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catena-Poly[tetraaquazinc(II)-μ-benzene-1,4-dioxyacetato-κ^2O:O']

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Key indicators

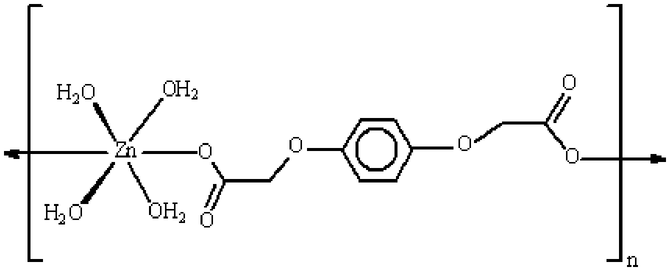
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.034
wR factor = 0.090
Data-to-parameter ratio = 14.0

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

In the title complex, $[Zn(1,4\text{-BDOA})(H_2O)_4]_n$ or $[Zn(C_{10}H_8O_6)(H_2O)_4]_n$ (where 1,4-BDOA^{2-} is the benzene-1,4-dioxyacetate dianion), the Zn^{II} atom and the 1,4-BDOA^{2-} ligand build up a one-dimensional polymer chain along c. The Zn^{II} atom, located on an inversion center, shows an octahedral coordination geometry, defined by two carboxyl O atoms of different benzene-1,4-dioxyacetate ligands and four water molecules. Adjacent Zn^{II} atoms are bridged by bis-monodentate carboxylate groups of the centrosymmetric 1,4-BDOA^{2-} ligands, to furnish the one-dimensional chain along the c axis; the Zn$\cdots$Zn separation within the polymer is 14.717 (3) Å. A hydrogen-bonded supramolecular architecture is formed *via* O—H$\cdots$O intermolecular hydrogen bonds.

Comment

Recently, we have reported some coordination polymers constructed by benzene-1,4-dioxyacetic acid (1,4-BDOAH$_2$), in which the 1,4-BDOA^{2-} group shows the capability of acting as bridging ligand in various coordination modes, including bidentate (Gao, Liu, Huo, Zhao & Ng, 2004*a*), tridentate (Gao, Liu, Huo, Zhao & Zhao, 2004*a*,*c*,*d*) and tetradentate (Gao, Liu, Huo, Zhao & Ng, 2004*b*). The $[Co(1,4\text{-BDOA})(H_2O)_4]_n$ polymer gives a good example of the 1,4-BDOA^{2-} dianion acting as a bidentate bridging ligand (Gao, Liu, Huo, Zhao & Zhao, 2004*b*). The title Zn^{II} complex, $[Zn(1,4\text{-BDOA})(H_2O)_4]_n$, (I), was synthesized under similar reaction conditions; complex (I) is isomorphous with the Co^{II} analog.



(I)

As shown in Fig. 1, the Zn^{II} atom and the centroid of the 1,4-BDOA^{2-} ligand occupy different inversion centers [($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$) for the Zn atom and ($-\frac{1}{2}$, $\frac{1}{2}$, 0) for the centroid of the ligand]. Each Zn^{II} atom is six-coordinated by two carboxyl O atoms from different 1,4-BDOA^{2-} ligands [Zn—O = 2.093 (2) Å] and four water molecules [mean Zn—O = 2.100 (2) Å], displaying an octahedral geometry. However, in the previously reported one-dimensional chain polymer, $[Zn(1,3\text{-BDOA})(H_2O)_2]_n$, (II), the Zn^{II} atom is four-coordinate, with a

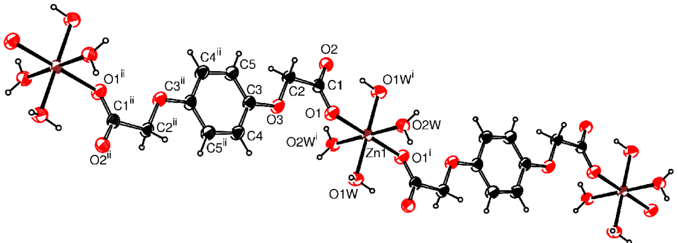


Figure 1
*ORTEP*III plot of (I), with the atom-numbering scheme. Displacement ellipsoids are shown at the 50% probability level. [Symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $-1 - x, 1 - y, -z$.]

