ESI

Two unprecedented 10-connected bct topological metal-organic frameworks constructed from cadmium clusters

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Materials, Methods, Syntheses and Characterizations

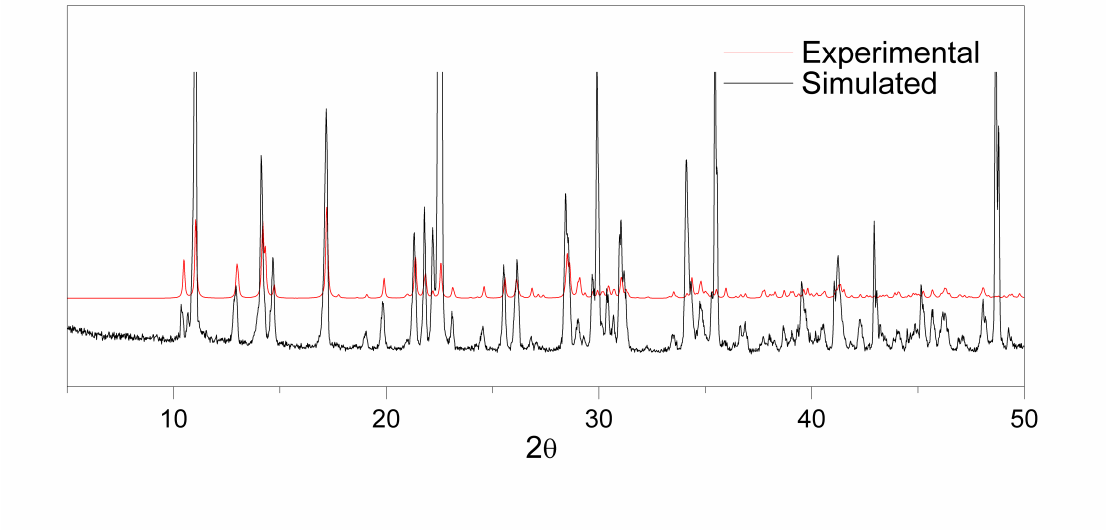
All the reagents for synthesis were obtained commercially and used as received.

The ligand 5-(4-pyridyl)tetrazole was prepared from NaN_3 and 4-cyanopyridine according to a reported procedure [Detert, H.; Schollmeier, D. *Synthesis* **1999**, 999].

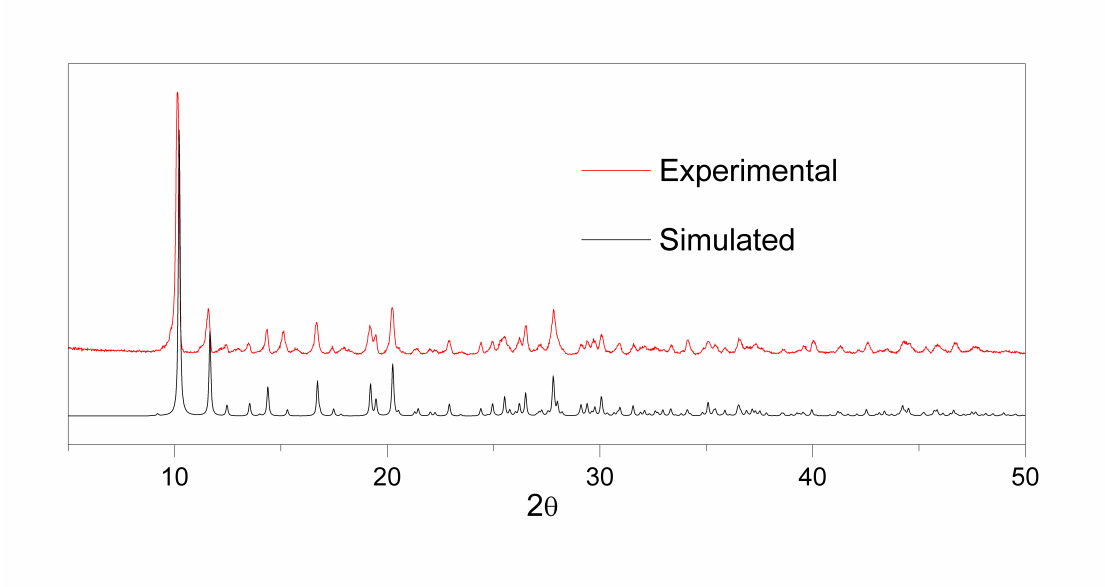
Elemental analyses were performed on a Perkin-Elmer 240C analyzer. The FT-IR spectra were recorded from KBr pellets in the range 4000-400 cm^{-1} on a TENSOR 27 (Bruker) spectrometer. Emission spectra in solid state at room temperature were taken on a Cary Eclips fluorescence spectrophotometer. The X-ray powder diffraction (XRPD) was recorded on a Rigaku D/Max-2500 diffractometer at 40 kV, 100 mA for a Cu target tube and a graphite monochromator. Simulation of the XRPD spectra was carried out by the single-crystal data and diffraction-crystal module of the commercially available *Cerius2* program (*Cerius2*, Molecular Simulation Incorporated, San Diego, CA, 2001). XRPD patterns are shown in Fig. S1. The thermogravimetric analysis (TGA) was done on a standard TG-DTA analyzer under air atmosphere at a heating rate of 10 °C/min for all measurements (Fig. S7). For **2**, the initial weight loss from 25 to 100°C may be ascribed to the surface absorption of moisture.

