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Bis[2-(cyclohexyliminomethyl)-6-methoxyphenolato]nickel(II)

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Key indicators

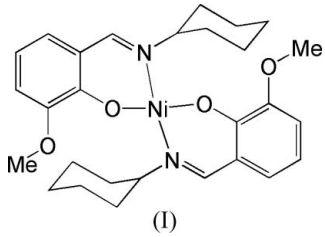
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.063
wR factor = 0.163
Data-to-parameter ratio = 18.0

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

In the title mononuclear nickel(II) complex, [Ni($C_{14}H_{18}NO_2$)$_2$], the Ni^{II} atom is four-coordinated in a square-planar geometry by two phenolate O atoms and two imine N atoms from two Schiff base ligands. The Ni atom lies on a centre of inversion.

Comment

Nickel(II) complexes with Schiff base ligands have received much attention in recent years (Marganian *et al.*, 1995). Some of the complexes have been found to have pharmacological and catalytic properties (Harrop *et al.*, 2003; Brückner *et al.*, 2000). Nickel is present in the active sites of several important classes of metalloproteins, as either a homodinuclear or a heterodinuclear species. In order to further develop the coordination chemistry of such nickel complexes, the title nickel(II) complex, (I), is reported here.



(I)

The Ni^{II} atom in (I) is coordinated by two phenolate O and two imine N atoms from two Schiff base ligands, forming a four-coordinate square-planar geometry (Fig. 1). The Ni atom

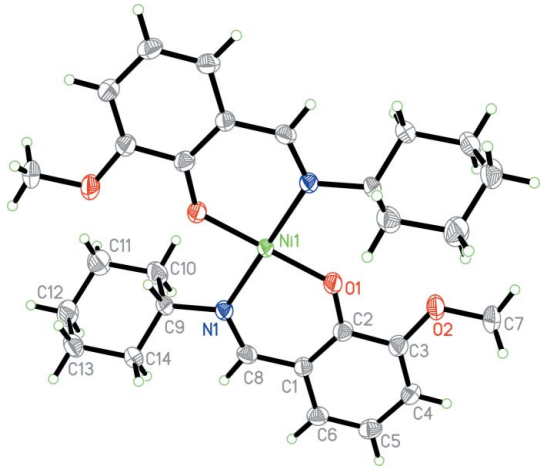


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are related to labelled atoms by $-x$, $-y$, $-z$.

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lies on a centre of inversion. All the bond lengths and angles (Table 1) subtended at the Ni centre are comparable with the values observed in other Schiff base nickel(II) complexes (Liu *et al.*, 2006; Yu, 2006; Zhu *et al.*, 2004). There are no significant intermolecular interactions in the crystal structure (Fig. 2).

Experimental

3-Methoxysalicylaldehyde (1.0 mmol, 152.3 mg), cyclohexylamine (1.0 mmol, 99.2 mg) and $Ni(CH_3COO)_2{\cdot}4H_2O$ (0.5 mmol, 124.3 mg) were dissolved in MeOH (80 ml). The mixture was stirred at room temperature for about 1 h, giving a red solution. After allowing the solution to stand in air for 12 d, red block-shaped crystals were formed.

Crystal data

$[Ni(C_{14}H_{18}NO_2)_2]$
M_r = 523.30
Monoclinic, $P2_1/c$
a = 11.043 (1) Å
b = 18.041 (4) Å
c = 6.465 (2) Å
β = 99.990 (3)°
V = 1268.5 (5) Å^3
Z = 2
D_x = 1.370 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.80 mm^{-1}
T = 298 (2) K
Block, red
0.32 × 0.27 × 0.23 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.784, T_{max} = 0.837
10730 measured reflections
2890 independent reflections
1739 reflections with $I > 2\sigma(I)$
R_{int} = 0.083
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.163
S = 1.02
2890 reflections
161 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0691P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.97 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.872 (3)	Ni1—N1	2.019 (3)
O1—Ni1—O1^{i}	180	O1—Ni1—N1	91.37 (11)
O1—Ni1—N1^{i}	88.63 (11)	N1^{i}—Ni1—N1	180

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

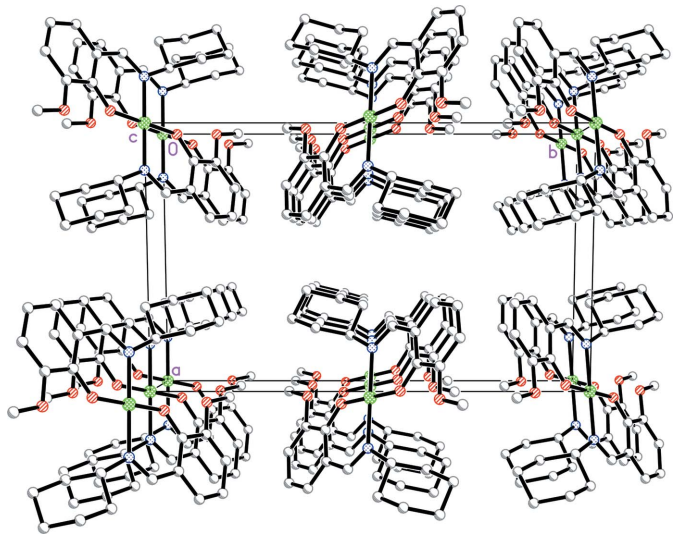

Figure 2
The crystal packing of (I). H atoms have been omitted.

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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