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catena-Poly[[[tripyridinecopper(II)]-μ-*m*-phenylenedioxydiacetato] monohydrate]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
Disorder in solvent or counterion
R factor = 0.051
wR factor = 0.132
Data-to-parameter ratio = 14.8

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

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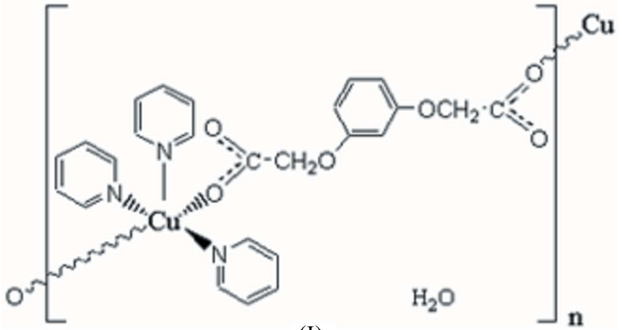
In the title compound, $[Cu(C_{10}H_8O_6)(C_5H_5N)_3]\cdot H_2O$, the coordination geometry around the Cu^{II} atom is distorted square-pyramidal, and the Cu—N bond at the apical position lies on a twofold axis. The *m*-phenylenedioxydiacetate ligand also has twofold symetry and acts as bridge to link Cu atoms to form infinite chains along the *c* axis. The solvent water molecule connects two adjacent carboxylate groups of the *m*-phenylenedioxydiacetates on the same chain *via* hydrogen bonds.

Comment

In recent years, metal–organic coordination polymers have been of great interest, due to their interesting topological structures and potential applications, such as new nanomaterials (Bai *et al.*, 2002). However, studies of copper(II) benzeneoxyacetate or benzenedioxyacetate are relatively scarce (Bickley *et al.*, 2004). A search of the Cambridge Structural Database (May 2005 update; Allen, 2002) for structures containing [Cu(pyridine)(phenyleneoxyacetato)] yielded 18 hits, but only one example involving benzene-1,3-dioxyacetate, namely $[Cu(H_2O)(py)_2$(benzene-1,3-dioxyacetate)] (Gao *et al.*, 2004). The title compound, (I), is reported here; it is a novel linear coordination polymer of Cu^{II} involving *m*-phenylenedioxydiacetate.



(I)

The asymmetric unit of (I) consists of one Cu^{II} ion, one and a half pyridine ligands and half a benzene-1,3-dioxyacetate ligand (Fig. 1). There is a twofold axis passing through atoms Cu1, N2 and C8, and another twofold axis through atoms C13 and C14 in the benzene ring of the ligand. The Cu^{II} ion is five-coordinated in a distorted square-pyramidal arrangement, by two O atoms of different carboxylate groups and two N atoms of two pyridine ligands in basal positions [N1, N1^{i}, O1 and O1^{i}; symmetry code: (i) $x, \frac{1}{2} - y, \frac{1}{2} - z$], and a pyridine N atom at the apex (N2). The Cu1—N2 bond length at the apex is longer than the Cu1—N1 bond at the equatorial position (Table 1).

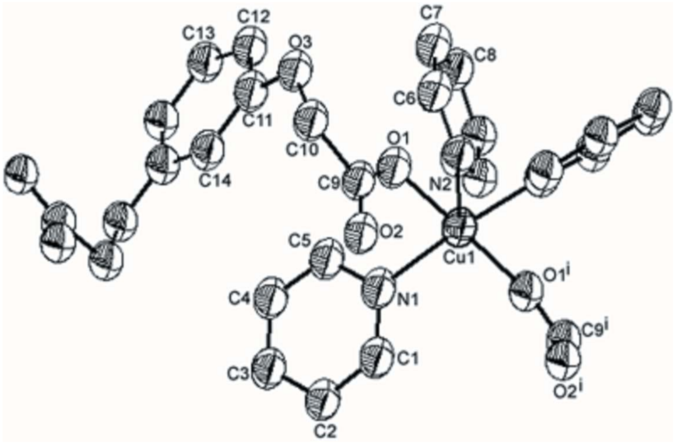


Figure 1
A view of (I) with the atom-numbering scheme, showing displacement ellipsoids at the 50% probability level. H atoms and the solvent water molecule have been omitted for clarity. [Symmetry code: (i) $x, \frac{1}{2} - y, \frac{1}{2} - z$.]