Single-crystal X-ray diffraction measurements for **1** and **2** were carried out on a scx-mini diffractometer equipped with a graphite crystal monochromator situated in the incident beam for

data collection at 293(2) K. Data collections and cell refinement were performed with RAPID-AUTO (Rigaku. *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan, 2004). Data reduction was carried out using CrystalStructure (Rigaku/MSC. CrystalStructure. Rigaku/MSC Inc. The Woodlands, Texas, USA, 2004). The structure was solved by direct methods using the SHELXS program of the SHELXTL package and refined with SHELXL (Sheldrick, G. M., *SHELXTL Version 6.1. Program for Solution and Refinement of Crystal Structures*, University of Göttingen, Germany, 1998). The final refinement was performed by full matrix least-squares methods with anisotropic thermal parameters for non-hydrogen atoms on F^2. Crystallographic data (excluding structure factors) for **1** and **2** have also been deposited on the Cambridge Crystallographic Data Centre as supplementary publication (no. CCDC 764835 - 764836).



(a)



(b)

Fig. S1 XRPD patterns for **1** (a) and **2** (b).

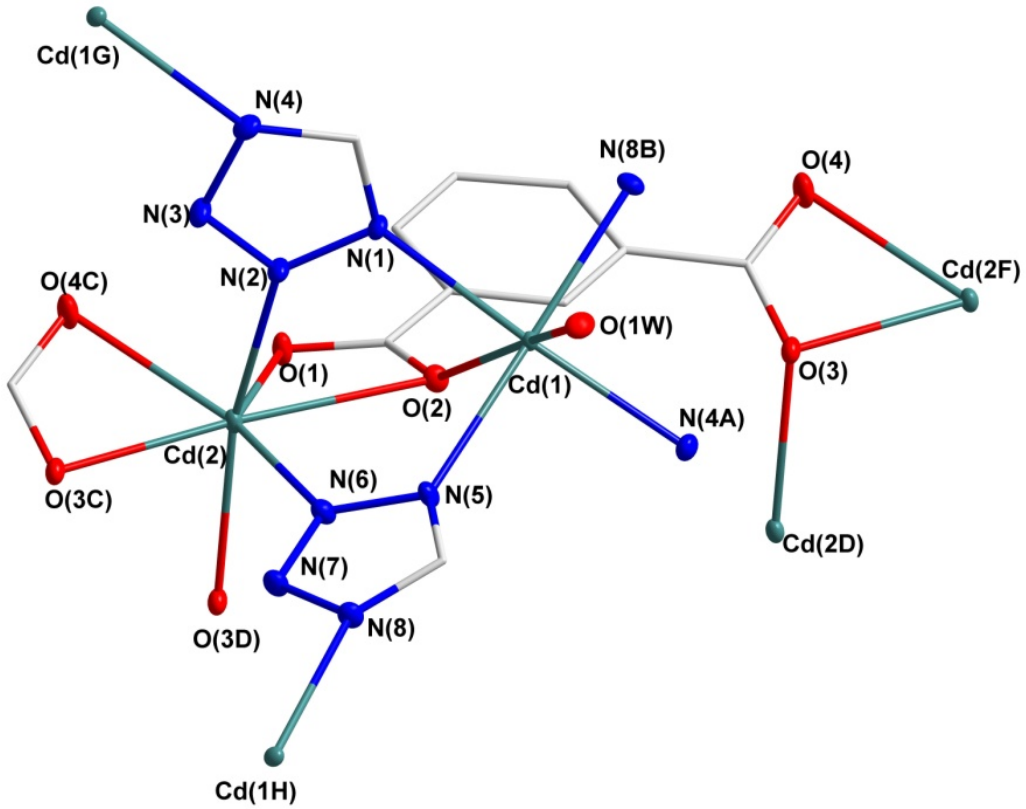


Fig. S2 Linkage and coordination mode in **1** (Symmetry codes: A: x, -y+3/2, z-1/2; B: x-1, -y+3/2, z-1/2; C: x+1, y, z+1; D: -x+2, -y+1, -z; F: x-1, y, z-1; G: x, -y+3/2, z+1/2; H: x+1, -y+3/2, z+1/2).

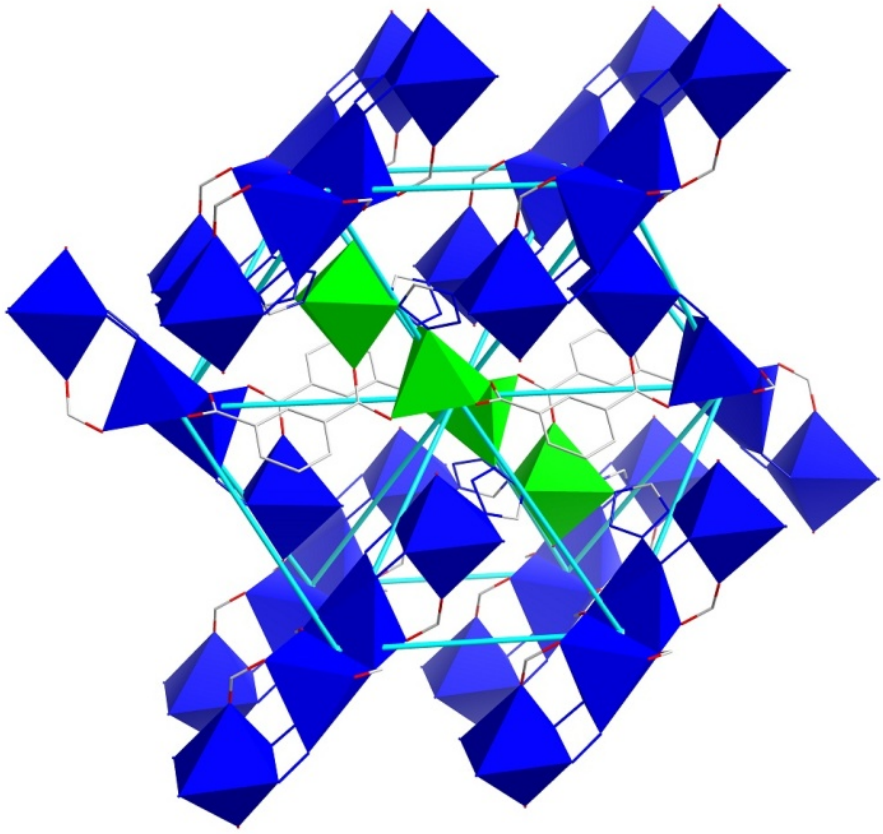


Fig. S3 View of the linkages of a tetranuclear cadmium core (green) with ten adjacent cores (blue) in **1**.

