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Aqua{2,2′-[propane-1,3-diylbis(nitrilomethylidyne)]diphenolato}zinc(II)

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Key indicators

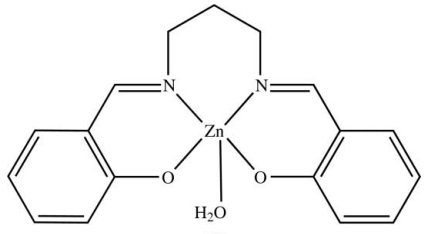
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.018
wR factor = 0.054
Data-to-parameter ratio = 16.3

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

In the title compound, $[Zn(C_{17}H_{16}N_2O_2)(H_2O)]$, the Zn^{II} atom has a distorted pentacoordinate square-pyramidal geometry. A mirror plane passes through the Zn^{II} atom, the central C atom of the propyl group and the O atom of the coordinated water molecule. The two planar Schiff base groups make a dihedral angle of 39.49 (6)°. The crystal packing is stabilized by weak intermolecular interactions *via* the coordinated water molecule.

Comment

To date, it has been reported that Zn^{II} and its complexes exhibit insulinomimetic activity *in vitro* and anti-diabetic effects in animals (Chen *et al.*, 1998; Song *et al.*, 2001; Sakurai *et al.*, 2002). It has also been reported that several vanadium complexes of the tetradentate Schiff base salen-type [*N*,*N*′-bis(salicylidene)-1,2-ethylenediamine] ligands show insulin-enhancing properties (Durai & Saminathan, 1997; Correia *et al.*, 2004). As part of a study aimed to design new insulinomimetic Zn^{II} complexes, we have synthesized the title compound, (I), in which bis(*N*,*N*′-salicylidene)propane-1,3-diamine (salpr) behaves as a tetradentate Schiff base ligand.



(I)

The crystal structure and the atom-numbering scheme of (I) are shown in Fig.1. Selected geometric parameters are shown in Table 1. The Zn^{II} atom is in a pentacoordinate distorted square-pyramidal geometry, defined by two N atoms and two O atoms of the salpr ligand as the basal plane and by one apical O atom of a water molecule. The Zn^{II} atom sits in the body of the pyramid 0.3539 (7) Å from the O1/N1/N1^{i}/O1^{i} basal plane [symmetry code: (i) $x, \frac{1}{2} - y, z$]. A mirror plane passes through the Zn^{II} atom, the central C9 atom of the propyl group and the O2 atom of the coordinated water molecule. The two planar Schiff base groups (r.m.s. deviation of fitted atoms of O1/C1–C6/C7/N1 and O1^{i}/C1^{i}–C6^{i}/C7^{i}/N1^{i} = 0.0207 Å) make a dihedral angle of 39.49 (6)°. The six-membered chelate ring composed of Zn^{II} and the propanediamine group has a chair conformation with out-of-plane Zn^{II} and C9 atoms.

In the crystal structure, complex molecules are weakly linked with one another along the *a* axis *via* the coordinated

water molecules. The water molecule makes bifurcated O—H···O hydrogen bonds with two O atoms of a neighboring salpr ligand. Atom C8 of the propyl group makes another C—H···O contact with O2 of the water molecule of a neighboring complex (Fig. 2 and Table 2).

Experimental

N,*N*′-Bis(salicylidene)propane-1,3-diamine (5 mg) was dissolved in 80% (*v*/*v*) EtOH–water (5 ml) and zinc chloride (1.2 mg) dissolved in a small amount of water was added at room temperature. Colorless platelet-shaped crystals appeared from this mixture after a few days by evaporation at room temperature.

Crystal data

$[Zn(C_{17}H_{16}N_2O_2)(H_2O)]$
M_r = 363.72
Orthorhombic, *Pnma*
a = 8.731 (7) Å
b = 24.06 (2) Å
c = 7.488 (7) Å
V = 1573 (2) Å^3
Z = 4
D_x = 1.536 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 13198 reflections
θ = 3.4–27.5°
μ = 1.58 mm^{-1}
T = 296.1 K
Platelet, colorless
0.20 × 0.20 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.668, T_{max} = 0.854
15638 measured reflections
1845 independent reflections
1579 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.016
θ_{max} = 27.5°
h = −11 → 11
k = −31 → 31
l = −9 → 9

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.054
S = 1.10
1845 reflections
113 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0353P)^2 + 0.1946P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	2.027 (2)	Zn1—N1	2.112 (2)
Zn1—O2	2.012 (1)		
O1—Zn1—O1^{i}	86.05 (3)	O2—Zn1—N1	99.70 (3)
O1—Zn1—O2	100.00 (3)	N1—Zn1—N1^{i}	94.06 (4)
O1—Zn1—N1	86.59 (3)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*w*···O1^{ii}	0.88	1.77	2.590 (3)	154
C8—H8*b*···O2^{iii}	0.97	2.63	3.407 (2)	137

Symmetry codes: (ii) $x-\frac{1}{2}, y, -z+\frac{3}{2}$; (iii) $x-\frac{1}{2}, -y+\frac{1}{2}, -z+\frac{3}{2}$.

All H atoms, except for those of the water molecule, were located in difference Fourier maps and were placed at ideal positions and treated 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 methylene H atoms]. H atoms of the water molecule were located in difference Fourier maps and treated as riding [U_{iso}(H) = 1.5U_{eq}(O)].

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*.

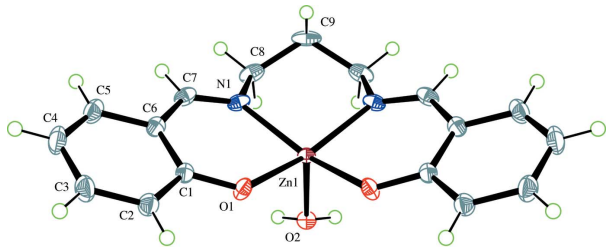


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are shown at the 50% probability level and H atoms are shown as spheres of arbitrary radii. Unlabeled atoms are related to labeled atoms by the symmetry operation $x, \frac{1}{2}-y, z$.

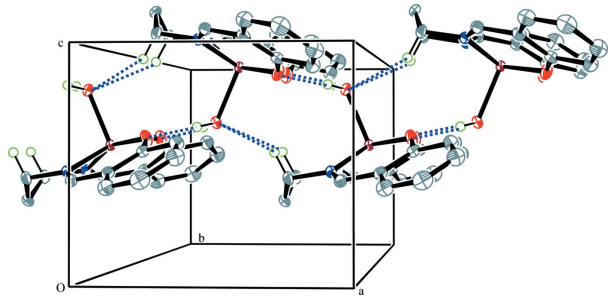


Figure 2
A view of the crystal packing of (I). Dashed lines indicate hydrogen bonds and intermolecular contacts.

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