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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.030
 wR factor = 0.071
Data-to-parameter ratio = 14.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**catena-Poly[[bis(isothiocyanato- κ N)copper(II)]-bis(μ -1,1'-methylenedi-1*H*-imidazole- κ N³: κ N^{3'})]**

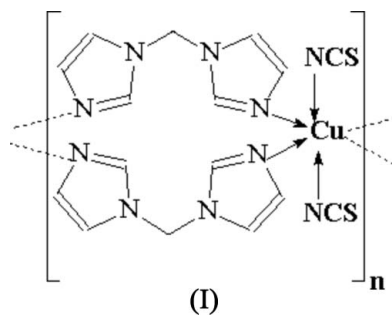
The title crystal structure, $[\text{Cu}(\text{NCS})_2(\text{C}_7\text{H}_8\text{N}_4)_2]_n$, comprises one-dimensional chains propagating in the a -axis direction. The Cu^{II} atoms, which have crystallographic $2/m$ site symmetry, are coordinated by six N atoms from four 1,1'-methylenedi-1*H*-imidazole ligands and two NCS^- anions, giving a slightly distorted octahedral coordination geometry. The 1,1'-methylenedi-1*H*-imidazole ligand adopts a bismonodentate bridging mode, linking the Cu^{II} atoms.

Received 1 February 2006

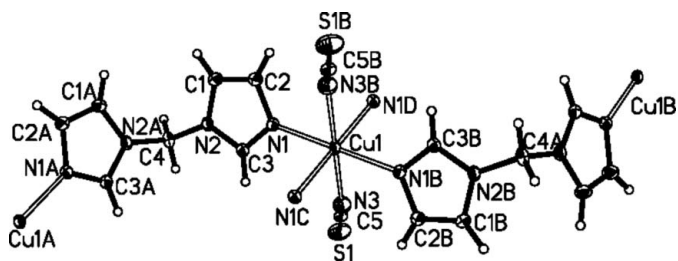
Accepted 9 February 2006

Comment

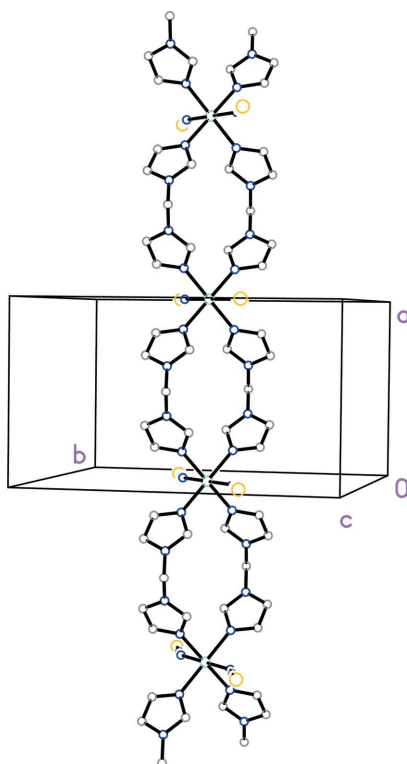
Copper complexes with imidazole ligands are of considerable interest as models for the active site of copper proteins such as haemocyanin, azurin and plastocyanin (Chen *et al.*, 1994; Kirchner & Krebs, 1987). Some metal complexes with alkyl-linked bisimidazole ligands have been used successfully to construct three-dimensional networks (Wu *et al.*, 1997; Ma *et al.*, 2004; Cui *et al.*, 2005). In order to further examine the structural features of copper complexes with this class of ligand, the crystal structure determination of the title compound, (I), was carried out.



