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Bis{1-[*N*-(2-methoxyphenyl)iminomethyl]naphthalen-2(1*H*)-onato-κ^3O,N,O'}zinc(II) ethanol solvate

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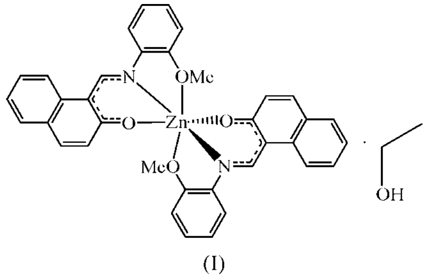
In the crystal structure of the title compound, $[Zn(C_{18}H_{14}NO_2)_2]\cdot C_2H_6O$, the Zn atom displays a highly distorted octahedral coordination involving the O and N atoms of two molecules of the Schiff base 1-[*N*-(2-methoxyphenyl)iminomethyl]naphthalen-2(1*H*)-one, which acts as an *O*,*N*,*O'*-tridentate ligand. The ethanol molecule is bound to the methoxy group of one ligand molecule *via* a hydrogen bond.

Comment

Schiff bases derived from 2-hydroxy-1-naphthaldehyde are interesting ligands with excellent donor abilities. Such derivatives having N, O or other heteroatom donors are good chelating agents (Elerman *et al.*, 1992; Elmali *et al.*, 1993; Bashirpoor *et al.*, 1997; Cindrić *et al.*, 2004; Popović, Roje, Pavlović, Matković-Čalogović & Giester, 2001; Popović, Roje, Pavlović, Matković-Čalogović, Rajić & Giester, 2001; Popović *et al.*, 2004).



(I)

In the crystal structure of the title compound, (I), the Zn atom displays a highly distorted octahedral coordination involving four O and two N atoms of two molecules of the Schiff base acting as a tridentate ligand (Fig. 1). Coordination of the Zn^{II} ion by the two methoxy O atoms is weakened, which is reflected in the lengthening of the Zn—O(methoxy) distances [2.4778 (18) and 2.556 (2) Å] in comparison with the Zn—O(oxo) bond lengths [1.9674 (18) and 1.9722 (18) Å]. In the previously reported structure of bis(salicylal-*o*-anisidinato)zinc(II) (Shol'nikova *et al.*, 1970), the Zn—O bond distances were also found in a wide range (1.965–2.406 Å). The Zn—N [2.025 (2) and 2.0260 (19) Å] distances in (I) are comparable with the corresponding values reported in the literature (Mukherjee *et al.*, 2000; Rajsekhar *et al.*, 2003).

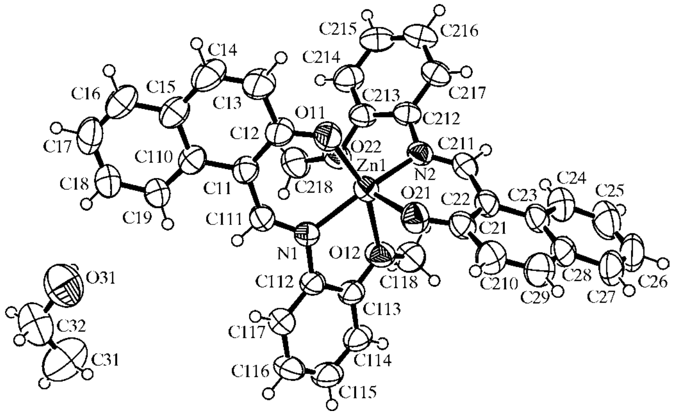


Figure 1
A plot of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

Delocalization of the π electrons accounts for the O11—C12, O21—C22, N1—C111 and N2—C211 bond lengths [1.285 (3), 1.305 (3), 1.299 (3) and 1.288 (3) Å, respectively] being intermediate between single- and double-bond values (Allen *et al.*, 1987). Bond lengths in the naphthalene moieties are mostly as expected; shortening of the C13—C14 and C23—C24 bonds [1.353 (4) and 1.342 (4) Å] is consistent with the quinoid effect (Exelby & Grinter, 1965).

The six-membered chelate rings, Zn1/O11/C12/C11/C111/N1 and Zn1/O21/C22/C21/C211/N2, are almost planar. The angles between the planes of the naphthalene rings and the phenyl rings of the phenyliminomethyl substituents [40.11 (8) and 53.55 (8)°] indicate non-planarity of the Schiff base ligands.

In addition to van der Waals interactions, the crystal packing in (I) is stabilized by weak intermolecular C—H···O hydrogen bonds. The ethanol solvent molecule is linked to the methoxy group of one ligand molecule by an O—H···O hydrogen bond (Table 2).

