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Bis(dimethylammonium) aquadioxalatocuprate(II) monohydrate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.002 Å
R factor = 0.025
wR factor = 0.073
Data-to-parameter ratio = 14.1

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

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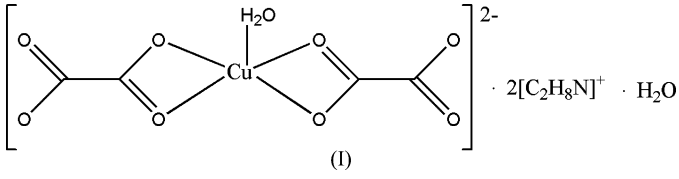
In the title compound, $(C_2H_8N)_2[Cu(C_2O_4)_2(H_2O)]\cdot H_2O$, the cations, anions and water molecules are linked by hydrogen bonds into a network structure. Two oxalate dianions and one water molecule are coordinated to the Cu atom and the geometry is square pyramidal.

Comment

The design and synthesis of supramolecular inorganic architectures exhibiting novel properties provide 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)

Compound (I) consists of dimethylammonium cations, $[Cu(C_2O_4)_2H_2O]^{2-}$ anions and solvent water molecules. The geometry around the Cu atom is square pyramidal, arising from coordination by two oxalate dianions and a water molecule (Fig. 1). The cations, anions and water molecules interact through O—H···O and N—H···O hydrogen bonds (Table 2) to generate a three-dimensional network (Fig. 2).

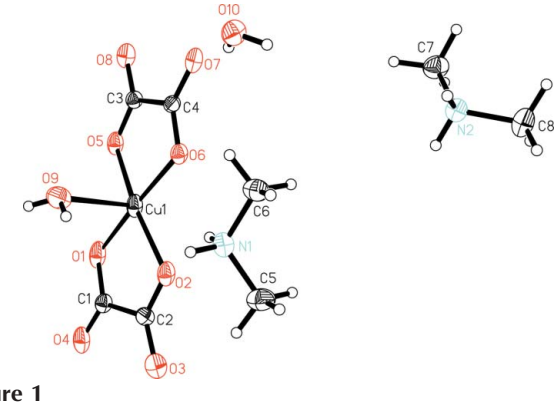


Figure 1
The asymmetric unit of (I) with the atom numbering, showing displacement ellipsoids at the 50% probability level.

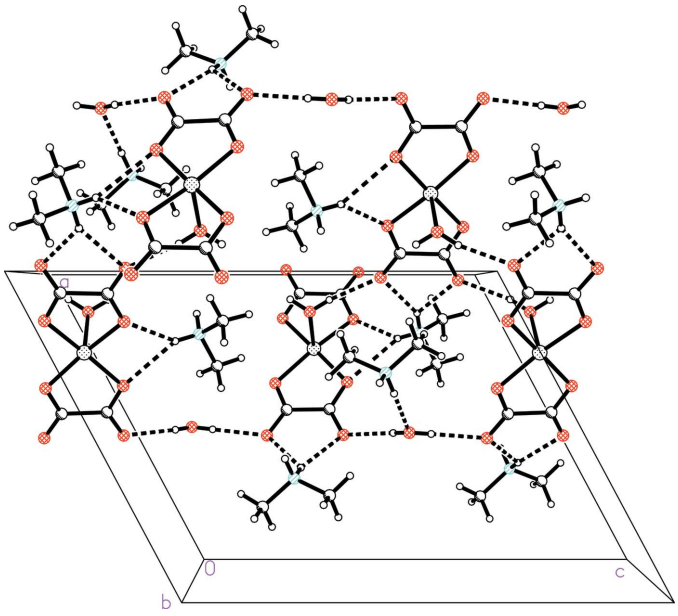


Figure 2
A perspective view of the molecular packing of (I), with hydrogen bonds shown as dashed lines.

Experimental

Copper(II) chloride dihydrate (0.04 g, 0.2 mmol) was dissolved in aqueous dimethylamine (40%, 10 ml), and the solution was mixed with a dimethylformamide solution (10 ml) of oxalic acid dihydrate (0.03 g, 0.2 mmol) and 2,2′-dithiosalicylic acid (0.07 g, 0.2 mmol). The reaction mixture was filtered. Blue prism-shaped crystals separated from the solution after about a month.

Crystal data

$(C_2H_8N)_2[Cu(C_2O_4)_2(H_2O)]\cdot H_2O$
M_r = 367.81
Monoclinic, $P2_1/c$
a = 11.7600 (16) Å
b = 9.5328 (13) Å
c = 15.3997 (16) Å
β = 118.103 (8)°
V = 1522.9 (3) Å^3
Z = 4
D_x = 1.604 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2706 reflections
θ = 2.0–25.1°
μ = 1.48 mm^{-1}
T = 298 (2) K
Prism, blue
0.50 × 0.27 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.63, T_{max} = 0.81
7740 measured reflections
2706 independent reflections
2436 reflections with $I > 2\sigma(I)$
R_{int} = 0.020
θ_{max} = 25.1°
$h = -14 \rightarrow 14$
$k = -11 \rightarrow 11$
$l = -18 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.073
S = 1.06
2706 reflections
192 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2 + 0.272P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0288 (13)

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.9334 (12)	Cu1—O6	1.9480 (11)
Cu1—O2	1.9640 (12)	Cu1—O9	2.3540 (15)
Cu1—O5	1.9377 (12)		
O1—Cu1—O2	84.57 (5)	O2—Cu1—O6	94.82 (5)
O1—Cu1—O5	94.58 (5)	O2—Cu1—O9	93.74 (5)
O1—Cu1—O6	176.01 (6)	O5—Cu1—O6	85.34 (5)
O1—Cu1—O9	95.78 (6)	O5—Cu1—O9	96.19 (6)
O2—Cu1—O5	170.07 (6)	O6—Cu1—O9	88.19 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
O10—H10B···O7	0.81	1.97	2.7443 (18)	160
O10—H10A···O8^{i}	0.81	2.03	2.8415 (18)	174
N2—H2B···O8^{i}	0.90	2.25	2.929 (2)	132
N2—H2B···O7^{i}	0.90	2.13	2.907 (2)	144
N2—H2A···O10^{ii}	0.90	1.88	2.776 (2)	175
N1—H1B···O3^{iii}	0.90	2.24	3.065 (2)	152
N1—H1B···O4^{iii}	0.90	2.14	2.809 (2)	130
N1—H1A···O6	0.90	2.48	3.2006 (19)	137
N1—H1A···O2	0.90	2.12	2.896 (2)	143
O9—H9B···O3^{iii}	0.82	2.05	2.8525 (19)	167
O9—H9A···O4^{iv}	0.82	1.99	2.7722 (19)	158

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

All H atoms were positioned geometrically and allowed to ride on their parent atoms, at distances of 0.82 (O—H), 0.90 (N—H) and 0.96 Å (C—H), and with U_{iso}(H) = 1.2U_{eq}(parent atom).

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*.

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