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# *catena*-Poly[[[tetraaquacopper(II)]-$\mu$-4,4′-bipyridine-$\kappa^2N$:$N'$] 4-sulfonatobenzoate]

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**Key indicators**

Single-crystal X-ray study
$T$ = 295 K
Mean $\sigma$(C–C) = 0.003 Å
$R$ factor = 0.031
$wR$ factor = 0.083
Data-to-parameter ratio = 11.8

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

The title complex, $\{[\mathrm{Cu}(\mathrm{C_{10}H_8N_2})(\mathrm{H_2O})_4](\mathrm{C_7H_4O_5S})\}_n$, shows the cation to form a linear chain in which each Cu centre exists in a distorted octahedral geometry. Interactions between the cations and anions are mediated by hydrogen bonding, which gives rise to a three-dimensional architecture.

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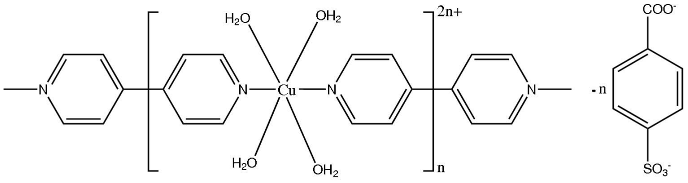
## Comment

The structural chemistry of complexes with the $[\mathrm{Co}(4,4'\text{-bipy})(\mathrm{H_2O})_4]^{2+}$ (4,4′-bipy is 4,4′-bipyridine) cation have been extensively studied (He *et al.*, 2005; Shen *et al.*, 2004; Dong *et al.*, 2000; Wang *et al.*, 2002) but, by contrast, only one analogous $[\mathrm{Cu}(4,4'\text{-bipy})(\mathrm{H_2O})_4]^{2+}$ complex has been characterized to date (Wang *et al.*, 1999). Recently, we have directed our attention to the structural systematics of 4-sulfobenzoate (sb) complexes and constructed a number of interesting topological architectures (Fan, Xiao, Zhang *et al.*, 2004; Fan, Xiao, Zhang & Zhu, 2004; Fan *et al.*, 2005; Zhang *et al.*, 2005*a*,*b*; Zhang & Zhu, 2005). As part of our investigations of metal–sb complexes, the title cation–anion complex, $[\mathrm{Cu}(4,4'\text{-bipy})(\mathrm{H_2O})_4]^{2+}\cdot[\mathrm{C_7H_4O_5S}]^{2-}$, (I), has been characterized and the results are presented here.



(I)

The title complex comprises a cation and an anion (Fig. 1 and Table 1). In the cation, the Cu atom adopts a distorted octahedral geometry defined by four O-donors, from four water molecules, and two N-donors, from two 4,4′-bipyridine ligands, so that the donor set is *trans*-$\mathrm{N_2O_4}$. The coordination mode of the 4,4′-bipy ligand leads to a linear cationic chain (Fig. 2). The two rings of the 4,4′-bipyridine molecule have a dihedral angle of 11.3 (2)°.

The anion is doubly deprotonated and does not coordinate to the Cu atom. The anion interacts with the cation through hydrogen bonds, so that the coordinated water molecules interact with sb through both the sulfonate and carboxyl groups to generate a three-dimensional hydrogen-bonding architecture (Table 2).

## Experimental

Crystals of (I) were obtained by the layer method using three layered solutions in a slender tube. The upper layer solution was $\mathrm{CH_3OH}$

(5 ml) containing 0.025 *M* 4,4′-bipyridine. The bottom layer was an aqueous solution (5 ml; pH = 6, adjusted by 1 *M* NaOH) containing 0.025 *M* $Cu(CH_3COO)_2\cdot H_2O$ and 0.025 *M* potassium hydrogen 4-sulfobenzoate. The middle layer was a $CH_3OH–H_2O$ (5 ml, *v*/*v*, 3:2) mixed solvent system. After standing for three weeks, blue block-shaped crystals of (I) were obtained and collected by suction filtration.

