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## Key indicators

Single-crystal X-ray study

T = 295 K

Mean  $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$ 

R factor = 0.032

wR factor = 0.085

Data-to-parameter ratio = 12.8

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**catena-Poly[[[aqua(2,2'-bipyridine)copper(II)]- $\mu$ -3-sulfonatobenzoato] monohydrate]**

In the title polymeric complex,  $\{[\text{Cu}(\text{C}_7\text{H}_4\text{O}_5\text{S})(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]\cdot\text{H}_2\text{O}\}_n$ , each Cu atom is coordinated by a water molecule, two 3-sulfonatobenzoate ligands and two N atoms from one 2,2'-bipyridine molecule, in the shape of a square pyramid. The bridging 3-sulfonatobenzoate ligands extend the molecular structure into a one-dimensional chain. The coordinated water molecule forms an intramolecular hydrogen bond with the carboxyl group and an intermolecular hydrogen bond with the solvent water molecule. The extensive hydrogen-bonding network between the sulfonate groups and the solvent water molecules of two polymer chains generates ring structures, which form an infinite ladder-like pattern extending along the *a* axis.

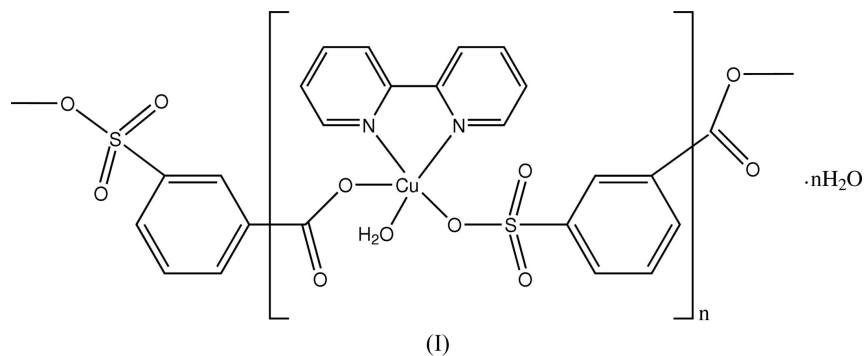
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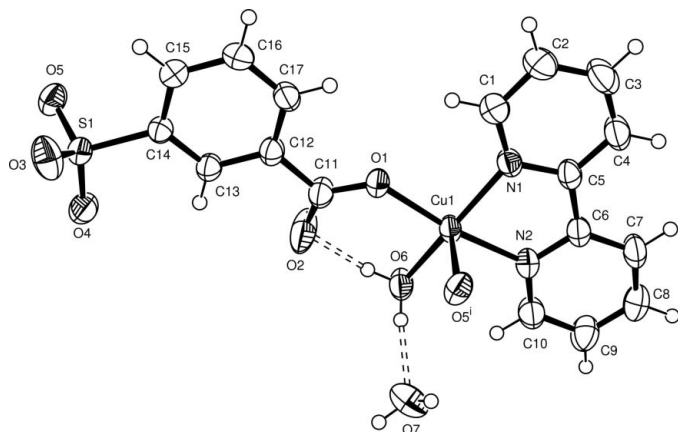
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## Comment

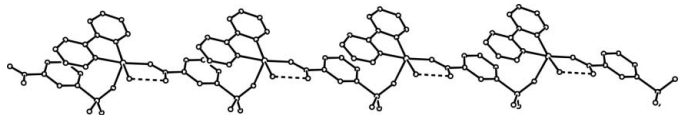
In recent years, numerous metal complexes with ditopic ligands, such as 1,4-benzenedicarboxylate (bdc) or 4,4'-bipyridine, have been extensively investigated owing to their potential application as functional materials (Chisholm, 2003; Yaghi *et al.*, 2003; Zhu & Kitagawa, 2002). However, metal complexes with sulfobenzoate, a ligand with a combination of sulfonate and carboxylate groups, are sparse (Zhang & Zhu, 2005). In the related reaction system of 4-sulfobenzoate (4-sb), copper(II), 2,2'-bipyridine (2,2'-bipy) and water, a dimer structure is formed (Fan *et al.*, 2004). In the title complex, (I), using 3-sulfobenzoate (3-sb) instead of 4-sulfobenzoate, a polymeric species is formed.



