Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

A new microporous metal-organic framework with open metal sites and exposed carboxylic acid groups for selective separation of CO_2/CH_4 and C_2H_2/CH_4

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Table S1. Equation parameters for the DSLF isotherm model.

Adsorbates	N_1^{max} (mmol/g)	b_1 (kPa^{-1})	n_1	N_2^{max} (mmol/g)	b_2 (kPa^{-1})	n_2
C_2H_2(273 K)	1.3482	0.00288	1.05418	11.52941	0.06215	1.33581
CH_4 (273 K)	4.2875	0.00293	0.00293	1.26519	0.00125	1.03086
CO_2(273 K)	12.84527	0.00284	1.05839	10.42661	0.00935	1.14162
C_2H_2(298 K)	4.95847	0.00289	0.99848	8.1522	0.05423	1.11579
CH_4 (298 K)	2.90927	0.00281	0.93687	3.74395	0.00067397	0.98588
CO_2(298 K)	10.11099	0.00331	1.03233	7.37523	0.00627	1.32127

Table1 S2. Crystallographic Data Collection and Refinement Results for **ZJU-72.**

	ZJU-72
Chemical formla	$C_{69}H_{27}Cu_6O_{36}$
Formula weight	1813.14
Temperature(K)	296(2)
Wavelength(Å)	0.71073
Crystal system	Orthorhombic
Space group	C mcm
a(Å)	24.8419 (17)
b(Å)	33.5320 (17)
c(Å)	18.7099(16)
V($Å^3$)	15579.0(19)
Z	4
Density(calculated g/cm^3)	0.773
Absorbance coefficient(mm^{-1})	0.849
F(000)	3612
Crystal size(mm^3)	0.22X0.27X0.20
Goodness of fit on F^2	0.809
R_1,wR_2[$I>2\sigma(I)$]	0.0587, 0.1512
R_1,wR_2(all data)	0.1459, 0.1725
Largest difference peak and hole($e/Å^3$)	0.812, -0.324

Table S3. IAST selectivities of C_2H_2/CH_4 (C_2H_2/CH_4 = 50:50) and CO_2/CH_4 (CO_2/CH_4 = 50:50)

mixture	Temperature (K)	component proportion	IAST selectivity
C_2H_2/CH_4	273	50:50	36.3
CO_2/CH_4	273	50:50	8.2
C_2H_2/CH_4	298	50:50	39.7
CO_2/CH_4	298	50:50	6.8

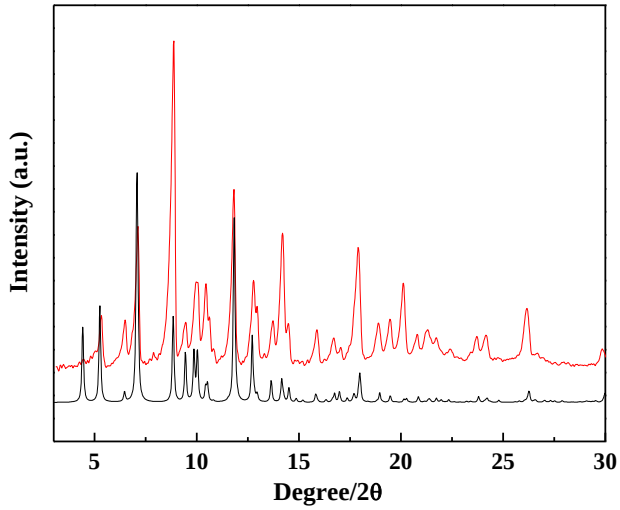

Fig. S1. PXRD patterns of as-synthesized MOF **ZJU-72** (red) and the simulated from single crystal structure (black).

