Electronic Supplementary Material (ESI) for Dalton Transactions.

A Metal-Organic Framework Based on a Custom-Designed Diisophthalate Ligand Exhibiting Excellent Hydrostability and Highly Selective Adsorption of C_2H_2 and CO_2 over CH_4

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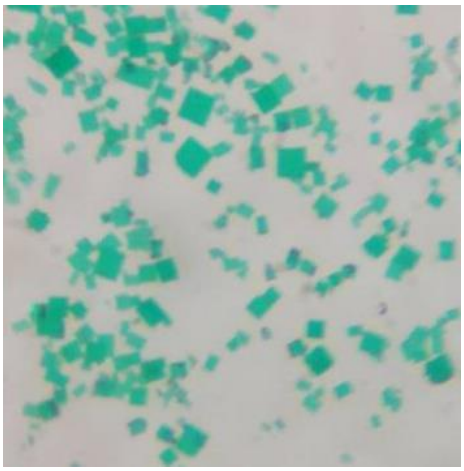


Fig. S1 The electronic photograph of the as-synthesized **ZJNU-51**.

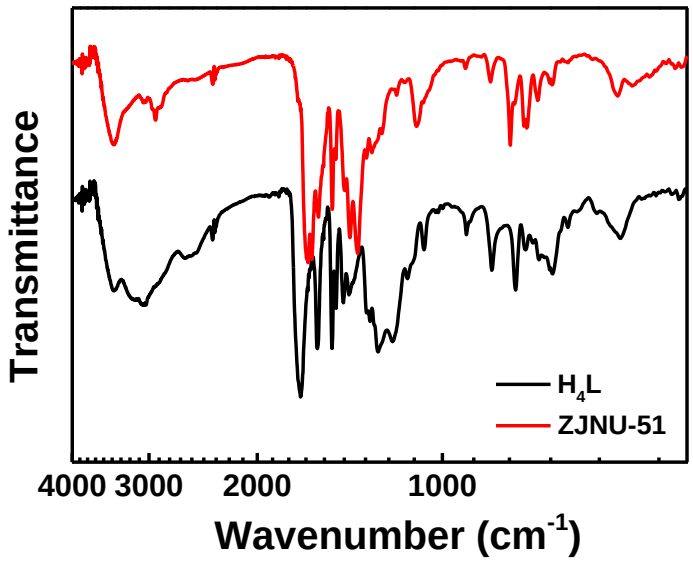


Fig. S2 FTIR spectra of the organic ligand H_4L (black) and the as-syntheiszed **ZJNU-51** (red).

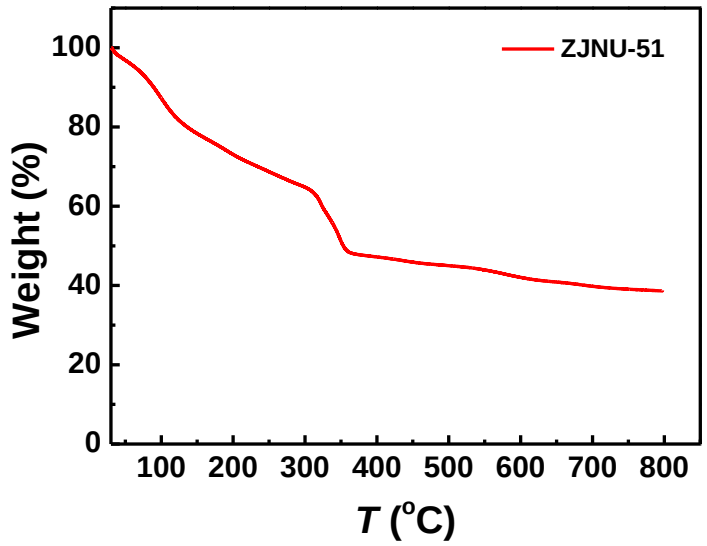


Fig. S3 TGA curve of the as-synthesized **ZJNU-51** under nitrogen atmosphere.

