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Crystallographic report

Crystal structure of a one-dimensional zinc(II) coordination polymer containing 4,4′-biphenyldicarboxylate hemihydrate

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A one-dimensional zinc(II) coordination polymer has been constructed from zinc(II), 4,4′-biphenyldicarboxylate and pyridine in which each zinc(II) atom is coordinated by two pyridine ligands and two monodentate 4,4′-biphenyldicarboxylate ligands that define a distorted tetrahedral geometry. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: 4,4′-biphenyldicarboxylate; crystal structure; zinc; coordination polymer

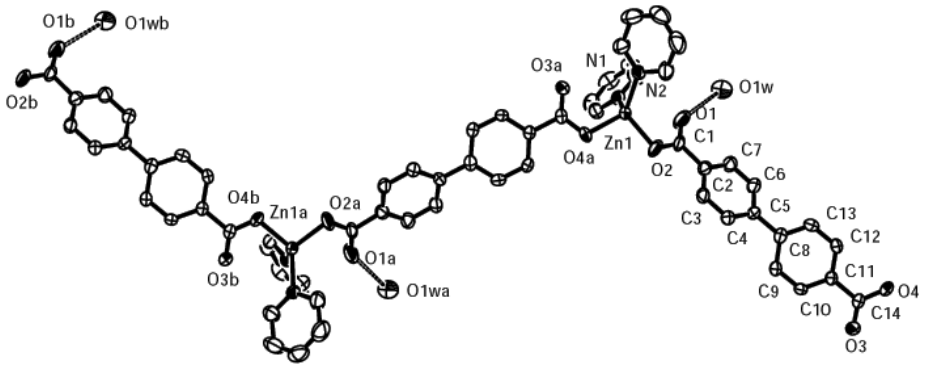

Figure 1. The one-dimensional chain structure of [Zn(pyridine)$_2$(4,4′-biphenyldicarboxylate)]·0.5H$_2$O. Key geometric parameters: Zn1–O2 1.986(3), Zn1–O4a 1.946(3), Zn1–N1 2.061(4), Zn1–N2 2.036(4) Å; O2–Zn1–N1 119.60(18), O2–Zn1–N2 111.45(17), O2–Zn1–O4a 99.28(16), O4a–Zn1–N1 103.87(16), O4a–Zn1–N2 120.93(16), N1–Zn1–N2 102.62(18)°. Hydrogen bond: O1w···O1c 2.809(7) Å. Symmetry operation: (a) $-x+1/4, y+1/4, z+1/4$, (b) $-x+1/4, y-1/4, z-1/4$.

COMMENT

Self-assembled metal coordination polymers formed through the deliberate selection of metal ions and multifunctional ligands have received considerable recent attention in materials chemistry, as they demonstrate intriguing network topologies and generate a new class of materials with potential functions.[1,2] However, to achieve a predictable combination of structural features remains a great challenge.[3,4] Herein, the construction of a one-dimensional coordination polymer from the dianion derived from the rigid ligand 4,4′-biphenyldicarboxylic acid and zinc(II) is reported. Crystallography shows zinc(II) exists in a distorted

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tetrahedral geometry defined by two pyridine ligands and one oxygen atom from each end of the bidentate bridging 4,4′-biphenyldicarboxylate. This arrangement generates a one-dimensional structure along the *c* axis, as shown in Fig. 1. The lattice water molecule hydrogen bonds to the non-coordinated oxygen atom of each carboxylate group (O1w $\cdots$ O1 = 2.809(7) Å; $-x+1, -y, z$).

EXPERIMENTAL

Synthesis

The title complex was synthesized by hydrothermal reaction of zinc nitrate (0.29 g, 1 mmol) and 4,4′-biphenyldicarboxylic acid (0.24 g, 1 mmol) in pyridine solution (15 ml) at around pH 6. The mixture was heated to 180 °C at a rate of 5 °C h^{-1}, was kept at this temperature for 100 h and then cooled to room temperature at a rate of 5 °C h^{-1}. Colorless crystals, suitable for X-ray crystallography, were obtained in a yield of 76% (0.36 g).

Crystallography

Intensity data were collected at 298 K on Smart Apex 2000 diffractometer for a colorless crystal $0.25 \times 0.34 \times 0.46$ mm^3. $C_{24}H_{19}N_2O_{4.50}Zn$, $M = 472.78$, orthorhombic, *Fdd*2, $a = 13.5612(18)$, $b = 52.231(7)$, $c = 11.9567(16)$ Å, $V = 8470(2)$ $Å^3$, $Z = 16$; 3945 unique data ($\theta = 26.0°$), 3856 data with $I > 2\sigma(I)$. $R_1 = 0.051$, $wR_2 = 0.120$; Flack parameter: 0.038(18), $\rho_{max} = 0.63$ e^- $Å^{-3}$. Programs used: SHELXL and ORTEP. CCDC deposition number: 200315.

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