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{*N*,*N*′-Bis[(5-chloro-2-hydroxyphenyl)-phenylmethylene]ethylendiaminato}-nickel(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.058
wR factor = 0.148
Data-to-parameter ratio = 13.1

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

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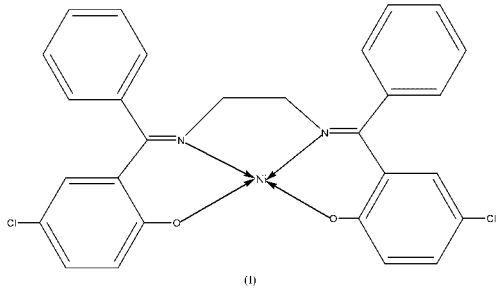
In the title complex, $[Ni(C_{28}H_{20}Cl_2N_2O_2)]$, the Ni^{II} atom exists in a square-planar environment, coordinated by four atoms from the tetradentate ligand. Molecules are held together by intermolecular C—H···O hydrogen bonds, which link the molecules in a chain along the *a* axis.

Comment

This work continues our studies of transition metal complexes with Schiff base ligands. In earlier papers, we reported salicylaldehyde (Bian, Gu *et al.*, 2003), acetylacetone (Bian, Xu *et al.*, 2003) and pyridine-2-carboxaldehyde (Wang *et al.*, 2004) Schiff base complexes. The present paper details the crystal structure of the nickel(II) complex with the Schiff base that is obtained by condensing 5-chloro-2-hydroxybenzophenone with ethylenediamine. The Ni^{II} atom is in a square-planar geometry as it is coordinated by the two N atoms and two O atoms from the tetradentate ligand (Fig. 1). The two ligand fragments O1/C13/C8/C7/N1 and O2/C14/C19/C20/N2 are inclined at an angle of 10.00 (2)° angle to each other. The Ni atom is in the O_2N_2 square and none of the five atoms deviates by more than 0.08 Å from it. In the crystal structure, the H atoms of C1 and C26 are involved in hydrogen bonding with atoms O1 and O2 of a neighboring molecule. These weak hydrogen bonds lead to the formation of a chain along the *a* axis.



(I)

Experimental

Crystal data

$[Ni(C_{28}H_{20}Cl_2N_2O_2)]$
M_r = 546.07
Triclinic, $P\overline{1}$
a = 10.168 (5) Å
b = 10.945 (5) Å
c = 11.492 (6) Å
α = 68.232 (7)°
β = 89.066 (8)°
γ = 85.532 (8)°
V = 1184.0 (10) Å^3
Z = 2
D_x = 1.532 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 840 reflections
θ = 3.3–25.1°
μ = 1.08 mm^{-1}
T = 293 (2) K
Prism, red
0.18 × 0.12 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.620, T_{max} = 0.898
6084 measured reflections
4133 independent reflections
2641 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 25.0°
$h = -12 \rightarrow 6$
$k = -13 \rightarrow 13$
$l = -13 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.148
S = 1.00
4133 reflections
316 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.074P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.831 (3)	Ni1—N1	1.859 (4)
Ni1—O2	1.830 (3)	Ni1—N2	1.854 (4)
O1—Ni1—O2	85.11 (15)	O2—Ni1—N1	173.87 (18)
O1—Ni1—N1	93.53 (16)	O2—Ni1—N2	93.92 (16)
O1—Ni1—N2	174.79 (18)	N1—Ni1—N2	87.96 (17)

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O1^{i}	0.93	2.51	3.385 (7)	157
C26—H26···O2^{ii}	0.93	2.52	3.371 (7)	152

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

H atoms were positioned geometrically and refined using a riding model, with C-H distances of 0.93 Å for aromatic H atoms and 0.97 Å for H atoms on secondary C atoms.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

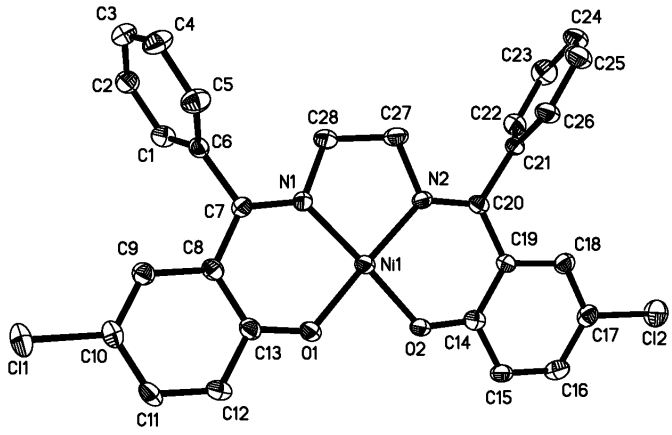


Figure 1
A view of the molecular structure of (I), with the atom-numbering scheme and 30% displacement ellipsoids. H atoms have been omitted.

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