

Diaqua(1,10-phenanthroline)(3-sulfonato-  
benzoato)copper(II) monohydrateLei Cai<sup>a</sup> and Long-Guan Zhu<sup>b\*</sup><sup>a</sup>Department of Polymer Science and Engineering, Zhejiang University, Hangzhou 310027, People's Republic of China, and<sup>b</sup>Department of Chemistry, Zhejiang University, Hangzhou 310027, People's Republic of China

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The title compound,  $[\text{Cu}(\text{C}_7\text{H}_4\text{O}_5\text{S})(\text{C}_{12}\text{H}_8\text{N}_2)(\text{H}_2\text{O})_2]\cdot\text{H}_2\text{O}$ , contains a monomeric zwitterion in which the  $\text{Cu}^{\text{II}}$  atom displays a square-pyramidal geometry defined by two N atoms of one 1,10-phenanthroline, one O atom from the carboxylate group of the 3-sulfonatobenzoate, and two O atoms from two water molecules. Extensive  $\text{O}-\text{H}\cdots\text{O}$  intermolecular hydrogen bonds generate a two-dimensional network, enhancing the stability of the structure.

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## Key indicators

Single-crystal X-ray study

 $T = 295 \text{ K}$ Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$ 

Disorder in main residue

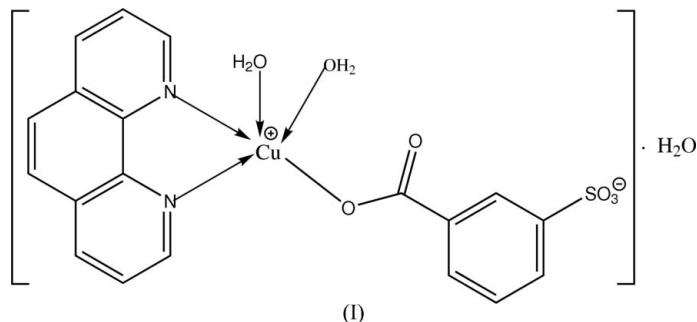
 $R$  factor = 0.033 $wR$  factor = 0.090

Data-to-parameter ratio = 11.5

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

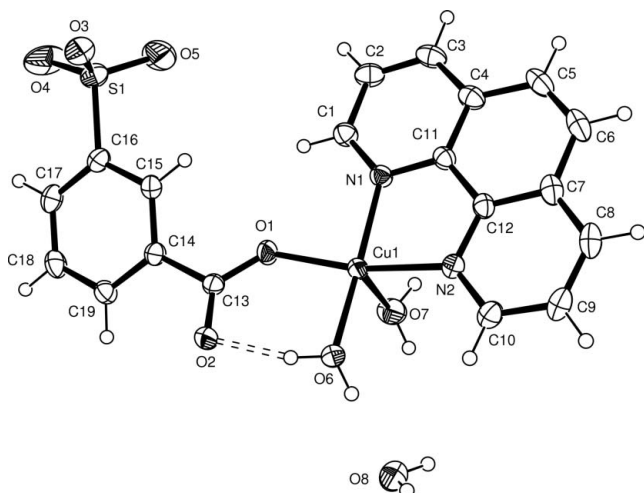
## Comment

Recently, several 4-sulfonatobenzoate metal compounds with interesting topologies have been synthesized in our laboratory (Fan, Xiao, Zhang & Zhu, 2004; Fan *et al.*, 2005; Zhang *et al.*, 2005, 2005*a,b*). The 4-sulfonatobenzoate (4-sb)/ $\text{Cu}^{\text{II}}$ /1,10-phenanthroline (phen) system under hydrothermal conditions yielded a polymeric compound (Fan, Xiao, Zhang, Cai & Zhu, 2004),  $[\text{Cu}(4\text{-sb})(\text{phen})(\text{H}_2\text{O})]_n$ , (II). However, a similar synthesis with 3-sulfonatobenzoate (3-sb) instead of 4-sb leads to the mononuclear title compound, (I).



