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Key indicators

Single-crystal X-ray study
 T = 293 K
 Mean $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$
 R factor = 0.051
 wR factor = 0.108
 Data-to-parameter ratio = 19.9

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

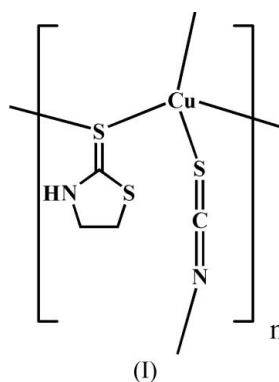
Poly[μ -1,3-thiazolidine-2-thione- $\kappa^2\text{S}^2:\text{S}^2$ - μ -thiocyanato- $\kappa^2\text{S}:\text{N}$ -copper(I)]

The title compound, $[\text{Cu}(\text{SCN})(\text{C}_3\text{H}_5\text{NS}_2)]_n$, was prepared from the direct reaction between copper(I) thiocyanate and 1,3-thiazolidine-2-thione. The structure is an infinite two-dimensional polymer, parallel to the *ac* plane, with tetrahedrally distorted Cu atoms which are coordinated by the S and N atoms of the thiocyanate ions, and by the thione S atom of 1,3-thiazolidine-2-thione molecules.

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Comment

Heterocyclic thione compounds have received much attention due to their wide range of applications (Rapper, 1985, 1994, 1996, 1997; Akrivos, 2001; Bell *et al.*, 2004). Neutral thione molecules can coordinate to metal atoms in a variety of ways (Aslanidis *et al.*, 2004). Likewise, the metal atoms in group IB are also interesting for use in synthesis with these ligands; the complexes have been applied in optical, electrical, magnetic and luminescent materials (Huang *et al.*, 2004).



For this work, we used copper(I) thiocyanate as a starting material to interact directly with 1,3-thiazolidine-2-thione under mild reaction conditions. The structure of the title complex, (I), is depicted in Fig. 1. The title complex is a two-dimensional polymeric structure, the Cu centre having a distorted tetrahedral geometry and being coordinated by two 1,3-thiazolidine-2-thione molecules and two thiocyanate groups. Each 1,3-thiazolidine-2-thione molecule is bonded to Cu atoms *via* the thione S atom. The thiocyanate groups bridge two Cu centres. As a result, 12-membered rings are formed. The crystal packing shows a weak N—H \cdots N hydrogen bond (Table 1).

Experimental

1,3-Thiazolidine-2-thione (0.125 g, 0.985 mmol) was dissolved in CH_3CN (30 ml); CuSCN (0.120 g, 0.985 mmol) was then added as a powder to the solution. The mixture was heated to 343 K and refluxed

until the grey solid had changed colour to yellow (around 7 h). The yellow solid was filtered off and the yellow solution was kept at room temperature and allowed to evaporate slowly. Colourless needle-like crystals of the title complex were obtained.

Crystal data

[Cu(SCN)(C ₃ H ₅ NS ₂)]	$V = 781.17 (18) \text{ \AA}^3$
$M_r = 240.82$	$Z = 4$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 5.8370 (7) \text{ \AA}$	$\mu = 3.52 \text{ mm}^{-1}$
$b = 19.992 (3) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 6.9779 (9) \text{ \AA}$	$0.23 \times 0.05 \times 0.02 \text{ mm}$
$\beta = 106.391 (2)^\circ$	

Data collection

Bruker SMART APEX diffractometer	6767 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 1997)	1871 independent reflections
$T_{\min} = 0.671, T_{\max} = 0.940$	1573 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.039$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.051$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.108$	
$S = 1.15$	$\Delta\rho_{\text{max}} = 0.73 \text{ e \AA}^{-3}$
1871 reflections	$\Delta\rho_{\text{min}} = -0.54 \text{ e \AA}^{-3}$
94 parameters	

Table 1

Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1\cdots N2^i$	0.877 (19)	2.69 (3)	3.486 (5)	151 (4)

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

H atoms bonded to C atoms were placed in geometrically idealized positions and refined using a riding model, with $C-H = 0.97 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The H atom bonded to nitrogen was located in a difference Fourier map. Its position was refined with a distance restraint [$N-H = 0.89 (2) \text{ \AA}$] and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$.

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT and SHELXTL (Bruker, 1997); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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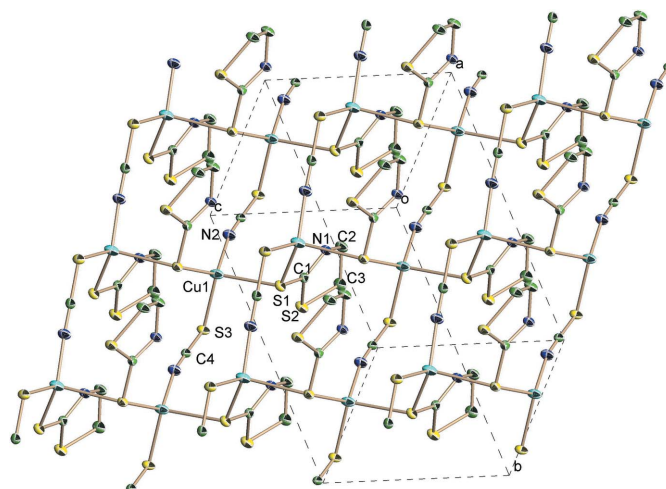


Figure 1

The polymeric sheet structure of title complex, showing the atom-labelling. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

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References

- Akrivos, P. D. (2001). *Coord. Chem. Rev.* **181**, 181–210.
- Aslanidis, P., Cox, P. J., Divanidis, S. & Karagiannidis, P. (2004). *Inorg. Chim. Acta*, **357**, 2677–2686.
- Bell, N. A., Clegg, W., Coles, S. J., Constable, C. P., Harington, R. W., Hursthouse, M. B., Light, M. E., Raper, E. S., Sammon, C. & Walker, M. R. (2004). *Inorg. Chim. Acta*, **357**, 1063–1076.
- Bruker (1997). SMART (Version 5.631), SAINT (Version 6.02A), SADABS (Version 2.0) and SHELXTL (Version 6.14). Bruker AXS Inc., Madison, Wisconsin, USA.
- Huang, Z., Song, H.-B., Du, M., Chem, S.-T. & Wang, S. (2004). *Inorg. Chem.* **43**, 931–944.
- Rapper, E. S. (1985). *Coord. Chem. Rev.* **61**, 115–184.
- Rapper, E. S. (1994). *Coord. Chem. Rev.* **129**, 91–156.
- Rapper, E. S. (1996). *Coord. Chem. Rev.* **153**, 199–255.
- Rapper, E. S. (1997). *Coord. Chem. Rev.* **165**, 475–567.
- Sheldrick, G. M. (1997). SHELXL97 and SHELXS97. University of Göttingen, Germany.