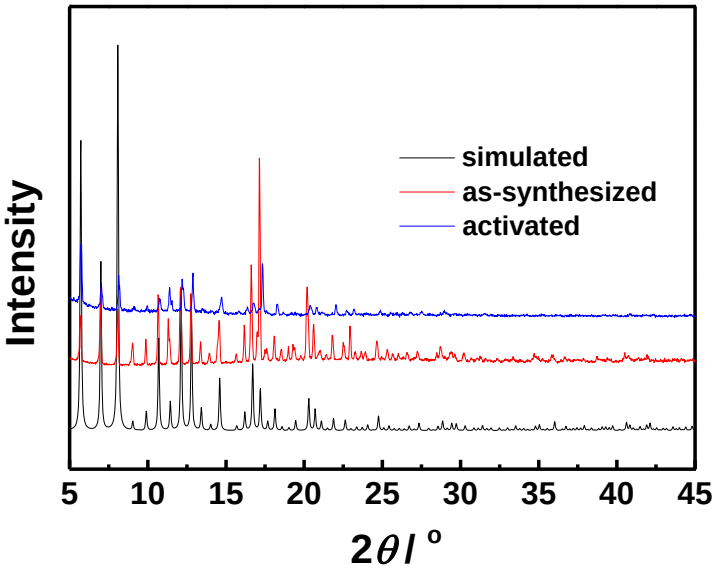
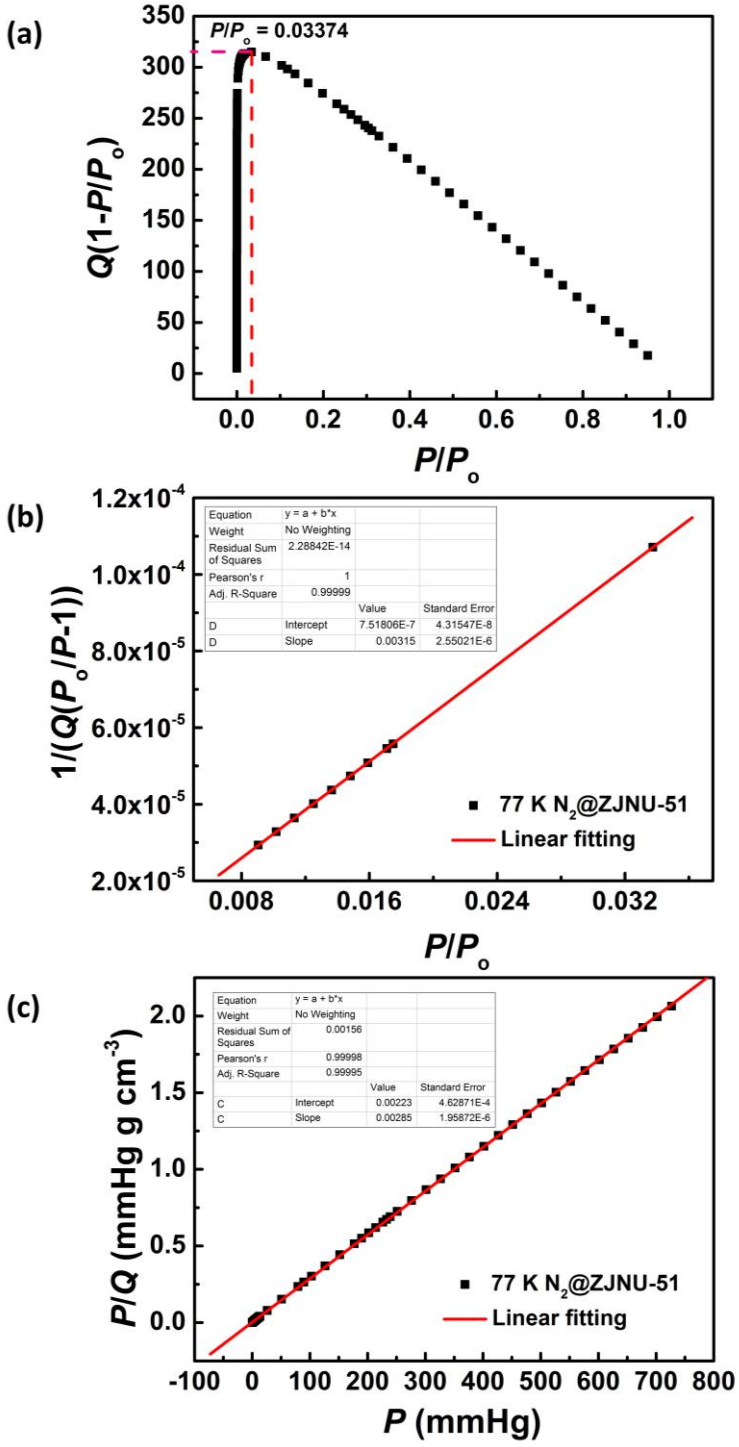


Fig. S4 The experimental and simulated PXRD patterns for **ZJNU-51**.



S_{BET} = 1/(7.51806 ×10^{-7}+ 0.00315)/22414 × 6.023 × 10^{23} × 0.162 × 10^{-18} = 1382 m^2 g^{-1}

$S_{Langmuir}$= (1/0.00285)/22414 × 6.023 × 10^{23} × 0.162 × 10^{-18} = 1527 m^2 g^{-1}

BET constant C = 1 + 0.00315/7.51806 ×10^{-7} = 4191

$$(P/P_o)_{n_m} = \frac{1}{\sqrt{C}+1} = 0.015212$$

Fig. S5 The consistency (a), BET (b), and Langmuir (c) plots for **ZJNU-51**.

