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Bis[1-(2-hydroxyethyliminomethyl)-2-naphtholato-κ^2N,O]nickel(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.052
wR factor = 0.124
Data-to-parameter ratio = 12.4

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

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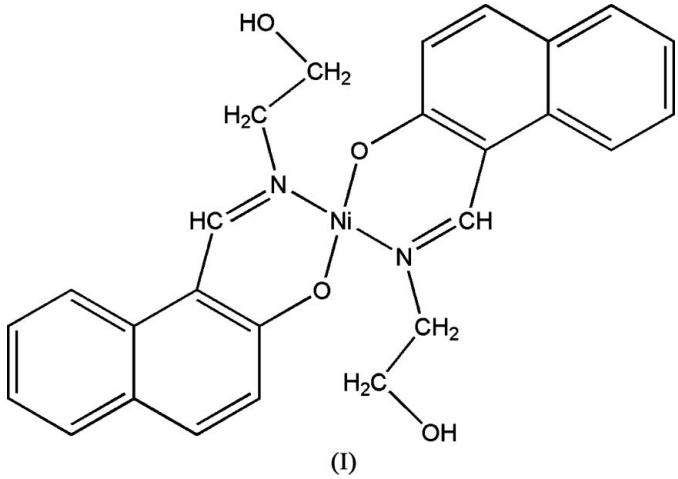
The title nickel(II) complex, $[Ni(C_{13}H_{12}NO_2)_2]$, has been synthesized by the reaction of a Schiff base ligand derived from 2-hydroxy-1-naphthaldehyde and 2-ethanolamine with $Ni(CH_3COO)_2\cdot4H_2O$. The asymmetric unit consists of half each of two independent molecules which have similar geometries, with the Ni atom of each of the two neutral complex molecules lying on an inversion centre. The coordination geometry around each Ni atom is square planar, with the two bidentate chelate Schiff base ligands coordinated through their imine N and phenol O atoms in a mutually *trans* configuration. The hydroxy O atoms do not coordinate to the Ni atom.

Comment

Schiff bases are of considerable current interest due to their biological activity (Garnovskii *et al.*, 1993; Costamagna *et al.*, 1992; Walsh & Orme-Johnson, 1987). Apart from this, photochromism is another characteristic of these materials, leading to applications in various areas such as the control and measurement of radiation intensity, display systems and optical computers (Hadjoudis *et al.*, 1987; Elmali *et al.*, 1999). We report here the crystal structure of the title compound, (I) (Fig. 1 and Table 1).



(I)

The asymmetric unit of (I) consists of half each of two independent molecules which have similar geometries, with the Ni atom of each of the two neutral complex molecules lying on an inversion centre. The hydroxy O atoms are not involved in coordination to nickel, with the Schiff base acting as a bidentate chelate ligand, coordinating to nickel through the phenol O and imine N atoms. The geometry at the Ni atom is essentially square planar, as has been observed previously in

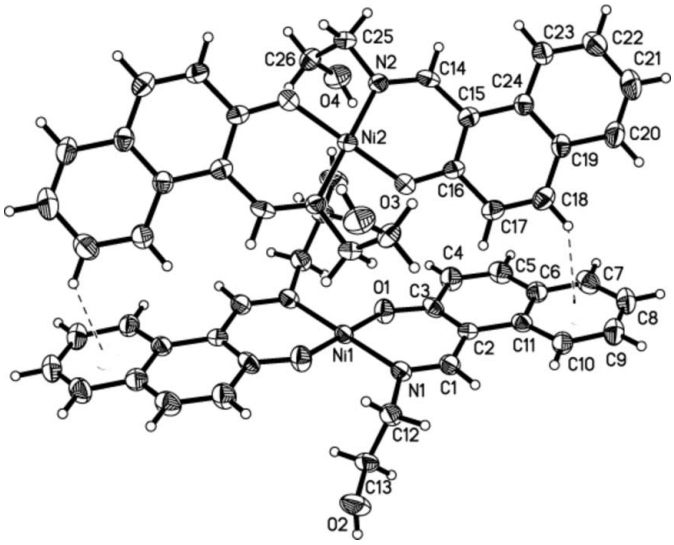


Figure 1
The two independent molecules of (I), showing 40% probability displacement ellipsoids and the atom-numbering scheme. The dashed line represents the C—H···π interaction between the two molecules. Unlabelled atoms are related to labelled atoms by the symmetry operations ($-x$, $-y$, $-z$) for the Ni1 molecule and ($-x$, $1-y$, $-z$) for the Ni2 molecule.

