Acta Crystallographica Section E
**Structure Reports**
**Online**

ISSN 1600-5368

# Bis($\mu$-2-aminoethanesulfonato)-$\kappa^3N,O:O'$;$\kappa^3O':N,O$-bis[(bipyridine-$\kappa^2N,N'$)(perchlorato-$\kappa O$)copper(II)]

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Received 1 September 2004
Accepted 11 October 2004
Online 22 October 2004

The dimeric molecule of the hydrothermally synthesized binuclear complex [$Cu_2(C_2H_6NO_3S)_2(ClO_4)_2(C_{10}H_8N_2)_2$], a tauride complex, occupies a special position on an inversion centre. The Cu atom has a severely distorted octahedral coordination, with four short and two substantially longer bonds. The four short bonds involve two bipyridine and one taurine N atoms [$Cu—N_{bipyridine}$ = 1.990 (3) and 2.025 (3) Å, $Cu—N_{taurine}$ = 1.992 (3) Å] as well as one of the taurine O atoms [Cu—O = 1.964 (3) Å]. The second taurine O atom belonging to the second bridging molecule forms a much longer Cu—O bond [2.363 (4) Å], and the perchlorate O atom participates in the longest Cu—O bond [2.675 (3) Å]. The molecules are linked *via* N—H···O bonds into infinite chains running along the *a* axis of the crystal structure.

**Key indicators**

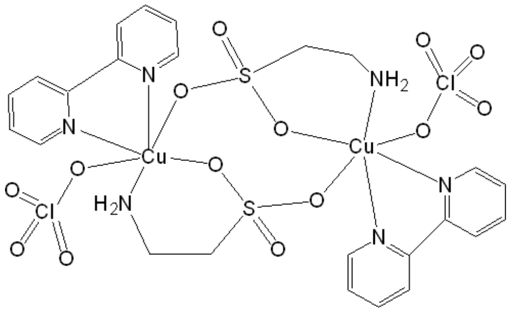
Single-crystal X-ray study
*T* = 293 K
Mean σ(C–C) = 0.006 Å
*R* factor = 0.038
*wR* factor = 0.166
Data-to-parameter ratio = 15.9

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

## Comment

Copper is especially important in the nervous system of higher eukaryotes, appearing in proteins responsible for the biogenesis of both catecholamine and peptidic hormones (Kinman, 1996). Metal β-alaninesulfonates, also known as taurides, are of substantial interest because of their applications in medicine and biochemistry (Bottari & Festa, 1996; Bottari & Festa, 1998).

The title compound, (I), is a copper complex with two metal atoms bridged by two chelate bridging tauride ligands (Fig. 1). The molecule of the complex occupies a special position on a crystallographic inversion centre, which coincides with the centre of the eight-membered $Cu_2S_2O_4$ ring formed by the atoms of two bridging ligands and the Cu atoms; the distance between the two Cu atoms is 4.868 (12) Å. A similar eight-membered cycle was reported earlier in the copper complex [$Cu(C_9H_9NSO_4)(H_2O)$]$_2$ ($C_9H_9NSO_4$ = taurine salicylic Schiff base; Jiang & Zhang, 2003).



(I)

Atom Cu1 has a distorted octahedral coordination, formed by atom O4 of the perchlorate anion, atoms N1 and N2 of the

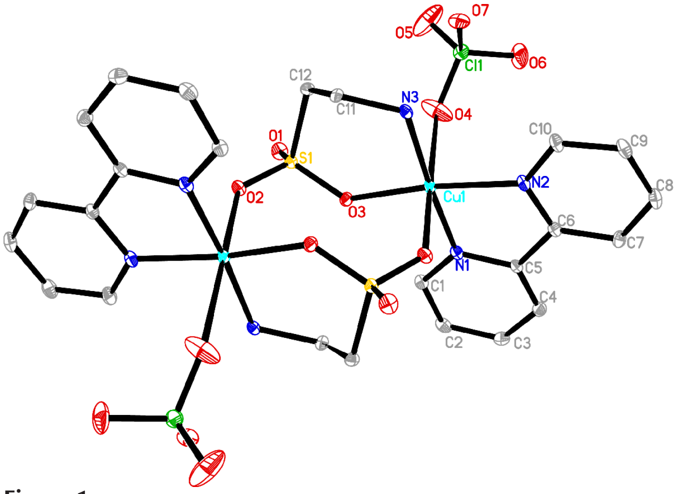


**Figure 1**
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level; H atoms have been omitted. Unlabelled atoms are related to labelled atoms by $-x, 1-y, 1-z$.

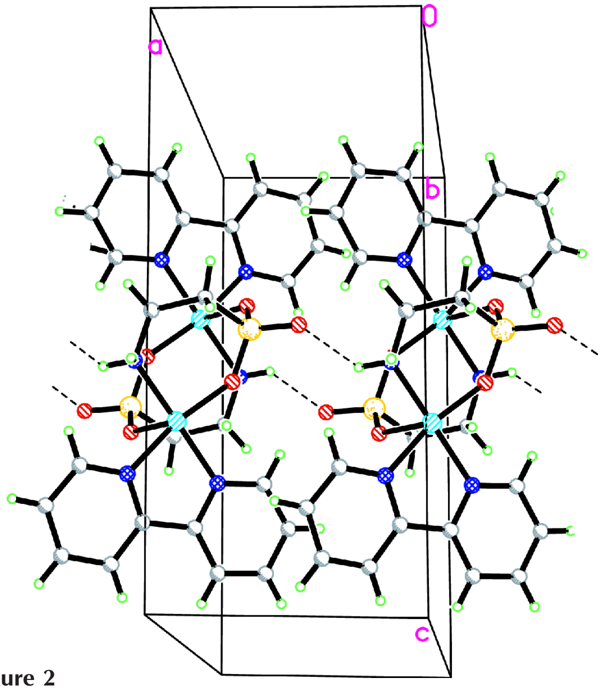


**Figure 2**
A fragment of the crystal structure of (I), showing a polymeric hydrogen-bonded chain (dashed lines) of Cu complexes running along the *a* axis.