In (I), each  $\text{Cu}^{\text{II}}$  atom adopts a square-pyramidal geometry defined by two N-atom donors from one 2,2'-bipyridine molecule, two O atoms from two 3-sb ligands and one O atom from a water molecule. Atoms O1, O6, N1, and N2 occupy the basal plane, while atom O5<sup>i</sup> [symmetry code: (i)  $-1 + x, y, z$ ] occupies the apical position (Fig. 1 and Table 1). The coordination geometry of (I) is similar to that of the dimer  $[\text{Cu}(4\text{-sb})\text{-(2,2'-bipy)}(\text{H}_2\text{O})]_2$ , (II) (Fan *et al.*, 2004). The Cu—



**Figure 1**  
ORTEP-3 (Farrugia, 1997) view of a segment of (I). Displacement ellipsoids are drawn at the 40% probability level. Hydrogen bonds are shown as dashed lines. [Symmetry code: (i)  $-1 + x, y, z$ .]



**Figure 2**  
A view of the one-dimensional chain of (I). H atoms and solvent water molecules have been omitted for clarity. Hydrogen bonds are shown as dashed lines.

O(carboxylate), Cu–N and Cu–O(SO<sub>3</sub><sup>−</sup>) distances in (I) are remarkably close to those in (II), and the Cu–O(carboxylate) and Cu–N distances in (I) are also similar to those in reported one-dimensional bdc/1,10-phen/Cu<sup>2+</sup> complexes, such as [Cu(bdc)(phen)] (Sun *et al.*, 2001), [Cu<sub>2</sub>(bdc)(phen)<sub>2</sub>(N<sub>3</sub>)<sub>2</sub>] (Li *et al.*, 2001) and [Cu(bdc)(phen)(H<sub>2</sub>O)](H<sub>2</sub>O)(DMF) (Zhu *et al.*, 2004). The 3-sb ligand in (I) acts as a bridge in the bis-monodentate coordination mode and the Cu···Cu separation by the 3-sb ligand is 9.5843 (5) Å, which is slightly shorter than that of (II) [9.7495 (8) Å] and significantly shorter than those of reported one-dimensional bdc/1,10-phen/Cu<sup>2+</sup> complexes (about 11.0 Å). The dihedral angle between the planes of the 3-sb ring and its carboxylate group is 12.1 (3)°, which is larger than that of (II) [4.0 (4)°]. In (II), the two *cis*-arranged 4-sb ligands around the Cu atom are strictly parallel and lead to a cyclic dimer. However, in (I), the two 3-sb ligands around the copper centre are arranged in a *trans* fashion, and a one-dimensional chain is formed (Fig. 2), including an intramolecular hydrogen bond between the coordinated water molecule and the uncoordinated carboxyl O atom. The solvent water molecule forms three hydrogen bonds with the coordinated water molecule and two sulfonate groups from two neighbouring chains, and thus the molecular structure is assembled into a ladder-like pattern (Fig. 3 and Table 2), in which the shortest Cu···Cu separation is 6.9967 (6) Å.

## Experimental

A mixture of Cu(CH<sub>3</sub>COO)<sub>2</sub>·H<sub>2</sub>O (0.093 g, 0.47 mmol), sodium hydrogen 3-sulfobenzoate (0.129 g, 0.58 mmol) and 2,2'-bipyridine (0.070 g, 0.45) in an aqueous solution (10 ml) was sealed in a 20 ml

stainless steel reactor with a Teflon liner, and heated at 423 K for 72 h. After being cooled to room temperature, the resulting mixture was kept in the closed reactor for 2 d; green prismatic crystals of (I) were then separated by suction filtration.

## Crystal data

[Cu(C<sub>7</sub>H<sub>4</sub>O<sub>5</sub>S)(C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>)(H<sub>2</sub>O)]·  
H<sub>2</sub>O  
*M<sub>r</sub>* = 455.92  
Monoclinic, *P*2<sub>1</sub>/*n*  
*a* = 9.5843 (5) Å  
*b* = 17.8784 (9) Å  
*c* = 10.6912 (6) Å  
*β* = 93.094 (1)°  
*V* = 1829.29 (17) Å<sup>3</sup>  
*Z* = 4