### *Crystal data*

$[Cu(C_{10}H_8N_2)(H_2O)_4](C_7H_4O_5S)$
$M_r = 491.95$
Triclinic, $P\overline{1}$
$a = 7.6210$ (4) Å
$b = 10.4049$ (6) Å
$c = 13.1550$ (8) Å
$\alpha = 68.003$ (1)°
$\beta = 85.642$ (1)°
$\gamma = 78.651$ (1)°
$V = 948.28$ (9) Å$^3$
$Z = 2$
$D_x = 1.723$ Mg m$^{-3}$
Mo *Kα* radiation
Cell parameters from 4069 reflections
$\theta = 2.7–28.2°$
$\mu = 1.32$ mm$^{-1}$
$T = 295$ (2) K
Block, blue
0.31 × 0.18 × 0.10 mm

### *Data collection*

Bruker APEX area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.685$, $T_{max} = 0.879$
7042 measured reflections
3479 independent reflections
3249 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 25.5°$
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -15 \rightarrow 15$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.083$
$S = 1.05$
3479 reflections
295 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0464P)^2 + 0.4714P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å$^{-3}$
$\Delta\rho_{min} = -0.35$ e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Cu1—O1 | 1.9961 (16) | Cu1—O4 | 2.3733 (17) |
| Cu1—O2 | 2.4556 (19) | Cu1—N1 | 2.0093 (17) |
| Cu1—O3 | 2.0072 (17) | Cu1—N2 | 2.0131 (17) |
| | | | |
| O1—Cu1—O2 | 91.35 (7) | O2—Cu1—N2 | 88.58 (7) |
| O1—Cu1—O3 | 178.38 (7) | O3—Cu1—O4 | 95.80 (7) |
| O1—Cu1—O4 | 85.79 (7) | O3—Cu1—N1 | 90.20 (7) |
| O1—Cu1—N1 | 90.11 (7) | O3—Cu1—N2 | 86.90 (7) |
| O1—Cu1—N2 | 92.76 (7) | O4—Cu1—N1 | 90.19 (7) |
| O2—Cu1—O3 | 87.06 (7) | O4—Cu1—N2 | 91.27 (7) |
| O2—Cu1—O4 | 177.13 (6) | N1—Cu1—N2 | 176.87 (7) |
| O2—Cu1—N1 | 90.10 (7) | | |

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1*A*···O5$^{i}$ | 0.84 (3) | 1.75 (3) | 2.587 (2) | 177 (3) |
| O3—H3*B*···O8$^{ii}$ | 0.84 (1) | 1.87 (1) | 2.704 (3) | 168 (3) |
| O2—H2*B*···O7$^{iii}$ | 0.84 (1) | 2.13 (1) | 2.941 (3) | 160 (3) |

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

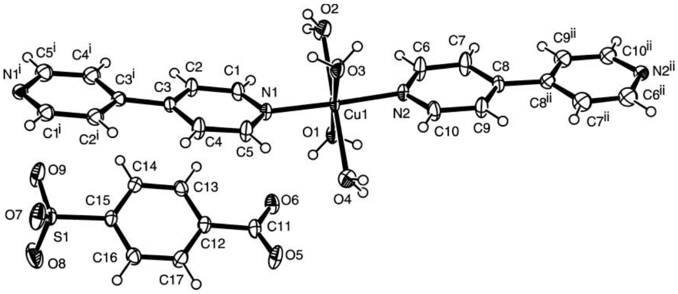


**Figure 1**
A view of a segment of the cationic chain in (I) and the independent sb dianion. Displacement ellipsoids are drawn at the 50% probability level. Symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $2 - x, 2 - y, 2 - z$.

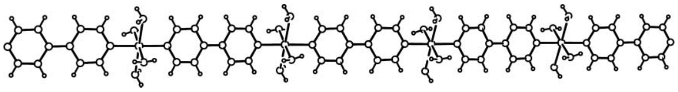


**Figure 2**
A view of the linear chain motif formed by the cation in (I).

Aromatic H atoms were positioned geometrically and were included in the refinement in the riding-model approximation, with C—H = 0.93 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$. Water H atoms were located in a difference Fourier map and were refined with a distance restraint of O—H = 0.85 (1) Å and with a fixed isotropic displacement parameter of $U_{iso}(H) = 0.05$ 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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