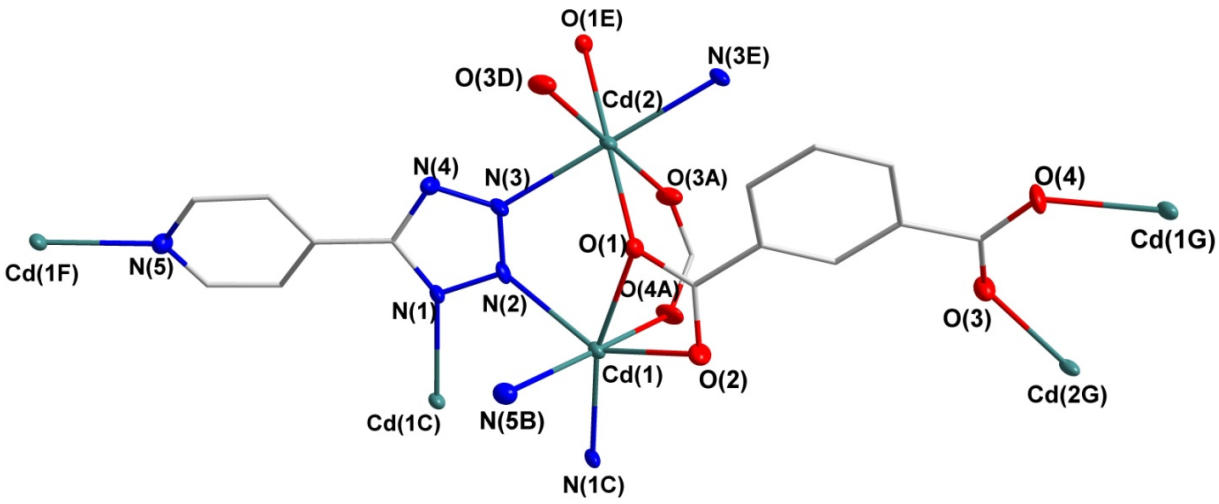


Fig. S4 Linkage and coordination mode in **2** (Symmetry codes: A: -x+1, y-1/2, -z-1/2; B: -x+2, y+1/2, -z+1/2; C: -x+2, -y+1, -z; D: x, -y+3/2, z+1/2; E: -x+1, -y+1, -z; F: -x+2, y-1/2, -z+1/2; G: -x+1, y+1/2, -z-1/2).

