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Key indicators

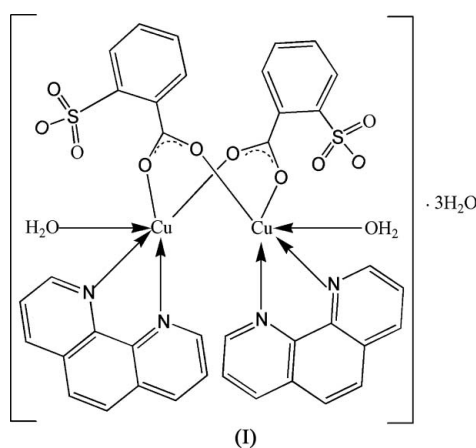
Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
 R factor = 0.038
 wR factor = 0.101
Data-to-parameter ratio = 13.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Di- μ -2-sulfonatobenzoato-bis[aqua(1,10-phenanthroline)copper(II)] trihydrate

In the title compound, $[\text{Cu}_2(\text{C}_7\text{H}_4\text{O}_5\text{S})_2(\text{C}_{12}\text{H}_8\text{N}_2)_2(\text{H}_2\text{O})_2] \cdot 3\text{H}_2\text{O}$, each copper(II) atom is coordinated by two N atoms from one 1,10-phenanthroline molecule, two carboxylate O atoms from two 2-sulfonatobenzoato dianions and one aqua O atom in a distorted square pyramidal geometry. The 2-sulfonatobenzoato dianions function as μ_2 -bridging ligands in the formation of a dinuclear complex. Intermolecular hydrogen-bond interactions link the dinuclear units into a two-dimensional network structure.

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Comment

Sulfobenzoic acids (obs) such as 4-sulfobenzoic acid (Fan *et al.*, 2004; Zhang, Zhu & Xiao, 2005) and 2-sulfobenzoic acid (*o*-H₂sb) (Li & Yang, 2004; Xiao, 2005; Xiao, Li & Hu, 2005; Xiao, Shi & Cheng, 2005; Su *et al.*, 2005), are suitable ligands for the preparation of metal-organic coordination polymers owing to their diverse structural motifs. As part of our ongoing investigation on the coordination properties of sulfobenzoic acids, we have used 2-sulfobenzoic acid, copper(II) and 1,10-phenanthroline (phen) in a mixed ethanol and water solvent to give a mononuclear complex $[\text{CuCl}(\text{phen})_2] \cdot (\text{o-Hsb}) \cdot \text{H}_2\text{O}$ (Zhang, Wang, Chen & Xiao, 2005). The title complex, $[\text{Cu}_2(\text{H}_2\text{O})_2(\text{phen})_2(\text{o-sb})_2] \cdot 3\text{H}_2\text{O}$ (I), was obtained by using $\text{Cu}(\text{CH}_3\text{CO}_2)_2 \cdot \text{H}_2\text{O}$ instead of $\text{CuCl}_2 \cdot 2\text{H}_2\text{O}$ and with aqueous *N,N*-dimethylformamide as solvent.



In (I), each Cu(II) atom is in a distorted square pyramidal geometry defined by one aqua O atom, two O atoms belonging to two 2-sulfonatobenzoato dianions and two N atoms from one 1,10-phenanthroline molecule (Fig. 1 and Table 1). The *o*-sb dianions function as μ_2 -bridging ligands between the two copper(II) atoms to form a dinuclear complex having a $\text{Cu} \cdots \text{Cu}$ distance of 3.175 (2) Å. In the reported complex,

