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catena-Poly[[(*N*,*N*-diethylethane-1,2-diamine)-thiocyanatocopper(II)]-*μ*-thiocyanato]

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The title compound, $[Cu(NCS)_2(C_6H_{16}N_2)]_n$, is a thiocyanate-bridged polynuclear copper(II) complex. The Cu^{II} atom is five-coordinate in a square-pyramidal geometry, with two N atoms of the *N*,*N*-diethylethane-1,2-diamine ligand and two N atoms from two thiocyanate ligands defining the basal plane, and one S atom of another thiocyanate ligand occupying the apical position. The $[Cu(NCS)_2(C_6H_{16}N_2)]$ units are linked by bridging thiocyanate ligands, forming chains running along the *a* axis.

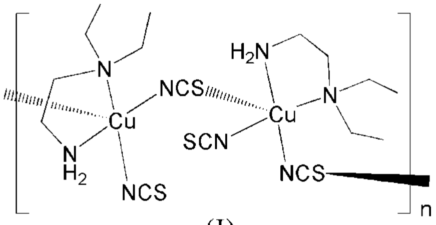
Key indicators

Single-crystal X-ray study
T = 298 K
Mean *σ*(C–C) = 0.004 Å
R factor = 0.025
wR factor = 0.057
Data-to-parameter ratio = 22.2

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

Comment

Thiocyanate groups play an important role in the formation of polynuclear complexes (Navarro *et al.*, 1997; Zurowska *et al.*, 2002; Dey *et al.*, 2004). Complexes derived from polyamine ligands are also very interesting, either for their structures or applications (Dapporto *et al.*, 2000; Lamarque *et al.*, 2001). Recently, a mononuclear zinc(II) complex derived from *N*,*N*-diethylethane-1,2-diamine was reported (Hong, 2007). As an extension of our work on the structural investigation of these complexes (Li & Wang, 2007), the title copper(II) complex, (I), is reported here.



(I)

Compound (I) is a thiocyanate-bridged polynuclear copper(II) complex (Fig. 1). The Cu atom is five-coordinate in a square-pyramidal geometry, with two N atoms of the *N*,*N*-diethylethane-1,2-diamine ligand and two N atoms from two thiocyanate ligands defining the basal plane, and one terminal S atom of another thiocyanate ligand occupying the apical position. The significant distortion of the square pyramid is revealed by the bond angles between the apical and basal atoms (Table 1). The apical bond is much longer than the basal bonds, indicating that the Cu—S bond is not very strong. The Cu—N bond lengths are comparable to those observed in a similar copper(II) complex (Wang, 2007).

In the crystal structure, the [(*N*,*N*-diethylethane-1,2-diamino)thiocyanato]copper(II) units are linked by bridging thiocyanate ligands, forming polymeric chains running along the *a* axis. The chains are further linked through N—H···S intermolecular hydrogen bonds (Table 2), forming a three-dimensional network (Fig. 2).

Experimental

A methanol solution (5 ml) of *N*,*N*-diethylethane-1,2-diamine (0.1 mmol, 11.2 mg) was added to a stirred aqueous solution (5 ml) of NH_4NCS (0.2 mmol, 15.2 mg) and $Cu(OAc)_2{\cdot}H_2O$ (0.1 mmol, 19.9 mg). After stirring for about 30 min, the deep-blue solution was filtered and the filtrate was left to stand undisturbed. Blue block-shaped crystals of (I) were formed by slow evaporation of the solvent after 3 d.

