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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 = 0.030
 wR factor = 0.099
Data-to-parameter ratio = 13.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

Diaquabis(pyridine-2,3-dicarboxylato)copper(II)

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The centrosymmetric title copper(II) complex, $[\text{Cu}(\text{C}_7\text{H}_4\text{NO}_4)_2(\text{H}_2\text{O})_2]$, was synthesized *via* the hydrothermal method at a mild temperature (353 K). The Cu^{II} ion has a distorted octahedral coordination environment, with two N and two O atoms from the pyridine-2,3-dicarboxylate ligands in a common plane and with two water molecules in axial positions. Hydrogen bonds play an important role in the formation of the three-dimensional structure.

Comment

The rational design and controlled crystallization of coordination complexes have received much attention (Kuduva *et al.*, 1999; Muthuraman *et al.*, 2001). A series of such complexes has been synthesized and characterized. Among the ligands, multidentate N- or O-donor ligands such as pyridine-dicarboxylic acids (pydcH₂) have drawn extensive attention (Harmon & Shaw, 1999; Puntus *et al.*, 2004; Du *et al.*, 2006), because they can be regarded not only as hydrogen-bond acceptors and donors, depending upon the number of deprotonated carboxylic groups, but also because π - π stacking interactions are also possible (Chen *et al.*, 2003). We present here the crystal structure of the title complex, (I).

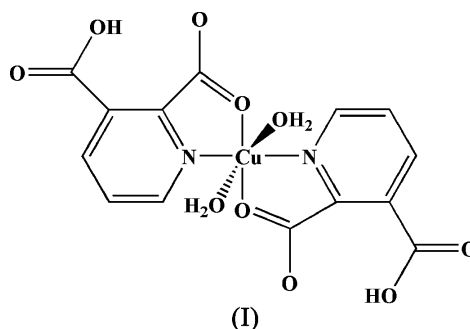
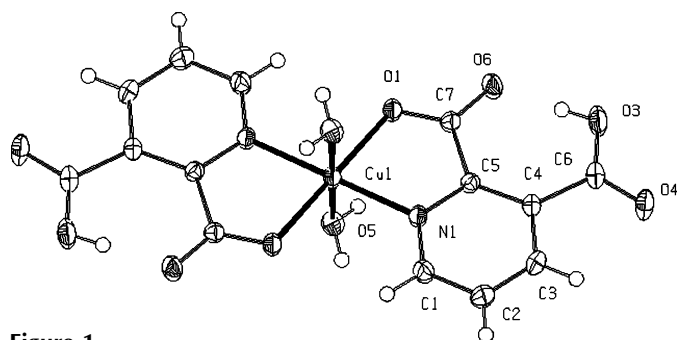
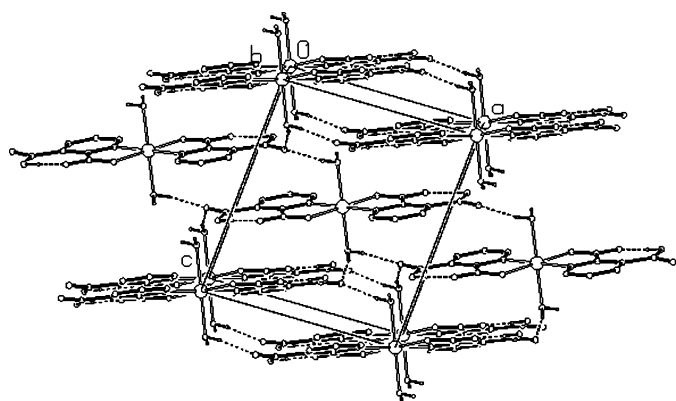


Fig. 1 shows the coordination environment of the Cu^{II} ion of (I), which lies on a special position of site symmetry $\bar{1}$ and has a distorted octahedral coordination environment. The equatorial plane is occupied by two pyridine-2,3-dicarboxylate ligands coordinating through the pyridine N and one O atom of the deprotonated 2-carboxyl group.

