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Aquabis(chloroacetato-κ*O*)bis(pyridine-κ*N*)copper(II)

Lesław Sieroń

Institute of General and Ecological Chemistry, Technical University of Łódź, Żeromskiego 116, 90-924 Łódź, Poland

Correspondence e-mail: lsieron@p.lodz.pl

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In the title compound, $[Cu(C_2H_2ClO_2)_2(C_5H_5N)_2(H_2O)]$, the Cu^{II} atom has a slightly distorted square-pyramidal coordination made up of two N atoms of the pyridine ligands and two O atoms of monodentate chloroacetate anions in the basal plane, as well as the water O atom in the apical position. Both the Cu and the O_{water} atoms occupy special positions on a twofold rotation axis. $O_{water}—H\cdots O_{carboxy}$ hydrogen bonds link molecules in the crystal structure into infinite chains, which run along the *b* axis, resulting in a $C_1^2(6)[R_1^2(10)]$ graph-set motif.

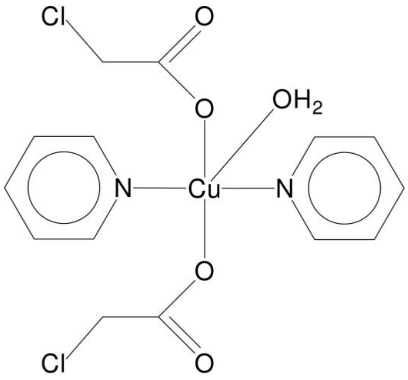
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.028
wR factor = 0.069
Data-to-parameter ratio = 13.4

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

Comment

The structure determination of the title compound, (I), was undertaken to study the influence of the chlorosubstituted acetate ligand on the stereochemistry of $[Cu(C_5H_5N)_2(H_2O)]$-type complexes. The crystal structure of (I) is built up of mononuclear $[Cu(CH_2ClCOO)_2(C_5H_5N)_2(H_2O)]$ complexes (Fig. 1), with the Cu atom and the O atom of the water molecule occupying special positions on a twofold rotation axis. The chloroacetate group coordinates to the central atom *via* one of its O atoms (O1), the distance between the Cu atom and the uncoordinated atom O3 being 3.151 (2) Å. Atom O3 participates in a strong O—H$\cdots$O hydrogen bond involving the O1 water molecule (Table 2). These hydrogen bonds link the complex molecules into infinite chains running along the [010] direction (Fig. 2), which may be described as a $C_1^2(6)[R_1^2(10)]$ graph set (Etter, 1990).



(I)

The bond valences around Cu^{II} were computed according to Brown (1994) and O'Keeffe & Brese (1991) as $\nu_{ij} = \exp[(R_{ij} - d_{ij})/0.37]$, where R_{ij} is the bond-valence parameter (in the formal sense, it is the single-bond length between the *i* and *j* atoms) and d_{ij} is the observed bond length. The application of this correlation allows the comparison of the relative impor-

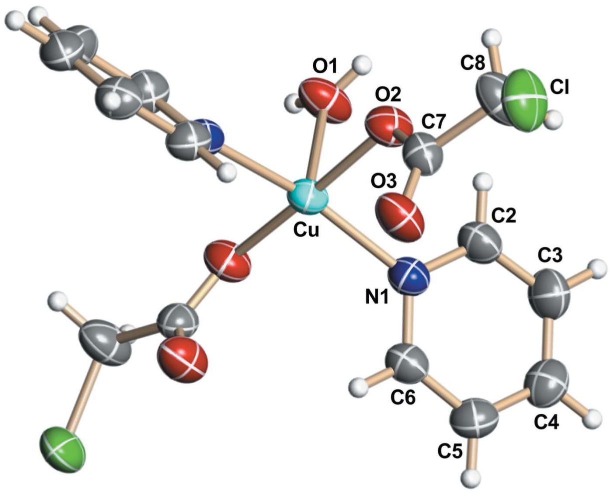


Figure 1
The molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are depicted as spheres of arbitrary radii. Unlabelled atoms are related to the corresponding labelled atoms by the symmetry code $(-x + 1, y, -z + \frac{3}{2})$.