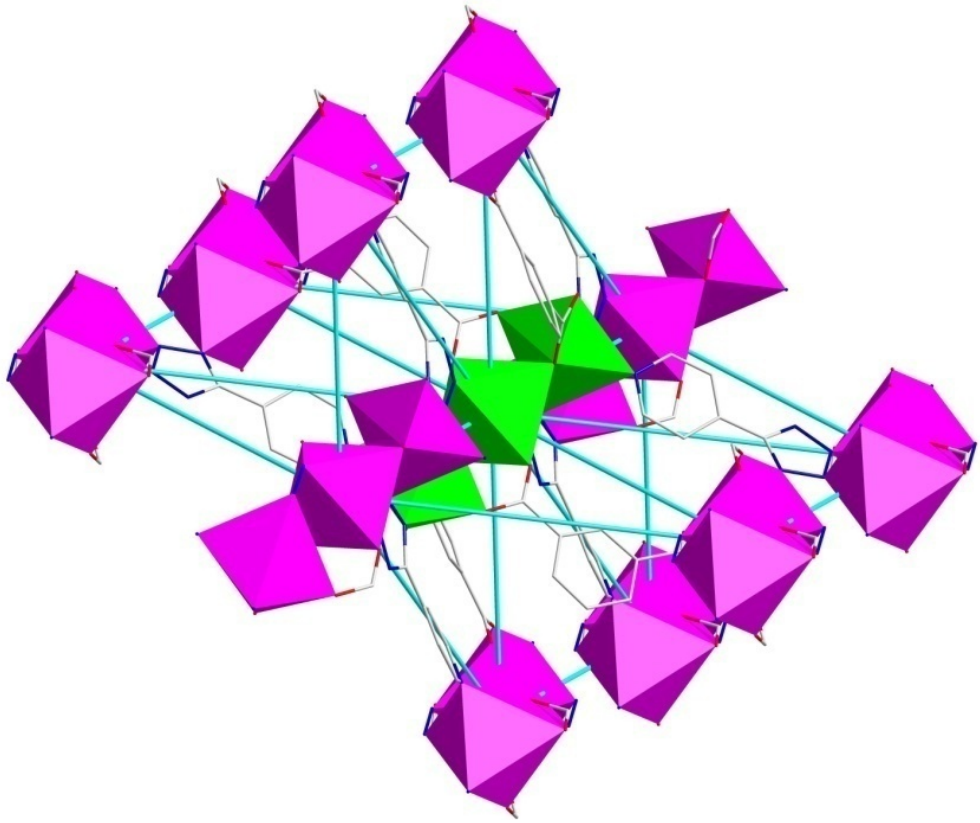


Fig. S5 View of the linkages of a trinuclear cadmium core (green) with ten adjacent cores (pink) in **2**.

