Electronic Supplementary Material (ESI) for CrystEngComm.

A NbO-type MOF based on an aromatic-rich and N-functionalized diisophthalate ligand for high-performance acetylene storage and purification

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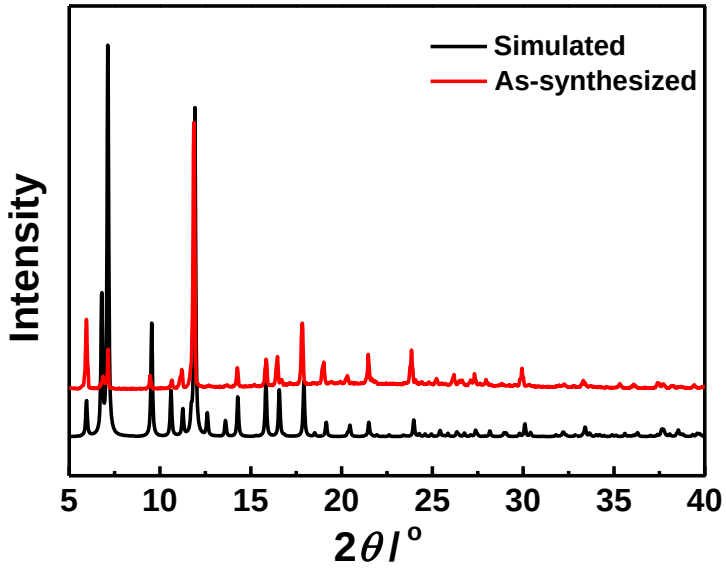


Fig. S1 Comparison of the simulated (black) and experimental (red) PXRD patterns of **ZJNU-93**.

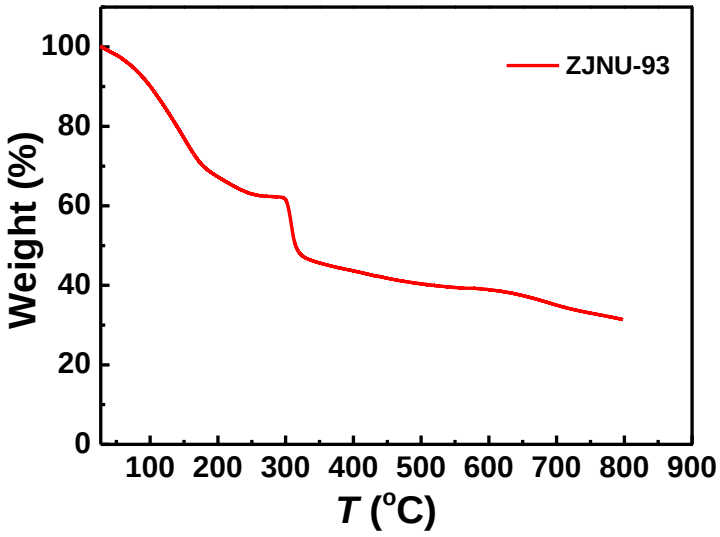


Fig. S2 TGA curve of **ZJNU-93** under nitrogen atmosphere.

