Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis{1-[3-(cyclohexylamino)propyliminomethyl]-naphth-2-olato}nickel(II)

Yi-Jun Wei

Department of Chemistry, Huainan Normal College, Huainan 232001, People's Republic of China

Correspondence e-mail: huainanweiyijun@163.com

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.071
wR factor = 0.186
Data-to-parameter ratio = 17.7

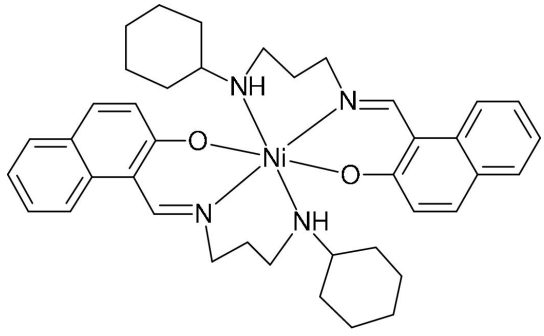
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 14 April 2005
Accepted 19 April 2005
Online 14 May 2005

In the title centrosymmetric mononuclear nickel(II) complex, $[Ni(C_{20}H_{25}N_2O)_2]$, the Ni^{II} ion has octahedral geometry and is coordinated by two O atoms and four N atoms from two Schiff bases.

Comment

Nickel complexes are very important in biology, for example, functioning as the active site of hydrolytic enzymes such as ureases (Carlsson *et al.*, 2004; Brown *et al.*, 2001). As part of an investigation of the structures of such nickel compounds, the title centrosymmetric mononuclear nickel(II) complex, (I), is reported here.



(I)

The molecular structure of (I) is illustrated in Fig. 1. The Ni^{II} ion, lying on an inversion center, is in an octahedral geometry and is six-coordinated by two O atoms and four N atoms from two Schiff bases. Selected bond distances and angles are given in Table 1. All the bond lengths are in normal ranges (Allen *et al.*, 1987). The bond lengths involving the Ni^{II} ion are comparable to the corresponding values observed in other nickel(II) complexes (Zhu *et al.*, 2004; Gomes *et al.*, 2000). The bond angles around the central metal ion show very slight deviations from ideal octahedral geometry, ranging from 89.66 (10) to 90.34 (10)°. The three *trans* bond angles are 180°, from symmetry.

Experimental

2-Hydroxy-1-naphthaldehyde (0.1 mmol, 17.5 mg) and *N*-cyclohexyl-1,3-diaminopropane (0.1 mmol, 15.5 mg) were dissolved in MeOH (15 ml). The mixture was stirred for about 30 min to give an orange solution. To the solution was added an MeOH solution (15 ml) of $Ni(CH_3COO)_2{\cdot}4H_2O$ (0.1 mmol, 25.4 mg), with stirring. The resulting solution was kept in air for 13 d, after which time green block-shaped crystals were formed.

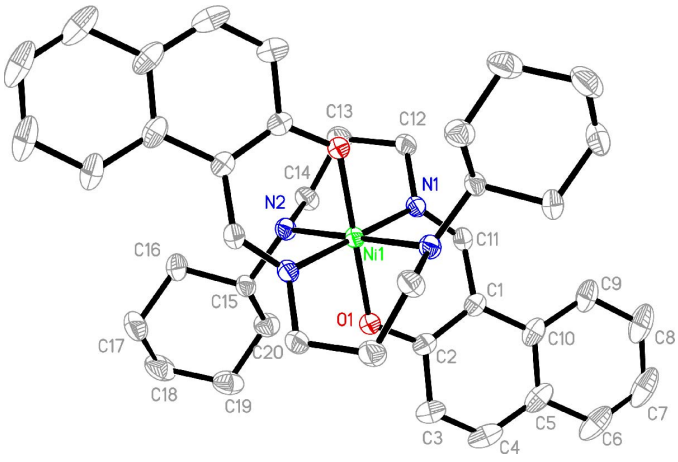


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. Unlabelled atoms are related to labelled atoms by $(1-x, 1-y, 1-z)$.