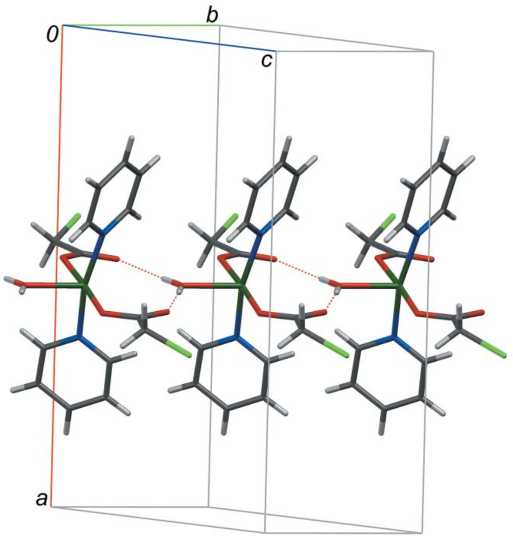


Figure 2
Hydrogen-bonded polymeric chains, running along the [010] direction and viewed approximately down the [01$\bar{1}$] direction. Hydrogen bonds are drawn as dashed lines.

tance of Cu—O and Cu—N bonds of Cu polyhedra and the checking of the valence-sum rule for Cu^{II} (Brown, 2002). R_{Cu-O} and R_{Cu-N} were taken as 1.679 and 1.713 Å, respectively (Sieroń & Bukowska-Strzyżewska, 1999). The computed bond valences of the Cu^{II} atom of (I) show that the Cu—O bond is distinctly stronger than the Cu—N bond (ν_{Cu-O2} = 0.474 v.u. and ν_{Cu-N1} = 0.423 v.u.). The valence of the apical Cu—O1 bond is 0.234 v.u. The valence of the very long Cu···O3 contact is only 0.019 v.u., indicating a lack of interaction. Finally, the valence of the five-coordinated Cu atom is consistent with the valence-sum rule ($V_i = \Sigma\nu_{ij}$), which gives here V_{Cu} = 2.03 v.u.

The observed square-pyramidal (SQP) environment of Cu^{II} is slightly distorted towards trigonal–bipyramidal (TBP) coordination, with the trigonality parameter τ = 0.162 [as defined by Addison *et al.* (1984), τ is equal to 0 for a regular SQP structure and 1 for TBP].

The molecular packing and geometry of the Cu^{II} coordination environment are consistent with those found in two similar octanoate [(II); Petrič *et al.*, 1995] and crotonate [(III); Baggio *et al.*, 2000] complexes. The pyridine ring is inclined to the Cu coordination basal plane, with a dihedral angle of 58.45 (6)°. The corresponding angles for (II) and (III) are 58.2 (1) and 59.3 (1)°, respectively, indicating that the structure of the carboxylic acid chain most probably has no influence on this parameter.

Experimental

The title compound was obtained by adding pyridine (1 mmol) dropwise to a boiling solution of copper(II) monochloroacetate (1 mmol) in water (30 ml). A deep-blue solution was formed and after a few days prismatic crystals precipitated.

Crystal data

$[Cu(C_2H_2ClO_2)_2(C_5H_5N)_2(H_2O)]$
M_r = 426.74
Monoclinic, $C2/c$
a = 16.3650 (6) Å
b = 5.8030 (2) Å
c = 18.3458 (6) Å
β = 90.511 (3)°

V = 1742.16 (10) $Å^3$
Z = 4
Mo $K\alpha$ radiation
μ = 1.59 mm^{-1}
T = 295 K
0.5 × 0.3 × 0.1 mm

Data collection

Kuma KM-4 CCD area-detector diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006)
T_{min} = 0.612, T_{max} = 0.862

7787 measured reflections
1525 independent reflections
1522 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.069
S = 1.12
1525 reflections
114 parameters

H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.38 e $Å^{-3}$

Table 1
Selected geometric parameters (Å, °).

Cu—O1	2.217 (2)	O2—C7	1.272 (3)
Cu—O2	1.9549 (16)	O3—C7	1.218 (3)
Cu—N1	2.0311 (18)		
O1—Cu—O2	87.99 (5)	O2—Cu—O2^{i}	175.98 (8)
O1—Cu—N1	96.87 (5)	O2—Cu—N1^{i}	91.43 (7)
O2—Cu—N1	89.05 (7)	N1—Cu—N1^{i}	166.26 (7)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O3^{ii}	0.78 (3)	1.98 (3)	2.759 (2)	174 (3)

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

All H atoms were initially located in a difference Fourier synthesis. The aromatic and methylene H atoms were then positioned geometrically, with C—H = 0.93 and 0.97 Å, respectively, and included in the refinement in the riding-model approximation, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). Atom H1 of the water molecule was refined isotropically [O1—H1 = 0.78 (3) Å].

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *PLATON* (Spek, 2003) and *publCIF* (Westrip, 2007).

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