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Tetrapyridinedithiocyanatocopper(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.045
wR factor = 0.146
Data-to-parameter ratio = 17.1

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

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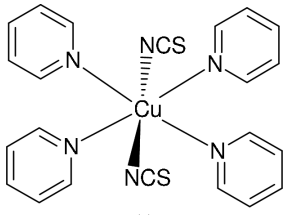
The title compound, $[Cu(NCS)_2(C_5H_5N)_4]$, is a mononuclear copper(II) complex. The Cu^{II} atom, lying on an inversion center, is six-coordinated by four pyridine N atoms and by another two N atoms of two thiocyanate anions in a slightly distorted octahedral geometry.

Comment

Transition metal complexes play an important role in the development of coordination chemistry. Since copper complexes have potential applications in the design and construction of new magnetic materials, the study of copper complexes is of great interest in various aspects of chemistry. As an extension of work on the structural characterization of copper(II) complexes, a mononuclear copper(II) complex, (I), is reported here.



(I)

The title compound, (I), is a centrosymmetric copper(II) complex (Fig. 1). The Cu^{II} ion in the complex is in an octahedral geometry and is six-coordinated by four N atoms of four pyridine ligands and by another two N atoms of two thiocyanate anions. The thiocyanate anion is a monodentate ligand and coordinates to the Cu atom *via* the terminal N atom. The three *trans* angles for the copper(II) octahedron are all 180° (Table 1), from symmetry, and all other angles around the Cu^{II} atom are close to 90°, varying from 86.97 (9) to 93.03 (9)°, indicating a slightly distorted octahedral geometry of the Cu^{II} atom. The Cu1—N1 bond length of 2.203 (2) Å is much longer than the value of 1.946 (2) Å observed in another copper(II) complex (Andac *et al.*, 2002). The Cu1—N3 bond length is a little longer than the value of 1.938 (4) Å observed in yet another copper(II) complex (Jiang *et al.*, 2004).

Experimental

Pyridine (0.2 mmol, 15.8 mg) and ammonium thiocyanate (0.1 mmol, 6.0 mg) were dissolved in methanol (5 ml) and a methanol solution (10 ml) of $Cu(CH_3COO)_2{\cdot}2H_2O$ (0.1 mmol, 21.7 mg) was added with stirring. The mixture was stirred for 1 h at room temperature to give a clear blue solution. The solution was allowed to stand in air for 18 d,

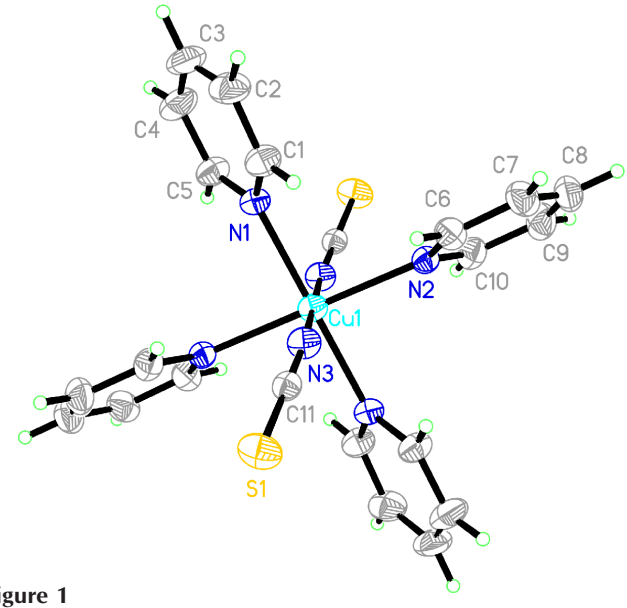


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms are related to labelled atoms by the symmetry operation $\frac{1}{2}-x, \frac{1}{2}-y, 1-z$.

whereupon blue block-shaped crystals formed on slow evaporation of the solvent.

Crystal data

$[Cu(NCS)_2(C_5H_5N)_4]$	D_x = 1.408 Mg m^{-3}
M_r = 496.10	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 3236 reflections
a = 12.420 (2) Å	θ = 2.3–27.3°
b = 12.999 (2) Å	μ = 1.13 mm^{-1}
c = 15.180 (3) Å	T = 298 (2) K
β = 107.245 (3)°	Block, blue
V = 2340.7 (7) Å^3	0.26 × 0.23 × 0.18 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2425 independent reflections
	2117 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.019
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 26.5°
	$h = -7 \rightarrow 15$
T_{min} = 0.757, T_{max} = 0.822	$k = -16 \rightarrow 16$
6801 measured reflections	$l = -19 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0816P)^2 + 3.7197P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.045	
$wR(F^2)$ = 0.146	
S = 1.07	$(\Delta/\sigma)_{max} < 0.001$
2425 reflections	$\Delta\rho_{max}$ = 0.54 e Å^{-3}
142 parameters	$\Delta\rho_{min}$ = −0.47 e Å^{-3}
H-atom parameters constrained	

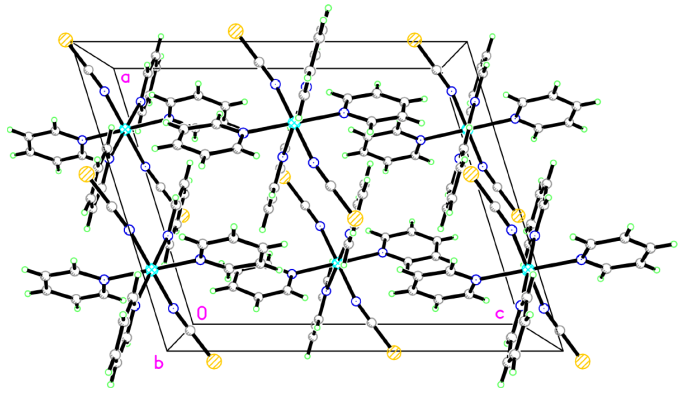


Figure 2
The crystal packing of (I), viewed along the b axis.

Table 1
Selected geometric parameters (Å, °).

Cu1—N3	2.077 (2)	Cu1—N2	2.219 (2)
Cu1—N1	2.203 (2)		
N3^i—Cu1—N3	180	N1—Cu1—N2^i	86.97 (9)
N3^i—Cu1—N1	89.25 (10)	N3—Cu1—N2	90.54 (10)
N3—Cu1—N1	90.75 (10)	N1—Cu1—N2	93.03 (9)
N1—Cu1—N1^i	180	N2^i—Cu1—N2	180
N3—Cu1—N2^i	89.46 (10)		

Symmetry code: (i) $\frac{1}{2}-x, \frac{1}{2}-y, 1-z$.

All H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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