Supplementary Material (ESI) for Chemical Communications

Supporting information for

An unprecedented nanoporous and fluorescent supramolecular framework with $SrAl_2$ topology controllably synthesized from a flexible ditopic acid

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Experimental Section.

(a) The ligand H_2BDOA was prepared according to the described method. (J. -F. Zhang, Y. -H. Hu, D. -Z. Wang, *J. Cent. South Univ. Technol.* (*Chin. Ed.*) **2001**, *32*, 146-149.)

(b) Crystal data of the complexes were measured on a Bruker SMART Apex2 diffractometer at 291K using graphite-monochromated $Mo_{K\alpha}$ radiation, respectively. Data reduction was performed with the Bruker SAINT package. The structures were solved with direct methods and refined with full-matrix least-squares technique using the SHELXS-97 and SHELXL-97 programs, respectively (References: Sheldrick, G. M. *SHELXS-97, Program for Crystal Structure Solution*; Göttingen University: Göttingen, Germany, **1997**; Sheldrick, G. M. *SHELXL-97, Program for Crystal Structure Refinement*; Göttingen University: Göttingen, Germany, **1997**.). The coordinates of the non-hydrogen atoms were refined anisotropically, and hydrogen atoms were located in the calculated positions.

(c) Fluorescence measurements were performed on an AMINCO-BOWMAN Series AB2 luminescence spectrometer. The as-synthesized samples were characterized by thermogravimetric analysis (TGA) on a thermoflex analyzer (Rigaku) up to 1073 K using a heating rate of 20 K min-1 for _10 mg samples open to air.

(d) XRD measurements were performed on a Bruker D8 Advance X-ray diffractometer using Cu KR radiation (0.15418 nm), in which the X-ray tube was operated at 35 kV and 20 mA.

Table S1. Selected Bond Lengths (in Å) and Angles (deg) for complex **1**.

Ca(1)-O(2B)	2.370(2)	O(1W)-Ca(1)-O(2)	131.10(7)
Ca(1)-O(1W)	2.411(2)	O(1WC)-Ca(1)-O(1W)	88.92(10)
Ca(1)-O(2C)	2.506(2)	O(2A)-Ca(1)-O(1W)	94.32(7)
Ca(1)-O(3)	2.517(2)	O(2B)-Ca(1)-O(1WC)	94.32(7)
Ca(1)-O(1WC)	2.411(2)	O(2B)-Ca(1)-O(2)	72.36(8)
Ca(1)-O(2)	2.506(2)	O(2A)-Ca(1)-O(1WC)	156.27(7)
Ca(1)-O(3C)	2.517(2)	O(2)-Ca(1)-O(2C)	144.59(10)
		O(2)-Ca(1)-O(3)	52.11(7)
		O(2B)-Ca(1)-O(2C)	83.16(5)
		O(1W)-Ca(1)-O(2C)	77.10(7)
		O(2A)-Ca(1)-O(3C)	124.42(7)
		O(1WC)-Ca(1)-O(3C)	79.22(7)
		O(2)-Ca(1)-O(3C)	142.10(6)
		O(2A)-Ca(1)-O(3)	80.44(6)
		O(1WC)-Ca(1)-O(3)	77.09(7)

Symmetry codes: A:x, -y, z-1/2; B:-x+2, -y, -z+2; C:-x+2, y, -z+3/2; D:-x+2, -y, -z+1.

Table S2. Hydrogen bonding geometry for complex **1** (in Å and deg).

