Electronic Supplementary Material (ESI) for RSC Advances.
This journal is © The Royal Society of Chemistry 2017

Supporting Information

An amino-coordination metal-organic framework for highly selective C_2H_2/CH_4 and C_2H_2/C_2H_4 separations through the appropriate control of window sizes

Ling Zhang,[a] Xili, Cui,[b] Huabin Xing,[b] Yu Yang,[a] Yuanjing Cui,[a] Banglin Chen*[a,c] and Guodong Qian*[a]

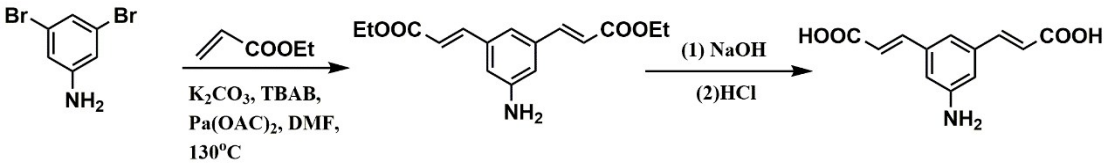
[a] *State Key Laboratory of Silicon Materials, Cyrus Tang Center for Sensor Materials and Applications, Department of Materials Science & Engineering, Zhejiang University, Hangzhou 310027, China. E-mail: gdqian@zju.edu.cn.*

[b] *College of Chemical and Biological Engineering, Zhejiang University, Hangzhou 310027, China.*

[C] *Department of Chemistry, University of Texas at San Antonio, One UTSA Circle, San Antonio, Texas 78249-0698, USA. E-mail: banglin.chen@utsa.edu; Fax: (+1) 210-458-7428.*

1. Synthesis of the organic linker 5-amino-H_2L.

5-amino-H_2L was synthesized via Heck cross-coupling,[1] followed by hydrolysis and acidification as shown in Scheme S1.



Scheme S1. Synthetic routes to the organic linker 5-amino-H_2L.

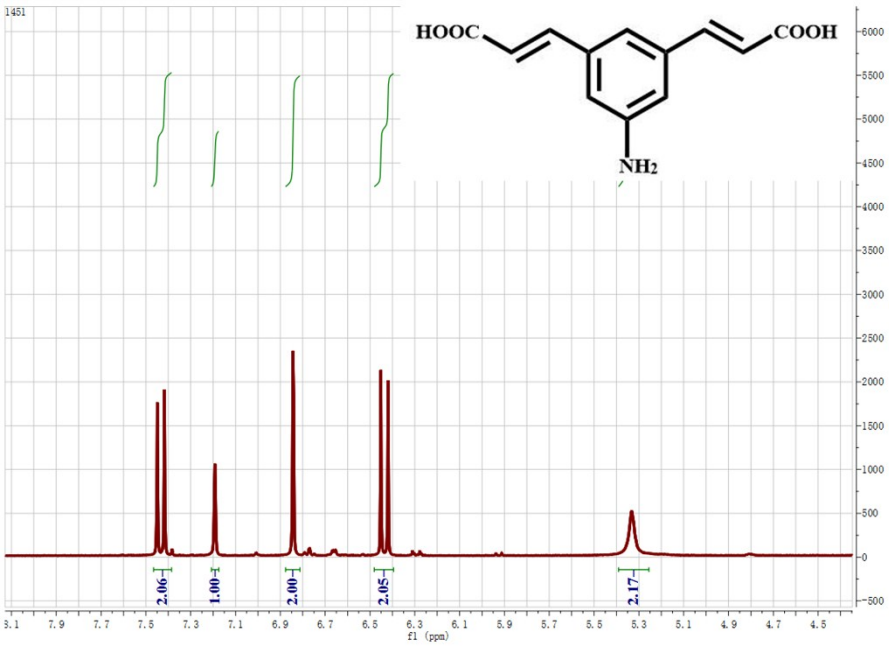


Figure S1. 1H (DMSO-d6, 500MHz) spectra of the ligand 5-amino-H_2L.