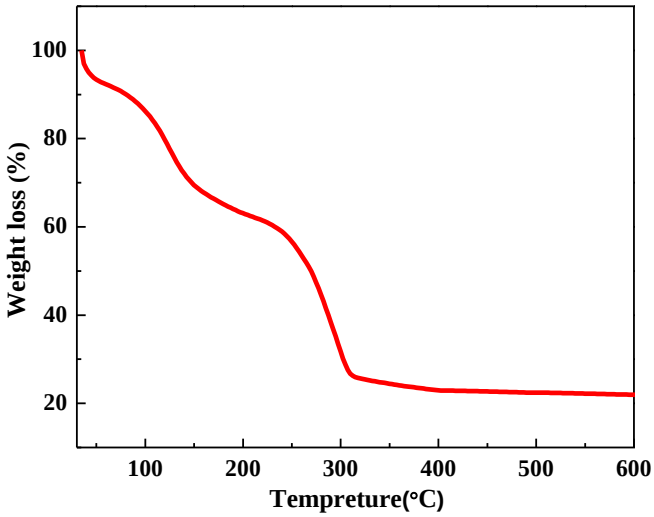

Fig. S2. TGA curves of as-synthesized **ZJU-72.**

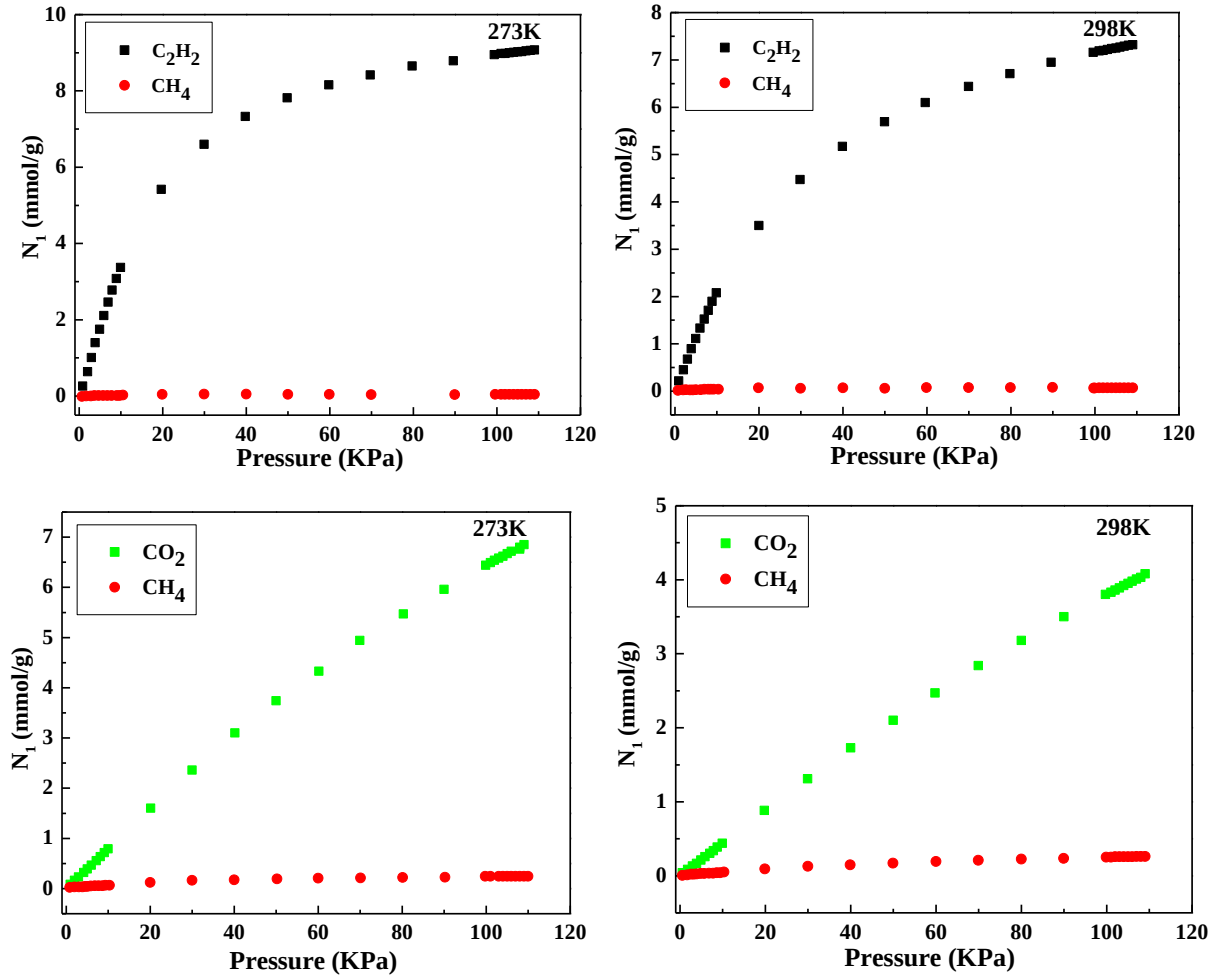

Fig. S3. Mixture adsorption isotherms predicted by IAST of **ZJU-72a** for C_2H_2/CH_4=50/50 and CO_2/CH_4=50/50 at 273 and 298 K, respectively.