D-H···A	<DHA	d(D···A)
O(5W)-H(5WB) ···O(5W)[a]	125.1	3.1238(4)
O(5W)-H(5WD) ···O(4W)[b]	169.5	2.883(3)
O(4W)-H(4WC) ···O(5W)[c]	111.1	2.883(3)
O(4W)-H(4WC) ···O(5W)[d]	117.7	2.883(3)
O(3W)-H(3WB) ···O(2W)[e]	133.3	2.898(6)
O(2W)-H(2WA) ···O(1W)[f]	130.3	2.995(3)
O(2W)-H(2WD) ···O(5)	118.8	2.903(3)
O(4W)-H(4WA) ···O(2W)[g]	132.5	2.694(5)
O(1W)-H(1WB) ···O(5)[g]	121.4	2.724(3)

Symmetry codes: [a]x, -y+2, z+1/2; [b]x-1/2, y+1/2, z; [c]x+1/2, y-1/2, z; [d]-x+3/2, y-1/2, -z+1/2; [e]x, y, z-1; [f]x-1/2, -y+1/2, z+1/2; [g]-x+3/2, -y+1/2, -z+1.

Fig. S1. Coordination environment of the Ca ion in complex **1**. Solvent molecules are omitted for clarity. Symmetry codes: A, 2-*x*, *y*, 3/2-*z*; B, 2-*x*, -*y*, 2-*z*; C, *x*, -*y*, -1/2+*z*.

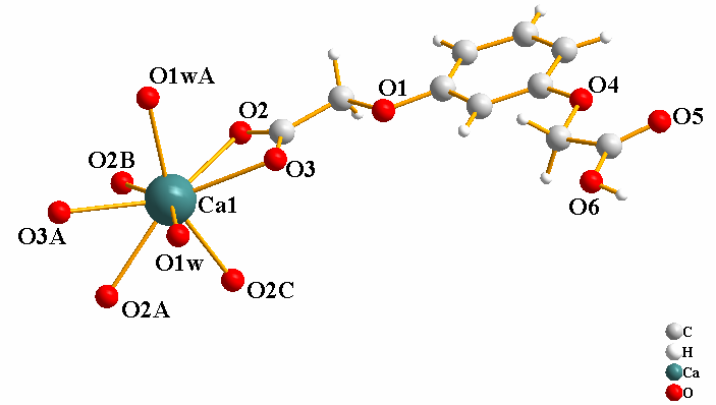
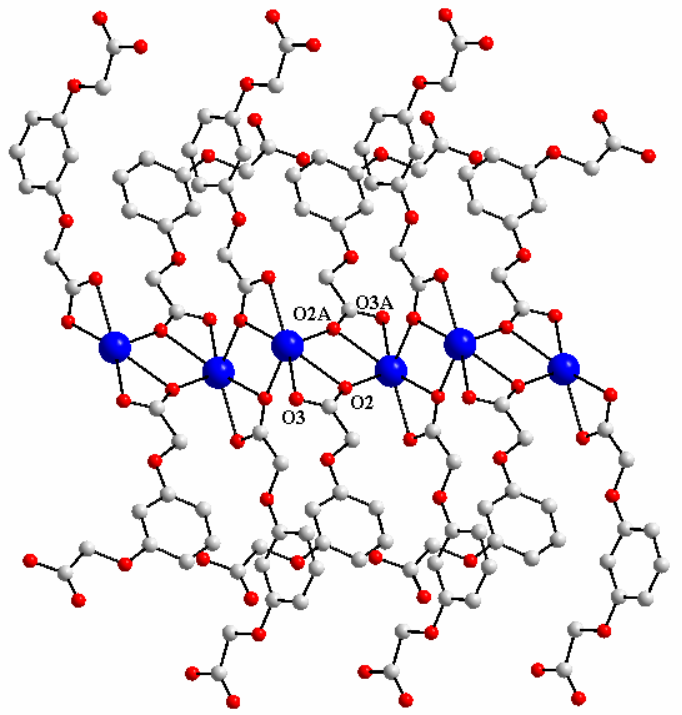
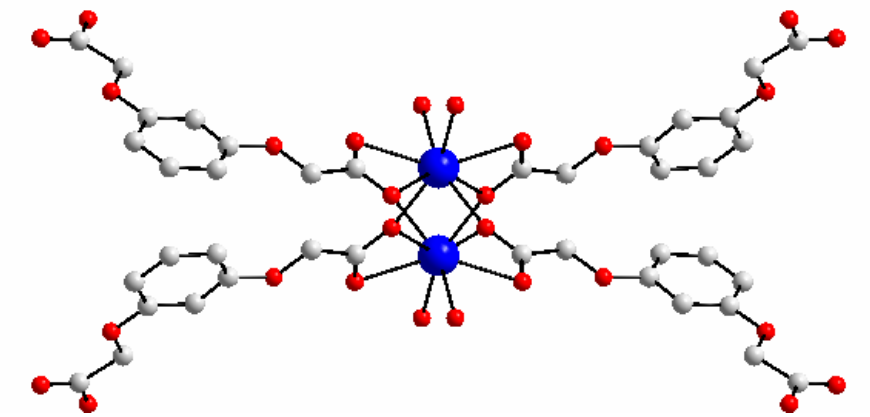


