Rational construction and remarkable gas adsorption properties of a HKUST-1-like *tbo*-type MOF based on a tetraisophthalate linker

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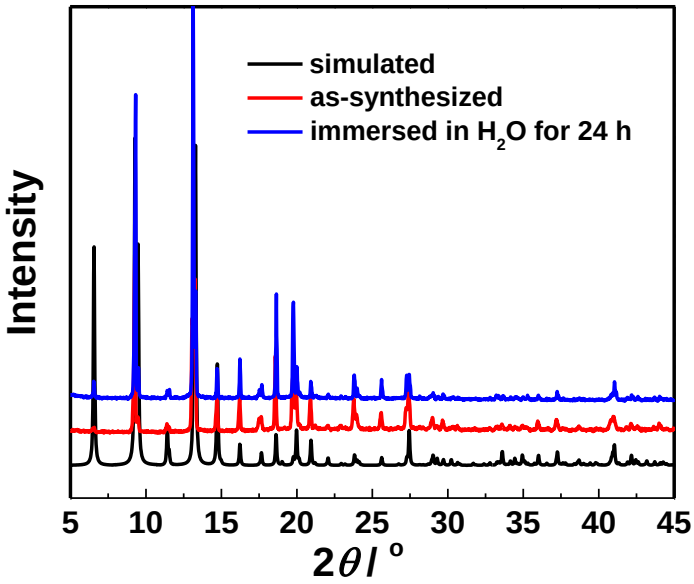


Fig. S1 PXRD patterns of **ZJNU-10**.

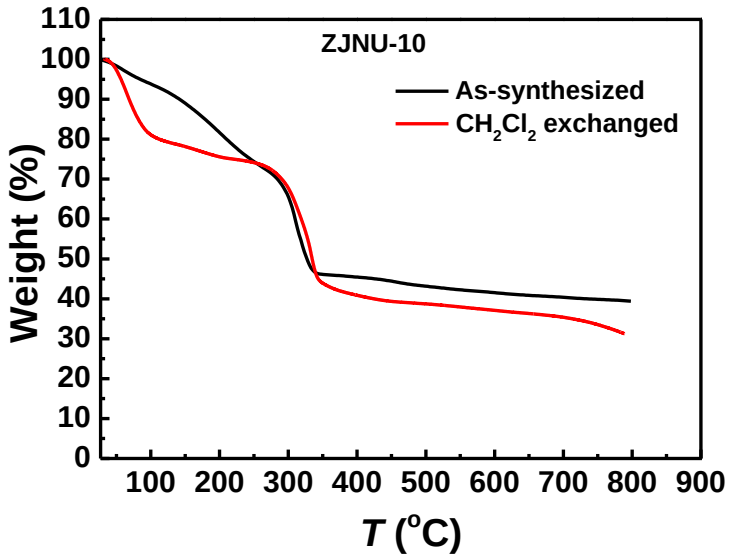


Fig. S2 TGA curves of as-synthesized and CH_2Cl_2-exchanged **ZJNU-10** under nitrogen atmosphere.