Crystal data

$[Cu(NCS)_2(C_6H_{16}N_2)]$	$V = 1339.1$ (2) Å^3
$M_r = 295.91$	$Z = 4$
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation
$a = 9.5219$ (9) Å	$\mu = 1.92$ mm^{-1}
$b = 9.9083$ (9) Å	$T = 298$ (2) K
$c = 14.1931$ (13) Å	0.33 × 0.31 × 0.27 mm

Data collection

Bruker SMART CCD area-detector diffractometer	8106 measured reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)	3064 independent reflections
$T_{min} = 0.542$, $T_{max} = 0.594$	2786 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$	$\Delta\rho_{max} = 0.26$ e Å^{-3}
$wR(F^2) = 0.057$	$\Delta\rho_{min} = -0.34$ e Å^{-3}
$S = 1.02$	Absolute structure: Flack (1983), 1295 Friedel pairs
3064 reflections	Flack parameter: 0.022 (11)
138 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—N3	1.940 (2)	Cu1—N2	2.090 (2)
Cu1—N1	1.974 (2)	Cu1—S2^i	2.8240 (7)
Cu1—N4	1.991 (2)		
N3—Cu1—N1	174.68 (8)	N4—Cu1—N2	149.56 (8)
N3—Cu1—N4	93.49 (8)	N1—Cu1—S2^i	85.21 (8)
N1—Cu1—N4	90.66 (8)	N2—Cu1—S2^i	107.90 (8)
N3—Cu1—N2	93.36 (8)	N3—Cu1—S2^i	90.70 (8)
N1—Cu1—N2	84.70 (7)	N4—Cu1—S2^i	101.64 (8)

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{3}{2}, -z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···S1^{ii}	0.90	2.55	3.396 (2)	156
N1—H1A···S1^{iii}	0.90	2.56	3.413 (2)	158

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

All H atoms were placed in idealized positions and constrained to ride on their parent atoms, with N—H = 0.90, C—H = 0.96–0.97 Å and $U_{iso}(H) = 1.2U_{eq}$(C,N) or $1.5U_{eq}$(methyl C).

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

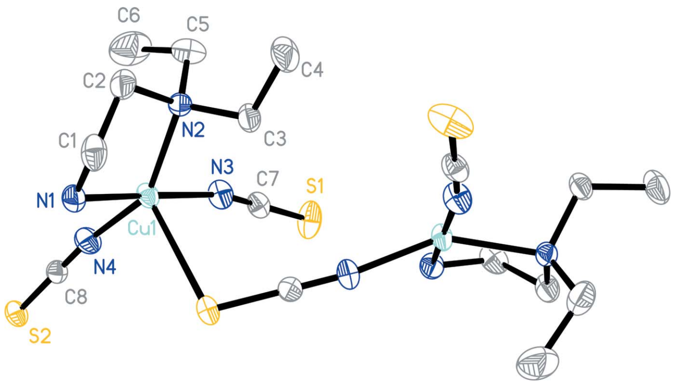


Figure 1
Part of the polymeric structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operation ($\frac{1}{2}+x, \frac{3}{2}-y, -z$).

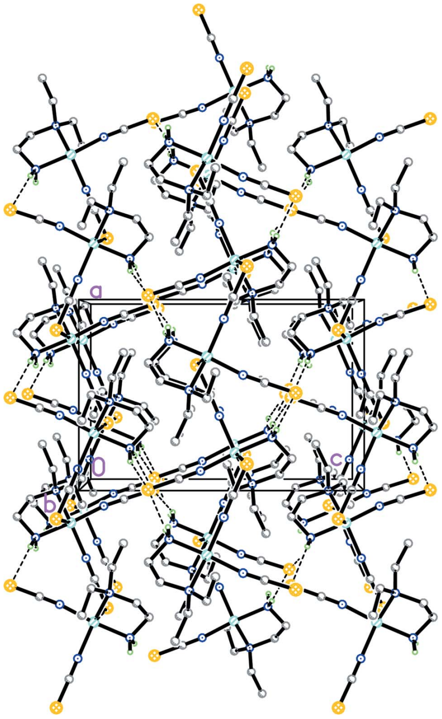


Figure 2
The crystal structure of (I), viewed along the *b* axis. Intermolecular N—H···S hydrogen bonds are shown as dashed lines.

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