Fig. S2. A perspective view of a section of the polymeric network along the *c* (a) and *b* (b) axis, respectively. Solvent molecules and hydrogen atoms have been omitted for clarity.



(a)



(b)

Fig. S3. A perspective view of the hydrogen-bonded network of complex 1 along the c axis, showing the hydrogen bonding interactions between the adjacent chains.

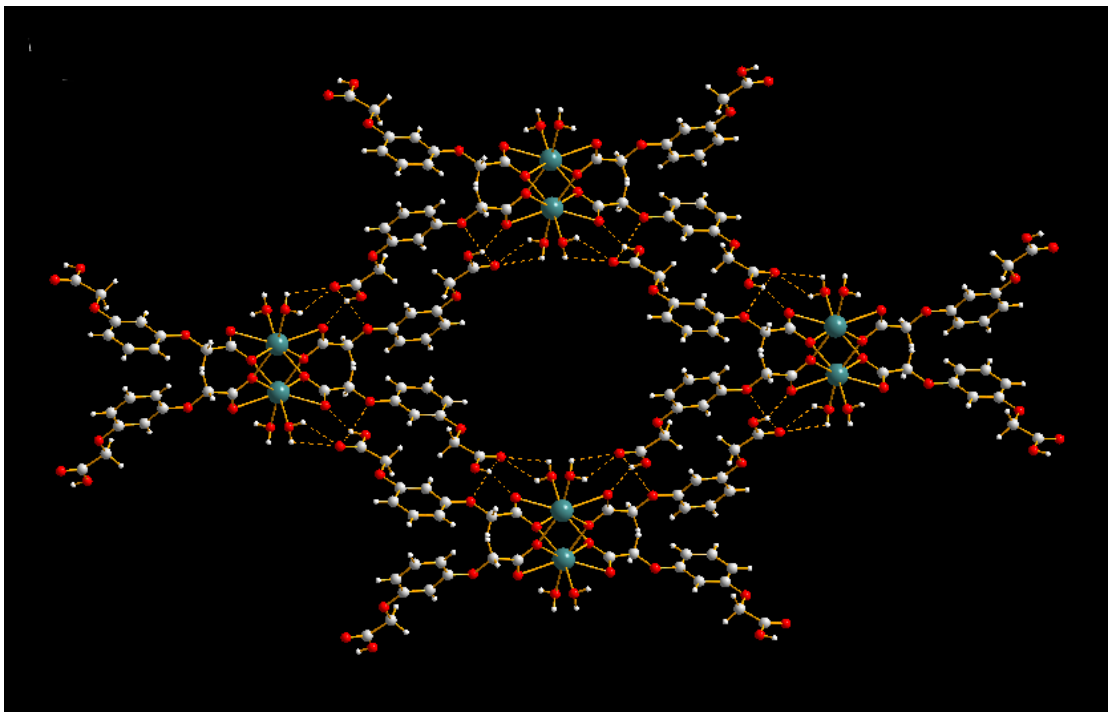