*D<sub>x</sub>* = 1.655 Mg m<sup>−3</sup>  
Mo *Kα* radiation  
Cell parameters from 4969  
reflections  
*θ* = 2.2–27.7°  
*μ* = 1.35 mm<sup>−1</sup>  
*T* = 295 (2) K  
Prism, green  
0.39 × 0.27 × 0.19 mm

## Data collection

Bruker SMART APEX area-  
detector diffractometer  
*φ* and *ω* scans  
Absorption correction: multi-scan  
(*SADABS*; Bruker, 2002)  
*T<sub>min</sub>* = 0.621, *T<sub>max</sub>* = 0.783  
9836 measured reflections

3402 independent reflections  
3069 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.020  
*θ<sub>max</sub>* = 25.5°  
*h* = −11 → 11  
*k* = −21 → 11  
*l* = −12 → 12

## Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.032  
*wR*(*F*<sup>2</sup>) = 0.085  
*S* = 1.05  
3402 reflections  
265 parameters  
H atoms treated by a mixture of  
independent and constrained  
refinement

$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.7756P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
(*Δ*/σ)<sub>max</sub> = 0.001  
*Δρ*<sub>max</sub> = 0.34 e Å<sup>−3</sup>  
*Δρ*<sub>min</sub> = −0.27 e Å<sup>−3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Cu1–O1	1.9606 (16)	Cu1–N2	2.0044 (19)
Cu1–O5 <sup>i</sup>	2.2877 (17)	S1–O3	1.4434 (19)
Cu1–O6	1.9582 (17)	S1–O4	1.4409 (19)
Cu1–N1	2.0027 (19)	S1–O5	1.4543 (17)
O1–Cu1–O5 <sup>i</sup>	92.39 (6)	O6–Cu1–N1	164.95 (8)
O6–Cu1–O1	93.30 (7)	O6–Cu1–N2	92.00 (8)
O1–Cu1–N1	92.39 (8)	N1–Cu1–N2	81.07 (8)
O1–Cu1–N2	172.09 (7)	O4–S1–O3	113.90 (13)
O6–Cu1–O5 <sup>i</sup>	99.01 (7)	O4–S1–O5	113.14 (11)
N1–Cu1–O5 <sup>i</sup>	94.66 (7)	O3–S1–O5	110.68 (12)
N2–Cu1–O5 <sup>i</sup>	92.58 (7)		

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

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
O7–H7A···O3 <sup>ii</sup>	0.86 (3)	1.96 (1)	2.795 (3)	165 (3)
O7–H7B···O4 <sup>i</sup>	0.87 (2)	1.91 (2)	2.714 (3)	154 (2)
O6–H6A···O2	0.86 (1)	1.66 (1)	2.523 (2)	174 (3)
O6–H6B···O7	0.84 (3)	1.81 (3)	2.620 (3)	164 (3)

Symmetry codes: (i)  $x - 1, y, z$ ; (ii)  $-x + 2, -y + 2, -z + 2$ .

All aromatic H atoms were positioned geometrically and refined as riding atoms, with C–H = 0.93 Å and *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C). The water

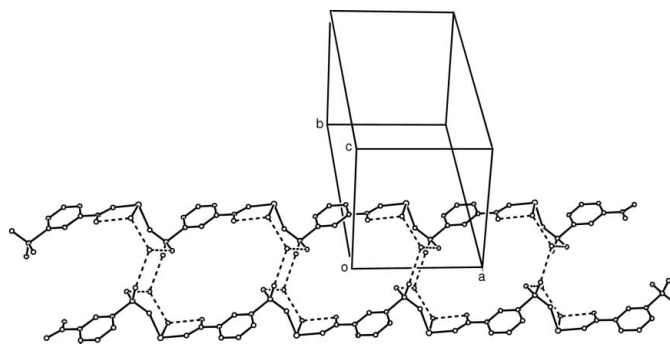
H atoms were located in difference Fourier maps and were refined with a distance restraint of O–H = 0.85 (1) Å and fixed isotropic displacement parameters of 0.08 Å<sup>2</sup>.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINTE* (Bruker, 2002); data reduction: *SAINTE*; 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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**Figure 3**

A view of the ladder-like hydrogen-bonded pattern in (I). H atoms and 2,2'-bipyridine ligands have been omitted for clarity. Hydrogen bonds are shown as dashed lines.

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