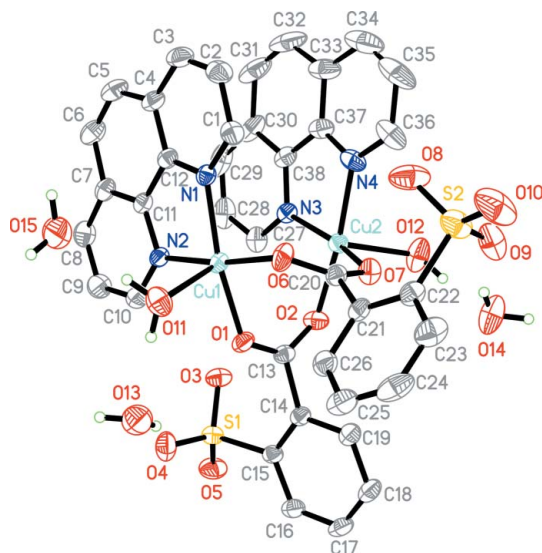


Figure 1
The structure of (I), with the atom numbering, showing displacement ellipsoids at the 30% probability level. C-bound H atoms have been omitted.

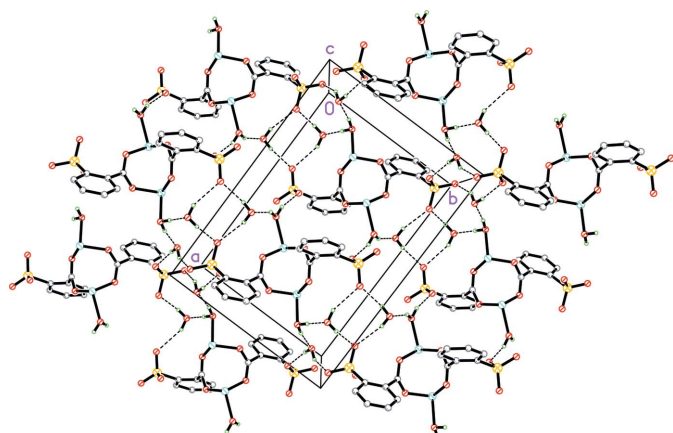


Figure 2
The two-dimensional hydrogen-bonded (dashed lines) network in (I). H atoms not involved in the interactions shown have been omitted.

$[\text{CuCl}(\text{phen})_2] \cdot (\text{o-Hsb}) \cdot \text{H}_2\text{O}$, the anion does not coordinate to the Cu atom (Zhang, Wang, Chen & Xiao, 2005).

The structure shows a short interplanar distance of 3.56 Å between two 1,10-phenanthroline rings in the dinuclear complex, an indication of π - π stacking. Intermolecular O-H...O hydrogen bonds are found in the crystal structure (Table 2). The interactions link the dinuclear units into a two-dimensional network structure and enhance its stability (Fig. 2).

Experimental

An aqueous solution (10 ml) containing $\text{Cu}(\text{CH}_3\text{CO}_2)_2 \cdot \text{H}_2\text{O}$ (0.30 mmol, 0.059 g) was added slowly to a solution (10 ml) of *N,N*-dimethylformamide containing 1,10-phenanthroline (0.30 mmol, 0.054 g) and 2-sulfobenzoic acid (0.30 mmol, 0.061 g). Blue crystals suitable for X-ray analysis were obtained on standing the solution at room temperature for two weeks.

Crystal data

$[\text{Cu}_2(\text{C}_7\text{H}_4\text{O}_5\text{S})_2(\text{C}_{12}\text{H}_8\text{N}_2)_2 \cdot (\text{H}_2\text{O})_2] \cdot 3\text{H}_2\text{O}$
 $M_r = 977.89$
 Monoclinic, $P2_1/c$
 $a = 15.7402$ (8) Å
 $b = 11.0625$ (6) Å
 $c = 22.8274$ (12) Å
 $\beta = 97.334$ (1)°
 $V = 3942.3$ (4) Å³
 $Z = 4$

$D_x = 1.648$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 6431 reflections
 $\theta = 2.4$ – 25.4 °
 $\mu = 1.26$ mm⁻¹
 $T = 298$ (2) K
 Prism, blue
 $0.28 \times 0.22 \times 0.14$ mm

Data collection

Bruker APEX area-detector diffractometer
 φ and ω scan
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
 $T_{\text{min}} = 0.719$, $T_{\text{max}} = 0.843$
 20723 measured reflections