The  $\text{Cu}^{\text{II}}$  atom adopts a square-pyramidal geometry defined by two N-atom donors from one phen ligand, one O atom from the carboxylate group of 3-sb, and two O atoms from two water molecules. Atoms N1, N2, O1, and O6 occupy the basal plane, whereas atom O7 occupies the apical position. The coordination environment and bond lengths of (I) are similar to those of (II), although the structures are very different. In (II), 4-sb is a bis-monodentate link, whereas in (I) 3-sb is a monodentate ligand. The apical position taken by the O atom of the sulfonyl in (II) is replaced by a water molecule in (I), which implies that hydrogen bonds between the sulfonate group and water molecules prevent the coordination of the sulfonate to the metal atom.

There is an intramolecular hydrogen bond between the water molecule (O6) and the free carboxylate O atom (Table 2). Extensive  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds between the coordinated water molecule (O6) and uncoordinated water molecule, between the coordinated water molecule (O7) and



**Figure 1**

A view of the molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines and the minor part of the disordered sulfonate group is not shown.

the sulfonate group, and between the sulfonate group and the solvent water molecule, extend the structure into layers (Fig. 2 and Table 2).

## Experimental

A mixture of  $\text{Cu}(\text{NO}_3)_2 \cdot 3\text{H}_2\text{O}$  (0.125 g, 0.52 mmol), sodium hydrogen 3-sulfonatobenzoate (0.128 g, 0.57 mmol), 1,10-phenanthroline hydrate (0.094 g, 0.47 mmol) and water (15 ml) was sealed in a 30 ml Teflon-lined stainless steel autoclave and heated at 423 K for 51 h. After cooling to room temperature, blue plate-shaped crystals of (I) were obtained and collected by suction filtration.

### Crystal data

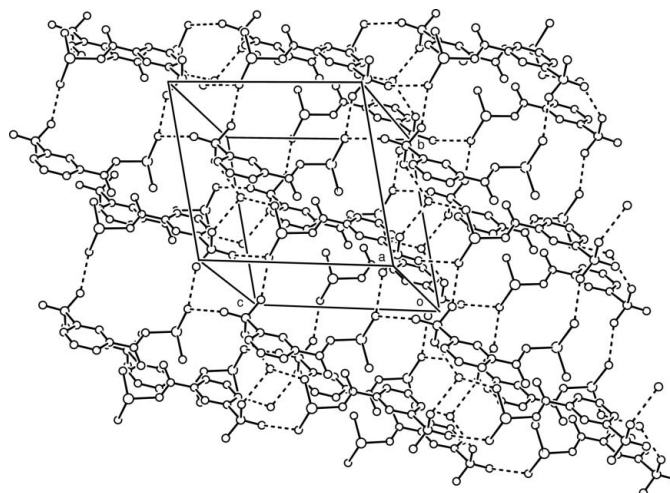
$[\text{Cu}(\text{C}_7\text{H}_4\text{O}_5\text{S})(\text{C}_{12}\text{H}_8\text{N}_2) \cdot (\text{H}_2\text{O})_2] \cdot \text{H}_2\text{O}$	$Z = 2$
$M_r = 497.95$	$D_x = 1.717 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 8.6047 (9) \text{ \AA}$	Cell parameters from 3706 reflections
$b = 10.5469 (11) \text{ \AA}$	$\theta = 2.5\text{--}28.1^\circ$
$c = 11.7021 (13) \text{ \AA}$	$\mu = 1.30 \text{ mm}^{-1}$
$\alpha = 79.123 (1)^\circ$	$T = 295 (2) \text{ K}$
$\beta = 84.585 (1)^\circ$	Plate, blue
$\gamma = 67.500 (1)^\circ$	$0.30 \times 0.13 \times 0.11 \text{ mm}$
$V = 963.25 (18) \text{ \AA}^3$	

