Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information for the Manuscript

A Flexible Doubly Interpenetrated Metal−Organic Framework with Gate Opening Effect for Highly Selective C_2H_2/C_2H_4 Separation at Room Temperature

*Di-Ming Chen, Xiao-Hui Liu, Jia-Hui Zhang and Chun-Sen Liu**

Henan Provincial Key Lab of Surface & Interface Science, Zhengzhou University of Light Industry, Zhengzhou 450002, Henan, China

Corresponding Author E-mail: chunsenliu@zzuli.edu.cn

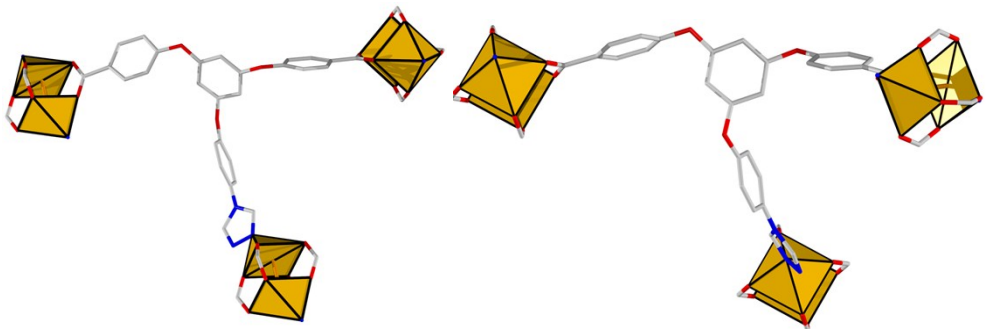

Fig. S1 View for the coordination surroundings for the H_2TPPB ligand.

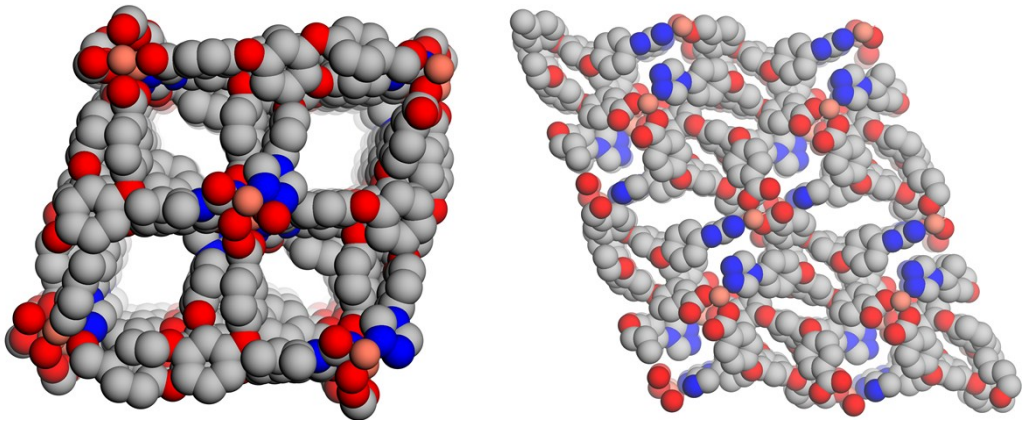

Fig. S2 View for the two different pore structures of **1**.