Fig S4. Detailed arrangement of the water molecules in the water column. Symmetry codes to generate atoms: A, 1/2 + *x*, 1/2 - *y*, -1/2 + *z*; B, 1/2 + *x*, 1/2 - *y*, 1/2 + *z*; C, 1/2 + *x*, 3/2 - *y*, 1/2 + *z*; D, 2 - *x*, 1 - *y*, 1 - *z*; E, 3/2 - *x*, 1/2 + *y*, 3/2 - *z*; F, 3/2 - *x*, 1/2 + *y*, 1/2 - *z*; G, 3/2 - *x*, -1/2 + *y*, 1/2 - *z*; H, 3/2 - *x*, 1/2 - *y*, 1 – *z*.

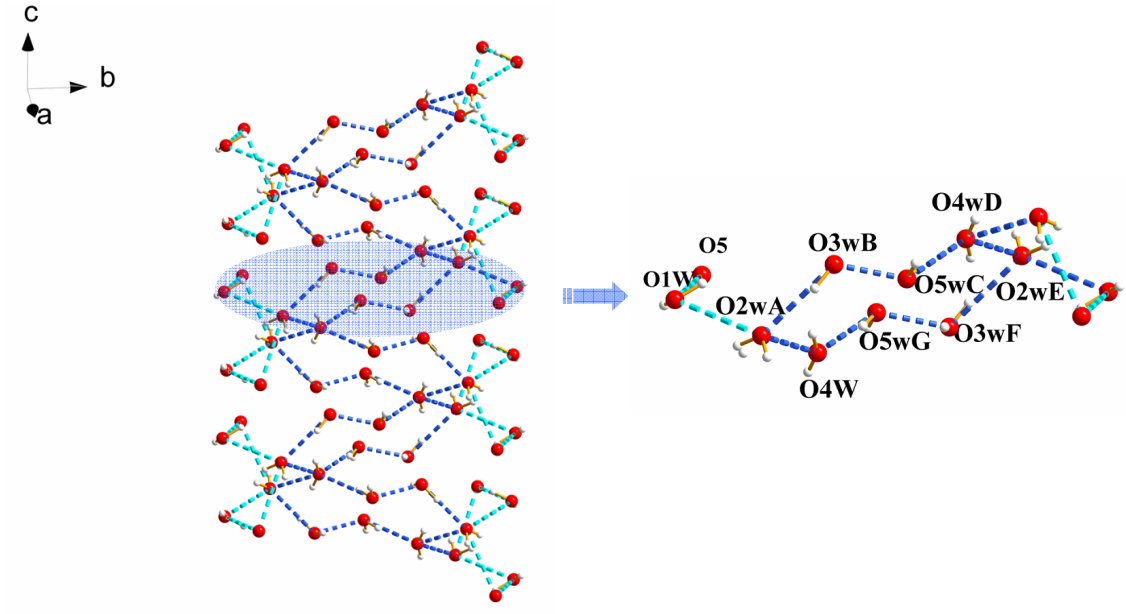


Fig S5. TG curve of complex **1**.

