Centrosymmetric and Chiral Porous Thorium Organic Frameworks Exhibiting Uncommon Thorium Coordination Environments

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Contents

S1. Elemental analysis. Elemental analyses (C, N, and H) were performed with a Vario EL CHNOS elemental analyzer.

Table S1. The elemental analysis for compound **2**.

Name	Wight. [mg]	Date Time	C/N Ratio	Content [%]	Peak Area	Daily Factor
Compound **2**	2.9510	15.10.15	15.38	N: 1.944	1940	0.9478
				C: 29.90	22607	0.9744
				H: 2.932	6381	1.0814

S2. Powder X-ray diffraction. PXRD data were collected from 5° to 50° with a step of 0.02° on a Bruker D8 Advance diffractometer with Cu Kα radiation (λ=1.54056 Å) and a Lynxeye one-Dimensional detector.

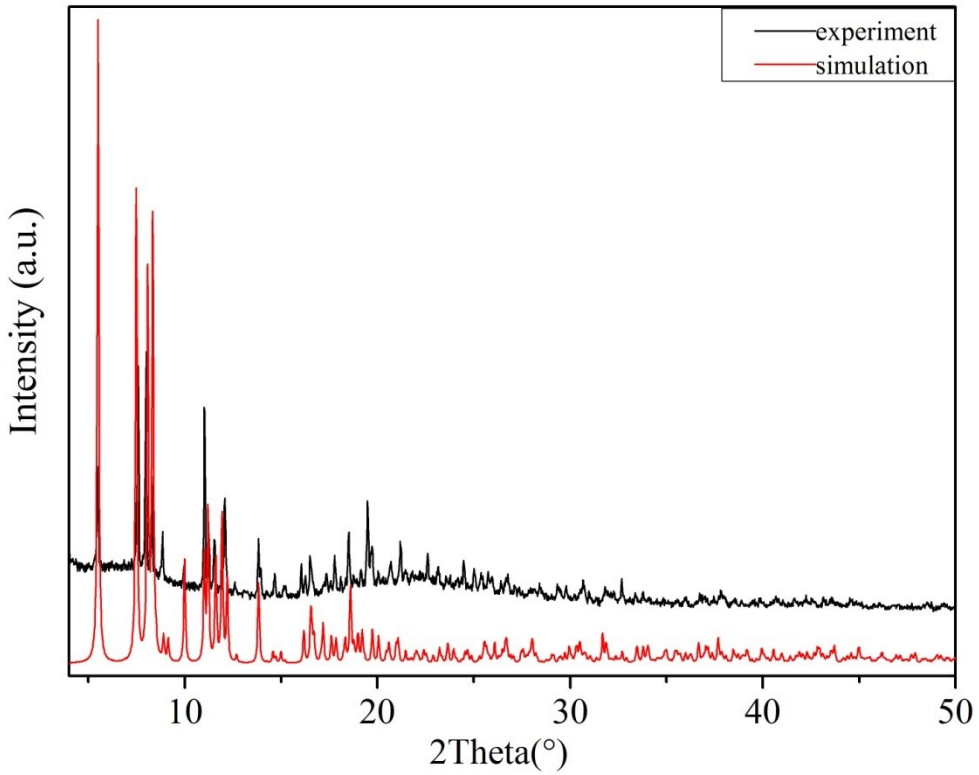

Figure S1. The powder X-ray diffraction (PXRD) for compound **2.**

S3. Thermogravimetric analysis. The compound 2 were heated at a rate 10 K/min in nitrogen from 30ºC to 900ºC. Only one weight loss step is observed in compound 2 (found. 23.8 %, cal. 34.7 %), which can be attributed to the lost of free water.

