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A new one-dimensional coordination polymer: $\{[Cu(C_{10}H_9NO_5S)(H_2O)]\cdot H_2O\}_n$

Ju-Lan Zeng,[a]* Yi-Min Jiang[a] and Kai-Bei Yu[b]

[a]College of Chemistry and Chemical Engineering, Guangxi Normal University, Guilin, Guangxi 541004, People's Republic of China, and [b]Analysis and Test Center, Chinese Academy of Sciences, Chengdu, Sichuan 610041, People's Republic of China

Correspondence e-mail: julan_zeng@163.com

Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.004 Å
R factor = 0.029
wR factor = 0.073
Data-to-parameter ratio = 11.9

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

The title compound, *catena*-poly[[copper(II)-μ-2-{[(*E*)-(5-formyl-2-oxidophenyl)methylidene]amino}-1-ethanesulfonato(2−)] monohydrate], $\{[Cu(L)(H_2O)]\cdot H_2O\}_n$, where H_2L = 2-{[(*E*)-(5-formyl-2-hydroxyphenyl)methylidene]amino}-1-ethanesulfonic acid ($C_{10}H_{11}NO_5S$), was synthesized in water–methanol solution and the crystal structure determined by X-ray diffraction analysis. The Cu atom is five-coordinate, forming a distorted square-pyramidal geometry. This geometry includes a weak bond between the Cu atom and the O atom of the formyl group of another ligand, giving a one-dimensional infinite chain structure. The structure is further stabilized by intermolecular hydrogen bonds.

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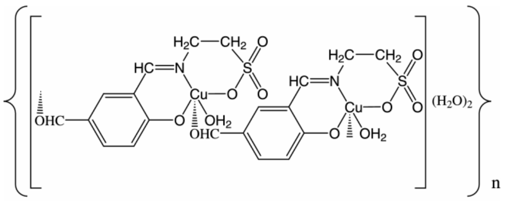
Comment

5-Formylsalicylaldehyde is an important organic synthetic intermediate that can be used to synthesize macrocyclic complexes (Badri *et al.*, 1990) and photochromic compounds of spiropyrans (Sharmila & Bhaskar, 1996). Studies of Schiff base complexes containing sulfur and complexes of amino acid Schiff bases (Casella & Gullotti, 1981; Wang *et al.*, 1994; Casella & Gullotti, 1986) have aroused more and more interest because of their antiviral, anticancer and antibacterial activities. Recently, Zhang & Jiang (2002) have reported a Schiff base complex derived from taurine, an amino acid containing sulfur. We report here the synthesis and crystal structure of a new Schiff base copper(II) complex, (I), prepared by the reaction of $CuSO_4\cdot 5H_2O$ and the potassium salt of the Schiff base ligand 2-{[(*E*)-(2-hydroxy-5{[(2-sulfoethyl)imino]methyl}phenyl)methylidene]amino}-1-ethanesulfonic acid, derived in turn from the reaction of taurine and 5-formylsalicylaldehyde.



(I)

As shown in Figs. 1 and 2, the one-dimensional infinite chain of the title compound, (I), is assembled from $[Cu(C_{10}H_9NO_5S)(H_2O)]\cdot H_2O$ units, in which the Cu atom is five-coordinate with two O atoms and one N atom of the tridentate ligand L, one O atom of the coordinated water and one O atom of the formyl group belonging to the ligand on an adjacent unit [symmetry code: (i) $1 + x, y, z$], giving a distorted square-pyramidal geometry. The plane O1/N/O4/O6 is the base of the pyramid, while $O5^i$ is the apex. The distance from