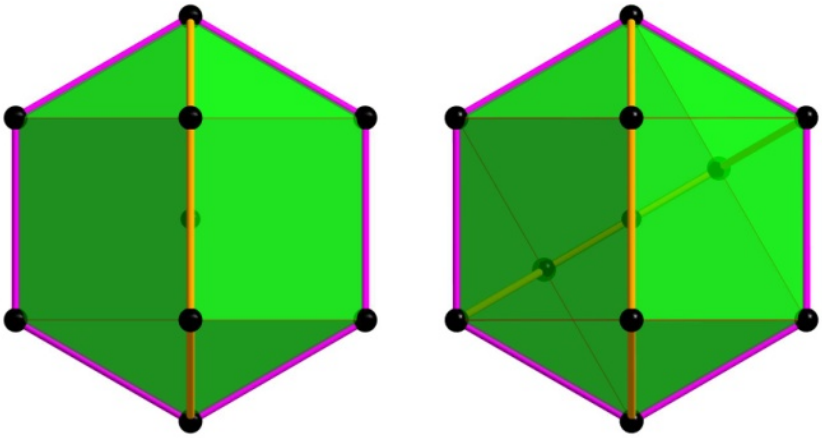
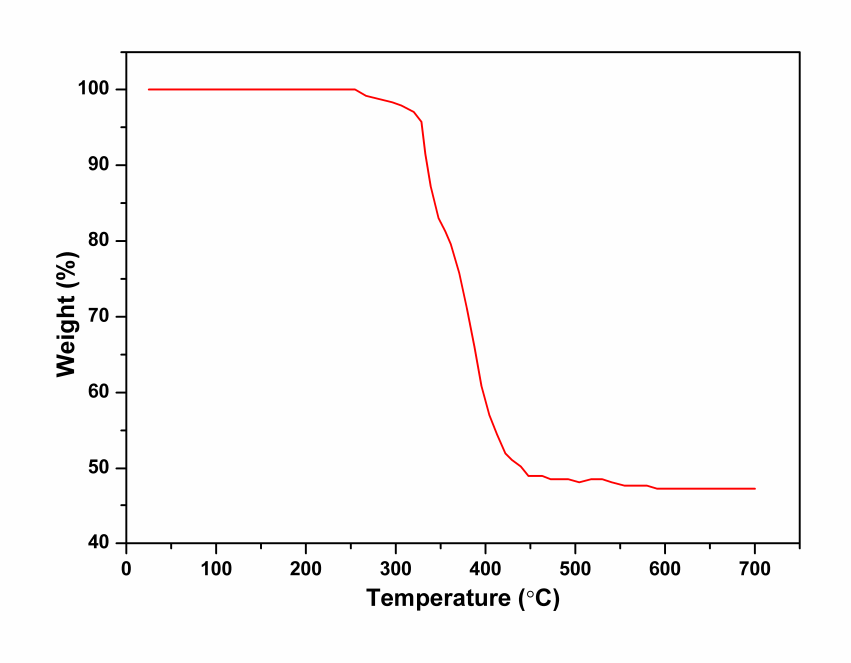
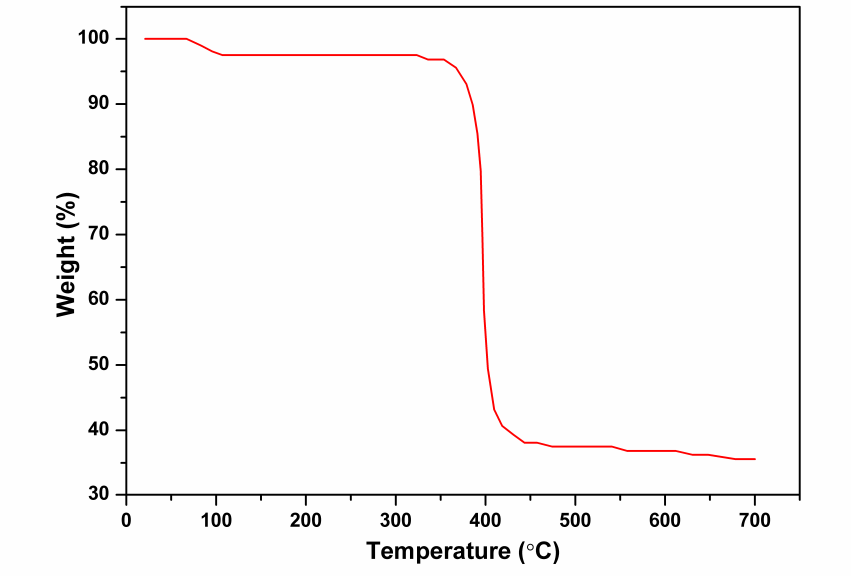


