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Poly[2-aminopyridinium [aquacuprate(II)-μ_4-5-sulfonatosalicylato]]

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.034
wR factor = 0.078
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.

The title complex, $\{[Cu(C_7H_3O_6S)(H_2O)](C_5H_7N_2)\}_n$, consists of a polymeric anionic chain and protonated 2-aminopyridine. In the chain, each Cu^{II} atom has a distorted octahedral environment. The fully deprotonated 5-sulfonatosalicylate ligand acts as a μ_4-bridging link, resulting in a dinuclear Cu_2O_6 motif. N—H···O hydrogen bonds between cations and anions lead to a two-dimensional architecture.

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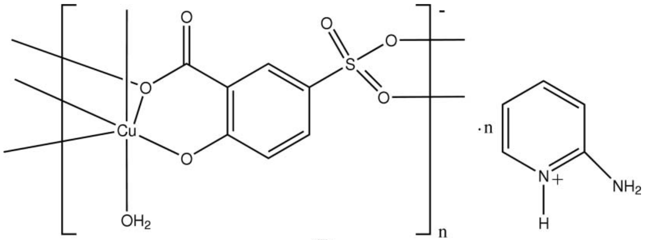
Comment

5-Sulfosalicylic acid possesses three functional groups which can be partly or fully deprotonated to give rise to interesting topologies (Ma *et al.*, 2003). A search of the Cambridge Structural Database (Version 5.26 of November 2004 Allen, 2002) and recent references revealed that about 40 crystal structures of 5-sulfosalicylate–metal complexes have been reported, among which are seven metal complexes containing fully deprotonated 5-sulfosalicylate (ssal^{3-}) (Fan & Zhu, 2005*a*,*b*; Fan *et al.*, 2005; Marzotto *et al.*, 2001; Sun *et al.*, 1995; Wang, Zhang, Li *et al.*, 2004; Wang, Zhang, Song & Ju, 2004). We present here another metal complex with ssal^{3-} in a new coordination mode, (I).



(I)

The complex consists of a polymeric anion and protonated 2-aminopyridine cations. In the polyanion, the Cu atom adopts a distorted octahedral geometry defined by five O atoms from two carboxylate, one phenolate and two sulfonate groups of four different ssal^{3-} ligands and one O atom from one water molecule (Fig. 1 and Table 1). The ssal^{3-} ligand serves as a μ_4-bridging link through carboxylate, phenolate and sulfonate groups. Both the sulfonate and the mono-oxygen of the carboxylate act in a bridging mode to form a Cu_2O_6 dimeric unit that is different from the Cu_2O_8 unit in $[Cu_2(CH_3COO)_4(H_2O)_2]$ (Brown & Chidambaram, 1973). Such a dimeric motif is the first example in 5-sulfosalicylate metal complexes. The Cu···Cu separation in this unit is 2.9961 (7) Å, significantly longer than that in $[Cu_2(CH_3COO)_4(H_2O)_2]$. As expected, the structure is extended into a chain by the bridging ssal^{3-} ligands (Fig. 2). The cations, *viz*. protonated 2-aminopyridine, interact with the anionic polymeric chains through N—H···O hydrogen bonds (Table 2) and the extended hydrogen-bonding network adopts a layer structure.

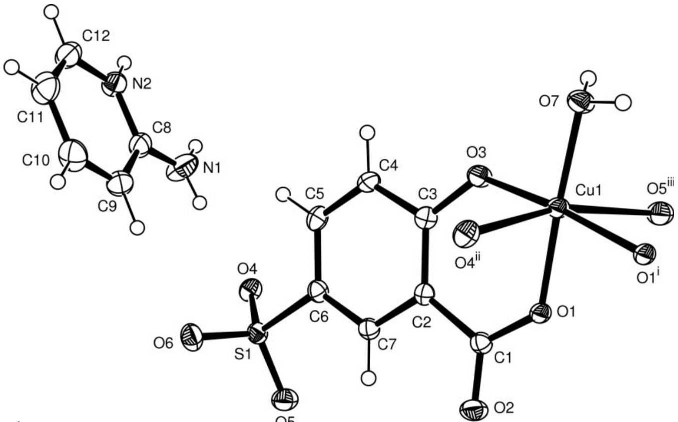


Figure 1
A view of a segment of (I). Displacement ellipsoids are drawn at the 40% probability level. [Symmetry codes (i): $1 - x, -y, 1 - z$; (ii): $x, -1 + y, z$; (iii) $1 - x, 1 - y, 1 - z$.]

