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Key indicators

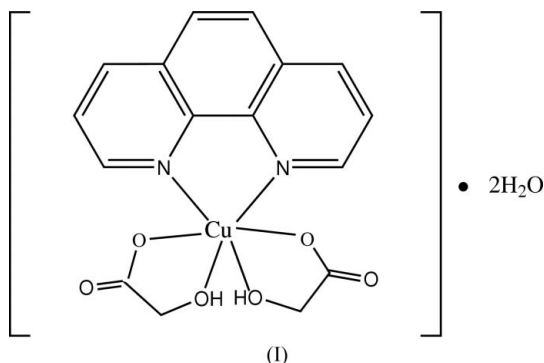
Single-crystal X-ray study
 $T = 273$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.021
 wR factor = 0.059
Data-to-parameter ratio = 16.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Bis(glycolato- $\kappa^2\text{O},\text{O}'$)(1,10-phenanthroline- $\kappa^2\text{N},\text{N}'$)copper(II) dihydrate

The title mononuclear complex, $[\text{Cu}(\text{C}_2\text{H}_3\text{O}_3)_2(\text{C}_{12}\text{H}_8\text{N}_2)] \cdot 2\text{H}_2\text{O}$, is isostructural with its zinc(II) analogue. The Cu atom in the complex exists in a distorted octahedral coordination environment, defined by four O atoms and two N atoms. O—H...O hydrogen bonds and π – π stacking interactions help to consolidate the crystal packing.

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Comment

The chemistry of glycolic acid complexes has grown substantially since the initial report in 1969 (Fischinger & Webb, 1969). The title complex, (I), is isostructural with its Zn^{II} analogue (Gao *et al.*, 2004).



As shown in Fig. 1, the geometry about the six-coordinated Cu^{II} atom can be described as a distorted octahedron. The two glycolate ligands act as two bidentate ligands in a distorted *cis*- CuO_4N_2 octahedral geometry, coordinating to the metal ions through their $\text{O}_{\text{carboxy}}$ and $\text{O}_{\text{C}-\text{OH}}$ atoms, forming five-membered chelating rings. The two carboxy O atoms occupy the pseudo-axial positions, while the two hydroxyl O atoms and the two N atoms of the 1,10-phenanthroline ligand are in a pseudo-plane, with an r.m.s. deviation of 0.1417 Å out of the plane.

The dihedral angle between the two five-membered chelating rings ($\text{Cu}1/\text{O}2^1/\text{C}7^1/\text{C}8/\text{O}3$ and $\text{Cu}1/\text{O}2/\text{C}7/\text{C}8^1/\text{O}3^1$) is $81.66(3)^\circ$ [symmetry code: (i) $-x, y, \frac{3}{2} - z$]. The $\text{Cu}-\text{O}_{\text{carboxy}}$ distances are relatively short [2.046 (1) Å], while the $\text{Cu}-\text{O}_{\text{C}-\text{OH}}$ bond lengths are longer [2.163 (1) Å] (Table 1).

Hydrogen-bonding interactions between the water molecules and carbonyl groups are observed (Fig. 2 and Table 2). The adjacent 1,10-phenanthroline planes are parallel to each other and the centroid-to-centroid distance between the central aromatic ring and the pyridyl ring of a neighbouring complex is 3.56 (2) Å.

Experimental

The title compound was obtained as blue blocks by slow evaporation at room temperature of a water–methanol (1: 2) solution of copper(II) acetate monohydrate [Cu(CH₃COO)₂·H₂O], 1,10-phenanthroline and glycolic acid in a 1:1:2 molar ratio.

Crystal data

[Cu(C₂H₃O₃)₂(C₁₂H₈N₂)]·2H₂O
M_r = 429.86
 Monoclinic, *C*₂/*c*
a = 8.3000 (6) Å
b = 24.534 (2) Å
c = 9.1356 (7) Å
 β = 109.660 (1)°
V = 1751.9 (2) Å³
Z = 4
D_x = 1.630 Mg m⁻³
 Mo *K*α radiation
 μ = 1.30 mm⁻¹
T = 273 (2) K
 Block, blue
 0.28 × 0.23 × 0.19 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.709, *T_{max}* = 0.786
 10361 measured reflections
 2154 independent reflections
 2025 reflections with *I* > 2σ*I*
R_{int} = 0.017
 θ_{max} = 28.3°

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.021
wR (*F*²) = 0.059
S = 1.00
 2154 reflections
 129 parameters
 H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.037P)^2 + 0.7037P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 (Δ/σ)_{max} < 0.001
 Δρ_{max} = 0.29 e Å⁻³
 Δρ_{min} = -0.31 e Å⁻³

Table 1 Selected geometric parameters (Å, °).

