

Aqua(2,2'-bipyridyl)(6-carboxypyridine-2-carboxylato)copper(II) nitrate monohydrate

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Key indicators

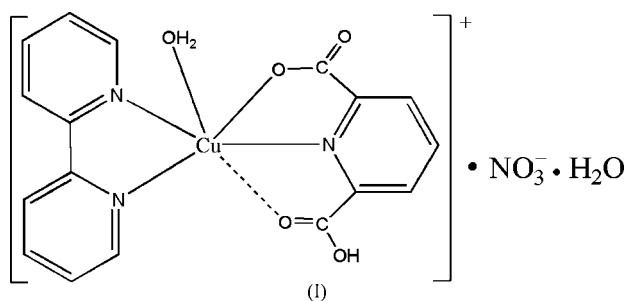
Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.008\text{ \AA}$
 R factor = 0.060
 wR factor = 0.125
Data-to-parameter ratio = 11.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the title compound, $[\text{Cu}(\text{C}_7\text{H}_4\text{NO}_4)(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})]\text{NO}_3 \cdot \text{H}_2\text{O}$, the Cu^{II} ion exhibits a distorted octahedral geometry. The Cu^{II} ion is coordinated by one water O atom, two bipyridyl N atoms, and one N atom, one carboxyl O atom, and one carboxylate O atom from 6-carboxypyridine-2-carboxylate.

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Comment

Transition-metal complexes with phen (1,10-phenanthroline) or bpy (2,2'-bipyridyl) as ligands have been important in the study of nucleic acids and in the development of new diagnostic and therapeutic agents (Chen & Yang, 2002). Chakravarty and coworkers have used several copper(II) complexes of diimines to cleave DNA by double-strand scission under physiological conditions (Dhar *et al.*, 2003). For these reasons, we have designed and synthesized the title copper complex, (I), which crystallized as a monohydrated nitrate salt.

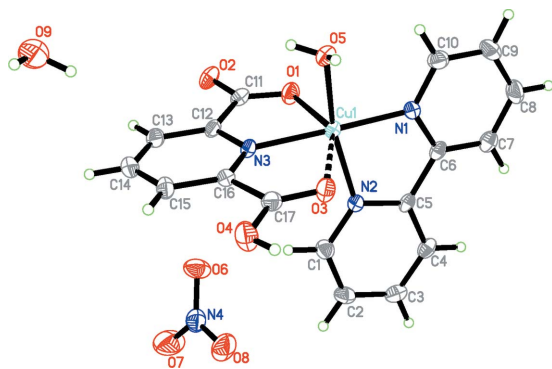


A displacement ellipsoid drawing of (I) is shown in Fig. 1. Selected bond lengths and angles are listed in Table 1. The Cu^{II} ion exhibits a distorted octahedral geometry. The coordination of Cu is formed by atoms N1, N2, N3 and O5 as equatorial atoms, and O1 [$\text{Cu1}-\text{O1} = 2.258(4)\text{ \AA}$] and O3 [$\text{Cu1}-\text{O3} = 2.543(4)\text{ \AA}$] as axial atoms.

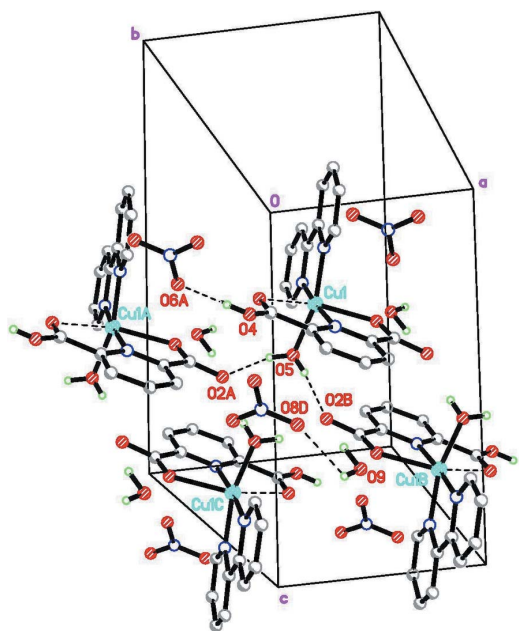
The packing of (I) is mainly governed by electrostatic forces and $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds (Fig. 2). These hydrogen bonds are formed between nitrate and a neighbouring cation, and between the water molecule of crystallization and nitrate. The coordinated water molecule is involved in two types of hydrogen bonds, joining three cations together. Details of the hydrogen-bond geometry are listed in Table 2.

