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trans-Dichlorobis[2-(*o*-tolyliminomethyl)-phenolato-κ*O*]nickel(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.053
wR factor = 0.138
Data-to-parameter ratio = 14.3

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

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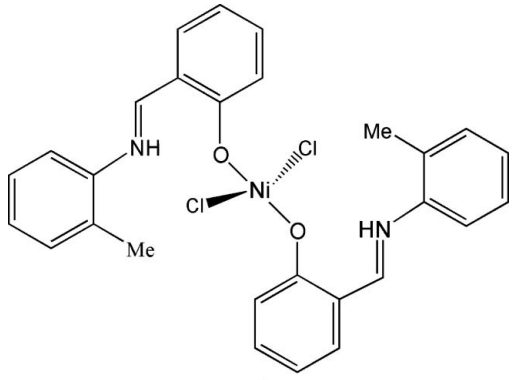
In the title compound, $[NiCl_2(C_{14}H_{13}NO)_2]$, the Ni^{II} atom is four-coordinated by two phenolate O atoms from two 2-(*o*-tolyliminomethyl)phenol ligands and two Cl anions, giving an approximately tetrahedral geometry. The Ni atom lies on a crystallographic twofold rotation axis. A strong intramolecular N—H···O hydrogen bond forms an *S*(6) ring.

Comment

Schiff base compounds play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Costamagna *et al.*, 1992; Bhatia *et al.*, 1981). Recently, we have reported a Schiff base compound (Cheng *et al.*, 2006). As an extension of our work on the structural characterization of Schiff base complexes, the title compound, (I), is reported here.



(I)

The Ni^{II} atom of (I) is four-coordinated by two Cl atoms and two phenolate O atoms from the Schiff base ligand 2-(*o*-tolyliminomethyl)phenol (Fig. 1). The Ni atom lies on a crystallographic twofold rotation axis. The angles around the Ni^{II} atom are in the range 103.7 (2)–115.4 (1)° (Table 1), indicating that the Ni^{II} atom is in a slightly distorted tetrahedral geometry. The Ni—O bond length of 1.981 (3) Å is a little shorter than the corresponding bond distance of 2.038 (2) Å observed in the six-coordinated Ni^{II} complex $[Ni(C_{16}H_{24}N_2O)_2(N_3)_2]$ (You *et al.*, 2004). The C7═N1 and C8—N1 bond lenths (Table 1) conform to the values for double and single bonds, respectively (Allen *et al.*, 1986).

The strong intramolecular N—H···O hydrogen bond (Table 2) results in the formation of a pseudo-six-membered planar ring, C1/C6/C7/N1/H1/O1 (Fig. 1). There are no significant intermolecular hydrogen bonds, so that van der Waals interactions are effective in the molecular packing (Fig. 2).

Experimental

Salicylaldehyde and *o*-toluidine were available commercially and were used without further purification. Salicylaldehyde (2.0 mmol, 244 mg) and *o*-toluidine (2.0 mmol, 214 mg) were dissolved in methanol (100 ml) and the mixture was stirred for 1 h to give a clear yellow solution. To the solution was added a methanol solution (30 ml) of $NiCl_2·6H_2O$ (1.0 mmol, 237 mg) with stirring. After keeping the resulting solution at room temperature in air for 10 d, large red block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent. The crystals were isolated, washed three times with methanol and dried in a vacuum desiccator using P_4O_{10} (yield 88.7%). Analysis, found: C 60.94, H 4.69, N 5.03%; calculated for $C_{28}H_{26}Cl_2N_2O_2Ni$: C 60.91, H 4.75, N 5.07%.