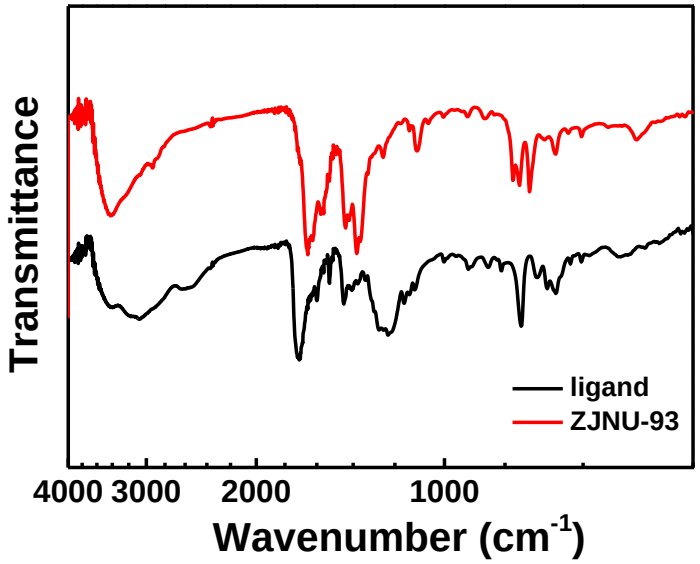
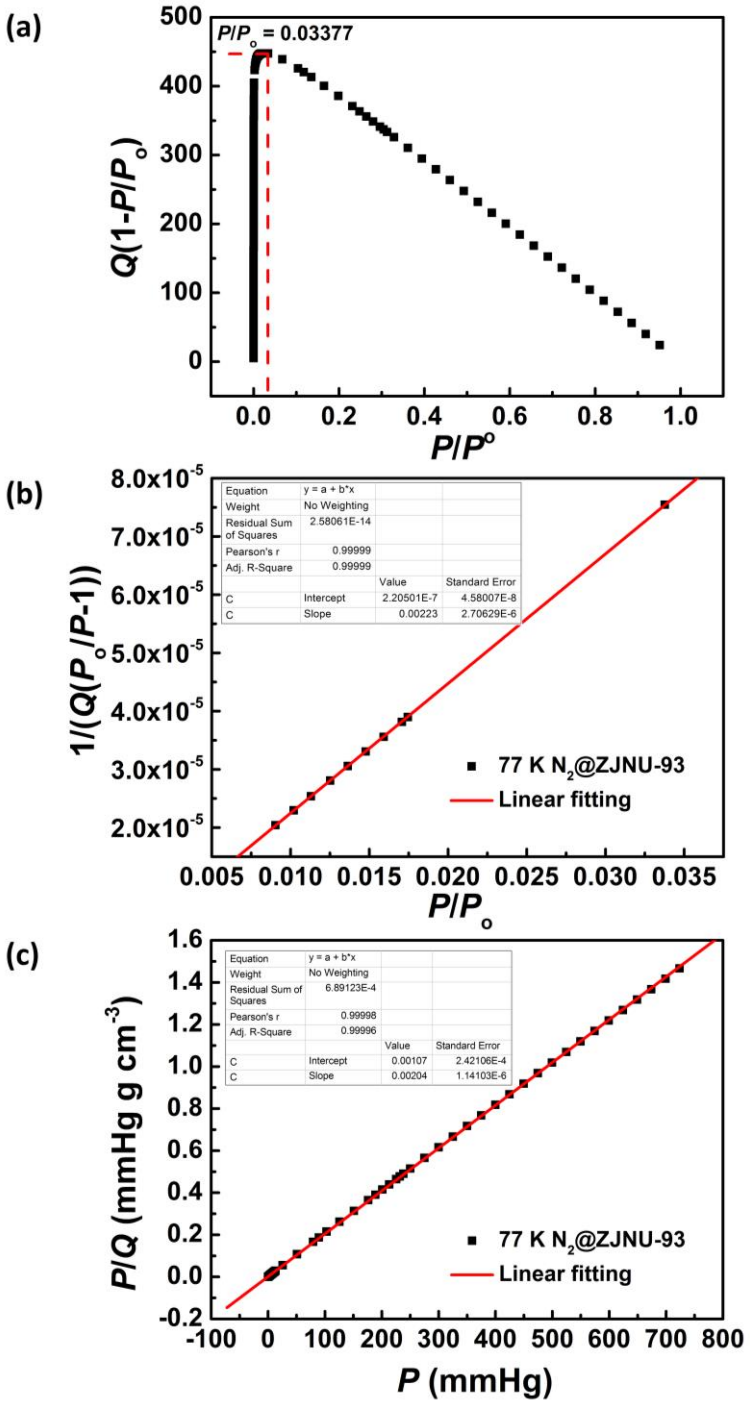


Fig. S3 Comparison of FTIR spectra of **ZJNU-93** and its organic ligand.



