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catena-Poly[[aquazinc(II)]-*μ*-2-carboxylato-phenoxyacetato]

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Key indicators

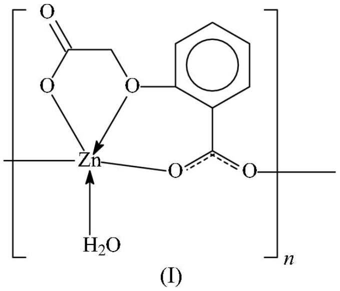
Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.022
wR factor = 0.060
Data-to-parameter ratio = 13.7

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

The $-OCH_2CO_2$ arm of the ligand in the title compound, $[Zn(C_9H_6O_5)(H_2O)]_n$, uses the single-bond carboxyl O atom, as well as the ether O atom, to chelate to the Zn atom; the other $-CO_2$ arm bridges adjacent Zn atoms into a helical chain that propagates by means of a 2_1 screw axis. The $-OCH_2CO_2$ arm features distinct single- and double-bond C—O distances; in the other $-CO_2$ arm, the C—O distances are interpreted in terms of a delocalized carboxyl group. The coordination about zinc is completed by a water molecule, resulting a distorted ZnO_5 square-pyramidal arrangement in which the apical position is occupied by water.

Comment

A number of divalent first-row transition metal derivatives of the isomeric carboxyphenoxyacetic acids have been crystallographically authenticated. Derivatives of the 4-isomer include the hydrated Mn (Gu *et al.*, 2004; Huo *et al.*, 2005), Co (Kennard *et al.*, 1984), Ni (Chen *et al.*, 2004; Kennard *et al.*, 1984) and Cu (Gao, Yue *et al.*, 2004) complexes; the derivatives of the 3-isomer, the Co (Li *et al.*, 2004) and Ni (Gao, Liu *et al.*, 2004) complexes, also exist as water-coordinated compounds. Only one derivative of the 2-isomer, a tetraaquacopper compound, has been reported (Kennard *et al.*, 1986).



(I)

The present monoaqua derivative of zinc, (I), represents a variation on the hitherto reported motifs as the metal atom is chelated by the oxyacetate $-OCH_2CO_2$ arm of the $O_2C-C_6H_4-OCH_2$ dianion (Fig. 1), the ether O atom (O3) to zinc dative interaction being surprisingly short at 2.268 (1) Å. The $-OCH_2CO_2$ and $-CO_2$ groups both engage in bridging; however, whereas the first of these features long and short C—O distances, the two C—O bond lengths in the latter group are indistinguishable from each other (Table 1). This ligand-bonding motif results in a polymeric chain propagating along [010] (Fig. 2). The Zn atom is displaced out of the square plane formed by atoms O1, O2^{i} (see Table 1 for symmetry code), O3 and O5 by 0.437 (1)° in the direction of the apical water O

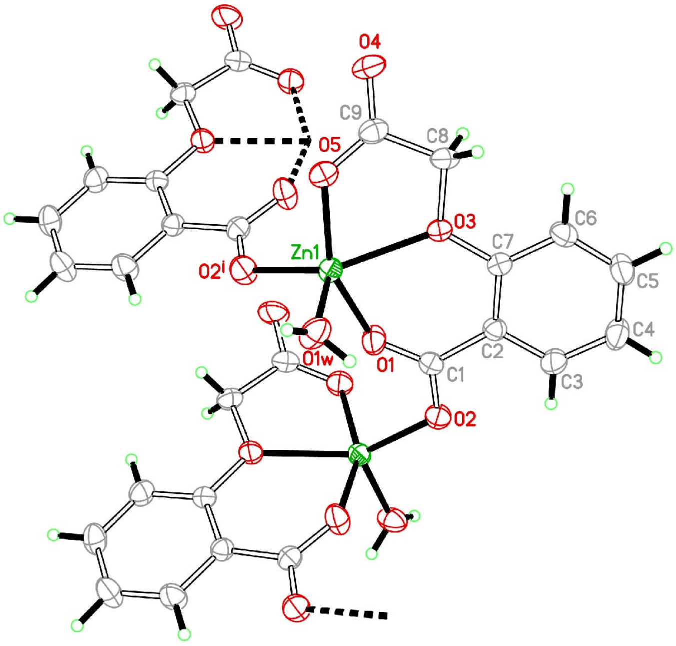


Figure 1
View of a portion of (I), showing 50% displacements ellipsoids (arbitrary spheres for the H atoms). The heavy dashed lines indicate bonds to adjacent Zn atoms in the chain. The symmetry code is as in Table 1.

