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catena-Poly[[tri-μ_2-benzoato-dizinc(**II**)]-μ_2-hydroxy]

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.051
wR factor = 0.129
Data-to-parameter ratio = 18.2

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

In the crystal structure of the title compound, $[Zn_2(C_7H_5O_2)_3(OH)]$, the two Zn atoms are bridged by the carboxyl groups of three benzoate anions. Adjacent dinuclear units are linked into a chain through the hydroxy groups to confer tetrahedral geometries on the metal atoms.

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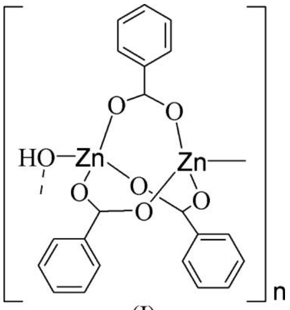
Comment

Zinc(II) benzoate and other arylcarboxylates adopt structures in which the anion binds in the bridging mode to confer tetrahedral coordination on the metal atom. The compound with the zinc dibenzoate formulation exists as polymeric $[Zn_2(\mu\text{-}O_2CC_6H_5)_3(O_2CC_6H_5)]$ (Guseinov *et al.*, 1984), which features a dinuclear $[Zn_2(\mu\text{-}O_2CC_6H_5)_3]$ unit having three *syn–syn* carboxylate bridges. The fourth benzoate anion (which balances the +1 charge) links adjacent dinuclear units into a chain. The compound formulated as dizinc tetrakis(2-chlorobenzoate) (Clegg *et al.*, 1990) adopts a similar chain motif. For this compound, the fourth 2-chlorobenzoate anion appears to be readily replaced by adventitious hydroxide ions present in the aqueous acetone medium used for recrystallization. The resulting hydroxide, $[Zn_2(\mu\text{-}O_2CC_6H_4Cl)_3(OH)(H_2O)]\cdot H_2O$, is stabilized by extensive hydrogen bonding with the coordinated and uncoordinated water molecules (Nakacho *et al.*, 1976). Three arylcarboxylate anions binding to two transition metal atoms is an unusual feature in the structural chemistry of transition metal carboxylates, as noted from a search for such compounds in the Cambridge Structural Database (Version 5.25; Allen, 2002). Possibly, two metal atoms prefer to be bridged by four instead of three anions and the difficulty appears to be one of packing.



(I)

In the title compound, (I), Zn^{2+} cations combined hydrothermally with benzoate anions to generate the $[Zn_2(\mu\text{-}O_2CC_6H_5)_3]$ unit, the charge of which is balanced by a hydroxide ion (Fig. 1). The geometry of both Zn atoms is tetrahedral. There is no interaction between the Zn atoms, as

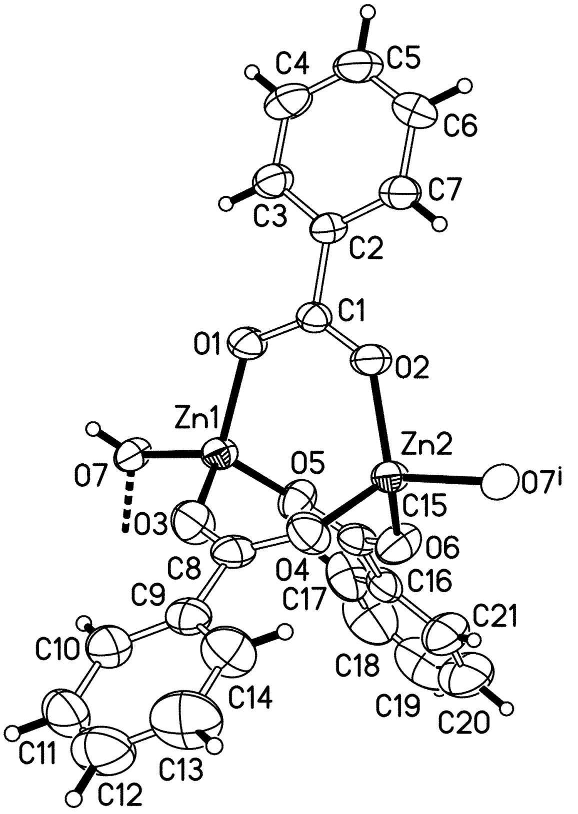


Figure 1
A plot of the asymmetric unit of (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. [Symmetry code (i): $\frac{1}{2} + x, \frac{1}{2} - y, 1 - z$.]

