

**Zhong-Lu You**

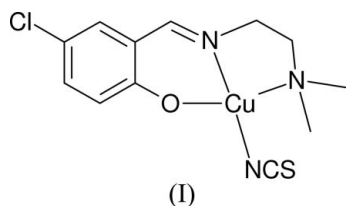
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youzhonglu@yahoo.com.cn**Key indicators**Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$   
Disorder in main residue  
 $R$  factor = 0.035  
 $wR$  factor = 0.100  
Data-to-parameter ratio = 15.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**{4-Chloro-2-[(2-dimethylaminoethylimino)methyl]-phenolato}thiocyanatocopper(II)**

The title compound,  $[\text{Cu}(\text{C}_{11}\text{H}_{14}\text{ClN}_2\text{O})(\text{NCS})]$ , is a mononuclear Schiff base copper(II) complex. The  $\text{Cu}^{\text{II}}$  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. The molecule possesses crystallographic mirror symmetry.

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Recently, the author has reported a series of Schiff base complexes (You, 2005*a,d,e*). As an extension of the work on the structural characterization of Schiff base complexes, the synthesis and structure of a new copper(II) compound, (I), is reported here.



The molecular structure of complex (I), a mononuclear copper(II) compound, 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*b,c*). The Cu 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 molecule possesses crystallographic mirror symmetry, with almost all atoms lying in the crystallographic mirror plane. The angles at Cu indicate a slightly distorted square-planar coordination. The Cu—O and Cu—N bond lengths (Table 1) are comparable to the corresponding values observed in other Schiff base copper(II) complexes (MacLachlan *et al.*, 1996; Colacio *et al.*, 2000) and, as expected, the 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 *b* axis and the crystal packing is shown in Fig. 2.

**Experimental**

5-Chlorosalicylaldehyde (0.1 mmol, 15.6 mg) and *N,N'*-dimethylethane-1,2-diamine (0.1 mmol, 8.8 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature for 20 min to give a yellow solution. To the above solution was added an aqueous solution (2 ml) of  $\text{NH}_4\text{NCS}$  (0.1 mmol, 6.5 mg) and an MeOH solu-

tion (3 ml) of  $\text{Cu}(\text{CH}_3\text{COO})_2 \cdot \text{H}_2\text{O}$  (0.1 mmol, 19.9 mg), with stirring. The mixture was stirred for another 20 min at room temperature. The filtrate was kept in air for 9 d, during which time blue block-shaped crystals were formed.

## Crystal data

$[\text{Cu}(\text{C}_{11}\text{H}_{14}\text{ClN}_2\text{O})(\text{NCS})]$

$M_r = 347.31$

Orthorhombic, *Pnma*

$a = 19.172$  (2) Å

$b = 6.764$  (1) Å

$c = 11.334$  (1) Å

$V = 1469.8$  (3) Å<sup>3</sup>

$Z = 4$

$D_x = 1.570$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

Cell parameters from 4650 reflections

$\theta = 2.8\text{--}27.2^\circ$

$\mu = 1.80$  mm<sup>-1</sup>

$T = 298$  (2) K

Block, blue

$0.22 \times 0.20 \times 0.20$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer

$\omega$  scans

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)

$T_{\text{min}} = 0.692$ ,  $T_{\text{max}} = 0.714$

12043 measured reflections

1827 independent reflections

1558 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\text{max}} = 27.5^\circ$

$h = -24 \rightarrow 24$

$k = -8 \rightarrow 8$

$l = -14 \rightarrow 14$

## Refinement

Refinement on  $F^2$

$R[F^2 > 2\sigma(F^2)] = 0.035$

$wR(F^2) = 0.100$

$S = 1.05$

1827 reflections

117 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.053P)^2 + 0.9005P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.77$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.60$  e Å<sup>-3</sup>

Extinction correction: *SHELXL97*

Extinction coefficient: 0.0051 (8)

**Table 1**

Selected geometric parameters (Å, °).

Cu1—O1	1.906 (2)	Cu1—N3	1.932 (3)
Cu1—N1	1.925 (3)	Cu1—N2	2.071 (3)
O1—Cu1—N1	93.02 (10)	O1—Cu1—N2	177.79 (11)
O1—Cu1—N3	91.56 (12)	N1—Cu1—N2	84.76 (12)
N1—Cu1—N3	175.41 (12)	N3—Cu1—N2	90.65 (13)

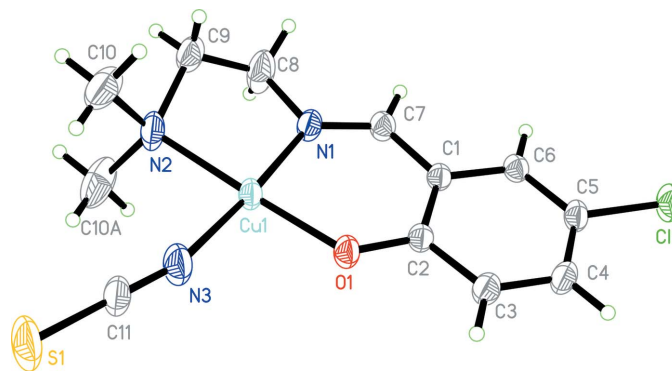
All non-H atoms except C9 and C10 lie in a crystallographic mirror plane. Atom C9 is disordered across the mirror plane and as a result the occupancy factor for the disordered components were fixed at 0.50 each. The H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.96 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{C})$ .

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*.

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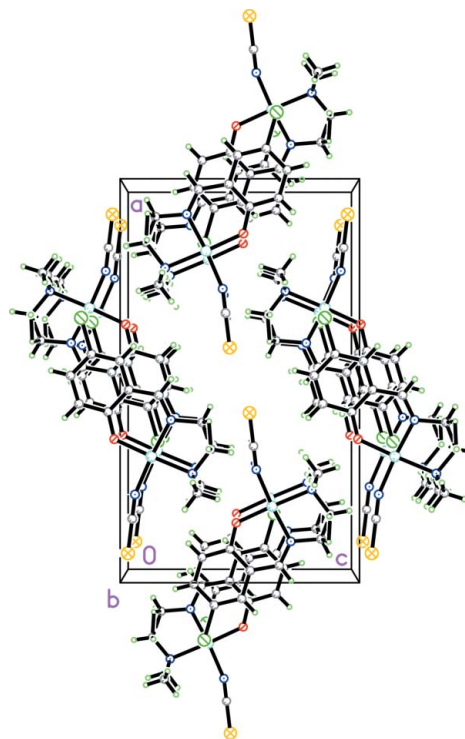
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**Figure 1**

The molecular structure of compound (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 30% probability level. The atom labelled with the suffix A is at the symmetry position  $(x, \frac{1}{2} - y, z)$ . Only one component of the disordered C9 group is shown.



**Figure 2**

The crystal packing of compound (I), viewed along the *b* axis.

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