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catena-Poly[[bis(2-nitrobenzoato-κ*O*)copper(**II**)]-di-μ-3-pyridylmethanol-$\kappa^2N,O;\kappa^2O:N$]

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Key indicators

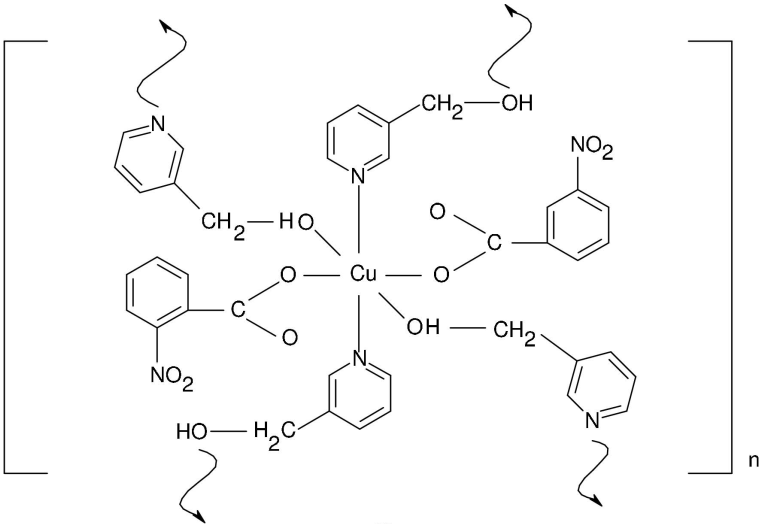
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.025
wR factor = 0.065
Data-to-parameter ratio = 12.1

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

The crystal structure of the title compound, $[\mathrm{Cu(C_7H_4NO_4)_2(C_6H_7NO)_2}]_n$, has been studied at 100 (2) K. The structure contains a linear polymeric chain of Cu$^{\rm II}$ atoms, which lie on centres of inversion and are doubly bridged by 3-pyridylmethanol molecules. Two coordination positions on each Cu centre are occupied by O atoms from 3-pyridylmethanol, with two other positions occupied by piridyl N atoms. Monodentate 2-nitrobenzoate anions bind to Cu in axial positions so that the copper(II) chromophore is *trans*-$[\mathrm{CuO_2N_2O'_2}]$. The axially bound 2-nitrobenzoate anions form strong intramolecular O—H···O hydrogen bonds with the OH groups of the 3-pyridylmethanol molecules. The resulting linear chains are held together by weak van der Waals interactions.

Comment

As a part of our study of copper(II) carboxylate complexes with molecular ligands showing biologically interesting properties, the title compound, (I) (Fig. 1), has been prepared and its structure determined.



(I)

The 3-pyridylmethanol ligands prefer to bridge metal centres rather than act as monodentate ligands, as was found with tetrakis(2-acetato)bis(3-pyridylmethanol)dicopper(II) dichloromethane solvate (Melník *et al.*, 1998, 2000). Selected bond distances and bond angles of (I) are summarized in Table 1. The asymmetric unit consists of a Cu atom located on an inversion centre, one 2-nitrobenzoato anion and one 3-pyridylmethanol molecule. The coordination environment around the Cu$^{\rm II}$ atom is nearly octahedral. The tetragonal

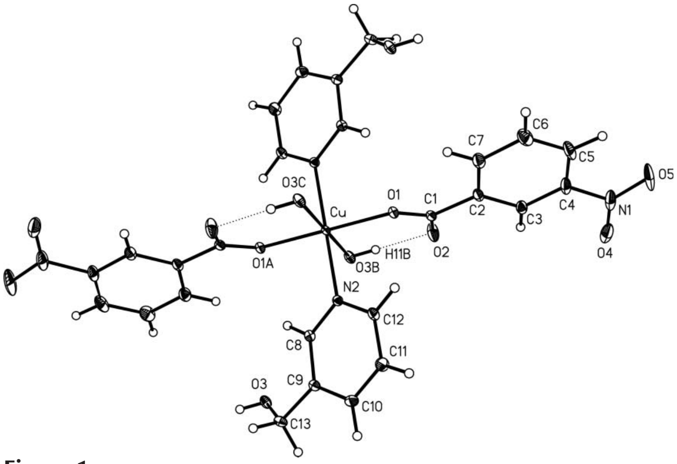


Figure 1
A section of the polymeric structure of (I), with displacement ellipsoids drawn at the 40% probability level and H atoms shown as spheres of arbitrary radii. Hydrogen bonds are drawn as dotted lines.

plane comprises a pair of monodentate 2-nitrobenzoate ligands bound through their carboxylate O atoms [Cu—O1 = 1.9860 (12) Å] and a pair of neutral ronicol molecules (ronicol = ron = 3-pyridylmethanol) coordinated *via* the N atoms of the pyridine ring [Cu - N2 = 2.0368 (13) Å]. These ligands are mutually *trans*. The axial positions are occupied by two hydroxy O atoms [Cu—O3*C* = 2.3724 (11) Å] from two adjacent molecules of ronicol (symmetry positions of the ronicol ligands: $x - 1, y, z$ and $1 - x, -y, -z$).