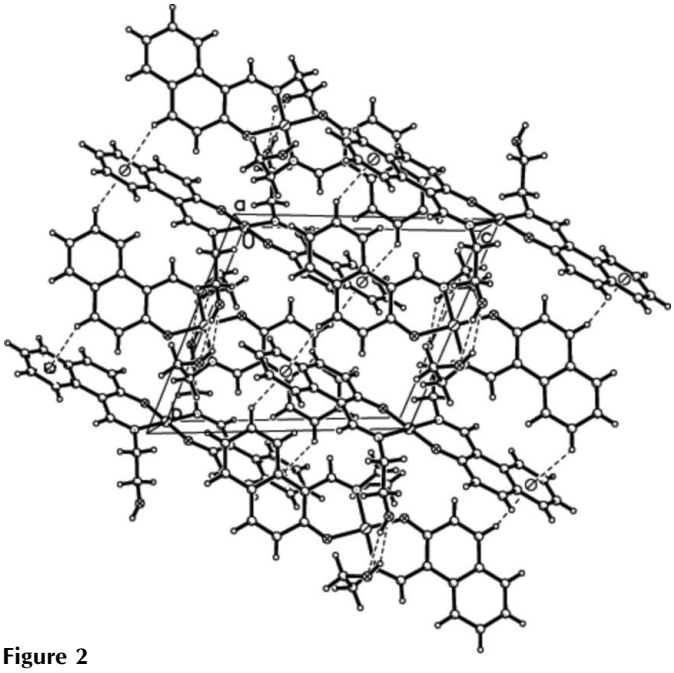


Figure 2
A molecular packing diagram of (I). Hydrogen bonds and C—H···π interactions are shown as dashed lines.

similar molecules (Liu *et al.*, 2004; Nepveu, & Paulus, 1985). The dihedral angle between the N1/C1–C13/O1 plane and N2/C14–C24/O3 planes is 51.43 (8)°. The largest deviation from the least-squares plane through all the atoms of the Ni1 complex (except Ni1, and the atoms of the pendant ethanol substituent, *viz*. O2, C12 and C13) is 0.0931 (3) Å for atom C1. Atom Ni1 lies −0.4661 (2) Å from that plane. The second complex deviates further from planarity, the dihedral angle between the C14—C-24 and Ni2/O3/N2 planes being 23.61 (10)°.

O—H···O hydrogen bonds and C—H···π interactions involving the C6–C11 benzene ring stabilize the structure (Fig. 2 and Table 2).

Experimental

The title compound, (I), was prepared by reacting $Ni(CH_3COO)_2{\cdot}4H_2O$ with salicylaldehyde and 2-hydroxy-1-naphthaldehyde (1:2:2 molar ratio) in ethanol. Single crystals of (I) suitable for X-ray study were obtained by recrystallization from a dimethylformamide–methanol (2:1 *v*/*v*) solution.

Crystal data

$[Ni(C_{13}H_{12}NO_2)_2]$
M_r = 487.18
Triclinic, $P\overline{1}$
a = 10.227 (4) Å
b = 10.288 (4) Å
c = 12.119 (5) Å
α = 105.941 (6)°
β = 109.636 (6)°
γ = 103.438 (6)°
V = 1077.9 (8) Å^3
Z = 2
D_x = 1.501 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.94 mm^{-1}
T = 298 (2) K
Plate, brown
0.43 × 0.15 × 0.07 mm

Data collection

Bruker CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.689, T_{max} = 0.937
5658 measured reflections
3748 independent reflections
2236 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.124
S = 1.01
3748 reflections
303 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.826 (3)	Ni2—O3	1.818 (3)
Ni1—N1	1.904 (4)	Ni2—N2	1.907 (4)
O1^{i}—Ni1—O1	180	O3^{ii}—Ni2—O3	180
O1—Ni1—N1	91.47 (15)	O3—Ni2—N2	91.40 (15)
N1^{i}—Ni1—N1	180	N2—Ni2—N2^{ii}	180

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O4^{i}	0.82	2.01	2.813 (5)	164
O4—H4···O2^{i}	0.82	2.22	2.813 (5)	129
C18—H18···Cg	0.93	2.76 (1)	3.4914 (11)	136
C22—H22···Cg^{iii}	0.93	3.06 (1)	3.6071 (12)	119

Symmetry codes: (i) $-x$, $-y$, $-z$; (iii) x, $y+1$, z. Cg is the centroid of the C6–C11 benzene ring.

All H atoms were refined using a riding model, with C—H = 0.93–0.97 Å, O—H = 0.82 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ and $1.5U_{eq}(O)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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References

Bruker (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1998). *SMART*. Version 5.0. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Costamagna, J., Vargas, J., Latorre, R., Alvarado, A. & Mena, G. (1992). *Coord. Chem. Rev.* **119**, 67–88.
Elmali, A., Kabak, M., Kavlakoglu, E., Elerman, Y. & Durlu, T. N. (1999). *J. Mol. Struct.* **510**, 207–214.
Garnovskii, A. D., Nivorozhkin, A. L. & Minkin, V. I. (1993). *Coord. Chem. Rev.* **126**, 1–69.
Hadjoudis, E., Vittorakis, M. & Moustakali-Mavridis, I. (1987). *Tetrahedron*, **43**, 1345–1360.
Liu, H., Wang, H., Niu, D. & Lu, Z. (2004). *Acta Cryst.* E**60**, m1941–m1942.
Nepveu, F. & Paulus, H. (1985). *Acta Cryst.* C**41**, 858–860.
Sheldrick, G. M. (1996). *SADABS*. Version 2.05. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Walsh, C. T. & Orme-Johnson, W. H. (1987). *Biochemistry*, **26**, 4901–4906.