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Diaquabis(malato-$\kappa^2 O^1,O^2$)copper(II)

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In the title compound, $[Cu(C_6H_5O_5)_2(H_2O)_2]$, the Cu^{II} atom, located on an inversion center, is coordinated by four O atoms from two malate ligands forming the equatorial plane and two water molecules in axial positions, resulting in an elongated octahedral geometry. The structure of this compound has been reported previously [Polyanskaya *et al.* (1982). *Zh. Strukt. Khim.* **23**, 117–118], but the quality of the refinement has been improved. The packing is governed by intermolecular O—H···O hydrogen bonds, forming an intricate three-dimensional network.

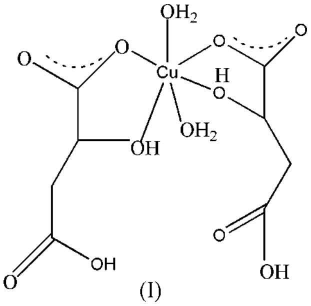
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.022
wR factor = 0.060
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.

Comment

Some hydroxypolycarboxylic acids are present in fruits and living cells and they also play an important role in biological processes (Kotsakis *et al.*, 2003). Hydroxypolycarboxylic acids can act not only as hydrogen-bond acceptors, but also as hydrogen-bond donors, depending on the number of deprotonated carboxyl groups. The structure of the title compound, (I), has been reported previously (Polyanskaya *et al.*, 1982), but the results of this new study are of higher precision.



(I)

The Cu^{II} atom, located on an inversion center, is coordinated by four O atoms from two malate ligands which form the equatorial plane of a distorted octahedron; two water molecules occupy the axial postions with a rather long Cu—O1W distance of 2.515 (1) Å (Fig. 1). Intermolecular O—H···O hydrogen bonds (Table 2) result in an intricate three-dimensional network.

Experimental

Malic acid (0.05 g, 0.82 mmol) and $Cu(CH_3COO)_2$ (0.18 g, 1.23 mmol) were added to a mixed solvent (15 ml) of ethanol and acetonitrile (2:1) and the resulting mixture was heated for 5 h under reflux. During the process, stirring and refluxing were required. The resulting solution into which diethyl ether was allowed to diffuse in a closed vessel. A week later some single crystals of a size suitable for X-ray diffraction analysis were obtained.

Crystal data

$[Cu(C_6H_5O_5)_2(H_2O)_2]$
$M_r = 365.73$
Monoclinic, $P2_1/c$
$a = 8.4762$ (5) Å
$b = 7.4377$ (4) Å
$c = 10.3117$ (6) Å
$\beta = 10.268$ (10)°
$V = 634.23$ (6) Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 1.79$ mm^{-1}
$T = 293$ (2) K
0.25 × 0.18 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.663$, $T_{\max} = 0.775$
3281 measured reflections
1243 independent reflections
1075 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.016$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$
$wR(F^2) = 0.060$
$S = 1.04$
1243 reflections
98 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{\max} = 0.27$ e Å^{-3}
$\Delta\rho_{\min} = -0.21$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2$^{\rm i}$	0.83	1.80	2.6254 (17)	171
O5—H5···O1$W^{\rm ii}$	0.82	1.88	2.6874 (19)	171
O1W—H1W···O2$^{\rm iii}$	0.83	2.02	2.8353 (19)	166
O1W—H2W···O4$^{\rm iv}$	0.83	2.04	2.842 (2)	161

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

All H atoms attached to C and hydroxyl O atoms were positioned geometrically and treated as riding, with C—H = 0.98 (methine) or 0.97 Å (methylene) and O—H = 0.82 Å, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) and 1.5$U_{\rm eq}$(O). Carboxylic H atoms were located in difference Fourier maps, but they were treated as riding on their parent O atoms, with O—H = 0.82–0.83 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(O).

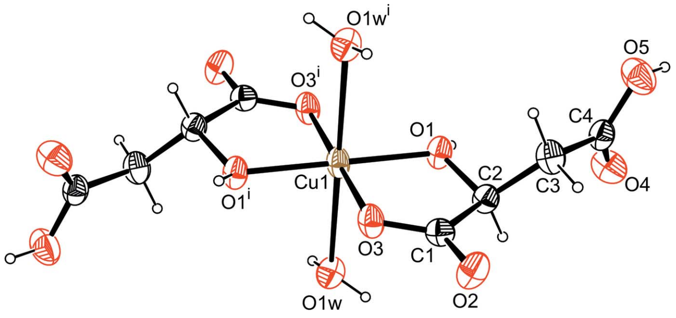


Figure 1
The molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented as small spheres of arbitrary radius. [Symmetry code: (i) $1-x, 1-y, 1-z$.]

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXTL* (Bruker, 1998).

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