Supporting information for

An unprecedented (4, 10)-connected porous metal-organic framework containing two rare large second building units (SBUs)†

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Experimental Section

General Remarks. All of the chemicals are commercially available and used without further purification. Elemental analyses were determined using Elementar Vario EL elemental analyser. The IR spectra were recorded in the 4000 to 400 cm^{-1} region using KBr pellets and a Bruker EQUINOX 55 spectrometer. The Powder X-ray diffraction patterns were recorded on D8 ADVANCE X-Ray Diffractometer. The thermogravimetric analyses (TGA) was carried out on Netzsch TG-209 Thermogravimetry Analyzer in air atmosphere. The fluorescent measurement was conducted on a RF-5301PC spectrometer. The single crystal data were collected on a Bruker Smart 1000 CCD diffractometer.

X-ray Crystallography. Single-crystal data for **1** were collected on a Bruker Smart 1000 CCD diffractometer, with Mo-Kα radiation (λ = 0.71073 Å). All empirical absorption corrections were applied using the SADABS program.[1] The structure was solved using direct methods, which yielded the positions of all non-hydrogen atoms. These were refined first isotropically and then anisotropically. The hydrogen atoms attached to the ligands were placed in calculated position, with fixed isotropic thermal parameters and included in the structure factor calculation in the final stage of full-matrix least-squares refinement. The hydrogen atoms of lattice H_2O molecules were not added. All calculations were performed using the SHELXTL system of computer programs.[2]

Topological Analysis by TOPOS 4.0.

Atom coordinates (C1 = 4-connected SBUA, C2 = 10-connected SBUB)

Topology for C1

The links to atom C1

C1	0.3824	0.5000	0.5000	(0 0 0)	0.764 Å
C1	0.3824	-0.5000	0.5000	(0 -1 0)	0.764 Å
C2	0.0000	0.0000	0.0000	(0 0 0)	1.021 Å
C2	0.0000	0.0000	1.0000	(0 0 1)	1.021 Å

Topology for C2

The links to atom C2

C1	0.1176	0.0000	0.5000	(0 0 0)	1.021
C1	0.1176	0.0000	-0.5000	(0 0-1)	1.021
C1	-0.1176	0.0000	0.5000	(0 0 0)	1.021
C1	-0.1176	0.0000	-0.5000	(0 0-1)	1.021
C2	0.0000	-1.0000	0.0000	(0-1 0)	1.094
C2	0.0000	1.0000	0.0000	(0 1 0)	1.094
C2	-0.5000	-0.5000	0.0000	(-1-1 0)	1.146
C2	0.5000	0.5000	0.0000	(0 0 0)	1.146
C2	0.5000	-0.5000	0.0000	(0-1 0)	1.146
C2	-0.5000	0.5000	0.0000	(-1 0 0)	1.146

Coordination sequences

C1	1	2	3	4	5	6	7	8	9	10
Num	4	19	60	122	206	304	422	556	710	880
Cum	5	24	84	206	412	716	1138	1694	2404	3284

C2	1	2	3	4	5	6	7	8	9	10
Num	10	38	82	146	226	326	442	578	730	902
Cum	11	49	131	277	503	829	1271	1849	2579	3481

Vertex symbols for selected sublattice

C1 Point (Schlafli) symbol:$\{4^5\cdot5\}$

Extended point symbol:[4·4·4·4·4·5(2)]

C2 Point (Schlafli) symbol:$\{3^6\cdot4^{16}\cdot5^{11}\cdot6^{10}\cdot8^2\}$

Extended point symbol:

[3·3·3·3·3·3·4·4·4·4·4·4·4·4·4·4·4·4·4·4·4·4·4·5(2)·5(2)·5(2)·5(2)·5(2)·5(2)·5(2)·5(2)

·5(2)·5(2)·5(2)·6(2)·6(2)·6(5)·6(5)·6(5)·6(5)·6(5)·6(5)·6(5)·6(5)·8(20)·8(20)]

Point (Schlafli) symbol for net: $\{3^6\cdot4^{16}\cdot5^{11}\cdot6^{10}\cdot8^2\}\{4^5\cdot5\}_2$

4,10-c net with stoichiometry (4-*c*)$_2$(10-*c*); 2-nodal net

New topology, please contact the authors (78739 types in 10 databases)

Elapsed time: 19.67 sec.

References

1 G. M. Sheldrick, *SADABS, Program for Empirical Absorption Correction of Area Detector Data*; University of Göttingen: Göttingen, 1996.

