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catena-Poly[[di-μ-thiocyanato-κ^4S:S-argentate(I)]-di-μ-thiocyanato-κ^4S:N-bis[diamminecopper(II)]-di-μ-thiocyanato-κ^4N:S]

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Key indicators

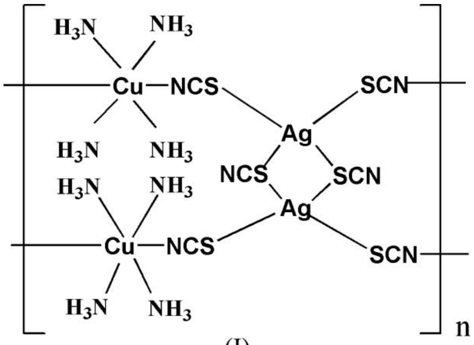
Single-crystal X-ray study
T = 298 K
Mean σ(N–C) = 0.007 Å
R factor = 0.021
wR factor = 0.082
Data-to-parameter ratio = 15.9

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

The title compound, $[\mathrm{Cu^{II}Ag^{I}(SCN)_3(NH_3)_4}]_n$, consists of two single chains of $\mathrm{CuN_6}$ Jahn–Teller-distorted octahedra and $\mathrm{AgS_4}$ tetrahedra connected by thiocyanate groups. Both metal atoms are located on twofold rotation axes. The two single chains are connected, forming a double chain along the *a* axis. Adjacent double chains are linked into a three-dimensional network by N—H···N hydrogen bonds.

Comment

In recent years, considerable attention has been paid to the investigation of the structures and properties of heteropolynuclear complexes of transition metal ions containing the thiocyanate ligand (Wrzeszcz *et al.*, 2002; Krautscheid *et al.*, 1998; Kovbasyak *et al.*, 1998; Ribas *et al.*, 1998; Potvin *et al.*, 1987; Singh, 1980). Transition metal thiocyanates (Singh & Singh, 2002; Carlson *et al.*, 1988) play a central role in the construction of molecular materials which display unusual conducting and magnetic properties and find wide applicability in materials chemistry because of the *N*,*S*-bridging coordination modes of thiocyanate which afford fascinating structures of different dimensionalities. To the best of our knowledge, only a few inorganic heteropolynuclear complexes including the thiocyanate ligand have been reported in the literature, and even fewer have been studied by single-crystal X-ray crystallography (Costes *et al.*, 2006; Bala *et al.*, 2006; Geng *et al.*, 2005; Güneş & Valkonen, 2002, 2004; Wang *et al.*, 2003; Jiang *et al.*, 2003; Güneş *et al.*, 2002; Xu *et al.*, 1999). In this contribution, we report the preparation and X-ray crystallographic structure of a new example of an inorganic heteropolynuclear complex, (I), including the thiocyanate ligand.



(I)

In the title compound, the Cu and Ag atoms are located on twofold rotation axes. The copper(II) metal exhibits a Jahn–Teller-distorted octahedral geometry defined by the N atoms

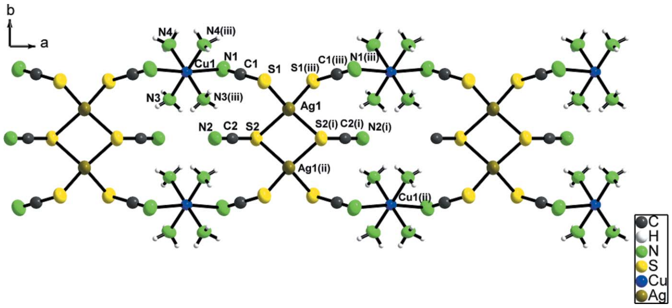


Figure 1
The double-chain of the title compound running along the *a* axis, showing the atom-labelling scheme and 70% probability displacement ellipsoids. [Symmetry codes: (i) $1 - x, y, 1 - z$; (ii) $1 - x, 1 - y, 1 - z$; (iii) $-x, y, 1 - z$.]

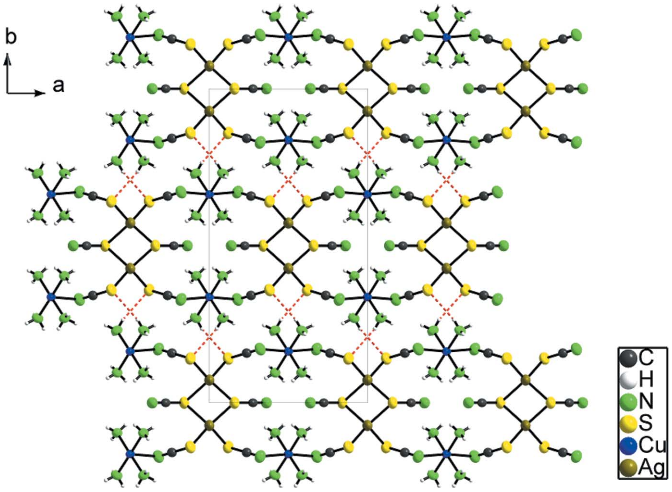


Figure 2
Packing diagram of the title compound, viewed along [001], shown with 70% probability displacement ellipsoids. Dashed lines indicate hydrogen bonds.