Crystal data

$[NiCl_2(C_{14}H_{13}NO)_2]$
M_r = 552.10
Monoclinic, $C2/c$
a = 16.0580 (2) Å
b = 10.4430 (1) Å
c = 15.7520 (3) Å
β = 104.507 (2)°
V = 2557.29 (7) Å^3
Z = 4
D_x = 1.434 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.00 mm^{-1}
T = 293 (2) K
Block, red
0.32 × 0.22 × 0.11 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.769, T_{max} = 0.896
6793 measured reflections
2285 independent reflections
1401 reflections with $I > 2\sigma(I)$
R_{int} = 0.065
θ_{max} = 25.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.138
S = 1.01
2285 reflections
160 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0589P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.981 (3)	N1—C7	1.298 (5)
Ni1—Cl1	2.2322 (13)	N1—C8	1.426 (5)
O1—Ni1—O1^{i}	103.73 (19)	O1—Ni1—Cl1	105.91 (9)
O1—Ni1—Cl1^{i}	115.36 (10)	O1^{i}—Ni1—Cl1	115.36 (10)
O1^{i}—Ni1—Cl1^{i}	105.91 (9)	Cl1^{i}—Ni1—Cl1	110.66 (8)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.86	1.91	2.601 (4)	137

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with N—H = 0.86 Å and C—H = 0.93–0.96 Å, and with U_{iso}(H) = 1.2U_{eq}(C,N).

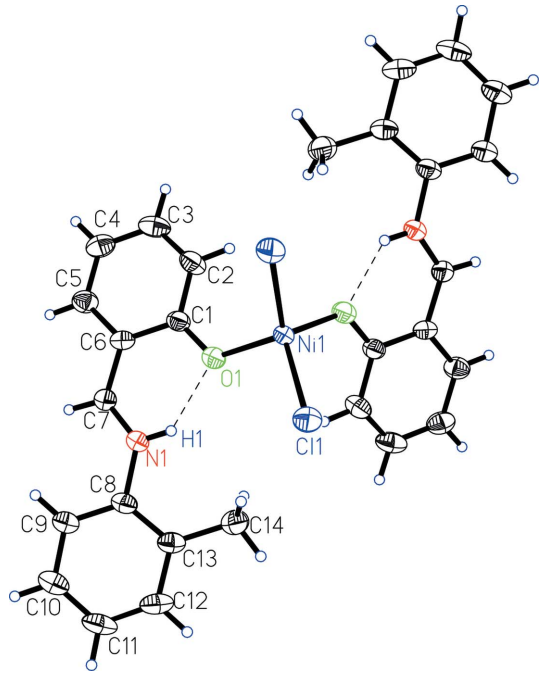


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Hydrogen bonds are indicated by dashed lines. Unlabelled atoms are related to labelled atoms by the symmetry operator $(-x+1, y, -z+\frac{1}{2})$.

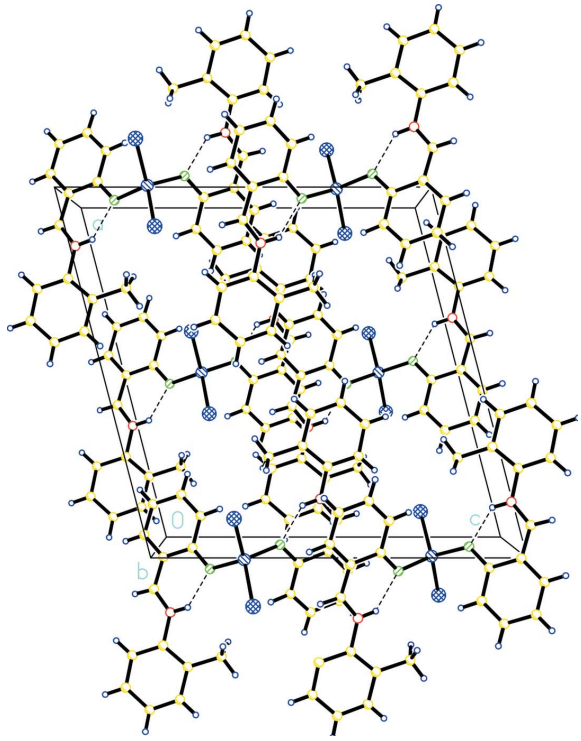


Figure 2
The crystal packing of (I), viewed along the *b* axis. Dashed lines indicate hydrogen bonds.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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*.

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