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Bis(ethylenediamine-κ^2N,N')(thiosulfato-κS)-copper(II)

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Key indicators

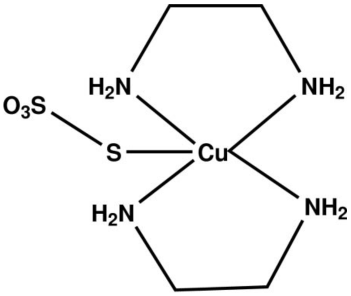
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.038
wR factor = 0.099
Data-to-parameter ratio = 14.9

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

The title complex, $[Cu(S_2O_3)(C_2H_8N_2)_2]$, exhibits a slightly distorted square-pyramidal geometry. The copper(II) atom is five-coordinated by four N atoms from two ethylenediamine molecules, and one S-atom from the thiosulfate anion. The crystal structure is stabilized by weak intermolecular Cu···S interactions and N—H···O hydrogen bonds.

Comment

The asymmetric unit of the title compound, (I), contains one monomeric five-coordinate cupric complex. The molecular structure of (I) is illustrated in Fig. 1 and selected bond distances and angles are given in Table 1. The Cu atom is coordinated by two ethylenediamine ligands *via* atoms N1, N2, N3 and N4 [Cu—N bond distances range from 2.016 (3) to 2.023 (3) Å], and one thiosulfate anion *via* atom S2 atom [Cu1—S2 = 2.8614 (13) Å]. Other bond lengths and angles are normal.



(I)

The complex exhibits a slightly distorted square-pyramidal geometry about the copper(II) atom, with the apical position occupied by atom S2 of the thiosulfate ligand. The Cu atom is displaced by 0.095 (1) Å from the basal plane defined by atoms N1, N2, N3 and N4. This situation is different from that in the similar compound aquadichloro(2,9-dimethyl-1,10-phenanthroline-κ^2N,N')copper(II) (Lemoine *et al.*, 2003), where the Cu atom is displaced by 0.3074 (6) Å out of the basal plane defined by atoms N, O and two Cl atoms. There the distance between the apical N atoms and the Cu atom is 2.230 (2) Å, compared to 2.8614 (13) Å in (I) for distance Cu1—S2.

The distance Cu1···S2^{i} (see Table 1 for symmetry code) is 3.2304 (14) Å, showing that there are weak intermolecular Cu···S interactions that link the molecules together (Fig. 2). All the ethylenediamine amino H atoms and the three thiosulfate O atoms participate in intra- and intermolecular N—H···O hydrogen bonds (Table 2 and Fig. 2). In this manner, the crystal structure is stabilized and a two-dimensional

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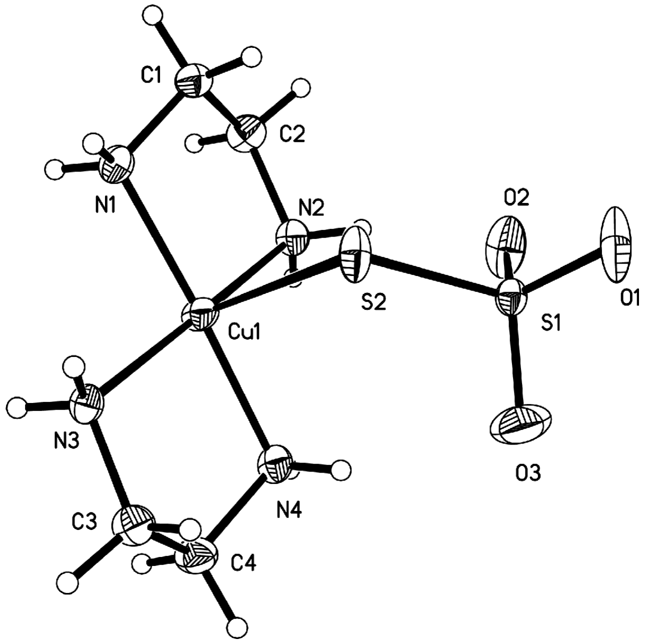

Figure 1
The structure of the title compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