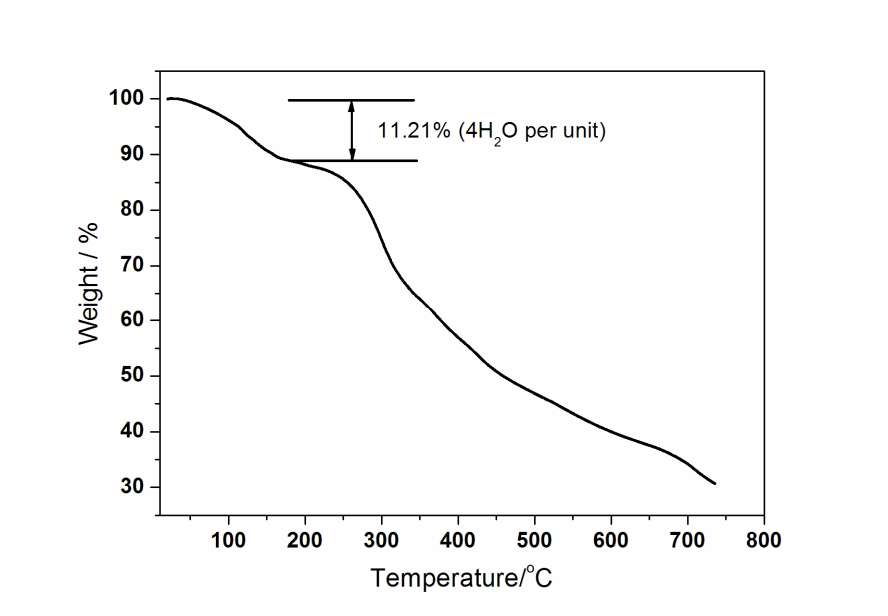


Fig. S6. XPRD results for complex **1**: (a) Simulated; (b) as-synthesized sample; (c) sample dried at 90°C under reduced pressure for 2 h; (d) sample dried at 100°C under reduced pressure for 2 h; (e) sample dried at 140°C under reduced pressure for 2 h; (f) sample immersed in H_2O for 7 days after dehydration.

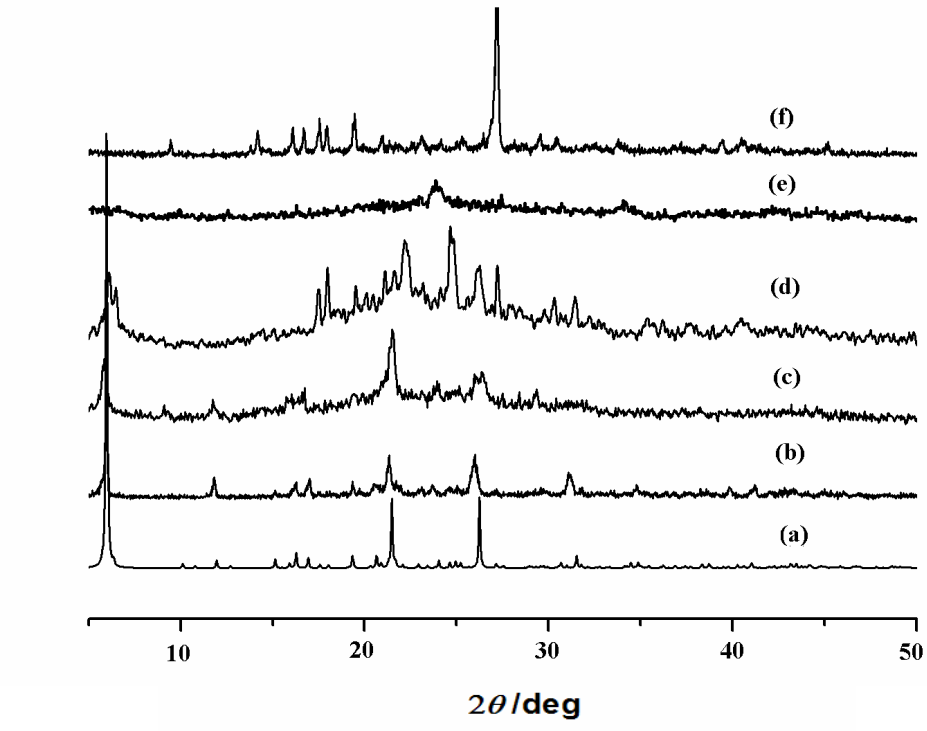


Fig. S7. Photoluminent emission of as-synthesized sample upon excitation at 346 nm (a), the partly dehydrated sample upon excitation at 348 nm (b) and the completely dehydrated sample upon excitation at 364 nm (c) of complex **1** at room temperature, respectively.