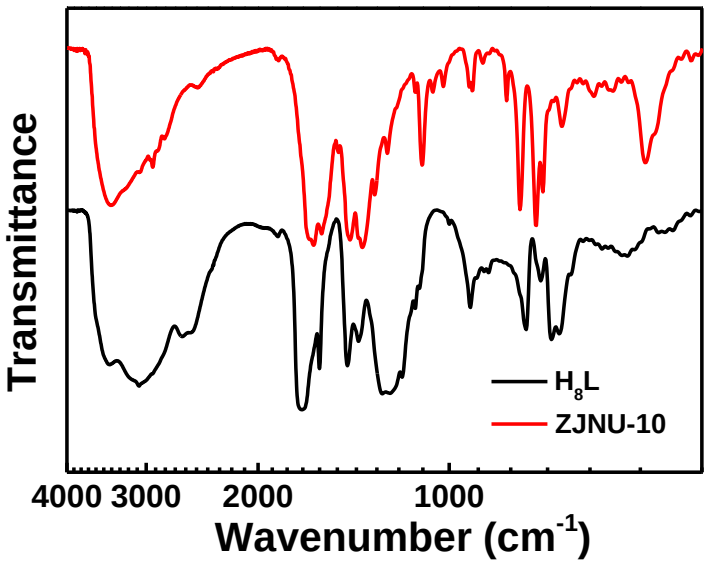
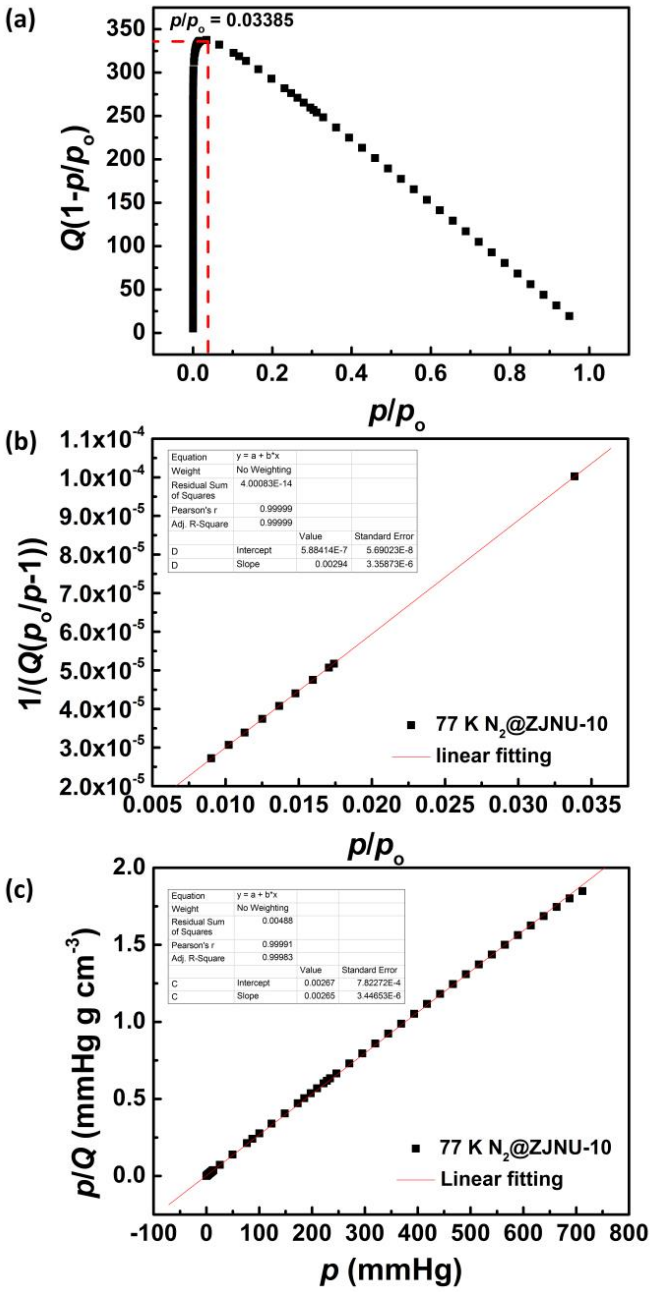


Fig. S3 Comparison of FTIR spectra of as-synthesized **ZJNU-10** (red) and its corresponding ligand H_8L (black).



S_{BET} = 1/(5.88414×10^{-7}+ 0.00294)/22414 × 6.023 × 10^{23} × 0.162 × 10^{-18} = 1480 m^2 g^{-1}

$S_{Langmuir}$ = (1/0.00265)/22414 × 6.023 × 10^{23} × 0.162 × 10^{-18} = 1643 m^2 g^{-1}

BET constant C = 1 + 0.00294/5.88414×10^{-7} = 4997

$$(p/p_o)_{n_m} = \frac{1}{\sqrt{C}+1} = 0.01395$$

Fig. S4 The consistency plot (a), BET surface area plot (b), and Langmuir surface area plot (c) for **ZJNU-10**.