S_{BET} = 1/(2.20501 ×10^{-7}+ 0.00223)/22414 × 6.023 × 10^{23} × 0.162 × 10^{-18} = 1952 m^2 g^{-1}

$S_{Langmuir}$= (1/0.00204)/22414 × 6.023 × 10^{23} × 0.162 × 10^{-18} = 2134 m^2 g^{-1}

BET constant C = 1 + 0.00223/2.20501 ×10^{-7} = 10114

$$(p/p_o)_{n_m} = \frac{1}{\sqrt{C}+1} = 0.009845$$

Fig. S4 The consistency (a), BET (b), and Langmuir (c) plots for **ZJNU-93a**.

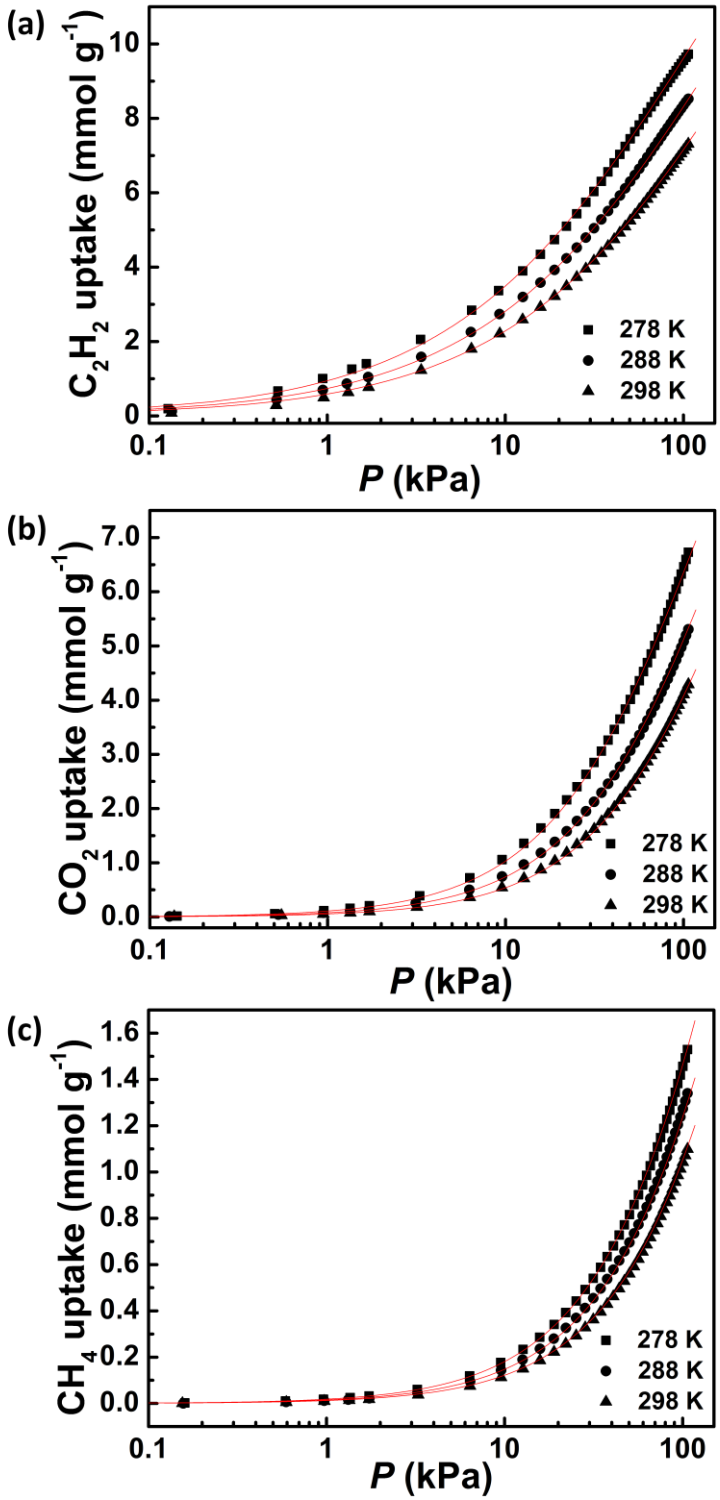
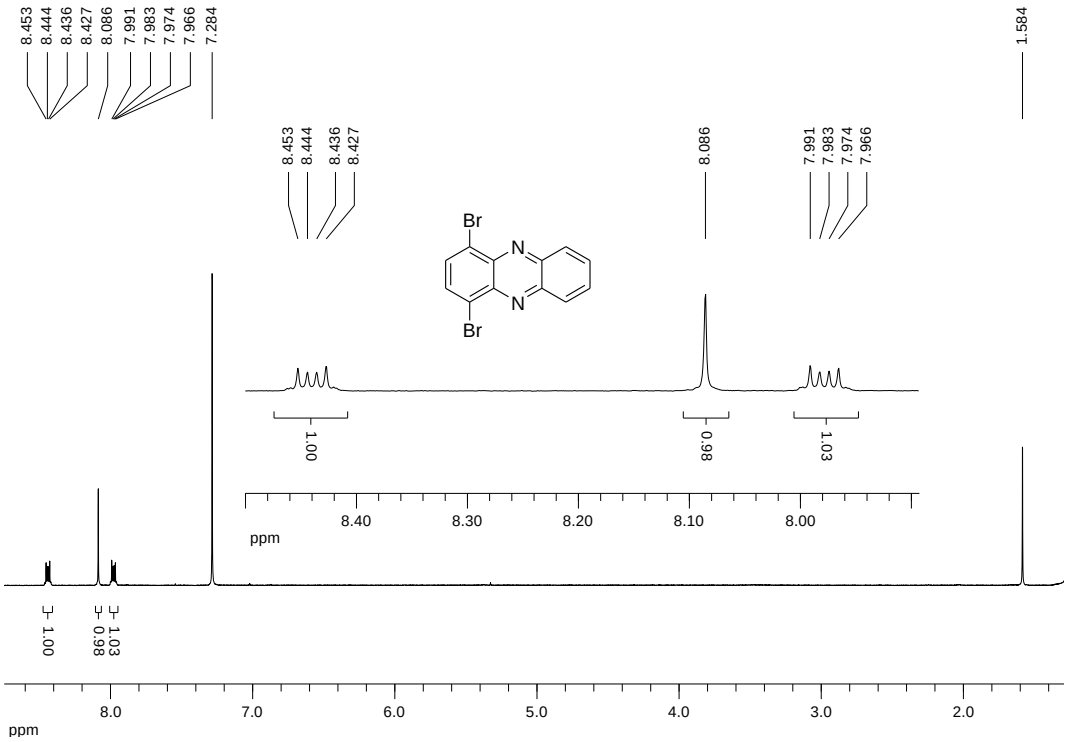
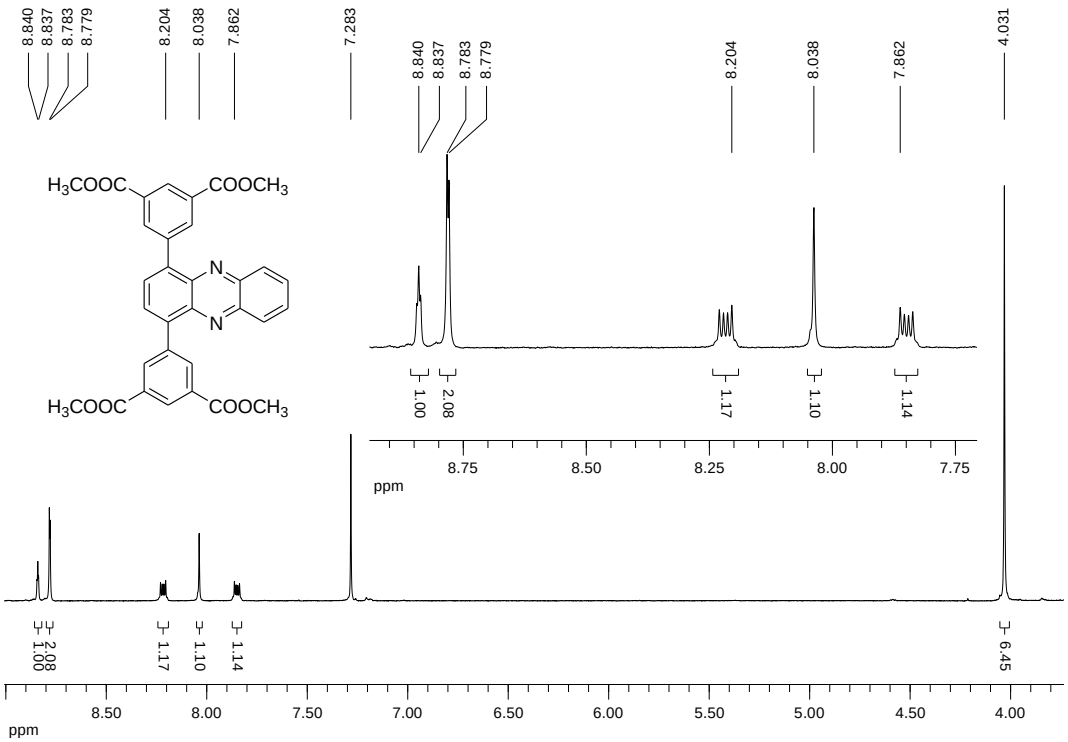


