Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{1-[2-(Methylamino)ethyliminomethyl]naphthalen-2-olato}thiocyanatocopper(II)

Han-Na Hou

Department of Chemistry, Hubei Institute of Education, Wuhan 430205, People's Republic of China

Correspondence e-mail: houhanna@163.com

The title compound, $[Cu(C_{14}H_{15}N_2O)(NCS)]$, is a mononuclear copper(II) complex, with two molecules in the asymmetric unit. The Cu^{II} ion is coordinated by one O and two N atoms of a Schiff base ligand, and by one N atom of a thiocyanate anion, forming a square-planar geometry.

Received 30 May 2006
Accepted 7 June 2006

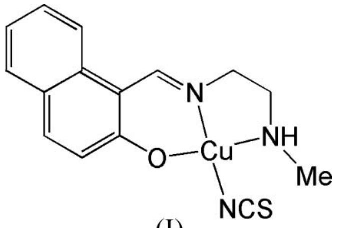
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.047
wR factor = 0.124
Data-to-parameter ratio = 17.4

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

Comment

Copper(II) complexes derived from Schiff base ligands have been studied extensively due to their interesting structures and wide applications (Bhaduri, *et al.*, 2003; Rospendowski & Smith, 1988; Dominguez-Vera *et al.*, 1998; Hebbachi & Benali-Cherif, 2005; Butcher *et al.*, 2003). As part of an investigation of the structures of Schiff base copper(II) complexes, the title mononuclear copper(II) complex, (I), is reported here.



(I)

Complex (I) is a mononuclear copper(II) compound, as shown in Fig. 1. The asymmetric unit consists of two molecules. Each Cu^{II} ion is in a square-planar geometry and is four-coordinated by one O and two N atoms of a Schiff base ligand, and by one N atom of a thiocyanate anion. The bond lengths and angles (Table 1) are within normal ranges and comparable to the values in other copper(II) complexes (Marek *et al.*, 2003; Akitsu & Einaga, 2004; Ali *et al.*, 2004).

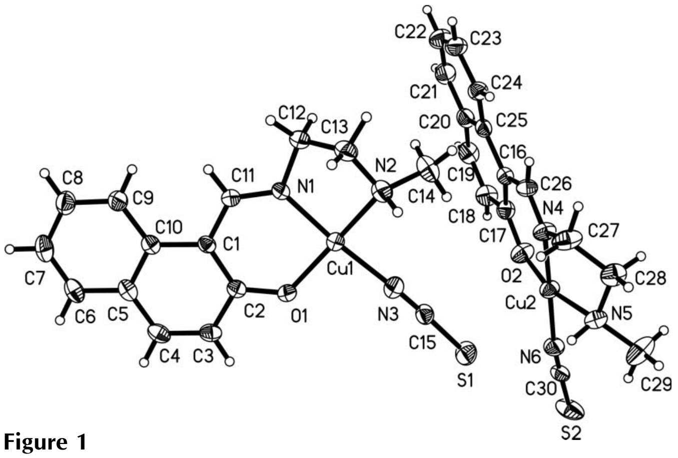


Figure 1
The asymmetric unit of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

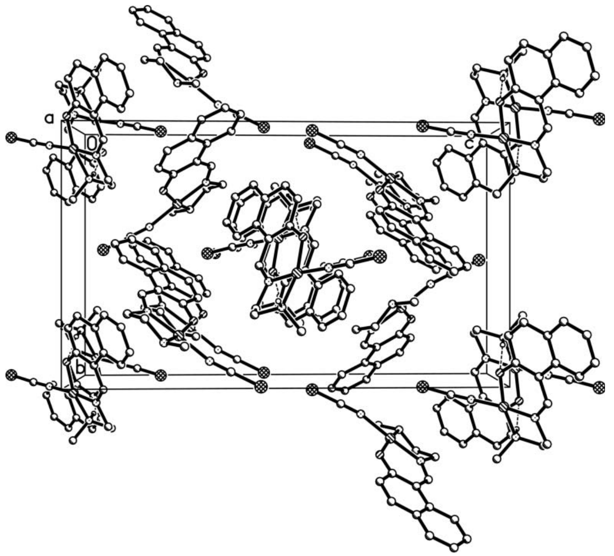


Figure 2
The crystal packing of (I), viewed along the *a* axis. Intermolecular hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

In the crystal structure, adjacent molecules are linked through intermolecular N—H···O hydrogen bonds (Table 2), forming dimers (Fig. 2).