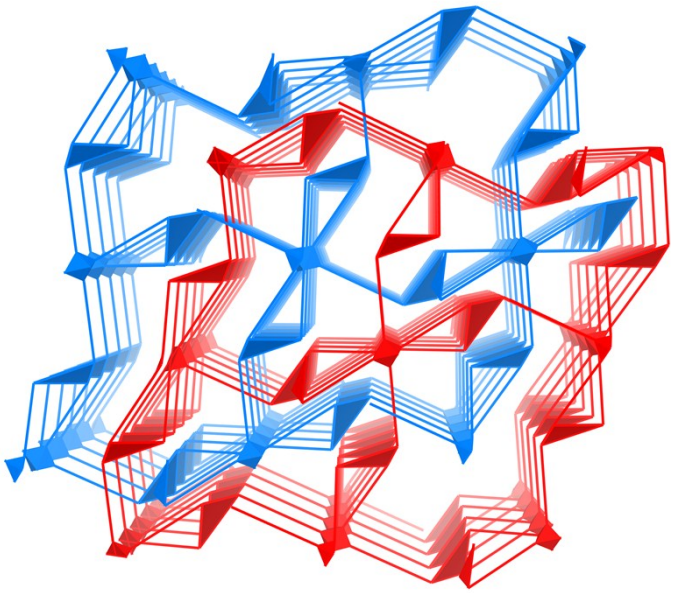

Fig. S3 The simplified 2-fold interpenetrated **rtl**-type (3,6)-connected net for **1**.

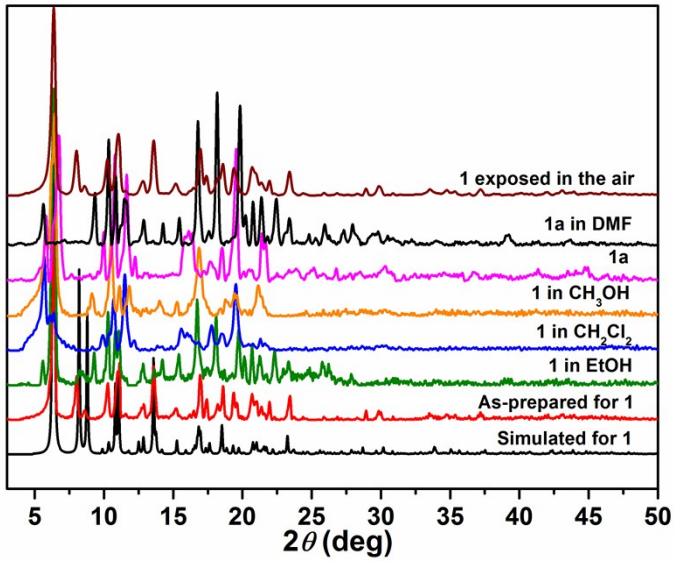

Fig. S4 PXRD patterns of **1**.

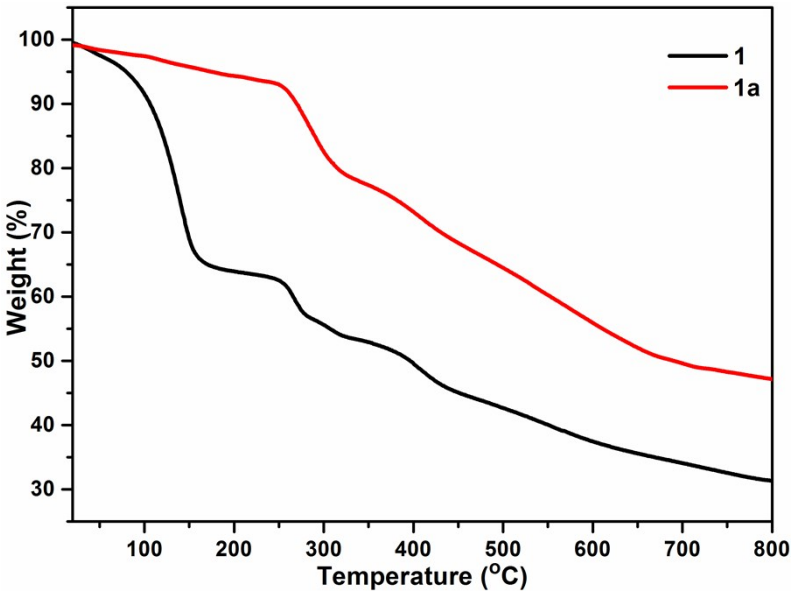

Fig. S5 Thermogravimetric curves of **1**.

