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Aqua(2,2′-bipyridine-κ^2N,N')(L-malato-κ^3O,O',O'')-copper(II)

Long He

College of Pharmaceutical Sciences, Zhejiang University of Technology, Hangzhou 310014, People's Republic of China

Correspondence e-mail:
chemhelong@yahoo.com.cn

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In the title complex, $[Cu(C_4H_4O_5)(C_{10}H_8N_2)(H_2O)]$, the chiral L-malate group, which acts as a tridentate ligand, the bidentate 2,2′-bipyridine ligand and the water molecule provide an octahedral coordination of the Cu^{II} atom with strong Jahn–Teller distortion. Intermolecular O—H···O hydrogen bonds stabilize the crystal packing.

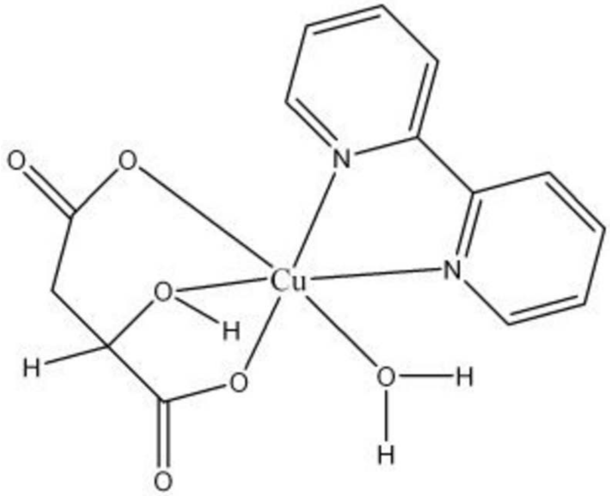
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.028
wR factor = 0.070
Data-to-parameter ratio = 13.8

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

Comment

Copper complexes with organic acids and other donor ligands are important for living things, being involved in a number of chemical and biochemical catalytic systems (King, 1994). The crystal structures of several copper–carboxylate complexes are known (Du *et al.*, 2004; Hu *et al.*, 2004; Li & Xiao, 2004). However, the structural aspects of copper complexes containing chiral organic acids are notably less studied. In this paper, we report the synthesis and X-ray crystal structure of a new mononuclear copper–L-malate acid complex with 2,2′-bipyridine.



(I)

In the title compound, (I) (Fig. 1), the Cu^{II} atom is six-coordinated by the two N atoms from 2,2′-bipyridine, three O atoms from the chiral L-malate group and atom O6 from the water molecule. The bond lengths and angles around the Cu atom (Table 1) clearly show a distorted octahedral coordination environment caused by a strong Jahn–Teller effect; the equatorial Cu—N and Cu—O bond lengths[1.9264 (14)–2.0090 (18) Å] are substantially shorter than the axial Cu—O bonds [2.4301 (18) and 2.468 (2) Å]. The S configuration of the chiral C atom (C12) in (I) is identical to that in L-malic acid.

The crystal packing (Fig. 2) is stabilized by intermolecular O—H···O hydrogen bonds (Table 2).

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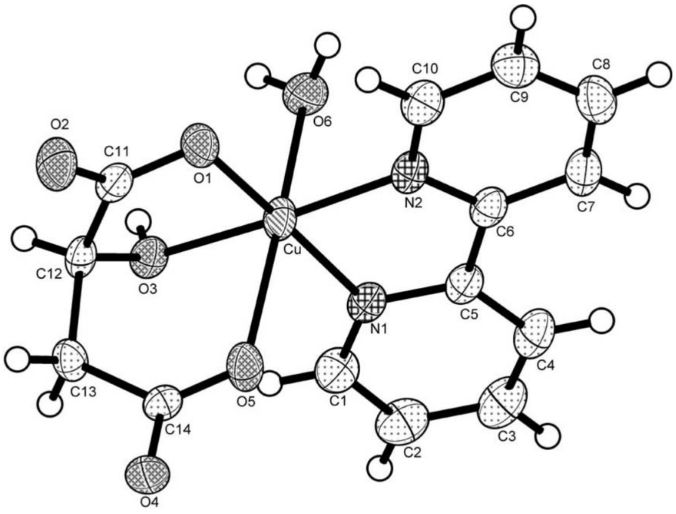

Figure 1
View of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

Experimental

L-Malic acid (270 mg, 2.0 mmol) and copper basic carbonate (240 mg, approximately 1.0 mmol) were dissolved in water (10 ml) with stirring. An ethanol solution (4 ml) of 2,2′-bipyridine (310 mg, 2.0 mmol) was added to the solution with stirring. After filtration, the filtrate was allowed to stand at room temperature and single crystals suitable for X-ray analysis were obtained after two weeks. Analysis calculated: C 45.47, H 3.82, N 7.58%; found: C 45.62, H 3.98, N 7.62%. IR (KBr, ν cm^{-1}): 791, 1315, 1401, 1557, 1625, 3246.

