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Bis(pyridine-2,4-dicarboxylato)copper(II) dihydrate

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Key indicators

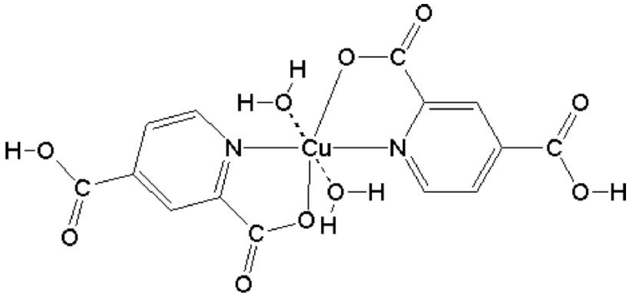
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.036
wR factor = 0.098
Data-to-parameter ratio = 10.3

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

A mononuclear copper(II) coordination complex, [Cu(Hpydc)$_2$]·2H$_2$O (pydc = 2,4-pyridinedicarboxylate, $C_7H_4NO_4$), has been prepared from the hydrothermal reaction of CuO and H$_2$pydc in H$_2$O. The complex consists of discrete [Cu(Hpydc)$_2$] and two uncoordinated water molecules, the copper(II) displaying a typical planar four-coordinate geometry. All Cu—O and Cu—N distances range from 1.945 (2) to 1.975 (2) Å. The discrete structure is further extended into a three-dimensional structure by weak hydrogen bonds.

Comment

Research into transition metal complexes has been rapidly expanding because of their fascinating structural diversity and potential applications as functional materials and enzymes. The key step in the design of polymeric transition metal complexes is to select suitable multidentate bridging ligands containing certain features, such as flexibility, versatile binding modes and the ability to form hydrogen bonds. With these criteria in mind, we chose pyridine-2,5-dicarboxylic acid as ligand. It reacts with transition metals or rare earths; a series of novel complexes having infinite or discrete structures has been obtained and reported (Liang *et al.*, 2000, 2001). In this paper, we report the synthesis and crystal structure of a mononuclear copper(II) compound, (I), *i.e.* [Cu(Hpydc)$_2$]·2H$_2$O, (I), where pydc is pyridine-2,4-dicarboxylate.



(I)

The coordination complex [Cu(Hpydc)$_2$]·2H$_2$O was prepared by the hydrothermal reaction of CuO and H$_2$pydc in H$_2$O. The crystallographic analysis reveals that the compound is a discrete [Cu(Hpydc)$_2$] molecule, in which the Cu^{II} atom is coordinated by the two N and two O atoms of two Hpydc ligands to form a distorted planar four-coordinate geometry, as shown in Fig. 1. There is a weak interaction between the Cu and hydrate O atoms, with an average Cu—O distance of 2.602 Å. Other Cu—O and Cu—N distances are listed in Table

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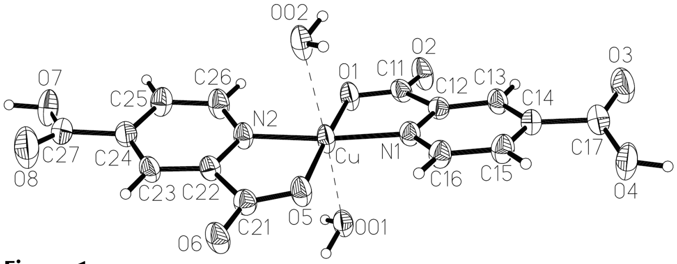

Figure 1
The structure of $[Cu(Hpydc)_2]\cdot 2H_2O$. Displacement ellipsoids are plotted at the 50% probability level.

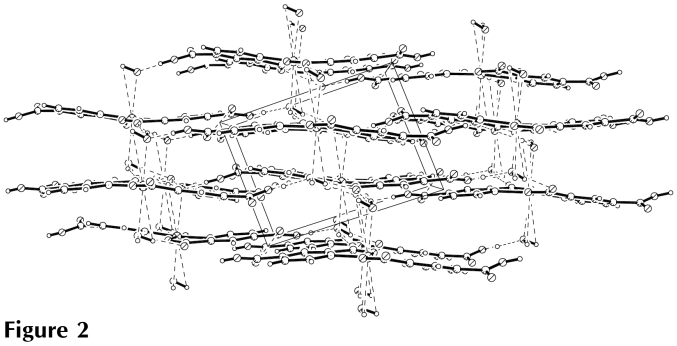

Figure 2
Packing diagram of $[Cu(Hpydc)_2]\cdot 2H_2O$. Dashed lines indicate the hydrogen bonds.