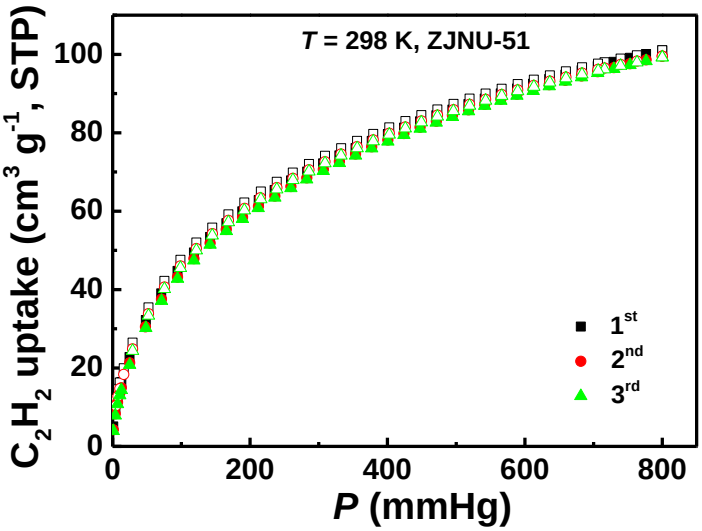


Fig. S6 Three cycles of C_2H_2 adsorption and desorption in **ZJNU-51** without reactivation between any two consecutive cycles. The solid and open symbols represent adsorption and desorption, respectively. STP = standard temperature and pressure.

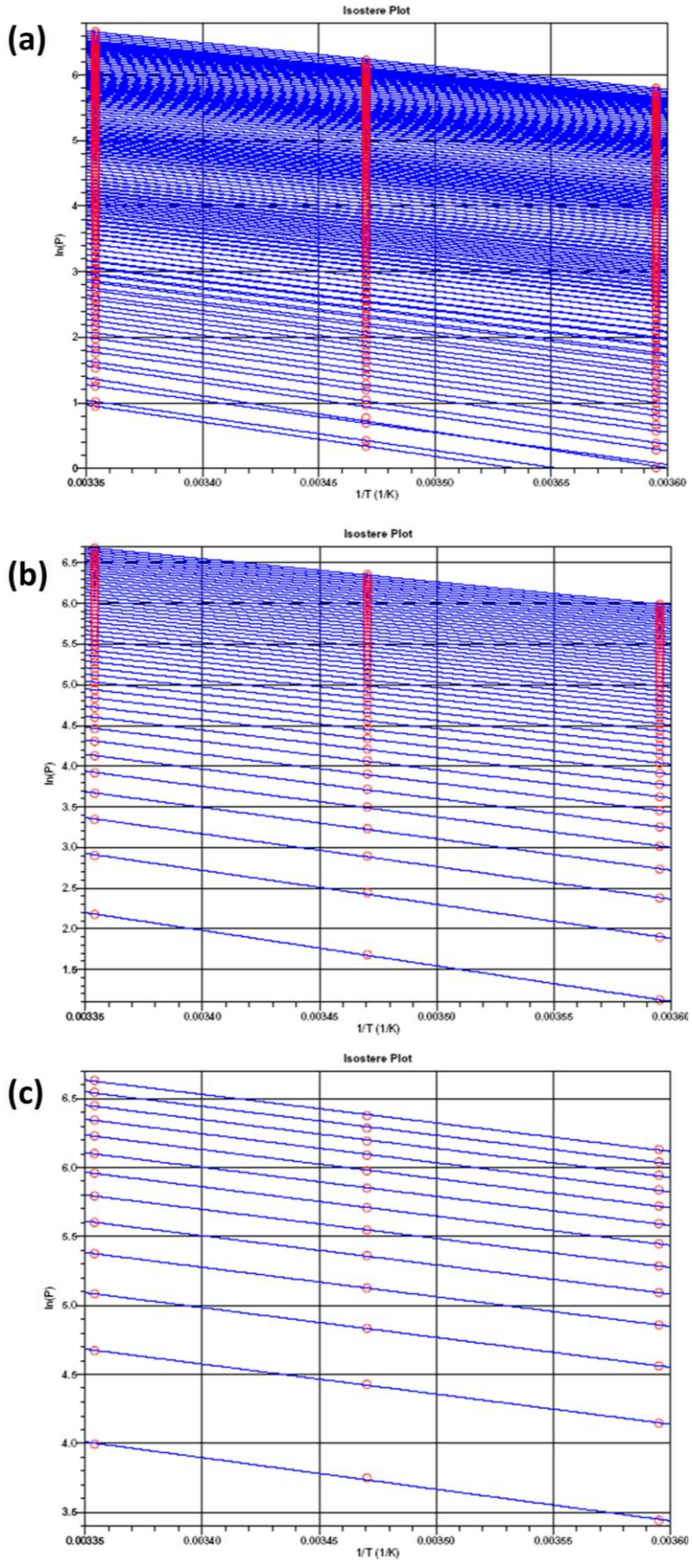


Fig. S7 Isostere plots for (a) C_2H_2, (b) CO_2, and (c) CH_4 adsorption in **ZJNU-51**.

