Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[diaquazinc(II)-μ-benzene-1,3-dioxyacetate] dihydrate]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
H-atom completeness 51%
R factor = 0.038
wR factor = 0.093
Data-to-parameter ratio = 9.2

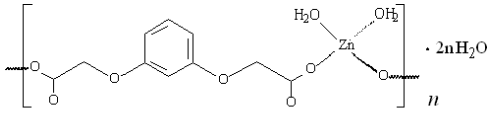
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 19 November 2003
Accepted 18 December 2003
Online 10 January 2004

The title coordination polymer, $\{[Zn(C_{10}H_8O_6)(H_2O)_2]\cdot 2H_2O\}_n$, was synthesized and characterized by X-ray crystallography. The crystal structure reveals the asymmetric unit to consist of the zinc(II) complex $[Zn(1,3\text{-BDOA})(H_2O)_2]$ and two uncoordinated water molecules. The zinc(II) ion displays a four-coordinate distorted tetrahedral geometry, formed by two carboxylate O atoms of two benzene-1,3-dioxyacetate ligands and two coordinated water molecules. The zinc(II) ions are bridged by carboxylate groups, forming a one-dimensional chain structure. The Zn—O bond distances lie in the range 1.941 (4)–1.981 (4) Å and the Zn···Zn separation within the polymer is 14.627 (3) Å.

Comment

Coordination polymers have been of great interest, due not only to their fascinating structural diversity, but also to their potential applications. Phenylenedioxydiacetic acids, which have been known to show biological activities and are widely used in agriculture, are a family of flexible multidentate ligands with versatile binding ability. The structures of several divalent metal complexes with the benzene-1,2-dioxyacetate acid ligand have been reported (McCann *et al.*, 1995, 1996; Kennard *et al.*, 1984, 1986). They are either six- or seven-coordinate. The zinc(II) complex with benzene-1,2-dioxyacetate has been reported previously (Smith *et al.*, 1987); the Zn^{II} atom is in a pentagonal bipyramidal geometry. However, complexes of benzene-1,3-dioxyacetate are rare. Recently, we synthesized a new zinc(II) coordination polymer, (I), with the benzene-1,3-dioxyacetate ligand, in which the zinc(II) ion center has a tetrahedral geometry.



(I)

As shown in Fig. 1, the structure of the coordination polymer consists of the zinc(II) complex $[Zn(1,3\text{-BDOA})(H_2O)_2]$ and uncoordinated water molecules. The average Zn—O(carboxylate) length is 1.946 (4) Å, which is slightly shorter than the average Zn—O(H_2O) distance of 1.963 (4) Å. Each benzene-1,3-dioxyacetate acts as a bidentate ligand, linking two zinc(II) ions through the carboxylate O atoms. As a result, one-dimensional infinite chains are formed (see Fig. 2). The Zn···Zn separation in the chain is 14.627 (3) Å. In addition, the chains are connected through intermolecular hydrogen bonds, formed between the water molecules and carboxylate O atoms, yielding a hydrogen-bonding network.

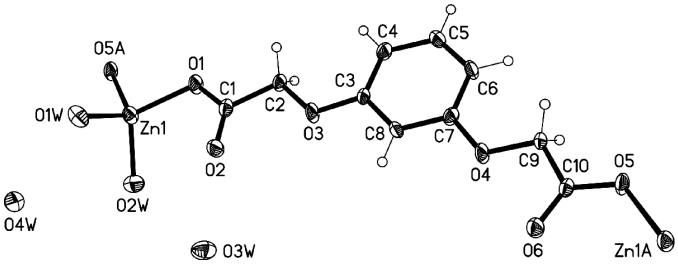


Figure 1
View of the title compound, (I), showing 30% probability ellipsoids and the atom labeling. The suffix *A* denotes a symmetry-generated atom.

