

{1-[2-(Dimethylamino)ethyliminomethyl]-2-naphtholato}thiocyanatonickel(II)**Zhong-Lu You**Department of Chemistry and Chemical
Engineering, Liaoning Normal University,
Dalian 116029, People's Republic of ChinaCorrespondence e-mail:
youzhonglu@yahoo.com.cn**Key indicators**Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.007$ Å
 R factor = 0.062
 wR factor = 0.151
Data-to-parameter ratio = 18.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The title compound, $[\text{Ni}(\text{C}_{15}\text{H}_{17}\text{N}_2\text{O})(\text{NCS})]$, is a mononuclear Schiff base nickel(II) complex. The Ni^{II} atom is coordinated by one O and two N atoms of the Schiff base ligand, and by one N atom of the thiocyanate ligand, forming a square-planar coordination.

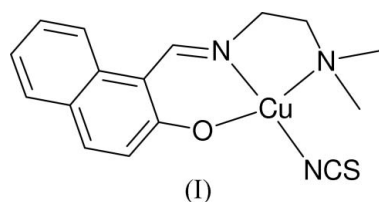
Received 6 September 2005

Accepted 7 September 2005

Online 14 September 2005

Comment

Schiff base complexes are of great interest in coordination chemistry (Goswami & Eichhorn, 1999; Dominguez-Vera *et al.*, 1998; Bernardo *et al.*, 1996). Recently, we have reported a few Schiff base complexes (You, 2005*a,b,c,d,e,f*; You & Zhu, 2005*a,b*). As an extension of our work on the structural characterization of Schiff base complexes, the new title Schiff base nickel(II) complex, (I), is reported.



Complex (I) is a mononuclear nickel(II) compound (Fig. 1). The Ni atom is four-coordinated in a slightly distorted square-planar coordination by one O and two N atoms of the Schiff base ligand, and by one N atom of the thiocyanate anion (Table 1). The Ni–O and Ni–N bond lengths are comparable to the corresponding values observed in other Schiff base nickel(II) complexes (You, 2005*g,h,i*) and, as expected, the bond involving amine atom N2 is longer than that involving imine atom N1. The thiocyanate group is nearly linear and shows almost linear coordination to the metal atom.

Experimental

2-Hydroxy-1-naphthaldehyde (0.2 mmol, 17.2 mg) and *N,N*-dimethylethane-1,2-diamine (0.2 mmol, 17.6 mg) were dissolved in MeOH (10 ml). The mixture was stirred for 20 min to give a clear yellow solution. To the solution were added an aqueous solution (5 ml) of NH_4NCS (0.1 mmol, 7.6 mg) and an MeOH solution (10 ml) of $\text{Ni}(\text{ClO}_4)_2 \cdot 7\text{H}_2\text{O}$ (0.1 mmol, 38.4 mg), with stirring. The mixture was stirred at room temperature for about 30 min and filtered. After keeping the green filtrate in air for 7 d, green block-shaped crystals were formed.

Crystal data

[Ni(C₁₅H₁₇N₂O)(NCS)]
M_r = 358.10
 Monoclinic, *P*₂₁/*n*
a = 8.413 (2) Å
b = 6.167 (2) Å
c = 30.683 (6) Å
 β = 93.04 (3)°
V = 1589.7 (7) Å³
Z = 4

D_x = 1.496 Mg m⁻³
 Mo Kα radiation
 Cell parameters from 1147 reflections
 θ = 2.5–21.3°
 μ = 1.36 mm⁻¹
T = 298 (2) K
 Block, green
 0.31 × 0.22 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.679, *T_{max}* = 0.802
 12963 measured reflections

3617 independent reflections
 2051 reflections with *I* > 2σ(*I*)
R_{int} = 0.086
 θ_{max} = 27.5°
h = -10 → 10
k = -8 → 8
l = -39 → 39

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.062
wR (*F*²) = 0.151
S = 1.00
 3617 reflections
 201 parameters

