Supplementary Material (ESI) for Chemical Communications

Support information

Organically Templated Metal-Organic Framework with 2-fold Interpenetrated $\{3^3.5^9.6^3\}$-lcy Net

Ye-Yan Qin, Jian Zhang, Zhao-Ji Li, Lei Zhang, Xin-Yi Cao, Yuan-Gen Yao *

State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, The Chinese Academy of Sciences, Fuzhou, Fujian 350002, China. E-mail: yyg@fjirsm.ac.cn

Experimental Details

All the syntheses were performed in polytetrafluoroethylene-lined stainless steel autoclaves under autogenous pressure. Reagents were purchased commercially and were used without further purification. Elemental analyses were performed on a Vario EL III elemental analyzer. IR (KBr pellet) spectra were recorded on a Nicolet Magna 750 FT-IR spectrometer. Fluorescence measurements were performed on an Edinburgh FLS920 fluorescence spectrometer. TG-MS analysis was carried out on preweighted samples in a nitrogen stream using a Netzsch STA449C-QMS403C apparatus.

X-ray intensity of compound **1** was collected on a Rigaku Mercury CCD diffractometer equipped with graphite monochromated MoKa radiation (λ = 0.71073 Å) at 293(2)K. Empirical absorption corrections were applied to the data using the SADABS program. The structures were solved by the direct methods and refined by the full-matrix least-squares on F^2 using the SHELXTL–97 program. All of the non-hydrogen atoms were refined anisotropically.

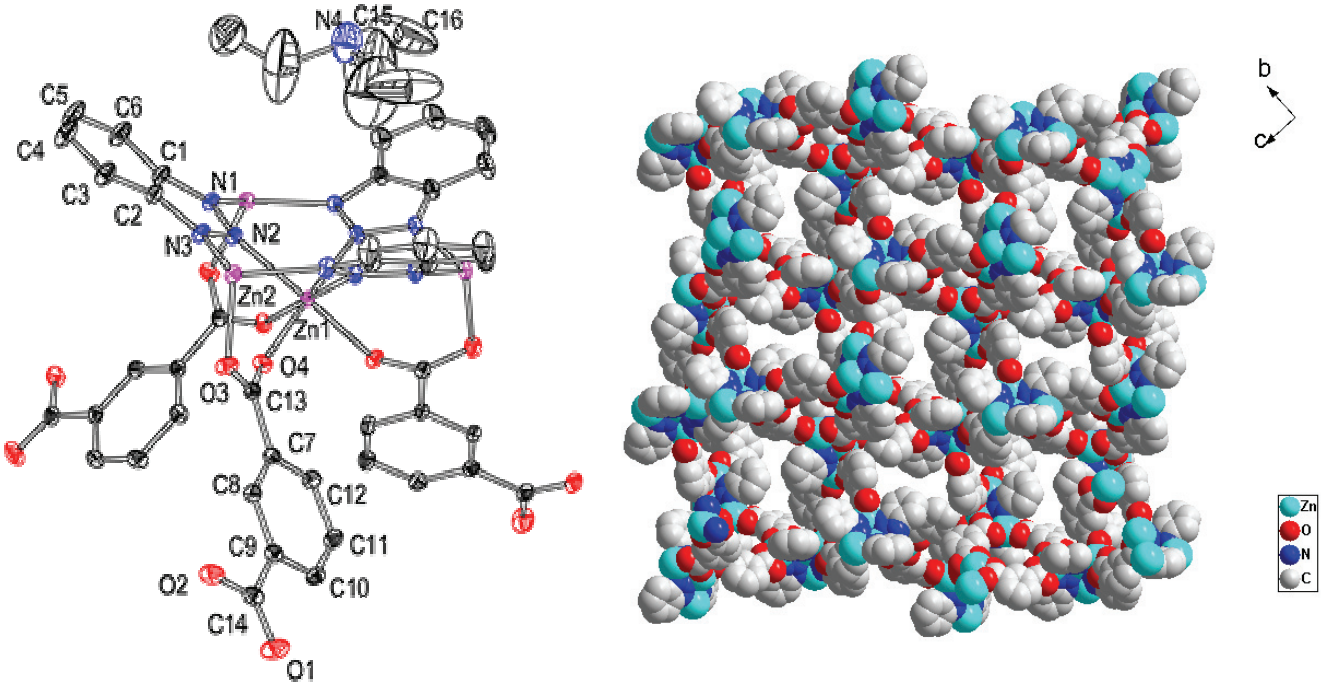


Figure S1. (a) ORTEP drawing of the molecular structure of compound **1;** (b) Packing diagram of compound **1**

