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[*N*,*N*′-Bis(2-hydroxynaphthylmethylene)-1,2-ethanediaminato]zinc(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.051
wR factor = 0.137
Data-to-parameter ratio = 15.9

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

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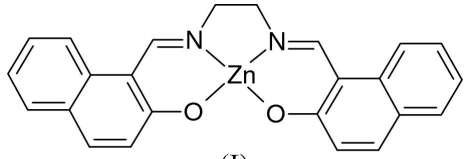
The title compound, $[Zn(C_{24}H_{18}N_2O_2)]$, is a mononuclear zinc(II) complex. The crystal is isostructural with the previously studied Ni and Co analogues. The Zn atom has a slightly distorted square-planar coordination formed by two O and two N atoms of the tetradentate Schiff base ligand.

Comment

Zinc(II) complexes play important roles in numerous biological systems, where they usually function as the active sites of hydrolytic enzymes (Casella & Gullotti, 1981; Leussing & Leach, 1971). As a part of our investigations of the structures of zinc derivatives, we prepared a new Zn^{II} complex, *viz.* the title compound, (I); its structure is reported here.



(I)

Compound (I) is a mononuclear zinc(II) complex (Fig. 1). The crystals of (I) are isostructural with those of the previously studied Ni and Co analogues (Freiburg *et al.*, 1980; Akhtar, 1981; Ma *et al.*, 2004). Atom Zn1 has a slightly distorted square-planar coordination formed by atoms O1, O2, N1 and N2 of the tetradentate Schiff base ligand. The bond lengths involving atom Zn1 (Table 1) are comparable to the corresponding values observed in other zinc(II) complexes (Hou, 2005; Chisholm *et al.*, 2001; Erxleben, 2001). The bond angles at atom Zn1 show some deviations from ideal square-planar geometry. The two *trans* bond angles N2—Zn1—O1 and N1—Zn1—O2 are 176.90 (10) and 178.54 (10)°, respectively. All other bond angles at atom Zn1 are close to 90°, ranging from 86.52 (9) to 93.49 (10)°. The molecule as a whole is almost planar, with the notable exception of the dimethylene fragment, whose conformation may be characterized by the N1—C12—C13—N2 torsion angle [−34.0 (3)°].

Experimental

1,2-Diaminoethane (0.1 mmol, 6.0 mg) and 2-hydroxy-1-naphthaldehyde (0.2 mmol, 34.3 mg) were dissolved in MeOH (15 ml), and the mixture was stirred for about 20 min to give a clear yellow solution. An MeOH solution (5 ml) of $Zn(ClO_4)_2{\cdot}7H_2O$ (0.1 mmol, 39.1 mg) was then added, and the mixture was stirred for another 20 min. The resulting colourless solution was left to stand; colourless block crystals precipitated after 5 d.

Crystal data

$[Zn(C_{24}H_{18}N_2O_2)]$
M_r = 431.77
Monoclinic, $P2_1/c$
a = 17.681 (1) Å
b = 8.184 (1) Å
c = 12.957 (1) Å
β = 99.92 (1)°
V = 1846.9 (3) Å^3
Z = 4
D_x = 1.553 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2849 reflections
θ = 2.7–26.9°
μ = 1.35 mm^{-1}
T = 298 (2) K
Block, colourless
0.33 × 0.30 × 0.22 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.663, T_{max} = 0.755
9152 measured reflections
4153 independent reflections
3029 reflections with $I > 2\sigma(I)$
R_{int} = 0.061
θ_{max} = 27.5°
$h = -21 \rightarrow 22$
$k = -10 \rightarrow 9$
$l = -15 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.137
S = 1.01
4153 reflections
262 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0753P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	1.836 (2)	Zn1—O1	1.848 (2)
Zn1—N2	1.836 (2)	Zn1—O2	1.849 (2)
N1—Zn1—N2	86.91 (11)	N1—Zn1—O2	178.54 (10)
N1—Zn1—O1	93.49 (10)	N2—Zn1—O2	93.16 (10)
N2—Zn1—O1	176.90 (10)	O1—Zn1—O2	86.52 (9)
N1—C12—C13—N2	−34.0 (3)		

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

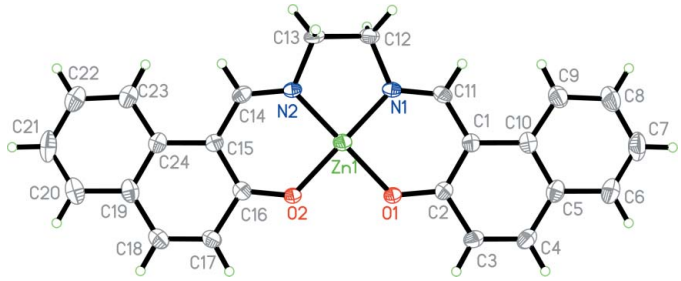


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level; H atoms are shown as small spheres of arbitrary radius.

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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