  and  $q_j$  respectively. The LJ parameter of the atom in MOFs is mainly from the DREIDING field, with a small number of parameters from the UFF field, mainly because the DREIDING field has no information about this part of the atom. During the simulation, all atom charges of MOFs were calculated by EQeq algorithm<sup>7</sup>. The MOFs is considered to be the rigid structure. The chemical potential, volume and temperature were kept constant throughout the simulation. Lorentz-Berthelot rule is used to calculate the interaction between MOF and adsorbent molecules. The shear distance of truncated intermolecular interaction is set to 12 Å, and the length of each boundary of MOF is not less than 24 Å. Each simulation consists of 1000000 GCMC cycles, with the first 500000 cycles used to balance the simulation system and the last 500000 cycles used to calculate the accumulation of the average. Balance is achieved by performing translation, rotation, swap, regeneration, and insert and delete operations in each cycle.



**Figure S15.** Sorption density distribution and possible binding sites calculated by GCMC simulation at 298 K and 1.0 bar for SF<sub>6</sub> (a) and N<sub>2</sub> (b) in Sc-cage-MOF.



**Figure S16.** The simulated SF<sub>6</sub> (a) and N<sub>2</sub> (b) density distribution in the Sc-cage-MOF

## 8. References

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