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Key indicators

Single-crystal X-ray study
 T = 293 K
 Mean $\sigma(C-C)$ = 0.004 Å
 Disorder in main residue
 R factor = 0.047
 wR factor = 0.099
 Data-to-parameter ratio = 15.3

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

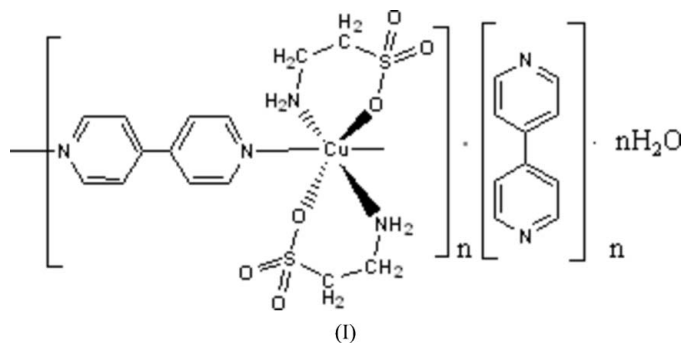
catena-Poly[[[bis(2-aminoethanesulfonato- κ^2N,O)-copper(II)]- μ -4,4'-bipyridine- $\kappa^2N:N'$] 4,4'-bipyridine monohydrate]

The title compound, $\{[Cu(C_2H_6NO_3S)_2(C_{10}H_8N_2)] \cdot C_{10}H_8N_2 \cdot nH_2O\}_n$, was obtained by the hydrothermal reaction of $Cu(CH_3COO)_2 \cdot 2H_2O$, 4,4'-bipyridine and taurine at 380 K. The 4,4'-bipyridine ligands bridge Cu^{II} ions, forming polymeric chains, in which Cu^{II} ions and the bridging ligands lie on twofold axes. Two taurine anions chelate to the Cu^{II} ion by the terminal N and O atoms, completing the distorted octahedral coordination. The uncoordinated bipyridine molecule is located on an inversion center.

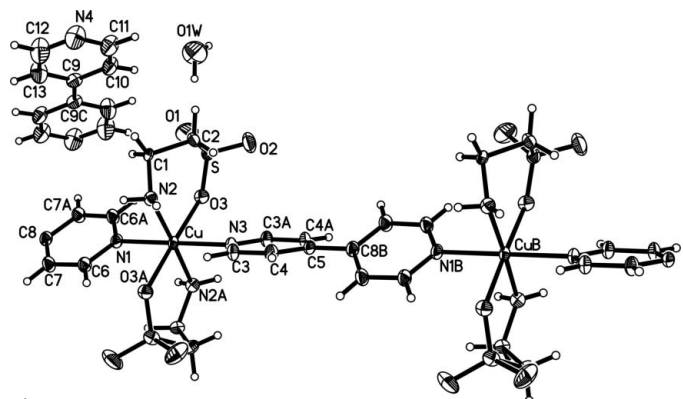
Received 7 November 2005
 Accepted 6 December 2005
 Online 10 December 2005

Comment

Several Schiff bases derived from taurine have recently been prepared in our laboratory (Zhang & Jiang, 2002; Zeng *et al.*, 2003; Jiang *et al.*, 2004) because of the important physiological properties of taurine. As part of our ongoing investigation on taurine derivatives, we report here the synthesis and crystal structure of the title taurine-copper(II) complex, (I).



The crystal structure of (I) consists of one-dimensional complex chains, uncoordinated 4,4-bipyridine (bipy) and water molecules. The bipy ligands bridge neighboring Cu^{II} ions, forming infinite polymeric chains along the crystal-



lographic b axis (Fig. 1). The Cu^{II} ions and bridging ligands lie on twofold axes. Two taurine anions chelate to the Cu^{II} ion by terminal N and O atoms to complete the distorted octahedral coordination. The longer Cu—O3 bond distance (Table 1) shows the typical Jahn–Teller distortion effect for the Cu^{II} ion. Within the bridging bipy ligand, the two pyridine rings are twisted with respect to each other; the dihedral angle is $53.11(4)^\circ$.