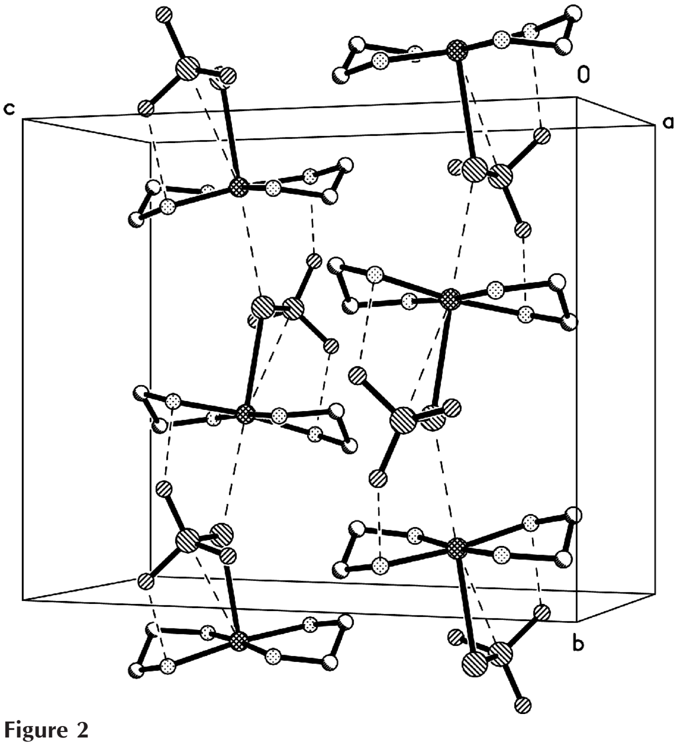

Figure 2
Crystal packing of (I), showing the weak intermolecular Cu···S interactions, and the N···O hydrogen-bonded interactions, as dashed lines. H atoms have been omitted for clarity.

hydrogen-bonded network is formed extending in the *ab* plane.

Experimental

The title compound was synthesized as follows: to a methanol solution of ethylenediamine (1.0 mmol) and $Na_2S_2O_3\cdot5H_2O$ (0.5 mmol) was added a methanol solution of $CuSO_4\cdot6H_2O$ (0.5 mmol), with stirring at reflux. The mixture was stirred continuously for 6 h, and then cooled and filtered. Slow evaporation of the solution give a blue crystalline compound (I). Crystals suitable for X-ray analysis were obtained by diffusion of diethyl ether into an acetonitrile solution of (I) over a period of six days.

Crystal data

$[Cu(S_2O_3)(C_2H_8N_2)_2]$
$M_r = 295.87$
Monoclinic, $P2_1/n$
$a = 6.613$ (2) Å
$b = 11.858$ (4) Å
$c = 13.936$ (5) Å
$\beta = 94.216$ (4)°
$V = 1089.8$ (6) Å^3
$Z = 4$
$D_x = 1.803$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1942 reflections
$\theta = 2.9$–$26.4°$
$\mu = 2.38$ mm^{-1}
$T = 293$ (2) K
Block, blue
0.29 × 0.17 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.535$, $T_{max} = 0.703$
5507 measured reflections
1893 independent reflections
1356 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 25.0°$
$h = -6 \rightarrow 7$
$k = -11 \rightarrow 14$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.099$
$S = 0.93$
1893 reflections
127 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0621P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.56$ e Å^{-3}
$\Delta\rho_{min} = -0.76$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—N4	2.016 (3)	Cu1—N2	2.023 (3)
Cu1—N1	2.017 (3)	Cu1—S2	2.8614 (13)
Cu1—N3	2.018 (3)	Cu1—S2^{i}	3.2304 (14)
N4—Cu1—N1	175.32 (11)	N3—Cu1—S2	91.24 (8)
N4—Cu1—N3	84.79 (11)	N2—Cu1—S2	94.89 (9)
N1—Cu1—N3	95.39 (11)	N4—Cu1—S2^{i}	88.98 (8)
N4—Cu1—N2	94.85 (11)	N1—Cu1—S2^{i}	86.37 (8)
N1—Cu1—N2	84.47 (11)	N3—Cu1—S2^{i}	86.07 (8)
N3—Cu1—N2	173.87 (11)	N2—Cu1—S2^{i}	87.80 (9)
N4—Cu1—S2	92.16 (8)	S2—Cu1—S2^{i}	176.975 (16)
N1—Cu1—S2	92.51 (8)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*B*···O2^{ii}	0.90	2.09	2.955 (4)	161
N2—H2*A*···O2	0.90	2.03	2.889 (4)	160
N2—H2*B*···O1^{iii}	0.90	2.46	3.164 (4)	135
N3—H3*B*···O1^{iv}	0.90	2.04	2.888 (4)	156
N4—H4*A*···O1^{iii}	0.90	2.00	2.840 (4)	155
N4—H4*B*···O3	0.90	2.33	3.201 (5)	163

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

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

References

Lemoine, P., Viossat B. & Daran, J.-C. (2003). *Acta Cryst.* E**59**, m17–m19.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1996). *SADABS.* University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL*97. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL.* Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT.* Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.