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Key indicators

Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.052
 wR factor = 0.112
Data-to-parameter ratio = 15.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Poly[[*cis*-diaqua(2,2'-bipyridine)copper(II)]- μ -3-carboxylato-4-hydroxybenzenesulfonato]

The title complex, $[\text{Cu}(\text{C}_7\text{H}_4\text{O}_6\text{S})(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2]_n$, consists of a polymeric neutral chain involving the 3-carboxylato-4-hydroxybenzenesulfonate ligand. The Cu atom shows a distorted octahedral coordination geometry, defined by two N atoms of the bipyridine, two O atoms of water molecules and the carboxyl O atom as well as one sulfonyl O atom of a symmetry-related bridging ligand. H atoms of water molecules are involved in $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonding, building a three dimensional network.

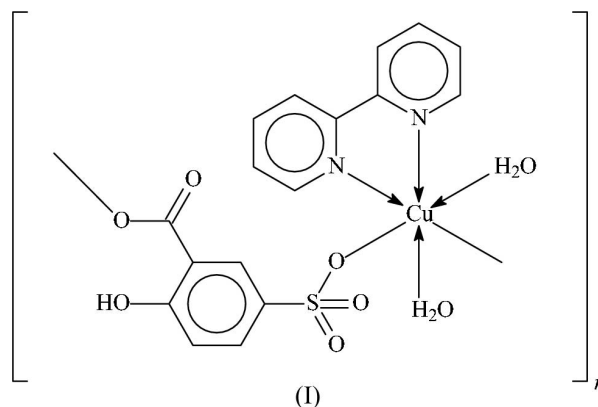
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Comment

In a recent report on metal 3-carboxy-4-hydroxybenzenesulfonates, the authors reacted copper(II) bis(3-carboxy-4-hydroxybenzenesulfonate) (prepared *in situ*) with two molar equivalents of 2,2'-bipyridine and obtained the expected bis-chelated compound but, of the two monoanions, only one is coordinated to the Cu atom, which is only five-coordinate (Gao *et al.*, 2005). Without an abstracting reagent, a similar synthesis yielded the monochelated compound, but the 3-carboxy-4-hydroxybenzenesulfonate behaves here as a dianion (Fig. 1).



In the title compound, (I), the doubly deprotonated 3-carboxylato-4-hydroxybenzenesulfonate group acts as a μ_2 -bridging ligand linking Cu atoms, forming a polymeric zigzag chain. The compound is isostructural with the cobalt(II) analog, whose structure has been described recently (Fan *et al.*, 2005). H atoms of water molecules are involved in intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonding, building a three-dimensional network (Table 1 and Fig. 2). There are also intramolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds between the hydroxyl group and the carboxyl O atom coordinated to copper, and between one of the water molecules and the second carboxyl O atom (Table 1).

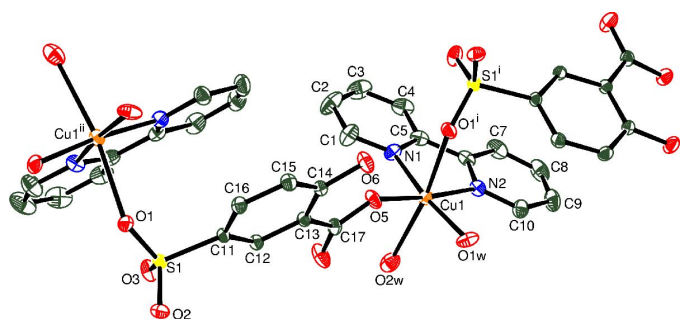


Figure 1
 ORTEP (Burnett & Johnson, 1996) plot of a fragment of the polymeric chain of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) $x - \frac{1}{2}, \frac{1}{2} - y, z - \frac{1}{2}$; (ii) $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$.]