The uncoordinated bipy is located on an inversion center and displays a planar configuration. Weak C—H \cdots O hydrogen bonding occurs between the bipy and the water molecules. Classical O—H \cdots O hydrogen bonding is also observed between the water and the complex chain (Table 2).

Experimental

A methanol solution (10 ml) of taurine (1.5 mmol) and KOH (1.5 mmol) was mixed with another methanol solution (10 ml) of $\text{Cu}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ (0.5 mmol). After stirring for 10 min, 4,4'-bipyridine (1 mmol) was added slowly to the mixture, which was then dropped into a 25 ml Teflon-stainless steel reactor and heated at 380 K for 5 d. After cooling the reactor to room temperature, single crystals of (I) were obtained (yield 65%). Analysis found (%): C 44.87, H 4.66, N 13.05, S 9.98; calculated (%): C 44.84, H 4.67, N 13.08, S 9.97. IR (KBr, cm^{-1}): ν 1033.3, 1168.1, 1237.4 (— SO_3), 3258.4, 3304.3 (N—H).

Crystal data

$[\text{Cu}(\text{C}_2\text{H}_6\text{NO}_3\text{S})_2(\text{C}_{10}\text{H}_8\text{N}_2)] \cdot$ $\text{C}_{10}\text{H}_8\text{N}_2 \cdot \text{H}_2\text{O}$	$D_x = 1.537 \text{ Mg m}^{-3}$
$M_r = 642.2$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 2887 reflections
$a = 9.8647(11) \text{ \AA}$	$\theta = 3.3\text{--}27.5^\circ$
$b = 11.3846(9) \text{ \AA}$	$\mu = 0.99 \text{ mm}^{-1}$
$c = 12.9516(14) \text{ \AA}$	$T = 293(2) \text{ K}$
$\beta = 107.446(5)^\circ$	Prism, blue
$V = 1387.6(2) \text{ \AA}^3$	$0.25 \times 0.20 \times 0.15 \text{ mm}$
$Z = 2$	

Data collection

Rigaku Mercury CCD diffractometer	3176 independent reflections
φ and ω scans	2681 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.039$
$T_{\text{min}} = 0.775$, $T_{\text{max}} = 0.860$	$\theta_{\text{max}} = 27.5^\circ$
10598 measured reflections	$h = -11 \rightarrow 12$
	$k = -14 \rightarrow 14$
	$l = -16 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.031P)^2 + 1.3917P]$
$R[F^2 > 2\sigma(F^2)] = 0.047$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.099$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.08$	$\Delta\rho_{\text{max}} = 0.42 \text{ e \AA}^{-3}$
3176 reflections	$\Delta\rho_{\text{min}} = -0.40 \text{ e \AA}^{-3}$
208 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (\AA , $^\circ$).

Cu—N1	2.166 (3)	Cu—N3	2.127 (3)
Cu—N2	1.990 (2)	Cu—O3	2.3067 (19)
N2—Cu—N2 ⁱ	177.17 (13)	N2—Cu—N3	91.42 (6)

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

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
O1W—H1C \cdots O1	0.88	1.96	2.827 (8)	169
O1W—H1D \cdots O1 ⁱⁱ	0.92	1.81	2.693 (7)	159
N2—H2A \cdots O2 ⁱⁱⁱ	0.88	2.20	2.971 (3)	145
N2—H2B \cdots N4 ^{iv}	0.85	2.21	3.021 (4)	160

Symmetry codes: (ii) $-x + 1, y, -z + \frac{3}{2}$; (iii) $x, -y + 1, z - \frac{1}{2}$; (iv) $-x + 1, y, -z + \frac{1}{2}$.

The methylene group of aminomethylenesulfonate is disordered over two sites with 0.5 site-occupancy factors. The water molecule is located close to the twofold axis and has a 0.5 site-occupancy factor. H atoms on N and O atoms were located in a difference Fourier map and refined as riding in their as-found relative positions, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$. Other H atoms were placed in calculated positions, with C—H = 0.93 (aromatic) or 0.97 \AA (methylene), and refined using a riding-model approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *CrystalClear* (Rigaku, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Natural Science Foundation of Guangxi Chuang Autonomous Region of China (grant No. 0339034) and the Science Research Foundation of Guangxi University.

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