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Diaquadithiocyanatocopper(II)

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(N–C) = 0.004 Å
R factor = 0.032
wR factor = 0.086
Data-to-parameter ratio = 14.5

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

The Cu atom in the title compound, $[Cu(NCS)_2(H_2O)_2]$, exists in a *trans*-N_2O_2Cu square-planar geometry and the molecule lies on a crystallographic mirror plane. A weak intermolecular Cu···S interaction of 3.0185 (2) Å is also observed.

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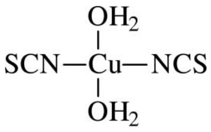
Comment

A number of copper(I)–thiocyanate complexes have been crystallographically characterized, as noted from the Cambridge Structural Database (Version 5.26; Allen, 2002). Cuprous thiocyanate exists in several forms (Smith & Saunders, 1981, 1982). Our interest in this compound comes from our studies on the related cupric thiocyanate analog, for which fewer complexes have been reported (Hou *et al.*, 2005), but the attempt to synthesize the cuprous compound yielded a cupric compound. Copper dithiocyanate exists as an aqua-coordinated compound, (I), in which the Cu atom shows a distorted octahedral geometry, with two long Cu···S interactions (Fig. 1). The water molecules participate in hydrogen-bonding interactions to give a three-dimensional network.



$$\begin{array}{c} OH_2 \\ | \\ SCN—Cu—NCS \\ | \\ OH_2 \end{array}$$

(I)

Experimental

The title compound was the oxidized product of the reaction of copper(I) nitride and ammonium thiocyanate (molar ratio 3:1) in water. The two solutions were placed in the two arms of a fritted U-tube; more water was added to equalize the hydrostatic pressures. Crystals deposited from the solution after 10 d.

Crystal data

$[Cu(NCS)_2(H_2O)_2]$
M_r = 215.73
Orthorhombic, *Pnma*
a = 13.962 (1) Å
b = 6.009 (1) Å
c = 8.877 (1) Å
V = 744.78 (9) Å^3
Z = 4
D_x = 1.924 Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 2400 reflections
θ = 2.7–28.0°
μ = 3.42 mm^{-1}
T = 295 (2) K
Column, blue
0.24 × 0.13 × 0.12 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.564, T_{max} = 0.684
4463 measured reflections

928 independent reflections
876 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 27.5°
$h = -16 \rightarrow 17$
$k = -7 \rightarrow 7$
$l = -10 \rightarrow 11$

doi:10.1107/S1600536805019215

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.086$
$S = 1.06$
928 reflections
64 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 0.2079P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.99$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.007 (1)

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.979 (3)	S1—C1	1.637 (3)
Cu1—N2	1.970 (3)	S2—C2	1.628 (3)
Cu1—O1	2.011 (3)	N1—C1	1.157 (4)
Cu1—O2	2.008 (3)	N2—C2	1.150 (4)
N1—Cu1—N2	179.3 (1)	O1—Cu1—O2	179.1 (1)
N1—Cu1—O1	90.9 (1)	C1—N1—Cu1	173.5 (3)
N1—Cu1—O2	90.0 (1)	C2—N2—Cu1	179.2 (3)
N2—Cu1—O1	89.8 (1)	N1—C1—S1	179.9 (3)
N2—Cu1—O2	89.3 (1)	N2—C2—S2	179.0 (3)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···S2^{i}	0.86 (1)	2.81 (2)	3.627 (2)	159 (3)
O2—H2···S2^{ii}	0.86 (1)	2.90 (1)	3.757 (2)	177 (3)

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

The H atoms were located in a difference Fourier map and were refined with distance restraints of O—H = 0.85 (1) Å and H···H = 1.39 (1) Å.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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*.

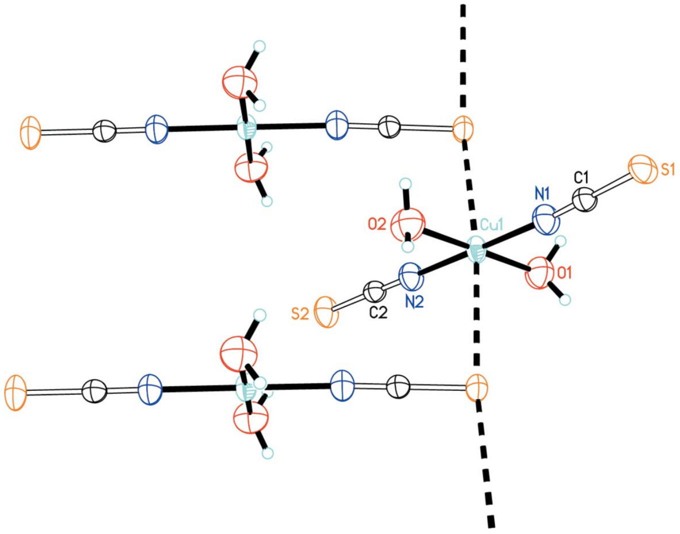


Figure 1
ORTEPII (Johnson, 1976) plot of (I). Probability ellipsoids are shown at the 50% probability level. The Cu1 atom is 3.0185 (2) Å from the symmetry-related S1 atom [at ($\frac{1}{2}-x, -y, z-\frac{1}{2}$) or ($\frac{1}{2}-x, 1-y, z-\frac{1}{2}$)]. The dashed line represents a weak Cu···S interaction.

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