Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

catena-Poly[[μ-1,2-di-4-pyridylethylene-κ^2N,N'-[aqua(2-sulfonatobenzoato-κ^2O,O')copper(**II**)]] *N*,*N*-dimethylformamide]

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Received 4 April 2005
Accepted 13 April 2005
Online 16 April 2005

In the title compound, $[Cu(C_{12}H_8N_2)(C_7H_4SO_5)(H_2O)]\cdot C_3H_7NO$, the Cu^{II} atom has a square-pyramidal coordination geometry formed by three O atom and two N atoms. The 1,2-di-4-pyridylethylene ligands function as μ_2-bridging ligands to form a zigzag chain. The 2-sulfonatobenzoate ligands protrude on alternate sides of the chain. Intermolecular O—H···O hydrogen bonds link the chains into a two-dimensional network structure.

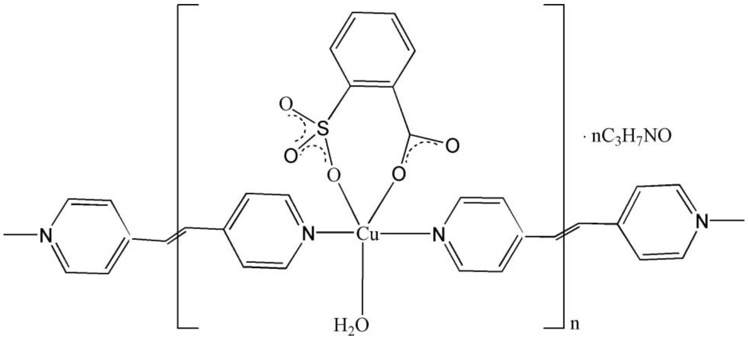
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.009 Å
R factor = 0.094
wR factor = 0.170
Data-to-parameter ratio = 13.2

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

Comment

The 2-sulfobenzoic acid (*o*-H$_2$sb) ligand, containing one sulfonate group and one carboxyl group, exhibits diverse coordination behaviour in the preparation of metal–organic coordination polymers (Li & Yang, 2004; Su *et al.*, 2005; Xiao *et al.*, 2005). Numerous novel coordination polymers with the 1,2-di-4-pyridylethylene (bpe) ligand have been synthesized in recent years (Hong & You, 2004; Kondo *et al.*, 2004; Yin & Xiao, 2005). Here, we present the crystal structure of the title compound, (I), from the same family.



(I)

In compound (I), the Cu^{II} atom has a square-pyramidal environment defined by one water O atom, two O atoms belonging to the 2-sulfonatobenzoate ligand and two N atoms from the two bpe ligands (Fig. 1). In the basal plane, the N2^i—Cu1—N1 [symmetry code: (i) $x, \frac{1}{2} - y, z - \frac{1}{2}$] and O1—Cu1—O6 bond angles are 163.59 (19) and 179.47 (19)°, respectively, while the other angles around the Cu^{II} centre are in the range 86.00 (17)–104.44 (17)°. The apical position is occupied by sulfonate atom O3, with an axial Cu—O bond distance of 2.268 (4) Å (Table 1). The *o*-sb ligand chelates to the Cu^{II} centre to form a six-membered ring, leading to a coordination mode observed previously in $[Ni(o\text{-}sb)(bpe)(H_2O)_2]\cdot 0.25H_2O$ (Xiao *et al.*, 2005). The dihedral angle between the planes of the *o*-sb ring and its carboxylate group is 62.5 (2)°. The C13—O1 bond [1.307 (7) Å] is longer than C13—O2 [1.212 (7) Å], indicating more keto character in the latter. Bpe ligands function as μ_2-bridging ligands, forming a zigzag polymeric chain. The *o*-sb ligands protrude on alternate sides of this chain (Fig. 2). Intermolecular O—H···O hydrogen bonds (Table 2) link the chains into a two-dimensional network structure (Fig. 3).

Experimental

An aqueous solution (10 ml) containing $Cu(ClO_4)_2\cdot 6H_2O$ (0.25 mmol, 0.910 g) was added slowly to a solution (10 ml) of *N*,*N*-dimethylformamide containing 1,2-di-4-pyridylethylene (0.25 mmol, 0.991 g) and 2-sulfobenzoic acid (0.25 mmol, 0.g). The mixture was left to stand at room temperature. Blue crystals of (I) were obtained after 5 d.