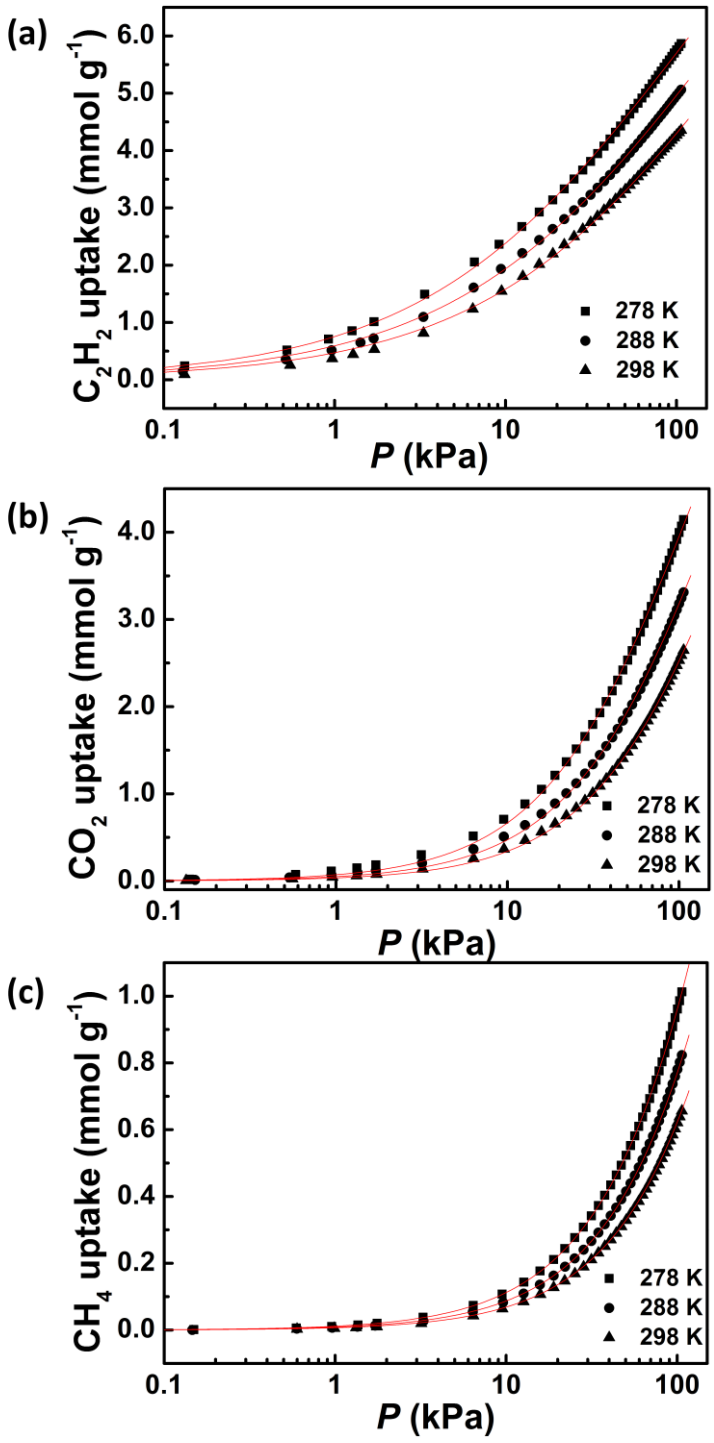


Fig. S8 Comparison of the pure-component isotherm data for (a) C_2H_2, (b) CO_2, and (c) CH_4 in **ZJNU-51** with the fitted isotherms at 278 K, 288 K and 298 K.

