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Key indicators

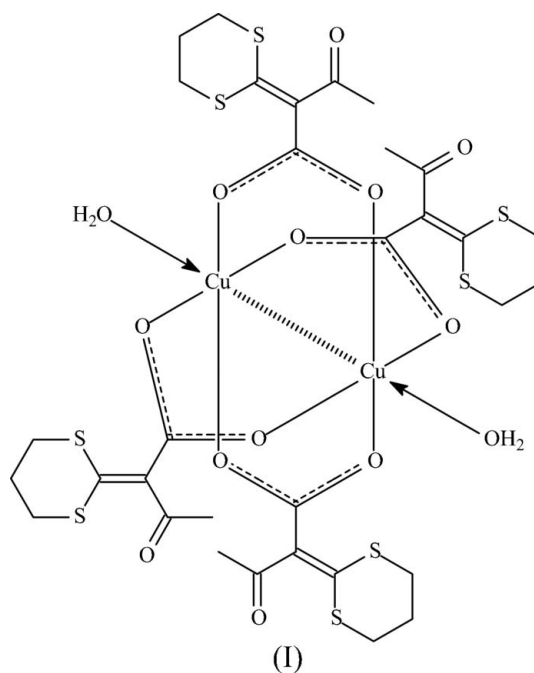
Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
Disorder in main residue
R factor = 0.034
wR factor = 0.092
Data-to-parameter ratio = 17.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Tetrakis[μ -2-(1,3-dithian-2-ylidene)-3-oxo-butanoato- $\kappa^2\text{O}:\text{O}'$]bis[aquacopper(II)]

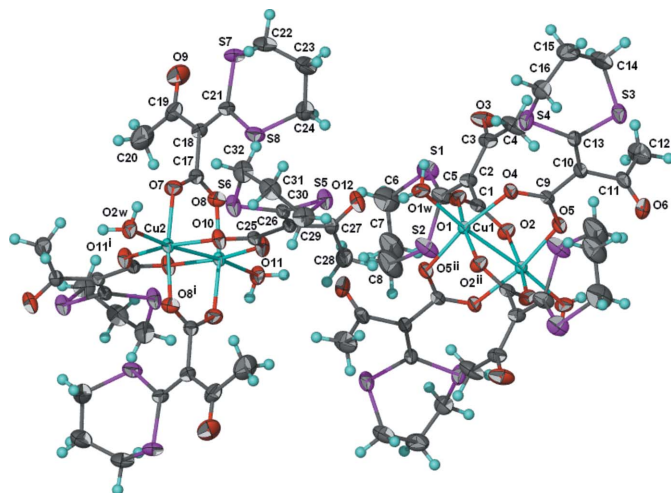
The two independent dinuclear molecules of the title compound, $[\text{Cu}_2(\text{C}_8\text{H}_9\text{O}_3\text{S}_2)_4(\text{H}_2\text{O})_2]$, lie on different inversion sites. In both molecules, two Cu atoms are bridged by four carboxylate groups, and the fifth coordination site of the square pyramid is occupied by the water molecule. Adjacent molecules are linked by hydrogen bonds into a three-dimensional network architecture.

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Comment

Among copper dicarboxylates, a common feature is the existence of a centrosymmetric dinuclear molecule whose Cu atoms are bridged by four carboxylate units, the O atoms of the units comprising a square around the metal atom. One coordination site above the plane is occupied by a donor ligand; the other Cu atom exists on the other side of the square plane at a distance that is indicative of a metal–metal bond. The structural literature has numerous such examples [Cambridge Structural Database (CSD), Version 5.25, November 2005; Allen, 2002]. The donor ligand is water if no other donor ligands are present in the synthesis. The tetrakis(μ -acetato)bis(aquacopper) (Kita *et al.*, 1992; de Meester *et al.*, 1973; Shamuratov *et al.*, 1994; van Niekerk & Schoening, 1953) homologue exemplifies this structural feature.




