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Key indicators

Single-crystal X-ray study
T = 100 K
Mean $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$
R factor = 0.032
wR factor = 0.087
Data-to-parameter ratio = 16.9

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

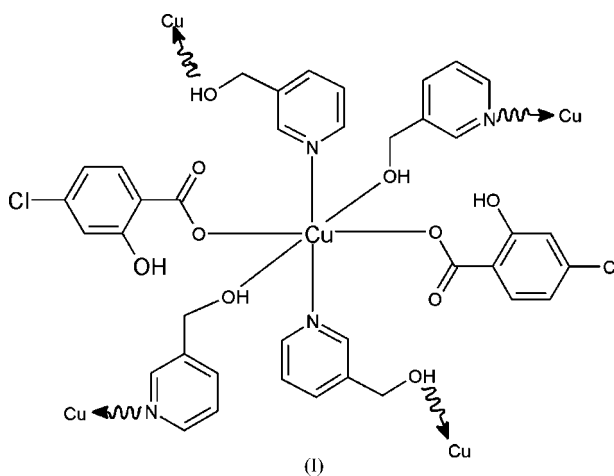
Poly[[bis(4-chlorosalicylato- κO)copper(II)]-di- μ -3-pyridylmethanol- $\kappa^2\text{N}:\text{O};\kappa^2\text{O}:\text{N}$]

The polymeric structure of the title complex, $[\text{Cu}(\text{C}_7\text{H}_4\text{ClO}_3)_2(\text{C}_6\text{H}_7\text{NO})_2]_n$, at 100 (2) K contains two-dimensional sheets parallel to the *ac* plane. The Cu^{II} atom, lying on an inversion centre, has an octahedral coordination environment. It is bonded in a *trans*-square-planar arrangement to the N atoms of two 3-pyridylmethanol molecules and one carboxylate O atom from each of two 4-chlorosalicylate anions. The axial positions are also occupied by 3-pyridylmethanol, but coordinated through O rather than the pyridyl N atom.

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Comment

3-Pyridylmethanol (also known as ronicol and abbreviated as 3-pyme) is known for its ability to be bonded as a monodentate ligand and/or bridging ligand (Stachová *et al.*, 2005) that can form linear chains of copper(II) atoms bridged by two 3-pyme molecules, as well as two-dimensional sheets. Recently, another mode of 3-pyme bridging, namely the formation of one-dimensional ‘accordion chains’ with copper(II) atoms bridged by one 3-pyme ligand, has been reported (Moncol *et al.*, 2005). As part of our systematic study of copper(II) carboxylate complexes with biologically interesting molecular ligands, we report here the crystal structure of the title compound, (I).



The asymmetric unit of (I) consists of a Cu^{II} atom located on an inversion centre, one 4-chlorosalicylate anion and one 3-pyridylmethanol molecule (Fig. 1). The coordination environment around the Cu^{II} atom is nearly octahedral. The equatorial plane consists of a pair of monodentate 4-chlorosalicylate ligands bound through their carboxylate O atoms [$\text{Cu}-\text{O}1 = 1.9787(12) \text{ \AA}$] and a pair of neutral 3-pyme molecules coordinated *via* the N atoms of the pyridine ring [$\text{Cu}-$

$N1 = 2.0194(15) \text{ \AA}$]. The axial positions are occupied by two hydroxy O atoms [$\text{Cu}-\text{O4B} = \text{Cu}-\text{O4C} = 2.560(3) \text{ \AA}$] from two adjacent symmetry-related 3-pyme molecules. Each Cu^{II} complex unit is connected to another four units through the 3-pyme ligands to form two-dimensional layers parallel to the *ac* plane.

The crystal structure of (I) can be compared with others of the general formula $[\text{Cu}X_2(3\text{-pyme})_2]_n$, where *X* is salicylate (Hoang *et al.*, 1992), niflumate (Valach *et al.*, 1997), clofibrate (Moncol *et al.*, 2001), flufemate (Lörinc *et al.*, 2004) and 2-chlorobenzoate (Moncol *et al.*, 2005).

Experimental

2-Pyridylmethanol (2 mmol) was added to copper(II) acetate (1 mmol) in aqueous solution (20 ml). 3,5-Dinitrobenzoic acid (2 mmol) was then added with stirring. The powdery blue product was filtered off, washed with a small amount of water and dried at room temperature. Blue prismatic crystals of (I) suitable for X-ray analysis were obtained from the mother liquor after slow room-temperature crystallization over a period of a few weeks.

