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Key indicators

Single-crystal X-ray study
 T = 298 K
 Mean σ (C–C) = 0.009 Å
 R factor = 0.044
 wR factor = 0.108
 Data-to-parameter ratio = 20.3

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

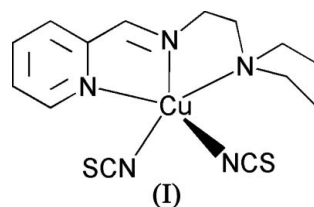
[*N,N*-Diethyl-*N'*-(2-pyridylmethylene)ethane-1,2-diamine]dithiocyanatocopper(II)

The title compound, [Cu(NCS)₂(C₁₂H₁₉N₃)], is a mononuclear copper(II) complex. The Cu^{II} ion is five-coordinated in a square-pyramidal configuration by three N atoms of the Schiff base ligand, and by two terminal N atoms from two thiocyanate anions.

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Comment

Recently, we have reported the crystal structures of a few Schiff base copper(II) compounds (You, 2005, 2006; You & Zhu, 2006). As an extension of the work on the structural characterization of these compounds, the new title copper(II) compound, (I), is reported here.



Compound (I) is a mononuclear copper(II) complex (Fig. 1). The Cu^{II} atom is five-coordinated by three N atoms from a Schiff base ligand, and by two terminal N atoms from two thiocyanate anions, forming a square-pyramidal geometry. The Cu–N bond lengths and angles (Table 1) are comparable to the values observed in the Schiff base copper(II) complexes cited above. There are no significant intermolecular interactions in the crystal structure.

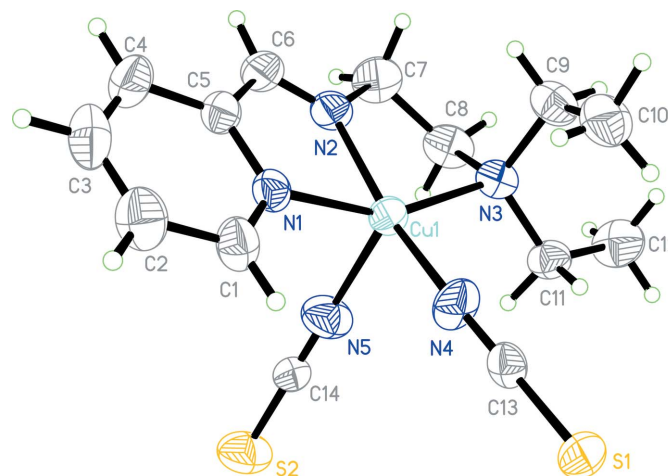


Figure 1
 The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Experimental

N,N-Diethylethane-1,2-diamine and pyridylaldehyde were available commercially and were used without further purification. *N,N*-Diethylethane-1,2-diamine (0.1 mmol, 13.5 mg) and pyridylaldehyde (0.1 mmol, 10.7 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. To this solution was added an aqueous solution (2 ml) of NH_4NCS (0.1 mmol, 7.6 mg) and an MeOH solution (5 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 resulting mixture was stirred for another 10 min at room temperature. After keeping the filtrate in air for 11 d, blue block-shaped crystals were formed at the bottom of the vessel. Analysis found: C 43.50, H 5.07, N 18.02%; calculated for $\text{C}_{14}\text{H}_{19}\text{CuN}_5\text{S}_2$: C 43.67, H 4.97, N 18.19%.

Crystal data

$[\text{Cu}(\text{NCS})_2(\text{C}_{12}\text{H}_{19}\text{N}_3)]$	Mo $K\alpha$ radiation
$M_r = 385.00$	Cell parameters from 3609 reflections
Tetragonal, $P4_1$	$\theta = 2.4\text{--}25.1^\circ$
$a = 7.294$ (1) Å	$\mu = 1.46$ mm $^{-1}$
$c = 33.549$ (3) Å	$T = 298$ (2) K
$V = 1784.9$ (4) Å 3	Block, blue
$Z = 4$	$0.35 \times 0.12 \times 0.10$ mm
$D_x = 1.433$ Mg m $^{-3}$	

Data collection

Bruker SMART CCD area-detector diffractometer	4084 independent reflections
ω scan	2778 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996)	$R_{\text{int}} = 0.031$
$T_{\text{min}} = 0.629$, $T_{\text{max}} = 0.868$	$\theta_{\text{max}} = 27.5^\circ$
15425 measured reflections	$h = -9 \rightarrow 9$
	$k = -9 \rightarrow 9$
	$l = -43 \rightarrow 43$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0581P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.044$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.108$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 0.97$	$\Delta\rho_{\text{max}} = 0.33$ e Å $^{-3}$
4084 reflections	$\Delta\rho_{\text{min}} = -0.24$ e Å $^{-3}$
201 parameters	Absolute structure: Flack (1983);
H-atom parameters constrained	1995 Friedel pairs
	Flack parameter: 0.027 (15)

Table 1

Selected geometric parameters (Å, °).

Cu1—N4	1.921 (4)	Cu1—N3	2.096 (4)
Cu1—N2	1.954 (3)	Cu1—N5	2.151 (5)
Cu1—N1	2.053 (4)		
N4—Cu1—N2	166.1 (2)	N1—Cu1—N3	155.49 (15)
N4—Cu1—N1	95.02 (18)	N4—Cu1—N5	97.2 (2)
N2—Cu1—N1	79.66 (18)	N2—Cu1—N5	96.25 (19)
N4—Cu1—N3	99.01 (17)	N1—Cu1—N5	98.6 (2)
N2—Cu1—N3	82.00 (17)	N3—Cu1—N5	99.4 (2)

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{C})$. The U_{eq} values of the N and S atoms of the NCS groups are high compared to those of the C atoms. This may be a result of unresolved disorder or twinning [$F^2(\text{observed})$ is greater than $F^2(\text{calculated})$ for the reflections with greatest discrepancies].

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1998); data reduction: *SAINTE*; 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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