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{1,1′-[1,3-Propanediylbis(nitrilomethylidyne)]-di-2-naphtholato}zinc(II), containing a square-planar ZnO_2N_2 group

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Key indicators

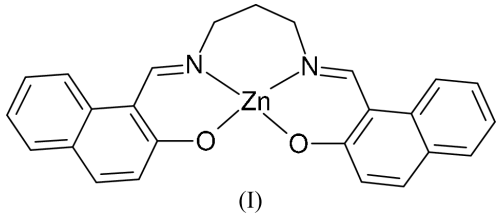
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.005 Å
R factor = 0.041
wR factor = 0.124
Data-to-parameter ratio = 14.2

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

The title compound, $[Zn(C_{24}H_{18}N_2O_2)]$, is a mononuclear zinc(II) complex. The Zn atom is located on a mirror plane and is coordinated by two N atoms and two O atoms from a Schiff base ligand in a slightly distorted square-planar geometry.

Comment

The synthesis and structure of the title compound, (I), is reported, as part of ongoing studies of model zinc complexes related to those with biological functions (Wu, 2004).



(I)

Compound (I) is a mononuclear zinc(II) complex (Fig. 1). The central Zn atom, located on a mirror plane, is coordinated by two O atoms and two N atoms of the Schiff base ligand. This ZnO_2N_2 coordination has a slightly distorted square-planar geometry [both *trans*-O—Zn—N angles are 173.59 (11)°], with the Zn atom displaced by 0.011 (2) Å from the plane of the four donor atoms. The Zn—O bond length in (I) (Table 1) is much shorter than the value of 2.058 (3) Å observed in a related Schiff base zinc complex (Tatar *et al.*, 2002), although in the latter case, another O atom is coordinated to Zn, resulting in a distorted square-pyramidal geometry about the Zn atom. The Zn—N bond length in (I) is also much shorter than the value of 2.040 (3) Å observed in

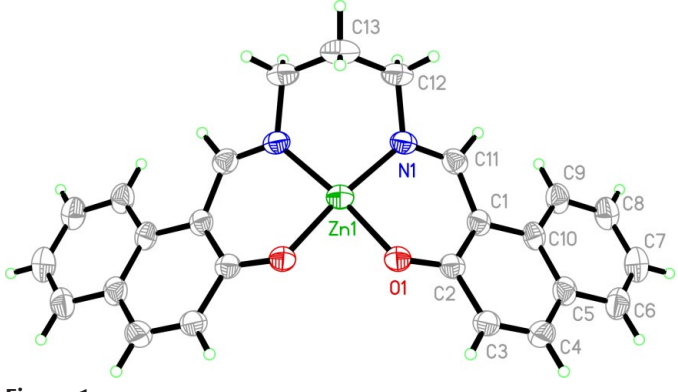


Figure 1
View of (I), with displacement ellipsoids drawn at the 30% probability level and H atoms shown as small spheres of arbitrary radii. Unlabelled atoms are related to labelled atoms by $1 - x, y, z$.

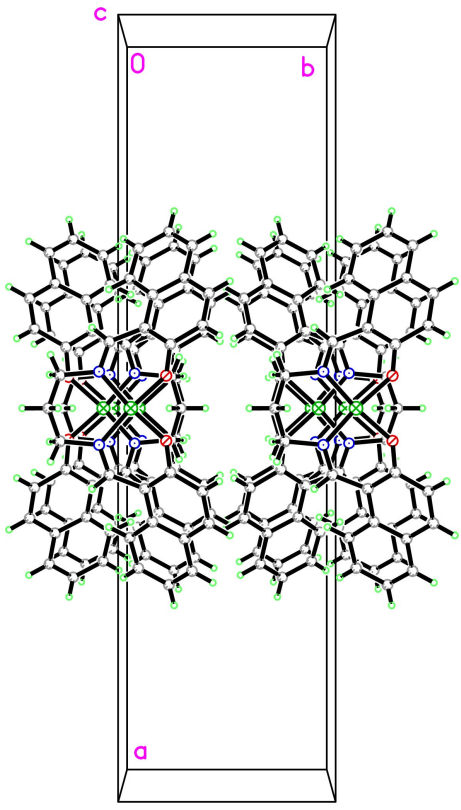


Figure 2
The crystal packing of (I), viewed along the *c* axis.

the same related Schiff base zinc complex (Tatar *et al.*, 2002). The dihedral angle between the two naphthalene rings in (I) is 52.6 (4)°.

Experimental

1,2-Diaminoethane (0.2 mmol, 12.1 mg) and 2-hydroxy-1-naphthaldehyde (0.4 mmol, 68.9 mg) were dissolved in EtOH (15 ml). The mixture was stirred for 30 min to give a clear yellow solution. An EtOH solution (15 ml) of $Zn(CH_3COO)_2{\cdot}2H_2O$ (0.2 mmol, 44.1 mg) was added with stirring. The mixture was stirred for another 30 min and filtered. The filtrate was left to stand at room temperature in air for 14 d, whereupon colourless block-shaped crystals were formed.

Crystal data

$[Zn(C_{25}H_{20}N_2O_2)]$
M_r = 445.80
Orthorhombic, $Cmc2_1$
a = 30.601 (4) Å
b = 8.4526 (11) Å
c = 7.7465 (10) Å
V = 2003.7 (5) Å^3
Z = 4
D_x = 1.478 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3565 reflections
θ = 2.5–27.2°
μ = 1.25 mm^{-1}
T = 273 (2) K
Block, colourless
0.27 × 0.22 × 0.19 mm

Data collection

Bruker SMART 1000 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.729, T_{max} = 0.797
5623 measured reflections
1983 independent reflections
1908 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 26.5°
$h = -37 \rightarrow 37$
$k = -7 \rightarrow 10$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.124
S = 1.11
1983 reflections
140 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0924P)^2 + 0.1608P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0049 (10)
Absolute structure: Flack (1983), 844 Friedel pairs
Flack parameter = 0.09 (2)

Table 1
Selected geometric parameters (Å, °).

Zn1—O1	1.851 (2)	Zn1—N1	1.871 (3)
O1—Zn1—O1^{i}	82.42 (14)	O1^{i}—Zn1—N1	173.59 (11)
O1—Zn1—N1	91.20 (12)	N1—Zn1—N1^{i}	95.17 (18)

Symmetry code: (i) $1-x, y, z$.

All H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with C—H distances of 0.93–0.97 Å and with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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