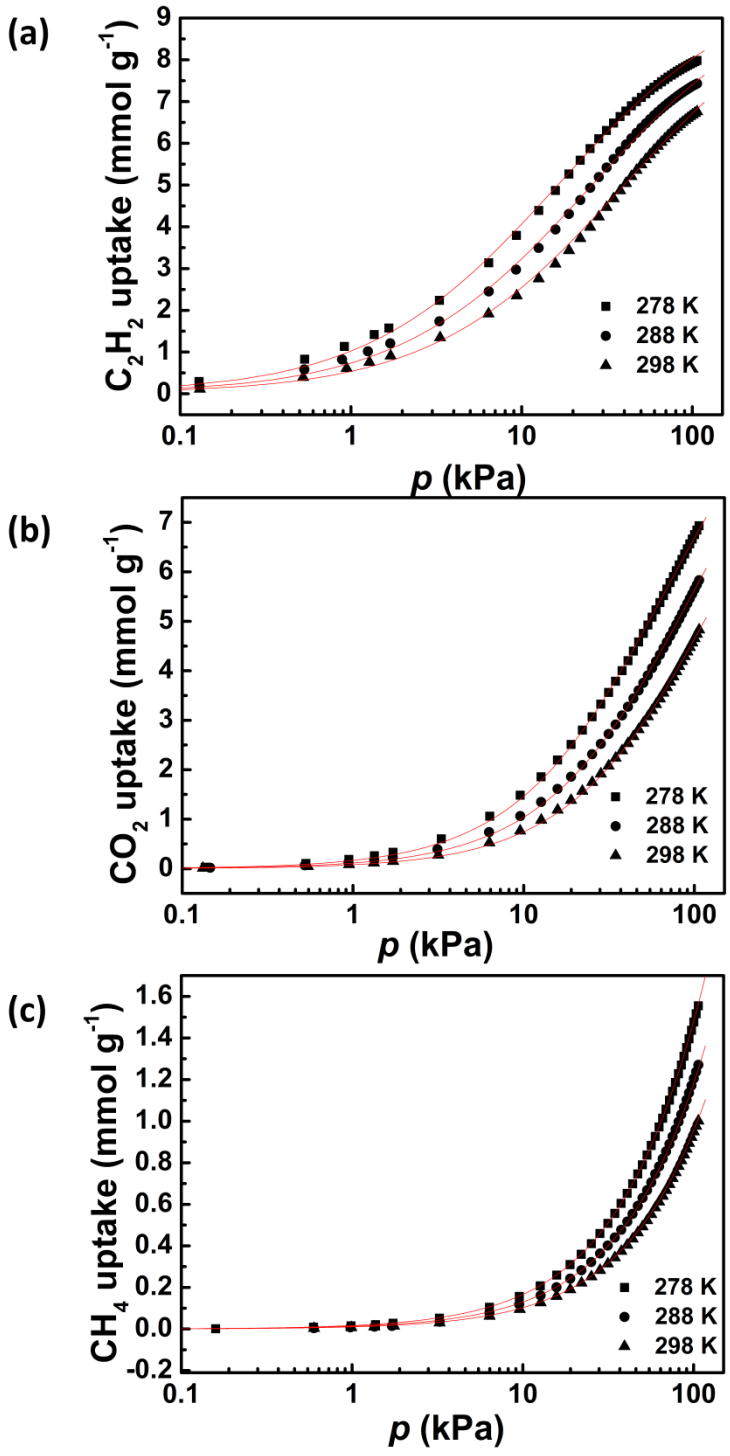
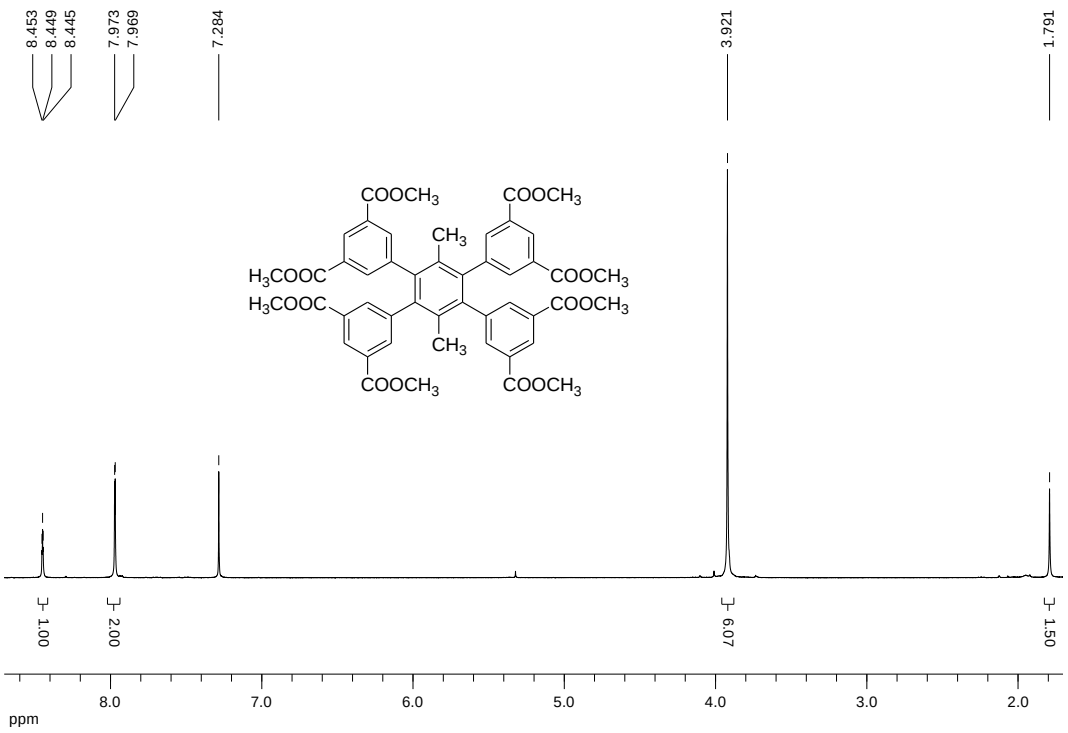
