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Supporting Information

A New Multi-Functional Cu(II)-Organic Framework as a Platform for Selective Carbon Dioxide Chemical Fixation and Separation of Organic Dyes

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Table S1. Selected bond lengths (Å) and bond angles (º) for **1**

Complex **1**			
Cu(1)-O(2)#2	1.959(3)	O(2)#1-Cu(1)-Cu(1)#1	83.66(14)
Cu(1)-O(2)#1	1.959(3)	O(2)#1-Cu(1)-O(2)#2	89.44(18)
Cu(1)-O(1)	1.962(3)	O(2)#1-Cu(1)-O(1)#3	90.21(14)
Cu(1)-O(1)#3	1.962(3)	O(2)#2-Cu(1)-O(1)	90.21(14)
Cu(1)-O(5)	2.146(8)	O(2)#1-Cu(1)-O(1)	168.22(18)
Cu(1)-O(2)#2	1.959(3)	O(2)#2-Cu(1)-O(1)#3	168.22(18)
O(2)#2-Cu(1)-Cu(1)#1	83.66(14)	O(2)#2-Cu(1)-O(5)	95.3(2)
O(2)#1-Cu(1)-O(5)	95.3(2)	O(1)#3-Cu(1)-O(5)	96.5(2)
O(1)#3-Cu(1)-Cu(1)#1	84.60(14)	O(5)-Cu(1)-Cu(1)#1	178.5(2)
O(1)-Cu(1)-Cu(1)#1	84.60(14)	O(1)-Cu(1)-O(1)#3	87.7(2)
O(1)-Cu(1)-O(5)	96.5(2)		

Symmetrical codes: #1 -x+1/2, -y+3/2, -z+1/2; #2 -x+1/2, y, -z+1/2; #3 x, -y+3/2, z; #4 -y+5/4, -x+5/4, -z+3/4.

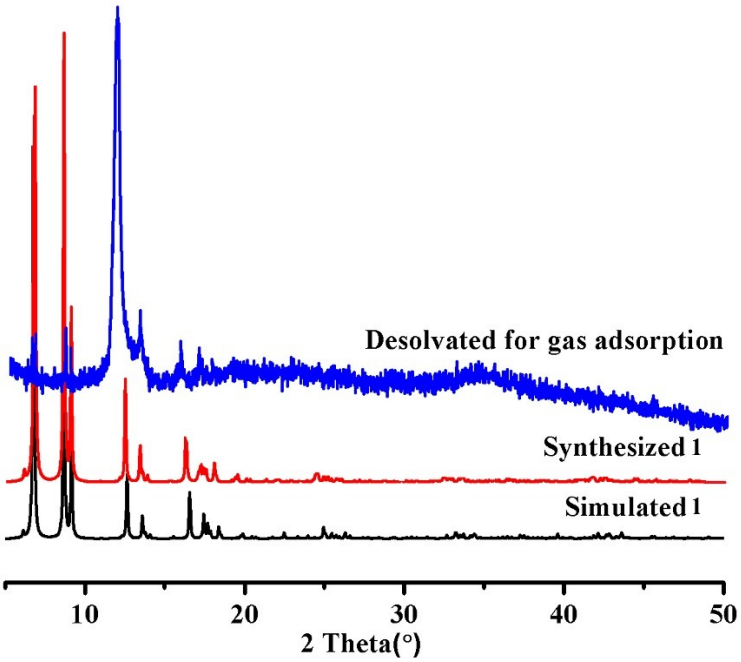

Fig. S1. PXRD patterns of **1** simulated from the X-ray single-crystal structure, experimental samples and desolvated samples (**1a**).

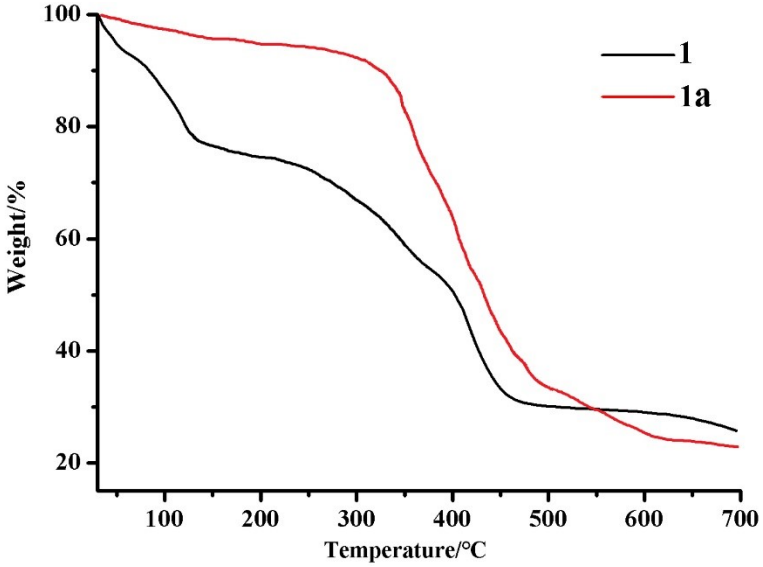

Fig. S2. TGA plots of complex **1** and **1a**.