chelate 2,2′-bipyridine ligand and atoms O3 and N3 of one of the bridging taurides, as well as atom O2$^i$ [symmetry code: (i) $-x, 1-y, 1-z$] of the second bridging tauride ligand. The Cu1 coordination shows a typical tetragonal distortion, with four short 'equatorial' coordination bonds involving both N atoms of the bipyridine ligand [Cu1—N1 = 1.990 (3) Å and Cu1—N2 = 2.025 (3) Å] and the chelating Cu1—N3 [1.992 (3) Å] and Cu1—O3 [1.964 (3) Å] bonds with one of the bridging taurides. The 'axial' Cu1—O2$^i$ and Cu1—O4 bonds involving the second bridging tauride and the perchlorate ligand, respectively, are considerably longer [2.363 (3) and 2.675 (3) Å]; the O4—Cu1—O2$^i$ angle formed by the long 'axial' bonds is 175.97 (12)°.

In the structure of the title compound there are two symmetry-independent 'active' H atoms; both of them belong to the $NH_2$ group of the tauride ligand (at atom N3). Atom H2N3 forms an intramolecular hydrogen bond with sulfonate atom O7. Atom H1N3 participates in an intermolecular hydrogen bond with atom O1$^{ii}$ [symmetry code (ii): $x+1, y, z$]. The latter hydrogen bond is responsible for the formation of infinite chains of molecules of the complex running along the *a* axis of the crystal structure (Fig. 2 and Table 2).

## Experimental

A solution of taurine (1.0 mmol) and NaOH (1.0 mmol) in anhydrous methanol (10 ml) was added slowly to a solution of $CuClO_4 \cdot 6H_2O$ (1.0 mmol) in anhydrous methanol (10 ml). After stirring for 10 min, bipyridine (1.0 mmol), dissolved in methanol (5 ml) and $H_2O$ (5 ml), was added slowly to the mixture. It was then dropped into a 25 ml Teflon-lined stainless steel reactor and heated at 383 K for four days. Thereafter, the reactor was slowly cooled to room temperature and blue prism-shaped crystals suitable for X-ray diffraction were collected.

### *Crystal data*

$[Cu_2(C_2H_6NO_3S)_2(ClO_4)_2(C_{10}H_8N_2)_2]$
$M_r = 886.65$
Monoclinic, $P2_1/c$
$a = 6.741$ (3) Å
$b = 15.58$ (3) Å
$c = 15.126$ (6) Å
$\beta = 91.401$ (12)°
$V = 1588$ (3) Å$^3$
$Z = 2$
$D_x = 1.855$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 105 reflections
$\theta = 1.9$–27.5°
$\mu = 1.72$ mm$^{-1}$
$T = 293$ (2) K
Prism, blue
0.34 × 0.10 × 0.05 mm

### *Data collection*

Siemens *P*4 diffractometer
$\omega$ scans
Absorption correction: multi-scan (*XPREP* in *SHELXTL*; Siemens, 1994)
$T_{min} = 0.814$, $T_{max} = 0.918$
12 077 measured reflections
3601 independent reflections
3102 reflections with $I > 2\sigma(I)$
$R_{int} = 0.031$
$\theta_{max} = 27.5°$
$h = -7 \rightarrow 8$
$k = -20 \rightarrow 20$
$l = -19 \rightarrow 19$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.166$
$S = 1.13$
3601 reflections
226 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1151P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.78$ e Å$^{-3}$
$\Delta\rho_{min} = -0.86$ e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cu1—O2$^i$ | 2.363 (3) | Cu1—N1 | 1.990 (3) |
| Cu1—O3 | 1.964 (3) | Cu1—N2 | 2.025 (3) |
| Cu1—O4 | 2.675 (3) | Cu1—N3 | 1.992 (3) |
| | | | |
| O3—Cu1—N1 | 88.58 (12) | O3—Cu1—O2$^i$ | 98.37 (12) |
| O3—Cu1—N3 | 93.95 (12) | O4—Cu1—O2$^i$ | 175.97 (12) |
| N1—Cu1—N3 | 175.65 (12) | N1—Cu1—O2$^i$ | 93.45 (12) |
| O3—Cu1—N2 | 169.53 (12) | N3—Cu1—O2$^i$ | 89.69 (13) |
| N1—Cu1—N2 | 81.21 (13) | N2—Cu1—O2$^i$ | 84.68 (12) |
| N3—Cu1—N2 | 96.09 (13) | | |

Symmetry code: (i) $-x, 1-y, 1-z$.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H1N3···O1$^{ii}$ | 0.90 | 2.15 | 2.872 (7) | 137 |
| N3—H2N3···O7 | 0.90 | 2.16 | 3.009 (7) | 157 |

Symmetry code: (ii) $1 + x, y, z$.

H atoms were positioned geometrically (C—H = 0.93–0.97 Å and N—H = 0.90 Å) and included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}$(carrier atom).

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Siemens, 1994); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was supported by the Natural Science Foundation of the Guangxi Chuang Autonomous Region of the People's Republic of China (grant No. 0339034) and the Science Research Foundation of Guangxi Universities of the People's Republic of China.

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