

Supporting Information

An Unprecedented (3,10)-Connected 2-D Metal-Organic Framework Constructed from Octanuclear Cobalt(II) Clusters and a New Bifunctional Ligand

Wen-Qiang Zou,^{†,‡} Ming-Sheng Wang,[†] Yan Li,^{†,‡} A-Qing Wu,^{†,‡} Fa-Kun Zheng,^{*,†} Qi-Yong Chen,^{†,‡} Guo-Cong Guo,^{*,†} and Jin-Shun Huang[†]

State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China, and Graduate School, Chinese Academy of Sciences, Beijing 100039, P. R. China

Lists of Supporting Information

S1: the crystallographic information file (CIF) of **1** (see the attached [complex 1.CIF](#) file)

S2: [Materials and Measurements](#)

S3: [Crystal structure analyses](#)

S4: [Scheme S1](#) showing coordination modes of the carboxylate groups in **1** (see below).

S5: [Figure S1](#) showing experimental and simulated powder X-ray diffraction patterns for **1** (see below).

S5: [Figure S2](#) showing TGA curve of **1**.

S6: [Figure S3](#) showing coordination modes of DCPPT ligands in **1** characterized with Harris notation (see below).

S7: [Figure S4](#) showing the “double-bridges” in **1** [a\)](#) and the (4,4) net constructed by them [b\)](#)

S7: [Figure S5](#) showing the interlayer π - π interactions of **1** along a direction. (see below).

* Author to whom correspondence should be addressed. E-mail: zfk@fjirsm.ac.cn

† State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China

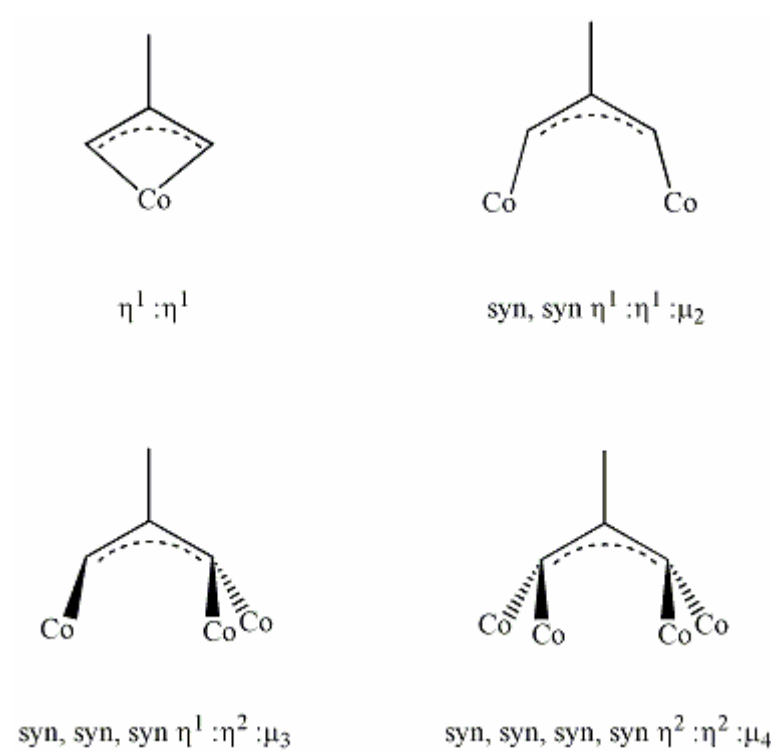
‡ Graduate School of Chinese Academy of Sciences, Beijing 100039, P. R. China

Materials and Measurements. All the chemicals except DCPPT were used as purchased without further purification. The powder X-ray diffraction pattern was collected with a Rigaku DMAX2500 diffractometer at 40 kV and 100 mA for Cu- $K\alpha$ ($\lambda = 1.5406 \text{ \AA}$), with a scan speed of $5^\circ/\text{min}$ at room temperature. The simulated pattern was produced using the Mercury program and single-crystal reflection diffraction data. Magnetic susceptibilities were measured by using a Quantum Design MPMS-7 super-conducting quantum interference device (SQUID) magnetometer in the temperature range of 5–300 K at a field of 1.0T, and diamagnetic corrections were made using Pascal's constants. Elemental analyses (C, H, N) were determined on an Elementar Vario ELIII analyzer. IR spectra were measured as KBr pellets on a Nicolet Magna 750 FT-IR spectrometer in the range of $400\text{--}4000 \text{ cm}^{-1}$.