IAST adsorption selectivity calculation

The experimental isotherm data for pure CO_2 and CH_4 (measured at 273 and 298 K) were fitted using a Langmuir-Freundlich (L-F) model

$$q = \frac{a * b * p^c}{1 + b * p^c}$$

Where q and p are adsorbed amounts and pressures of component i, respectively. The adsorption selectivities for binary mixtures of CO_2/CH_4 at 273 and 298 K and CO_2/N_2 at 298 K., defined by

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

Where *qi* is the amount of *i* adsorbed and *pi* is the partial pressure of *i* in the mixture.

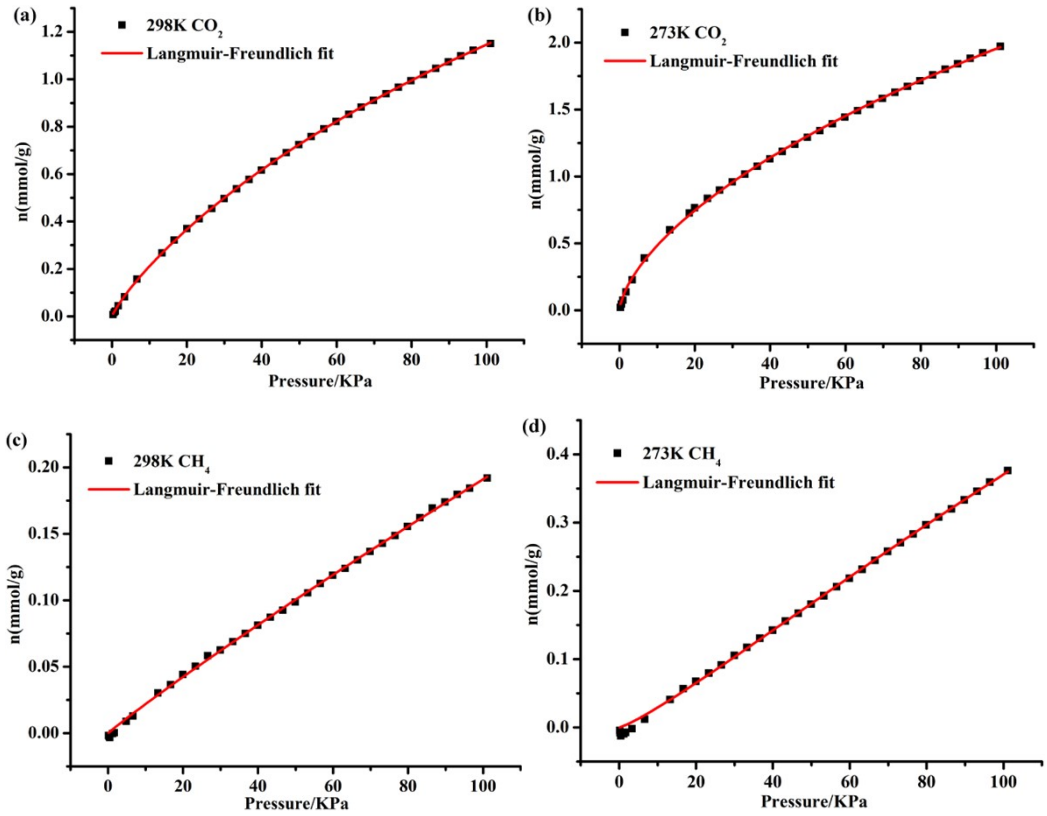

Fig. S3. CO_2 adsorption isotherms of **1a** at 273K with fitting by L-F model: a = 15.652, b = 0.0071, c =0.6510, Chi^2 = 1.75 ×10^{-4}, R^2 = 0.99951; CO_2 adsorption isotherms of **1a** at 298K with fitting by L-F model: a = 4.0308, b = 0.0076, c =0.8568, Chi^2 = 6.18 ×10^{-6}, R^2 = 0.99995; CH_4 adsorption isotherms of **1a** at 273K with fitting by L-F model: a = 2.04506, b = 9.47 ×10^{-4}, c =1.18421, Chi^2 = 2.24 ×10^{-5}, R^2 = 0.99856; CH_4 adsorption isotherms of **1a** at 298K with fitting by L-F model: a = 4.18026, b = 5.7768, c = 0.95923, Chi^2 = 3.24 ×10^{-6}, R^2 = 0.99918.

