

Poly[*diaquabis*(3-pyridylpropionato)copper(II)]

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Key indicators

Single-crystal X-ray study

$T = 293\text{ K}$

Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$

R factor = 0.032

wR factor = 0.072

Data-to-parameter ratio = 13.0

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

The title compound, $[\text{Cu}(\text{C}_8\text{H}_8\text{NO}_2)_2(\text{H}_2\text{O})_2]_n$, is a novel material consisting of a Cu^{II} atom bonded to two O and two N atoms from four distinct 3-pyridylpropionate anions. The Cu^{II} atom lies on an inversion center. The connectivity gives rise to two-dimensional sheets in the (101) plane.

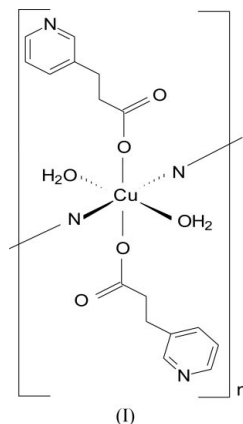
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Comment

The title compound, (I), was found as a side product of an attempt to synthesize a heteronuclear framework material containing both copper and neodymium centers (Cahill *et al.*, 2003). We were able, however, to reproduce the compound without the use of neodymium. Copper, on an inversion center, is found in square-planar coordination and is bonded to O1 and N1, as well as their symmetry equivalents. The carboxylate end of the 3-pyridylpropionate ligand is bonded in a monodentate fashion through O1 to the copper center. The flexibility in the aliphatic section of the ligand allows the copper centers to be connected into buckled layers with coordinated water molecules between the layers. Atoms N1 and O1 (*cis* to each other) are at comparable distances from the Cu^{II} site [2.021 (2) and 1.998 (1) Å, respectively], whereas the water molecule (O3) is 2.476 (2) Å away from the Cu^{II} site, completing an elongated octahedral coordination geometry.



Experimental

Copper nitrate hexahydrate and 3-pyridinepropionic acid are available commercially and were used without any further purification. Copper nitrate hexahydrate (0.116 g) and 3-pyridinepropionic acid (0.076 g) were dissolved in water (1.36 g) in the presence of concentrated ammonium hydroxide (0.07 g) in the molar ratio 1:1:151:2. The solution (pH = 7.70) was prepared in a 23 ml Teflon-

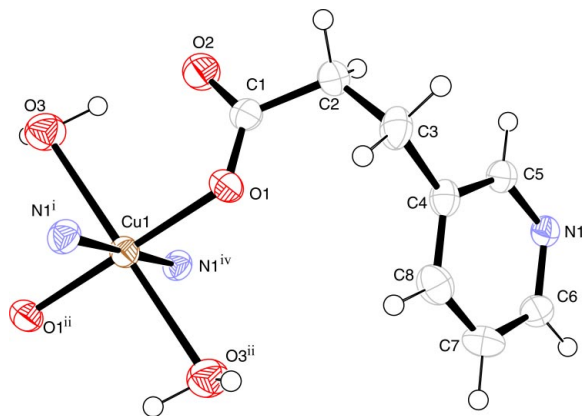


Figure 1
The asymmetric unit of the title compound, together with symmetry equivalent atoms to complete the coordination of Cu, showing 50% probability ellipsoids and the atom-numbering scheme. Symmetry codes are as in Tables 1 and 2, with the addition of (iv) $\frac{1}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$.

