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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>.

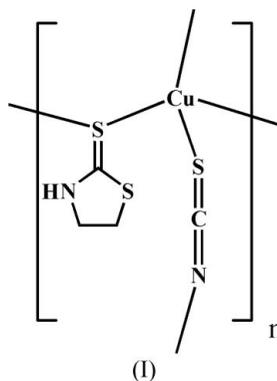
Poly[μ -1,3-thiazolidine-2-thione- $\kappa^2\text{S}^2:\text{S}^2$ - μ -thiocyanato- $\kappa^2\text{S}:\text{N}$ -copper(I)]

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···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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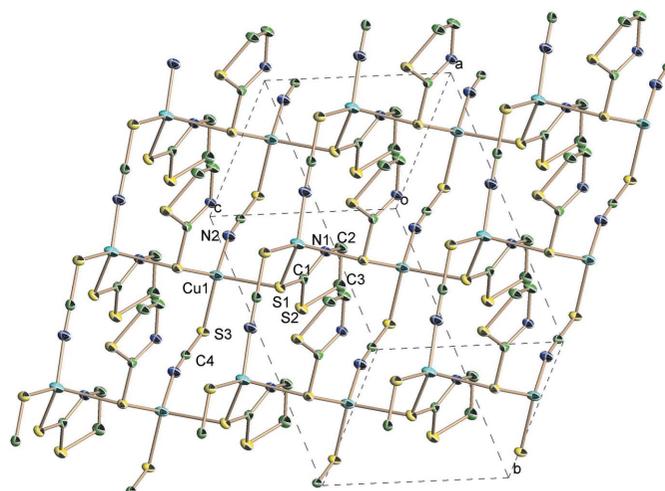


Figure 1

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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supporting information

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Poly[μ -1,3-thiazolidine-2-thione- κ^2 S²:S²- μ -thiocyanato- κ^2 S:N-copper(I)]

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Poly[μ -1,3-thiazoline-2-thione- κ^2 S²:S²- μ -thiocyanato- κ^2 S:N-copper(I)]

Crystal data

[Cu(SCN)(C₃H₅NS₂)]

$M_r = 240.82$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 5.8370$ (7) Å

$b = 19.992$ (3) Å

$c = 6.9779$ (9) Å

$\beta = 106.391$ (2)°

$V = 781.17$ (18) Å³

$Z = 4$

$F(000) = 480$

$D_x = 2.048$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71074$ Å

Cell parameters from 1484 reflections

$\theta = 3.2$ – 24.0 °

$\mu = 3.52$ mm⁻¹

$T = 293$ K

Needle, colorless

$0.23 \times 0.05 \times 0.02$ mm

Data collection

Bruker AXS D8

diffractometer

Radiation source: sealed X-ray tube

Graphite monochromator

Detector resolution: 8.366 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 1997)

$T_{\min} = 0.671$, $T_{\max} = 0.940$

6767 measured reflections

1871 independent reflections

1573 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.039$

$\theta_{\max} = 28.2$ °, $\theta_{\min} = 2.0$ °

$h = -7 \rightarrow 7$

$k = -25 \rightarrow 26$

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.051$

$wR(F^2) = 0.108$

$S = 1.15$

1871 reflections

94 parameters

1 restraint

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 0.9712P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.73$ e Å⁻³

$\Delta\rho_{\min} = -0.54$ e Å⁻³

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.17403 (10)	0.30184 (3)	1.19916 (9)	0.0394 (2)
S1	0.04782 (19)	0.29292 (5)	0.81538 (16)	0.0296 (2)
S2	0.1806 (2)	0.43839 (5)	0.82671 (18)	0.0359 (3)
N1	0.4138 (6)	0.34760 (17)	0.7097 (5)	0.0312 (8)
H1	0.453 (8)	0.3078 (13)	0.676 (7)	0.037*
N2	0.5112 (7)	0.3246 (2)	1.2443 (6)	0.0430 (9)
C1	0.2285 (7)	0.35495 (19)	0.7778 (6)	0.0255 (8)
C2	0.5562 (8)	0.4071 (2)	0.7042 (8)	0.0399 (11)
H2A	0.6123	0.4068	0.5860	0.048*
H2B	0.6935	0.4088	0.8213	0.048*
C3	0.3971 (8)	0.4660 (2)	0.7007 (8)	0.0408 (11)
H3A	0.3177	0.4792	0.5643	0.049*
H3B	0.4883	0.5037	0.7701	0.049*
S3	-0.06175 (18)	0.38930 (5)	1.25329 (17)	0.0335 (3)
C4	-0.3110 (7)	0.3499 (2)	1.2486 (6)	0.0288 (9)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0300 (3)	0.0270 (3)	0.0662 (4)	0.0021 (2)	0.0215 (3)	0.0067 (3)
S1	0.0331 (5)	0.0212 (5)	0.0393 (6)	-0.0044 (4)	0.0178 (4)	-0.0041 (4)
S2	0.0378 (6)	0.0227 (5)	0.0548 (7)	-0.0044 (4)	0.0252 (5)	-0.0055 (5)
N1	0.0290 (17)	0.0251 (17)	0.044 (2)	0.0006 (14)	0.0175 (16)	0.0001 (16)
N2	0.0254 (18)	0.055 (2)	0.050 (2)	-0.0006 (18)	0.0129 (17)	0.001 (2)
C1	0.0303 (19)	0.0214 (19)	0.026 (2)	-0.0002 (16)	0.0104 (16)	0.0003 (15)
C2	0.030 (2)	0.039 (3)	0.056 (3)	-0.0020 (19)	0.022 (2)	0.005 (2)
C3	0.040 (2)	0.029 (2)	0.059 (3)	-0.0071 (19)	0.023 (2)	0.006 (2)
S3	0.0271 (5)	0.0261 (5)	0.0489 (7)	0.0013 (4)	0.0132 (5)	-0.0051 (5)
C4	0.026 (2)	0.032 (2)	0.028 (2)	0.0071 (17)	0.0073 (16)	0.0001 (17)