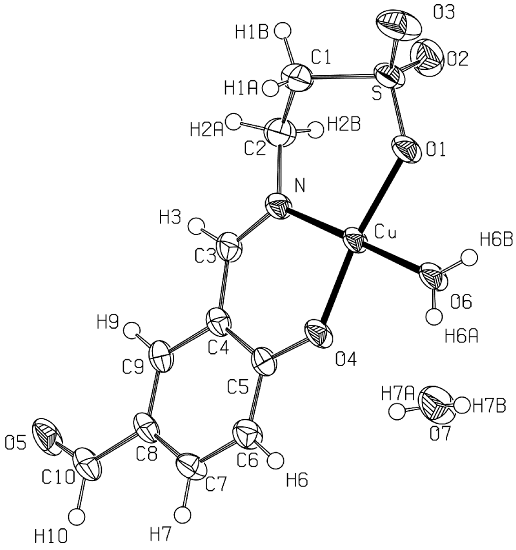


Figure 1
View of the asymmetric unit of the title compound, with displacement ellipsoids drawn at the 50% probability level.

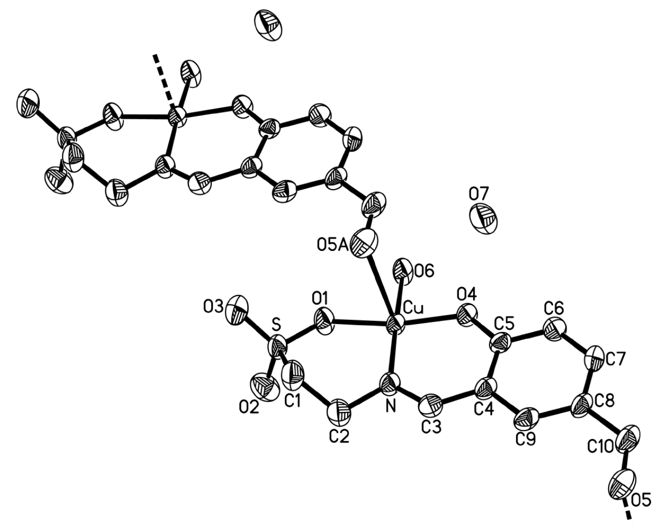


Figure 2
View of the interactions between adjacent molecules. H atoms have been omitted for clarity.

Cu to the least-squares plane O1/N/O4/O6 is 0.0133 (1) Å. The length of the bond Cu—O5^{i}, which links the structural units to form a one-dimensional infinite chain structure, is 2.877 (3) Å. This bond is much longer than a normal coordinate bond length, so can be called a partly coordinated bond (Procter *et al.*, 1968). The Cu atom forms two six-membered chelate rings with the ligand. The bond length of Cu—O4 [1.8786 (18) Å] is the shortest coordinate bond in (I), while Cu—O1 is 1.9526 (18) Å, indicating that the sulfonate group can coordinate to the metal ion in competition with water molecules.

There are a number of hydrogen bonds in (I). The hydrogen bond involving the coordinated and uncoordinated water molecules is O6—H6*A*···O7. The polymer chains are linked by four intermolecular hydrogen bonds (Table 2) O6—H6*B*···O5^{i}, O7—H7*A*···O2^{ii}, O7—H7*B*···O3^{iii} and C10—H10···O1^{iv} (symmetry codes as in Table 2) to form a three-dimensional structure. This is why, despite the weakness of the Cu—O5^{i} bond, the polymer is stable.

Fig. 1 also shows that there is only one imine group in the complex. This is because, in the case of the imine *ortho* to the hydroxyl, the imino-N, hydroxy-O and Cu can form a six-membered chelate ring that can stabilize the imine, while the other imine has no such effect; as a result, the C═N double bond is broken down by attack of water molecules.