Experimental

For the preparation of the ligand, 2-hydroxy-1-naphthaldehyde (1.72 g, 10 mmol) and *o*-anisidine (1.23 g, 10 mmol) were dissolved in ethanol (40 ml) and the solution was refluxed for 1 h. The resulting yellow product was filtered off, washed with ethanol and dried *in vacuo* (yield 2.12 g, 76.5%). Elemental analysis found (calculated) for $C_{18}H_{15}NO_2$: C 77.86 (77.96), H 5.68 (5.45), N 5.00% (5.05%). The title compound was prepared by mixing zinc(II) acetate dihydrate (0.25 g, 1.14 mmol), the above ligand (0.63 g, 2.28 mmol) and triethylamine (0.23 g, 2.28 mmol) in ethanol (45 ml). After refluxing for 3 h, the reaction mixture was left to stand at room temperature for about a week. Only a few yellow single crystals of (I) were obtained. After a

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period of time, the crystals deteriorated into a yellow powder. Elemental analysis found (calculated) for $C_{36}H_{28}N_2O_4Zn$: C 70.28 (69.96), H 5.04 (4.57), N 4.32% (4.53%). Elemental analyses (CHN) were performed at the Central Analytical Laboratory of the Ruer Bošković Institute, Zagreb, Croatia.

Crystal data

$[Zn(C_{18}H_{14}NO_2)_2]\cdot C_2H_6O$
$M_r = 664.06$
Triclinic, $P\overline{1}$
$a = 10.2078$ (15) Å
$b = 10.9122$ (14) Å
$c = 16.7214$ (10) Å
$\alpha = 96.550$ (16)°
$\beta = 98.113$ (8)°
$\gamma = 115.592$ (12)°
$V = 1630.8$ (4) Å^3

$Z = 2$
$D_x = 1.352$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 60 reflections
$\theta = 10.2$–18.0°
$\mu = 0.80$ mm^{-1}
$T = 295$ K
Needle, yellow
0.58 × 0.11 × 0.09 mm

Data collection

Philips PW1100 diffractometer, upgraded by Stoe
ω scans
Absorption correction: ψ scan (*X-RED*; Stoe & Cie, 1995)
$T_{\min} = 0.90$, $T_{\max} = 0.93$
9774 measured reflections
9462 independent reflections
5673 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.091$
$\theta_{\max} = 30.0°$
$h = -14 \rightarrow 14$
$k = -15 \rightarrow 15$
$l = 0 \rightarrow 23$
5 standard reflections
frequency: 120 min
intensity decay: 4.1%

Table 1
Selected geometric parameters (Å, °).

Zn1—O11	1.9674 (18)	N2—C212	1.420 (3)
Zn1—O12	2.4778 (18)	N1—C111	1.299 (3)
Zn1—O21	1.9722 (18)	N1—C112	1.423 (3)
Zn1—O22	2.556 (2)	O12—C113	1.363 (3)
Zn1—N1	2.0260 (19)	O22—C213	1.378 (3)
Zn1—N2	2.025 (2)	O11—C12	1.285 (3)
O21—C22	1.305 (3)	C23—C24	1.342 (4)
N2—C211	1.288 (3)	C14—C13	1.353 (4)
O11—Zn1—O21	109.25 (9)	N2—Zn1—N1	150.26 (8)
O11—Zn1—N2	104.67 (8)	O11—Zn1—O12	155.69 (8)
O21—Zn1—N2	90.74 (8)	O21—Zn1—O12	92.20 (7)
O11—Zn1—N1	91.26 (8)	N2—Zn1—O12	85.80 (7)
O21—Zn1—N1	107.75 (8)	N1—Zn1—O12	70.78 (7)

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O31—H31$\cdots$O21$^{\rm i}$	0.82	1.97	2.781 (4)	169
C23—H23$\cdots$O31$^{\rm ii}$	0.93	2.53	3.263 (6)	136
C27—H27$\cdots$O31$^{\rm iii}$	0.93	2.48	3.225 (6)	137

Symmetry codes: (i) $x-1, y, z$; (ii) $x+1, y, z$; (iii) $x+1, y-1, z$.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.165$
$S = 1.03$
9462 reflections
419 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1019P)^2 + 0.0196P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.69$ e Å^{-3}
$\Delta\rho_{\min} = -0.63$ e Å^{-3}

All H atoms were positioned geometrically, each riding on their carrier atom, with C—H distances in the range 0.93–0.97 Å and an O—H distance of 0.82 Å, and with $U_{\rm iso}$(H) = 1.5 (for methyl and hydroxyl H atoms) or 1.2 (for methylene and aromatic H atoms) times $U_{\rm eq}$ of the parent atom.

Data collection: *STADI4* (Stoe & Cie, 1995); cell refinement: *STADI4*; data reduction: *X-RED* (Stoe & Cie, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: AV1245). Services for accessing these data are described at the back of the journal.

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