Strong intramolecular hydrogen bonding interactions [O2—H11*B*···O3*C;* O2···O3*C* = 2.618 (3) Å] stabilize the structure, forming one-dimensional chains. The structure of (I) can be compared with others with the general formula $[\mathrm{Cu}X_2(\mathrm{ron})_2]_n$, where *X* is salicylate (Hoang *et al.*, 1992), niflumate (Valach *et al.*, 1997), clofibriate (Moncol̓ *et al.*, 2001), trichloracetate (Múdra *et al.*, 2003), dichloracetate (Múdra *et al.*, 2003) and flufenamate (Lörinc *et al.*, 2004). The $\mathrm{Cu—O_{eq}}$ (O atom of the carboxylate group), $\mathrm{Cu—N_{eq}}$ (N atom of the pyridine ring of ronicol) and $\mathrm{Cu—O_{ax}}$ (O atom of the hydroxy group of ronicol) bond lengths are 1.944 (4), 2.039 and 2.622 (4) Å for salicylate, 1.946 (3), 2.038 (3) and 2.573 (3) Å for niflumate, 1.989 (2), 2.008 (2) and 2.441 (1) Å for clofibriate, 2.013 (1), 2.012 (2) and 2.359 (1) Å for trichloracetate, 1.983 (1), 2.023 (2) and 2.471 (2) Å for dichloracetate, and 1.974 (2), 2.028 (2) and 2.404 (1) Å for flufenamate. In the present crystal structure, the corresponding bond lengths are consistent with these values (Table 1). This class of compounds displays polymeric structures with axially elongated tetragonal bipyramidal geometry about each $\mathrm{Cu^{II}}$ atom of the $\mathrm{CuO_4N_2}$ chromophore, commensurate with Jahn–Teller distortion.

Experimental

The title compound was prepared by reaction of ronicol (2 mmol) with copper(II) acetate (1 mmol) in aqueous solution. 2-Nitrobenzoic acid (2 mmol) was added, and the final blue powder was filtered and dried at room temperature. Blue crystals were obtained from the mother liquor after one week at room temperature.

Crystal data

$[\mathrm{Cu(C_7H_4NO_4)_2(C_6H_7NO)_2}]$
$M_r = 614.03$
Triclinic, $P\overline{1}$
$a = 6.6920$ (13) Å
$b = 7.6470$ (15) Å
$c = 12.997$ (3) Å
$\alpha = 83.72$ (3)°
$\beta = 77.11$ (3)°
$\gamma = 80.69$ (3)°
$V = 637.9$ (2) Å^3

$Z = 1$
$D_x = 1.598$ Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 25 reflections
$\theta = 3.9$–11.6°
$\mu = 0.92$ mm^{-1}
$T = 100$ (2) K
Prism, blue
0.4 × 0.3 × 0.2 mm

Data collection

Kuma KM-4 CCD diffractometer
ω scans
Absorption correction: part of the refinement model (Δ*F*) (COSABS99; Starynowicz, 1999)
$T_{\min} = 0.724$, $T_{\max} = 0.831$
4407 measured reflections

2788 independent reflections
2663 reflections with $I > 2\sigma(I)$
$R_{\mathrm{int}} = 0.018$
$\theta_{\max} = 28.3°$
$h = -8 \rightarrow 8$
$k = -10 \rightarrow 6$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.065$
$S = 1.09$
2788 reflections
231 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 0.2981P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.32$ e Å^{-3}
$\Delta\rho_{\min} = -0.53$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu—O1	1.9860 (12)	Cu—O3$^{\mathrm{i}}$	2.3724 (11)
Cu—N2	2.0368 (13)		
O1—Cu—N2	89.73 (5)	O1—Cu—O3$^{\mathrm{i}}$	93.57 (5)

Symmetry code: (i) $-x + 1, -y, -z$.

H atoms were located in difference Fourier syntheses and refined independently [C—H = 0.91 (2)–0.98 (2) Å and O—H = 0.78 (2) Å].

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2001); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2001); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP* (Johnson, 1965); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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