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Bis{μ-2,2′-[ethane-1,3-diylbis(nitrilomethylidyne)]diphenolato}dizinc(II)

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The crystal structure of the title compound, $[Zn_2(C_{16}H_{14}N_2O_2)_2]$, shows the dimeric complex to be centrosymmetric. Distorted pentacoordinate square-pyramidal geometry is formed around Zn^{II}, defined by two N atoms and two O atoms of the *N*,*N*′-bis(salicylidene)-1,2-ethylenediamine (salen) ligand and one bridging O atom of the adjacent ligand. Two salen ligands in this dimeric complex are twisted in opposite directions to each other.

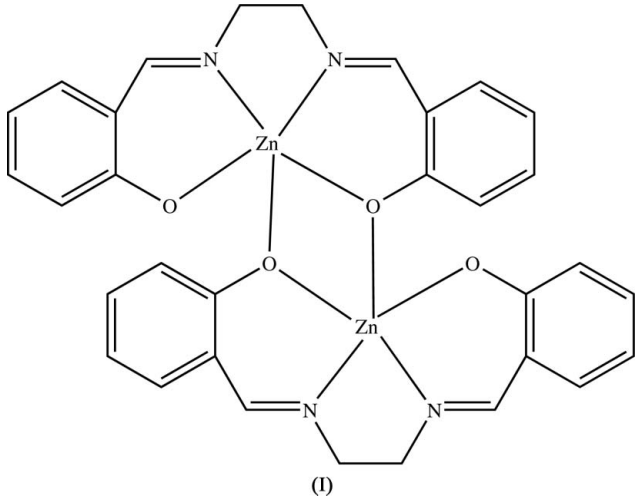
Key indicators

Single-crystal X-ray study
T = 123 K
Mean σ(C–C) = 0.011 Å
R factor = 0.071
wR factor = 0.200
Data-to-parameter ratio = 16.0

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

Comment

Zinc(II), a trace element for mammals, is essential for the various biochemical and physiological processes. Until now, Zn^{II} and its complexes have been found to exhibit *in vitro* insulinomimetic activity and anti-diabetic effects in animals (Chen *et al.*, 1998; Song *et al.*, 2001; Sakurai *et al.*, 2002). Several vanadium complexes with tetradentate Schiff base salen-type [salen is *N*,*N*′-bis(salicylidene)-1,2-ethylenediamine] ligands have been studied for use as insulin-enhancing agents (Durai & Saminathan, 1997; Correia *et al.*, 2004). In the present study, aimed to design new insulinomimetic Zn^{II} compounds, we have synthesized the title compound, (I), which has salen as the tetradentate Schiff base ligand, and analysed its crystal structure.



(I)

The crystal structure of (I) is shown in Fig. 1 with the atom-numbering scheme. Selected geometric parameters are given in Table 1. (I) is a centrosymmetric dimeric complex, rather than monomeric as in $[Zn^{II}(salen)\cdot H_2O]$ (Hall & Moore, 1966) and $[Zn^{II}(salen)py]$ (py = pyridine; Reglinski *et al.*, 2002). $[Zn^{II}(salen)]$ units in (I) are connected by the oxygen bridges Zn1—O1^{i} and O1—Zn1^{i} [symmetry code: (i) $\frac{3}{2}-x, \frac{1}{2}-y, 1-$

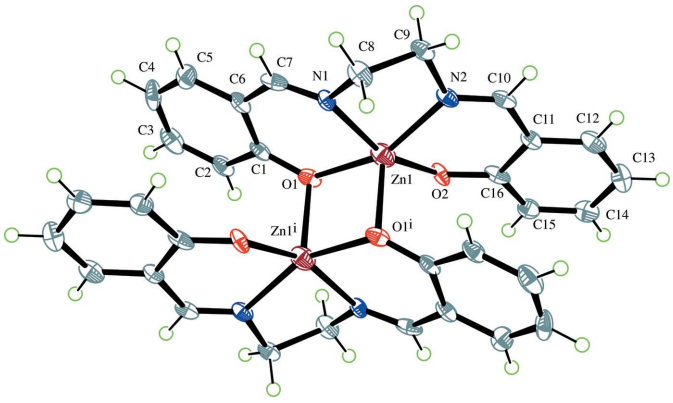


Figure 1
A view of the structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are shown at the 50% probability level and H atoms are shown as spheres of arbitrary radii. Symmetry code: (i) $\frac{3}{2}-x$, $\frac{1}{2}-y$, $1-z$.]