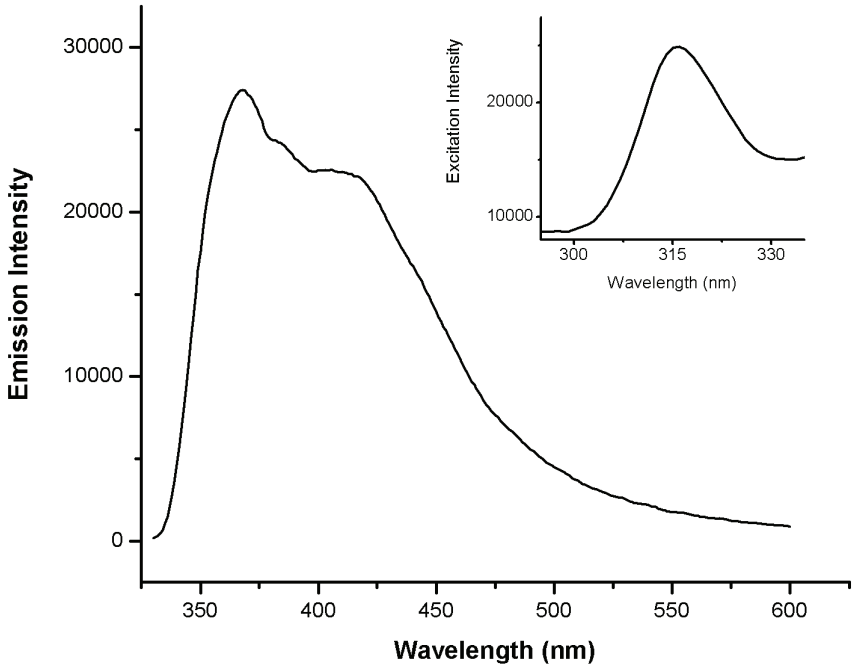
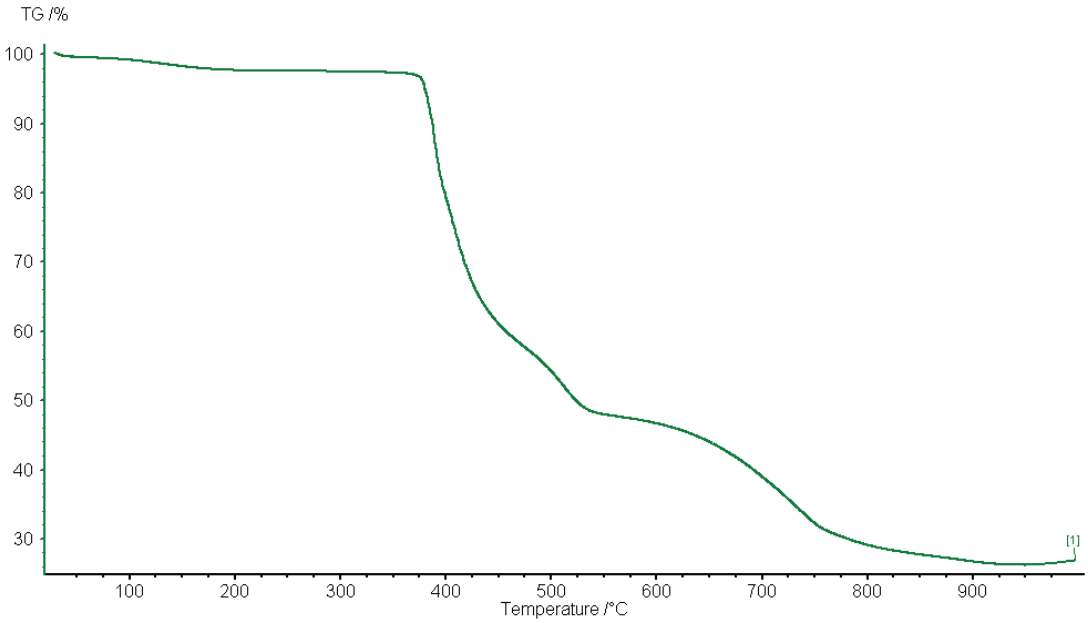
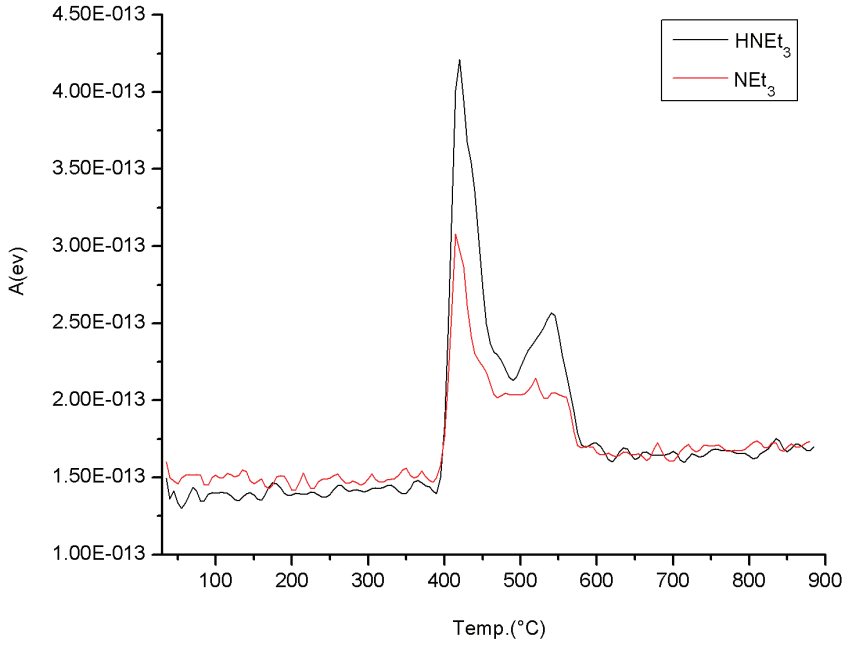