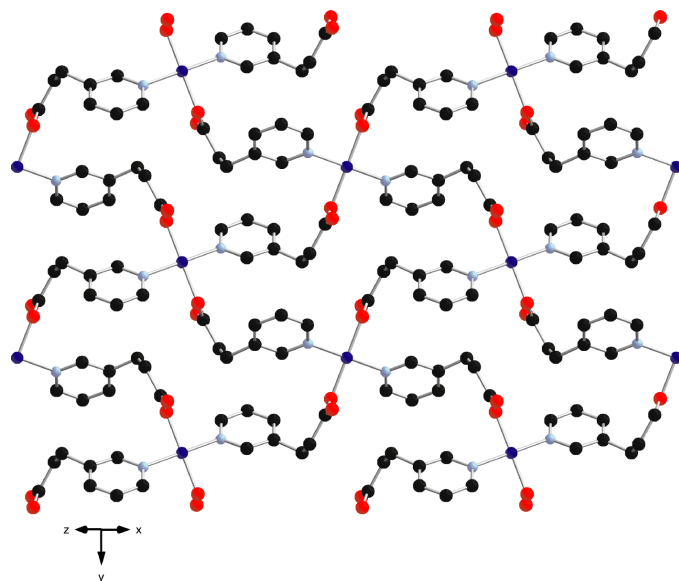


Figure 2
A single (101) layer of (I). Coordinated water molecules and H atoms have been omitted for clarity. Color codes: dark-blue Cu, light-blue N, red O, and black C.

lined Parr bomb then heated at 393 K under autogenous pressure for 3 d. Light-blue crystals formed *in situ* and are insoluble in water, ethanol and acetone. Phase purity was confirmed by comparison of the observed and calculated powder X-ray diffraction patterns.

Crystal data

[Cu(C₈H₈NO₂)₂(H₂O)₂]
 $M_r = 399.88$
 Monoclinic, $P2_1/n$
 $a = 9.4199$ (5) Å
 $b = 8.6557$ (5) Å
 $c = 10.1261$ (7) Å
 $\beta = 99.872$ (4)°
 $V = 813.41$ (9) Å³
 $Z = 2$

$D_x = 1.633$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 17 349 reflections
 $\theta = 1.5$ – 28.3 °
 $\mu = 1.38$ mm⁻¹
 $T = 293$ (2) K
 Prism, light blue
 $0.14 \times 0.11 \times 0.06$ mm

Data collection

Rigaku R-Axis RAPID diffractometer
 ω scans
 Absorption correction: numerical
CrystalClear (Rigaku/MSC, 2003)
 $T_{\min} = 0.855, T_{\max} = 0.922$
 13 951 measured reflections

2020 independent reflections
 1654 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.048$
 $\theta_{\max} = 28.3$ °
 $h = -12 \rightarrow 12$
 $k = -11 \rightarrow 11$
 $l = -13 \rightarrow 13$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.072$
 $S = 1.06$
 2020 reflections
 155 parameters
 All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.022P)^2 + 0.74P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.27$ e Å⁻³
 $\Delta\rho_{\min} = -0.31$ e Å⁻³

Table 1

Selected geometric parameters (Å).

Cu1—O1	1.9976 (14)	Cu1—O3	2.4763 (17)
Cu1—N1 ⁱ	2.0207 (17)		

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

Table 2

Hydrogen-bonding geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O3—H1 \cdots O2 ⁱⁱ	0.95 (3)	1.80 (3)	2.727 (2)	164 (3)
O3—H2 \cdots O2 ⁱⁱⁱ	0.83 (4)	2.11 (4)	2.936 (2)	172 (3)

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

Refined C—H distances range from 0.93 (3)–1.01 (3) Å.

Data collection: *CrystalClear* (Rigaku/MSC, 2003); cell refinement: *HKL* (Otwinowski & Minor, 1997); data reduction: *HKL*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *CrystalMaker* (CrystalMaker, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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References

- Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
 Cahill, C. L., Borkowski, L. A., Frisch, M. & Gunning, N. (2003). 226th American Chemical Society National Meeting, Abstracts of Papers, INOR-677.
 CrystalMaker (2003). *CrystalMaker*. Version 5.1.3. PO Box 183, Bicester, Oxfordshire, OX26 3TA, England.
 Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
 Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
 Rigaku/MSC (2003). *CrystalClear*. Version 1.3.5. Rigaku/MSC, 9009 New Trails Drive, The Woodlands, TX 77381–5209, USA.
 Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. Release 97-2. University of Göttingen, Germany.