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Key indicators

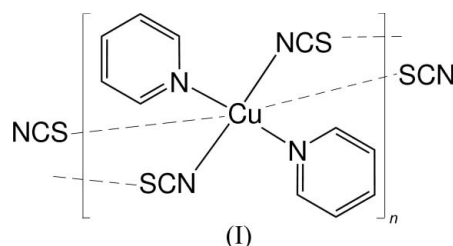
Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.036
 wR factor = 0.099
Data-to-parameter ratio = 18.3For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.*catena*-Poly[[dipyridylcopper(II)]-di- μ -thiocyanato]

The title complex, $[\text{Cu}(\text{NCS})_2(\text{C}_5\text{H}_5\text{N})_2]_n$, is a polymeric copper(II) compound. Each Cu^{II} atom of the complex has a primary coordination by four N atoms from two pyridyl and two thiocyanate ligands in mutually *trans* orientations, which define the equatorial plane. Two weakly coordinated S atoms from the thiocyanate ligands of adjacent complexes occupy axial positions, giving each Cu^{II} atom an axially distorted octahedral geometry and forming one-dimensional polymeric chains along the c axis. There are three molecules in the triclinic unit cell with one of the Cu^{II} atoms lying on a centre of inversion.

Received 27 October 2005
Accepted 10 November 2005
Online 30 November 2005

Comment

Transition metal complexes are very important in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures (Costamagna *et al.*, 1992; Bhatia *et al.*, 1981). As a part of our investigations of the structures of copper(II) derivatives, we have prepared a new Cu^{II} compound, (I) with pyridine and thiocyanate ligands, and its structure is reported here.



In complex (I), the unit cell in the crystal contains three $[\text{Cu}(\text{C}_5\text{H}_5\text{N})_2(\text{NCS})_2]$ groups, as one of the Cu^{II} atoms lies on a centre of inversion. Each Cu^{II} ion is coordinated by four N atoms from two pyridyl and two N-bound thiocyanate ligands, each in a mutually *trans* orientation, forming a square plane. Additional semi-coordinate binding by the thiocyanate S atoms of adjacent complexes, with $\text{Cu}-\text{S}$ distances of 2.991 (2) and 3.085 (2) \AA , leads to an axially distorted octahedral coordination environment for each Cu^{II} atom and the formation of one-dimensional polymeric chains along the c axis.

Experimental

Pyridine (0.2 mmol, 15.8 mg), NH_4NCS (0.2 mmol, 15.2 mg) and $\text{Cu}(\text{CH}_3\text{COO})_2 \cdot \text{H}_2\text{O}$ (0.1 mmol, 19.9 mg) were dissolved in EtOH (20 ml). The mixture was stirred for 30 min at room temperature and filtered. After the filtrate had been kept in air for 12 d, blue crystals were formed.

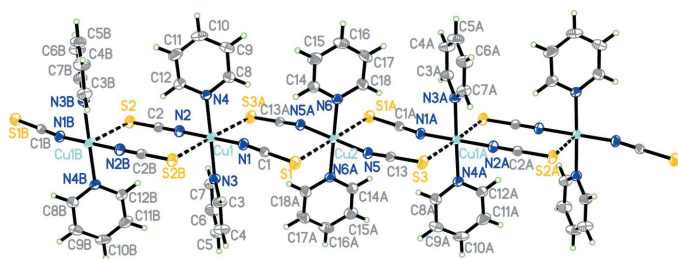


Figure 1

The structure of (I). Displacement ellipsoids are drawn at the 30% probability level. Atoms labelled with the suffixes A and B are related to atoms without a suffix by the symmetry codes ($2-x, 2-y, 2-z$) and ($1-x, 1-y, 1-z$), respectively.

Crystal data

$[\text{Cu}(\text{NCS})_2(\text{C}_5\text{H}_5\text{N})_2]$	$Z = 3$
$M_r = 337.90$	$D_x = 1.579 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 8.528 (2) \text{ \AA}$	Cell parameters from 2902 reflections
$b = 9.128 (1) \text{ \AA}$	$\theta = 2.5\text{--}28.1^\circ$
$c = 15.371 (1) \text{ \AA}$	$\mu = 1.82 \text{ mm}^{-1}$
$\alpha = 91.737 (1)^\circ$	$T = 293 (2) \text{ K}$
$\beta = 97.043 (1)^\circ$	Block, blue
$\gamma = 115.639 (1)^\circ$	$0.32 \times 0.28 \times 0.23 \text{ mm}$
$V = 1065.9 (3) \text{ \AA}^3$	

Data collection

Bruker SMART CCD area-detector diffractometer	4737 independent reflections
ω scans	3626 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.018$
$T_{\text{min}} = 0.594, T_{\text{max}} = 0.680$	$\theta_{\text{max}} = 27.5^\circ$
9264 measured reflections	$h = -11 \rightarrow 9$
	$k = -11 \rightarrow 11$
	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.036$	$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2]$
$wR(F^2) = 0.099$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{\text{max}} < 0.001$
4737 reflections	$\Delta\rho_{\text{max}} = 0.27 \text{ e \AA}^{-3}$
259 parameters	$\Delta\rho_{\text{min}} = -0.57 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters ($\text{\AA}, ^\circ$).

Cu1—N2	1.932 (2)	Cu1—S3 ⁱⁱ	3.045 (2)
Cu1—N1	1.936 (2)	Cu2—N5	1.933 (2)
Cu1—N4	2.049 (2)	Cu2—N6	2.044 (2)
Cu1—N3	2.055 (2)	Cu2—S1	3.085 (2)
Cu1—S2 ⁱ	2.991 (2)		
N2—Cu1—N1	179.93 (6)	S3 ⁱⁱ —Cu1—N3	89.9 (2)
N2—Cu1—N4	88.88 (7)	S3 ⁱⁱ —Cu1—N4	89.36 (5)
N1—Cu1—N4	91.06 (7)	S2 ⁱ —Cu1—S3 ⁱⁱ	176.1 (2)
N2—Cu1—N3	89.46 (7)	N5—Cu2—N5 ⁱⁱ	180
N1—Cu1—N3	90.60 (7)	N5—Cu2—N6	89.70 (7)
N4—Cu1—N3	178.19 (6)	N5 ⁱⁱ —Cu2—N6	90.30 (7)
S2 ⁱ —Cu1—N1	84.7 (2)	N6—Cu2—N6 ⁱⁱ	180
S2 ⁱ —Cu1—N2	95.2 (2)	S1—Cu2—N5	87.7 (2)
S2 ⁱ —Cu1—N3	90.3 (2)	S1—Cu2—N5 ⁱⁱ	92.3 (2)
S2 ⁱ —Cu1—N4	90.6 (2)	S1—Cu2—N6	89.1 (2)
S3 ⁱⁱ —Cu1—N1	91.4 (2)	S1—Cu2—N6 ⁱⁱ	90.9 (2)
S3 ⁱⁱ —Cu1—N2	88.7 (2)	S1—Cu2—S1 ⁱⁱ	180

Symmetry codes: (i) $-x+2, -y+2, -z+2$; (ii) $-x+1, -y+1, -z+1$.

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93 \AA and with $U_{\text{iso}}(\text{H})$ values set to $1.2U_{\text{eq}}(\text{C})$.

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.

We thank Qufu Normal University for support of this research.

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