from two thiocyanate and four NH_3 molecules. The Ag atom is tetrahedrally coordinated by the S atoms from four thiocyanate groups (Fig. 1). In the asymmetric unit there are two crystallographically independent thiocyanate groups. One group is bonded to the Ag atom through the S atom at one end, and to the Cu atom through the N atom at the other end, forming a single-chain structure. The other thiocyanate group lies on a mirror plane and bridges two centrosymmetrically related Ag atoms through the S atom, forming a double chain running along the *a* axis (Fig. 2), which is stabilized by a weak N—H⋯S hydrogen-bond interaction (Table 2). The average S—C and C—N distances are 1.65 (3) and 1.15 (5) Å, respectively. The N—C—S bond angles of the thiocyanate groups are close to 180° (Table 1).

In the crystal packing, N—H⋯N hydrogen bonds link adjacent chains into a three-dimensional network (Table 2).

Experimental

To a vigorously stirred solution containing $Cu(NO_3)_2\cdot 3H_2O$ (0.241 g, 1 mmol) and $AgNO_3$ (0.169 g, 1 mmol) with KSCN (0.582 g, 6 mmol) in H_2O (5 ml), an excess of concentrated ammonia (15 *M*) was added dropwise. The mixture was sealed in a 23 ml Teflon-lined stainless steel autoclave and heated at 353 K for 2 d. After cooling at a rate of 9 K h^{-1} to 296 K, green crystals of the title compound suitable for X-ray analysis were isolated from the solution by filtration.

Crystal data

$[CuAg(SCN)_3(NH_3)_4]$
$M_r = 413.79$
Monoclinic, $C2/m$
$a = 11.485 (2)$ Å
$b = 21.440 (4)$ Å
$c = 5.5973 (11)$ Å
$\beta = 109.77 (3)°$
$V = 1297.0 (5)$ Å^3
$Z = 4$
$D_x = 2.119$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 3.61$ mm^{-1}
$T = 298 (2)$ K
Parallelepiped, green
0.18 × 0.07 × 0.06 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
φ and ω scans
Absorption correction: multi-scan (*RAPID-AUTO*; Rigaku, 1998)
$T_{min} = 0.562$, $T_{max} = 0.812$
5870 measured reflections
1523 independent reflections
1301 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.021$
$wR(F^2) = 0.082$
$S = 1.01$
1523 reflections
96 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0556P)^2 + 0.7288P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -0.63$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.004681

Table 1
Selected geometric parameters (Å, °).

Ag1—S1	2.5848 (10)	S2—C2	1.660 (4)
Ag1—S2	2.6344 (12)	S2—Ag1^{i}	2.6344 (12)
Cu1—N4	2.014 (3)	N1—C1	1.158 (4)
Cu1—N3	2.016 (2)	N2—C2	1.153 (6)
S1—C1	1.643 (3)		
S1—Ag1—S1^{ii}	110.60 (5)	N4^{iii}—Cu1—N3	179.02 (11)
S1—Ag1—S2	108.71 (3)	N4—Cu1—N3	91.17 (12)
S1^{ii}—Ag1—S2	110.43 (3)	N4^{iii}—Cu1—N3^{iii}	91.17 (12)
S2—Ag1—S2^{i}	107.92 (4)	N3—Cu1—N3^{iii}	88.14 (15)
S1—Ag1—Ag1^{i}	124.70 (2)	N1—C1—S1	177.0 (3)
N4^{iii}—Cu1—N4	89.53 (17)	N2—C2—S2	176.6 (4)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N4—H6⋯S1^{iv}	0.86 (6)	2.75 (5)	3.596 (3)	168 (4)
N3—H3⋯N1^{v}	0.87 (3)	2.38 (3)	3.255 (4)	175 (2)
N4—H4⋯N1^{v}	0.82 (5)	2.29 (5)	3.095 (4)	168 (5)

Symmetry codes: (iv) $-x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$; (v) $-x, y, -z$.

All H atoms were found in difference density maps and refined freely, except that the H atoms attached to N3 were assigned $U_{iso}(H) = 1.5U_{eq}(N)$.

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Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1993); software used to prepare material for publication: *SHELXL97/2* (Sheldrick, 1997).

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