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Bis(1-methyl-1*H*-imidazole-κN^3)dithiocyanato-copper(II)

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In the title compound, $[Cu(NCS)_2(C_4H_6N_2)_2]$, each Cu atom is located on an inversion center, in a distorted octahedral environment. The equatorial plane is occupied by four N atoms from two 1-methylimidazole ligands and two thiocyanate anions. Thiocyanate S atoms are weakly coordinated to Cu in the axial positions, linking the copper centers to form extended zigzag chains.

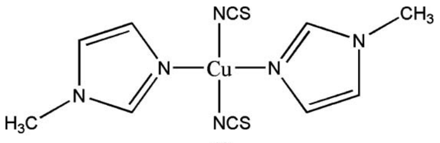
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.034
wR factor = 0.114
Data-to-parameter ratio = 17.7

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

Comment

Imidazole is of considerable interest as a ligand in many biological systems in which it provides a potential binding site for metal ions (Brooks & Davidson, 1960). Imidazole itself is a monodentate ligand and forms complexes with metal ions through its tertiary nitrogen atoms. It has been reported that a large number of imidazole derivatives possesses diverse pharmacological effects, including anti-inflammatory, anti-malarial and antitumor activities (Eilbeck *et al.*, 1967; Davis & Smith, 1971). Furthermore, the thiocyanate anion is a versatile inorganic ligand in the synthesis of coordinated compounds. Therefore, it appeared to be interesting to study the conditions of the formation of thiocyanate-containing copper(II) complexes with imidazole derivatives and to investigate the influence of steric properties on the stoichiometry as well as on the stoichiometry of the resulting species (Maslejova *et al.*, 1997). In this paper, we report the crystal structure of the title compound, (I).



(I)

In this structure, each Cu atom is located in a distorted octahedral environment. The equatorial plane is occupied by N atoms from the two 1-methylimidazole ligands and the two thiocyanate groups (Fig. 1). S atoms from the thiocyanate ligands are weakly coordinated to Cu in the axial positions, linking the copper centers to form extended zigzag chains (Fig. 2). The *trans* N—Cu—N angles are all 180° as required by symmetry, while the *cis* angles are 89.88 (10) and 90.12 (10)°, respectively. The Cu1—N2 bond length of 2.013 (2) Å and Cu1—N3 bond length of 1.963 (2) Å are comparable to Cu—N distances reported previously (Battaglia *et al.*, 1983; Li *et al.*, 2003). The Cu—S bond length of 3.221 (1) Å is shorter than the sum of van der Waals radii of Cu and S atoms (3.4 Å) and also comparable to the similar distances reported previously (Bie *et al.*, 2003; Carmen *et al.*, 1999).

Experimental

The title compound was prepared by the reaction of 1-methylimidazole (0.82 g, 10 mmol) with $CuCl_2{\cdot}2H_2O$ (0.85 g, 5 mmol) and potassium thiocyanate (0.98 g, 10 mmol) by means of hydrothermal synthesis in a stainless steel reactor with a Teflon liner at 383 K for 24 h. Elemental analysis calculated for title compound: C 34.92, H 3.52, N 24.44%; found: C 34.78, H 3.46, N 24.38%.

Crystal data

$[Cu(NCS)_2(C_4H_6N_2)_2]$
M_r = 343.95
Monoclinic, $P2_1/c$
a = 5.7200 (11) Å
b = 15.020 (3) Å
c = 8.4340 (17) Å
β = 91.46 (3)°
V = 724.4 (2) Å^3
Z = 2
D_x = 1.577 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 4–14°
μ = 1.79 mm^{-1}
T = 293 (2) K
Block, blue
0.35 × 0.25 × 0.25 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
1723 measured reflections
1573 independent reflections
1164 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.017
$\theta_{\rm max}$ = 27.0°
$h = 0 \rightarrow 7$
$k = 0 \rightarrow 19$
$l = -10 \rightarrow 10$
3 standard reflections every 100 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.114
S = 0.97
1573 reflections
89 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.08P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max}$ = 0.52 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.49 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C5—N3	1.154 (4)	N3—Cu1	1.963 (2)
C5—S1	1.624 (3)	Cu1—S1$^{\rm i}$	3.221 (1)
N2—Cu1	2.013 (2)		
N3—C5—S1	178.8 (3)	C5—N3—Cu1	167.8 (2)
C4—N2—Cu1	127.0 (2)	N3$^{\rm ii}$—Cu1—N2	90.12 (10)
C3—N2—Cu1	128.4 (2)	N3—Cu1—N2	89.88 (10)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4A···N3	0.93	2.52	2.959 (4)	109

