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Diisothiocyanatobis(1-vinyl-1*H*-imidazole-κN^3)-copper(II)

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Key indicators

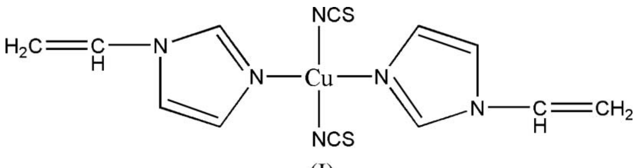
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.011 Å
R factor = 0.063
wR factor = 0.179
Data-to-parameter ratio = 16.1

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

In the title compound, $[Cu(NCS)_2(C_5H_6N_2)_2]$, each Cu atom is coordinated by two N atoms from two Eim (Eim = 1-vinyl-1*H*-imidazole) ligands and two N atoms from two isothiocyanate groups. The Cu atom adopts a square-planar geometry. The mean Cu—N(Eim) and Cu—N(NCS) distances are 1.960 (6) and 1.993 (6) Å, respectively.

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 N atoms. It has been reported that a large number of imidazole derivatives possess diverse pharmacological effects, including anti-inflammatory, antimalarial and antitumor activities (Eilbeck *et al.*, 1967; Davis & Smith, 1971). The isothiocyanato anion is a versatile inorganic ligand in the synthesis of coordination compounds. It was, therefore, of interest to study the conditions of formation of thiocyanate-containing copper(II) complexes with imidazole derivatives and to investigate the influence of steric properties on the stoichiometry of the resulting species (Maslejova *et al.*, 1997). The crystal structure of $[Cu(NCS)_2(C_4H_6N_2)_2]$ has been reported (Li *et al.*, 2006). In this paper, we report the crystal structure of the title compound, (I).



(I)

The coordination of the Cu atom is nearly square planar, with four N atoms, two from two Eim ligands and the other two from two monodentate thiocyanate groups, forming the CuN_4 chromophore. The N3—Cu1—N5 angle (Table 1) shows the largest deviation from the ideal square-planar value. The Cu—N bond lengths are in agreement with those observed in a similar structure (Li *et al.*, 2006). As expected, the two imidazole rings are planar and the angle between them is 62.00 (3)°. The NCS groups are almost linear, while a significant bending is displayed at the Cu—N—C—S linkage.

Experimental

The title compound was prepared by the reaction of 1-vinylimidazole (1.88 g, 20 mmol) with $CuCl_2\cdot 2H_2O$ (0.85 g, 5 mmol) and potassium thiocyanate (0.98 g, 10 mmol) by hydrothermal synthesis in a stainless-steel reactor with a Teflon liner at 383 K for 24 h. Single crystals suitable for X-ray diffraction measurements were obtained by recrystallization from methanol at room temperature.

Crystal data

$[Cu(NCS)_2(C_5H_6N_2)_2]$
$M_r = 367.97$
Orthorhombic, *Pbca*
$a = 9.849$ (2) Å
$b = 17.665$ (4) Å
$c = 18.044$ (4) Å
$V = 3139.3$ (12) Å^3
$Z = 8$
$D_x = 1.557$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.66$ 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
3073 measured reflections
3073 independent reflections
2038 reflections with $I > 2\sigma(I)$
$\theta_{max} = 26.0°$
3 standard reflections every 100 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.179$
$S = 1.01$
3073 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0993P)^2 + 2.7846P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.038$
$\Delta\rho_{max} = 0.89$ e Å^{-3}
$\Delta\rho_{min} = -0.67$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0061 (8)

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.960 (5)	S2—C2	1.617 (6)
Cu1—N2	1.959 (5)	N1—C1	1.148 (7)
Cu1—N3	1.987 (5)	N2—C2	1.157 (7)
Cu1—N5	1.998 (5)	C6—C7	1.300 (9)
S1—C1	1.624 (6)	C11—C12	1.177 (8)
N1—Cu1—N2	176.9 (2)	N3—Cu1—N5	173.3 (2)
N1—Cu1—N3	88.04 (19)	C1—N1—Cu1	163.0 (5)
N2—Cu1—N3	90.1 (2)	C2—N2—Cu1	163.9 (5)
N1—Cu1—N5	89.9 (2)	N1—C1—S1	178.8 (6)
N2—Cu1—N5	92.3 (2)	N2—C2—S2	178.0 (6)

H atoms were positioned geometrically and allowed to ride on their attached atoms, with C—H = 0.93–0.96 Å and $U_{iso}(H) = 1.2$ or 1.5 times $U_{eq}(C)$. There is some disorder that could not be resolved for atoms C11 and C12.

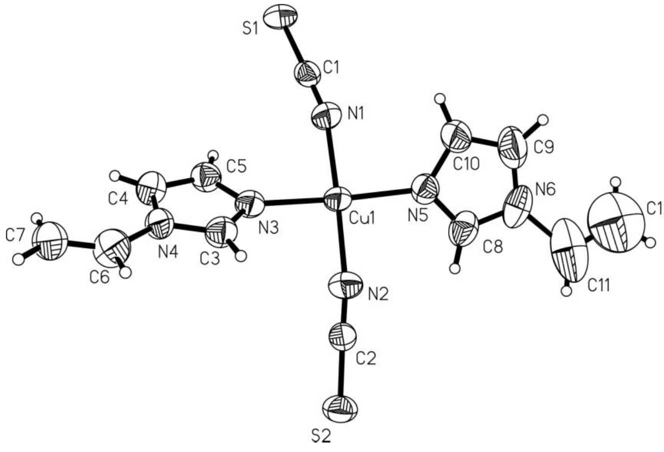


Figure 1
The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

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, 1997); 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).

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