H-atom parameters constrained
w = 1/[σ²(*F_o*²) + (0.0615*P*)²]
 where *P* = (*F_o*² + 2*F_c*²)/3
 (Δ/σ)_{max} < 0.001
 Δρ_{max} = 0.49 e Å⁻³
 Δρ_{min} = -0.41 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ni1—O1	1.818 (3)	Ni1—N3	1.875 (4)
Ni1—N1	1.833 (4)	Ni1—N2	1.926 (4)
O1—Ni1—N1	92.64 (15)	N1—Ni1—N2	87.54 (16)
O1—Ni1—N3	88.33 (17)	N3—Ni1—N2	92.16 (17)
N1—Ni1—N3	174.52 (18)	C16—N3—Ni1	170.4 (4)
O1—Ni1—N2	172.86 (16)	N3—C16—S1	179.2 (5)

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.96 Å, and with *U*_{iso}(H) = 1.2 or 1.5*U*_{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.

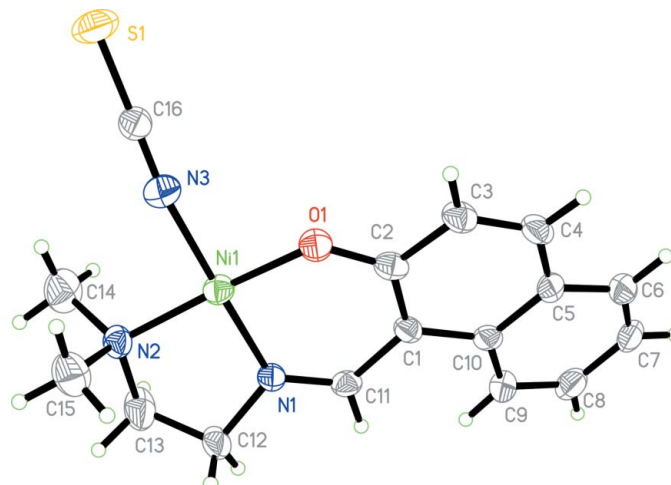


Figure 1

The structure of (1), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

The author thanks Liaoning Normal University for funding this study.

References

- Bernardo, K., Leppard, S., Robert, A., Commenges, G., Dahan, F. & Meunier, B. (1996). *Inorg. Chem.* **35**, 387–396.
 Bruker (1998). SMART (Version 5.628) and SAINT (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
 Dominguez-Vera, J. M., Camara, F., Moreno, J. M., Colacio, E. & Stoeckli-Evans, H. (1998). *Inorg. Chem.* **37**, 3046–3050.
 Goswami, N. & Eichhorn, D. M. (1999). *Inorg. Chem.* **38**, 4329–4333.
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (1997a). SHELXL97 and SHELXS97. University of Göttingen, Germany.
 Sheldrick, G. M. (1997b). SHELXTL. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
 You, Z.-L. (2005a). *Acta Cryst.* **C61**, m359–m360.
 You, Z.-L. (2005b). *Acta Cryst.* **C61**, m406–m408.
 You, Z.-L. (2005c). *Acta Cryst.* **C61**, m432–m434.
 You, Z.-L. (2005d). *Acta Cryst.* **C61**, m295–m297.
 You, Z.-L. (2005e). *Acta Cryst.* **C61**, m339–m341.
 You, Z.-L. (2005f). *Acta Cryst.* **C61**, m383–m385.
 You, Z.-L. (2005g). *Acta Cryst.* **E61**, m1601–m1603.
 You, Z.-L. (2005h). *Acta Cryst.* **E61**, m1637–m1638.
 You, Z.-L. (2005i). *Acta Cryst.* **E61**, m1807–m1809.
 You, Z.-L. & Zhu, H.-L. (2005a). *Acta Cryst.* **C61**, m421–m423.
 You, Z.-L. & Zhu, H.-L. (2005b). *Acta Cryst.* **C61**, m397–m399.