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Tetraaquabis(4,4′-bipyridine)copper(II) 2,6-naphthalenedicarboxylate trihydrate

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The Cu atom in $[Cu(C_{10}H_8N_2)_2(H_2O)_4](C_{12}H_6O_4)\cdot 3H_2O$ exists in a *trans*-N_2O_4 octahedral coordination polyhedron that is formed by the N atoms of two 4,4′-bipyridine heterocycles and the O atoms of four water molecules. The carboxylate groups of the centrosymmetric anions interact indirectly with the Cu atoms through the coordinated water molecules. The cations and anions are linked by hydrogen bonds into a network motif. The Cu atom lies at a site of 2 symmetry.

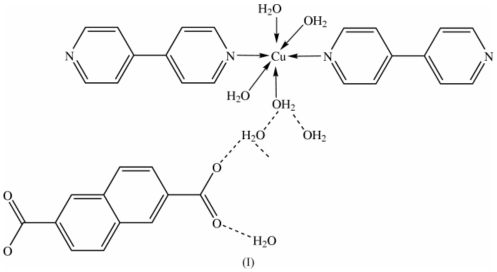
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.120
Data-to-parameter ratio = 15.7

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

Comment

The 4,4′-bipyridine spacer ligand has been used to react with a range of copper(II) salts; the products adopt a number of topologies such as squares, rectangles or rhombuses (Yuan *et al.*, 2003). At other times, the ligand links adjacent Cu atoms into a linear chain, and in one instance, the ligand merely interacts with the Cu atom through only one N site, the other being involved with hydrogen-bonding interactions (Abu-Shandi *et al.*, 2001). The structure of the 1/1 adduct with copper dibenzoate has not been authenticated, but a substituted derivative furnishes a heterocycle-coordinated compound in which the Cu atom is covalently linked to the carboxylate entity (He & Zhu, 2003). However, the extension of this study to copper terephthalate, a dicarboxylate compound, gave instead a tetraaquacopper complex in which the carboxylate anion interacts with the six-coordinate Cu atom through the coordinated water molecules (Long, 2003).



(I)

In the title compound, (I), the Cu atom, which lies on a twofold axis, is coordinated by four water molecules. The geometry is tetragonally distorted as the two Cu—O_{water} distances [2.385 (3) and 2.457 (3) Å] are significantly longer than the pairs of Cu—O [2.005 (2) Å] and Cu—N [2.079 (2) Å] bonds. The coordinated water molecules interact with the uncoordinated water molecules, which, in turn, interact with the dicarboxylate dianion. One of them also interacts with the coordinated heterocycle. The cations and anions are linked by hydrogen bonds into a network motif (Table 2).

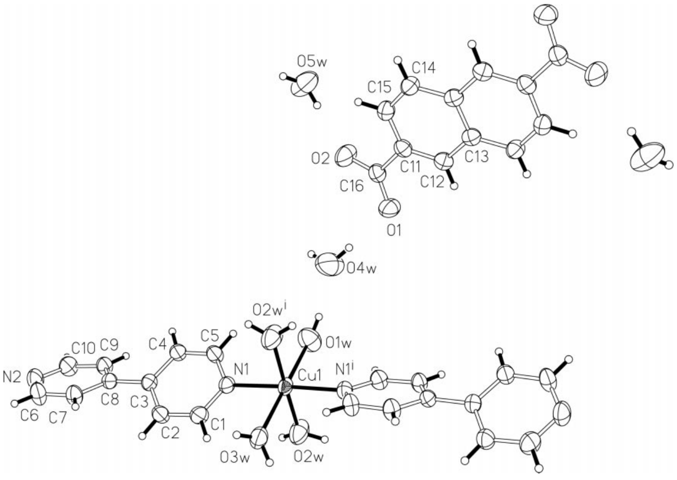


Figure 1

*ORTEP*II (Johnson, 1976) plot of the title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as circles of arbitrary radii. [Symmetry code: (i) $1 - x, y, \frac{1}{2} - z$.]