1, as are N—Cu—N, O—Cu—O and O—Cu—N angles. The molecules are connected by hydrogen-bonding interactions between the carboxylate groups and H_2O, with an average O···O distance of 2.675 Å, to form a three-dimensional network, as shown in Fig. 2.

Experimental

A mixture of CuO (0.080 g, 2.0 mmol), $[H_2pydc]\cdot H_2O$ (0.185 g, 1.0 mmol) and H_2O (16 ml) in a molar ratio of *ca* 2:1:890 was sealed in a 25 ml stainless-steel reactor with Teflon liner. The reaction system was heated at 443 K for 72 h. Slowly cooling the system to room temperature yielded needle-like green crystals of the complex and some blue–green precipitate. The organic H atoms were positioned geometrically (C—H bond fixed at 0.96 Å) and allowed to ride on their parent C atoms before the final cycle of refinement. The hydrate H atoms were located from difference maps and refined with isotropic displacement parameters.

Crystal data

$[Cu(C_7H_4NO_4)_2]\cdot 2H_2O$
$M_r = 431.80$
Triclinic, $P\overline{1}$
$a = 7.212$ (3) Å
$b = 10.139$ (3) Å
$c = 11.337$ (5) Å
$\alpha = 73.67$ (3)°
$\beta = 82.67$ (3)°
$\gamma = 85.04$ (3)°
$V = 787.8$ (5) Å^3

$Z = 2$
$D_x = 1.820$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4087 reflections
$\theta = 1.9$–25.0°
$\mu = 1.45$ mm^{-1}
$T = 293$ (2) K
Needle, green
0.42 × 0.10 × 0.04 mm

Data collection

SMART CCD diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.586$, $T_{max} = 0.944$
4087 measured reflections
2754 independent reflections

2345 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 25.0°$
$h = -8 \rightarrow 6$
$k = -11 \rightarrow 12$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.098$
$S = 1.04$
2754 reflections
268 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0527P)^2 + 0.4456P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.61$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—O5	1.945 (2)	O2—O01^{ii}	2.736 (3)
Cu—O1	1.948 (2)	O4—O02^{iii}	2.575 (3)
Cu—N2	1.972 (2)	O6—O02^{iv}	2.721 (3)
Cu—N1	1.975 (2)	O6—O01^{v}	2.764 (3)
O2—O02^{i}	2.716 (3)	O7—O01^{vi}	2.600 (3)
O5—Cu—O1	174.94 (9)	C11—O1—Cu	114.43 (17)
O5—Cu—N2	83.63 (9)	C21—O5—Cu	114.81 (17)
O1—Cu—N2	96.47 (9)	C16—N1—Cu	128.61 (19)
O5—Cu—N1	97.05 (9)	C12—N1—Cu	111.75 (18)
O1—Cu—N1	83.40 (9)	C26—N2—Cu	128.11 (19)
N2—Cu—N1	173.73 (10)	C22—N2—Cu	111.84 (18)

Symmetry codes: (i) $3 - x, 3 - y, 1 - z$; (ii) $2 - x, 3 - y, 1 - z$; (iii) $x, 1 + y, z$; (iv) $3 - x, 3 - y, -z$; (v) $2 - x, 3 - y, -z$; (vi) $x, y - 1, z$.

The organic H atoms were positioned geometrically (C—H bond fixed at 0.96 Å) and allowed to ride on their parent C atoms before the final cycle of refinement. The hydrate H atoms were located from difference maps and refined with isotropic displacement parameters.

Data collection: *SMART* (Siemens, 1994); cell refinement: *SMART* and *SAINT* (Siemens, 1994); data reduction: *XPREP* (Siemens, 1994); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXL*97; software used to prepare material for publication: *SHELXL*97.

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