Figure 1

The two independent dinuclear molecules of (I), showing displacement ellipsoids drawn at the 50% probability level (H atoms are drawn as spheres of arbitrary radii). Only one disorder component of a dithiane ring is shown. [Symmetry codes (i): $-x, 1 - y, 1 - z$; (ii) $1 - x, 1 - y, 1 - z$.]

thioacetylation, has water as the donor ligand (Fig. 1). The two independent dinuclear molecules lie on different inversion sites. In both molecules, the Cu atoms are bridged by four carboxylate anions. The geometry is a square pyramid whose apical site is occupied by the water molecule. There is a short Cu...Cu distance [2.6434 (7) and 2.6407 (7) Å] in each independent molecule. The water molecules in the two dinuclear molecules interact with other Lewis acceptor sites (Table 2) to generate a three-dimensional network motif.

Experimental

2-(1,3-Dithian-2-ylidene)-3-oxobutanoic acid was synthesized as described in the literature (Liu *et al.*, 2003; Dong *et al.*, 2005). The acid (109 mg, 0.5 mmol) was added to a solution of copper(II) chloride dihydrate (43 mg, 0.25 mmol) dissolved in water (20 ml). The solution was heated to dissolve the reactants. Blue crystals separated from the solution after several days (about 60% yield, based on Cu).

Crystal data

[Cu₂(C₈H₉O₃S₂)₄(H₂O)₂]
M_r = 1032.20
 Monoclinic, *P*₂₁/*c*
a = 19.573 (5) Å
b = 12.050 (2) Å
c = 18.269 (4) Å
 β = 105.23 (1)°
V = 4157.5 (16) Å³

Z = 4
D_x = 1.649 Mg m⁻³
 Mo *K*α radiation
 μ = 1.49 mm⁻¹
T = 293 (2) K
 Block, blue
 0.45 × 0.38 × 0.21 mm

Data collection

Rigaku R-AXIS RAPID IP
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
T_{min} = 0.432, *T_{max}* = 0.745

39510 measured reflections
 9497 independent reflections
 8103 reflections with *I* > 2σ(*I*)
R_{int} = 0.031
θ_{max} = 27.5°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.034
wR (*F*²) = 0.092
S = 1.02
 9497 reflections
 540 parameters
 H atoms treated by a mixture of
 independent and constrained
 refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0513P)^2 + 2.5306P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.86 \text{ e } \text{Å}^{-3}$$

$$\Delta\rho_{\min} = -0.54 \text{ e } \text{Å}^{-3}$$

Table 1

Selected bond lengths (Å).

Cu1—O1	1.954 (2)	Cu2—O7	1.984 (2)
Cu1—O4	1.976 (2)	Cu2—O10	1.953 (2)
Cu1—O1W	2.140 (2)	Cu2—O2W	2.137 (2)

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1W—H1W1...O3 ⁱ	0.84 (1)	1.94 (2)	2.745 (3)	159 (3)
O1W—H1W2...O12	0.85 (1)	2.02 (1)	2.847 (3)	166 (3)
O2W—H2W1...O6 ⁱⁱ	0.86 (1)	1.96 (1)	2.790 (3)	165 (3)
O2W—H2W2...O9 ⁱⁱⁱ	0.85 (1)	1.98 (2)	2.804 (3)	162 (3)

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

One of the dithiane rings is disordered over two sites of occupancy 0.535 (6) and 0.465 (6). The occupancies of the unprimed and primed atoms were later fixed at 0.50 each. Pairs of 1,2-related distances were restrained to within 0.01 Å of each other. The displacement parameters of the primed atoms were set equal to those of the unprimed atoms. The water H atoms were located in a difference Fourier map and were refined with distance restraints of O—H = 0.85 (1) Å and H...H = 1.39 (1) Å; the atomic displacement parameters were refined. C-bound H atoms were positioned geometrically, with C—H = 0.96 or 0.97 Å, and were included in the riding-model approximation, with *U*_{iso}(H) = 1.2–1.5*U*_{eq}(C). The methyl groups were rotated to fit the electron density.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97* and publCIF (Westrip, 2006).

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