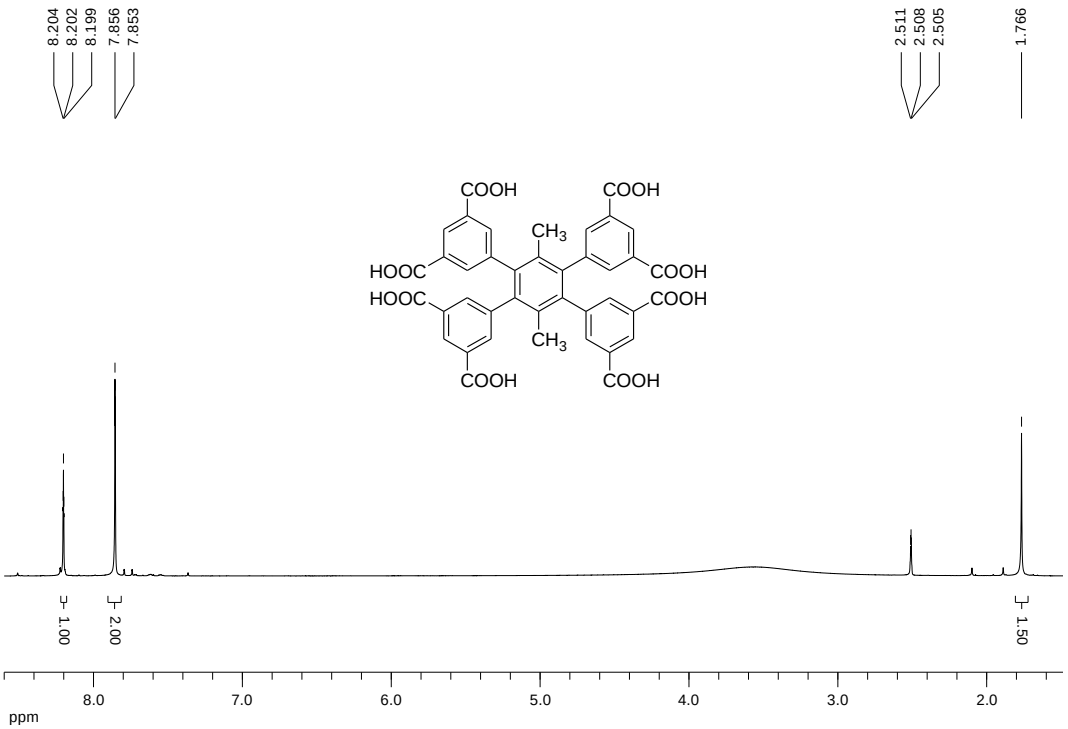


