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catena-Poly[[[tetraaquacopper(II)]-μ-sulfato-κ^2O:O'-[bis(malonamide-κ^2O,O')copper(II)]-μ-sulfato-κ^2O:O'] dihydrate]

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Key indicators

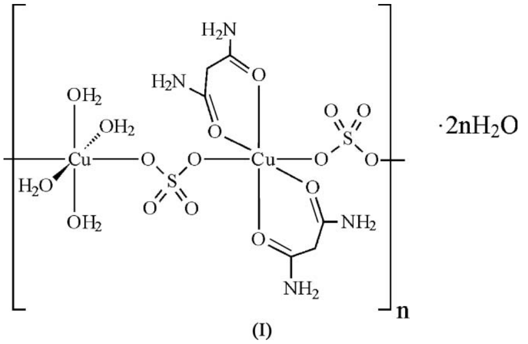
Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.005 Å
Some non-H atoms missing
R factor = 0.039
wR factor = 0.097
Data-to-parameter ratio = 13.5

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

In the title compound, $\{[Cu_2(SO_4)_2(C_3H_6N_2O_2)_2(H_2O)_4]\cdot 2H_2O\}$, two differently coordinated Cu atoms are bridged by the sulfate groups, forming a polymeric chain extending along the c axis. One Cu atom is coordinated by two malonamide molecules and two sulfate groups, while the other is coordinated by four water molecules and two sulfate groups. Both Cu atoms lie on centers of symmetry. An extensive three-dimensional hydrogen-bonding network involves the uncoordinated water molecules and stabilizes the crystal packing.

Comment

In our search for new compounds exhibiting biological activity, copper complexes containing the amide group are of interest. We report here the synthesis and crystal structure of the title compound, (I), a product of the reaction of $CuSO_4$ with malonamide (ML).



(I)

Two differently coordinated Cu atoms are bridged by the sulfate groups, forming a $–Cu(ML)_2–SO_4–Cu(H_2O)_4–SO_4–$ polymeric chain (Fig. 1) extending along the c axis. Both Cu atoms occupy centers of symmetry and adopt an octahedral geometry, being coordinated by two bridging sulfate groups and two chelating ML ligands for Cu1, and by four water molecules and two sulfate groups for Cu2 (Fig. 1). Atom Cu2 has an almost ideal octahedral coordination, while for atom Cu1 the deviation is more pronounced (Table 1). The bond lengths (Table 1) are in good agreement with those observed in similar complexes (Orpen *et al.*, 1989). An extensive three-dimensional hydrogen-bond network (Table 2) involves the uncoordinated water molecules and stabilizes the crystal packing.

Experimental

Saturated aqueous solutions of copper sulfate and malonamide (molar ratio 1:2) were mixed at room temperature. Blue crystals

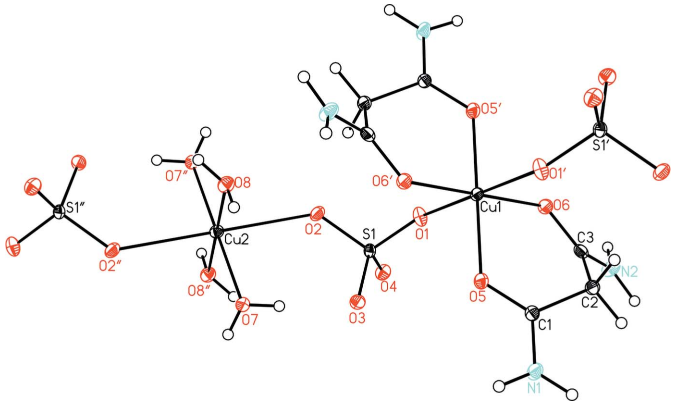


Figure 1
View of (I), showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. The primed and double primed labels are used for the atoms generated by the symmetry codes ($1 - x, -y, -z$) and ($1 - x, -y, -1 - z$), respectively. The uncoordinated water molecules have been omitted for clarity.

suitable for the X-ray analysis were obtained by isothermal evaporation of the solution at room temperature.

Crystal data

$[Cu_2(SO_4)_2(C_3H_6N_2O_2)_2$-
$(H_2O)_4]\cdot 2H_2O$
$M_r = 631.50$
Triclinic, $P\overline{1}$
$a = 6.7953$ (10) Å
$b = 7.1236$ (11) Å
$c = 12.2249$ (19) Å
$\alpha = 78.692$ (3)°
$\beta = 77.817$ (3)°
$\gamma = 64.214$ (2)°
$V = 517.18$ (14) Å^3
$Z = 1$
$D_x = 2.028$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 2.35$ mm^{-1}
$T = 120$ (2) K
Prism, blue
0.15 × 0.15 × 0.1 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
$T_{min} = 0.684$, $T_{max} = 0.790$
4014 measured reflections
1996 independent reflections
1813 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.098$
$S = 1.00$
1996 reflections
148 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.045P)^2 + 2.25P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.92$ e Å^{-3}
$\Delta\rho_{min} = -1.12$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	2.304 (2)	Cu2—O2	2.415 (2)
Cu1—O5	1.962 (2)	Cu2—O7	1.964 (2)
Cu1—O6	1.969 (2)	Cu2—O8	1.975 (2)
O1—Cu1—O5	95.63 (9)	O2—Cu2—O7	87.63 (9)
O1—Cu1—O6	84.49 (9)	O2—Cu2—O8	89.39 (9)
O5—Cu1—O6	93.11 (10)	O7—Cu2—O8	88.91 (10)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7*A*···O3	0.82	1.80	2.618 (3)	175
O7—H7*B*···O1*W*^{i}	0.82	1.95	2.714 (3)	156
O8—H8*A*···O1*W*^{ii}	0.82	1.97	2.765 (3)	162
O8—H8*B*···O4^{iii}	0.82	1.92	2.704 (3)	159
N1—H1*N*1···O4^{iv}	0.90	2.07	2.949 (4)	166
N1—H2*N*1···O5^{v}	0.90	2.14	3.029 (4)	171
N2—H1*N*2···O3^{iv}	0.90	2.12	2.985 (4)	162
N2—H2*N*2···O1^{vi}	0.90	2.18	2.943 (4)	143
O1*W*—H1*W*1···O4	0.82	2.05	2.798 (3)	151
O1*W*—H2*W*1···O2^{vii}	0.82	2.00	2.761 (3)	155

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

The H atoms of the NH_2 groups and of water molecules were found in a difference Fourier synthesis and fixed at distances of 0.90 and 0.82 Å from the N and O atoms, respectively. The C-bound H atoms were positioned geometrically, with C—H = 0.99 Å. All H atoms were refined as riding with $U_{iso}(H) = 1.2$–$1.5U_{eq}$(parent atom). The deepest residual density hole is located at 0.79 Å from atom Cu1.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1998); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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