2. The TGA curves of ZJU-198.

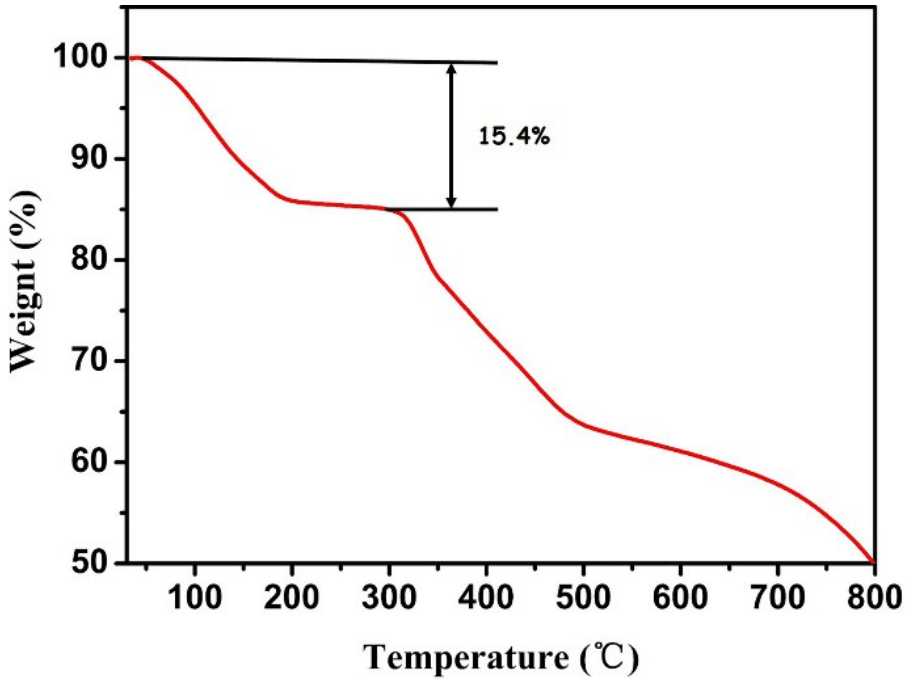


Figure S2. Thermogravimetric analysis (TGA) curves of as-synthesized **ZJU-198**. It's demonstrated the remarkable thermostability of **ZJU-198**, with no decomposition of framework occurring up to at least 300°C.

3. The IR spectra of the ligand 5-amino-H_2L and ZJU-198.

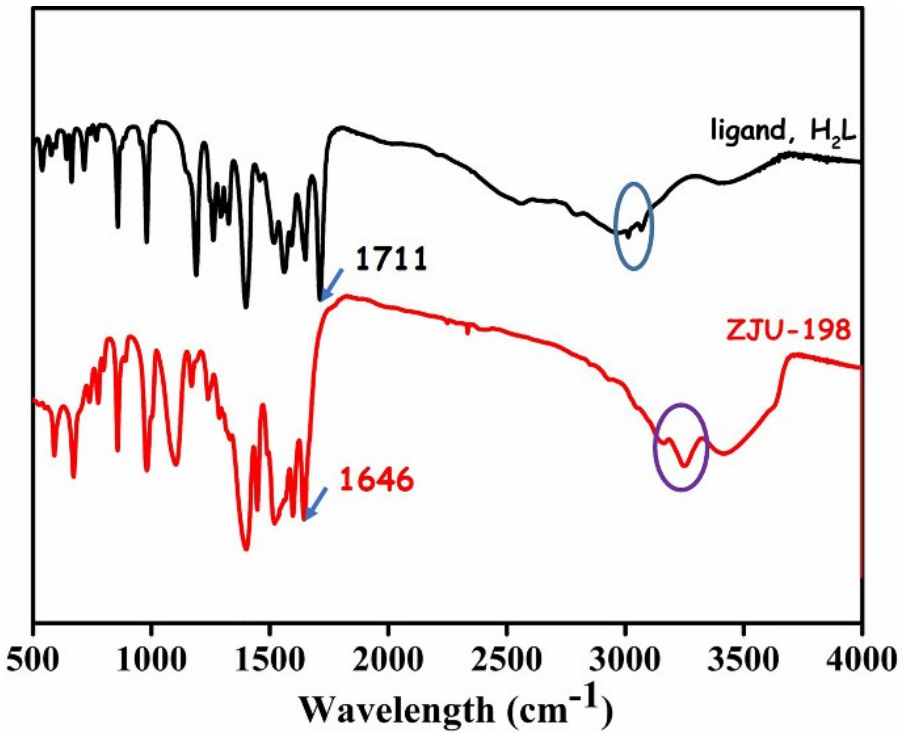


Figure S3. Infrared spectrum (IR) curves of ligand (H_2L), as-synthesized **ZJU-198**. It's clear to see that the adsorption peak of carbonyl changes from 1711 cm^{-1} of ligand to 1646 $cm^{-1}$of **ZJU-198** and the double-peak of amino varies from 3075 cm^{-1} to 3254 cm^{-1} during the deprotonation process.

