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catena-Poly[bis[aquacopper(I)-μ-4,4′-bipyridine-κ^2N:N'] terephthalate dihydrate]

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The 4,4′-bipyridine spacer in the crystal structure of the title compound, $\{[\mathrm{Cu}(\mathrm{C}_{10}\mathrm{H}_8\mathrm{N}_2)_2(\mathrm{H}_2\mathrm{O})]_2(\mathrm{C}_8\mathrm{H}_4\mathrm{O}_4)\cdot 2\mathrm{H}_2\mathrm{O}\}_n$, links the water-coordinated Cu^{I} atoms into a linear chain in which the metal atom exists in a T-shaped environment [N—Cu—N = 156.6 (1)°]. Interacting through the coordinated water molecules, the chains connect with the centrosymmetric terephthalate dianions and uncoordinated water molecules to form a three-dimensional network structure.

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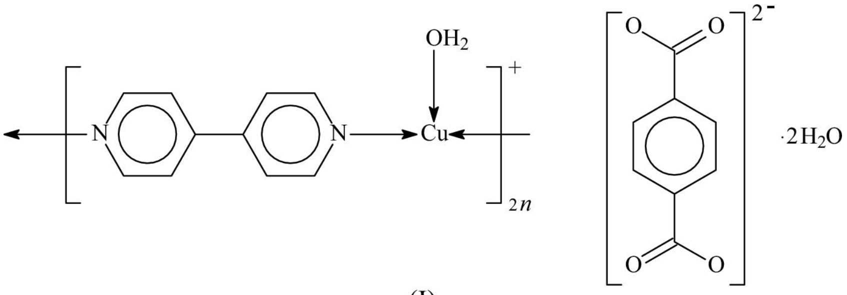
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.113
Data-to-parameter ratio = 14.9

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

Comment

In the presence of copper(II) ions and under hydrothermal conditions, 1,10-phenanthroline forms a phenanthrolinol that is isolated as the copper derivative; 2,2′-bipyridine also undergoes hydroxylation under hydrothermal conditions (Tao *et al.*, 2002; Zhang *et al.*, 2002; Zheng *et al.*, 2004). Hydroxide ions that are contributed by sodium hydroxide appear to be crucial, and the present study explores an analogous synthesis with 4,4′-bipyridine, which typically functions as a spacer, in place of the chelating 2,2′-bipyridine analogue. A previous study of the hydrothermal reaction of copper(II) nitrate, terephthalic acid and this heterocycle in the absence of sodium hydroxide reported the formation of the co-crystal $[\mathrm{Cu}(\mathrm{C}_8\mathrm{H}_4\mathrm{O}_4)(\mathrm{C}_{10}\mathrm{H}_8\mathrm{N}_2)]\cdot\mathrm{C}_8\mathrm{H}_6\mathrm{O}_4$ (Baeg & Lee, 2002). The synthesis of this copper(II) compound was aimed at duplicating the synthesis of the mixed-valence compound bis(4,4′-bipyridyl)tris(μ_2-terephthalato-κ^4O,O',O'',O''')tetracopper(I,II), which used an aqueous ethanol medium (Lo *et al.*, 2000). The present synthesis yielded *catena*-poly[bis[aquacopper(I)-μ-4,4′-bipyridine-κ^2N:N'] terephthalate dihydrate], (I), as the main phase (Fig. 1).



(I)

The cation exists as a linear chain with the spacer ligand functioning in the usual bridging mode; the three-coordinate copper(I) atom shows T-shaped coordination. The chains are linked to the terephthalate dianion (which lies on a centre of inversion) and the uncoordinated water molecule (Table 2), resulting in a three-dimensional network structure.

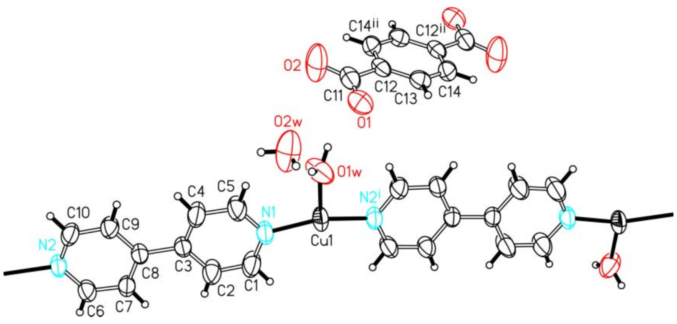


Figure 1

*ORTEP*II plot (Johnson, 1976) of a portion of the structure of (I). Displacement ellipsoids are shown at the 50% probability level and H atoms are drawn as spheres of arbitrary radii. [Symmetry codes: (i) $2 - x, \frac{1}{2} + y, \frac{3}{2} - z$; (ii) $1 - x, 2 - y, -z$].

Experimental

Copper(II) nitrate trihydrate (0.241 g, 1 mmol), 4,4′-bipyridine (0.078 g, 1 mmol), terephthalic acid (0.167 g, 1 mmol), sodium hydroxide (0.040 g, 1 mmol) and water (10 ml) were placed in a 23 ml Teflon-lined stainless steel Parr bomb. The bomb was then heated at 443 K for 2 d. After the bomb had cooled slowly to room temperature at a rate of 10 K h^{-1}, blue crystals of the copper(I) compound were isolated from the solution.

Crystal data

$[Cu(C_{10}H_8N_2)_2(H_2O)]_2(C_8H_4O_4)\cdot 2H_2O$
$M_r = 675.62$
Monoclinic, $P2_1/c$
$a = 9.4575$ (8) Å
$b = 21.398$ (2) Å
$c = 7.1568$ (6) Å
$\beta = 110.639$ (1)°
$V = 1355.4$ (2) Å^3
$Z = 2$

$D_x = 1.655$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2203 reflections
$\theta = 2.3$–27.4°
$\mu = 1.63$ mm^{-1}
$T = 295$ (2) K
Block, blue
0.35 × 0.26 × 0.23 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.468$, $T_{max} = 0.706$
8085 measured reflections

3062 independent reflections
2442 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 27.5°$
$h = -11 \rightarrow 12$
$k = -18 \rightarrow 27$
$l = -9 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.113$
$S = 1.03$
3062 reflections
206 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0639P)^2 + 0.208P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

Table 1

Selected geometric parameters (Å, °).

Cu1—O1*w*	2.185 (2)	Cu1—N2^i	1.915 (2)
Cu1—N1	1.912 (2)		
O1*w*—Cu1—N1	100.3 (1)	N1—Cu1—N2^i	156.6 (1)
O1*w*—Cu1—N2^i	102.7 (1)		

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

Table 2

Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*w*—H1*w*1···O1	0.84 (1)	1.85 (1)	2.657 (3)	162 (3)
O1*w*—H1*w*2···O2*w*	0.83 (1)	1.92 (2)	2.710 (3)	159 (3)
O2*w*—H2*w*1···O2^{iii}	0.85 (1)	2.07 (2)	2.834 (4)	151 (4)
O2*w*—H2*w*2···O2^{iv}	0.84 (1)	2.00 (2)	2.772 (3)	151 (3)

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

H atoms were placed in calculated positions (C—H = 0.93 Å) and were included in the refinement in the riding-model approximation, with U_{iso}(H) values set at 1.2 times U_{eq}(C). The water H atoms were located in difference Fourier maps and were refined with a distance restraint of O—H = 0.85 (1) Å.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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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