catena-Poly[[(di-2-pyridylamine-$\kappa^2 N$,N')copper(I)]-μ-isothiocyanato-$\kappa^2 S$:S]

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The NCS ligand in the title compound, $[Cu(NCS)(C_{10}H_9N_3)]_n$, bridges adjacent tetrahedral Cu^I atoms through the sulfur end into a linear chain that runs along the *b* axis of the orthorhombic unit cell.

Comment

An earlier study has reported the crystal structure of a copper(I) isothiocyanate adduct of 2,2′-biquinoline; the *N*-heterocycle chelates to the Cu^I and the NCS group links the heterocycle–Cu^I units into linear chains through the N and S atoms (Zhou & Ng, 2006). In the adduct with 2,2′-dipyridylamine, the NCS group links the *N*-heterocycle–Cu^I units into a chain, but the NCS group functions as a bridge through the S end only (Fig. 1). The chains are consolidated into layers by an inter-chain hydrogen bond (Table 2) between the amino group and the free N end of the NCS group.

(I)
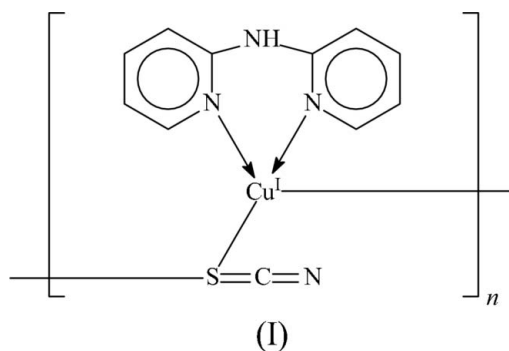
Experimental

A solution of 2,2′-dipyridylamine (0.171 g, 1.0 mmol) in DMF (10 ml) was layered over a solution of copper(I) isothiocyanate (0.125 g, 1.0 mmol) in saturated sodium thiocyanate dissolved in ethanol (10 ml). After two weeks, colourless needle-shaped crystals were formed in 40% yield based on Cu. Analysis calculated for $C_{11}H_9CuN_4S$: C 45.12, H 3.10, N 19.14%; found C 45.32, H 3.20, N 19.08%. A specimen was cut from a large needle for the diffraction measurements.

Crystal data

$[Cu(NCS)(C_{10}H_9N_3)]$	$Z = 4$
$M_r = 292.82$	$D_x = 1.749$ Mg m^{-3}
Orthorhombic, $Pca2_1$	Mo $K\alpha$ radiation
$a = 17.432$ (1) Å	$\mu = 2.13$ mm^{-1}
$b = 3.8123$ (3) Å	$T = 295$ (2) K
$c = 16.734$ (1) Å	Column, colourless
$V = 1112.1$ (2) Å^3	$0.15 \times 0.10 \times 0.07$ mm

Data collection

Bruker APEX area-detector
  diffractometer
φ and ω scans
Absorption correction: multi-scan
  (*SADABS*; Sheldrick, 1996)
  $T_{min} = 0.570$, $T_{max} = 0.865$

6277 measured reflections
2467 independent reflections
2299 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.105$
$S = 1.08$
2467 reflections
154 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0649P)^2]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.58$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}
Absolute structure: Flack (1983),
  1164 Friedel pairs
Flack parameter: 0.04 (2)

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	2.015 (3)	Cu1—S1	2.269 (1)
Cu1—N3	2.029 (3)	Cu1—S1^i	2.483 (1)
N1—Cu1—N3	94.8 (1)	N3—Cu1—S1	124.0 (1)
N1—Cu1—S1	118.4 (1)	N3—Cu1—S1^i	102.4 (1)
N1—Cu1—S1^i	109.1 (1)	S1—Cu1—S1^i	106.6 (1)

Symmetry code: (i) $x, y - 1, z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2N···N4^{ii}	0.86	2.14	2.981 (5)	166

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

H atoms were placed in calculated positions [C—H = 0.93 Å and N—H = 0.86 Å; U_{iso}(H) = 1.2U_{eq}(C,N)], and were included in the refinement in the riding model approximation.

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.
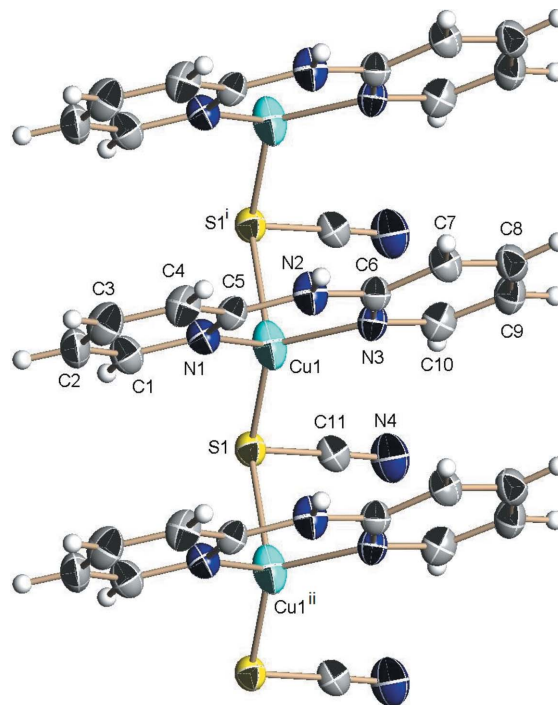
Figure 1
ORTEPII (Johnson, 1976) plot illustrating the coordination environment of Cu. Displacement ellipsoids are plotted at the 50% probability level, and H atoms as spheres of arbitrary radii. [Symmetry codes: (i) $x, \frac{3}{2} - y, z$; (ii) $x - \frac{1}{2}, y, \frac{3}{2} - z$.]

References

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