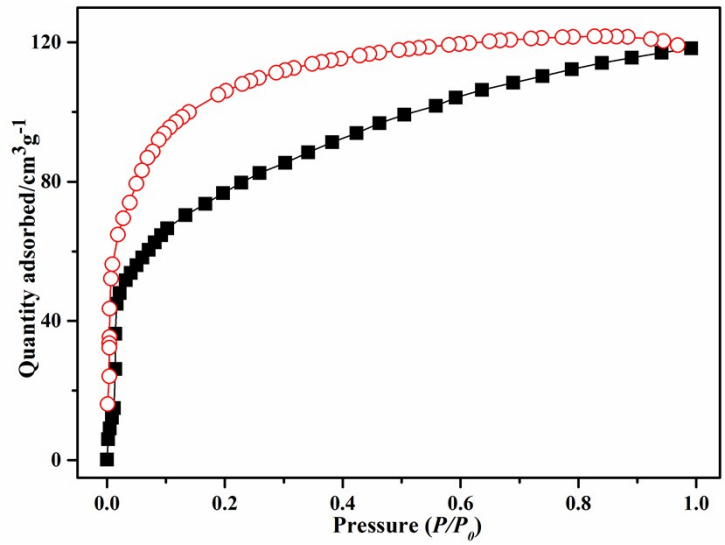

Fig. S6 The CO_2 sorption isotherm at 195 K.

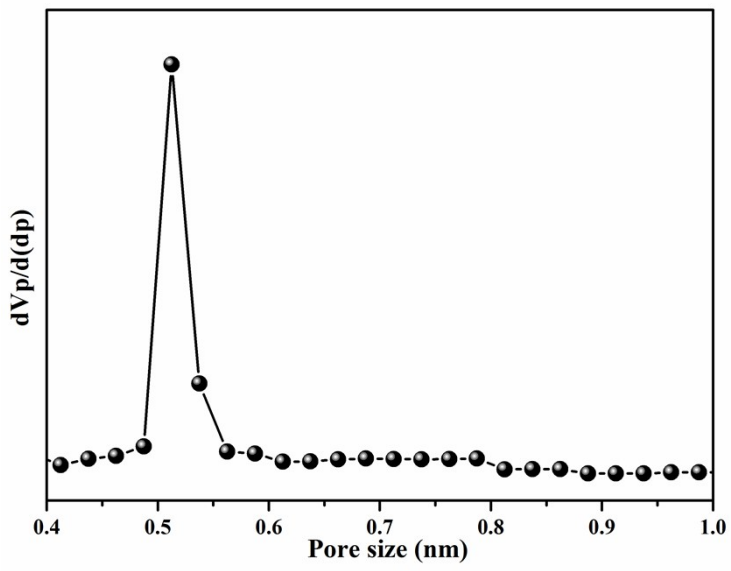

Fig. S7 The pore size distributing of 1a derived from the CO2 sorption isotherm at 195 K.

Calculation of Sorption Heat for C_2H_2 and C_2H_4 Uptake Using Virial Fitting.

$$\ln P = \ln N + 1/T\sum_{i=0}^{m} a_i N^i + \sum_{i=0}^{n} b_i N^i \qquad\qquad Q_{st} = -R\sum_{i=0}^{m} a_i N^i$$

The above virial expression was used to fit the combined isotherm data for **1a** at 273and 298 K, where P is the pressure, N is the adsorbed amount, T is the temperature, ai and bi are virial coefficients, and m and N are the number of coefficients used to describe the isotherms. Q_{st} is the coverage-dependent enthalpy of adsorption and R is the universal gas constant.