The structure of (I) comprises a one-dimensional neutral double $[\text{Cu}(\text{NCS})_2(L)_2]$ chain [L is 1,1'-methylenedi-1*H*-imidazole]. Within a chain, the coordination geometry of each Cu^{II} atom is slightly distorted octahedral (Fig. 1 and Table 1). The Cu^{II} atom, lying on a position of site symmetry $2/m$, is six-coordinated by four N atoms from four symmetry-related L ligands, with a unique $\text{Cu}-\text{N}$ distance of 2.0440 (17) Å. The coordination is completed by two N atoms from two NCS^- anions. The NCS^- anions are *trans*-coordinated to the Cu^{II} atoms, occupying the axial positions with a unique $\text{Cu}-\text{N}$ distance of 2.425 (3) Å; this is elongated, most likely due to Jahn-Teller effects. The *cis*- $\text{N}-\text{Cu}-\text{N}$ bond angles deviate only slightly from ideal octahedral values (90°) ranging from 87.55 (9) to 92.45 (9)°. Each L ligand coordinates to two Cu^{II} atoms, acting as a bridging ligand, forming an extended one-dimensional chain structure (Fig. 2). The distance between the


Figure 1

Part of the structure of (I), showing the coordination environment of atom Cu1. Displacement ellipsoids are drawn at the 30% probability level. [symmetry codes: (A) $-x + 1, -y + 1, -z$; (B) $x, -y + 1, -z$; (C) $-x + 1, y, z$; (D) $-x, y, z$].


Figure 2

A view of the one-dimensional chain structure of (I). H atoms have been omitted for clarity.

closest Cu^{II} atoms within a chain is 8.877 (2) Å and the dihedral angle between the two imidazole planes in one L ligand is 71.5 (2)°.

Experimental

The ligand *L* was prepared according to the reported procedure (Schütze & Schubert, 1959). A mixture of Cu(NO₃)₂ (0.126 g, 1 mmol) and KSCN (0.196 g, 2 mmol) in water (30 ml) was stirred at room temperature for 30 min. *L* (0.296 g, 2 mmol) was added and the resulting solution was refluxed for 3 h. The blue precipitate that was obtained was filtered off, washed with water and dissolved in a minimum amount of aqueous ammonia (14 M). Blue single crystals were obtained by slow evaporation of the ammoniacal solution of the solid at room temperature over three days (68% yield based on Cu).

Analysis calculated for C₁₆H₁₆CuN₁₀S₂: C 40.37, H 3.39, N 29.42%; found: C 40.31, H 3.34, N 29.21%.

Crystal data

[Cu(NCS)₂(C₇H₈N₄)₂]
 $M_r = 476.05$
 Orthorhombic, *Cmca*
 $a = 8.877$ (3) Å
 $b = 15.602$ (6) Å
 $c = 14.170$ (4) Å
 $V = 1962.5$ (12) Å³
 $Z = 4$
 $D_x = 1.611$ Mg m⁻³

Mo Kα radiation
 Cell parameters from 932 reflections
 $\theta = 2.6$ – 26.2°
 $\mu = 1.35$ mm⁻¹
 $T = 293$ (2) K
 Block, blue
 0.20 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.774, T_{\max} = 0.813$
 5534 measured reflections

1082 independent reflections
 872 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.044$
 $\theta_{\text{max}} = 26.5^\circ$
 $h = -11 \rightarrow 10$
 $k = -19 \rightarrow 19$
 $l = -17 \rightarrow 14$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.071$
 $S = 1.05$
 1082 reflections
 74 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 0.5699P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.24$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.30$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cu1–N1 ⁱ	2.0440 (17)	N1–C3	1.313 (2)
Cu1–N3	2.425 (3)	N2–C1	1.375 (3)
S1–C5	1.638 (4)	N2–C4	1.455 (2)
N1 ⁱ –Cu1–N1 ⁱⁱ	92.45 (9)	N1 ⁱⁱⁱ –Cu1–N3	90.77 (7)
N1 ⁱ –Cu1–N1 ⁱⁱⁱ	87.55 (9)	C3–N1–C2	105.88 (16)
N1 ⁱⁱ –Cu1–N1 ⁱⁱⁱ	180.00 (8)	C3–N1–Cu1	126.34 (13)
N1 ⁱ –Cu1–N3	89.23 (7)	C5–N3–Cu1	154.8 (2)

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

H atoms were placed in calculated positions, with C–H = 0.93 or 0.97 Å, and included in the final cycles of refinement using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1999); software used to prepare material for publication: SHELXTL.

The authors thank Hebei Polytechnic University for supporting this work. JR acknowledges financial support from the Spanish Government (grant No. BQU2003/00539).

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