

**{1-[2-(Methylamino)ethyliminomethyl]naphthalen-2-olato}thiocyanatonickel(II)****Chuan-Gao Zhu, Feng-Wu Wang\* and Yi-Jun Wei**

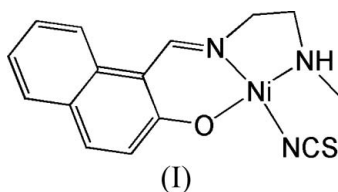
Department of Chemistry, Huainan Normal College, Huainan 232001, People's Republic of China

Correspondence e-mail:  
fengwu\_wang@126.com**Key indicators**Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å  
 $R$  factor = 0.051  
 $wR$  factor = 0.132  
Data-to-parameter ratio = 16.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title mononuclear nickel(II) complex,  $[\text{Ni}(\text{C}_{14}\text{H}_{15}\text{N}_2\text{O})(\text{NCS})]$ , the  $\text{Ni}^{\text{II}}$  atom is four-coordinated in a square-planar geometry by one Schiff base ligand and one thiocyanate anion. There are two molecules in the asymmetric unit.

Received 3 July 2006  
Accepted 9 July 2006**Comment**

Schiff base nickel(II) complexes have received much attention in recent years (Marganian *et al.*, 1995). Most of the complexes have been found to possess pharmacological and catalytic properties (Harrop *et al.*, 2003; Brückner *et al.*, 2000). In this paper, the structure of the title mononuclear nickel(II) complex, (I), is reported.



There are two crystallographically independent molecules in complex (I). The Ni1 molecules associate as dimers about a crystallographic centre of symmetry with an  $\text{Ni1} \cdots \text{Ni1}^i$  [symmetry code: (i)  $2 - x, -y, 2 - z$ ] distance of 3.389 (2) Å. The Ni atom in each of the molecules is four-coordinated by the Schiff base ligand and one thiocyanate anion, forming a square-planar geometry (Figs. 1 and 2). The Schiff base ligand acts as a tridentate ligand and coordinates to the metal *via* the NNO donor set. Despite the differences in packing geometries for the two independent molecules, the geometric parameters subtended at the metal centres (Table 1) are similar to each other, as well as to values observed for other Schiff base nickel(II) complexes (Liu *et al.*, 2006; Yu, 2006; Zhu *et al.*, 2004).

**Experimental**

A mixture of 2-hydroxy-1-naphthaldehyde (0.1 mmol, 17.2 mg) and *N*-methylethane-1,2-diamine (0.1 mmol, 7.4 mg) was dissolved in MeOH (10 ml). The mixture was stirred at room temperature for about 30 min. To this solution was added, with stirring, a MeOH solution (5 ml) of ammonium thiocyanate (0.1 mmol, 7.6 mg) and a MeOH solution (5 ml) of  $\text{Ni}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$  (0.1 mmol, 29.1 mg). The final mixture was stirred for another 30 min at room temperature to give a red solution. Red block-like crystals were formed after allowing the solution to stand in air for 5 d.

## Crystal data

[Ni(C<sub>14</sub>H<sub>15</sub>N<sub>2</sub>O)(NCS)] $M_r = 344.07$ Monoclinic,  $P2_1/n$  $a = 10.060$  (1) Å $b = 13.387$  (2) Å $c = 22.398$  (3) Å $\beta = 95.563$  (2)° $V = 3002.1$  (7) Å<sup>3</sup> $Z = 8$  $D_x = 1.523$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation $\mu = 1.43$  mm<sup>-1</sup> $T = 293$  (2) K

Block, red

 $0.28 \times 0.23 \times 0.22$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer

 $\omega$  scans

Absorption correction: multi-scan (SADABS; Bruker, 2000)

 $T_{\min} = 0.690$ ,  $T_{\max} = 0.744$ 

16751 measured reflections

6413 independent reflections

4635 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.031$  $\theta_{\max} = 27.0^\circ$ 

## Refinement

Refinement on  $F^2$  $R[F^2 > 2\sigma(F^2)] = 0.051$  $wR(F^2) = 0.132$  $S = 1.03$ 