Fig. S5 Comparison of the pure-component isotherm data for (a) C_2H_2, (b) CO_2, and (c) CH_4 in **ZJNU-10** with the fitted isotherms at 278 K, 288 K, and 298 K.


8.453
8.449
8.445
7.973
7.969
7.284
3.921
1.791
COOCH3
CH3
H3COOC
1.00
2.00
6.07
1.50
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm


8.204
8.202
8.199
7.856
7.853
2.511
2.508
2.505
1.766
COOH
CH3
HOOC
1.00
2.00
1.50
8.0
7.0
6.0
5.0
4.0
3.0
2.0
ppm

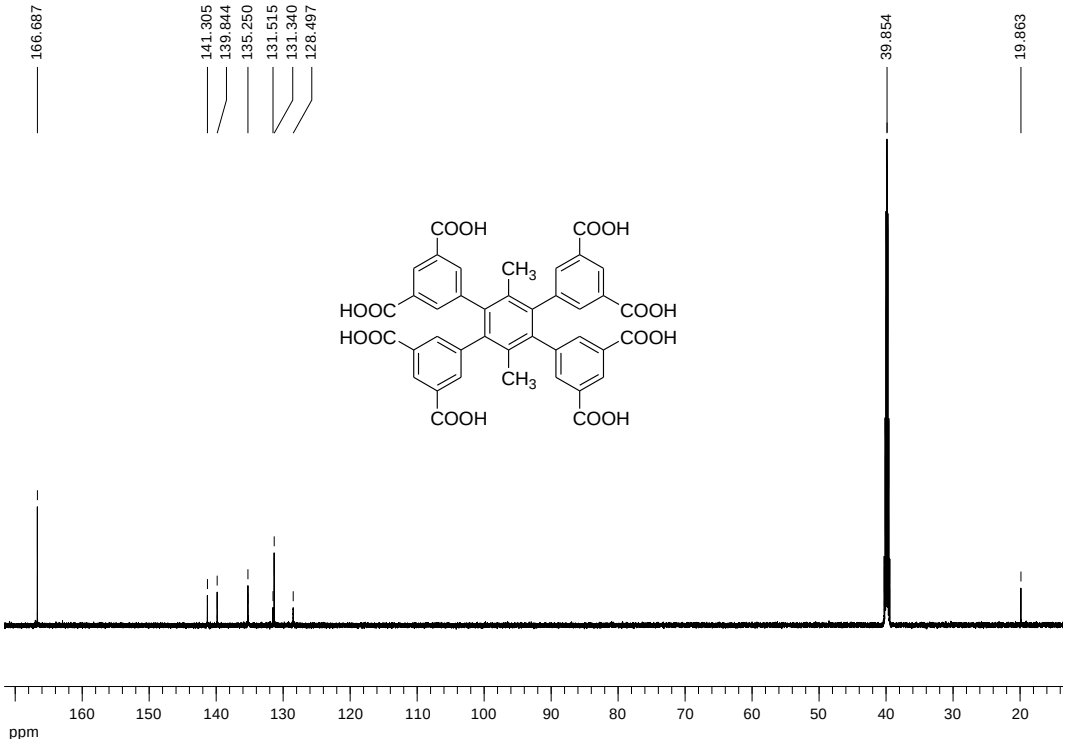


Fig. S6 ^{1}H and ^{13}C NMR spectra.

Table S1 Crystal data and structure refinement for **ZJNU-10**.

MOF	**ZJNU-10**
Empirical formula	$C_{52}H_{58}Cu_4N_4O_{26}$
Formula weight	1409.18
λ (Å)	0.71073
Crystal system	Tetragonal
Space group	*I4/mmm*
Unit cell dimensions	a = 19.0416(10) Å b = 19.0416(10) Å c = 18.6430(9) Å α = 90° β = 90° γ = 90°
V (Å^3)	6759.6(8)
Z	4
D_c (g cm^{-3})	1.385
μ (mm^{-1})	1.318
F(000)	2168
θ range for data collection (°)	2.185 to 26.371
Limiting indices	$-23 \le h \le 23$ $-15 \le k \le 21$ $-23 \le l \le 19$
Reflections collected / unique	9413 / 1979
R_{int}	0.0658
Max. and min. transmission	0.877 and 0.827
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	1979 / 37 / 86
Goodness-of-fit on F^2	1.063
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0488 wR_2 = 0.1394
R indices (all data)	R_1 = 0.0775 wR_2 = 0.1553
Largest diff. peak and hole (e·Å^{-3})	0.861 and -0.631
CCDC	1954395

Table S2 Langmuir-Freundlich parameters for adsorption of C_2H_2, CO_2, and CH_4 in **ZJNU-10**.

Adsorbate	q_{sat} (mmol g^{-1})	b_0 $(kPa)^{-v}$	E (kJ mol^{-1})	v	R^2
C_2H_2	9.96407	3.51054×10^{-6}	24.021	0.77938	0.99872
CO_2	11.08817	2.24662×10^{-7}	25.703	1	0.99971
CH_4	11.93825	9.95701×10^{-7}	16.776	1	0.99969