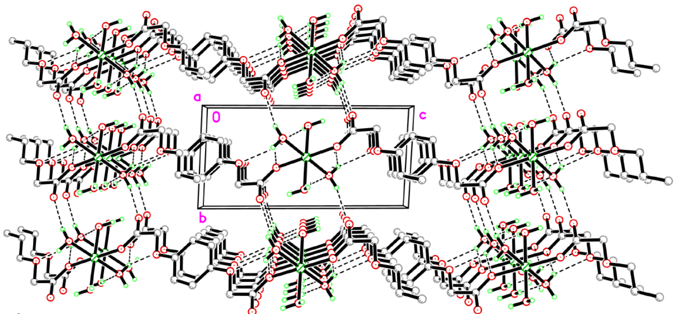


Figure 2
Packing diagram of the title complex showing the hydrogen-bonding network (dashed lines).

tetrahedral coordination sphere (Gao, Li *et al.*, 2004). In (I), the oxyacetate group and benzene ring are almost coplanar, with a C3—O3—C2—C1 torsion angle of −177.0 (2)°. Each 1,4-BDOA^{2-} group is in a bis-monodentate mode, bridging two Zn^{II} atoms and forming a one-dimensional chain along the *c* axis. In the chain, the shortest Zn···Zn distance of 14.717 (3) Å is somewhat longer than the shortest Co···Co distance [14.699 (2) Å] in the Co^{II} analog and the Zn···Zn distance [14.627 (3) Å] in (II). A hydrogen-bonded supramolecular network is constructed *via* O—H···O intermolecular hydrogen bonds, involving the water molecules and O atoms of the 1,4-BDOA^{2-} groups (Table 2 and Fig. 2).

Experimental

Benzene-1,4-dioxyacetic acid was prepared following the method described for the synthesis of benzene-1,2-dioxyacetic acid by Mirci (1990). The title complex was synthesized by the addition of zinc diacetate dihydrate (4.40 g, 20 mmol) and 3-hydroxypyridine (0.95 g,10 mmol) to a hot aqueous solution of 1,4-BDOAH$_2$ (4.52 g, 20 mmol). The solution was allowed to evaporate at room temperature, and colorless prismatic crystals were obtained after several days. Analysis calculated for $C_{10}H_{16}O_{10}Zn$: C 33.22, H 4.46%; found: C 33.40, H 4.39%.

Crystal data

$[Zn(C_{10}H_8O_6)(H_2O)_4]$
$M_r = 361.62$
Triclinic, $P\overline{1}$
$a = 4.9243$ (10) Å
$b = 5.7865$ (12) Å
$c = 11.843$ (2) Å
$\alpha = 92.21$ (3)°
$\beta = 95.08$ (3)°
$\gamma = 96.86$ (3)°
$V = 333.32$ (12) Å^3

$Z = 1$
$D_x = 1.801$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3048 reflections
$\theta = 3.9$–27.4°
$\mu = 1.89$ mm^{-1}
$T = 293$ (2) K
Prism, colorless
0.38 × 0.26 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.522$, $T_{max} = 0.712$
3198 measured reflections

1531 independent reflections
1475 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 27.5°$
$h = -6 \rightarrow 5$
$k = -7 \rightarrow 7$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.090$
$S = 1.02$
1531 reflections
109 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0685P)^2 + 0.0789P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.76$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.093 (2)	O1—C1	1.256 (3)
Zn1—O1*W*	2.051 (2)	O2—C1	1.254 (3)
Zn1—O2*W*	2.148 (2)		
O1^i—Zn1—O1	180	O1*W*^{i}—Zn1—O1*W*	180
O1^i—Zn1—O2*W*	91.72 (6)	O1*W*—Zn1—O2*W*	90.75 (7)
O1—Zn1—O2*W*	88.28 (6)	O1*W*^{i}—Zn1—O2*W*	89.25 (7)
O1*W*—Zn1—O1	88.40 (7)	O2*W*—Zn1—O2*W*^{i}	180
O1*W*^{i}—Zn1—O1	91.60 (7)		

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

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O2^i	0.85 (2)	1.91 (2)	2.694 (2)	154 (3)
O1*W*—H1*W*2···O2*W*^{iii}	0.84 (2)	2.07 (2)	2.855 (2)	155 (2)
O2*W*—H2*W*1···O1^{iii}	0.84 (2)	2.19 (2)	2.864 (2)	137 (2)
O2*W*—H2*W*1···O3^{iii}	0.84 (2)	2.23 (2)	2.985 (2)	150 (2)
O2*W*—H2*W*2···O2^{iv}	0.84 (2)	1.93 (2)	2.735 (2)	162 (3)

Symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (iii) $-x, 1 - y, 1 - z$; (iv) $1 - x, 2 - y, 1 - z$.

C-bound H atoms were placed in calculated positions and were refined in the riding-model approximation, with C—H = 0.93 or 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms of water molecules were located in a difference map and refined with O—H and H···H distance restraints of 0.85 (1) and 1.39 (1) Å, respectively, and $U_{iso}(H) = 1.5U_{eq}(O)$.

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC & Rigaku Corporation, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXS*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL*97.

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