Experimental

An aqueous solution (30 ml) of zinc(II) acetate dihydrate (20 mmol) was slowly added to an aqueous solution (20 ml) of sodium benzene-1,3-dioxyacetate (35 mmol). Colorless transparent single crystals were isolated over a period of 6 d.

Crystal data

$[Zn(C_{10}H_8O_6)(H_2O)_2]\cdot 2H_2O$
$M_r = 361.60$
Orthorhombic, $Pna2_1$
$a = 8.604$ (2) Å
$b = 27.271$ (6) Å
$c = 5.914$ (1) Å
$V = 1387.7$ (5) Å^3
$Z = 4$
$D_x = 1.731$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12865 reflections
$\theta = 3.5$–$27.4°$
$\mu = 1.82$ mm^{-1}
$T = 293$ (2) K
Plate, colorless
0.24 × 0.14 × 0.08 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.669$, $T_{max} = 0.868$
13 514 measured reflections
1743 independent reflections
1329 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 27.5°$
$h = -11 \rightarrow 11$
$k = -35 \rightarrow 35$
$l = -7 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.093$
$S = 0.92$
1743 reflections
190 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.15$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}
Absolute structure: Flack (1983), 1201 Friedel pairs
Flack parameter = 0.07 (3)

Table 1
Selected geometric parameters (Å, °).

Zn1—O5^{i}	1.941 (4)	Zn1—O1	1.950 (4)
Zn1—O2*W*	1.945 (4)	Zn1—O1*W*	1.981 (4)
O5^{i}—Zn1—O2*W*	111.5 (2)	O2*W*—Zn1—O1	115.5 (2)
O5^{i}—Zn1—O1	99.4 (1)	O5^{i}—Zn1—O1*W*	112.5 (2)

Symmetry code: (i) $x-1, y, z-2$.

The water H atoms were not located. Other H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$, and were included in the final cycles of refinement using a riding model.

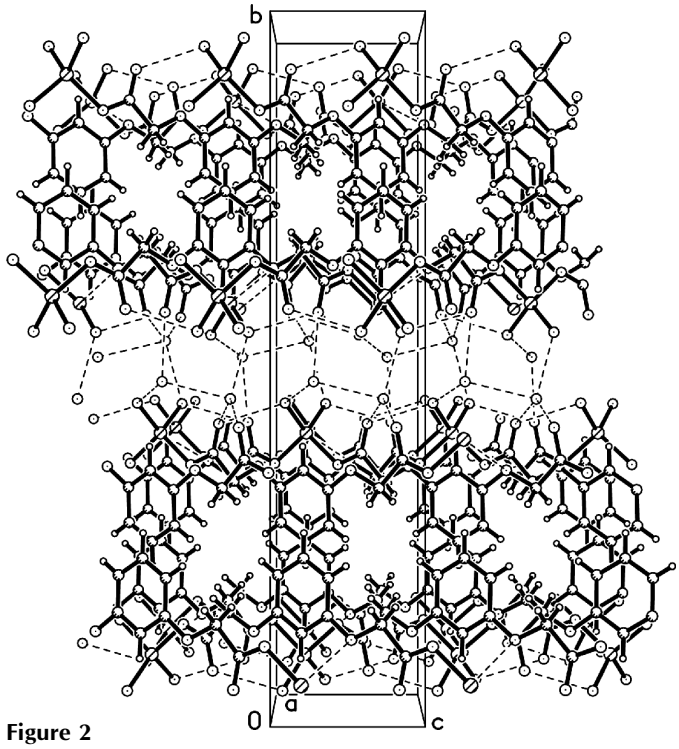


Figure 2
A crystal packing diagram for (I). Hydrogen bonds are shown as dashed lines.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXL*97; software used to prepare material for publication: *SHELXTL* (Sheldrick, 1997*b*).

The work was supported by the National Natural Science Foundation (No. 20101003) and Heilongjiang Province Natural Science Foundation (No. B0007).

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