Crystal structure analyses. The intensity data sets for the same crystal before and after UV irradiation were collected on a Saturn 70-CCD diffractometer equipped with a graphite monochromated Mo $K\alpha$ radiation ($\lambda = 0.71073 \text{ \AA}$) using ω scan technique at 133(2) K. The data sets were reduced by CrystalClear program. ^[1] The structures were solved by direct methods using the Siemens SHELXTLTM Version 5 package of crystallographic software. ^[2] The difference Fourier maps based on these atomic positions yield the other non-hydrogen atoms. The structures were refined using full-matrix least-squares refinement on F^2 . The hydrogen atoms were allowed to ride on their respective parent atoms and included in the structure factor calculations with assigned isotropic thermal parameters. Thermogravimetric analyses were carried out on a NETZSCH STA 449C unit at a heating rate of $15^\circ\text{C}/\text{min}$ under a nitrogen atmosphere.

Reference:

- [1] Rigaku. *CrystalClear*, version 1.35; Rigaku Corp.: Tokyo, Japan, 2002.
- [2] Siemens. *SHELXTL*, version 5; Reference Manual; Siemens Energy & Automation Inc.: Madison, WI, 1994.



Scheme S1. Coordination modes of the carboxylate groups in **1**.

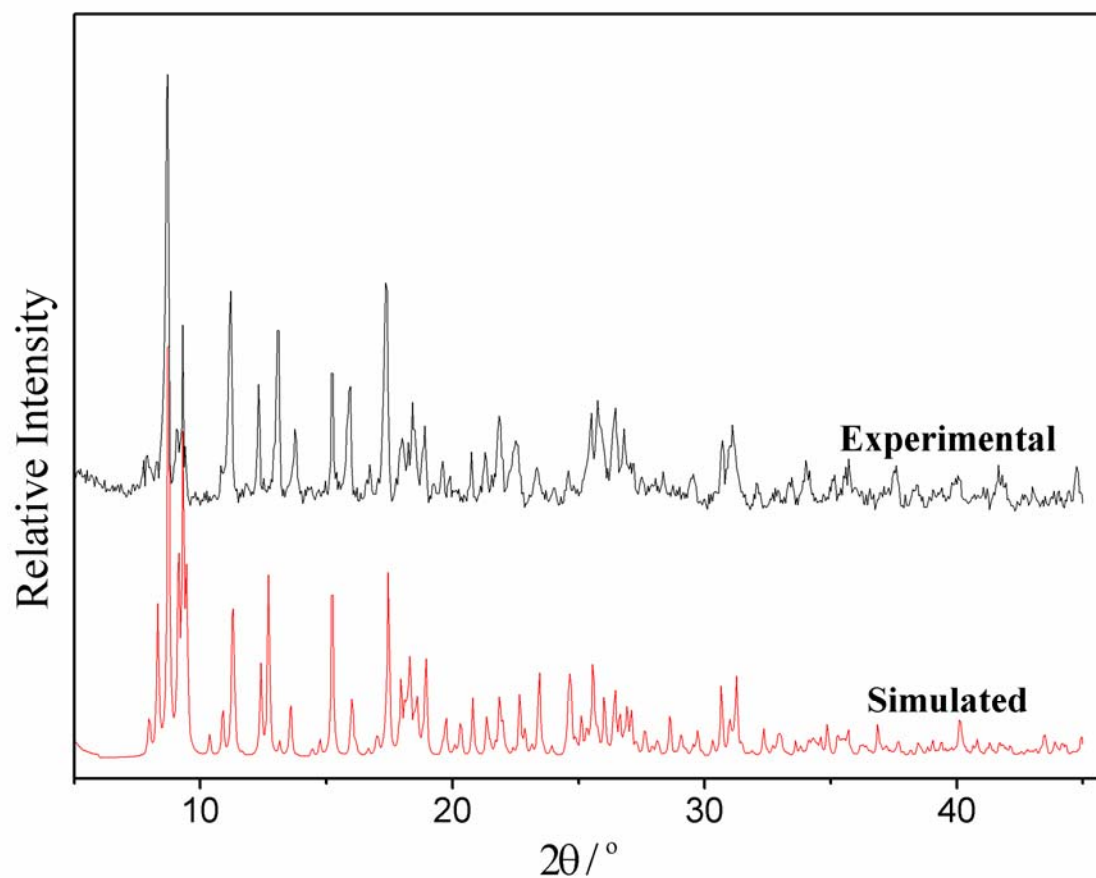


Figure S1. Experimental and simulated powder X-ray diffraction patterns for **1**

Notes: The most intense peaks observed in the X-ray powder diffraction patterns are consistent with those calculated from single-crystal diffraction data.