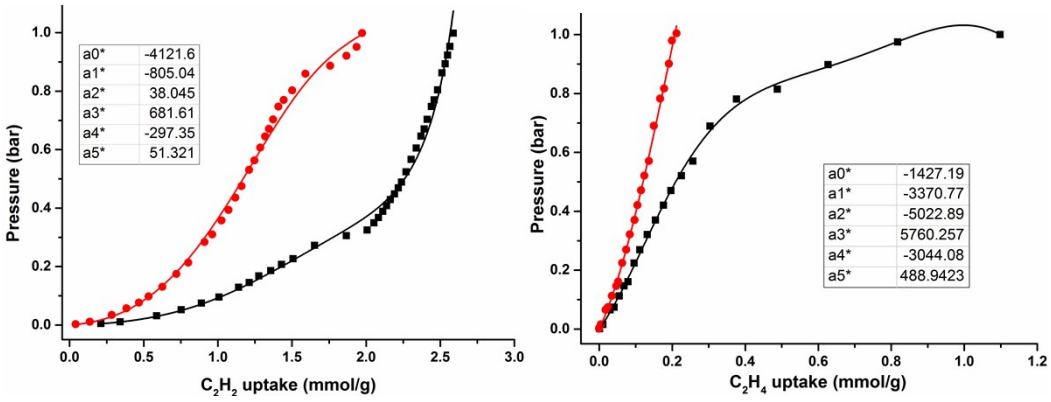

Fig. S8 Virial fitting for the C_2H_2 and C_2H_4 adsorption isotherms of **1a**.

Prediction of the C_2H_2/C_2H_4 Adsorption Selectivity by IAST.

We adopt the ideal adsorbed solution theory (IAST) based upon the experimental single gas adsorption measurements as listed in the main text, including C_2H_2 and C_2H_4 at 298 K, which is commonly used to predict binary mixture adsorption selectivity. Before calculation of the sorption and separation properties, the adsorption isotherms were fitted using single-site Langmuir (SSL) models:

$$\text{SSL:} \quad q = \frac{q_{sat} bp}{1 + bp}$$

Using the pure component isotherm fits, the adsorption selectivity is defined by:

$$S_{ads} = (q_1/q_2)/(p_1/p_2)$$

Where q_i is the amount of i adsorbed and p_i is the partial pressure of i in the mixture.

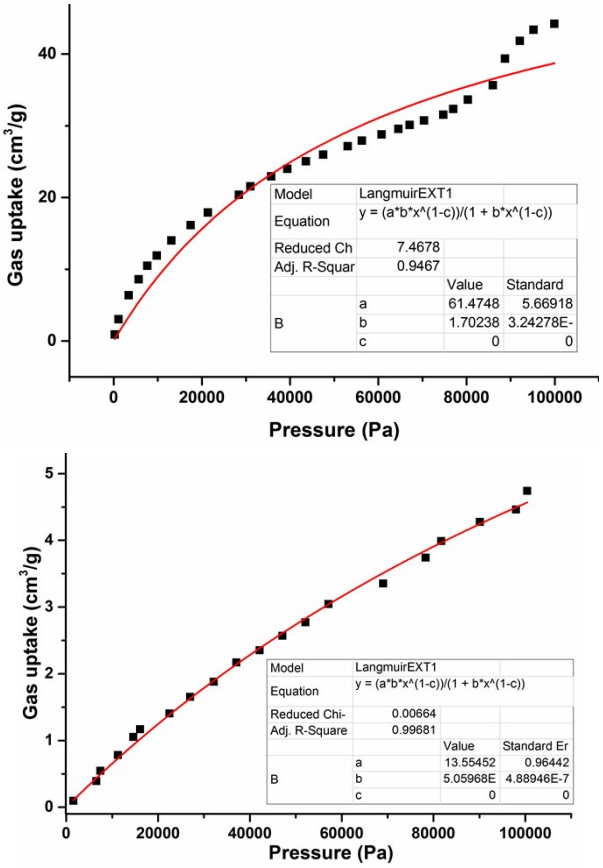

Fig. S9 The SSL fitting for the C_2H_2 and C_2H_4 adsorption isotherms of **1a**.

Table. S1 Crystal data and structure refinement for **1**.

Empirical formula	$C_{56}H_{34}Cu_2N_6O_{14}$
Formula weight	44.78
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	12.1088(4)
b/Å	16.9597(8)
c/Å	19.1362(4)
α/°	111.443(4)
β/°	91.846(3)
γ/°	95.794(3)
Volume/Å^3	3629.0(2)
Z	51
ρ_{calc}g/cm^3	1.045
μ/mm^{-1}	1.173
Radiation	CuKα (λ = 1.54184)
Goodness-of-fit on F^2	0.974
Final *R* indexes [I>=2σ (I)]	R_1 = 0.0832, wR_2 = 0.2366
Final *R* indexes [all data]	R_1 = 0.0935, wR_2 = 0.2573
Largest diff. peak/hole / e Å^{-3}	1.14/-0.74
CCDC number	1547691