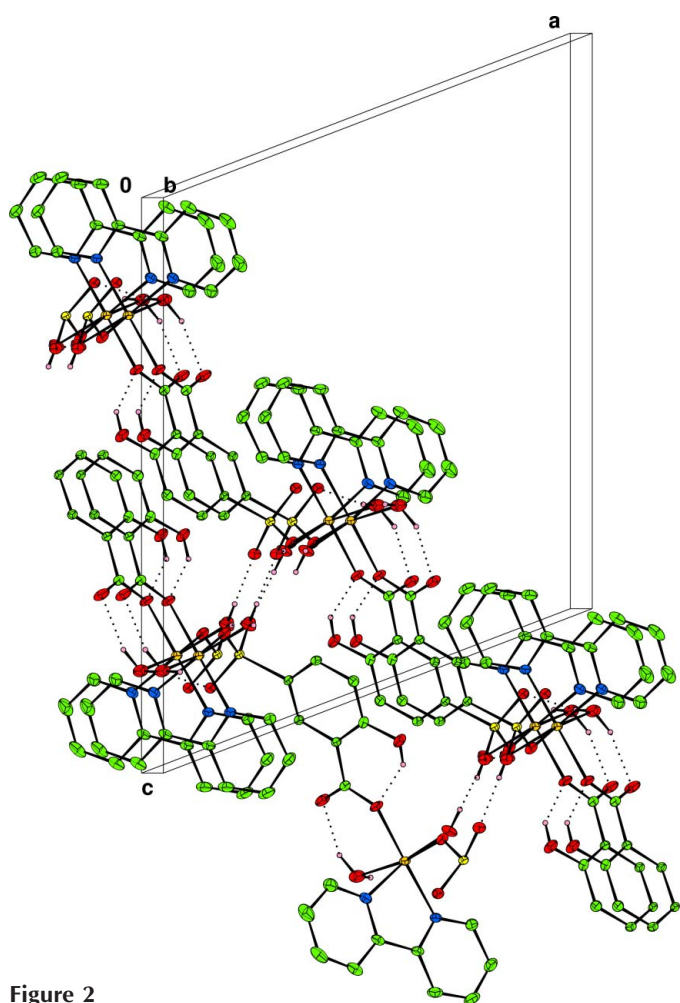


Figure 2
 CAMERON (Watkin *et al.*, 1993) view of the packing, showing the O—H...O hydrogen-bonded (dashed lines) three-dimensional network. H atoms not involved in hydrogen bonding have been omitted.

Experimental

A solution of copper acetate hydrate (0.041 g, 0.2 mmol) and 5-sulfosalicylic acid dihydrate (0.103 g, 0.4 mmol) dissolved in water (20 ml) was added to a methanol solution (5 ml) of 2,2'-bipyridyl (0.030 g, 0.2 mmol). The clear blue solution was left to stand for a day to allow the solvent to evaporate. Blue block-shaped crystals were

obtained. Analysis calculated for $C_{17}H_{16}CuN_2O_8S$: C 43.26, H 3.42, N 5.94%; found: C 42.63, H 3.47, N 5.96%.

Crystal data

[Cu(C₇H₄O₆S)(C₁₀H₈N₂)(H₂O)₂]
 $M_r = 471.92$
 Monoclinic, $P2_1/n$
 $a = 14.2339$ (8) Å
 $b = 7.7622$ (4) Å
 $c = 17.801$ (1) Å
 $\beta = 110.940$ (1)°
 $V = 1836.87$ (17) Å³
 $Z = 4$

$D_x = 1.707$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 4713 reflections
 $\theta = 2.3$ – 28.3 °
 $\mu = 1.35$ mm⁻¹
 $T = 295$ (2) K
 Block, blue
 $0.28 \times 0.26 \times 0.12$ mm

Data collection

Bruker SMART APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
 $T_{min} = 0.703$, $T_{max} = 0.854$
 10938 measured reflections

4143 independent reflections
 3855 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.024$
 $\theta_{max} = 27.5$ °
 $h = -18 \rightarrow 18$
 $k = -9 \rightarrow 10$
 $l = -23 \rightarrow 14$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.112$
 $S = 1.20$
 4143 reflections
 275 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0379P)^2 + 2.6968P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.63$ e Å⁻³
 $\Delta\rho_{min} = -0.40$ e Å⁻³

Table 1

Hydrogen-bonding geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W1...O2 ⁱ	0.821 (18)	1.870 (19)	2.688 (3)	174 (4)
O1W—H1W2...O2 ⁱⁱ	0.83 (4)	1.89 (4)	2.717 (3)	178 (4)
O2W—H2W1...O3 ⁱ	0.848 (17)	2.001 (19)	2.810 (4)	159 (3)
O2W—H2W2...O4	0.852 (18)	1.99 (2)	2.738 (4)	146 (3)
O6—H6...O5	0.82	1.89	2.599 (3)	143

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

Aromatic H atoms were positioned geometrically and were included in the refinement in the riding-model approximation [$C-H = 0.93$ Å and $U_{iso}(H) = 1.2U_{eq}(C)$]. The water and hydroxy H atoms were located in a difference Fourier map and refined with distance restraints of $O-H = 0.85$ (1) Å and $H\cdots H = 1.39$ (1) Å, and $U_{iso}(H) = 1.2U_{eq}(O)$.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP (Burnett & Johnson, 1996); software used to prepare material for publication: SHELXL97.

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