Calculation of sorption heat for CO_2 uptake using Virial 2 model

$$\ln P = \ln N + 1/T \sum_{i=0}^{m} aiN^i + \sum_{i=0}^{n} biN^i \quad Q_{st} = -R \sum_{i=0}^{m} aiN^i$$

The above equation was applied to fit the combined CO_2 isotherm data for desolvated **1a** at 273 and 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.

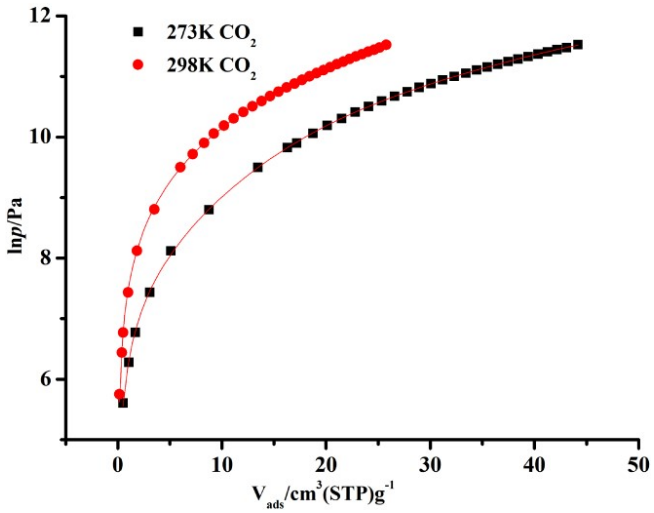

Fig. S4. Virial analysis of the CO_2 adsorption data at 273 and 298 K for **1a**. Fitting results: a0 = –3989.33，a1 = –32.37，a2 = 8.24，a3 = –0.24，a4 = 0.0014，Chi^2 = 0.00064，R^2 = 0.9997.

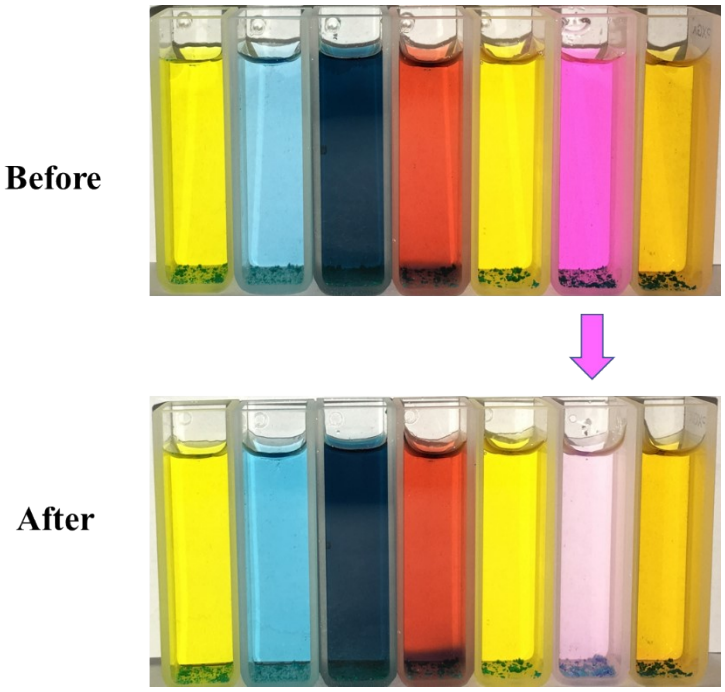

Fig. S5. Color differences of the H_2O solutions with complex **1** in various dyes.

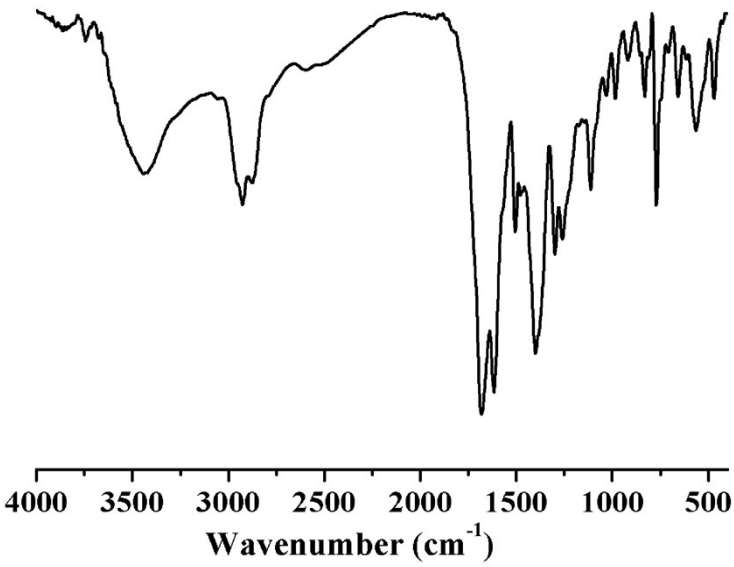

Fig. S6. The FT-IR spectra of complex **1**.