2 G. M. Sheldrick, *SHELXS 97*, *Program for Crystal Structure Refinement*; University of Göttingen, Göttingen, 1997.

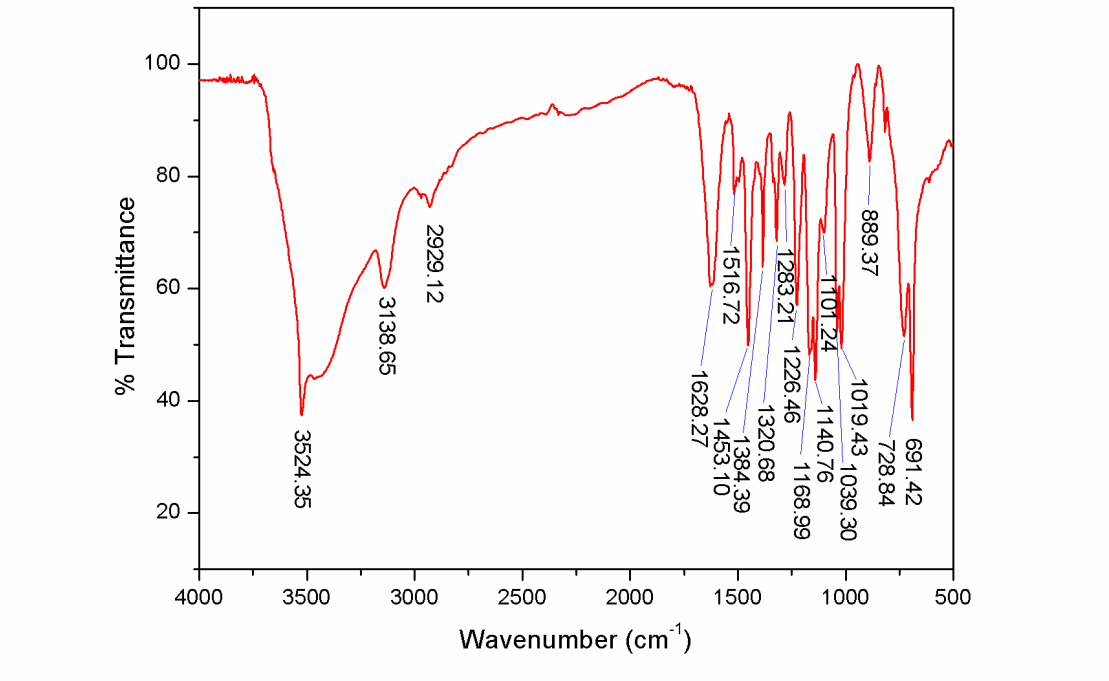

Fig. S1 The IR spectra of **1**

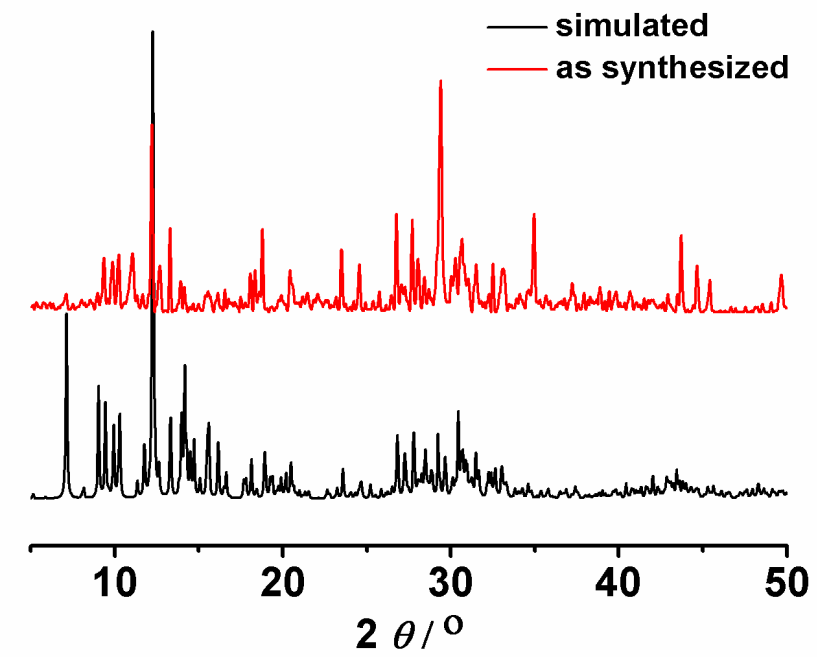

Fig. S2 The powder X-ray diffraction patterns for **1** measured at room temperature.

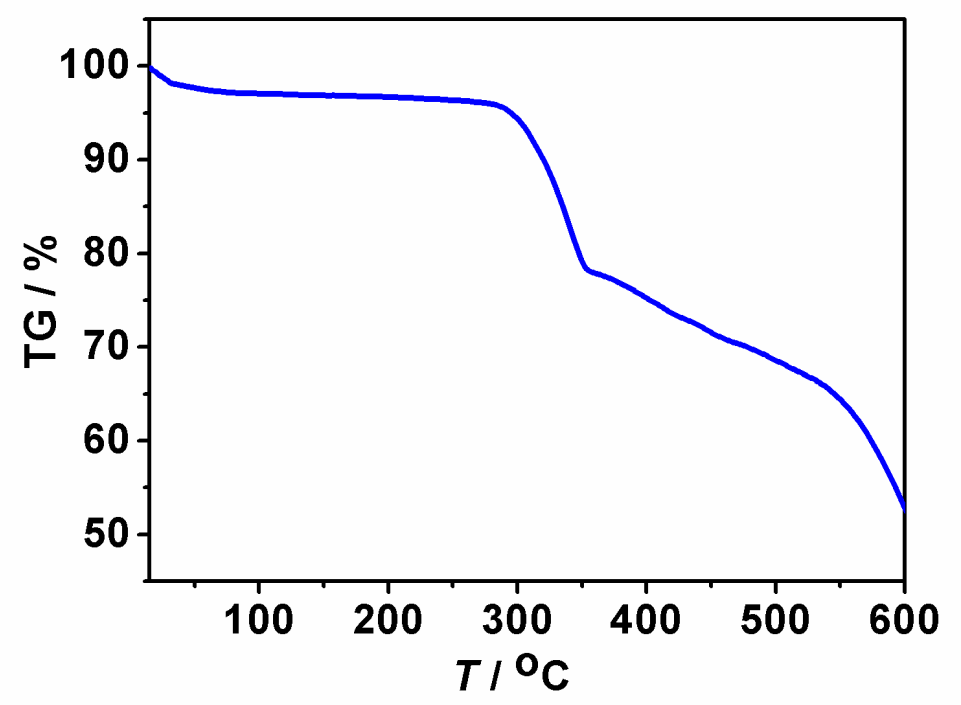

Fig. S3 The TGA curves for **1**.