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Crystallographic report

Diaqua(benzene-1,4-dioxyacetate)zinc(II): a one-dimensional zigzag chain

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The zinc(II) atom in the crystal structure of the title coordination polymer, $[Zn(p\text{-BDOA})\cdot 2H_2O]_n$ (p-$BDOA^{2-}$ = benzene-1,4-dioxyacetate), exists in a distorted trigonal prismatic geometry. Adjacent zinc(II) ions are linked by the p-$BDOA^{2-}$ ligands to furnish a one-dimensional (1-D) zigzag chain. A three-dimensional (3-D) network structure is stabilized by extended hydrogen bonds. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; zinc(II) coordination polymer; benzene-1,4-dioxyacetate; 1-D chain structure

COMMENT

Considerable effort has been devoted to the assembly of coordination polymers, and in this context a number of zinc carboxylate coordination polymers have been reported.[1–3] However, there is little knowledge of the coordination polymers with the flexible phendioxyacetic acid ligand.[4] Here, we report the synthesis and crystal structure of a coordination polymer, $[Zn(p\text{-BDOA})\cdot 2H_2O]_n$ (p-$BDOA^{2-}$ = benzene-1,4-dioxyacetate). In the structure, the zinc atom is located on a two-fold axis and the p-$BDOA^{2-}$ ligand is situated about a center of inversion. The zinc(II) atom is six-coordinate with a distorted trigonal prismatic geometry, being defined by four carboxylate oxygen atoms, of two bidentate chelating p-$BDOA^{2-}$ ligands, and two water molecules; Fig. 1. Each p-$BDOA^{2-}$ ligand connects two zinc(II) atoms through the carboxylate oxygen in an anti–anti configuration, and this leads to the formation of 1-D zigzag chains along the c axis; Fig. 2. In the chain, the adjacent Zn···Zn distance is 14.955(3) Å, and the interval Zn···Zn distance is 21.112(3) Å. A 3-D network structure is constructed by the intermolecular hydrogen bonds involving the water molecules and the oxygen atoms of the carboxyl groups.

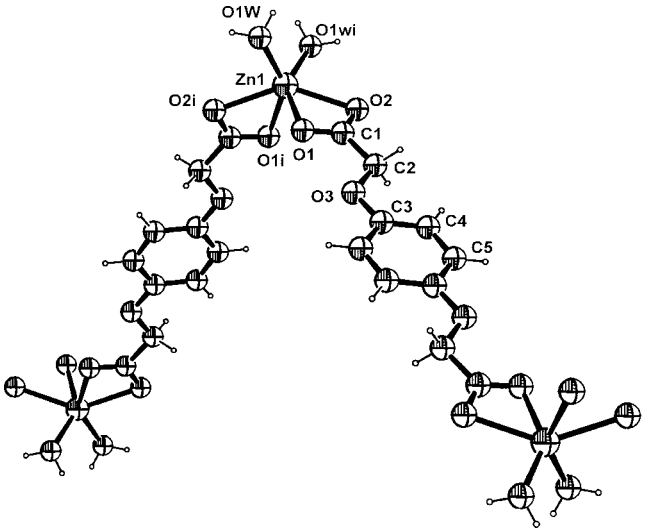

Figure 1. ORTEP plot of $[Zn(p\text{-BDOA})\cdot 2H_2O]_n$ with 30% probability ellipsoids. Key geometric parameters: Zn1–O1w 2.000(2), Zn1–O1 2.130(2), Zn1–O2 2.327(2) Å; O1w–Zn1–O1w^{i} 94.1(1), O1w–Zn1–O1^{i} 142.53(6), O1w–Zn1–O1 99.00(8), O1w–Zn1–O2^{i} 84.80(6), O1w–Zn1–O2 122.19(7), O1^{i}–Zn1–O1 91.61(8), O1–Zn1–O2 58.54(6), O1–Zn1–O2^{i} 94.00(6), O(2)^{i}–Zn(1)–O(2) 142.15(8)°. Symmetry operation i: $1-x$, y, $1/2-z$.

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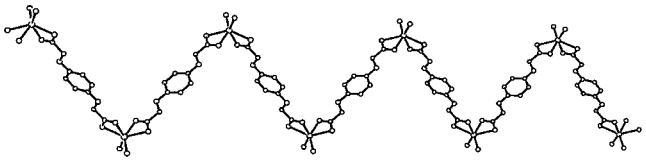

Figure 2. Packing diagram of $[Zn(p\text{-}BDOA)\cdot 2H_2O]_n$ along the *a* axis.

EXPERIMENTAL

An aqueous solution of zinc(II) acetate dihydrate (20 mmol) was slowly added to an aqueous solution of benzene-1,4-dioxyacetic acid (9.04 g, 40 mmol) and adjusted to pH 6 with 0.1 M sodium hydroxide. Colorless crystals were isolated from the filtered solution over several days. Anal. Found: C, 36.32; H, 6.19. Calc. for $C_{10}H_{12}O_8Zn$: C, 36.89; H, 3.72%. Intensity data were collected at 293 K on a Rigaku Raxis-Rapid diffractometer for a crystal $0.13 \times 0.22 \times 0.31$ mm^3. $C_{10}H_{12}O_8Zn$, $M = 325.59$, monoclinic, $C2/c$, $a = 11.611(2)$, $b = 5.2195(10)$, $c = 18.956(4)$ Å, $\beta = 96.32(3)°$, $V = 1141.8(4)$ Å^3, $Z = 4$; 1316 unique data ($\theta = 27.5$), 1102 data with $I \geq 2\sigma(I)$, $R_1 = 0.030$ (obs. data), $wR_2 = 0.077$ (all data). Programs used: SHELXL and ORTEPII. CCDC deposition number: 21 9643.

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