Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

{2,4-Dibromo-6-[(2-dimethylaminoethylimino)methyl]phenolato}(thiocyanato)-copper(II)

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Received 20 January 2006
Accepted 20 January 2006

In the mononuclear copper(II) title compound, [Cu($C_{11}H_{13}Br_2N_2O$)(NCS)], the Cu^{II} atom is four-coordinated by one imine N, one amine N, and one phenolate O atom of the Schiff base ligand, and by one N atom of a thiocyanate anion in a square planar geometry. In the crystal structure, adjacent molecules are linked through intermolecular C—H···Br hydrogen bonds, forming centrosymmetric dimers.

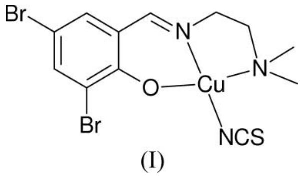
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.044
wR factor = 0.105
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

An extensive effort has been made to prepare and characterize a variety of coordination complexes in an attempt to model the physical and chemical behaviour of copper-containing enzymes (Reddy *et al.*, 2000). The peculiarity of copper lies in its ability to form complexes with coordination numbers of four, five, and six (Ray *et al.*, 2003; Arnold *et al.*, 2003; Raptopoulou *et al.*, 1998). As a continuation of our own work in this area (Wang & Li, 2005), the title compound, (I), a copper(II) complex is reported here.



(I)

Compound (I) is mononuclear, as shown in Fig. 1. The Cu atom is four-coordinated by one imine N, one amine N, and one phenolate O atom of the Schiff base ligand, and by one N atom of a thiocyanate anion, resulting in distorted square

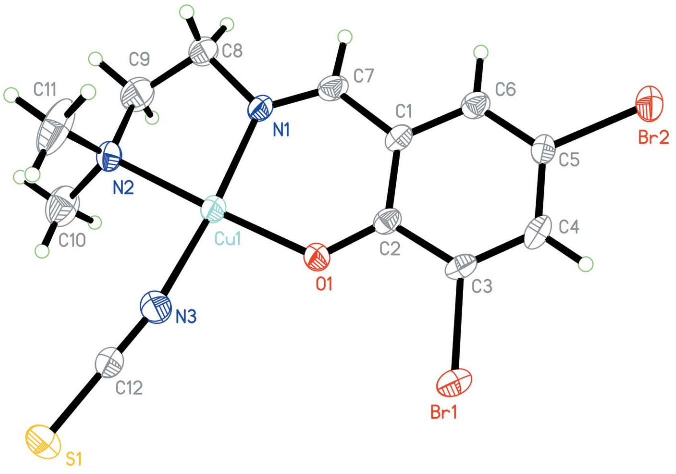


Figure 1
The structure of (I), showing 30% displacement ellipsoids (arbitrary spheres for the H atoms).

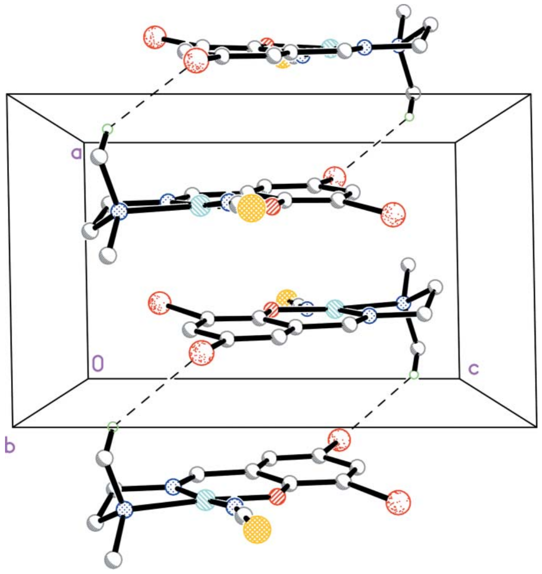


Figure 2
Part of the packing of (I). Intermolecular C—H···Br interactions are shown as dashed lines.

planar $CuON_3$ coordination (Table 1). The N1—Cu1—N2 bond angle deviates by some 5.61 (18)° from 90° as a result of the strain created by the five-membered chelate ring Cu1/N1/C8/C9/N2.

In the crystal structure, adjacent molecules are linked through intermolecular C—H···Br interactions (Table 2), forming centrosymmetric dimers (Fig. 2).

Experimental

3,5-Dibromosalicylaldehyde (0.1 mmol, 28.0 mg), *N*,*N*-dimethylethane-1,2-diamine (0.1 mmol, 8.8 mg), NH_4NCS (0.1 mmol, 7.6 mg) and $Cu(CH_3COO)_2\cdot H_2O$ (0.1 mmol, 19.9 mg) were dissolved in MeOH (15 ml). The mixture was stirred at room temperature for 1 h to give a red solution. The resulting solution was allowed to stand in air for 13 d, and red needle-shaped crystals of (I) were formed.

Crystal data

$[Cu(C_{11}H_{13}Br_2N_2O)(NCS)]$
$M_r = 470.67$
Monoclinic, $P2_1/n$
$a = 7.146$ (1) Å
$b = 19.213$ (3) Å
$c = 11.229$ (2) Å
$\beta = 91.026$ (2)°
$V = 1541.5$ (4) Å^3
$Z = 4$

$D_x = 2.028$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 1683 reflections
$\theta = 2.5–24.9°$
$\mu = 6.73$ mm^{-1}
$T = 298$ (2) K
Needle, red
0.42 × 0.08 × 0.04 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.164$, $T_{max} = 0.775$
12315 measured reflections

3180 independent reflections
2014 reflections with $I > 2\sigma(I)$
$R_{int} = 0.067$
$\theta_{max} = 26.5°$
$h = -8 \rightarrow 8$
$k = -24 \rightarrow 23$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.105$
$S = 1.01$
3180 reflections
183 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0345P)^2 + 0.8169P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.60$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.908 (3)	Cu1—N1	1.932 (4)
Cu1—N3	1.927 (5)	Cu1—N2	2.055 (4)
O1—Cu1—N3	91.61 (18)	O1—Cu1—N2	174.47 (18)
O1—Cu1—N1	92.55 (16)	N3—Cu1—N2	91.87 (19)
N3—Cu1—N1	173.3 (2)	N1—Cu1—N2	84.39 (18)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*A*···Br2^{i}	0.96	2.88	3.676 (5)	141

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

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 1.5 times $U_{eq}(C)$.

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 authors acknowledge the Lanzhou Jiaotong University, People's Republic of China, for funding this study.

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