Experimental

Copper nitrate trihydrate (0.12 g, 0.5 mmol) and 2,6-naphthalenedicarboxylic acid (0.11 g, 0.5 mmol) were placed in water (5 ml) and ammonium hydroxide was added until the reagents dissolved completely. 4,4′-Bipyridine (0.08 g, 0.5 mmol) was added, and water was added to make up a total volume of 10 ml. The mixture was heated in a Teflon-lined stainless-steel bomb at 413 K for 16 h. The title compound deposited from the solution as well formed crystals when the bomb was cooled to room temperature.

Crystal data

$[Cu(C_{10}H_8N_2)_2(H_2O)_4](C_{12}H_6O_4)\cdot 3H_2O$
$M_r = 716.19$
Orthorhombic, *Pbcn*
$a = 7.4063$ (5) Å
$b = 18.157$ (1) Å
$c = 23.801$ (2) Å
$V = 3200.7$ (4) Å^3
$Z = 4$
$D_x = 1.49$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2701 reflections
$\theta = 2.8$–$24.7°$
$\mu = 0.75$ mm^{-1}
$T = 298$ (2) K
Plate, blue
0.36 × 0.10 × 0.06 mm

Data collection

Bruker SMART area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.677$, $T_{max} = 0.914$
17 912 measured reflections
3768 independent reflections
2292 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 28.3°$
$h = -9 \rightarrow 8$
$k = -24 \rightarrow 17$
$l = -30 \rightarrow 31$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.120$
$S = 0.91$
3768 reflections
240 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0734P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.67$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ e Å^{-3}

Table 1

Selected geometric parameters (Å, °).

Cu1—O1*w*	2.385 (3)	Cu1—O3*w*	2.457 (3)
Cu1—O2*w*	2.005 (2)	Cu1—N1	2.079 (2)
O1*w*—Cu1—O3*w*	180	O2*w*—Cu1—N1	89.0 (1)
O1*w*—Cu1—O2*w*	88.8 (1)	O2*w*—Cu1—N1^{i}	91.1 (1)
O1*w*—Cu1—N1	91.6 (1)	O3*w*—Cu1—N1	88.4 (1)
O2*w*—Cu1—O2*w*^{i}	177.6 (1)	N1—Cu1—N1^{i}	176.9 (1)
O2*w*—Cu1—O3*w*	91.2 (1)		

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

Table 2

Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O4*w*^{i}	0.84	1.92	2.738 (3)	165
O2*w*—H2*w*1···N2^{ii}	0.87	2.34	3.202 (3)	169
O2*w*—H2*w*2···N2^{iii}	0.86	2.40	3.257 (3)	173
O3*w*—H3*w*1···O2^{iv}	0.85	1.96	2.799 (2)	174
O4*w*—H4*w*1···O1	0.85	1.95	2.792 (3)	168
O4*w*—H4*w*2···O2^{v}	0.85	2.17	2.955 (3)	153
O5*w*—H5*w*1···O2	0.85	1.94	2.790 (2)	177

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

The water H-atoms were located and refined subject to O—H = 0.85 (1) Å and H···H = 1.39 (1) Å. The C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and refined in the riding-model approximation; the displacement parameters of all H atoms were set to 1.2 times U_{eq} of the equivalent isotropic displacement parameters of the parent atoms.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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References

Abu-Shandi, K., Janiak, C. & Kersting, B. (2001). *Acta Cryst.* C**57**, 1261–1264.
Bruker (2001). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
He, H.-Y. & Zhu, L.-G. (2003). *Acta Cryst.* E**59**, o174–o176.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Long, L. S. (2003). Unpublished results.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Yuan, J. X., Hu, M. L. & Song, X. Y. (2003). *Z. Kristallogr. New Cryst. Struct.* **218**, 1–2.

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