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catena-Poly[[diaquazinc(II)]-μ-4-carboxylato-phenoxyacetato]

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The carboxylate dianion in the polymeric title compound, $[Zn(C_9H_6O_5)(H_2O)_2]_n$, which is disordered over a centre of inversion, links diaquazinc(II) units into a zigzag chain; the chains interact through hydrogen bonds to form layers. The six-coordinate metal atom lies on a special position of site symmetry 2.

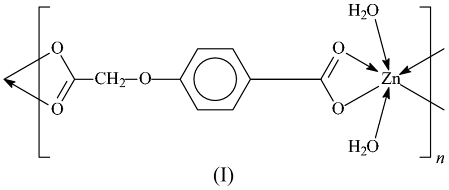
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(O–C) = 0.005 Å
Disorder in main residue
R factor = 0.045
wR factor = 0.114
Data-to-parameter ratio = 11.0

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

Comment

This report continues our studies of metal complexes of dicarboxylic acids having two carboxyl $-X-CH_2CO_2$ arms connected to an aromatic ring in the 1,4-positions. The diaquazinc derivative of phenylene-1,4-dioxyacetic acid adopts a zigzag structure; the metal atom lies on a twofold axis and the anion on a centre of inversion (Gao *et al.*, 2005). The six-coordinate geometry arises from chelation by the carboxyl $-CO_2$ unit. The present carboxylate, (I), has one ether linkage less, but the dianion also lies on a centre of inversion, so that a number of constraints and restraints had to be applied to the disordered model. The compound adopts a zigzag structure, and adjacent chains are linked to form sheets. The phenylene-1,4-dioxyacetate and the carboxyphenoxyacetate complexes (Fig. 1) are not isostructural, although their unit cells both have a short b axis. Disorder in the dianion is also noted in a related zinc complex (Gao *et al.*, 2004).



(I)

Experimental

Zinc(II) acetate dihydrate (2.20 g, 10 mmol) dissolved in water was mixed with 4-carboxyphenoxyacetic acid (1.96 g, 10 mmol) dissolved in water. The pH of the solution was raised to 6 with 0.1 M sodium hydroxide. Colourless crystals were isolated from the filtered solution after several days. Analysis found: C 36.73, H, 3.45%; calculated for $C_9H_{10}O_7Zn$: C 36.58, H 3.41%.

Crystal data

$[Zn(C_9H_6O_5)(H_2O)_2]$
M_r = 295.54
Monoclinic, $C2/c$
a = 11.853 (2) Å
b = 5.0520 (9) Å
c = 17.641 (3) Å
β = 102.720 (9)°
V = 1030.5 (3) Å^3
Z = 4

D_x = 1.905 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4330 reflections
θ = 3.8–27.4°
μ = 2.41 mm^{-1}
T = 295 (2) K
Block, colourless
0.34 × 0.25 × 0.18 mm

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Data collection

Rigaku R-AXIS RAPID diffractometer
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.441$, $T_{\max} = 0.671$
4588 measured reflections
1192 independent reflections
1048 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.033$
$\theta_{\max} = 27.5°$
$h = -15 \rightarrow 15$
$k = -6 \rightarrow 6$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.114$
$S = 1.09$
1192 reflections
108 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0475P)^2 + 5.0313P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.51$ e Å^{-3}
$\Delta\rho_{\min} = -0.39$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.445 (3)	Zn1—O1*W*	1.978 (3)
Zn1—O2	2.051 (3)		
O1—Zn1—O1$^{\rm i}$	139.3 (2)	O2—Zn1—O2$^{\rm i}$	96.6 (2)
O1—Zn1—O2	57.3 (1)	O2—Zn1—O1*W*	102.0 (1)
O1—Zn1—O2$^{\rm i}$	94.4 (1)	O2—Zn1—O1*W*$^{\rm i}$	137.1 (1)
O1—Zn1—O1*W*	128.1 (1)	O1*W*—Zn1—O1*W*$^{\rm i}$	90.0 (2)
O1—Zn1—O1*W*$^{\rm i}$	82.8 (1)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O1$^{\rm ii}$	0.85 (1)	1.83 (1)	2.665 (4)	171 (5)
O1*W*—H1*W*2···O2$^{\rm iii}$	0.85 (1)	1.89 (2)	2.723 (4)	166 (5)

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

The $C_9H_6O_5$ dianion is disordered over a centre of inversion (Wyckoff 4*d* site). Its benzene ring was refined as a rigid hexagon having 1.39 Å sides. The C1—C2 and C6—C1$^{\rm i}$ distances were restrained to 1.540 (2) Å; a rather small deviation had to be used. Additionally, the vibration of atom C6 of the ring was restrained to be approximately isotropic. Atoms O1 and O2, which are involved in coordination, are not disordered. The water H atoms were located and refined with distance restraints of O—H = 0.85 (1) Å and H···H = 1.39 (1) Å; their displacement parameters were set to 1.2 times $U_{\rm eq}$ of the O atom. The C-bound H atoms were placed in calculated positions (aromatic distance 0.93 Å and methylene distance 0.97 Å), and were included in the refinement in the riding-model approximation. Their displacement parameters were set to $1.2U_{\rm eq}$(C).

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: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

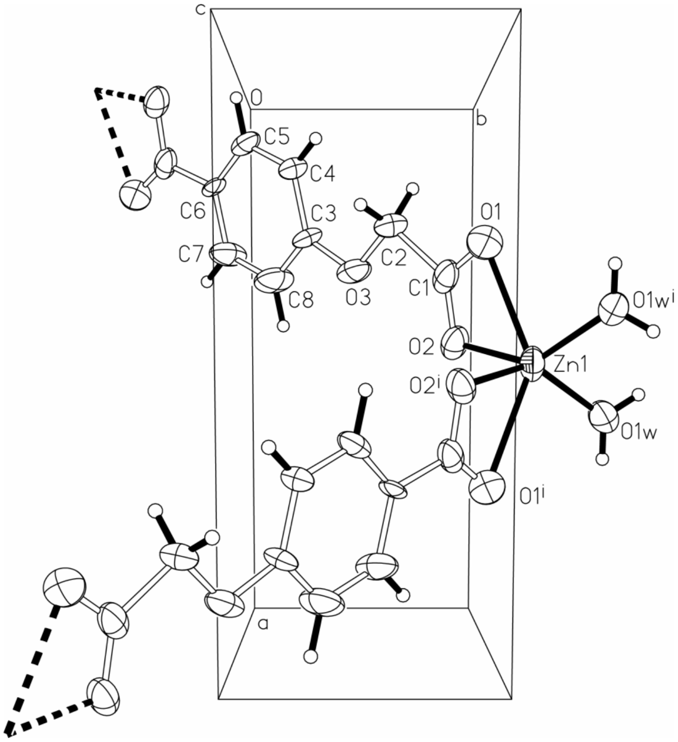

Figure 1
*ORTEP*II (Johnson, 1976) plot of the polymeric chain structure, with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

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