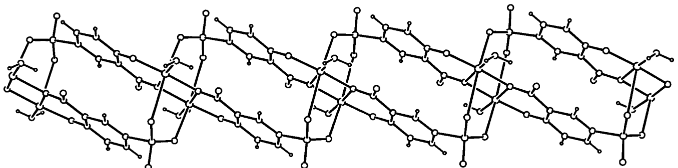


Figure 2
A view of the anionic one-dimensional chain in (I). H atoms have been omitted for clarity.

Experimental

$Cu(CH_3COO)_2\cdot H_2O$ (0.100 g, 0.50 mmol), 5-sulfosalicylic acid dihydrate (0.126 g, 0.50 mmol) and 2-aminopyridine (0.095 g, 1.0 mmol) were mixed in water (20 ml). The solution was set aside for the solvent to evaporate. After two weeks, green block-shaped crystals of (I) were obtained.

Crystal data

$[Cu(C_7H_3O_6S)(H_2O)](C_5H_7N_2)$
$M_r = 391.84$
Triclinic, $P\overline{1}$
$a = 7.7274$ (9) Å
$b = 8.0856$ (10) Å
$c = 12.1577$ (15) Å
$\alpha = 84.323$ (2)°
$\beta = 77.986$ (2)°
$\gamma = 69.051$ (1)°
$V = 693.62$ (15) Å^3
$Z = 2$
$D_x = 1.876$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2538 reflections
$\theta = 2.7$–28.2°
$\mu = 1.77$ mm^{-1}
$T = 295$ (2) K
Block, green
0.15 × 0.12 × 0.04 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\min} = 0.778$, $T_{\max} = 0.933$
5241 measured reflections
2554 independent reflections
2360 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$
$\theta_{\max} = 25.5°$
$h = -9 \rightarrow 9$
$k = -9 \rightarrow 9$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.078$
$S = 1.06$
2554 reflections
223 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0281P)^2 + 0.7674P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.38$ e Å^{-3}
$\Delta\rho_{\min} = -0.35$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.9392 (18)	Cu1—O7	1.937 (2)
Cu1—O1^{i}	1.9797 (18)	S1—O5	1.452 (2)
Cu1—O3	1.8771 (19)	S1—O4	1.455 (2)
Cu1—O4^{ii}	2.464 (2)	S1—O6	1.463 (2)
Cu1—O5^{iii}	2.779 (2)		
O1—Cu1—O1^{i}	80.27 (8)	O3—Cu1—O7	89.45 (9)
O1—Cu1—O4^{ii}	82.51 (7)	O4^{ii}—Cu1—O5^{iii}	167.09 (6)
O1^{i}—Cu1—O4^{ii}	88.64 (7)	O7—Cu1—O1	176.63 (8)
O1—Cu1—O5^{iii}	86.16 (7)	O7—Cu1—O1^{i}	96.36 (8)
O1^{i}—Cu1—O5^{iii}	83.35 (7)	O7—Cu1—O4^{ii}	97.25 (8)
O3—Cu1—O1	93.92 (8)	O7—Cu1—O5^{iii}	93.70 (8)
O3—Cu1—O1^{i}	174.14 (8)	O5—S1—O4	114.05 (13)
O3—Cu1—O4^{ii}	91.43 (8)	O5—S1—O6	112.24 (13)
O3—Cu1—O5^{iii}	95.51 (8)	O4—S1—O6	110.66 (12)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O7—H7$B\cdots$O3^{iv}	0.85 (3)	1.89 (3)	2.728 (3)	173 (3)
O7—H7$A\cdots$O2^{i}	0.84 (3)	1.88 (4)	2.667 (3)	155 (4)
N2—H3$N\cdots$O6^{v}	0.82 (4)	1.85 (4)	2.669 (3)	173 (4)
N1—H2$N\cdots$O5^{v}	0.82 (4)	2.27 (4)	3.076 (4)	168 (4)
N1—H1$N\cdots$O4	0.82 (4)	2.12 (4)	2.925 (4)	174 (4)

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

H atoms on C atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å and $U_{\rm iso}(H) = 1.2U_{\rm eq}(C)$. H atoms on O and N atoms were located in difference Fourier maps and were refined with distance restraints of O—H = 0.85 (1) Å and N—H = 0.82 (1) Å and fixed isotropic displacement parameters of $U_{\rm iso}(H) = 0.05$ Å^2.

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

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