Experimental

All chemicals were of reagent grade and commercially available from the Beijing Chemical Reagents Company of China, and were used without further purification. 2,2'-Bipyridine (0.5 mmol) and pyridine-2,6-dicarboxylic acid (0.5 mmol) were mixed together in a water-


Figure 1

The asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. The long, weak Cu1–O3 bond is shown dashed.


Figure 2

The molecular packing of the title compound [symmetry codes: (A) $x - 1, y, z$; (B) $-x + 1, y, z + 1$; (C) $-x, -y, -z + 1$; (D) $-x + 1, y + 1, z + 1$]. Hydrogen-bonding interactions are indicated by dashed lines; only atoms involved in the hydrogen bonds and metal ions are labelled, and other H atoms have been omitted.

methanol (1:1) solution, and an aqueous solution of copper(II) nitrate (0.5 mmol) was added slowly. The resulting mixture was stirred at 323 K for 3 h and then filtered. The filtrate was allowed to stand at room temperature for 6 weeks, affording blue crystals.

Crystal data

[Cu(C₇H₄NO₄)(C₁₀H₈N₂)(H₂O)]·
NO₃·H₂O
 $M_r = 483.88$
Triclinic, $P\bar{1}$
 $a = 7.081$ (7) Å
 $b = 11.390$ (12) Å
 $c = 12.952$ (13) Å
 $\alpha = 107.159$ (13)°
 $\beta = 95.004$ (13)°

$\gamma = 104.337$ (12)°
 $V = 952.5$ (17) Å³
 $Z = 2$
 $D_x = 1.687$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 1.21$ mm⁻¹
 $T = 298$ (2) K
Needle, blue
0.50 × 0.10 × 0.05 mm

Data collection

Bruker SMART 1000
diffractometer
 φ and ω scans
Absorption correction: multi-scan
(SADABS; Sheldrick, 2000)
 $T_{\min} = 0.583, T_{\max} = 0.942$

4540 measured reflections
3263 independent reflections
2446 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.031$
 $\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.060$
 $wR(F^2) = 0.125$
 $S = 1.06$
3263 reflections
281 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 0.2819P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.48 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.77 \text{ e \AA}^{-3}$

Table 1

Selected bond lengths (Å).

Cu1–N1	1.986 (4)	Cu1–N3	2.029 (4)
Cu1–O5	2.001 (3)	Cu1–O1	2.258 (4)
Cu1–N2	2.007 (4)	Cu1–O3	2.543 (4)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O9–H16 ⁱ ···O8 ⁱ	0.82	2.50	3.020 (7)	122
O5–H13 ⁱ ···O2 ⁱⁱ	0.85	1.85	2.674 (5)	164
O5–H14 ⁱ ···O2 ⁱⁱⁱ	0.82	1.89	2.702 (5)	170
O4–H12 ⁱ ···O6 ⁱⁱ	0.82	1.75	2.556 (5)	169

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

Water atoms H13, H14, H15 and H16 were located in a difference Fourier map and their positions and isotropic displacement parameters were refined, with O–H restraints which led to O–H values in the range 0.82–0.92 Å. They were subsequently refined as riding on the bonded O atom, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$. All other H atoms were positioned geometrically, treated as riding atoms and refined isotropically, with C–H = 0.93 Å, O–H = 0.82 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ and $1.5U_{\text{eq}}(\text{O})$.

Data collection: SMART (Bruker, 2000); cell refinement: SMART; data reduction: SAINT (Bruker, 2000); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2000); software used to prepare material for publication: SHELXTL.

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