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Poly[zinc(II)-μ_4-1,4-phenylenedioxydiacetato-$\kappa^2 O:O'$]

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The geometry of the Zn atom in the title compound, $[Zn(C_{10}H_8O_6)]_n$, is tetrahedral, but distorted towards trigonal–pyramidal by interaction with the ether O atom of one of the oxyacetate arms [Zn···O = 2.570 (2) Å].

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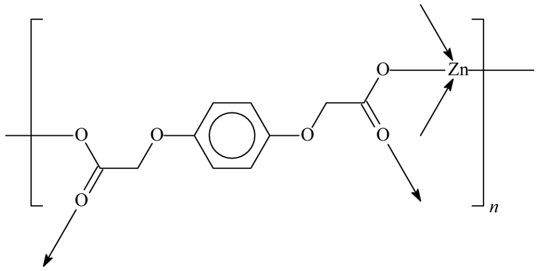
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.035
wR factor = 0.088
Data-to-parameter ratio = 14.1

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

Comment

The 1,4-phenylenedioxydiacetate dianion is an example of a structurally flexible dicarboxylate dianion that should easily link two metal atoms together. The present anhydrous zinc derivative, (I), was obtained in the attempted adduct formation with benzimidazole; a previous attempt at reacting zinc 1,4-phenylenedioxydiacetate with imidazole yielded the expected diimidazole complex as a tetrahydrate (Gao *et al.*, 2004*a*).



(I)

The direct synthesis of zinc 1,4-phenylenedioxydiacetate from the dicarboxylate dianion and Zn^{2+} under hydrothermal conditions affords the diaqua compound (Gao *et al.*, 2004*b*); the metal in the zigzag chain shows octahedral coordination as both carboxyl units chelate to it. In the anhydrous title compound (Fig. 1), the Zn atom is covalently bonded to the carboxyl O atoms of four 1,4-phenylenedioxydiacetate dianions in a distorted tetrahedral environment. The geometry is distorted towards trigonal-bipyramidal owing to an interaction with the ether O atom of one of the oxyacetate arms [Zn···O = 2.570 (2) Å] (Fig. 1). The dianion links adjacent Zn atoms, leading to a three-dimensional network.

Experimental

The title compound, not incorporating benzimidazole, was obtained in the attempted hydrothermal reaction between zinc 1,4-phenylenedioxydiacetate and the heterocyclic reagent. Zinc acetate dihydrate (4.38 g, 20 mmol), benzimidazole (2.34 g, 20 mmol) and 1,4-phenylenedioxydiacetic acid (4.52 g, 20 mmol), along with some water, were sealed in a Teflon-lined stainless-steel bomb. The bomb was heated at 393 K for 60 h. Crystals of (I) were obtained when the bomb was cooled to room temperature. Analysis calculated for $C_{10}H_8O_6Zn$: C 41.48, H 2.78%; found: C 41.66, H 2.90%.

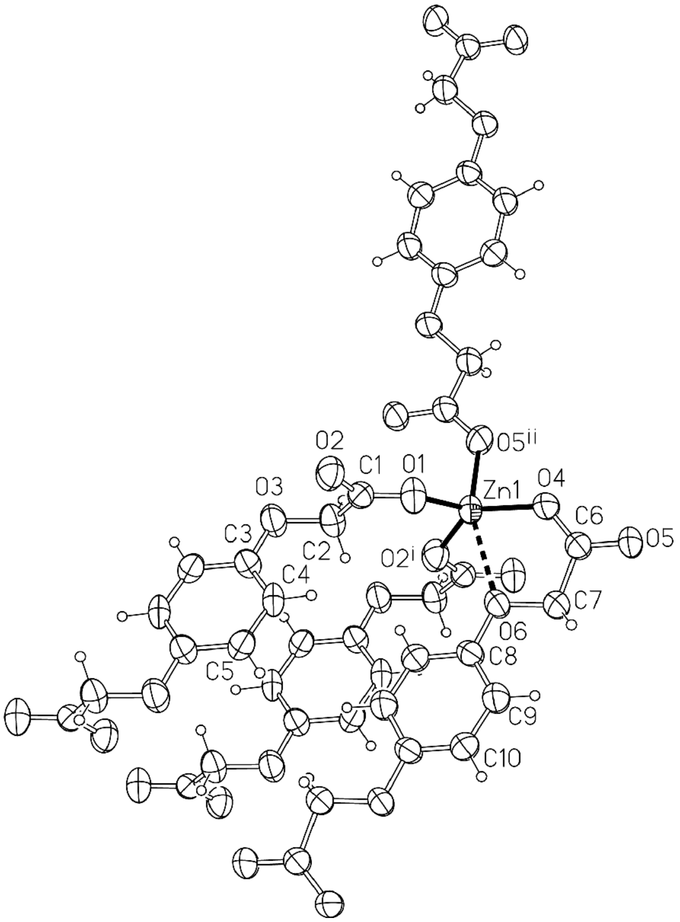


Figure 1
*ORTEP*II (Johnson, 1976) plot depicting a fragment of the polymeric structure of (I) at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. Only one disordered component is shown. The dashed line indicates the secondary Zn$\cdots$ether interaction. [Symmetry codes: (i) $x-1, y, z$; (ii) $x, \frac{1}{2}-y, z-\frac{1}{2}$.]

Crystal data

$[Zn(C_{10}H_8O_6)]$
$M_r = 289.53$
Monoclinic, $P2_1/c$
$a = 4.7934$ (9) Å
$b = 23.634$ (4) Å
$c = 9.340$ (1) Å
$\beta = 104.48$ (3)°
$V = 1024.5$ (3) Å^3
$Z = 4$
$D_x = 1.877$ Mg m$^{-3$}
Mo $K\alpha$ radiation
Cell parameters from 6462 reflections
$\theta = 4.1$–27.5°
$\mu = 2.41$ mm^{-1}
$T = 295$ (2) K
Prism, colorless
0.38 × 0.25 × 0.17 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.289$, $T_{\max} = 0.685$
9743 measured reflections
2348 independent reflections
2002 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.037$
$\theta_{\max} = 27.5°$
$h = -6 \rightarrow 5$
$k = -30 \rightarrow 30$
$l = -12 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.088$
$S = 1.07$
2348 reflections
166 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 0.9852P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.48$ e Å^{-3}
$\Delta\rho_{\min} = -0.40$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.967 (2)	Zn1—O4	1.957 (2)
Zn1—O2^{i}	1.956 (2)	Zn1—O5^{ii}	1.977 (2)
O1—Zn1—O2^{i}	105.5 (1)	O2^{i}—Zn1—O4	133.8 (1)
O1—Zn1—O4	111.8 (1)	O2^{i}—Zn1—O5^{ii}	102.9 (1)
O1—Zn1—O5^{ii}	106.3 (1)	O4—Zn1—O5^{ii}	92.0 (1)

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

The asymmetric unit contains two anions, both of which are disordered over centers of symmetry. The disorder affects only the unsubstituted C atoms of the phenylene rings (and not the methylene unit). The C—C distances were restrained to 1.390 (5) Å. The occupancy was fixed at 0.5 for the disordered atoms. The displacement parameters of the unprimed and primed atoms of both components were set to equal each other. The phenylene ring adopts two orientations along its 1,4-axis. The H atoms were placed in calculated positions [aromatic C—H = 0.93 Å and aliphatic C—H = 0.97 Å; $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$] and were included in the refinement in the riding-model approximation.

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); 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.

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