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Poly[[(2-iodopyrazine-κN^4)copper(I)]-μ_3-thiocyanato-$\kappa^3 N{:}S{:}S$]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.037
wR factor = 0.086
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.

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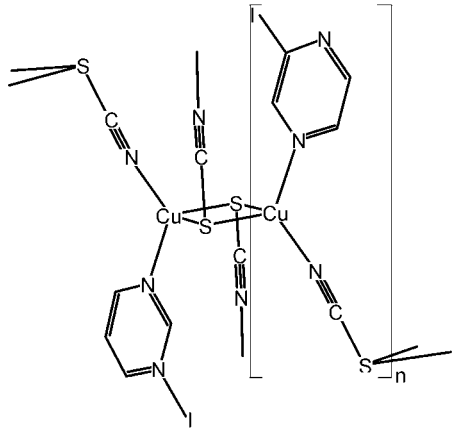
In the crystal structure of the title compound, $[Cu(NCS)(C_4H_3IN_2)]_n$, each Cu atom is coordinated by three thiocyanate anions and one 2-iodopyrazine ligand within a distorted tetrahedron. The Cu-coordinated units form dimers, which are connected into layers by the thiocyanate anions.

Comment

Recently, we have been interested in the synthesis, structures and thermal properties of coordination polymers based on copper(I) halides or pseudohalides and aromatic N-donor ligands. We have found that several of the ligand-rich compounds transform into ligand-poor compounds on heating. During these investigations, we have prepared several compounds using pyrazine derivatives such as 2-methylpyrazine or 2-chloropyrazine (Näther *et al.*, 2001, 2002). In further investigations, we have prepared coordination polymers with 2-iodopyrazine. With CuI, we have found two polymorphic modifications of CuI(2-iodopyrazine) (Näther *et al.*, 2003). We report here the structure of a compound, (I), with CuSCN and 2-iodopyrazine.



(I)

The asymmetric unit of (I) is built up of one Cu atom, one thiocyanate anion and one 2-iodopyrazine ligand. All atoms are located in general positions. The compound forms $(CuSCN)_2$ dimers in which the Cu atoms are connected *via* the S atoms of two symmetry-related thiocyanate anions (Fig. 1). Within the dimers, each Cu atom is coordinated by two S and one N atom of three symmetry-related thiocyanate anions and one N atom of the 2-iodopyrazine ligand, forming a distorted tetrahedron. In the 2-iodopyrazine ligand, only the N atom that is not adjacent to the bulky I atom is involved in copper coordination. The $(CuSCN)_2$ dimers are connected *via* the thiocyanate anions into layers (Fig. 2). These layers are

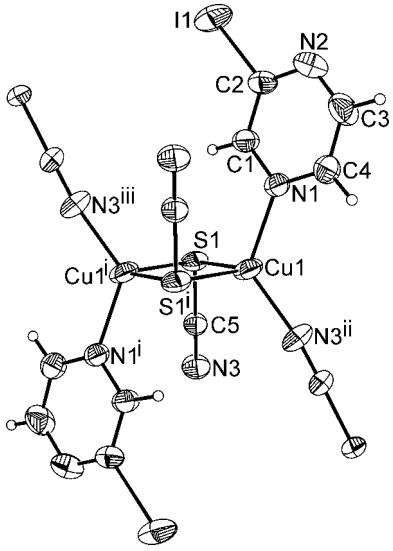


Figure 1
The centrosymmetric dimeric unit of (I), showing the copper coordination with the atom labelling and displacement ellipsoids drawn at the 50% probability level. [Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $-x+2, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.]

stacked in the direction of the *a* axis and are separated by the I atoms of the 2-iodopyrazine ligands (Fig. 3).

Experimental

The title compound was prepared by the reaction of CuSCN (172.4 mg) and 2-iodopyrazine (584.1 mg) in acetonitrile (3 ml). After 4 d, yellow single crystals suitable for single-crystal structure analysis had formed. The homogeneity of the product was confirmed by X-ray powder diffraction. The compound decomposes at about 403 K into CuSCN without the formation of a ligand-poor intermediate.