Experimental

2-Hydroxy-1-naphthaldehyde (1.0 mmol, 173.2 mg), *N*-methylethane-1,2-diamine (1.0 mmol, 74.1 mg), NH_4NCS (1.0 mmol, 76.2 mg) and $Cu(CH_3COO)_2\cdot H_2O$ (1.0 mmol, 199.3 mg) were dissolved in methanol (100 ml). The mixture was stirred at room temperature for 1 h to give a clear blue solution. After leaving the solution to stand in air for 13 days, blue block-shaped crystals were formed.

Crystal data

$[Cu(C_{14}H_{15}N_2O)(NCS)]$
$M_r = 348.90$
Monoclinic, $P2_1/n$
$a = 10.168$ (1) Å
$b = 13.237$ (1) Å
$c = 22.301$ (2) Å
$\beta = 93.679$ (1)°
$V = 2995.4$ (5) Å^3
$Z = 8$
$D_x = 1.548$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.60$ mm^{-1}
$T = 298$ (2) K
Block, blue
0.22 × 0.18 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.720$, $T_{max} = 0.773$
22106 measured reflections
6734 independent reflections
5081 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.125$
$S = 1.03$
6734 reflections
387 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 0.9166P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.80$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.902 (3)	Cu2—O2	1.908 (2)
Cu1—O1	1.910 (2)	Cu2—N4	1.926 (3)
Cu1—N3	1.942 (3)	Cu2—N6	1.945 (3)
Cu1—N2	2.040 (3)	Cu2—N5	2.056 (3)
N1—Cu1—O1	92.43 (9)	O2—Cu2—N4	91.11 (10)
N1—Cu1—N3	174.58 (11)	O2—Cu2—N6	91.12 (11)
O1—Cu1—N3	91.11 (11)	N4—Cu2—N6	177.33 (12)
N1—Cu1—N2	84.82 (11)	O2—Cu2—N5	166.31 (12)
O1—Cu1—N2	164.29 (11)	N4—Cu2—N5	83.82 (11)
N3—Cu1—N2	92.86 (13)	N6—Cu2—N5	94.32 (12)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.91 (3)	2.07 (2)	2.946 (4)	162 (4)
N5—H5···S1	0.90 (3)	2.78 (3)	3.481 (3)	135 (3)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Atoms H2 and H5 were located in a difference Fourier map and refined isotropically, with N—H distances restrained to 0.90 (1) Å. The other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.93–0.97 Å, and with $U_{iso}(H) = 1.2$ 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, 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*.

The author thanks the Hubei Institute of Education for funding this study.

References

Akitsu, T. & Einaga, Y. (2004). *Acta Cryst.* E**60**, m436–m438.
Ali, H., Khamis, N. A., Basirun, W. J. & Yamin, B. M. (2004). *Acta Cryst.* E**60**, m982–m983.
Bhaduri, S., Tasiopoulos, A. J., Bolcar, M. A., Abbound, K. A., Streib, W. E. & Christou, G. (2003). *Inorg. Chem.* **42**, 1483–1492.
Bruker (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Butcher, R. J., Mockler, G. M. & McKern, O. (2003). *Acta Cryst.* E**59**, m1104–m1106.
Dominguez-Vera, J. M., Camara, F., Moreno, J. M., Colacio, E. & Stoeckli-Evans, H. (1998). *Inorg. Chem.* **37**, 3046–3050.
Hebbachi, R. & Benali-Cherif, N. (2005). *Acta Cryst.* E**61**, m1188–m1190.
Marek, J., Vančo, J. & Švajlenová, O. (2003). *Acta Cryst.* C**59**, m509–m511.
Rospendowski, B. & Smith, W. E. (1988). *Inorg. Chem.* **27**, 4509–4511.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. V5.1. Bruker AXS, Inc., Madison, Wisconsin, USA.