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Bis(salicylaldehydo)zinc(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.042
wR factor = 0.121
Data-to-parameter ratio = 12.1

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

The title compound, $[Zn(C_7H_5O_2)_2]$, is a mononuclear zinc(II) complex. The Zn^{II} atom, lying on an inversion center, is coordinated by four O atoms from two salicylaldehyde ligands, forming a square planar geometry.

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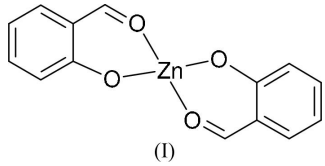
Comment

Zinc(II) complexes play a crucial biochemical role. Recently, we have found that some of these complexes have antifatigue properties. As part of a further investigation of these materials, here we report the synthesis and structure of the title complex, (I), a mononuclear zinc(II) complex (Fig. 1). The Zn1 atom (site symmetry $\bar{1}$) is in a slightly distorted square planar geometry, coordinated by four O atoms from two anionic salicylaldehydo ligands. All the bond lengths and angles are in normal ranges (Allen *et al.*, 1987).



(I)

Experimental

Salicylaldehyde (0.2 mmol, 24.2 mg) and $Zn(CH_3COO)_2{\cdot}2H_2O$ (0.1 mmol, 22.0 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for 1 h and then filtered. After keeping the colorless filtrate in air for 12 d, colorless block-shaped crystals of (I) were formed.

Crystal data

$[Zn(C_7H_5O_2)_2]$
M_r = 307.59
Monoclinic, $P2_1/n$
a = 8.804 (6) Å
b = 6.244 (5) Å
c = 11.419 (8) Å
β = 105.653 (10)°
V = 604.5 (8) Å^3
Z = 2
D_x = 1.690 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 554 reflections
θ = 2.2–22.1°
μ = 2.04 mm^{-1}
T = 298 (2) K
Block, colorless
0.31 × 0.24 × 0.14 mm

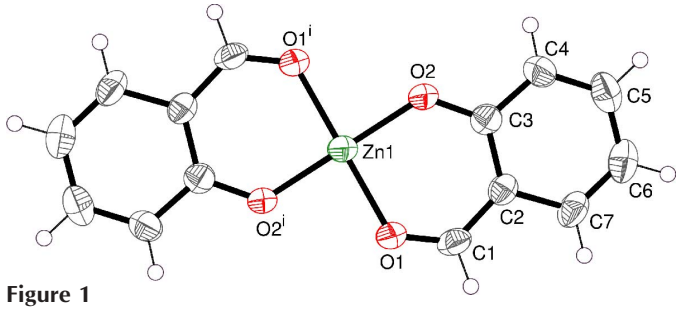


Figure 1
The structure of (I), showing 50% displacement ellipsoids (spheres of arbitrary radius for the H atoms). Symmetry code as in Table 1.

Data collection

Bruker SMART area-detector diffractometer	1063 independent reflections
ω scans	839 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.042$
$T_{min} = 0.560$, $T_{max} = 0.749$	$\theta_{max} = 25.0^\circ$
2945 measured reflections	$h = -10 \rightarrow 10$
	$k = -6 \rightarrow 7$
	$l = -13 \rightarrow 9$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.042$	$w = 1/[\sigma^2(F_o^2) + (0.083P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.121$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.97$	$\Delta\rho_{max} = 0.56$ e Å^{-3}
1063 reflections	$\Delta\rho_{min} = -0.39$ e Å^{-3}
88 parameters	

Table 1
Selected geometric parameters (Å, °).

Zn1—O2	1.887 (2)	Zn1—O1	1.947 (3)
O2—Zn1—O1^{i}	86.92 (11)		

Symmetry code: (i) $-x, -y, 2 - z$.

All H atoms were placed in geometrically idealized positions and refined as riding on their parent atom with d(C—H) = 0.93 Å, and with the constraint U_{iso}(H) = 1.2U_{eq}(C) applied.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998; data reduction: *SAINT*); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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