Fig. S6 The relations between the dodecahedral building unit in **bct** (left) and **gpu** (right) nets.



(a)



(b)

Fig. S7 Thermogravimetric curves for: (a) **1**, (b) **2**.

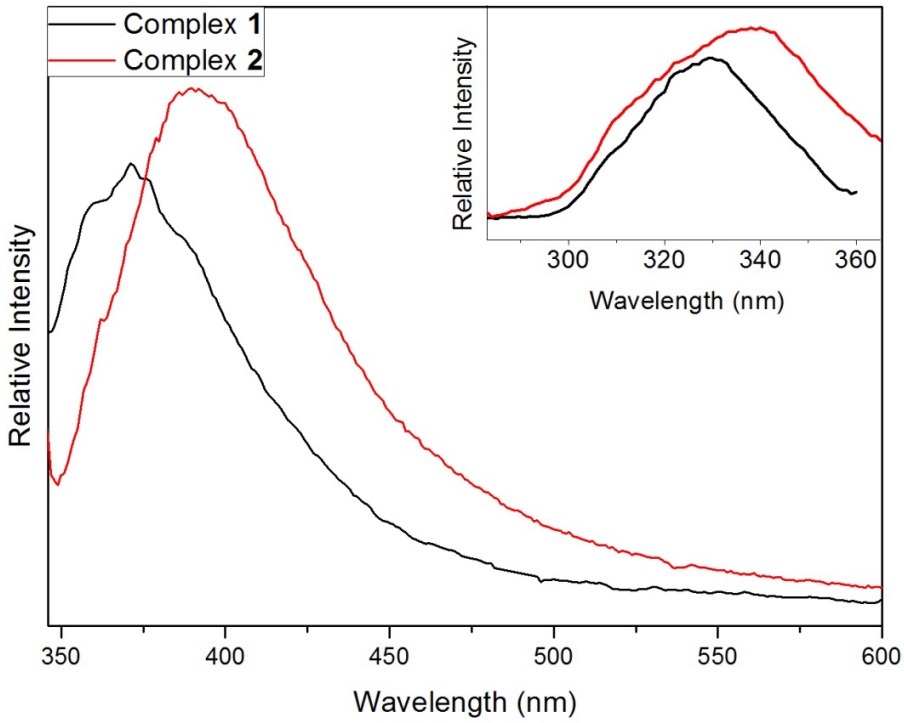


Fig. S8 Photoluminescence spectra and excitation spectra (inset) of **1** and **2** in the solid state at room temperature.