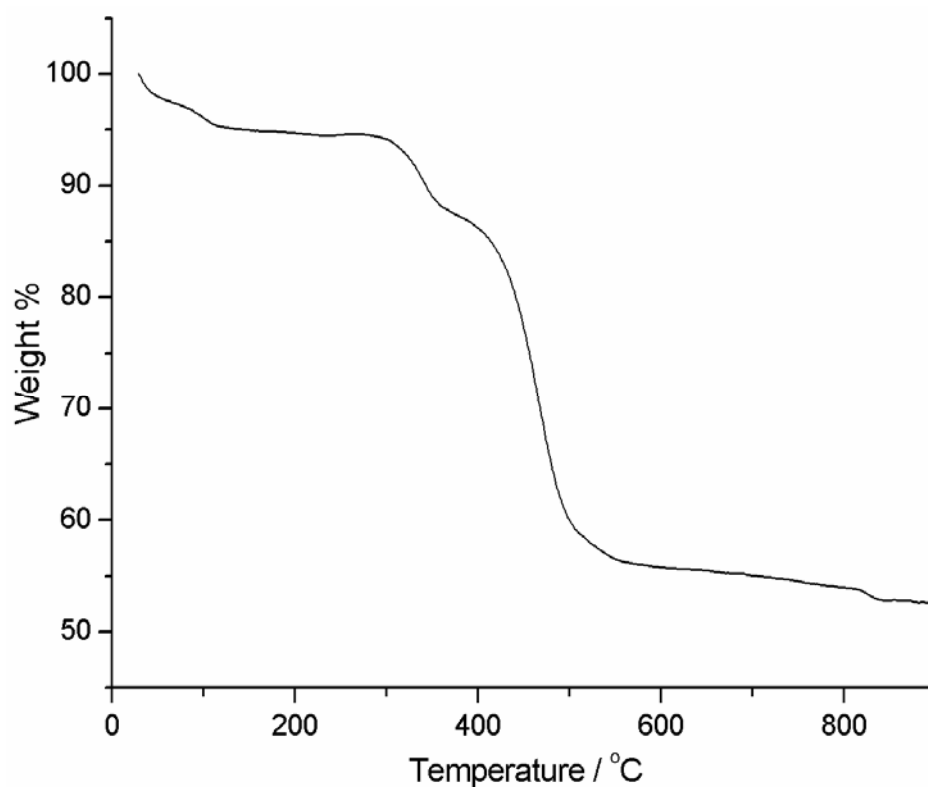


Figure S2. TGA curve of **1**

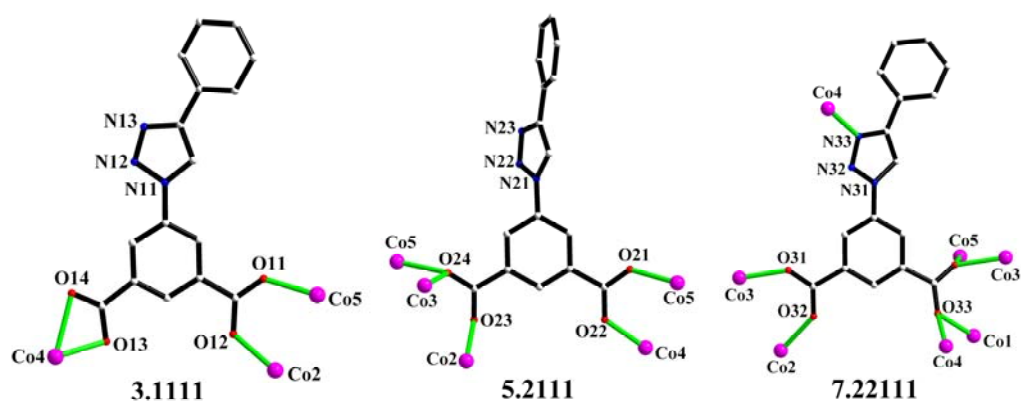


Figure S3. Coordination modes of DCPPT ligands in **1** characterized with Harris notation.