The molecules are connected by two types of hydrogen-bonding interactions. One is the interaction of the carboxylate groups and coordinated water molecules, which links the complexes to form a chain structure. The other is the interaction between neighbouring carboxylate groups (Fig. 2, Table 2).

**Figure 1**

The coordination environment of Cu^{II} in (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 70% probability level. Unlabelled atoms are generated by the symmetry operator (2 - x, -y, -z).

**Figure 2**

A packing diagram for (I), viewed approximately along the *b* axis. Dashed lines indicate hydrogen bonds.

Experimental

A mixture of CuO (0.0199 g, 0.25 mmol), 2,3-pydcH₂ (0.1025 g, 0.5 mmol) and H₂O (3 ml) was kept in a Teflon-lined autoclave at 353 K for 2 d and then cooled to room temperature. Block-like blue crystals of (I) were obtained in *ca* 78% yield based on CuO. The same product can also be obtained at a slightly higher temperature (393 K).

Crystal data

[Cu(C ₇ H ₄ NO ₄) ₂ (H ₂ O) ₂]	<i>Z</i> = 2
<i>M_r</i> = 431.80	<i>D_x</i> = 1.905 Mg m ⁻³
Monoclinic, <i>P</i> 2 ₁ / <i>n</i>	Mo <i>K</i> α radiation
<i>a</i> = 9.2115 (8) Å	<i>μ</i> = 1.52 mm ⁻¹
<i>b</i> = 7.9171 (6) Å	<i>T</i> = 273 (2) K
<i>c</i> = 10.3631 (9) Å	Block, blue
<i>β</i> = 94.945 (1)°	0.25 × 0.16 × 0.1 mm
<i>V</i> = 752.95 (11) Å ³	

Data collection

Bruker SMART CCD area-detector diffractometer	4841 measured reflections
<i>φ</i> and <i>ω</i> scans	1802 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1706 reflections with <i>I</i> > 2σ(<i>I</i>)
<i>T_{min}</i> = 0.703, <i>T_{max}</i> = 0.863	<i>R_{int}</i> = 0.012
	<i>θ_{max}</i> = 28.0°

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0615P)^2 + 0.6891P]$
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)] = 0.030	where $P = (F_o^2 + 2F_c^2)/3$
<i>wR</i> (<i>F</i> ²) = 0.099	(Δ/ <i>σ</i>) _{max} < 0.001
<i>S</i> = 1.04	Δ <i>ρ</i> _{max} = 0.47 e Å ⁻³
1802 reflections	Δ <i>ρ</i> _{min} = -0.68 e Å ⁻³
131 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997)
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.015 (3)

Table 1

Selected bond angles (°).

O1 ⁱ —Cu1—O1	180	N1—Cu1—O5 ⁱ	91.00 (6)
O1 ⁱ —Cu1—N1	79.17 (6)	O1—Cu1—O5	89.74 (5)
O1—Cu1—N1	100.83 (6)	N1—Cu1—O5	89.00 (6)
N1—Cu1—N1 ⁱ	180	O5 ⁱ —Cu1—O5	180
O1—Cu1—O5 ⁱ	90.26 (5)	C7—O1—Cu1	116.75 (12)

Symmetry code: (i) -x + 2, -y, -z.

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>
O5—H6...O4 ⁱⁱ	0.81 (1)	2.02 (1)	2.813 (2)	167 (3)
O3—H4...O6 ⁱ	0.82	1.58	2.398 (2)	178
O5—H5...O4 ⁱⁱⁱ	0.81 (1)	2.06 (1)	2.859 (2)	171 (3)

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

H atoms bonded to O atoms were located in a difference map and refined isotropically, with distance restraints of O—H = 0.82 (1) Å and H...H = 1.4 (1) Å. H atoms bonded to C atoms were placed in idealized locations, with C—H = 0.95 Å, and were refined using a riding model. For all H atoms, *U*_{iso}(H) = 1.2*U*_{eq}(C,O).

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

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