6413 reflections

381 parameters

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0563P)^2$  $+ 2.1613P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} < 0.001$  $\Delta\rho_{\max} = 0.80$  e Å<sup>-3</sup> $\Delta\rho_{\min} = -0.59$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Ni1—N1	1.834 (3)	Ni2—O2	1.827 (3)
Ni1—O1	1.837 (2)	Ni2—N3	1.837 (3)
Ni1—N5	1.874 (3)	Ni2—N6	1.880 (3)
Ni1—N2	1.927 (4)	Ni2—N4	1.918 (4)
N1—Ni1—O1	94.01 (12)	O2—Ni2—N3	93.58 (13)
N1—Ni1—N5	176.68 (13)	O2—Ni2—N6	89.50 (13)
O1—Ni1—N5	88.60 (13)	N3—Ni2—N6	176.78 (14)
N1—Ni1—N2	86.10 (14)	O2—Ni2—N4	178.47 (16)
O1—Ni1—N2	171.50 (18)	N3—Ni2—N4	86.28 (14)
N5—Ni1—N2	91.62 (16)	N6—Ni2—N4	90.66 (15)

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with N—H = 0.91 Å, C—H = 0.93–0.97 Å and  $U_{\text{iso}}(\text{H}) = 1.2$  or  $1.5U_{\text{eq}}(\text{C,N})$ .

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

The authors acknowledge the Education Office of Anhui Province, People's Republic of China, for research grant No. 2006kj166C.

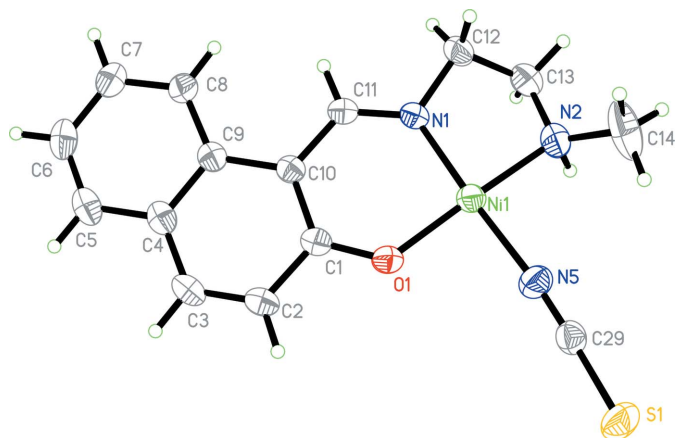


Figure 1

The structure of the Ni1 complex of (I). Displacement ellipsoids are drawn at the 30% probability level.

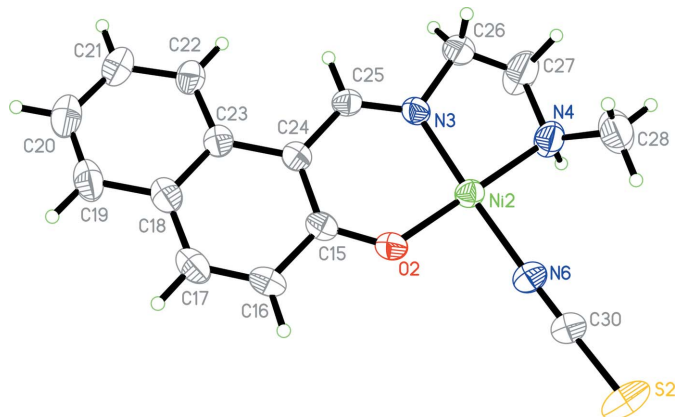


Figure 2

The structure of the Ni2 complex of (I). Displacement ellipsoids are drawn at the 30% probability level.

## References

- Brückner, C., Rettig, S. J. & Dolphin, D. (2000). *Inorg. Chem.* **39**, 6100–6106.
- Bruker (2000). SMART (Version 5.625), SAINT (Version 6.01), SHELXTL (Version 6.10) and SADABS (Version 2.03). Bruker AXS Inc., Madison, Wisconsin, USA.
- Harrop, T. C., Olmstead, M. M. & Mascharak, P. K. (2003). *Chem. Commun.* pp. 410–411.
- Liu, H.-Y., Gao, F., Lu, Z.-S. & Wang, H.-Y. (2006). *Acta Cryst.* **E62**, m1306–m1308.
- Marganian, C. A., Vazir, H., Baidya, N., Olmstead, M. M. & Mascharak, P. K. (1995). *J. Am. Chem. Soc.* **117**, 1584–1594.
- Yu, Y.-Y. (2006). *Acta Cryst.* **E62**, m948–m949.
- Zhu, B., Ruang, W. & Zhu, Z. (2004). *Acta Cryst.* **E60**, m634–m636.