Fig. S5 Comparison of the pure-component isotherm data for (a) C_2H_2, (b) CO_2, and (c) CH_4 in **ZJNU-93a** with the fitted isotherms at 278 K, 288 K, and 298 K.


8.453
8.444
8.436
8.427
8.086
7.991
7.983
7.974
7.966
7.284
1.584
Br
N
N
Br
1.00
0.98
1.03
ppm
8.0
7.0
6.0
5.0
4.0
3.0
2.0


8.840
8.837
8.783
8.779
8.204
8.038
7.862
7.283
4.031
H3COOC
COOCH3
N
N
H3COOC
COOCH3
1.00
2.08
1.17
1.10
1.14
6.45
ppm
8.50
8.00
7.50
7.00
6.50
6.00
5.50
5.00
4.50
4.00

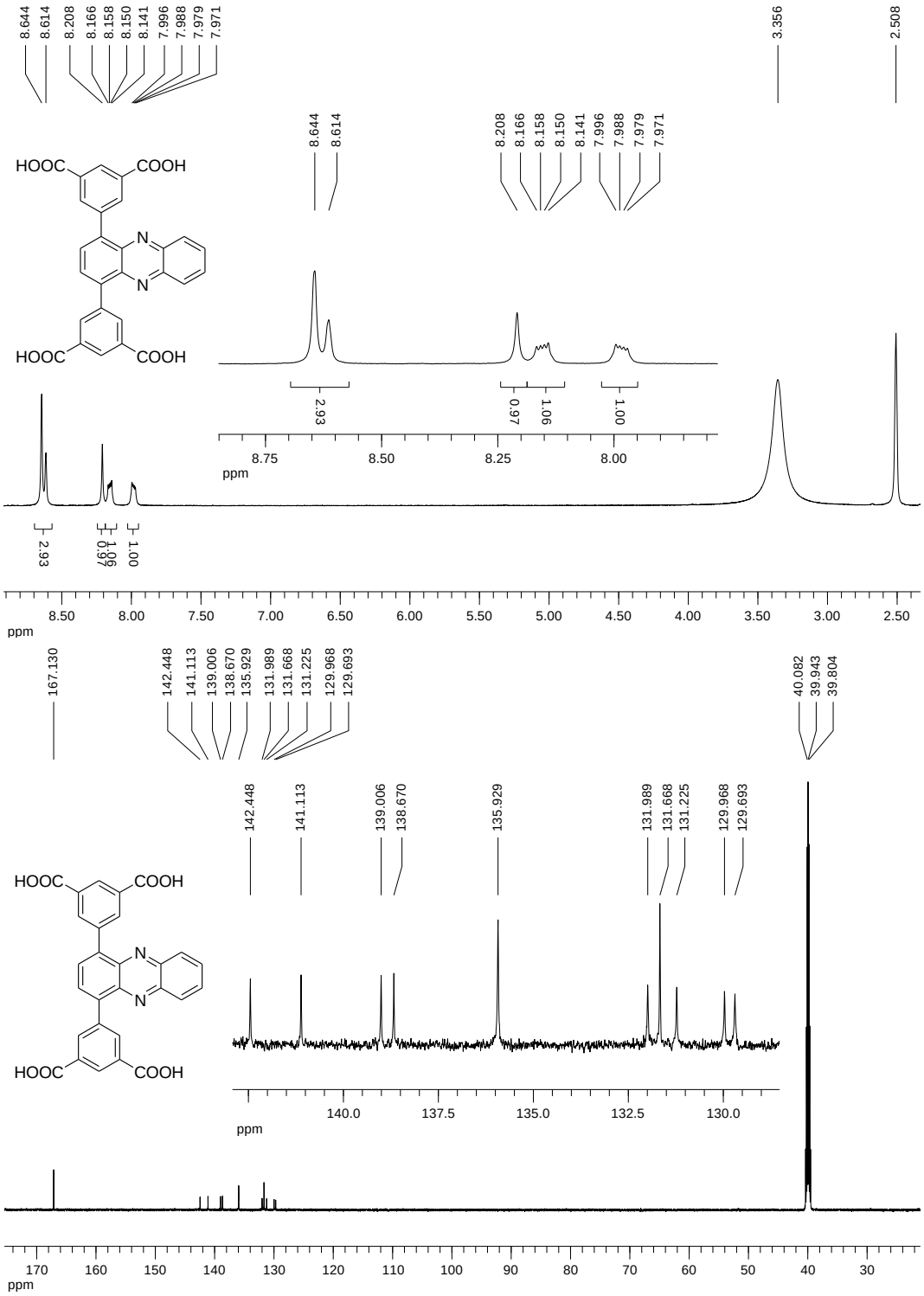


Fig. S6 ^{1}H and ^{13}C NMR spectra.

Table S1 Crystal data and structure refinement for **ZJNU-93**.

MOF	**ZJNU-93**
Empirical formula	$C_{28}H_{16}Cu_2N_2O_{10}$
Formula weight	667.51
λ (Å)	1.54178
Crystal system	Trigonal
Space group	*R-3m*
Unit cell dimensions	a = 18.5209(3) Å b = 18.5209(3) Å c = 39.0171(9) Å α = 90° β = 90° γ = 120°
V (Å^3)	11590.7(4)
Z	9