7158 independent reflections
 5901 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$
 $\theta_{\text{max}} = 25.3$ °
 $h = -18 \rightarrow 18$
 $k = -10 \rightarrow 13$
 $l = -24 \rightarrow 27$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.101$
 $S = 1.03$
 7158 reflections
 550 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 1.1268P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.49$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.29$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.9755 (18)	Cu2—O2	1.9404 (18)
Cu1—O6	1.9420 (18)	Cu2—O7	1.9943 (18)
Cu1—O11	2.183 (2)	Cu2—O12	2.134 (2)
Cu1—N1	2.010 (2)	Cu2—N3	2.012 (2)
Cu1—N2	1.995 (2)	Cu2—N4	1.995 (2)
O1—Cu1—O11	89.55 (8)	O2—Cu2—O7	88.36 (8)
O6—Cu1—O1	91.73 (8)	O2—Cu2—O12	92.33 (9)
O6—Cu1—O11	88.92 (8)	O7—Cu2—O12	90.83 (8)
O6—Cu1—N2	172.14 (9)	O2—Cu2—N4	173.68 (10)
O1—Cu1—N2	94.42 (8)	O2—Cu2—N3	92.39 (9)
O6—Cu1—N1	90.91 (9)	O7—Cu2—N3	161.02 (8)
O1—Cu1—N1	164.40 (8)	O7—Cu2—N4	95.80 (9)
N1—Cu1—O11	105.88 (8)	N4—Cu2—N3	82.13 (10)
N2—Cu1—N1	81.87 (8)	N3—Cu2—O12	108.08 (8)
N2—Cu1—O11	96.02 (8)	N4—Cu2—O12	92.37 (10)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O15—H15B...O10 ⁱ	0.85	2.37	3.115 (5)	146
O15—H15A...O8 ⁱⁱ	0.85	1.94	2.763 (4)	162
O14—H14A...O9	0.85	2.20	3.018 (4)	161
O14—H14B...O4 ⁱⁱⁱ	0.85	2.01	2.846 (3)	169
O13—H13B...O9 ⁱ	0.85	2.05	2.857 (4)	159
O13—H13A...O4	0.85	2.29	3.090 (3)	157
O12—H12B...O14	0.85	1.90	2.697 (3)	155
O12—H12A...O3 ^{iv}	0.85	1.88	2.700 (3)	161
O11—H11B...O13	0.85	1.95	2.800 (3)	174
O11—H11A...O15	0.85	1.89	2.733 (4)	171

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

All H atoms were positioned geometrically (C–H = 0.93 Å or O–H = 0.85 Å) and allowed to ride on their parent atoms, with $U_{\text{iso}}(\text{H})$ values equal to $1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{O})$.

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: *XP* in *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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References

- Bruker (2002). *SADABS* (Version 2.03), *SAINTE* (Version 6.02), *SMART* (Version 5.62) and *SHELXTL* (Version 6.10). Bruker AXS Inc., Madison, Wisconsin, USA.
- Fan, S. R., Xiao, H. P., Zhang, L. P., Cai, G. Q. & Zhu, L. G. (2004). *Acta Cryst.* **E60**, m1970–m1972.
- Li, X. H. & Yang, S. Z. (2004). *Acta Cryst.* **C60**, m423–m25.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Su, W., Bi, W. H., Li, X. & Cao, R. (2005). *Acta Cryst.* **C61**, m16–m18.
- Xiao, H. P. (2005). *Acta Cryst.* **E61**, m942–m944.
- Xiao, H. P., Li, X. H. & Hu, M. L. (2005). *Acta Cryst.* **E61**, m506–m508.
- Xiao, H. P., Shi, Q. & Cheng, Y. Q. (2005). *Acta Cryst.* **E61**, m907–m909.
- Zhang, L. P., Zhu, L. G. & Xiao, H. P. (2005). *Acta Cryst.* **E61**, m860–m862.
- Zhang, W. B., Wang, J. G., Chen, H. X. & Xiao, H. P. (2005). *Acta Cryst.* **E61**, m2559–m2560.