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Poly[diaqua-μ-oxalato-copper(II) monohydrate]

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Key indicators

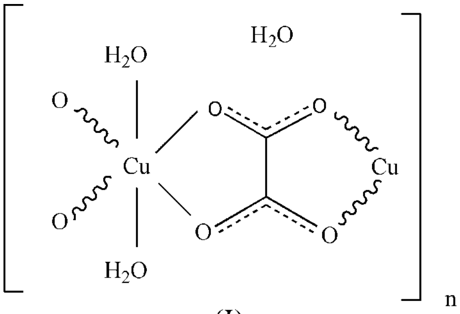
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.006 Å
R factor = 0.069
wR factor = 0.184
Data-to-parameter ratio = 12.7

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

The structure of the title compound, $\{[Cu(C_2O_4)(H_2O)_2]\cdot H_2O\}_n$, may be described as a one-dimensional zigzag chain, constructed of alternating bis-bidentate-bridged Cu atoms and oxalate groups. Two thirds of the water molecules coordinate to Cu atoms, and the rest are present as uncoordinated solvent. Intermolecular O—H···O hydrogen bonds link the molecules to form a three-dimensional supramolecular structure. The Cu atom and the uncoordinated water molecule lie on twofold rotation axes, and the oxalate ligand lies on an inversion centre.

Comment

Transition metal oxalate complexes exhibit diverse structure types, most of which could be classified as coordination polymers (Janiak, 2003). Among anhydrous or hydrated copper(II) oxalates, only β-CuC_2O_4 has been structurally characterized to date (Schmittler, 1968). We report here the synthesis and structure of the title compound, (I).



(I)

In the structure of (I) (Fig. 1 and Table 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The structure of (I) is similar to that of $[Mn(C_2O_4)]\cdot 3H_2O$ (Wu *et al.*, 2005). It may be described as a one-dimensional chain, constructed of alternating Cu atoms and oxalate groups, in which the oxalates are bis-bidentate-bridging to the Cu atoms, in a *cis* configuration, resulting in a zigzag chain structure. Two thirds of the water molecules are coordinated to Cu atoms, and the rest are present as uncoordinated solvent. The Cu atom and one uncoordinated water molecule lie on twofold rotation axes, and the oxalate ligand lies on an inversion centre.

As can be seen from the packing diagram (Fig. 2), intermolecular O—H···O hydrogen bonds (Table 2) link the molecules to form a three dimensional supramolecular structure; these hydrogen bonds may be effective in the stabilization of the crystal structure. Dipole–dipole and van der Waals interactions are also effective in the packing.

Experimental

The title compound was prepared from a mixture of $Cu(OAc)_2 \cdot H_2O$ (0.1996 g, 1 mmol), malonic acid (0.3122 g, 3 mmol), $(NH_4)_2C_2O_4 \cdot H_2O$ (0.1421 g, 1 mmol) and distilled water (15 ml), which was heated at 423 K for 72 h in a 23 ml Teflon-lined autoclave. The resulting crystals of (I) were washed with distilled water, collected by filtration, and then dried in air.

Crystal data

$[Cu(C_2O_4)(H_2O)_2] \cdot H_2O$
$M_r = 205.61$
Orthorhombic, *Pcca*
$a = 9.760$ (2) Å
$b = 6.6015$ (16) Å
$c = 10.500$ (3) Å
$V = 676.5$ (3) Å^3
$Z = 4$
$D_x = 2.019$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 3.21$ mm^{-1}
$T = 294$ (2) K
Needle, blue
0.35 × 0.10 × 0.06 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.658$, $T_{max} = 0.827$
1731 measured reflections
590 independent reflections
514 reflections with $I > 2\sigma(I)$
$R_{int} = 0.089$
$\theta_{max} = 25.1°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.070$
$wR(F^2) = 0.184$
$S = 1.62$
590 reflections
47 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0298P)^2 + 5.9975P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.86$ e Å^{-3}
$\Delta\rho_{min} = -1.19$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O3	2.162 (6)	C1—O1	1.242 (8)
Cu1—O1	2.182 (5)	C1—O2^{i}	1.246 (8)
Cu1—O2	2.204 (5)	C1—C1^{i}	1.574 (6)
O3—Cu1—O1	103.9 (2)	O1—Cu1—O2	75.1 (2)
O3—Cu1—O2	90.6 (2)	C1—O1—Cu1	116.7 (5)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3*B*···O4^{ii}	0.96	1.89	2.675 (8)	139
O3—H3*A*···O2^{iii}	0.96	1.92	2.827 (8)	156
O4—H4*A*···O1	0.96	1.85	2.751 (9)	154

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

H atoms were positioned geometrically, with O—H = 0.96 Å, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(O)$, where $x = 1.2$ and 1.5 for H atoms on O3 and O4, respectively. The deepest residual electron density hole is located 0.58 Å from atom Cu1.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

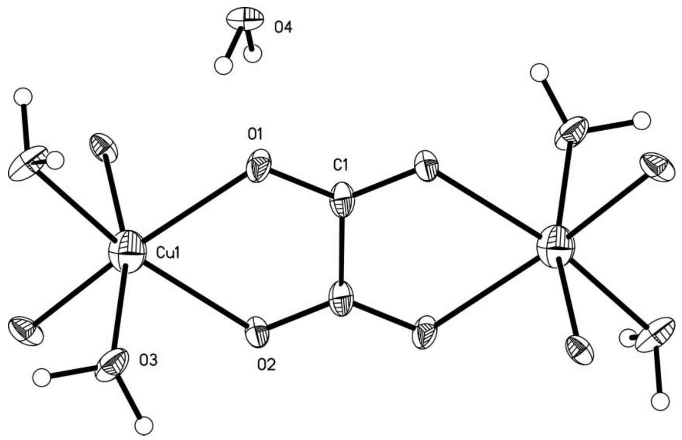


Figure 1
A fragment of the one-dimensional zigzag chain structure in (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

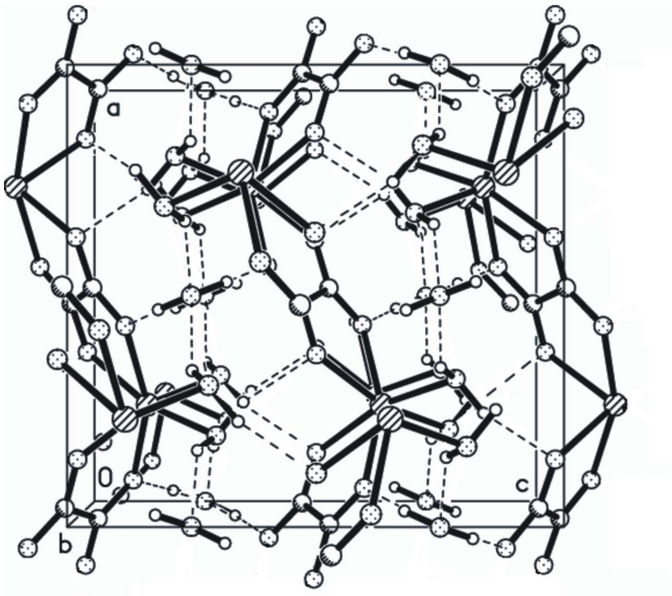


Figure 2
A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

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