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catena-Poly[[diaquacopper(II)]-μ-pyridine-2,4-dicarboxylato-$\kappa^3N,O^2:O^4$]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.037
wR factor = 0.097
Data-to-parameter ratio = 14.4

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

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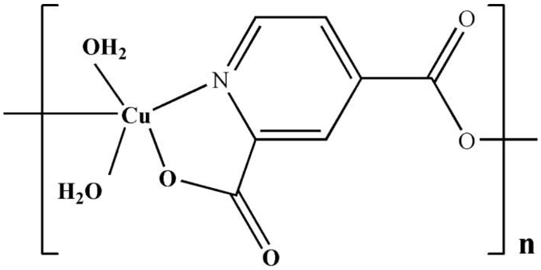
In the title polymer, $[Cu(C_7H_3NO_4)(H_2O)_2]_n$, the Cu^{II} ion is pentacoordinated and exhibits a distorted square-pyramidal environment formed by one N atom and two O atoms from pyridine-2,4-dicarboxylate ligands and two O atoms from coordinated water molecules. Each pyridine-2,4-dicarboxylate ligand bridges two Cu^{II} ions, to generate an infinite zigzag chain. Adjacent chains are linked by O—H···O hydrogen bonds, forming a three-dimensional network.

Comment

Pyridine-2,4-dicarboxylate, a non-linear multidentate ligand, can also be a good linker, because it can tolerate a distortion in its molecular geometry, resulting in an expansion of the angle between coordination sites (Min *et al.*, 2001; Liang *et al.*, 2002; Sileo *et al.*, 2003; Tong *et al.*, 2005). We report here the structure of such a pyridine-2,4-dicarboxylate-containing coordination polymer, the title compound, (I).



(I)

As shown in Fig. 1, the Cu^{II} ion in (I) adopts a square-pyramidal geometry and is coordinated by four O atoms, two of which belong to the two carboxylate groups of the pyridine-2,4-dicarboxylate ligand and two of which are from coordinated water molecules; one pyridine N atom completes the fivefold coordination environment around the metal centre. Geometric parameters (Table 1) are within normal ranges (Min *et al.*, 2001).

The pyridine-2,4-dicarboxylate ligand acts as a bridge *via* carboxylate atom O3, linking monomeric units in a head-to-tail fashion. This behaviour results in an infinite zigzag chain running along the [010] axis. Adjacent chains in the crystal structure are further extended into a three-dimensional network by extensive hydrogen bonds between coordinated water molecules and carboxylate O atoms (Fig. 2 and Table 2).

Experimental

$Cu(MeCO_2)_2\cdot H_2O$ (0.199 g, 1 mmol), pyridine-2,4-dicarboxylic acid (0.166 g, 1 mmol), sodium hydroxide (0.040 g, 1 mmol) and water

(14 ml) were placed in a 23 ml Teflon-lined autoclave, which was heated at 423 K for 3 d. After the mixture had cooled slowly to room temperature at a rate of 10 K h^{-1}, blue block-shaped crystals of (I) were isolated from the solution.

Crystal data

$[Cu(C_7H_3NO_4)(H_2O)_2]$
$M_r = 264.68$
Monoclinic, $P2_1/n$
$a = 7.1529$ (10) Å
$b = 13.5737$ (18) Å
$c = 9.1813$ (13) Å
$\beta = 107.797$ (2)°
$V = 848.8$ (2) Å^3

$Z = 4$
$D_x = 2.071$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 2.58$ mm^{-1}
$T = 293$ (2) K
Block, blue
0.27 × 0.22 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.522$, $T_{\max} = 0.620$

5016 measured reflections
1957 independent reflections
1620 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.041$
$\theta_{\max} = 28.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.097$
$S = 1.04$
1957 reflections
136 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 0.1458P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.004$
$\Delta\rho_{\max} = 0.81$ e Å^{-3}
$\Delta\rho_{\min} = -0.41$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1*W*	1.923 (2)	Cu1—N1	1.982 (2)
Cu1—O3$^{\rm i}$	1.9262 (19)	Cu1—O2*W*	2.345 (2)
Cu1—O1	1.9461 (19)		
O1*W*—Cu1—O3$^{\rm i}$	93.23 (8)	O1—Cu1—N1	82.79 (9)
O1*W*—Cu1—O1	91.46 (8)	O1*W*—Cu1—O2*W*	91.44 (9)
O3$^{\rm i}$—Cu1—O1	165.62 (9)	O3$^{\rm i}$—Cu1—O2*W*	89.16 (8)
O1*W*—Cu1—N1	174.24 (9)	O1—Cu1—O2*W*	104.31 (9)
O3$^{\rm i}$—Cu1—N1	92.26 (9)	N1—Cu1—O2*W*	90.37 (8)