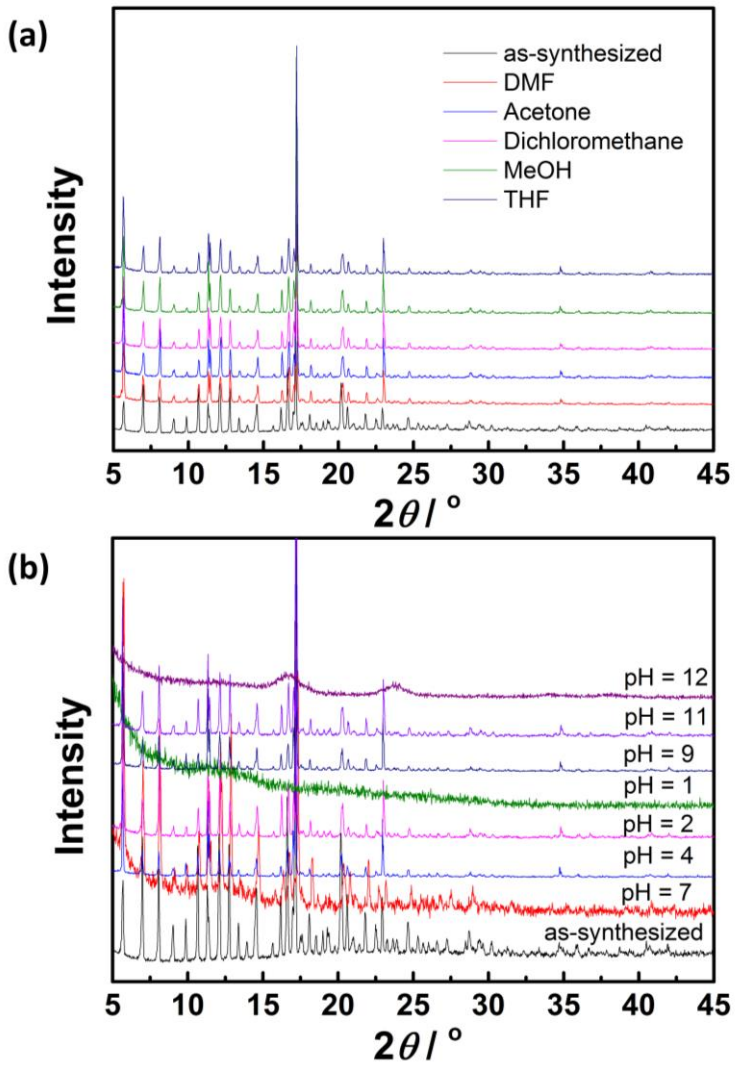


Fig. S9 PXRD patterns of **ZJNU-51** after immersion in (a) various organic solvents and (b) aqueous HCl/NaOH solutions for 36 h at room temperature.

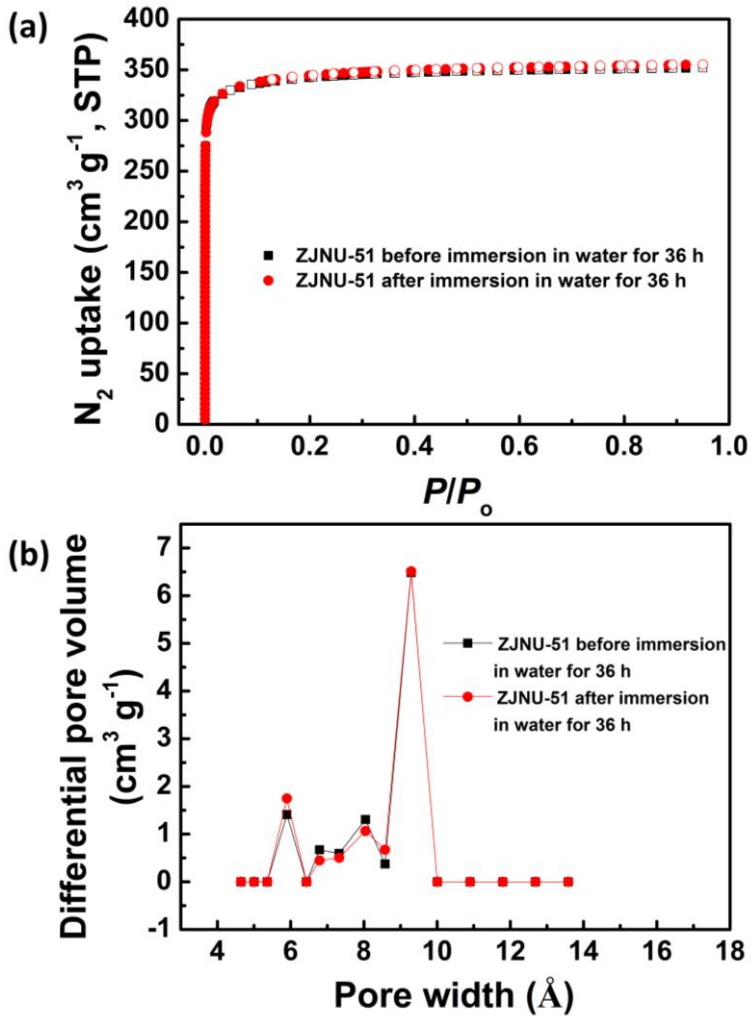
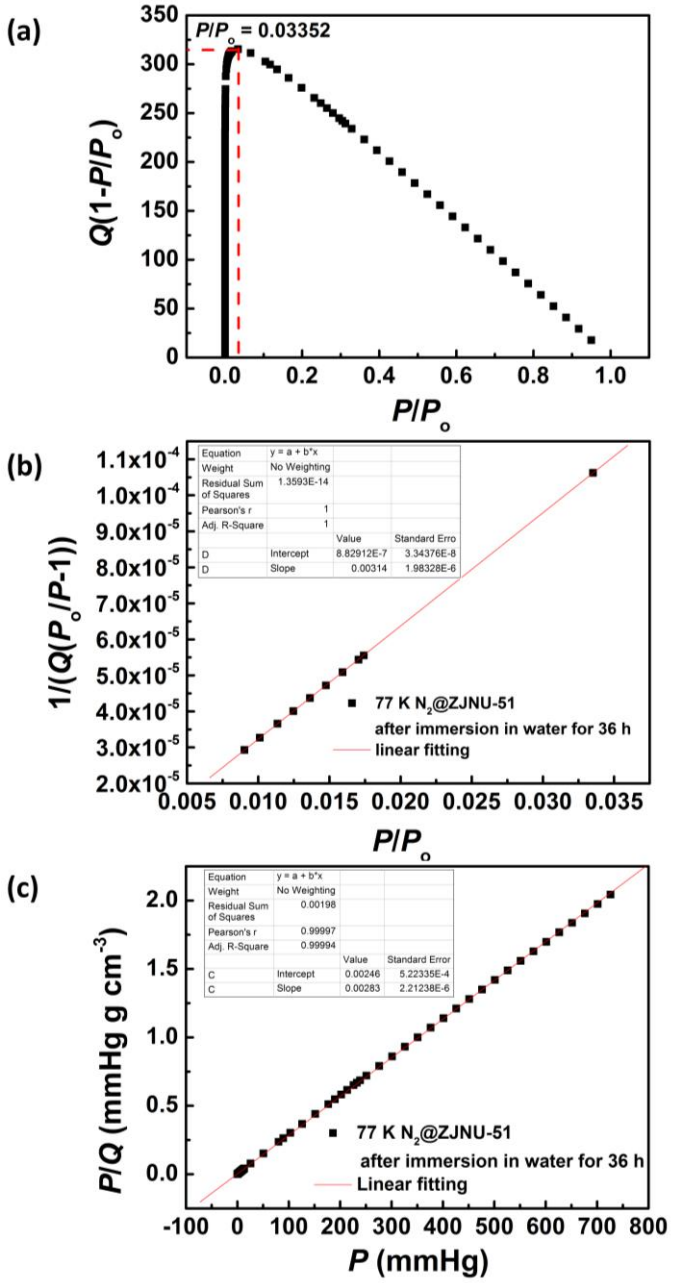