z]. Distorted pentacoordinate square-pyramidal geometry is formed around Zn^{II}, defined by two N atoms and two O atoms of the salen ligand as the basal plane and one bridging O atom of the adjacent ligand as the apical atom. Zn^{II} sits in the body of the pyramid, 0.375 (3) Å from the O1—N1—N2—O2 basal plane. The two planar (r.m.s. deviation of fited atoms = 0.0116 Å for O1/C1–C6/C7/N1 and 0.0425 Å for O10/C11–C16/C17/N2) Schiff base units are inclined at 21.9 (2)° in an umbrella-like conformation, similar to those in [Zn^{II}(salen)·H_2O] and [Zn^{II}(salen)py]. The two salen ligands in (I) are twisted in opposite directions to each other. The ethylenediamine group of the salen ligand is in a *gauche* conformation [N1—C8—C9—N2 — 45.0 (7)°], as seen in [Zn^{II}(salen)·H_2O].

The crystal packing of (I) is stabilized by van der Waals interactions between neighboring complexes.

Experimental

N,*N*′-Bis(salicylidene)-1,2-ethylenediamine (5 mg) was dissolved in MeOH (5 ml) and zinc perchlorate hexahydrate (3.4 mg) dissolved in a small amount of water was added at room temperature. Colorless needle-shaped crystals appeared from this mixture after evaporation over a few days at room temperature.

Crystal data

$[Zn_2(C_{16}H_{14}N_2O_2)_2]$	D_x = 1.646 Mg m^{-3}
M_r = 663.36	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 6984 reflections
a = 27.06 (5) Å	θ = 3.0–27.5°
b = 6.79 (1) Å	μ = 1.84 mm^{-1}
c = 14.70 (3) Å	T = 123.1 K
β = 97.67 (7)°	Needle, colorless
V = 2677 (8) Å^3	0.60 × 0.05 × 0.05 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	3063 independent reflections
ω scans	919 reflections with $F^2 > 2\sigma(F^2)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	R_{int} = 0.158
T_{min} = 0.197, T_{max} = 0.912	θ_{max} = 27.5°
12653 measured reflections	$h = -34 \rightarrow 34$
	$k = -8 \rightarrow 8$
	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)]$ = 0.071	$w = 1/[\sigma^2(F_o^2) + (0.0929P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.200	$(\Delta/\sigma)_{max}$ = 0.001
S = 0.89	$\Delta\rho_{max}$ = 0.97 e Å^{-3}
3063 reflections	$\Delta\rho_{min}$ = −1.06 e Å^{-3}
191 parameters	

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.053 (5)	Zn1—N1	2.072 (5)
Zn1—O1^i	2.053 (5)	Zn1—N2	2.078 (6)
Zn1—O2	1.973 (4)		
O1—Zn1—O1^i	88.3 (2)	O1^i—Zn1—N1	102.2 (2)
O1—Zn1—O2	98.0 (2)	O1^i—Zn1—N2	113.0 (2)
O1—Zn1—N1	86.2 (2)	O2—Zn1—N2	87.4 (2)
O1^i—Zn1—O2	100.4 (2)	N1—Zn1—N2	80.5 (2)

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

All H atoms were located in difference Fourier maps and then were placed in ideal positions and refined as riding [C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms; C—H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) for methine and methylene H atoms]. The crystal used for data collection was very poorly diffracting but it was the best that could be found. The highest electron-density peak was located close to atoms Zn1 and O2.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2005) and *CRYSTALS* (Betteridge *et al.*, 2003); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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