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Key indicators

Single-crystal X-ray study
$T = 298$ K
Mean σ(C–C) = 0.004 Å
R factor = 0.036
wR factor = 0.091
Data-to-parameter ratio = 12.7

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

Bis(μ-4-sulfamoylbenzoato)bis[chloro-(di-2-pyridylamine)copper(II)] dihydrate

In the title compound, $[Cu_2(C_7H_6NO_4S)_2Cl_2(C_{10}H_9N_3)_2]\cdot 2H_2O$, each Cu^{II} ion is six-coordinated by three O atoms, *viz.* carboxylate and sulfamoyl O atoms from two 4-sulfamoylbenzoate anions, by two N atoms from a di-2-pyridylamine ligand, and by a Cl atom. Each pair of Cu^{II} ions is bridged by two 4-sulfamoylbenzoate anions and each ion has the same coordination environment, forming a dinuclear ring. The dinuclear complex is centrosymmetric.

Comment

The design and synthesis of supramolecular inorganic architectures exhibiting novel properties provides exciting new opportunities (Swiegers & Malefetse, 2002; Johnson & Raymond, 2001; Hof *et al.*, 2002). In the synthesis of supramolecular inorganic architectures by design, the assembly of molecular units in predefined arrangements is a key goal (Desiraju, 1995, 1997; Braga *et al.*, 1998). Directional intermolecular interactions are the primary tools in achieving this goal and hydrogen bonding is currently the best among them (Zaworotko, 1997; Braga & Grepioni, 2000). We report here the structure of the title compound, (I).

(I)
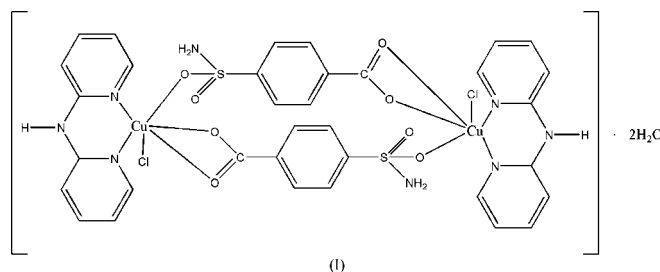
A dinuclear complex is formed, with each Cu^{II} ion coordinated by two O atoms from the carboxylate groups of a 4-sulfamoylbenzoate anion, one sulfamoyl O atom of a second 4-sulfamoylbenzoate anion, one Cl^- ion, and two N atoms from one 2,2′-dipyridylamine ligand, as shown in Fig. 1. The complex is centrosymmetric.

It should be noted that hydrogen-bonding interactions play an important role in the solid-state structure of (I), as shown in Fig. 2. Adjacent units are connected by hydrogen bonds to form a three-dimensional framework stucture (Table 2).

Experimental

Copper(II) chloride dihydrate (0.04 g, 0.2 mmol) was dissolved in water (10 ml), and the solution was mixed with a dimethylformamide solution (10 ml) of 2,2′-dipyridylamine (0.03 g, 0.2 mmol), 4-sulfamoylbenzoic acid (0.04 g, 0.2 mmol) and 2,2′-dithiosalicylic acid

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(0.07 g, 0.2 mmol). The reaction mixture was filtered and green block-shaped crystals of (I) were deposited from the solution after approximately one month.

Crystal data

$[Cu_2(C_7H_6NO_4S)_2Cl_2$-
$(C_{10}H_9N_3)_2]\cdot 2H_2O$
$M_r = 976.79$
Monoclinic, $P2_1/n$
$a = 8.4996 (6)$ Å
$b = 20.1067 (14)$ Å
$c = 11.7740 (8)$ Å
$\beta = 103.544 (1)°$
$V = 1956.2 (2)$ Å^3
$Z = 2$

$D_x = 1.658$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3474
reflections
$\theta = 2.2$–25.1°
$\mu = 1.40$ mm^{-1}
$T = 298 (2)$ K
Block, green
$0.39 \times 0.23 \times 0.20$ mm

Data collection

Bruker APEX area-detector
diffractometer
φ and ω scans
Absorption correction: multi-scan
(*SADABS*; Bruker, 2002)
$T_{min} = 0.685$, $T_{max} = 0.757$
10193 measured reflections

