Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{4-Bromo-2-[(2-diethylaminoethylimino)methyl]-phenolato}thiocyanatocopper(II)

Zhong-Lu You

Department of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, People's Republic of China

Correspondence e-mail: youzhonglu@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.036
wR factor = 0.091
Data-to-parameter ratio = 18.6

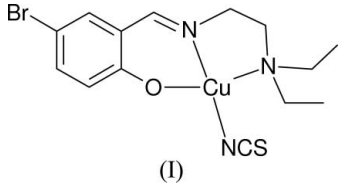
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, [Cu($C_{13}H_{18}BrN_2O$)(NCS)], is a mononuclear Schiff base copper(II) complex. The Cu^{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 30 November 2005
Accepted 2 December 2005
Online 7 December 2005

Comment

Recently, we have reported a series of Schiff base complexes (You, 2005*a*,*b*,*c*). As an extension of this work on the structural characterization of Schiff base complexes, we describe here the synthesis and structure of the title new copper(II) compound, (I).



(I)

The molecular structure of compound (I) is illustrated in Fig. 1, and selected bond distances and angles are given in Table 1. Compound (I) is structurally similar to the copper(II) compounds reported recently (You, 2005*d*,*e*). The Cu^{II} atom is four-coordinated, in a square-planar arrangement, by one O and two N atoms of the Schiff base ligand, and by one N atom of the thiocyanate anion. The values of the *trans* angles in the $CuON_3$ square plane are 176.48 (12) and 176.09 (10)°, indicating a slightly distorted square-planar coordination. The Cu—O and Cu—N bond lengths (Table 1) are comparable with the corresponding values observed in other Schiff base copper(II) complexes (You & Zhu, 2004) and, as expected, the

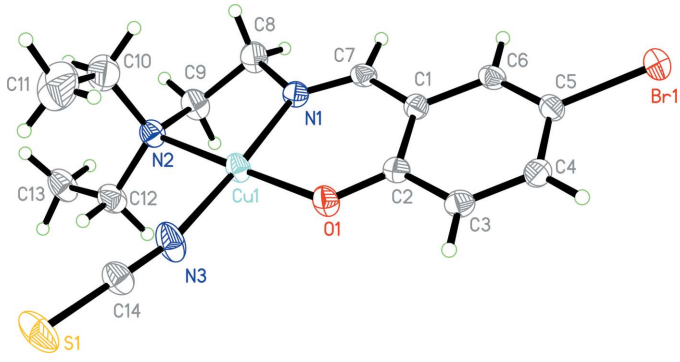


Figure 1
The molecular structure of compound (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

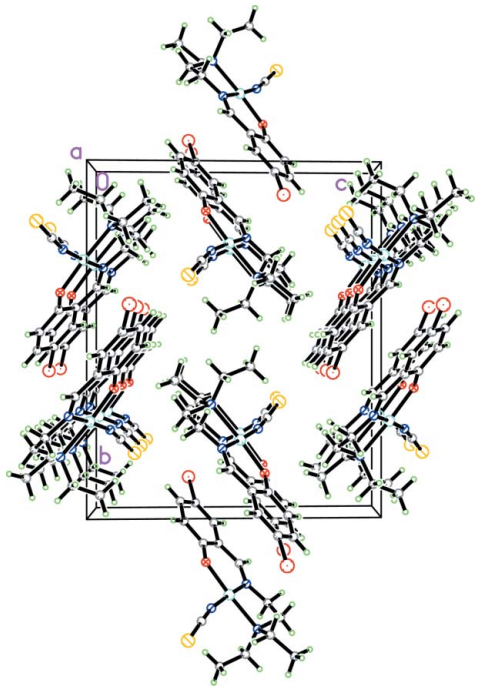


Figure 2
The crystal packing of compound (I), viewed along the *a* axis.

bond involving amine atom N2 is longer than that involving imine atom N1 (Mondal *et al.*, 2001).

In the crystal structure, the molecules stack along the *a* axis; the crystal packing is shown in Fig. 2.

Experimental

5-Bromosalicylaldehyde (0.1 mmol, 20.1 mg) and *N*,*N*′-diethylethane-1,2-diamine (0.1 mmol, 11.6 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature for 20 min to give a yellow solution. To this solution were added an aqueous solution (2 ml) of NH_4NCS (0.1 mmol, 6.5 mg) and a MeOH solution (3 ml) of $Cu(CH_3COO)_2{\cdot}H_2O$ (0.1 mmol, 19.9 mg), with stirring. The mixture was stirred for a further 20 min at room temperature and then filtered. The filtrate was kept in air for 5 d, during which time blue block-shaped crystals of (I) were formed.

Crystal data

$[Cu(C_{13}H_{18}BrN_2O)(NCS)]$	D_x = 1.726 Mg m^{-3}
M_r = 419.82	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 3328 reflections
a = 7.052 (1) Å	θ = 2.4–24.6°
b = 16.688 (2) Å	μ = 3.96 mm^{-1}
c = 13.775 (2) Å	T = 298 (2) K
β = 94.79 (1)°	Block, blue
V = 1615.4 (4) Å^3	0.25 × 0.18 × 0.17 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3564 independent reflections
ω scans	2787 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.031
T_{min} = 0.404, T_{max} = 0.510	θ_{max} = 27.5°
11427 measured reflections	$h = -8 \rightarrow 9$
	$k = -21 \rightarrow 21$
	$l = -16 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 0.4325P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.036	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.091	$\Delta\rho_{max}$ = 0.54 e Å^{-3}
S = 1.03	$\Delta\rho_{min}$ = −0.41 e Å^{-3}
3564 reflections	
192 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.902 (2)	Cu1—N3	1.938 (3)
Cu1—N1	1.928 (3)	Cu1—N2	2.103 (2)
O1—Cu1—N1	92.93 (9)	O1—Cu1—N2	176.09 (10)
O1—Cu1—N3	89.52 (11)	N1—Cu1—N2	84.27 (10)
N1—Cu1—N3	176.48 (12)	N3—Cu1—N2	93.41 (11)

The H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 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 Liaoning Normal University, People's Republic of China, for funding this study.

References

Bruker (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Mondal, N., Mitra, S., Gramilich, V., Ghodsi, S. O. & Malik, K. M. A. (2001). *Polyhedron*, **20**, 135–141.
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*. (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
You, Z.-L. (2005*a*). *Acta Cryst.* E**61**, m1571–m1573.
You, Z.-L. (2005*b*). *Acta Cryst.* E**61**, m1601–m1603.
You, Z.-L. (2005*c*). *Acta Cryst.* E**61**, m1637–m1638.
You, Z.-L. (2005*d*). *Acta Cryst.* E**61**, m2226–m2227.
You, Z.-L. (2005*e*). *Acta Cryst.* E**61**, m1963–m1964.
You, Z.-L. & Zhu, H.-L. (2004). *Z. Anorg. Allg. Chem.* **630**, 2754–2760.