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## Key indicators

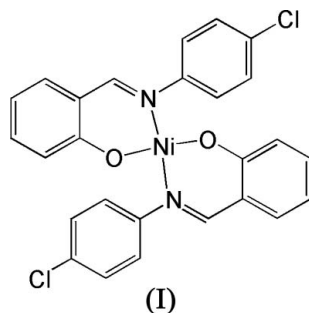
Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$   
 $R$  factor = 0.051  
 $wR$  factor = 0.120  
Data-to-parameter ratio = 17.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

## Bis[2-(4-chlorophenyliminomethyl)phenolato]-nickel(II)

In the title mononuclear nickel(II) complex,  $[\text{Ni}(\text{C}_{13}\text{H}_9\text{ClNO})_2]$ , the  $\text{Ni}^{\text{II}}$  atom lies on an inversion center and is coordinated by the N and O atoms of the two Schiff base ligands in a square-planar geometry. The dihedral angle between the two chlorophenyl rings is  $39.5(3)^\circ$ .

## Comment

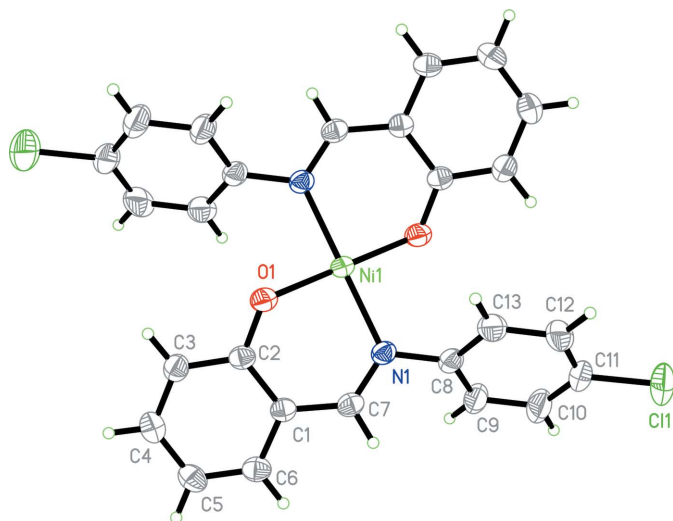
Nickel(II) compounds with Schiff bases have received much attention in recent years (Marganian *et al.*, 1995). Some of the compounds have been found to have pharmacological and catalytic properties (Harrop *et al.*, 2003; Brückner *et al.*, 2000). Nickel is present in the active sites of several important classes of metalloproteins, as either a homodinuclear or a heterodinuclear species. The active site of 2-mercaptoethanol-inhibited urease contains two Ni centers bridged by thiolate ligands. Similar bridging is observed between the Ni and Fe centers in Ni/Fe hydrogenases (Goswami & Eichhorn, 1999; Pearson *et al.*, 1997; Arnold *et al.*, 1998). The coordination sphere in both of these metalloenzyme systems contains N and S donor atoms in unusual five- or six-coordinate arrangements with significant distortions from regular geometry. These unusual structural features have led to increased interest in the synthesis of nickel complexes with various ligands as structural and spectroscopic models of the active sites (Rybak-Akimova *et al.*, 1998, 1999; Curtis *et al.*, 2006; Desrochers *et al.*, 2005; Edison *et al.*, 2004). In order to further develop the coordination chemistry of such nickel compounds, we have synthesized the title nickel(II) complex, (I), based on the Schiff base ligand 2-[(4-chlorophenylimino)methyl]phenol.