Cu1—O2	2.0456 (9)	Cu1—O3	2.1632 (10)
Cu1—N1	2.1334 (11)		
O2 ⁱ —Cu1—O2	160.38 (6)	O2—Cu1—O3	90.14 (4)
O2—Cu1—N1	96.13 (4)	N1—Cu1—O3	92.03 (4)
N1—Cu1—N1 ⁱ	78.07 (6)	N1 ⁱ —Cu1—O3	167.07 (4)
O2 ⁱ —Cu1—O3	77.06 (4)		

Symmetry code: (i) -*x*, *y*, -*z* + ½.

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—H1WA···O2	0.83	2.06	2.8622 (19)	165
O1W—H1WB···O1 ⁱⁱ	0.83	2.23	2.992 (2)	153
O3—H3B···O1 ⁱⁱⁱ	0.86 (2)	1.79 (2)	2.6469 (14)	174 (2)

Symmetry codes: (ii) -*x* + 1, *y*, -*z* + ½; (iii) -*x* + ½, -*y* + ½, -*z* + 2.

The H atoms of the solvent water molecules were located in a difference Fourier map and refined using a riding model, with an O—H distance restraint of 0.83 (6) Å. The H atom of the hydroxyl group was located in a difference Fourier map and refined isotropically. H atoms on all C atoms were included in calculated positions and constrained to an ideal geometry, with C—H distances of 0.93 or 0.97 Å and with *U*_{iso}(H) = 1.2*U*_{eq}(C).

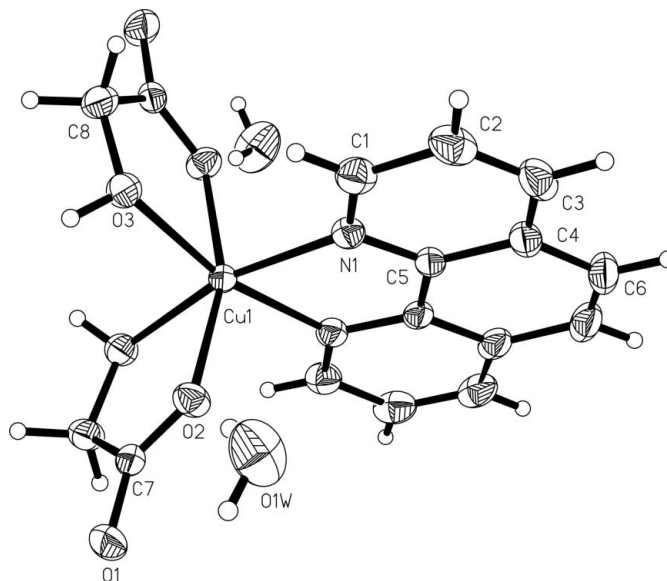


Figure 1 A view of the molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are shown at the 50% probability level. The unlabelled half of the molecule is generated by the symmetry operation (-*x*, *y*, ½ - *z*).

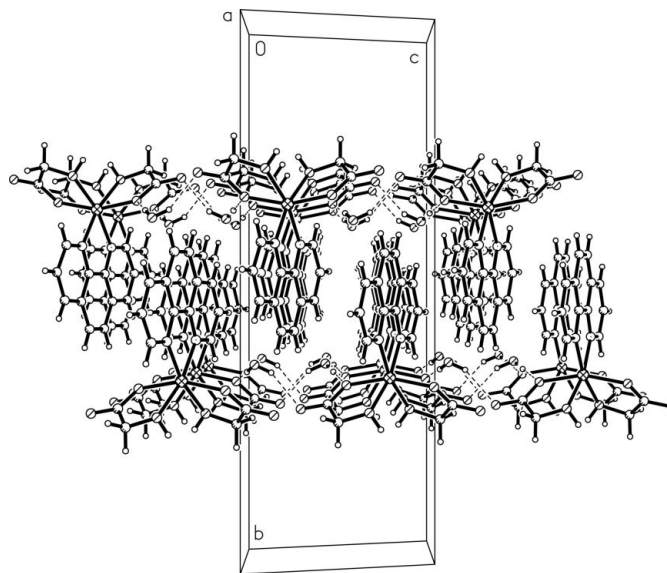


Figure 2 A partial packing diagram of complex (I), projected down the *a* axis. Weak intermolecular hydrogen bonds are shown as dashed lines.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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