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Key indicators

Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
R factor = 0.027
wR factor = 0.075
Data-to-parameter ratio = 11.4

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

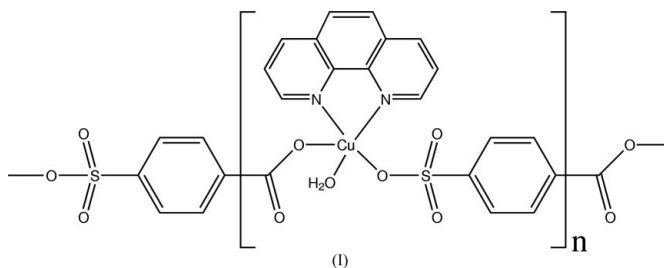
Poly[[aqua(1,10-phenanthroline- κ^2N,N')-copper(II)]- μ -4-sulfonatobenzoato- $\kappa^2O^4:O^1$]

The title compound, $[\text{Cu}(\text{C}_7\text{H}_4\text{O}_5\text{S})(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]_n$, a polymeric copper(II) complex, was obtained by the reaction of $\text{Cu}(\text{NO}_3)_2$ with potassium hydrogen 4-sulfobenzoate and 1,10-phenanthroline under hydrothermal condition. Each Cu^{II} atom displays a square-pyramidal geometry defined by three O atoms from one water molecule and two 4-sulfonatobenzoate ligands and two N atoms from one 1,10-phenanthroline ligand. The polymeric chains are linked into ladders by $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds.

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Comment

In the past decade, numerous 1,4-benzenedicarboxylate (bdc) complexes have been extensively studied due to their potential applications as functional materials (Yaghi *et al.*, 2003; Ohmura *et al.*, 2003; Chisholm, 2003). However, complexes with 4-sulfobenzoate (sb), a ligand with a combination of sulfonate and carboxyl groups, remain few (Yuan *et al.*, 2001; Xiong *et al.*, 2001). The sulfonate group could exhibit very different coordination behavior compared to the carboxyl group (Zheng *et al.*, 2003; Wang *et al.*, 2004; Starynowicz, 2000). We report here a one-dimensional coordination polymer with the sb ligand, $[\text{Cu}(\text{sb})(1,10\text{-phen})(\text{H}_2\text{O})]_n$ (1,10-phen is 1,10-phenanthroline), (I).



The Cu atom in (I) has a square-pyramidal geometry defined by one O atom from one water molecule, two N atoms from one 1,10-phenanthroline ligand, and two O atoms from two sb ligands. Atoms O1, O6, N1, and N2 occupy the basal plane, while atom O5ⁱ [symmetry code: (i) $x, y - 1, z$] occupies the apical position (Fig. 1 and Table 1). The coordination geometry of (I) is similar to that of $[\text{Cu}(\text{sb})(2,2'\text{-bipy})(\text{H}_2\text{O})_2]_2$, (II) (Fan *et al.*, 2004). The Cu—O(carboxylate), Cu—N, and Cu—O(SO_3^-) distances in (I) are remarkably similar to those in (II) and the Cu—O(carboxylate) and Cu—N distances in (I) are also close to those reported in one-dimensional bdc/1,10-phen/ Cu^{2+} complexes, such as $[\text{Cu}(\text{bdc})(\text{phen})]$, (III) (Sun *et al.*, 2001), $[\text{Cu}_2(\text{bdc})(\text{phen})_2(\text{N}_3)_2]$, (IV) (Li *et al.*, 2001), and $[\text{Cu}(\text{bdc})(\text{phen})(\text{H}_2\text{O})](\text{H}_2\text{O})(\text{DMF})$, (V) (Zhu *et al.*, 2004). In

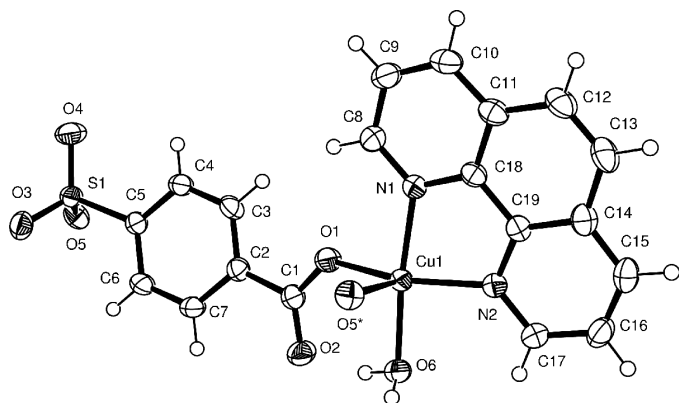


Figure 1
ORTEP-3 diagram (Farrugia, 1997) of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (*) $x, y - 1, z$].

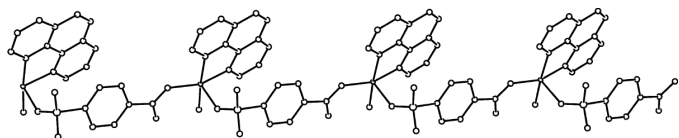


Figure 2
View of the one-dimensional chain of (I). H atoms have been omitted for clarity.

