[*N*,*N*-Dimethyl-*N*′-(2-pyridylmethylene)ethane-1,2-diamine]dithiocyanatocopper(II)

Guo-Ren Yue,* Xin-Jian Xu, Yu-Zhen Shi and Lei Feng

Chemical Department, Key Laboratory of Resources and Environment Chemistry of West China, Hexi University, Zhangye 734000, People's Republic of China

Correspondence e-mail: hxuygr@sohu.com

In the title Schiff base compound, $[Cu(NCS)_2(C_{10}H_{15}N_3)]$, the Cu^{II} atom is five-coordinated by three N atoms from the Schiff base ligand and by another two N atoms from two thiocyanate anions. The coordination geometry is best described as distorted square-pyramidal. In the crystal structure, there are no significant intermolecular interactions.
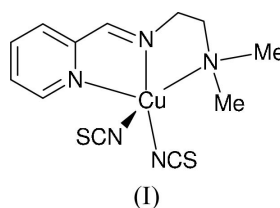
Comment

Investigations of copper(II) complexes have been of great interest in coordination chemistry (Dalai *et al.*, 2002; Bhaduri *et al.*, 2003). As an extension of work on the structural characterization of copper(II) complexes, we report here the structure of the title compound, (I).

(I)

Compound (I) (Fig. 1) is an electronically neutral mononuclear copper(II) compound. Selected bond distances and angles are given in Table 1. Atom Cu1 is coordinated by three N atoms from the Schiff base ligand and another two N atoms from the thiocyanate anions. Atom N4, of one of the thiocyante anions, acts as the apical atom of a highly distorted square-pyramidal geometry, as defined by the τ value (τ = 0.28) calculated according to the literature (Addison *et al.*, 1984).

The distortion of the square pyramid is also revealed by the bond angles between the apical and basal donor atoms [96.69 (11)–113.52 (11)°], which show a considerable deviation from the ideal 90° angle in a regular square pyramid. The smallest bond angles for the basal donor atoms [75.43 (10)° for N1—Cu1—N2 and 78.02 (10)° for N2—Cu1—N3] correlate with the strained ligand bite angle for the five-membered chelate rings. All the bond lengths involving atom Cu1 are in normal ranges.

In the crystal structure, the molecules pack in columns along the *b* axis, as shown in Fig. 2. There are no significant intermolecular interactions in the crystal structure.

Experimental

Pyridylaldehyde (0.1 mmol, 10.7 mg), *N*,*N*-dimethylethane-1,2-diamine (0.1 mmol, 8.8 mg), ammonium thiocyanate (0.2 mmol, 15.2 mg) and $Cu(CH_3COO)_2 \cdot H_2O$ (0.1 mmol, 19.9 mg) were

dissolved in methanol (10 ml). The mixture was stirred at room temperature for 1 h to give a clear blue solution. After keeping the solution in air for 5 d, blue block-shaped crystals were formed.

Crystal data

[Cu(NCS)$_2$(C$_{10}$H$_{15}$N$_3$)]
$M_r = 356.95$
Monoclinic, $P2_1/n$
$a = 10.216\ (1)$ Å
$b = 15.053\ (2)$ Å
$c = 10.610\ (1)$ Å
$\beta = 91.164\ (2)°$
$V = 1631.3\ (3)$ Å^3
$Z = 4$

$D_x = 1.453$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4575 reflections
$\theta = 2.4–24.7°$
$\mu = 1.59$ mm^{-1}
$T = 298\ (2)$ K
Block, blue
$0.23 \times 0.22 \times 0.18$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
$T_{min} = 0.703$, $T_{max} = 0.755$
18 130 measured reflections

3734 independent reflections
2649 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 27.5°$
$h = -13 \rightarrow 13$
$k = -19 \rightarrow 19$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.110$
$S = 1.02$
3734 reflections
183 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0501P)^2 + 0.4185P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.92$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

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Cu1—N5	1.958 (3)	Cu1—N1	2.211 (3)
Cu1—N4	1.963 (3)	Cu1—N3	2.222 (3)
Cu1—N2	2.061 (2)		
N5—Cu1—N4	111.20 (14)	N2—Cu1—N1	75.43 (10)
N5—Cu1—N2	135.15 (13)	N5—Cu1—N3	96.66 (11)
N4—Cu1—N2	113.52 (11)	N4—Cu1—N3	101.31 (11)
N5—Cu1—N1	96.34 (11)	N2—Cu1—N3	78.02 (10)
N4—Cu1—N1	96.69 (11)	N1—Cu1—N3	152.21 (9)

All 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 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, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.
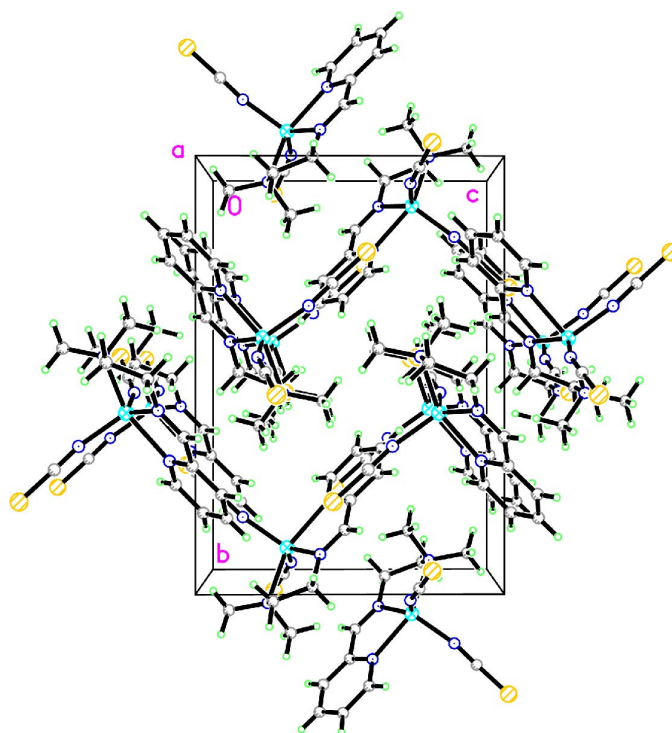
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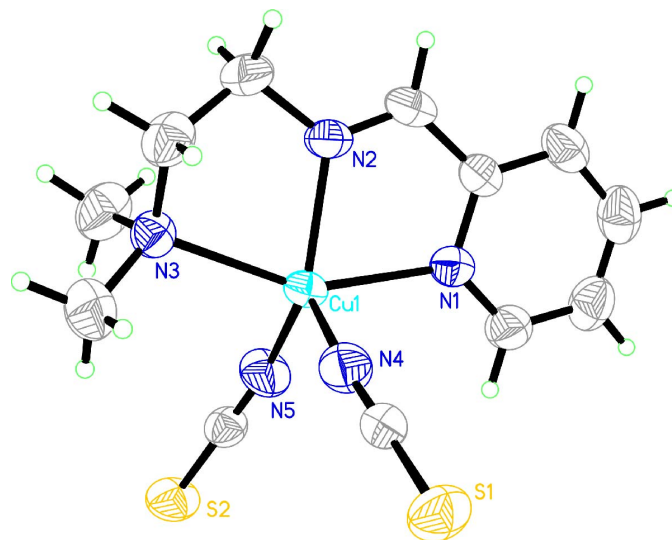
Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

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

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