3474 independent reflections
3110 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 25.1°$
$h = -7 \rightarrow 10$
$k = -23 \rightarrow 24$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.091$
$S = 1.05$
3474 reflections
274 parameters
H atoms treated by a mixture of
independent and constrained
refinement

$w = 1/[\sigma^2(F_o^2) + (0.044P)^2$
$+ 1.1581P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.28$ e Å^{-3}
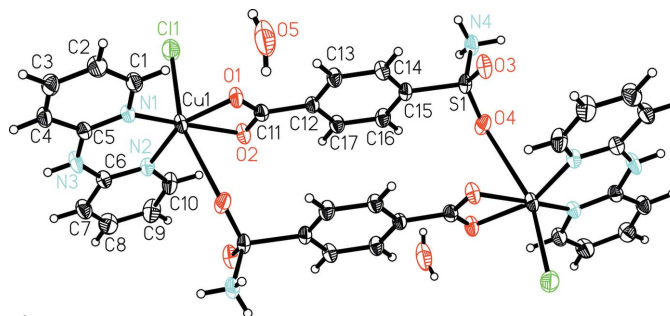$\Delta\rho_{min} = -0.33$ e Å^{-3}

Figure 1
The structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Unlabelled atoms are related to labelled atoms by the symmetry operator $(2 - x, 2 - y, 1 - z)$.
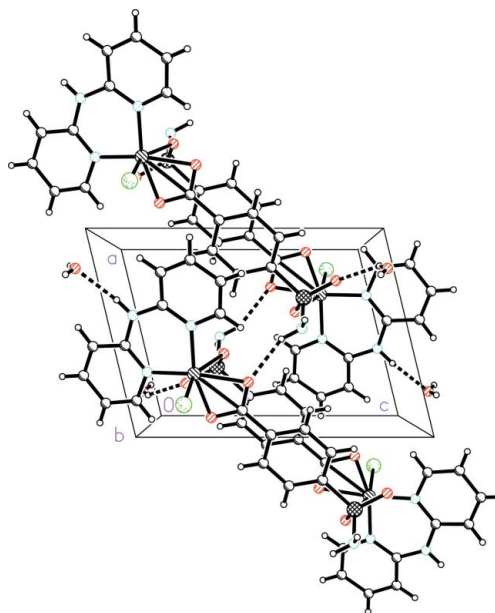

Figure 2
A perspective view of the molecular packing of (I) assembled *via* hydrogen bonds, which are shown as dashed lines.

Table 1
Selected geometric parameters (Å, °).

Cu1—N1	1.952 (2)	Cu1—O1	2.0815 (19)
Cu1—N2	1.972 (2)	Cu1—Cl1	2.5063 (9)
Cu1—O2	2.0093 (18)		
N1—Cu1—N2	94.10 (9)	N1—Cu1—Cl1	95.04 (7)
N1—Cu1—O2	162.82 (8)	N2—Cu1—Cl1	103.59 (7)
N2—Cu1—O2	98.59 (8)	O2—Cu1—Cl1	93.20 (6)
N1—Cu1—O1	100.31 (8)	O1—Cu1—Cl1	92.20 (6)
N2—Cu1—O1	157.61 (8)	C11—Cu1—Cl1	92.43 (7)
O2—Cu1—O1	64.28 (7)		

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O5—H5A$\cdots$O3^i	0.80 (3)	2.17 (3)	2.949 (4)	164 (7)
N4—H4B$\cdots$O1^{ii}	0.78 (4)	2.35 (4)	3.033 (3)	147 (4)
N3—H3N$\cdots$O5^{iii}	0.86	2.00	2.840 (4)	164

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

Water H atoms were refined subject to the restraint O—H = 0.82 (3) Å. The other H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of 0.86 (N—H), and 0.93 Å (C—H), with $U_{iso}(H) = 1.2U_{eq}$(parent atom). H atoms on N3 and N4 were all not refined and were positioned using the instruction AFIX 3 in *SHELXL97*, with N3—H = 0.86 Å and N4—H = 0.89 Å.

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: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97* (Sheldrick, 1997).

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