D_c (g cm^{-3})	0.861
μ (mm^{-1})	1.309
F(000)	3024
Crystal size (mm)	0.23 × 0.14 × 0.10
θ range for data collection (°)	5.31 to 73.86
Limiting indices	$-19 \le h \le 0$ $-19 \le k \le 0$ $-48 \le l \le 0$
Reflections collected / unique	2829 / 2829
R_{int}	0.0000
Max. and min. transmission	0.8803 and 0.7528
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	2829 / 192 / 178
Goodness-of-fit on F^2	1.015
Final R indices [$I > 2\sigma(I)$]	R_1 = 0.0480 wR_2 = 0.1413
R indices (all data)	R_1 = 0.0613, wR_2 = 0.1522
Largest diff. peak and hole (e·Å^{-3})	0.811 and -0.379
CCDC	1866277

Table S2 Langmuir-Freundich parameters for adsorption of C_2H_2, CO_2, and CH_4 in **ZJNU-93a**.

Guest	q_{sat} (mmol g^{-1})	b_0 $(kPa)^{-v}$	E (kJ mol^{-1})	v
C_2H_2	21.01408	3.13696×10^{-5}	16.903	0.62671
CO_2	14.9045	2.97705×10^{-7}	23.401	1
CH_4	6.85084	6.693×10^{-6}	13.878	1