# {2,4-Dichloro-6-[2-(dimethylamino)ethyl-iminomethyl]phenolato}thiocyanatonickel(II)
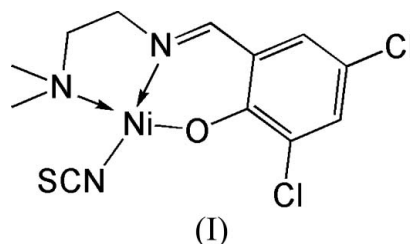
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In the title compound, [Ni(C$_{11}$H$_{12}$Cl$_2$N$_2$O)(NCS)], the Ni atom is four-coordinated in a square-planar geometry by one Schiff base ligand 2,4-dichloro-6-[2-(dimethylamino)ethyl-iminomethyl]phenol and by one terminal thiocyanate anion.

## Comment

Nickel(II) complexes are very important in bioinorganic chemistry and coordination chemistry (Suh *et al.*, 1996; Dey *et al.*, 2004; Angulo *et al.*, 2001; Ramadevi *et al.*, 2005; Edison *et al.*, 2004). As a further study of the structures of such complexes, the title nickel(II) complex, (I), is reported in this paper.



The Ni atom in (I) is four-coordinated by one O atom and two N atoms of the Schiff base ligand 2,4-dichloro-6-[2-(dimethylamino)ethyliminomethyl]phenol and by one N atom of the terminal thiocyanate anion, forming a square-planar geometry. The bond lengths and angles (Table 1) involving the Ni1 atom are within normal ranges and comparable with the corresponding values observed in other similar nickel(II) complexes (Zhu *et al.*, 2004; Wang, 2006; Wang & Wei, 2006; Liu *et al.*, 2006).

## Experimental

3,5-Dichloro-2-hydroxybenzaldehyde (0.4 mmol, 76.3 mg), *N*,*N*-dimethylethane-1,2-diamine (0.4 mmol, 35.7 mg) and ammonium thiocyanate (0.4 mmol, 26.2 mg) were dissolved in 10 ml methanol. To the mixture was added dropwise a 5 ml methanol solution of nickel(II) chloride hexahydrate (0.4 mmol, 95.0 mg) with stirring. The final solution was allowed to stand in air for a week, yielding red block-shaped crystals of (I).

*Crystal data*

| | |
|---|---|
| [Ni(C$_{11}$H$_{12}$Cl$_2$N$_2$O)(NCS)] | $Z = 4$ |
| $M_r = 376.92$ | $D_x = 1.671$ Mg m$^{-3}$ |
| Orthorhombic, *Pnma* | Mo $K\alpha$ radiation |
| $a = 19.308$ (1) Å | $\mu = 1.79$ mm$^{-1}$ |
| $b = 6.949$ (2) Å | $T = 291$ (2) K |
| $c = 11.169$ (2) Å | Block, red |
| $V = 1498.6$ (5) Å$^3$ | $0.41 \times 0.32 \times 0.27$ mm |

# metal-organic papers

## Data collection

Bruker SMART CCD area-detector
  diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan
  (*SADABS*; Sheldrick, 1996)
  $T_{min} = 0.528$, $T_{max} = 0.644$

12576 measured reflections
1978 independent reflections
1505 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 28.4°$

## Refinement

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.099$
$S = 1.04$
1978 reflections
123 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2$
  $+ 0.7298P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.39$ e Å$^{-3}$
$\Delta\rho_{min} = -0.46$ e Å$^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0043 (7)

## Table 1
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Ni1—O1 | 1.912 (3) | Ni1—N1 | 1.929 (3) |
| Ni1—N3 | 1.923 (4) | Ni1—N2 | 2.056 (3) |
| | | | |
| O1—Ni1—N3 | 91.78 (13) | O1—Ni1—N2 | 177.08 (12) |
| O1—Ni1—N1 | 92.39 (11) | N3—Ni1—N2 | 91.14 (14) |
| N3—Ni1—N1 | 175.83 (14) | N1—Ni1—N2 | 84.69 (13) |

H atoms were constrained to ideal geometries, with C—H = 0.93–0.96 Å and $U_{iso}$(H) = 1.2 or $1.5U_{eq}$(C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.
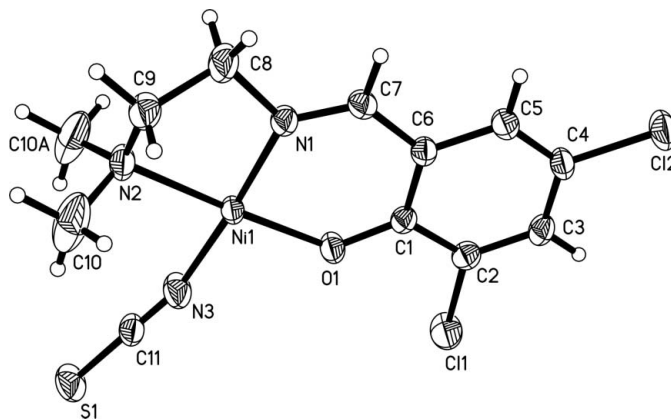
**Figure 1**
View of the molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level.

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