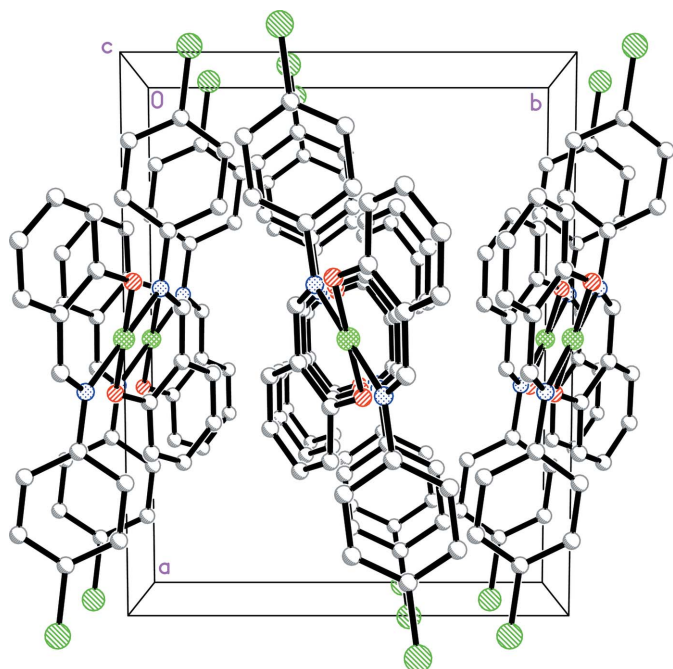
The  $\text{Ni}^{\text{II}}$  atom in (I) lies on an inversion center and is coordinated by the N and O atoms of the two Schiff base ligands in a square-planar geometry (Fig. 1). The dihedral angle between the C1–C6 and C8–C13 benzene rings is  $39.5(3)^\circ$ . The Ni–O and Ni–N bond lengths (Table 1) are comparable to the values in similar complexes (Chakraborty *et al.*, 2004; Skovsgaard *et al.*, 2005; Adams *et al.*, 2004; Bian *et al.*,

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**Figure 1**  
The molecular structure of (I), with anisotropic displacement ellipsoids drawn at the 30% probability level. Unlabeled atoms are related to labeled atoms by the symmetry code  $(1 - x, 2 - y, -z)$ .



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

2004). In the crystal structure, molecules stack in columns along the  $c$  axis (Fig. 2).

## Experimental

Salicylaldehyde (0.5 mmol, 61.1 mg) and 4-chlorophenylamine (0.5 mmol, 63.5 mg) were stirred into 50 ml of methanol. After 1 h,  $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$  (0.3 mmol, 87.3 mg) in methanol (20 ml) was added, and the stirring was continued for a further 1 h. The filtrate was kept at room temperature for about two weeks, depositing very thin, green, plate-like crystals of (I).

## Crystal data

$[\text{Ni}(\text{C}_{13}\text{H}_9\text{ClNO})_2]$   
 $M_r = 520.03$   
Monoclinic,  $P2_1/c$   
 $a = 13.568$  (2) Å  
 $b = 10.676$  (3) Å  
 $c = 8.168$  (4) Å  
 $\beta = 99.027$  (3)°  
 $V = 1168.5$  (7) Å<sup>3</sup>

$Z = 2$   
 $D_x = 1.478$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
 $\mu = 1.09$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
Plate, green  
 $0.12 \times 0.10 \times 0.04$  mm

## Data collection

Bruker SMART APEX CCD area-detector diffractometer  
 $\omega$  scans  
Absorption correction: multi-scan (SADABS; Bruker, 2000)  
 $T_{\min} = 0.881$ ,  $T_{\max} = 0.958$

9797 measured reflections  
2667 independent reflections  
1643 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.065$   
 $\theta_{\text{max}} = 27.5^\circ$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.051$   
 $wR(F^2) = 0.120$   
 $S = 1.02$   
2667 reflections  
151 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0217P)^2 + 0.3785P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.32$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.31$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Ni1—O1	1.878 (2)	Ni1—N1	2.020 (3)
O1—Ni1—O1 <sup>i</sup>	180	O1—Ni1—N1	90.94 (10)
O1—Ni1—N1 <sup>i</sup>	89.06 (10)	N1 <sup>i</sup> —Ni1—N1	180

Symmetry code: (i)  $-x + 1, -y + 2, -z$ .

H atoms were positioned geometrically and refined as riding atoms, with C—H distances of 0.93 Å and  $U_{\text{iso}}(\text{H})$  set to  $1.2U_{\text{eq}}(\text{C})$ .

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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