

Supporting Information For

A 6-fold Interpenetrated ThSi₂ Topological Metal–Organic Framework from a Nanosized Tripodal Aromatic Acid

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Materials and Measurements. All the solvents and reagents were commercially available and used as received without further treatment. Elemental analyses for C, H and N were performed on Perkin-Elmer 240C elemental analyzer. Thermogravimetric and differential thermal analyses (TG-DTA) were carried out in a nitrogen stream using Diamond TG/DTA thermal analyzer from room temperature to 800 °C with a heating rate of 10 °C min⁻¹. X-ray powder diffraction (XRPD) data were collected on a Bruker D8 Advance instrument using a Cu K α radiation ($\lambda = 1.54056 \text{ \AA}$) at room temperature. FT-IR spectra were obtained on a Nicolet Nexus 670 FTIR spectrometer with KBr pellets in the range 4000–400 cm⁻¹ region. The luminescence (emission) spectra for the powdered solid samples were measured at room temperature on LS-50B spectrofluorometer. The topological analysis was taken according to the TOPOS software.

Synthesis of Cd(C₃₃H₂₇O₉)(C₃H₇NO)(C₂H₈N)•0.5H₂O (**1**)

A mixture of CdBr₂·4H₂O (35.0 mg, 0.10 mmol), H₃L (76.4 mg, 0.13mmol) and NH₄Cl (12.0 mg, 0.22 mmol), N,N-Dimethylformamide (DMF) (2.5 ml) and H₂O (1.5 ml) was sealed into a 10 mL Teflon-lined autoclave and placed in an oven at 180 °C for 72 h, after slowly cooling to room temperature at a rate of 5 °C h⁻¹, a lot of colorless bulk crystals were obtained with a yield of 77% based on Cd, washed with absolute ethyl alcohol and ether, then dried in the air. Anal. Calcd. for C₃₈H₄₃CdN₂O_{10.50} (**1**): C, 56.47; H, 5.36; N, 3.48%, Found: C, 56.97; H, 5.42; N, 3.54%. IR (KBr, cm⁻¹): 3465 m, b, 2761 m, b, 2499 m, 1660 s, 1604 s, 1527 s, 1381 s, 1300 s, 1238 s, 1163 s, 1082 s, 987 s, 854 s, 784 s, 691 m, 655 s, 611 m, 526 w.

Crystallography. Colorless bulk crystals of compound **1** was mounted on a Bruker Smart APEX II CCD diffractometer with graphite-monochromated Mo-K α ($\lambda = 0.71073 \text{ \AA}$) radiation and the intensity data were collected at the temperature of 298 K. Data reductions and absorption corrections were performed using the SAINT and SADABS programs¹, respectively. All structures were solved by direct methods using the SHELXS-97 program and refined with full-matrix least squares on F² using the SHELXL-97 program². All non-hydrogen atoms were refined anisotropically, and the hydrogen atoms were placed in geometrically calculated positions. Selected bond distances and angles of compound **1** are shown in Table S1.

Crystallographic data (excluding structure factors) for the structure(s) reported in this paper have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC-862162. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [Fax: int. code + 44(1223)336-033; E-mail: deposit@ccdc.cam.ac.uk].

1 SMART, and SADABS, Bruker AXS Inc., Madison, Wisconsin, USA.
2 G. M. Sheldrick, *Acta. Cryst.*, 2008, **A64**, 112.

Table S1 Selected bond length [Å] and angles [°] of complex **1**.

Cd1–O1	2.321(4)	Cd1–O2	2.451(4)	Cd1–O4	2.452(4)	Cd1–O5	2.362(3)
Cd1–O7	2.257(4)	Cd1–O8	2.496(4)	Cd1–O10	2.375(4)		
O7–Cd1–O1	93.83(15)	O7–Cd1–O5	110.98(14)	O1–Cd1–O5	154.32(13)	O7–Cd1–O10	89.01(14)
O1–Cd1–O10	87.14(14)	O5–Cd1–O10	86.76(14)	O7–Cd1–O2	110.06(14)	O1–Cd1–O2	54.51(12)
O5–Cd1–O2	118.59(12)	O10–Cd1–O2	136.99(13)	O7–Cd1–O4	163.46(15)	O1–Cd1–O4	100.71(14)
O5–Cd1–O4	53.83(13)	O10–Cd1–O4	83.91(15)	O2–Cd1–O4	85.03(13)	O7–Cd1–O8	54.53(13)
O1–Cd1–O8	118.70(13)	O5–Cd1–O8	82.69(12)	O10–Cd1–O8	134.06(13)	O2–Cd1–O8	85.99(12)
O4–Cd1–O8	122.56(14)						

Symmetry codes for **1**: (i) 0.5+x, 1.5+y, z; (ii) x, 3-y, -0.5+z; (iii) x, 3-y, 0.5+z; (iv) -0.5+x, -1.5+y, z.
