Supporting materials

Supramolecular Borromean sheet consisting of threefold parallel interwoven 4^4-**sql** layers assembled by a flexible bipyridinium ligand

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Materials, Methods, Syntheses and Characterizations

1,1′-bis(4-carboxybenzyl)-4,4′-bipyridinium chloride ($H_2BpybcCl_2$) was synthesized based on the nucleophilic substitution reaction of 4,4′-bipyridine and 4-(chloromethyl)benzoic acid (refer to our paper published in Cryst. Growth Des. 2005, 5, 1939 for details). Other chemicals employed for synthesis were obtained commercially. Elemental analyses of C, H and N were carried out with a Vario EL III elemental analyzer. IR spectra were performed on a Spectrum One FT-IR spectrometer with KBr pellets in the range 4000–400 cm^{-1}. X-Ray powder diffraction (XRPD) data was obtained using a Rigaku DMAX 2500 powder diffractometer with Cu Kα radiation. Thermogravimetric analysis was performed with a Mettler Toledo TGA/SDTA 851^e analyzer.

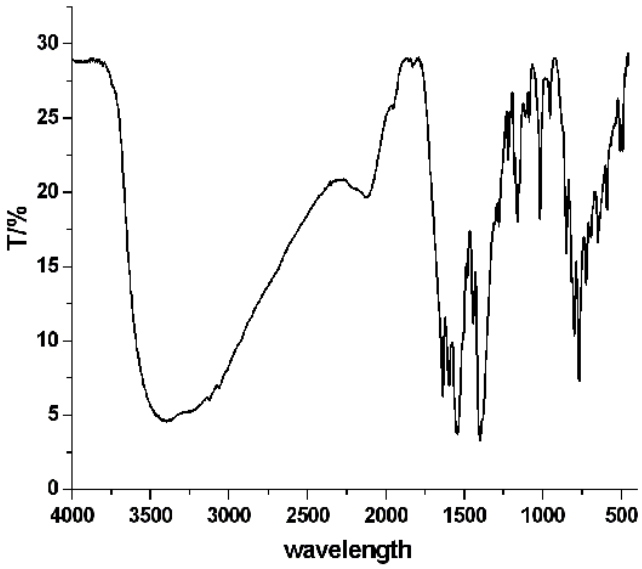

Fig. S1 IR spectrum of compound **1**.

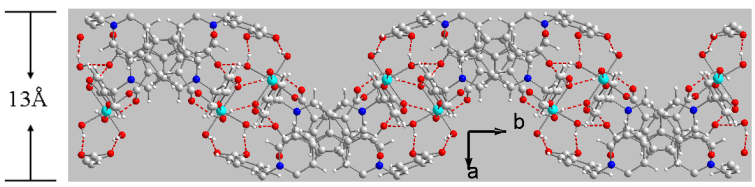

Fig. S2 The undulated layer with a thickness of about 13 Å..

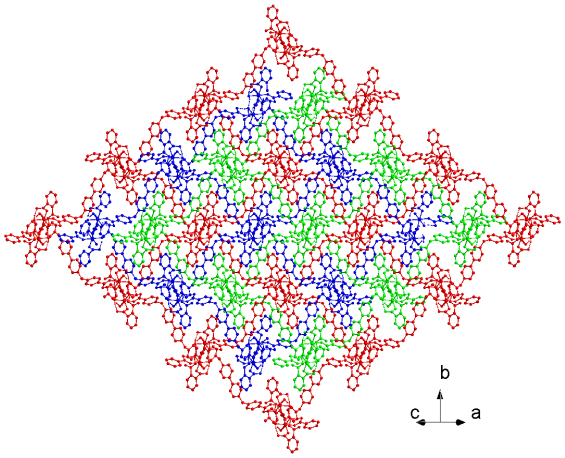

Fig. S3 A ball-and-stick projection along [101] showing the Borromean sheet consisting of three separate 4^4-**sql** layers (shown as red, blue and green color). Hydrogen atoms are omitted for clarity.

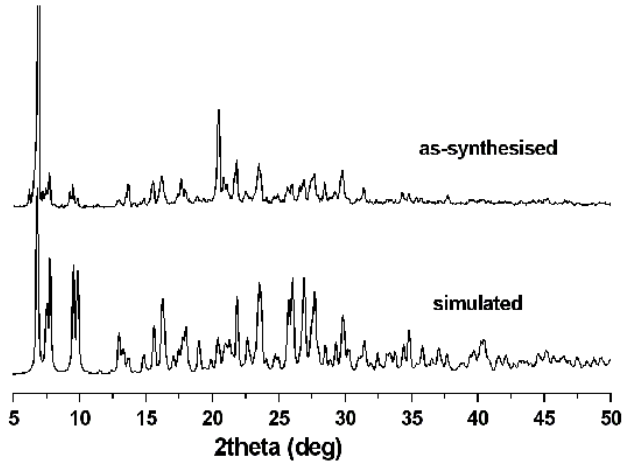

Fig. S4 Powder X-ray diffraction patterns of **1** as simulated from single-crystal XRD and as the prepared material.

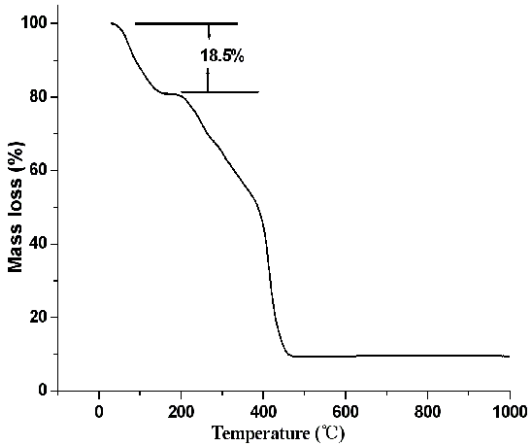

Fig. S5 TGA plot of **1** under N_2 atmosphere. The observed mass loss is about 18.5%, while the calculated is 26.55%. This is because some lattice water molecules are easily taken away by nitrogen flow.

Table S1. Hydrogen-bonding parameters in **1**.

D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (º)
O1W-H1W-O2	0.8635(2)	1.7322(5)	2.5769(7)	165.349(51)
O1W-H2W-O7	0.8534(1)	1.8701(3)	2.7083(5)	166.924(37)
O2W-H3W-O7A	0.8676(2)	1.8695(4)	2.7153(5)	164.446(37)
O2W-H4W-O4B	0.8550(2)	1.8242(4)	2.6288(6)	156.115(34)
O3W-H6W-O3B	0.8566(2)	1.9200(4)	2.7362(6)	158.803(46)
O4W-H7W-O1WA	0.8575(2)	1.9474(4)	2.7385(5)	152.825(33)
O4W-H8W-O6	0.8684(2)	1.7748(3)	2.6187(5)	163.362(32)

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