Fig. S10 Comparison of (a) N_2 adsorption-desorption isotherms at 77 K, and (b) DFT pore size distribution of **ZJNU-51** before and after immersion in water for 36 h. The solid and open symbols represent adsorption and desorption, respectively. STP = standard temperature and pressure.



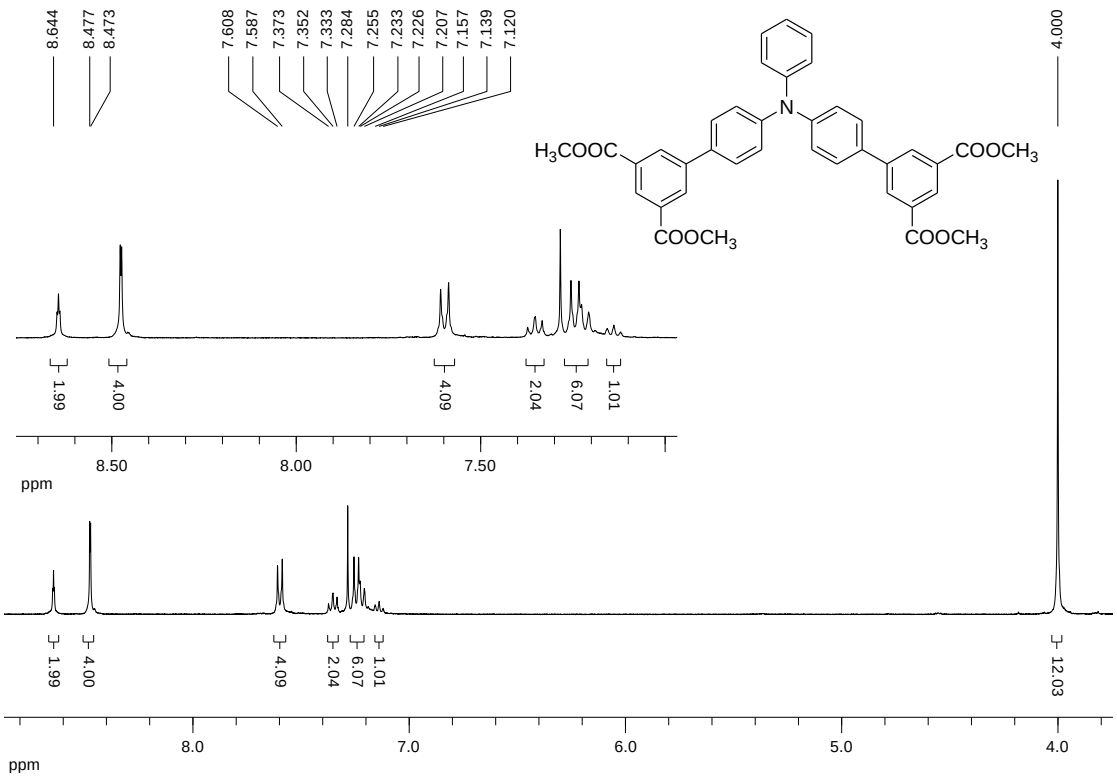
S_{BET} = 1/(8.82912 ×10^{-7}+ 0.00314)/22414 × 6.023 × 10^{23} × 0.162 × 10^{-18} = 1386 m^2 g^{-1}