4. The sorption isotherms for ZJU-198a.

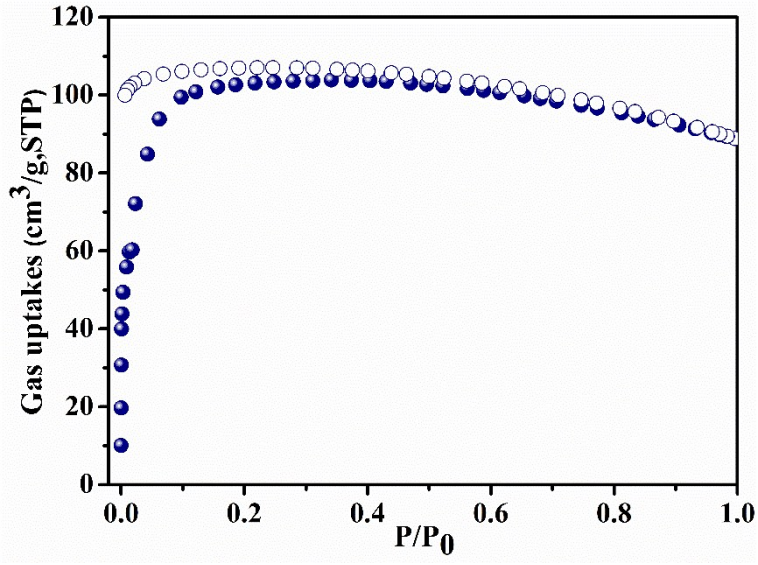


Figure S4. The CO_2 sorption isotherms for **ZJU-198a** at 196 K.

5. The PXRD patterns of as-synthesized ZJU-198 and ZJU-198a.

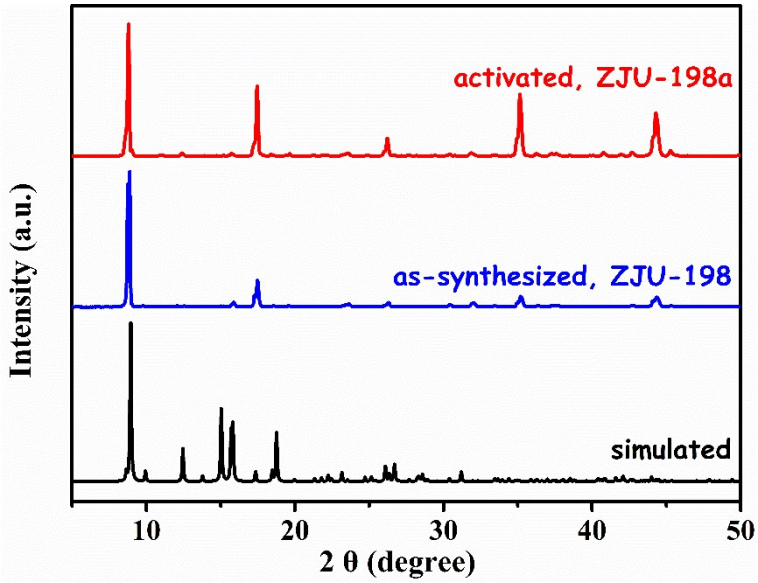


Figure S5. PXRD patterns of as-synthesized **ZJU-198** (blue) and activated **ZJU-198a** (red) along with the simulated XRD pattern from the single-crystal X-ray structure (black).

6. Breakthrough test of ZJU-198a.

The breakthrough experiments were accomplished by a dynamic gas breakthrough equipment.[2] The experiment was conducted using a stainless steel column (4.6 mm inner diameter × 50 mm). The weight of sample powder packed in the column was 0.62 g. The column packed with sample was firstly activated with He flow (15 ml min^{-1}) for 12 h at room temperature (298 K). After activation, the mixed gas (C_2H_2/C_2H_4: 1/99, v/v) flow was introduced at 1.26 ml min^{-1}. Outlet gas from the column was monitored using gas chromatography (GC-2010 plus, SHIMADZU). After the breakthrough experiment, the sample was regenerated with He flow (10 ml min^{-1}).

Reference

1. G. Q. Kong, Z. D. Han, Y. He, S. Ou, W. Zhou, T. Yildirim, R. Krishna, C. Zou, B. L. Chen, C.-D. Wu, *Chemistry*, 2013, **19**, 14886.

2. X. L. Cui, K. J. Chen, H. B. Xing, Q. W. Yang, R. Krishna, Z. B. Bao, H. Wu, W. Zhou, X. L. Dong, Y. Han, B. Li, Q. L. Ren, M. J. Zaworotko, B. L. Chen, *Science*. 2016, **353**: 141.