Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{2-Bromo-4-chloro-6-[2-(dimethylamino)-ethyliminomethyl]phenolato}thiocyanato-nickel(II)

Xiao-Fan Zhao

College of Chemistry & Chemical Engineering, Shaoxing University, Shaoxing 312000, People's Republic of China

Correspondence e-mail:
xiaofan_zhao@126.com

Received 12 December 2006
Accepted 5 January 2007

Key indicators

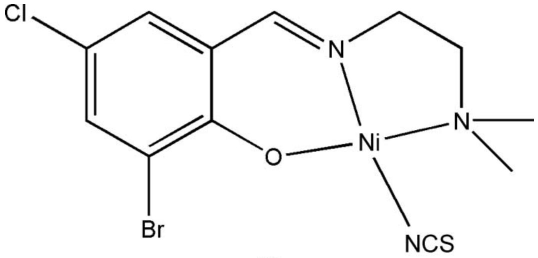
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.009 Å
Disorder in main residue
R factor = 0.043
wR factor = 0.109
Data-to-parameter ratio = 14.1

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

In the title mononuclear compound, $[Ni(C_{11}H_{13}BrClN_2O)(NCS)]$, the Ni^{II} atom is four-coordinated in a square-planar geometry by one O and two N atoms of the Schiff base ligand, and by one N atom of the thiocyanate anion. The molecule possesses crystallographic mirror symmetry.

Comment

Transition metal complexes play an important role in both bioinorganic chemistry and coordination chemistry (Chun & Bernal, 2001; Jackson *et al.*, 2003; Nakashima *et al.*, 2003). Recently, the author has reported the crystal structure of a mononuclear Schiff base cobalt(III) complex (Zhao, 2006). As part of a further study of the crystal structures of such complexes, the title mononuclear nickel(II) complex, (I), is reported here.



(I)

The molecule of compound (I) possesses crystallographic mirror symmetry, with all atoms except atoms H8*A*, H8*B* (both attached to C8), C9, H9*A*, H9*B* and the methyl groups lying on the crystallographic mirror plane. The Ni^{II} atom is four-coordinated in a square-planar geometry by the Schiff base ligand and the thiocyanate ligand (Fig. 1). The Schiff base acts as a tridentate ligand through the phenolate O atom, the imine N atom and the amine N atom. The two *trans* angles subtended at the Ni^{II} atom deviate slightly from 180° (Table 1), and the other angles around the Ni^{II} atom deviate slightly from the ideal value (90°) for a square-planar coordination, ranging from 83.9 (2) to 92.5 (2)°. The Ni—O and Ni—N bond lengths are typical and comparable to those in similar Schiff base–nickel(II) complexes (Gomes *et al.*, 1999; Jircitano *et al.*, 1990; Kabak *et al.*, 1997).

Experimental

3-Bromo-5-chloro-2-hydroxybenzaldehyde (0.2 mmol, 47.0 mg), *N*,*N*-dimethylethane-1,2-diamine (0.2 mmol, 17.6 mg), ammonium thiocyanate (0.2 mmol, 15.2 mg) and nickel nitrate hexahydrate (0.2 mmol, 58.2 mg) were dissolved in methanol (30 ml) with stirring.

The mixture was stirred for 30 min at room temperature to give a red solution which was allowed to stand in air for one week, yielding red block-shaped crystals of (I).

Crystal data

$[Ni(C_{11}H_{13}BrClN_2O)(NCS)]$
$M_r = 421.38$
Orthorhombic, *Pnma*
$a = 19.338$ (1) Å
$b = 6.994$ (1) Å
$c = 11.288$ (2) Å
$V = 1526.7$ (4) Å^3
$Z = 4$
$D_x = 1.833$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 4.20$ mm^{-1}
$T = 298$ (2) K
Block, red
0.17 × 0.15 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.536$, $T_{max} = 0.633$
11929 measured reflections
1717 independent reflections
1427 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 26.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.110$
$S = 1.05$
1717 reflections
122 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2 + 3.2149P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.82$ e Å^{-3}
$\Delta\rho_{min} = -1.00$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.915 (5)	Ni1—N1	1.934 (6)
Ni1—N3	1.925 (6)	Ni1—N2	2.068 (6)
O1—Ni1—N3	91.9 (2)	O1—Ni1—N2	176.4 (2)
O1—Ni1—N1	92.5 (2)	N3—Ni1—N2	91.7 (2)
N3—Ni1—N1	175.6 (2)	N1—Ni1—N2	83.9 (2)

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 or 0.96 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C). C9, H9*A* and H9*B* are disordered about the mirror plane, with site occupancy factors of 0.5.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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: *SHELXL97*.

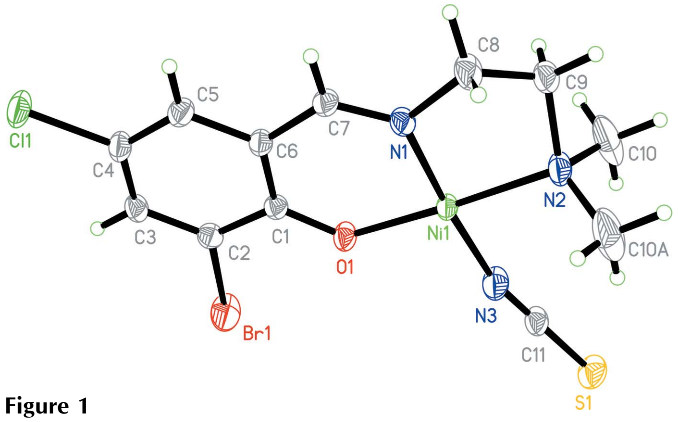


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Only one disorder component is shown. [Symmetry code: (A) $x, \frac{1}{2} - y, z$.]

Financial support from the Shaoxing University research fund is gratefully acknowledged.

References

Bruker (2002). *SAINT* (Version 6.02) and *SMART* (Version 5.62). Bruker AXS Inc., Madison, Wisconsin, USA.
Chun, H. & Bernal, I. (2001). *Cryst. Growth Des.* **1**, 143–149.
Gomes, L., Pinho, D., Freire, C. & de Castro, B. (1999). *Acta Cryst.* C**55**, 1425–1427.
Jackson, W. G., Rahman, A. F. M. M. & Craig, D. C. (2003). *Inorg. Chem.* **42**, 383–388.
Jircitano, A. J., Henry, R. F. & Hammond, R. R. (1990). *Acta Cryst.* C**46**, 1799–1802.
Kabak, M., Elmali, A. & Elerman, Y. (1997). *Acta Cryst.* C**53**, 868–870.
Nakashima, T., Mishiro, J., Ito, M., Kura, G., Ikuta, Y., Matsumoto, N., Nakajima, K. & Kojima, M. (2003). *Inorg. Chem.* **42**, 2323–2330.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Zhao, X.-F. (2006). *Acta Cryst.* E**62**, m3065–m3067.