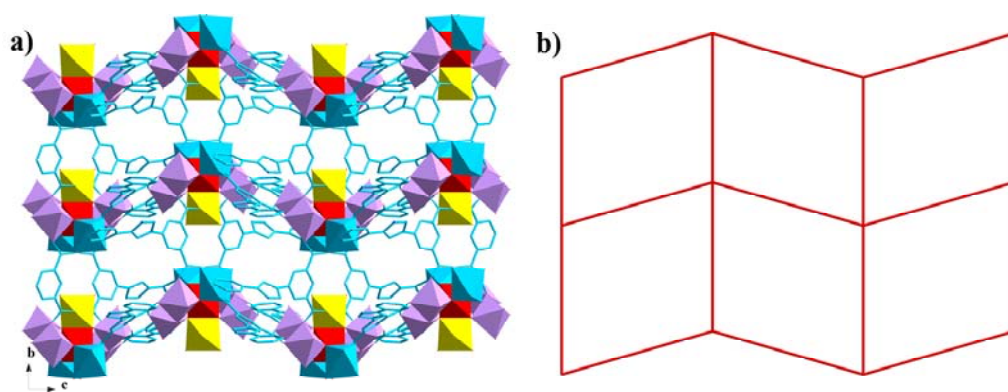


Figure S4. The “double-bridges” in **1** **a)** and the (4,4) net constructed by them **b)**.

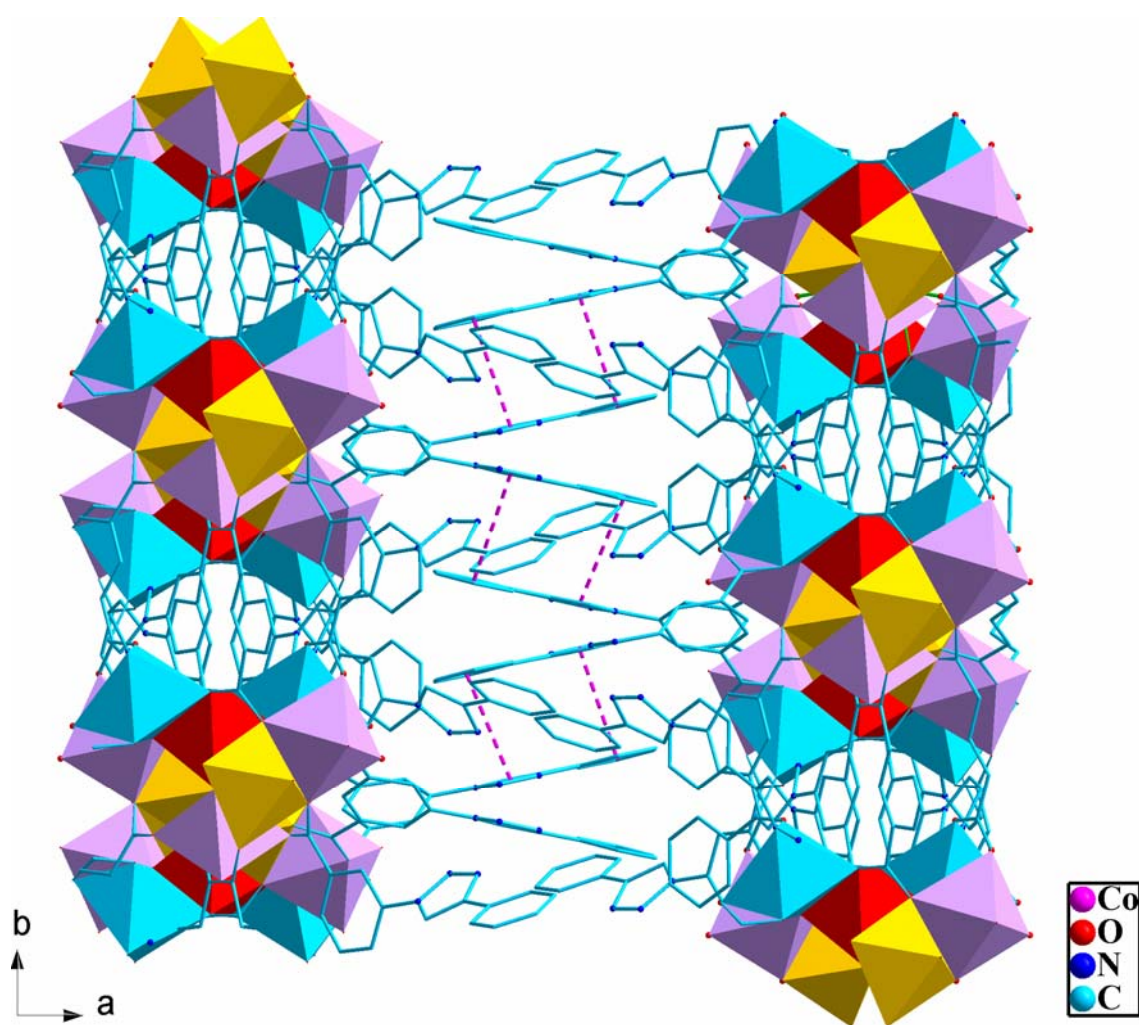


Figure S5. The interlayer π - π interactions of **1** along a direction.