Supplementary Information

A Nanotubular Metal-Organic Framework with Permanent Porosity: Structure Analysis and Gas Sorption Studies

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Preparation of PCN-19.

A mixture of H_2adc (0.005g) and $Ni(NO_3)_2$•$6H_2O$ (0.02 g) in 1.5 mL dimethylacetamide (DMA) with 3 drops of HBF_4 (30% aqua solution) was placed in a sealed Pyrex tube, and heated to 120 ^oC (temperature increasing rate 1 ^oC/min) in a programmable oven. The tube was allowed to stay at the temperature for 24 hours and was then cooled to 25 ^oC (temperature decreasing rate 0.1 ^oC/min). The light yellow green block crystals obtained were washed with DMA to give pure PCN-19 with the formula $Ni_3O(H_2O)_3(C_{28}H_{16}O_4)_3 \cdot 2(C_4H_{10}NO^+)$ (70% yield based on H_2adc). Elemental analysis calcd (%): C 55.35, H 4.15, N 2.30; found: C 54.65, H 4.23, N 2.35.

Single-crystal X-ray crystallography. Single crystal X-ray data were collected on a Bruker Smart Apex[1] diffractometer equipped with an Oxford Cryostream low temperature device and a fine-focus sealed-tube X-ray source (Mo-K_α radiation, λ = 0.71073 Å, graphite monochromated) operating at 45 kV and 35 mA. The crystals were protected with Paratone oil from air and moisture, and mounted on the tip of a glass fiber of a gonometer. Frames were collected with 0.3° intervals in φ and ω for 30 s per frame such that a hemisphere of data was collected. Raw data collection and refinement were done using SMART. Data reduction was performed using SAINT+ and corrected for Lorentz and polarization effects. The structure was solved by direct methods and refined by full-matrix least-squares on F^2 with anisotropic displacement using SHELX-97. Non-hydrogen atoms were refined with anisotropic displacement parameters during the final cycles. Hydrogen atoms on carbon were calculated in ideal positions with isotropic displacement parameters set to 1.2 × U_{eq} of the attached atom. In all cases solvent molecules were highly disordered, and attempts to locate and refine the solvent peaks were unsuccessful; contributions to scattering due to these solvent molecules were removed using the SQUEEZE routine of PLATON and refined further using the data generated.

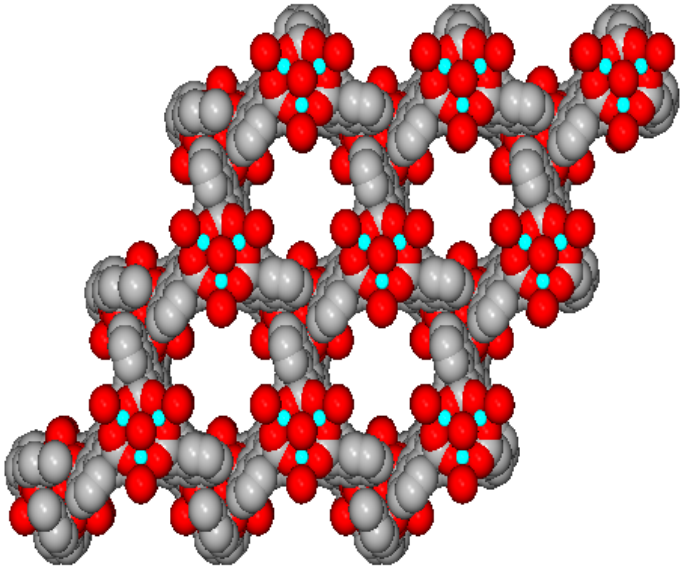

Fig. S1. 1D nanochannels with terminal aqua ligands of trinickel SBUs pointing toward the center.

1. Note: Certain commercial suppliers are identified in this paper to foster understanding. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.