Crystal data

$[\text{Cu}(\text{C}_7\text{H}_4\text{ClO}_3)_2(\text{C}_6\text{H}_7\text{NO})_2]$	$D_m = 1.555 \text{ Mg m}^{-3}$
$M_r = 624.91$	D_m measured by flotation
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 11.031(2) \text{ \AA}$	Cell parameters from 5225 reflections
$b = 12.815(3) \text{ \AA}$	$\theta = 3.7\text{--}28.6^\circ$
$c = 9.3410(2) \text{ \AA}$	$\mu = 1.12 \text{ mm}^{-1}$
$\beta = 104.16(3)^\circ$	$T = 100(2) \text{ K}$
$V = 1280.3(4) \text{ \AA}^3$	Prism, blue
$Z = 2$	$0.20 \times 0.15 \times 0.15 \text{ mm}$
$D_x = 1.621 \text{ Mg m}^{-3}$	

Data collection

Kuma KM4 CCD area-detector diffractometer	3002 independent reflections
ω scans	2536 reflections with $I > 2\sigma(I)$
Absorption correction: refined from ΔF (Parkin <i>et al.</i> , 1995)	$R_{\text{int}} = 0.030$
$T_{\text{min}} = 0.818$, $T_{\text{max}} = 0.846$	$\theta_{\text{max}} = 28.6^\circ$
8423 measured reflections	$h = -14 \rightarrow 14$
	$k = -17 \rightarrow 17$
	$l = -7 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0453P)^2 + 0.256P]$
$R[F^2 > 2\sigma(F^2)] = 0.032$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.087$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.17$	$\Delta\rho_{\text{max}} = 0.61 \text{ e \AA}^{-3}$
3002 reflections	$\Delta\rho_{\text{min}} = -0.57 \text{ e \AA}^{-3}$
178 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (\AA , $^\circ$).

Cu—O1	1.9787 (12)	Cu—N1	2.0194 (15)
$\text{O1}^i\text{—Cu—O1}$	180	$\text{N1}^i\text{—Cu—N1}$	180
O1—Cu—N1^i	90.11 (6)	C8—N1—Cu	119.97 (11)
O1—Cu—N1	89.89 (6)	C1—O1—Cu	123.24 (11)

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

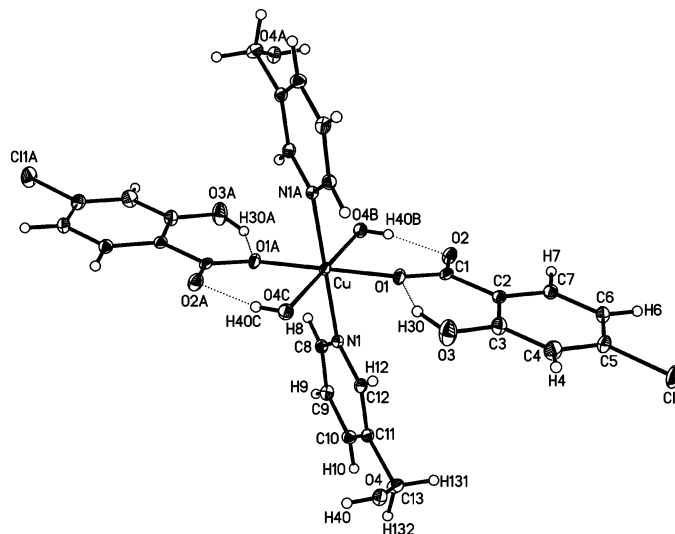


Figure 1

The monomer unit of (I). Displacement ellipsoids are drawn at the 40% probability level. Dotted lines represent O—H...O hydrogen bonds. Atoms labelled with the suffixes A, B and C are generated by the symmetry codes $(-x, -y, -z)$, $(x, -\frac{1}{2} - y, -\frac{1}{2} + z)$ and $(-x, \frac{1}{2} + y, \frac{1}{2} - z)$, respectively.

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D\text{—H}\cdots A$	$D\text{—H}$	$H\cdots A$	$D\cdots A$	$D\text{—H}\cdots A$
$\text{O3—H30}\cdots\text{O1}$	0.82	1.85	2.5705 (18)	146
$\text{O4—H40}\cdots\text{O2}^{\text{ii}}$	0.82	1.83	2.6400 (17)	168

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

H atoms were placed in geometrically calculated positions and allowed to ride on their parent atoms, with $\text{O—H} = 0.82 \text{ \AA}$ and $\text{C—H} = 0.93$ (aromatic) or 0.97 \AA (methylene). The $U_{\text{iso}}(\text{H})$ value for all H atoms was fixed at 0.05 \AA^2 .

Data collection: *KM-4 CCD System Software* (Kuma Diffraction, 1998); cell refinement: *KM-4 CCD System Software*; data reduction: *KM-4 CCD System Software*; 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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