### Data collection

Bruker APEX area-detector diffractometer	3735 independent reflections
$\varphi$ and $\omega$ scans	3288 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$R_{\text{int}} = 0.022$
$T_{\text{min}} = 0.697$ , $T_{\text{max}} = 0.871$	$\theta_{\text{max}} = 26.0^\circ$
7553 measured reflections	$h = -10 \rightarrow 10$
	$k = -12 \rightarrow 12$
	$l = -14 \rightarrow 14$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 0.5382P]$
$R[F^2 > 2\sigma(F^2)] = 0.033$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.090$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 0.92$	$\Delta\rho_{\text{max}} = 0.41 \text{ e \AA}^{-3}$
3735 reflections	$\Delta\rho_{\text{min}} = -0.32 \text{ e \AA}^{-3}$
326 parameters	
H atoms treated by a mixture of independent and constrained refinement	



**Figure 2**

A View of the two-dimensional hydrogen-bonding network of (I). Hydrogen bonds are shown by dashed lines and the H atoms and 1,10-phenanthroline ligands have been omitted.

**Table 1**

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

Cu1—O1	1.9427 (16)	Cu1—N1	2.0090 (19)
Cu1—O6	1.9518 (17)	Cu1—N2	2.0150 (19)
Cu1—O7	2.3141 (19)		
O1—Cu1—O6	91.97 (7)	N1—Cu1—N2	82.04 (8)
O1—Cu1—N1	89.23 (7)	O1—Cu1—O7	95.96 (8)
O6—Cu1—N1	170.77 (8)	O6—Cu1—O7	95.93 (7)
O1—Cu1—N2	167.56 (8)	N1—Cu1—O7	93.04 (7)
O6—Cu1—N2	95.26 (7)	N2—Cu1—O7	93.35 (8)

**Table 2**

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

$D\text{—}H \cdots A$	$D\text{—}H$	$H \cdots A$	$D \cdots A$	$D\text{—}H \cdots A$
O6—H6A...O2	0.84 (1)	1.77 (1)	2.587 (2)	165 (3)
O6—H6B...O8	0.85 (1)	1.81 (1)	2.647 (3)	170 (3)
O7—H7A...O5 <sup>i</sup>	0.85 (1)	1.87 (1)	2.701 (3)	169 (3)
O7—H7A...O5 <sup>ii</sup>	0.85 (1)	2.10 (3)	2.904 (19)	158 (3)
O7—H7B...O4 <sup>ii</sup>	0.84 (1)	2.04 (2)	2.877 (19)	173 (3)
O7—H7B...O4 <sup>iii</sup>	0.84 (1)	2.11 (2)	2.929 (6)	163 (3)
O8—H8A...O3 <sup>iii</sup>	0.85 (1)	1.94 (1)	2.778 (6)	169 (3)
O8—H8A...O4 <sup>iii</sup>	0.85 (1)	2.41 (3)	3.04 (3)	132 (2)
O8—H8A...O3 <sup>iii</sup>	0.85 (1)	2.49 (3)	3.33 (3)	170 (2)
O8—H8B...O3 <sup>iii</sup>	0.85 (3)	1.98 (1)	2.817 (6)	171 (3)
O8—H8B...O3 <sup>iii</sup>	0.85 (3)	2.12 (3)	2.95 (2)	166 (3)

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

C-bound H atoms were positioned geometrically and refined as riding atoms, with  $\text{C—H} = 0.93 \text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The water H atoms were located in difference Fourier maps and were refined with a distance restraint of  $\text{O—H} = 0.85 (1) \text{ \AA}$  and with a fixed isotropic displacement parameter of  $U_{\text{iso}}(\text{H}) = 0.05 \text{ \AA}^2$ . The sulfonate group is disordered over two positions and the occupancies were refined to a 0.830 (13):0.170 (13) ratio.

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:

*ORTEP3* for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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