Crystal data

$[Cu(C_{12}H_8N_2)(C_7H_4SO_5)(H_2O)]\cdot C_3H_7NO$
$M_r = 537.03$
Orthorhombic, *Pbca*
$a = 17.3586\ (19)$ Å
$b = 9.8854\ (11)$ Å
$c = 26.324\ (3)$ Å
$V = 4517.1\ (9)$ Å^3
$Z = 8$
$D_x = 1.579$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2377 reflections
$\theta = 2.5$–$21.8°$
$\mu = 1.11$ mm^{-1}
$T = 298\ (2)$ K
Prism, blue
0.20 × 0.17 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.809$, $T_{max} = 0.851$
22 879 measured reflections
4102 independent reflections
3679 reflections with $I > 2\sigma(I)$
$R_{int} = 0.071$
$\theta_{max} = 25.3°$
$h = -19 \rightarrow 20$
$k = -11 \rightarrow 11$
$l = -28 \rightarrow 31$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.094$
$wR(F^2) = 0.170$
$S = 1.42$
4102 reflections
310 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0339P)^2 + 17.9772P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.64$ e Å^{-3}
$\Delta\rho_{min} = -0.81$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.958 (4)	Cu1—O3	2.268 (4)
Cu1—N2^{i}	1.992 (5)	O1—C13	1.307 (7)
Cu1—O6	1.993 (4)	O2—C13	1.212 (7)
Cu1—N1	2.018 (5)		
O1—Cu1—N2^{i}	92.38 (19)	O6—Cu1—N1	90.7 (2)
O1—Cu1—O6	179.47 (19)	O1—Cu1—O3	94.43 (18)
N2^{i}—Cu1—O6	87.82 (19)	N2^{i}—Cu1—O3	104.44 (17)
O1—Cu1—N1	88.98 (19)	O6—Cu1—O3	86.00 (17)
N2^{i}—Cu1—N1	163.59 (19)	N1—Cu1—O3	91.76 (18)

Symmetry code: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O6—H6*B*···O1^{ii}	0.82	1.88	2.693 (6)	170
O6—H6*A*···O7^{iii}	0.82	1.84	2.642 (7)	164

Symmetry codes: (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, z$; (iii) $x, y-1, z+1$.

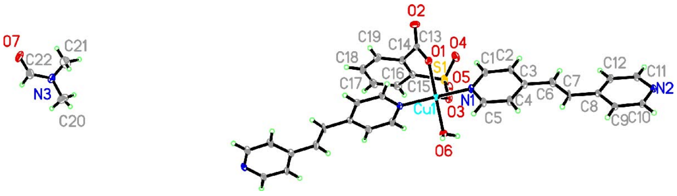


Figure 1
A view of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

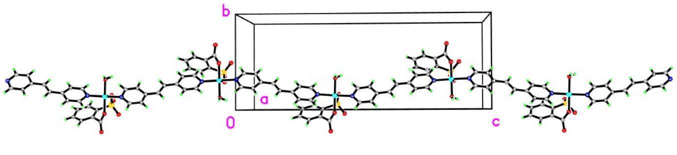


Figure 2
An illustration of the zigzag chain formed in the structure of (I).

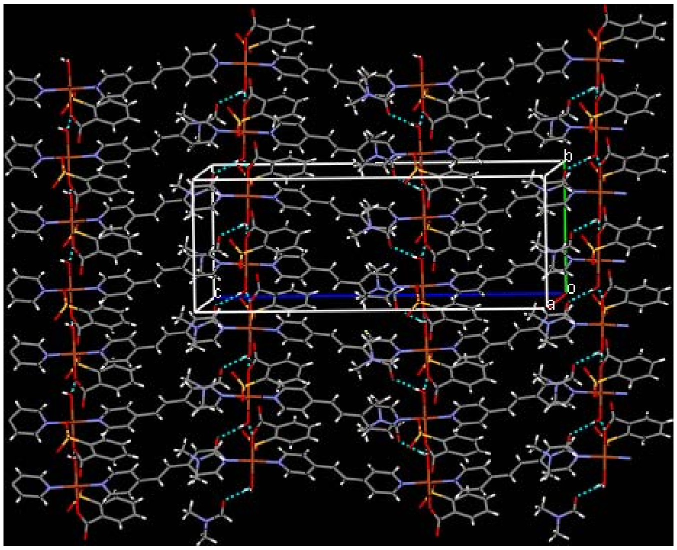


Figure 3
The two-dimensional network structure formed by O—H···O hydrogen bonds (dashed lines).

The H atoms of the water molecule were placed in calculated positions and refined using a riding model, with O—H distances of 0.82 Å and $U_{iso}(H) = 1.5U_{eq}(O)$. All H atoms of the dimethylformamide molecule were placed in calculated positions and refined using a riding-model approximation, with C–H distances of 0.93 Å for O═C—H and 0.96 Å for the methyl H atoms, and $U_{iso}(H) = 1.2$ (for CH) or 1.5 (for CH_3) times U_{eq}(parent atom). The remaining H atoms were positioned geometrically, with C—H = 0.93 Å, and allowed to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

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

The authors acknowledge financial support by the Zhejiang Provincial Natural Science Foundation (grant No. Y404294), the Wenzhou Science and Technology Project of China (grant

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