# Supporting Information

## A NbO Type Microporous Metal-Organic Frameworks Constructed from Naphthalene Derived Ligand for $CH_4$ and $C_2H_2$ storage at Room Temperature

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**Table S1**. Crystallographic Data Collection and Refinement Results for **ZJU-7**

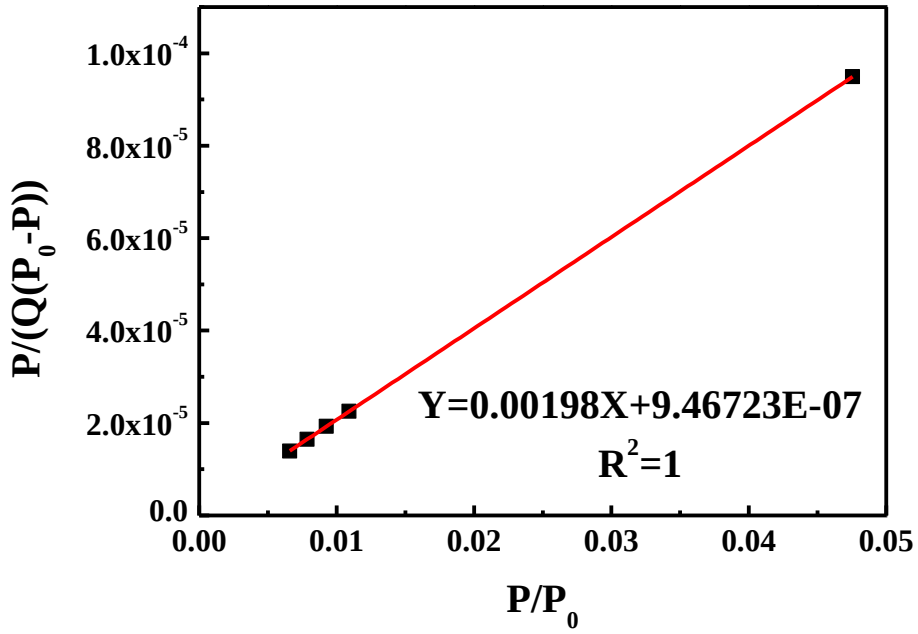
| | **ZJU-7** |
|---|---|
| Overall chemical formula | $C_{36}H_{44}Cu_2N_4O_{16}$ $[Cu_2(C_{26}H_{12}O_8)(H_2O)_2](DMF)_2(MeCN)_2(H_2O)_4$ |
| Overall formula weight | 915.83 |
| Framework chemical formula | $C_{26}H_{16}\,Cu_2O_{10}$ |
| Framework formula weight | 613.48 |
| Temperature(K) | 293(2) |
| Wavelength(Å) | 1.54178 |
| Crystal system | Trigonal |
| Space group | R-3m |
| *a*(Å) | 18.6843(7) |
| *b*(Å) | 18.6843(7) |
| *c*(Å) | 38.6052(12) |
| *V*(Å$^3$) | 11671.6(7) |
| Z | 9 |
| Density (calculated g/cm$^3$) | 1.173 |
| Absorbance coefficient(mm$^{-1}$) | 0.848 |
| No. of reflections measured | 39425 |
| No. of independent reflections | 2626 |
| *F*(000) | 4266 |
| Crystal size(mm$^3$) | 0.46×0.43×0.26 |
| R(int) | 0.0489 |
| Goodness of fit on $F_2$ | 1.057 |
| R1,wR2[$I$>2σ($I$)][a] | 0.0489, 0.0446 |
| R1,wR2(all data)[a] | 0.1380, 0.0586 |
| Largest difference peak and hole(e/Å$^3$) | 0.897,-0.381 |

[a] $\mathbf{R1} = \sum(|\mathbf{F_o}| - |\mathbf{F_c}|)/\sum|\mathbf{F_o}|\,;\ \mathbf{wR2} = \left[\frac{\sum \mathbf{w}(|\mathbf{F_o}|-|\mathbf{F_C}|^2)}{\sum \mathbf{wF_o^2}}\right]^{1/2}$

**Table S2**. $C_2H_2$ adsorption on various porous MOFs at room temperature and atmospheric pressure.

| Material | $S_{BET}$ [$m^2g^{-1}$] | $V_p$ [a] [$cm^3g^{-1}$] | $D_c$ [b] [g $cm^{-3}$] | $C_2H_2$ uptaked [$cm^3g^{-1}$]( [$cm^3cm^{-1}$]) | Ref. |
|---|---|---|---|---|---|
| **ZJU-7a** | 2198 | 0.8945 | 0.750 | 180 (135) | This work |
| ZJU-5a | 2823 | 1.074 | 0.679 | 193 (131) | S1 |
| MOF-505 | 1139 | 0.67 | 0.767 | 148 (137) | S2 |
| PCN-16 | 2273 | 1.06 | 0.724 | 176 (126) | S3 |
| NOTT-101 | 2805 | 1.080 | 0.6838 | 184 (126) | S4 |
| CoMOF-74 | 1018 | - | 1.169 | 197 (230) | S5 |
| MnMOF-74 | 695 | - | 1.085 | 168 (182) | S5 |
| MgMOF-74 | 927 | - | 0.909 | 184 (167) | S5 |
| ZnMOF-74 | 747 | - | 1.231 | 122 (150) | S5 |
| FeMOF-74 | 1350 | - | 1.126 | 156 (176) | S6 |
| HKUST-1 | 1401 | 0.76 | 0.879 | 201 (177) | S1 |

[a] Pore volume. [b] Crystal density calculated from the single-crystal structure without molecules and terminal ligands. [c]




$$S_{BET}= 1/( 0.00198+ 9.46723E-07)/22414\times6.023\times10^{23}\times0.162\times10^{-18}=2198\ m^2/g$$

**Figure S1.** The BET surface area of **ZJU-7a** obtained from $N_2$ adsorption isotherm at 77 K

## References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