Geometric parameters (\AA , $^\circ$)

Cu1—N2	1.957 (4)	N1—H1	0.877 (19)
Cu1—S1 ⁱ	2.2641 (11)	N2—C4 ⁱⁱⁱ	1.148 (5)
Cu1—S3	2.3211 (12)	C2—C3	1.495 (6)
Cu1—S1	2.5754 (13)	C2—H2A	0.9700
S1—C1	1.696 (4)	C2—H2B	0.9700
S1—Cu1 ⁱⁱ	2.2641 (11)	C3—H3A	0.9700
S2—C1	1.741 (4)	C3—H3B	0.9700
S2—C3	1.817 (4)	S3—C4	1.646 (4)

N1—C1	1.307 (5)	C4—N2 ^{iv}	1.148 (5)
N1—C2	1.458 (5)		
N2—Cu1—S1 ⁱ	123.44 (13)	S1—C1—S2	122.0 (2)
N2—Cu1—S3	114.47 (13)	N1—C2—C3	106.7 (3)
S1 ⁱ —Cu1—S3	107.71 (4)	N1—C2—H2A	110.4
N2—Cu1—S1	99.38 (12)	C3—C2—H2A	110.4
S1 ⁱ —Cu1—S1	106.74 (4)	N1—C2—H2B	110.4
S3—Cu1—S1	102.28 (4)	C3—C2—H2B	110.4
C1—S1—Cu1 ⁱⁱ	106.09 (14)	H2A—C2—H2B	108.6
C1—S1—Cu1	95.86 (14)	C2—C3—S2	105.5 (3)
Cu1 ⁱⁱ —S1—Cu1	113.82 (5)	C2—C3—H3A	110.6
C1—S2—C3	91.4 (2)	S2—C3—H3A	110.6
C1—N1—C2	117.0 (3)	C2—C3—H3B	110.6
C1—N1—H1	120 (3)	S2—C3—H3B	110.6
C2—N1—H1	123 (3)	H3A—C3—H3B	108.8
C4 ⁱⁱⁱ —N2—Cu1	165.4 (4)	C4—S3—Cu1	101.40 (15)
N1—C1—S1	126.1 (3)	N2 ^{iv} —C4—S3	177.6 (4)
N1—C1—S2	112.0 (3)		
N2—Cu1—S1—C1	-35.10 (19)	Cu1—S1—C1—N1	112.1 (4)
S1 ⁱ —Cu1—S1—C1	-164.36 (14)	Cu1 ⁱⁱ —S1—C1—S2	174.6 (2)
S3—Cu1—S1—C1	82.65 (14)	Cu1—S1—C1—S2	-68.5 (2)
N2—Cu1—S1—Cu1 ⁱⁱ	75.38 (14)	C3—S2—C1—N1	10.7 (3)
S1 ⁱ —Cu1—S1—Cu1 ⁱⁱ	-53.88 (8)	C3—S2—C1—S1	-168.8 (3)
S3—Cu1—S1—Cu1 ⁱⁱ	-166.87 (4)	C1—N1—C2—C3	-22.8 (5)
S1 ⁱ —Cu1—N2—C4 ⁱⁱⁱ	-178.7 (15)	N1—C2—C3—S2	27.9 (5)
S3—Cu1—N2—C4 ⁱⁱⁱ	-44.2 (16)	C1—S2—C3—C2	-22.4 (4)
S1—Cu1—N2—C4 ⁱⁱⁱ	64.0 (16)	N2—Cu1—S3—C4	-168.86 (19)
C2—N1—C1—S1	-175.1 (3)	S1 ⁱ —Cu1—S3—C4	-27.52 (15)
C2—N1—C1—S2	5.4 (5)	S1—Cu1—S3—C4	84.74 (15)
Cu1 ⁱⁱ —S1—C1—N1	-4.8 (4)		

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

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 ⁱⁱ	0.88 (2)	2.69 (3)	3.486 (5)	151 (4)

Symmetry code: (ii) $x, -y+1/2, z-1/2$.