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Bis(4-carboxamidopyridinium) diaquadioxalatocuprate(II)

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In the title compound, $(C_6H_7N_2O)_2[Cu(C_2O_4)_2(H_2O)_2]$, the Cu^{II} center (site symmetry $\bar{1}$) exhibits an octahedral coordination geometry arising from four O atoms of two oxalate dianions and two O atoms of water molecules. The protonated isonicotinamide cation interacts with the anion by O—H···O and N—H···O hydrogen bonds, generating a three-dimensional network.

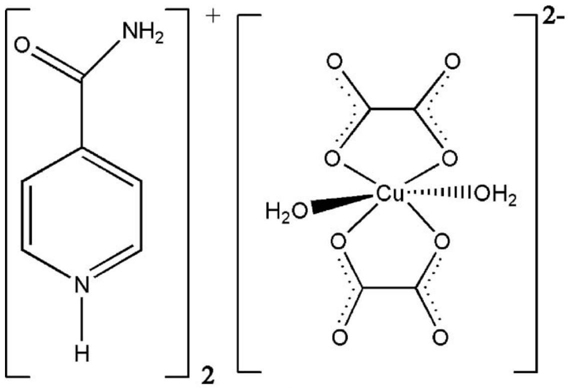
Key indicators

Single-crystal X-ray study
$T = 295$ K
Mean σ(C–C) = 0.003 Å
R factor = 0.025
wR factor = 0.067
Data-to-parameter ratio = 12.5

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

Comment

To extend our work (Gao *et al.*, 2006) on hydrogen-bonded supramolecular architectures (Eddaoudi *et al.*, 2002), we obtained the title compound, (I), by choosing oxalate dianions, isonicotinamide and Cu^{2+} cations as the starting materials.



(I)

Compound (I) contains $[Cu(C_2O_4)_2(H_2O)_2]^{2-}$ dianions and $[C_6H_7N_2O]^+$ cations, as shown in Fig. 1. The Cu^{II} atom (site symmetry $\bar{1}$) shows a distorted octahedral coordination geometry, being coordinated by four O atoms from two oxalate ligands and two O atoms from water molecules, with the Cu—O distances showing a typical Jahn–Teller distortion (Table 1).

The monoprotonated (at the pyridyl N atom) isonicotinamide cations balance the charge of the anionic complex ion. O—H···O and N—H···O hydrogen-bonding interactions (Table 2) play an important role in stabilizing the network in the crystal strcture of (I) (Fig. 2), resulting in a three-dimensional supramolecular network.

Experimental

A mixture of $CuSO_4$ (0.5 mmol), $K_2C_2O_4 \cdot H_2O$ (0.5 mmol) and isonicotinamide (1 mmol) was heated in 20 ml of water/ethanol (1:1 *v*/*v*) solution and continually stirred for about 30 min at 333 K. The pH value was adjusted to about 4.0 with 4 *M* HCl. The mixture was then cooled to room temperature and filtered. The filtrate was allowed to evaporate at room temperature. One week later, aquamarine-blue crystals of (I) were obtained.

Crystal data

$(C_6H_7N_2O)_2[Cu(C_2O_4)_2(H_2O)_2]$
$M_r = 521.89$
Triclinic, $P\overline{1}$
$a = 6.788$ (2) Å
$b = 6.957$ (2) Å
$c = 10.849$ (3) Å
$\alpha = 76.127$ (2)°
$\beta = 75.198$ (2)°
$\gamma = 79.483$ (3)°
$V = 476.9$ (2) Å^3
$Z = 1$
Mo $K\alpha$ radiation
$\mu = 1.23$ mm^{-1}
$T = 295$ (2) K
$0.43 \times 0.32 \times 0.24$ mm

Data collection

Bruker SMART CCD APEX II diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\min} = 0.635$, $T_{\max} = 0.750$
4061 measured reflections
1887 independent reflections
1822 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.012$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.067$
$S = 1.00$
1887 reflections
151 parameters
H-atom parameters constrained
$\Delta\rho_{\max} = 0.25$ e Å^{-3}
$\Delta\rho_{\min} = -0.46$ e Å^{-3}

Table 1
Selected bond lengths (Å).

Cu—O1	1.9428 (13)	Cu—OW1	2.4872 (16)
Cu—O2	1.9873 (13)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
OW1—HW1···O5^{v}	0.84	1.97	2.7959 (19)	170
OW1—HW2···O4^{ii}	0.79	1.94	2.733 (2)	175
N1—H1···O3^{iii}	0.86	1.91	2.675 (2)	148
N1—H1···O4^{iii}	0.86	2.31	2.963 (2)	132
N2—HN1···OW1^{iv}	0.86	2.04	2.837 (2)	154
N2—HN2···O2^{i}	0.86	2.31	3.078 (2)	149

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

The water H atoms were located in difference maps and refined as riding in their as-found relative positions (O—H = 0.79–0.84 Å), with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(O). The other H atoms were positioned geometrically and refined with a riding model (N—H = 0.86 Å and C—H = 0.93 Å), with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C,N).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

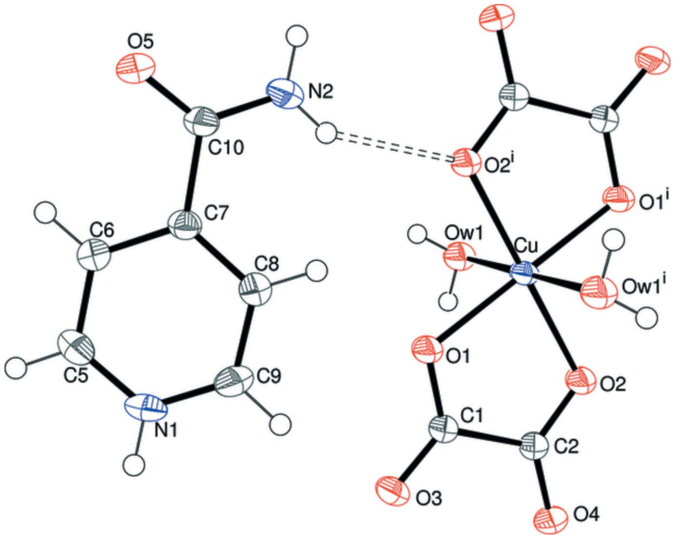


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids (arbitrary spheres for the H atoms). The hydrogen bond is shown as a double dashed line. [Symmetry code: (i) $1-x, 1-y, 1-z$.]

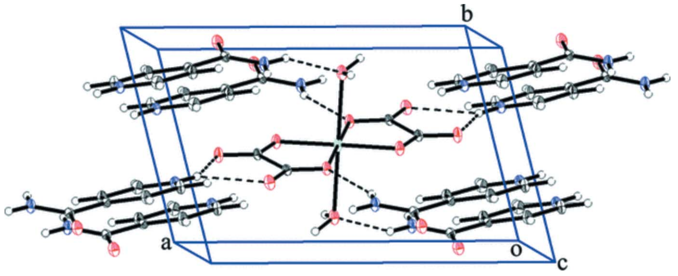


Figure 2
The unit cell packing for (I), showing the hydrogen bonds as dashed lines.

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