Experimental

A solution of 2.0 mmol of taurine and 2.0 mmol of KOH in 10 ml anhydrous methanol was dropped into a solution of 1.0 mmol of 5-formylsalicylaldehyde in 10 ml anhydrous methanol. The mixture was stirred and refluxed at 323 K for 2 h, and then was cooled to room temperature to give a yellow precipitate, which was collected by filtration, recrystallized from anhydrous methanol, washed successively with anhydrous methanol and ether, and dried *in vacuo* to yield 0.36 g of a yellow product. Analysis, found (%): C 32.85, H 3.12, N 6.27; $C_{12}H_{14}K_2N_2O_7S_2$ requires (%): C 32.73, H 3.18, N 6.36. IR (KBr, ν cm^{-1}): 1048.8, 1152.4, 1197.2 (ν SO$_3$), 1636.2 (ν C═N), 3442.3 (ν O—H). 1.0 mmol of the ligand, the potassium salt of 2-{[(*E*)-(2-hydroxy-5{[(2-sulfoethyl)imino]methyl}phenyl)methylidene]amino}-1-ethanesulfonic acid, was dissolved in 25 ml of aqueous methanol. To this solution, 1.0 mmol of $CuSO_4\cdot5H_2O$ was added, and the mixture was stirred and refluxed at 323 K for 6 h, then cooled to room temperature. After filtration, the filtrate was left to stand at room temperature. Dark-green crystals suitable for X-ray diffraction were obtained in a yield of 43%. Analysis, found (%): C 33.73, H 3.61, N 4.07; $C_{10}H_{13}CuNO_7S$ requires (%): C 33.82, H 3.66, N 3.95%. IR (KBr, ν cm^{-1}): 1039.5, 1129.8, 1156.1, 1182.8 (ν SO$_3$), 1619.52 (ν C═N), 3433.5 (ν O—H).

Crystal data

$[Cu(C_{10}H_{11}NO_5S)(H_2O)]\cdot H_2O$
$M_r = 354.81$
Monoclinic, $P2_1/c$
$a = 8.589$ (2) Å
$b = 17.585$ (2) Å
$c = 9.479$ (2) Å
$\beta = 115.69$ (1)°
$V = 1290.1$ (4) Å^3
$Z = 4$

$D_x = 1.827$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 33 reflections
$\theta = 3.5$–15.3°
$\mu = 1.89$ mm^{-1}
$T = 291$ (2) K
Plate, green
0.58 × 0.46 × 0.20 mm

Data collection

Siemens *P*4 diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.405$, $T_{\max} = 0.686$
2761 measured reflections
2409 independent reflections
1963 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.014$
$\theta_{\max} = 25.5°$
$h = 0 \rightarrow 10$
$k = 0 \rightarrow 21$
$l = -11 \rightarrow 10$
3 standard reflections
every 97 reflections
intensity decay: 5.2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.073$
$S = 1.04$
2409 reflections
202 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0403P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.34$ e Å^{-3}
$\Delta\rho_{\min} = -0.26$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0077 (7)

Table 1
Selected geometric parameters (Å, °).

Cu—O4	1.8786 (18)	Cu—N	1.960 (2)
Cu—O6	1.9346 (19)	Cu—O5^{i}	2.877 (3)
Cu—O1	1.9526 (18)		
O4—Cu—O6	84.54 (8)	O1—Cu—N	96.72 (8)
O4—Cu—O1	168.50 (8)	O4—Cu—O5^{i}	94.80 (8)
O6—Cu—O1	84.18 (8)	O6—Cu—O5^{i}	87.34 (8)
O4—Cu—N	94.68 (8)	O1—Cu—O5^{i}	82.43 (8)
O6—Cu—N	176.48 (10)	N—Cu—O5^{i}	96.16 (8)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O6—H6A···O7	0.813 (10)	1.842 (11)	2.654 (3)	177 (3)
O6—H6B···O5^{ii}	0.808 (10)	1.905 (11)	2.713 (3)	178 (3)
O7—H7A···O2^{iii}	0.820 (10)	2.078 (17)	2.866 (4)	161 (4)
O7—H7B···O3^{iv}	0.813 (10)	1.99 (2)	2.768 (3)	159 (6)
C10—H10···O1^{v}	1.02 (3)	2.58 (3)	3.417 (3)	139 (2)

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

The H atoms on O6, O7 and C10 were located in a difference Fourier map and their positions and isotropic displacement parameters were refined, with the O—H distance restrained to 0.82 Å; the C10—H10 refined distance is 1.02 (3) Å. All other H atoms were positioned geometrically and were treated as riding atoms, with C—H distances of 0.93—0.97 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C).

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*.

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