H atoms were positioned geometrically and allowed to ride on their attached atoms, with C—H distances of 0.93–0.96 Å, and with $U_{\rm iso}({\rm H}) = 1.2–1.5U_{\rm eq}({\rm C})$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

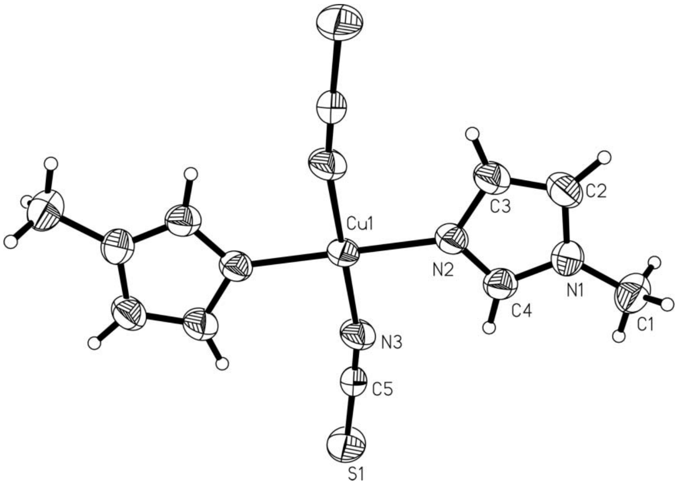


Figure 1
The structure of the title compound, showing 50% probability displacement ellipsoids for the non-H atoms and the atom-numbering scheme. [Symmetry code for unlabeled atoms: $1-x, 1-y, -z$.]

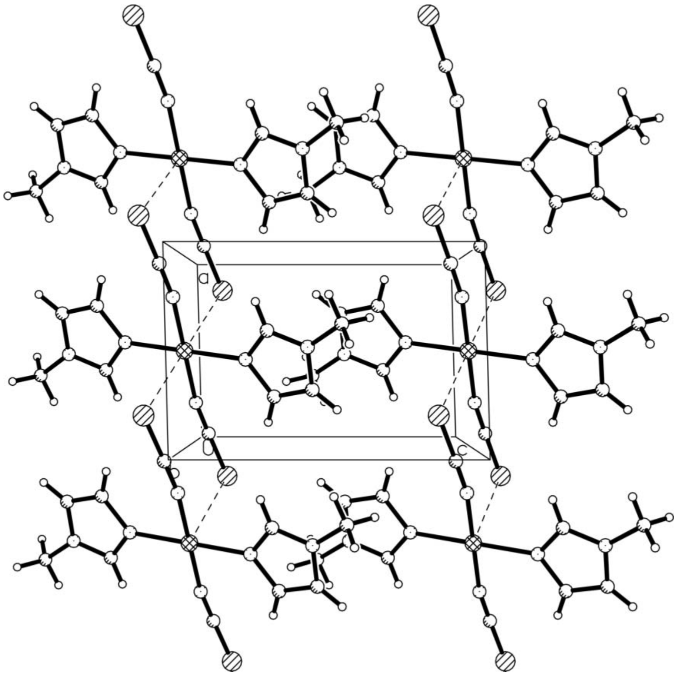


Figure 2
Packing diagram, down the b axis, of the title compound. Dashed lines indicate weak Cu···S axial coordination.

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