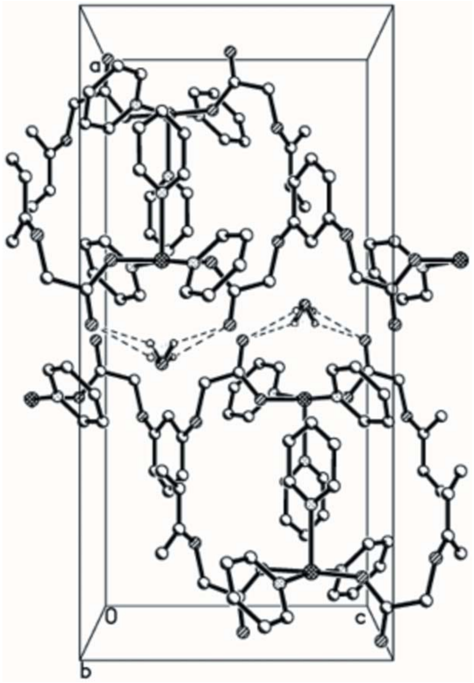


Figure 2
The crystal structure of (I), viewed down the *b* axis. H atoms have been omitted, except for those of the water molecule, which show positional disorder. Dashed lines indicate hydrogen bonds.

The pyridine ring at the apex of the pyramid is perpendicular to the basal plane of the pyramid.

The benzene-1,3-dioxyacetate ligands bridge the Cu^{II} ions to form infinite chains along the *c* axis (Fig. 2). Atom O1*W* of the solvent water molecule lies on a twofold axis and its H atoms show positional disorder. This water molecule connects two adjacent carboxylate groups of the benzene-1,3-dioxyacetate ligands in the same chain through a hydrogen bond (Table 2).

Experimental

Benzene-1,3-dioxyacetic acid was prepared according to the literature (Zhang *et al.*, 2001). Benzene-1,3-dioxyacetic acid (0.226 g, 1 mmol) and $Cu(NO_3)_2\cdot 6H_2O$ (0.371 g, 1.5 mmol) were dissolved in dimethylformamide (10 ml) and placed in a vial. The vial was then inserted into a larger container, which had previously been loaded with pyridine (3 ml). The larger container was sealed and the whole heated to 333 K, left undisturbed for 24 h, then cooled to room temperature and left undisturbed. Several days later, blue single crystals of (I) suitable for X-ray analysis were obtained (yield 15%). Compound (I) is stable in air and insoluble in water.

Crystal data

$[Cu(C_{10}H_8O_6)(C_5H_5N)_3]\cdot H_2O$
$M_r = 543.02$
Orthorhombic, *Pnna*
$a = 20.843$ (3) Å
$b = 11.964$ (1) Å
$c = 9.983$ (1) Å
$V = 2489.4$ (5) Å^3
$Z = 4$
$D_x = 1.449$ Mg m^{-3}

Mo *Kα* radiation
Cell parameters from 645 reflections
$\theta = 2.6$–19.6°
$\mu = 0.93$ mm^{-1}
$T = 293$ (2) K
Prism, blue
0.3 × 0.2 × 0.2 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.802$, $T_{max} = 0.833$
12469 measured reflections

2454 independent reflections
1392 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 26.0°$
$h = -24 \rightarrow 25$
$k = -13 \rightarrow 14$
$l = -12 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.132$
$S = 1.05$
2454 reflections
166 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.06P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.84$ e Å^{-3}
$\Delta\rho_{min} = -0.71$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.952 (2)	Cu1—N2	2.263 (5)
Cu1—N1	2.021 (3)		
O1—Cu1—O1^i	178.16 (15)	N1—Cu1—N1^i	170.97 (18)
O1—Cu1—N1	90.46 (11)	O1—Cu1—N2	90.92 (7)
O1—Cu1—N1^i	89.40 (11)	N1—Cu1—N2	94.51 (9)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1*W*—H1*WA*···O2^{ii}	0.85	2.07	2.772 (3)	139
O1*W*—H1*WB*···O2^{iii}	0.85	2.23	2.772 (4)	122

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

H atoms bonded to C atoms were positioned geometrically and refined as riding, with C—H distances in the range 0.93–0.97 Å and with $U_{iso}(H) = 1.2U_{eq}(C)$. The H atoms of the water molecule were

Acta Cryst. (2005). E**61**, m1556–m1558 Hong *et al.* • $[Cu(C_{10}H_8O_6)(C_5H_5N)_3]\cdot H_2O$ **m1557**

located in difference density maps and modified and constrained to maintain ideal geometry, with O—H = 0.85 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(O). Atom O1*W* lies on a twofold axis, and atoms H1*WA* and H1*WB* show positional disorder over two sites; the site occupancies of H1*WA* and H1*WB* are 50%.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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