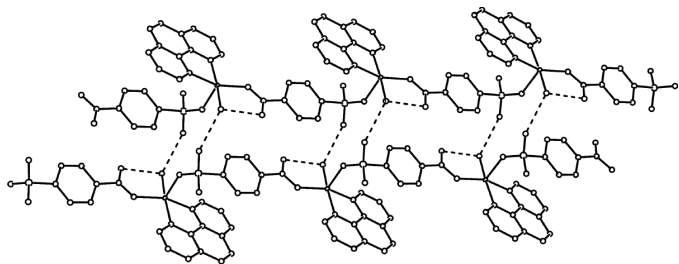


Figure 3
View of the one-dimensional hydrogen bonded ladder of (I). Hydrogen bonds are shown by dashed lines and the H atoms have been omitted for clarity.

(I), sb is in a bis-monodentate coordination mode, acting as a linker, and the Cu...Cu separation is 9.905 (1) Å, which is slightly longer than that in (II) [9.7495 (8) Å] and significantly shorter than those reported for one-dimensional bdc/1,10-phen/Cu²⁺ complexes (about 11.0 Å). The dihedral angle between the planes of the sb ring and its carboxyl group is 14.8 (5)°, which is larger than that of (II) [4.0 (4)°]. The C1—O1 bond length [1.275 (3) Å] is longer than the C1—O2 distance [1.245 (3) Å], indicating more keto character in the latter. In (II), the two *cis*-arranged sb ligands around the copper center are exactly parallel and lead to a dimeric species, while in (I), two sb ligands around the copper center are arranged *trans* and give a one-dimensional chain the structure (Fig. 2). There is an intramolecular hydrogen bond between the water molecule and the uncoordinated carboxyl O atom (Table 2).

The coordinated water molecule forms a hydrogen bond with atom O3(1 - x , 1 - y , 1 - z) of an adjacent chain,

thereby creating a one-dimensional hydrogen-bonded ladder (Fig. 3). The shortest Cu...Cu separation between neighboring chains in the ladder is 7.5943 (8) Å. Moreover, 1,10-phenanthroline ligands between neighboring hydrogen-bonded ladders are exactly parallel and exhibit π - π interaction with a distance of about 3.35 Å. From the above data, it is obvious that two sb ligands around the copper center in (I) and (II) are arranged *cis* and *trans*, respectively, and result in different assembly and extended hydrogen-bonded frameworks.

Experimental

A mixture of Cu(NO₃)₂·3H₂O (0.051 g, 0.21 mmol), potassium hydrogen 4-sulfobenzoate (0.053 g, 0.22 mmol), 1,10-phenanthroline (0.034 g, 0.17 mmol), and water (15 ml) was sealed in a 30 ml stainless steel reactor with a Teflon liner and heated to 423 K for 24 h. After cooling, blue block-shaped crystals of (I) were collected by filtration and washed with water.

Crystal data

[Cu(C₇H₄O₅S)(C₁₂H₈N₂)(H₂O)]

$M_r = 461.92$

Triclinic, $P\bar{1}$

$a = 9.6864$ (13) Å

$b = 9.9047$ (14) Å

$c = 10.8332$ (15) Å

$\alpha = 66.933$ (2)°

$\beta = 77.581$ (2)°

$\gamma = 64.206$ (2)°

$V = 859.7$ (2) Å³

$Z = 2$

$D_x = 1.784$ Mg m⁻³

Mo K α radiation

Cell parameters from 7411

reflections

$\theta = 4.0$ – 56.6 °

$\mu = 1.44$ mm⁻¹

$T = 293$ (2) K

Block, blue

$0.45 \times 0.23 \times 0.21$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

φ and ω scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

$T_{\min} = 0.678$, $T_{\max} = 0.739$

6272 measured reflections

3050 independent reflections

2895 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.013$

$\theta_{\max} = 25.1$ °

$h = -11 \rightarrow 11$

$k = -11 \rightarrow 11$

$l = -12 \rightarrow 12$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.075$

$S = 1.03$

3050 reflections

268 parameters

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0452P)^2 + 0.4913P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.29$ e Å⁻³

$\Delta\rho_{\min} = -0.35$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.9452 (15)	Cu1—N2	2.0103 (17)
Cu1—O6	1.9636 (15)	Cu1—O5 ⁱ	2.2372 (15)
Cu1—N1	2.0084 (17)		
O1—Cu1—O6	94.51 (6)	N1—Cu1—N2	81.94 (7)
O1—Cu1—N1	91.12 (7)	O1—Cu1—O5 ⁱ	97.76 (7)
O6—Cu1—N1	173.99 (7)	O6—Cu1—O5 ⁱ	91.45 (6)
O1—Cu1—N2	159.31 (7)	N1—Cu1—O5 ⁱ	89.85 (6)
O6—Cu1—N2	92.05 (7)	N2—Cu1—O5 ⁱ	101.66 (6)

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

Table 2

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O6-H6A\cdots O3^{ii}$	0.84 (1)	1.95 (1)	2.771 (2)	165 (3)
$O6-H6B\cdots O2$	0.84 (3)	1.73 (3)	2.551 (2)	163 (3)

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

H atoms bonded to C atoms were positioned geometrically and treated as riding, with C–H distances of 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(\text{parent})$. The water H atoms were located in difference Fourier maps and refined with restraints for O–H distances [0.85 (1) Å] and with $U_{iso}(H) = 0.05 \text{ \AA}^2$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE* and *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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