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Key indicators

Single-crystal X-ray study
 T = 295 K
 Mean $\sigma(C-C)$ = 0.007 Å
 R factor = 0.067
 wR factor = 0.147
 Data-to-parameter ratio = 15.5

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

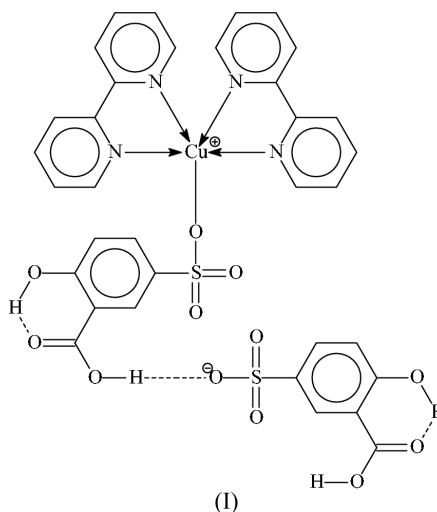
Bis(2,2'-bipyridine)(3-carboxy-4-hydroxybenzenesulfonato)copper(II) 3-carboxy-4-hydroxybenzenesulfonate

The Cu atom in the title compound, $[Cu(C_7H_5O_6S)(C_{10}H_8N_2)](C_7H_5O_6S)$, is chelated by the two N-heterocycles and is covalently bonded to the sulfonate O atom of the sulfosalicylate ion in a trigonal-bipyramidal geometry. The uncoordinated sulfosalicylate anion interacts with adjacent anions, forming a linear hydrogen-bonded chain; the mononuclear cations are appended to the chain by hydrogen bonds.

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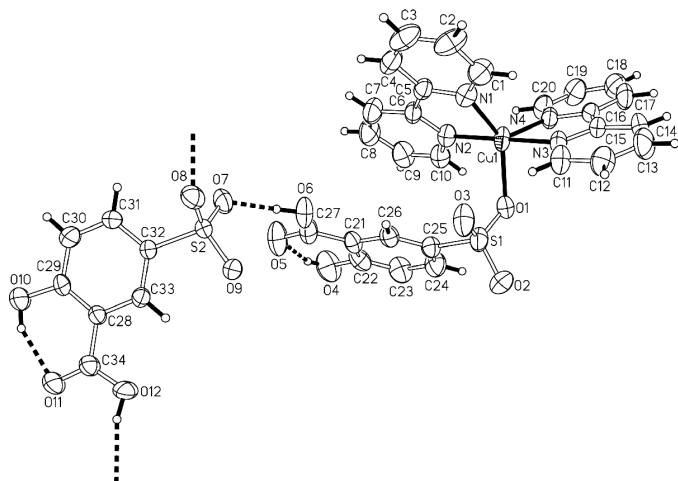
Comment

The reaction of copper diacetate, sulfosalicylic acid and 2,2'-bipyridine yields a centrosymmetric trinuclear complex, $[Cu_3(C_7H_3O_6S)_2(C_{10}H_8N_2)_2(H_2O)_4] \cdot 4H_2O$, which incorporates the sulfosalicylate entity as a completely deprotonated trianionic group. Two of the three Cu atoms are chelated by the heterocyclic ligand (Wang *et al.*, 2004).



However, a similar synthesis carried out with the sodium salt of the acid instead of the acid itself yields the mononuclear salt-like title compound, (I), containing two mono-deprotonated 3-carboxy-4-hydroxybenzenesulfonate groups. One of them is covalently bonded to the bis-chelated Cu atom, whereas the other exists in the outer coordination sphere resulting in a formulation of $[Cu(C_7H_5O_6S)(C_{10}H_8N_2)](C_7H_5O_6S)$ (Fig. 1). The trigonal-bipyramidal coordination about the Cu atom is completed by two bidentate 2,2'-bipyridine ligands, with atoms N2 and N3 in the axial positions (Table 1).

The uncoordinated anion uses its carboxylic acid H atom to form a hydrogen bond to the sulfonate O atom of another uncoordinated anion, resulting in a relatively strong hydrogen-bonded chain $[O \cdots O = 2.589(4) \text{ \AA}]$. The mononuclear cations are appended to the chain, also through a


Figure 1

View of the asymmetric unit of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii. Hydrogen bonds are indicated by dashed lines.

carboxylic acid/sulfonate hydrogen bond that is marginally weaker [$O \cdots O = 2.634(5) \text{ \AA}$] (Fig. 2 and Table 2).

Experimental

Copper nitrate hexahydrate (1.48 g, 5 mmol), 2,2'-bipyridine (1.60 g, 10 mmol), sodium hydroxide (0.20 g, 5 mmol) and sulfosalicylic acid (2.66 g, 10 mmol) were reacted in water to give a blue solution. The solution was filtered and then set aside for a week for the blue prismatic crystals of (I) to separate out. Analysis calculated for $C_{34}H_{26}CuN_4O_{12}S_2$: C 50.40, H 3.23, N 6.91%; found: C 50.33, H 3.28, N 6.89%.