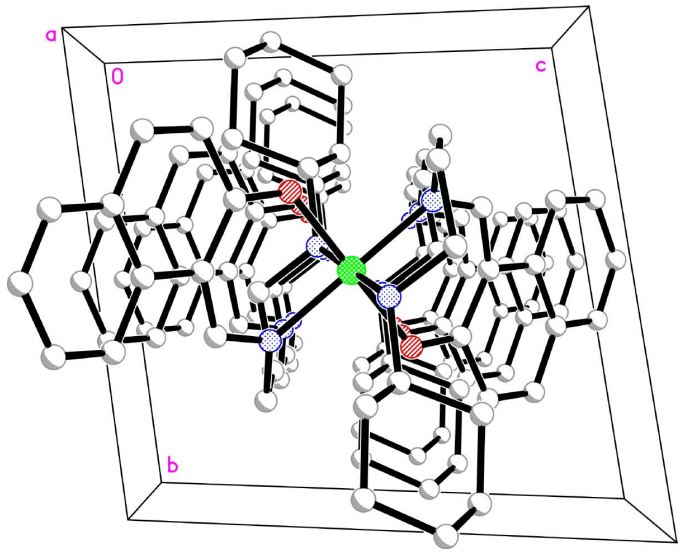


Figure 2
The crystal packing of (I), viewed along the *a* axis. H atoms have been omitted for clarity.

Crystal data

$[Ni(C_{20}H_{25}N_2O)_2]$	$Z = 1$
$M_r = 677.55$	$D_x = 1.149$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 9.248$ (2) Å	Cell parameters from 2530 reflections
$b = 10.272$ (2) Å	$\theta = 2.5$–$24.1°$
$c = 11.399$ (2) Å	$\mu = 0.53$ mm^{-1}
$\alpha = 79.155$ (2)°	$T = 298$ (2) K
$\beta = 67.425$ (2)°	Block, green
$\gamma = 81.923$ (2)°	0.20 × 0.20 × 0.09 mm
$V = 979.2$ (3) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3841 independent reflections
ω scans	3329 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.026$
$T_{min} = 0.901$, $T_{max} = 0.954$	$\theta_{max} = 26.5°$
7553 measured reflections	$h = -11 \rightarrow 11$
	$k = -12 \rightarrow 12$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.071$	$w = 1/[\sigma^2(F_o^2) + (0.1292P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.186$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.07$	$\Delta\rho_{max} = 1.36$ e Å^{-3}
3841 reflections	$\Delta\rho_{min} = -0.42$ e Å^{-3}
217 parameters	

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.890 (2)	Ni1—N2	2.023 (2)
Ni1—N1	1.926 (2)		
O1—Ni1—O1^i	180	N1—Ni1—N2^i	90.11 (11)
O1—Ni1—N1	90.28 (10)	O1—Ni1—N2	89.66 (10)
O1^i—Ni1—N1	89.72 (10)	N1—Ni1—N2	89.89 (11)
N1—Ni1—N1^i	180	N2^i—Ni1—N2	180
O1—Ni1—N2^i	90.34 (10)		

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

Atom H2 was located in a difference Fourier map and refined isotropically, with the N—H distance restrained to 0.90 (1) Å and U_{iso}(H) = 0.08 Å^2. The other 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). The structure contains solvent-accessible voids of 190 Å^3, which might accommodate a disordered MeOH molecule. An unassigned maximum residual density was observed 2.59 Å from atom H12*A*.

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*.

The author thanks the Education Office of Anhui Province, People's Republic of China, for research grant No. 2004kj326.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans.* 2, pp. S1–83.
Brown, D. A., Errington, W., Glass, W. K., Haase, W., Kemp, T. J., Nimir, H., Ostrovsky, S. M. & Werner, R. (2001). *Inorg. Chem.* **40**, 5962–5971.
Bruker (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Carlsson, H., Haukka, M., Bousseksou, A., Latour, J.-M. & Nordlander, E. (2004). *Inorg. Chem.* **43**, 8252–8262.
Gomes, L., Sousa, C., Freire, C. & de Castro, B. (2000). *Acta Cryst.* C**56**, 1201–1203.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Zhu, B., Ruang, W. & Zhu, Z. (2004). *Acta Cryst.* E**60**, m634–m636.