Crystal data

$[Cu(NCS)(C_4H_3IN_2)]$	$D_x = 2.494$ Mg m^{-3}
$M_r = 327.60$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 8000 reflections
$a = 10.6219$ (7) Å	$\theta = 3$–28°
$b = 7.6529$ (3) Å	$\mu = 6.22$ mm^{-1}
$c = 11.1018$ (7) Å	$T = 293$ (2) K
$\beta = 104.804$ (7)°	Block, yellow
$V = 872.49$ (9) Å^3	0.12 × 0.10 × 0.07 mm
$Z = 4$	

Data collection

Stoe IPDS diffractometer	1683 reflections with $I > 2\sigma(I)$
φ scans	$R_{int} = 0.041$
Absorption correction: numerical (*X-SHAPE*; Stoe & Cie, 1998)	$\theta_{max} = 27.9^\circ$
$T_{min} = 0.483$, $T_{max} = 0.653$	$h = -13 \rightarrow 13$
8241 measured reflections	$k = -10 \rightarrow 10$
2030 independent reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0294P)^2 + 3.1221P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.037$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.086$	$\Delta\rho_{max} = 1.55$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -1.34$ e Å^{-3}
2030 reflections	
100 parameters	
H-atom parameters constrained	

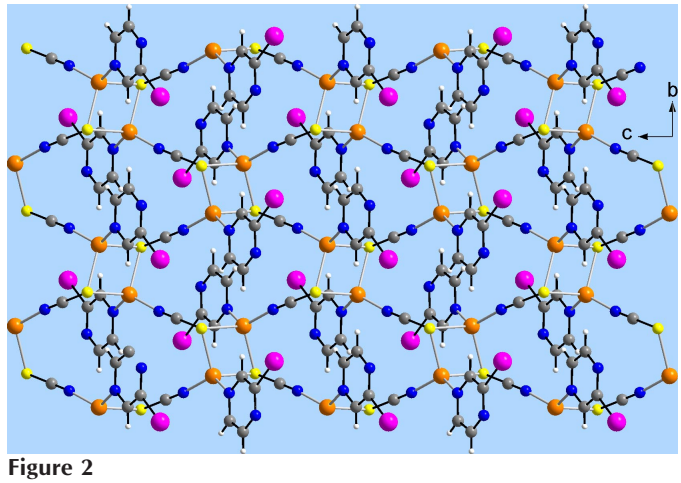


Figure 2
The crystal structure of (I), viewed in the direction of the *a* axis.

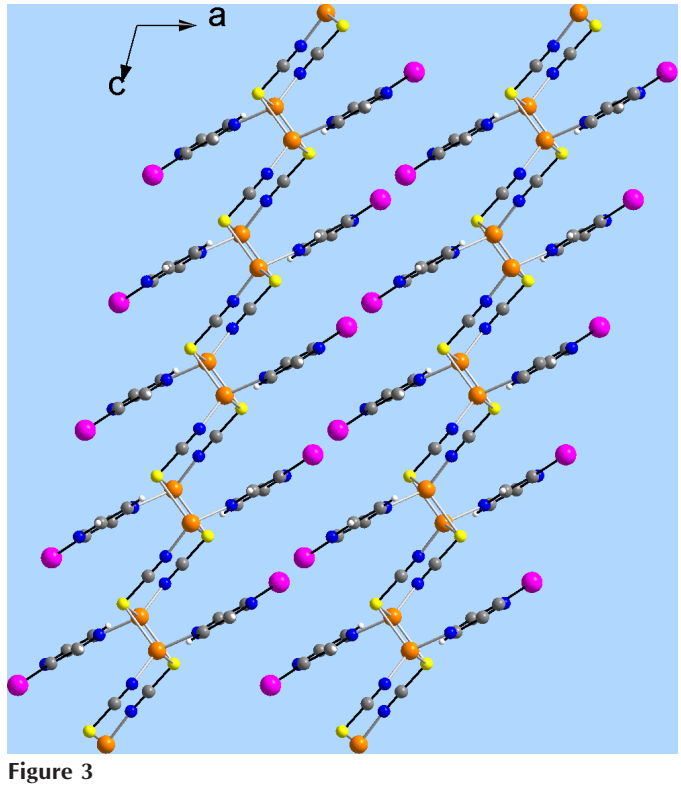


Figure 3
The crystal structure of (I), viewed in the direction of the *b* axis.

Table 1
Selected geometric parameters (Å, °).

Cu1—N3^{ii}	1.918 (4)	Cu1—S1^{i}	2.4396 (13)
Cu1—N1	2.026 (3)	Cu1—Cu1^{i}	2.8434 (12)
Cu1—S1	2.4064 (12)		
N3^{ii}—Cu1—N1	125.15 (18)	N3^{ii}—Cu1—S1^{i}	106.46 (13)
N3^{ii}—Cu1—S1	111.86 (14)	N1—Cu1—S1^{i}	102.03 (10)
N1—Cu1—S1	101.97 (11)	S1—Cu1—S1^{i}	108.15 (4)

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

The H atoms were positioned with idealized geometry (C—H = 0.93 Å) and refined using a riding model [U_{iso}(H) = 1.2U_{eq}(aromatic C)]. The highest peak in the difference map is located 0.78 Å from I1 and the deepest hole is located 0.78 Å from I1.

Data collection: *IPDS* (Stoe & Cie, 1998); cell refinement: *IPDS*; data reduction: *IPDS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *CIFTAB* in *SHELXL97*.

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