Crystal data

$[\text{Cu}(\text{C}_7\text{H}_5\text{O}_6\text{S})(\text{C}_{10}\text{H}_8\text{N}_2)] \cdot (\text{C}_7\text{H}_5\text{O}_6\text{S})$
 $M_r = 810.25$
 Triclinic, $P\bar{1}$
 $a = 8.343(2) \text{ \AA}$
 $b = 12.302(3) \text{ \AA}$
 $c = 17.540(4) \text{ \AA}$
 $\alpha = 98.82(3)^\circ$
 $\beta = 102.77(3)^\circ$
 $\gamma = 97.70(3)^\circ$
 $V = 1708.4(6) \text{ \AA}^3$

$Z = 2$
 $D_x = 1.575 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 12 885 reflections
 $\theta = 3.1\text{--}27.7^\circ$
 $\mu = 0.83 \text{ mm}^{-1}$
 $T = 295(2) \text{ K}$
 Prism, blue
 $0.32 \times 0.24 \times 0.15 \text{ mm}$

Data collection

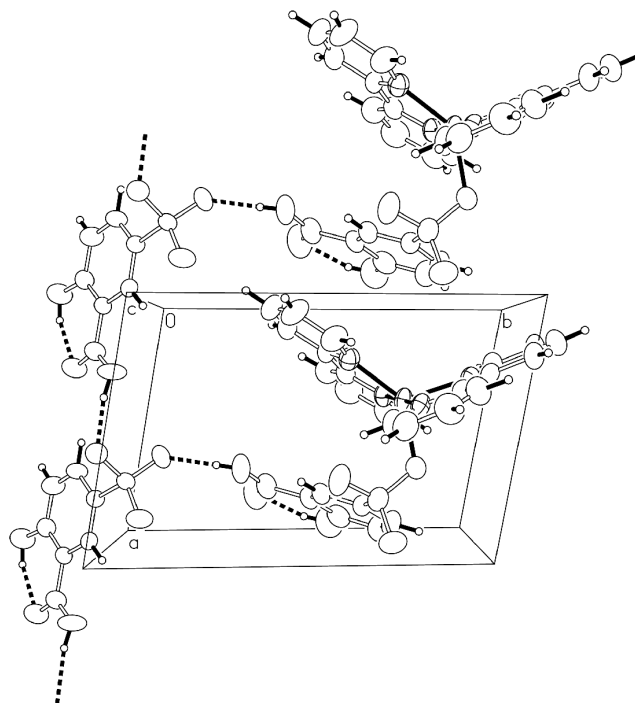
Rigaku R-AXIS RAPID diffractometer
 ω scans
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.407$, $T_{\max} = 0.885$
 15 414 measured reflections

7633 independent reflections
 4117 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.089$
 $\theta_{\text{max}} = 27.7^\circ$
 $h = -10 \rightarrow 10$
 $k = -15 \rightarrow 15$
 $l = -22 \rightarrow 22$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.067$
 $wR(F^2) = 0.147$
 $S = 1.00$
 7633 reflections
 494 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0627P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.46 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.42 \text{ e \AA}^{-3}$


Figure 2

Detail of (I), showing the hydrogen-bonded (dashed lines) structure.

Table 1

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

Cu1—O1	2.096 (3)	Cu1—N3	1.970 (3)
Cu1—N1	2.064 (4)	Cu1—N4	2.123 (4)
Cu1—N2	1.960 (4)		
O1—Cu1—N1	138.3 (1)	N1—Cu1—N3	96.4 (2)
O1—Cu1—N2	90.1 (1)	N1—Cu1—N4	124.1 (1)
O1—Cu1—N3	90.7 (1)	N2—Cu1—N3	176.4 (2)
O1—Cu1—N4	97.6 (1)	N2—Cu1—N4	103.4 (1)
N1—Cu1—N2	80.7 (2)	N3—Cu1—N4	80.0 (1)

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D\text{---}H \cdots A$	$D\text{---}H$	$H \cdots A$	$D \cdots A$	$D\text{---}H \cdots A$
O4—H4 α ...O5	0.85 (1)	1.82 (2)	2.625 (6)	158 (6)
O6—H6 α ...O7	0.85 (1)	1.78 (2)	2.609 (5)	164 (5)
O10—H10 α ...O11	0.85 (1)	1.87 (3)	2.634 (5)	149 (6)
O12—H12 α ...O8 ⁱ	0.85 (1)	1.77 (2)	2.589 (4)	163 (5)

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

The hydroxyl H atoms were found in a difference Fourier map and were refined with a distance restraint of $O\text{---}H = 0.85(1) \text{ \AA}$. The aromatic H atoms were placed at calculated positions ($C\text{---}H = 0.93 \text{ \AA}$) and were included in the refinement in the riding-model approximation with the constraint $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$ applied in all cases.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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