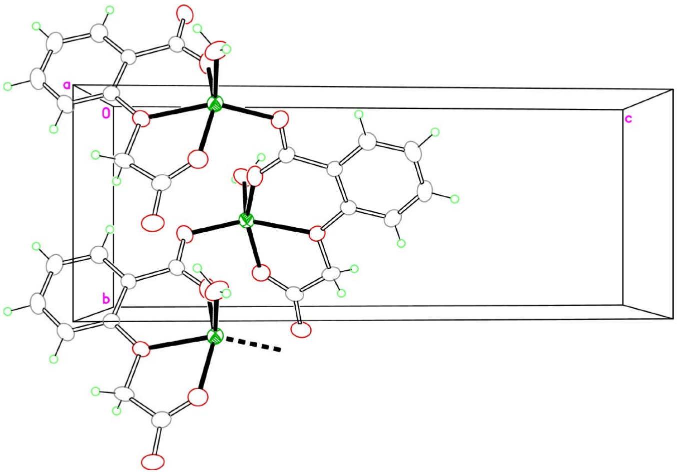


Figure 2
Detail of (I) showing a segment of the helical carboxylate-bridged chain motif.

atom (O1*w*). Two O—H···O hydrogen bonds (Table 2) link adjacent chains into a layered structure.

Experimental

Zinc nitrate hexahydrate (0.149 g, 0.5 mmol) and 2-carboxyphenoxyacetic acid (0.196 g, 1 mmol) were dissolved in a mixture of ethanol (3 ml) and water (15 ml). The solution was placed in a 23 ml Teflon-lined stainless steel hydrothermal bomb which was heated at 433 K for 120 h. The cooled mixture yielded colorless crystals of (I); these were washed with water and then dried in air (the yield was about 70%).

Crystal data

$[Zn(C_9H_6O_5)(H_2O)]$
$M_r = 277.52$
Monoclinic, $P2_1/n$
$a = 8.157$ (1) Å
$b = 6.7568$ (8) Å
$c = 17.451$ (2) Å
$\beta = 94.697$ (2)°
$V = 958.7$ (2) Å^3
$Z = 4$

$D_x = 1.923$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 853 reflections
$\theta = 2.3$–27.1°
$\mu = 2.57$ mm^{-1}
$T = 295$ (2) K
Block, colorless
0.50 × 0.36 × 0.28 mm

Data collection

Bruker SMART 1K CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{\min} = 0.331$, $T_{\max} = 0.487$
5672 measured reflections

2095 independent reflections
1880 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.021$
$\theta_{\max} = 27.1°$
$h = -10 \rightarrow 10$
$k = -8 \rightarrow 6$
$l = -22 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.022$
$wR(F^2) = 0.060$
$S = 1.02$
2095 reflections
153 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0304P)^2 + 0.4871P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.31$ e Å^{-3}
$\Delta\rho_{\min} = -0.36$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.961 (1)	C1—O1	1.257 (2)
Zn1—O2^{i}	1.969 (1)	C1—O2	1.256 (2)
Zn1—O3	2.268 (1)	C9—O4	1.232 (2)
Zn1—O5	1.996 (1)	C9—O5	1.267 (2)
Zn1—O1*w*	1.997 (1)		
O1—Zn1—O2^{i}	97.92 (6)	O2^{i}—Zn1—O5	97.64 (6)
O1—Zn1—O3	80.15 (5)	O2^{i}—Zn1—O1*w*	104.49 (6)
O1—Zn1—O5	153.75 (6)	O3—Zn1—O5	75.17 (5)
O1—Zn1—O1*w*	93.88 (7)	O3—Zn1—O1*w*	109.24 (6)
O2^{i}—Zn1—O3	146.27 (6)	O5—Zn1—O1*w*	102.50 (6)

Symmetry code: (i) $\frac{3}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O4^{ii}	0.85 (1)	1.80 (1)	2.644 (2)	176 (3)
O1*w*—H1*w*2···O5^{iii}	0.84 (1)	1.95 (1)	2.776 (2)	166 (2)

Symmetry codes: (ii) $x, y - 1, z$; (iii) $\frac{1}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$.

The carbon-bound H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with the constraint $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(carrier) applied. The water H atoms were located in a difference Fourier map and were freely refined.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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