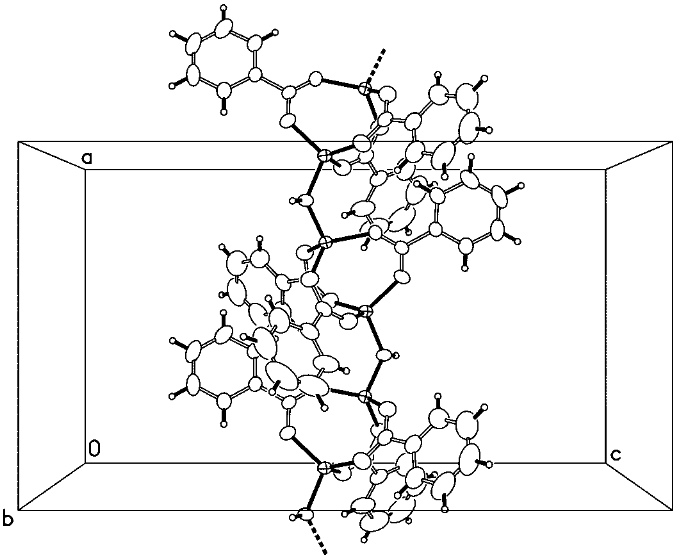


Figure 2
A plot of the polymeric chain of (I), propagating along the *a* axis of the orthorhombic unit cell.

they are >3.2 Å apart. The short hydroxide bridge links the cations into a chain (Fig. 2).

The dihydrated 4-diethylaminosulfonylbenzoate has a similar constitution of two Zn atoms, three carboxylate anions and a hydroxide ion, but only two of the anions chelate to the two Zn atoms (Guseinov *et al.*, 1987). The unusual structures of zinc arylcarboxylates are further illustrated by a terephthalate derivative, which also possesses a hydroxide bridge. However, the coordination number of Zn in $[Zn_4(OH)_2(C_8H_4O_4)_3(DMSO)_4]\cdot 2H_2O$ is raised, owing to coordination by the dimethylsulfoxide (DMSO) solvent (Wang *et al.*, 2001).

Experimental

Zinc(II) nitrate hexahydrate (0.30 g, 1.0 mmol) and sodium benzoate (0.29 g, 2.0 mmol) were dissolved in water (15 ml). The solution was placed in a Teflon-lined stainless steel bomb, which was heated to 473 K for 100 h. The bomb was allowed to cool slowly to room temperature and colourless plate-shaped crystals of (I) were deposited from the solution. IR (KBr, ν, cm^{-1}): 3652, 3064, 1641 (*s*), 1610 (*s*), 1571 (*s*), 1531 (*vs*), 1420 (*vs*), 719.

Crystal data

$[Zn_2(C_7H_5O_2)_3(OH)]$
$M_r = 511.08$
Orthorhombic, *Pbca*
$a = 11.9182$ (5) Å
$b = 16.5293$ (7) Å
$c = 21.1391$ (9) Å
$V = 4164.4$ (3) Å^3
$Z = 8$
$D_x = 1.630$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 6055 reflections
$\theta = 2.3$–26.5°
$\mu = 2.34$ mm^{-1}
$T = 298$ (2) K
Plate, colourless
0.30 × 0.25 × 0.04 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.540$, $T_{max} = 0.912$
34070 measured reflections

5015 independent reflections
3911 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 28.3°$
$h = -15 \rightarrow 15$
$k = -22 \rightarrow 21$
$l = -26 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.129$
$S = 1.05$
5015 reflections
275 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0586P)^2 + 3.2192P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.59$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.944 (2)	Zn2—O2	1.945 (2)
Zn1—O3	1.941 (3)	Zn2—O4	1.948 (3)
Zn1—O5	1.948 (3)	Zn2—O6	1.941 (2)
Zn1—O7	1.907 (2)	Zn2—O7^i	1.902 (2)
O1—Zn1—O3	113.6 (1)	O2—Zn2—O6	117.5 (1)
O1—Zn1—O5	111.6 (1)	O2—Zn2—O7^i	104.0 (1)
O1—Zn1—O7	110.4 (1)	O4—Zn2—O6	105.8 (1)
O3—Zn1—O5	112.9 (1)	O4—Zn2—O7^i	109.8 (1)
O3—Zn1—O7	108.4 (1)	O6—Zn2—O7^i	104.1 (1)
O5—Zn1—O7	99.0 (1)	Zn1—O7—Zn2^{ii}	121.3 (1)
O2—Zn2—O4	115.1 (1)		

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

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The aromatic H atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding. The hydroxy H atom was refined with the restraint O—H = 0.85 (1) Å. For all H atoms, $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C,O).

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: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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