Crystal data

$[Cu(C_4H_4O_5)(C_{10}H_8N_2)(H_2O)]$
$M_r = 369.81$
Monoclinic, $P2_1$
$a = 10.4874$ (6) Å
$b = 6.5998$ (3) Å
$c = 10.7986$ (4) Å
$\beta = 106.570$ (2)°
$V = 716.38$ (6) Å^3
$Z = 2$

$D_x = 1.714$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5265 reflections
$\theta = 3.7$–27.5°
$\mu = 1.56$ mm^{-1}
$T = 293$ (2) K
Prism, blue
0.30 × 0.23 × 0.09 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.657$, $T_{max} = 0.869$
6910 measured reflections

3102 independent reflections
2966 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 27.5°$
$h = -13 \rightarrow 13$
$k = -8 \rightarrow 8$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.070$
$S = 1.11$
3102 reflections
225 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.032P)^2 + 0.1622P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0326 (18)
Absolute structure: Flack (1983), 1318 Friedel pairs
Flack parameter: −0.028 (11)

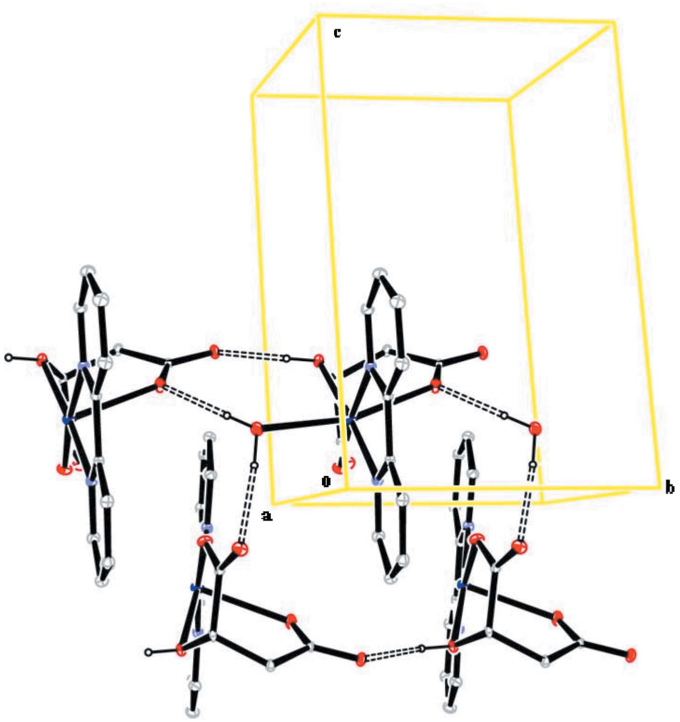

Figure 2
The molecular packing of (I), viewed approximately along the *a* axis. C-bound H atoms have been omitted for clarity. Dashed lines indicate hydrogen-bonding interactions.

Table 1
Selected geometric parameters (Å, °).

Cu—O1	1.9264 (14)	O1—C11	1.267 (3)
Cu—O3	2.0090 (18)	O2—C11	1.235 (3)
Cu—O5	2.4301 (18)	O3—C12	1.438 (3)
Cu—O6	2.468 (2)	O4—C14	1.254 (3)
Cu—N1	1.9850 (19)	O5—C14	1.244 (3)
Cu—N2	1.988 (2)		
O1—Cu—O3	83.87 (7)	O3—Cu—N2	175.88 (9)
O1—Cu—O5	88.45 (9)	O5—Cu—O6	166.12 (7)
O1—Cu—O6	100.98 (9)	O5—Cu—N1	86.73 (8)
O1—Cu—N1	174.12 (13)	O5—Cu—N2	104.38 (7)
O1—Cu—N2	96.17 (7)	O6—Cu—N1	84.38 (8)
O3—Cu—O5	79.74 (7)	O6—Cu—N2	84.88 (7)
O3—Cu—O6	91.05 (7)	N1—Cu—N2	81.81 (8)
O3—Cu—N1	98.55 (8)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H31···O4^{i}	0.78 (4)	1.84 (4)	2.551 (3)	151 (4)
O6—H61···O5^{i}	0.85 (3)	1.90 (3)	2.759 (3)	179 (4)
O6—H62···O2^{ii}	0.85 (2)	1.95 (2)	2.799 (3)	175 (3)

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

The hydroxyl H atom was located in a difference Fourier map and refined freely. The water H atoms were placed in idealized positions and refined with O—H distances restrained to 0.85 (3) Å, H···H distances of 1.39 (1) Å and U_{iso}(H) = 0.05 Å. The C-bound H atoms were positioned geometrically and refined as riding, with C—H distances of 0.93–0.98 Å and with U_{iso}(H) = 1.2–1.5U_{eq}(C).

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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