Figure S2. Photoluminescence spectra and excitation spectra (inset) of compound **1** in the solid state at room temperature.



(a)



(b)

Figure S3. TG-MS analysis of compound **1**: (a) TG curve; (b) MS curve

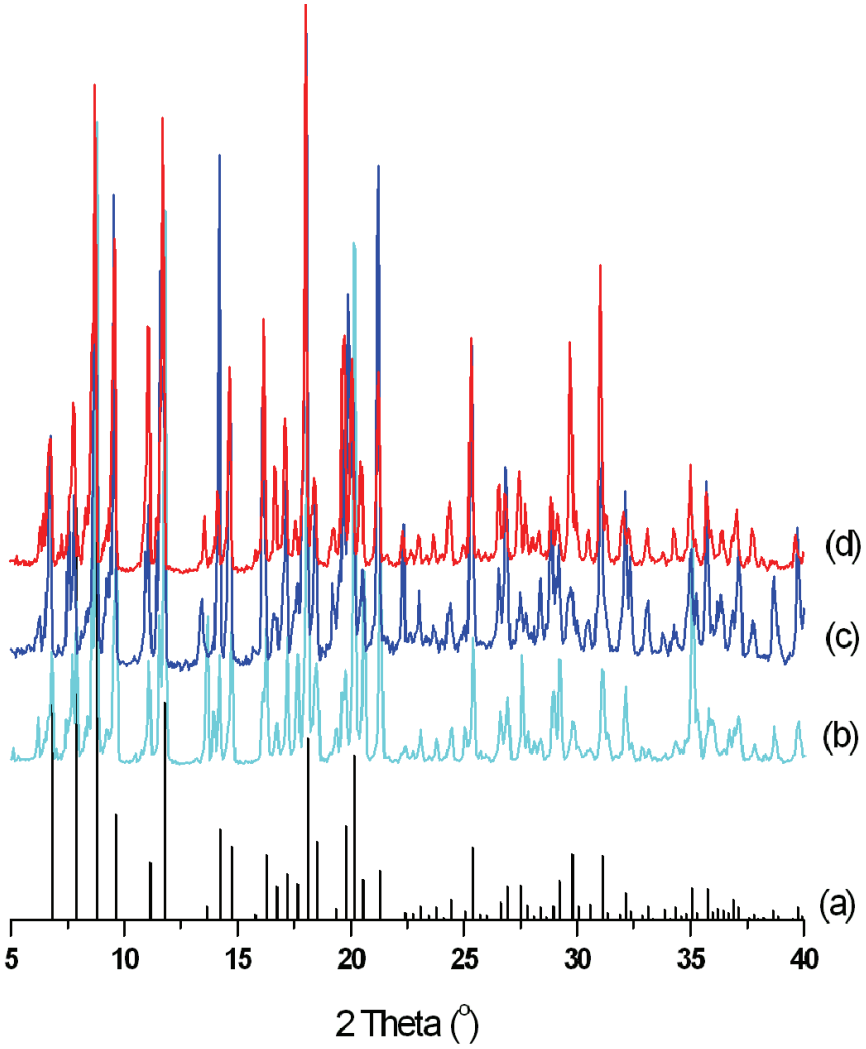


Figure S4 XPRD patterns for **1**. (a) Calculated on the basis of the structure determined by single-crystal X-ray diffraction; (b) taken at room temperature; (c) taken at 300 ^{o}C for 10 mins; (d) taken at 350 ^{o}C for 10 mins.