Symmetry code: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O1$^{\rm ii}$	0.86	1.82	2.664 (3)	169
O1*W*—H1*WA*···O2$^{\rm ii}$	0.86	2.65	3.139 (3)	118
O1*W*—H1*WB*···O4$^{\rm i}$	0.84	1.83	2.659 (3)	167
O2*W*—H2*WA*···O2$^{\rm iii}$	0.83	1.99	2.822 (3)	174
O2*W*—H2*WB*···O4$^{\rm iv}$	0.83	2.37	3.107 (3)	149

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+3, -y+2, -z+2$; (iii) $-x+\frac{5}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x+1, -y+2, -z+1$.

Water H atoms were located in a difference map and refined as riding in their as-found relative positions, with $U_{\rm iso}({\rm H}) = 1.5_{U\rm eq}({\rm O})$. Other H atoms were placed in calculated positions and refined as riding on their parent atoms, with C—H = 0.93 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

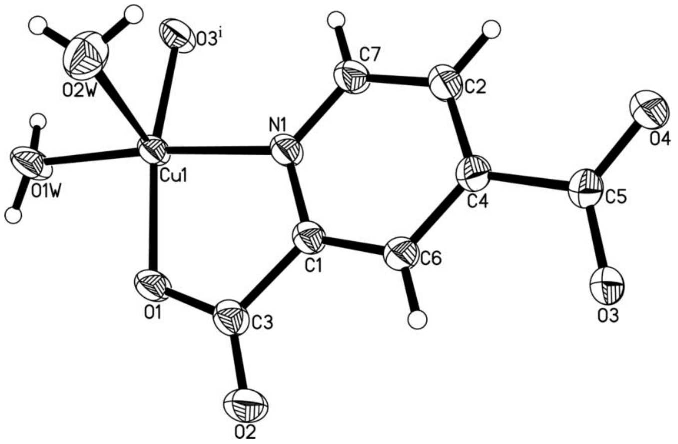


Figure 1
The asymmetric unit of (I), together with a symmetry-generated atom to complete the coordination of Cu1, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.]

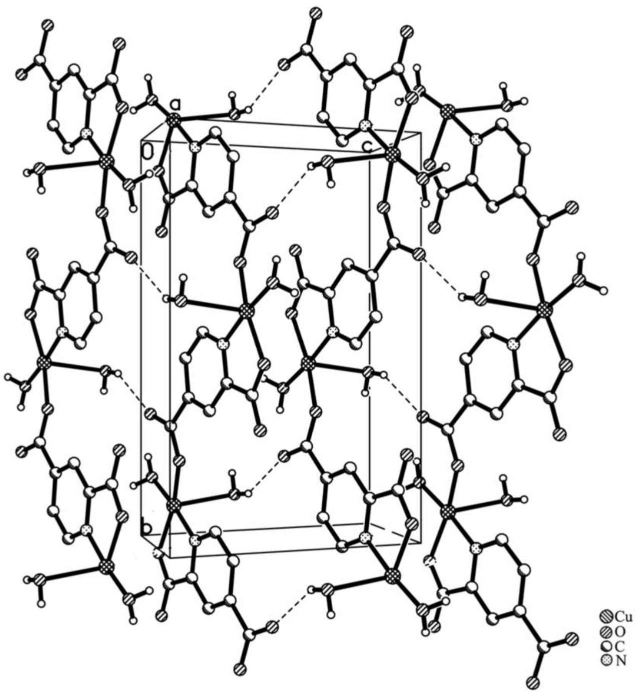


Figure 2
The hydrogen-bonding interactions (dashed lines) in the crystal packing of (I).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Siemens, 1998); software used to prepare material for publication: *SHELXTL-Plus*.

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