$S_{Langmuir}$= (1/0.00283)/22414 × 6.023 × 10^{23} × 0.162 × 10^{-18} = 1538 m^2 g^{-1}

BET constant C = 1 + 0.00314/8.82912 ×10^{-7} = 3557

$$(P/P_o)_{n_m} = \frac{1}{\sqrt{C}+1} = 0.01649$$

Fig. S11 The consistency (a), BET (b), and Langmuir (c) plots for **ZJNU-51** after immersion in water for 36 h.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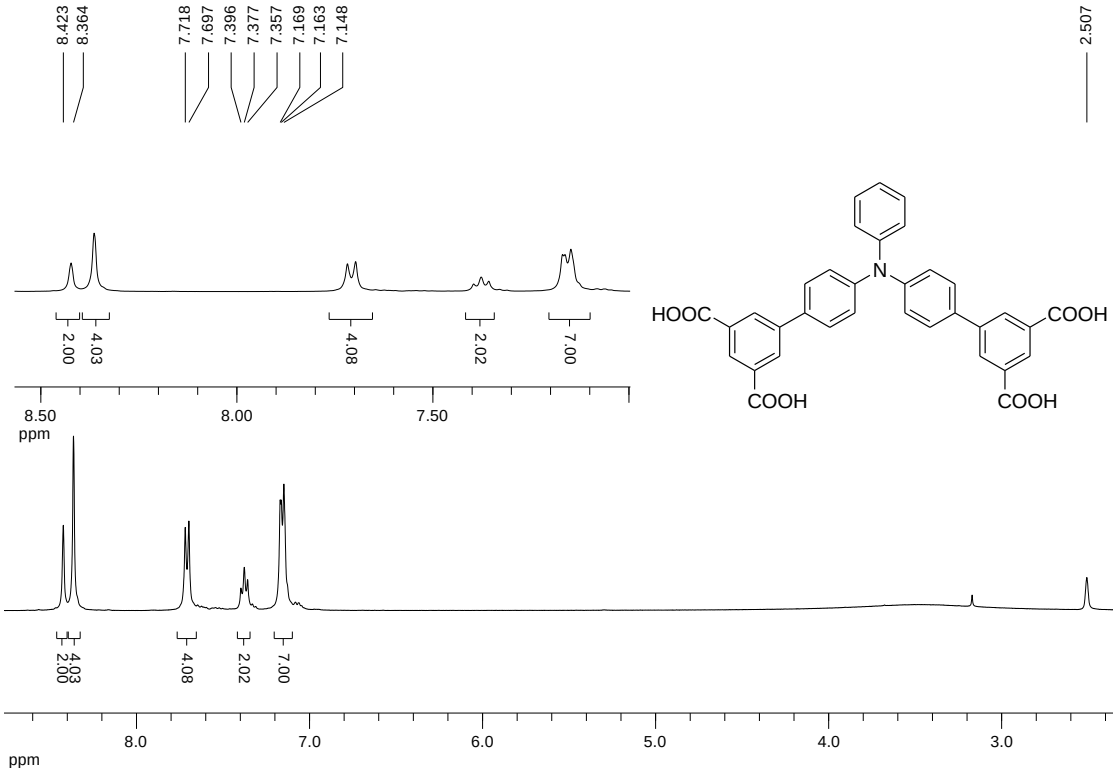
8.477
8.473
7.608
7.587
7.373
7.352
7.333
7.284
7.255
7.233
7.226
7.207
7.157
7.139
7.120
4.000
H3COOC
COOCH3
COOCH3
COOCH3
1.99
4.00
4.09
2.04
6.07
1.01
8.50
8.00
7.50
ppm
1.99
4.00
4.09
2.04
6.07
1.01
12.03
8.0
7.0
6.0
5.0
4.0
ppm


8.423
8.364
7.718
7.697
7.396
7.377
7.357
7.169
7.163
7.148
2.507
HOOC
COOH
COOH
COOH
2.00
4.03
4.08
2.02
7.00
8.50
8.00
7.50
ppm
2.00
4.03
4.08
2.02
7.00
8.0
7.0
6.0
5.0
4.0
3.0
ppm