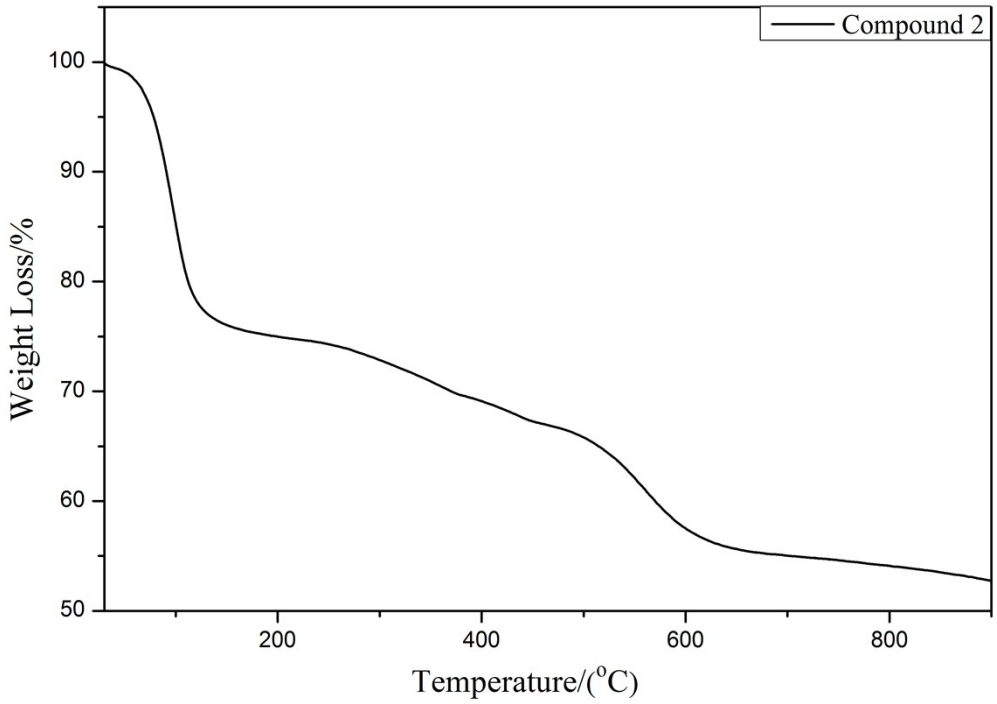

Figure S2. The TG curve for compound **2.**

S4. Surface area measurements. Volumetric gas adsorption measurements of compound 2 were measured at 77 K in a liquid nitrogen bath on a Quantachrome Autosorb Gas Sorption analyzer IQ2. The detecting pressures range from 0 to 760 Torr respectively. All the measurements were accomplished using ultra-high-purity N_2 (99.9999%). Methanol solution of $LiNO_3$ was added to the samples and soaked for 4 d to remove the solvent molecules. The sample was then treated with methanol to remove the excess $LiNO_3$. After decanting the methanol extract, the sample was dried at room temperature overnight. Before gas adsorption measurement, the sample was activated using the "outgas" function on the surface area analyzer for 10 h at 80℃.

S5. UV-vis absorption spectra.

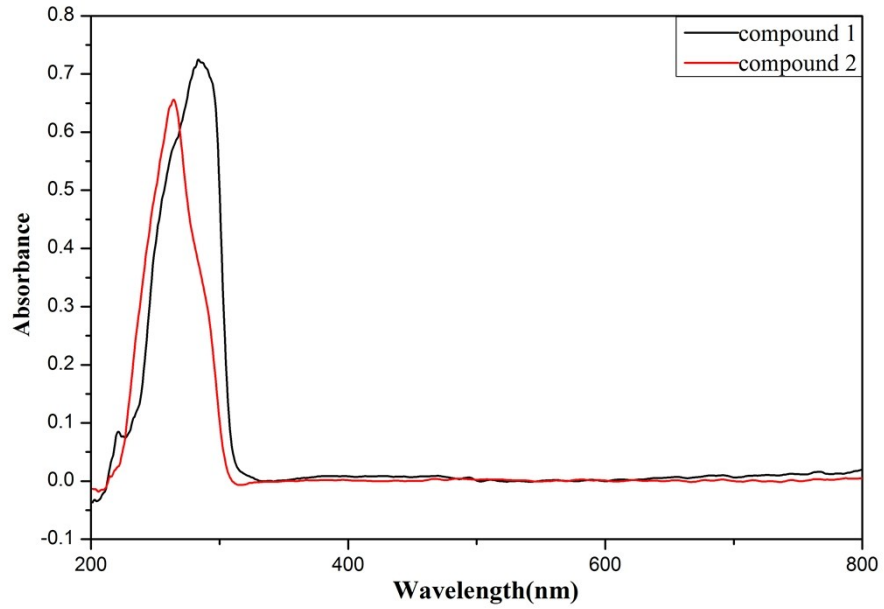

Figure S3. UV-vis absorption spectra for both compounds.

S6. Infrared spectrum

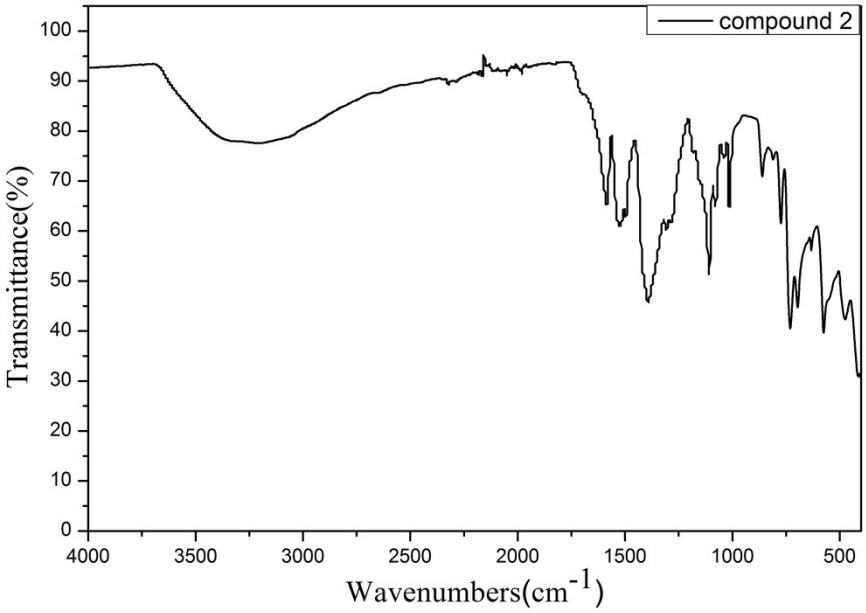

Figure S4. Infrared spectrum for compound **2**: 3307 cm^{-1} (s, water); 1588 cm^{-1} (s, C=C/C=N ring); 1390 cm^{-1} (s, P=O); 1108 cm^{-1} (s, C-H in-plane ring); 775 cm^{-1} (m, out-of-plane ring).[1,2]

Reference:

[1] K. Philipp, D. Richard, *Inorg. Chem.,* 2014, 43, 2803.

[2] D. Frank, J. Anne, B. Ingmar, *Eur. J. Org. Chem.,* 2008, 5571–5576.