Supporting Information

A 3D Chiral Nanoporous Coordination Framework Consisting of Homochiral Nanotubes Assembled from Octuple Helices

Xiang-Rong Hao, Xin-Long Wang, Chao Qin, Zhong-Min Su*, En-Bo Wang*, Ya-Qian Lan, and Kui-Zhan Shao

Institute of Functional Materials, Department of Chemistry and Key Laboratory of Polyoxometalates Science of Ministry of Education, College of Chemistry, Northeast Normal University, Changchun 130024, China. Email: zmsu@nenu.edu.cn wangenbo@public.cc.jl.cn
**X-ray structure analysis:** C$_{31}$H$_{38}$N$_3$O$_8$Cd: $M_r = 693.04$, hexagonal, space group $P6_122$, $a = b = 26.712(4)$ Å, $c = 15.919(3)$ Å, $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$, $V = 9837(3)$ Å$^3$, $Z = 12$, $\rho_{\text{calc}} = 1.404$ mg m$^{-3}$, Flack parameter = $-0.01(3)$, final $R1 = 0.0384$ for 9677 independent reflections [$I > 2\sigma(I)$]. The data were collected on a Bruker Apex CCD diffractometer at 133(2) K with graphite-monochromated Mo$_{K\alpha}$ radiation ($\lambda = 0.71073$ Å).

The data were collected on a Bruker Apex CCD diffractometer at 133(2) K with graphite-monochromated Mo$_{K\alpha}$ radiation ($\lambda = 0.71073$ Å). The structures were solved by direct method and refined by full-matrix least-squares methods with SHELXL.$^{[1]}$ The anion and DMA molecules were highly disordered and could not be modeled properly, thus the SQUEEZE routine, a part of the PLATON package of crystallographic software, was applied to calculate the solvent disorder area and remove its contribution to the overall intensity data. The refinements of the guest-free structure on the squeezed data gave the final $R1 = 0.0384$ and $wR2 = 0.0798$ ($R1 = 0.0463$ and $wR2 = 0.1322$ without employing PLATON/SQUEEZE). The final formula was calculated from the SQUEEZE results combined with the following characterization techniques. Despite the disorder, identification of the guest molecules is readily accomplished by $^1$H NMR spectroscopy. The $^1$H NMR spectrum of 1 recorded in D$_2$O exhibits a set of well-resolved proton signals. The signals at 2.88, 2.73 and 1.91 ppm attributed to three CH$_3$ groups of DMA,$^{[2]}$ while the signal at 2.54 ppm ascribes to the CH$_3$ group of dimethylamine. Furthermore, NMR analysis reveals that the relative molar ratio of dimethylamine and DMA is approximately 1:2. The IR
spectrum of 1, as expected, exhibits a sharp band at 1619 cm\(^{-1}\) corresponding to \(\tilde{\nu}_{C=O}\) stretching frequency, which is indicative of DMA molecule. According to the previous literature, the peaks of 1540 and 1398 cm\(^{-1}\) are attributed to the asymmetric and symmetric stretching vibrations of the carboxylate group of bpdc ligand.\(^3\) The peak at ca. 3419 cm\(^{-1}\) is attributed to the N-H absorption vibration of dimethylamine. Further information supporting the formula of 1 is obtained by thermogravimetric analysis, elemental analysis and the consideration of charge balance.

**S1-1.** Section of the X-ray crystal structure of 1, showing the coordination environments of Cd$^{2+}$ ions and their connectivity with bpdc anions. Color code: C black; O red; Cd green.

**S1-2.** Coordination modes of the bpdc ligands in the structure of 1. bpdc$^A$: chelating bis(bidentate), bpdc$^B$: bridging bis(bidentate). Color code: C black; O red; Cd green.
SI-3. An angle of 123.92° formed between the planes defined by the two C-O-Cd-O-C chelate rings at one metal center. Color code: C black; O red; Cd green.

SI-4. Perspective view of the trigonal channel that is surrounded by bpdc\(^B\) ligands. Color code: C black; O red; Cd green.
SI-5. The $^1$H NMR spectrum of 1 recorded in D$_2$O.

SI-6. FT-IR spectrum of as-synthesized 1.
SI-7. TG curve of 1.