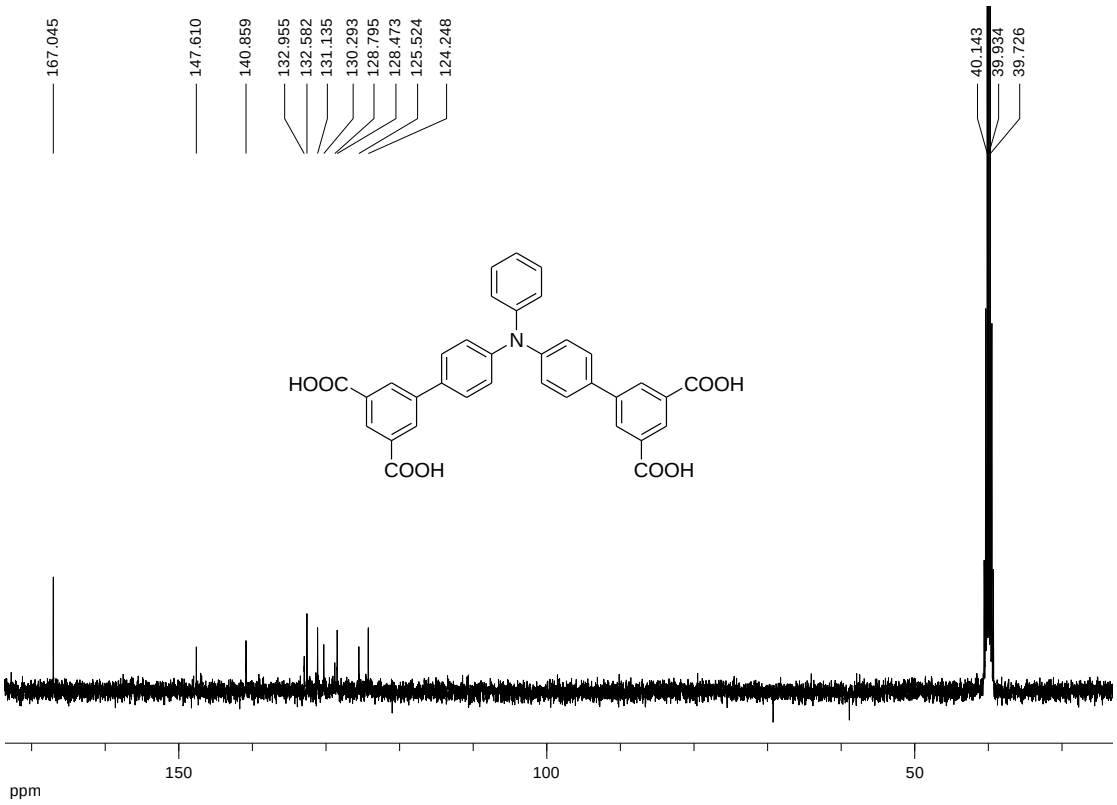


Fig. S12 ^{1}H and ^{13}C NMR spectra.

Table S1 Langmuir-Freundlich parameters for adsorption of C_2H_2, CO_2, and CH_4 in **ZJNU-51**.

	q_{sat} (mmol g^{-1})	b_0 $(kPa)^{-v}$	E (kJ mol^{-1})	v
C_2H_2	11.71149	4.46904×10^{-5}	16.963	0.56974
CO_2	8.70408	2.08651×10^{-7}	24.477	1
CH_4	5.97166	1.14047×10^{-6}	17.163	1

Table S2 Crystal data and structure refinement for **ZJNU-51**.

MOFs	**ZJNU-51**
Empirical formula	$C_{102}H_{69}N_3O_{30}Cu_6$
Formula weight	2197.84
λ (Å)	0.71073
Crystal system	Cubic
Space group	*I*4/m
Unit cell dimensions	a = 30.9140(7) Å b = 30.9140(7) Å c = 30.914 Å $\alpha = 90^o$ $\beta = 90^o$ $\gamma = 90^o$
V (Å^3)	29543.7(9)
Z	8
D_c (g cm^{-3})	0.988
μ (mm^{-1})	0.903
F(000)	8928
θ range for data collection (^{o})	2.083 to 27.282
Limiting indices	$-24 \le h \le 39$ $-35 \le k \le 39$ $-39 \le l \le 39$
Reflections collected / unique	64382 / 16780
R_{int}	0.0835
Max. and min. transmission	0.9232 and 0.8765
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	16780 / 781 / 732
Goodness-of-fit on F^2	1.096
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.1355 wR_2 = 0.3432
R indices (all data)	R_1 = 0.1658 wR_2 = 0.3786
Largest diff. peak and hole (e·Å^{-3})	1.978 and -1.318
CCDC	1826762