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A one-dimensional hydrogen-bonding chain of diacetatobis(3-hydroxypyridine)copper(II)

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Key indicators

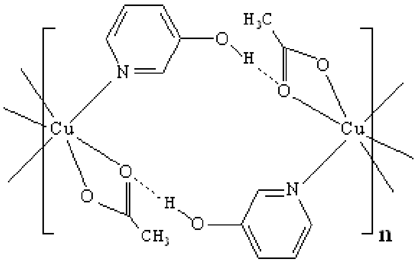
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.039
wR factor = 0.108
Data-to-parameter ratio = 16.4

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

The asymmetric unit of the title complex, $[Cu(C_2H_3O_2)_2(C_5H_5NO)_2]$, consists of two half-units of $[Cu(ac)_2(3\text{-PyOH})_2]$ (ac is acetate and 3-PyOH is 3-hydroxypyridine). The two molecules in the unit cell are held together *via* hydrogen bonds in a chain structure; the Cu$\cdots$Cu separation is 5.482 (2) Å. The Cu^{II} atoms in the two neutral units lie on special positions with inversion symmetry, and both show elongated octahedral geometry, defined by four acetate O atoms and two *endo*-N atoms of two 3-PyOH ligands.

Comment

In recent decades, a particularly active approach in the construction of supramolecular complexes with extended architectures has been focused on the utilization of non-covalent linkages, especially hydrogen-bonding interactions (Iglesias *et al.*, 2003; Braga *et al.*, 2003). In contrast to other weak linkages, hydrogen-bonding interactions between ligands are specific and directional, and have little dependence on the properties of metal ions, which play a critical role in the structures and functions of the products (Subramanian & Zaworotko, 1994). In this sense, bifunctional hydroxypyridine (PyOH) molecules, including 2-OH, 3-OH and 4-OH, are good candidates for the construction of supramolecular complexes, which not only are capable of binding to metal centers but also can form regular hydrogen bonds by functioning as both a hydrogen-bond donors and acceptors (Breeze & Wang, 1993). Among the isomers of PyOH, only 3-PyOH does not have the corresponding tautomeric form, *viz*. 3-pyridone; the N atom of this ligand is, therefore, a preferred binding site for metal ions, and the hydroxyl O atom may become a perfect hydrogen-bonding site. However, hydrogen-bonding supramolecular complexes based on 3-PyOH are relatively rare (Castillo *et al.*, 2000; Kawata *et al.*, 1997).



(I)

Recently, some hydrogen-bonding layer architectures of two cobalt(II) and one copper(II) complexes involving 3- or 4-PyOH ligands have been reported by our group (Gao, Zhang *et al.*, 2004; Gao, Lu *et al.*, 2004; Lu *et al.*, 2004). In this paper, a novel one-dimensional hydrogen-bonded complex,

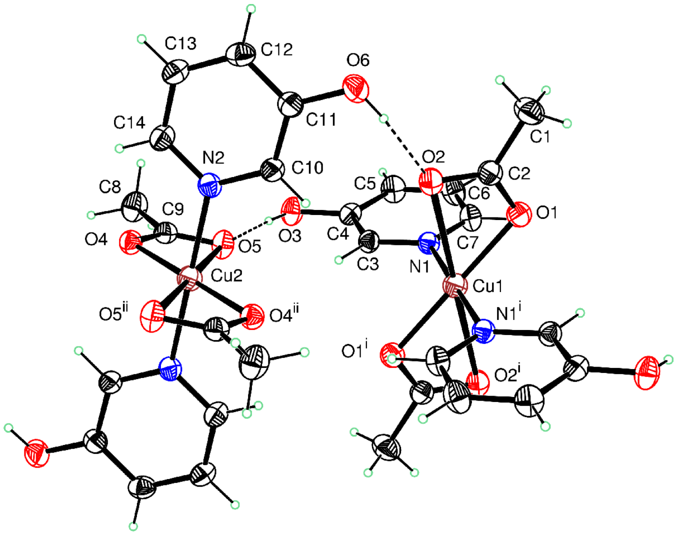


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), with 30% probability displacement ellipsoids.

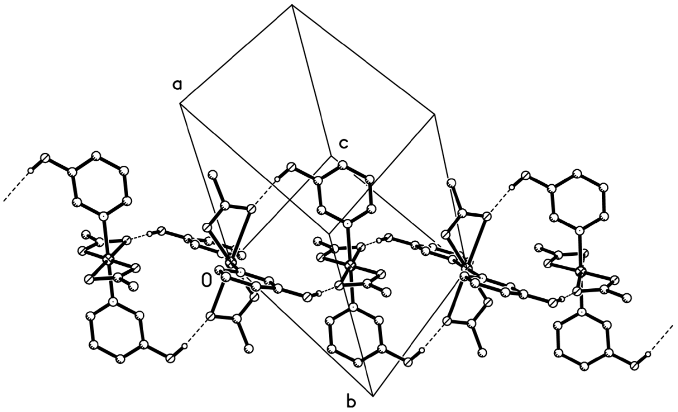


Figure 2
The packing of (I), with the O—H···O hydrogen bonds denoted by dashed lines. H atoms not involved in hydrogen bonding have been omitted.

$[Cu(ac)_2(3\text{-}PyOH)_2]_2$ (ac is acetate and 3-PyOH is 3-hydroxypyridine), (I), is described.

The asymmetric unit of (I) consists of half-units of $[Cu(ac)_2(3\text{-}PyOH)_2]$. The two molecules in the unit cell are held together *via* hydrogen bonds between the hydroxyl O atoms of the 3-PyOH ligand and the acetate O atoms (Fig. 1). The two Cu^{II} atoms are each located on an inversion center, displaying similar elongated octahedral environments defined by four acetate O atoms and two *endo*-N atoms of two 3-PyOH ligands. The Cu1—N1 bond length is 1.997 (2) Å, somewhat shorter than that for Cu2—N2 [2.014 (2) Å], while Cu1—O2 [2.586 (2) Å] is also shorter than Cu2—O5 [2.614 (2) Å].

The dihedral angle between the pyridine rings of the two neutral units is 76.41 (4)°. These mononuclear units are further linked sequentially to each other *via* O—H···O hydrogen bonds between the uncoordinated hydroxyl O atoms of 3-PyOH ligands and the O atoms of acetate groups into an infinite chain, with a Cu···Cu distance of 5.482 (2) Å. The O···O distances and O—H···O angles are in the ranges 2.618 (3)–2.632 (3) Å and 171 (4)–175 (4)°, respectively (Table 1 and Fig. 2).

Experimental

The title complex was prepared by the addition of $Cu(Ac)_2{\cdot}H_2O$ (2 mmol) to an ethanol solution of 3-PyOH (6 mmol). The mixed solution was allowed to evaporate at room temperature, and blue single crystals were isolated from the solution after 8 d. Analysis calculated for $C_{28}H_{32}Cu_2N_4O_{12}$: C 45.22, H 4.34, N 7.53%; found: C 44.98, H 4.50, N 7.56%

Crystal data

$[Cu(C_2H_3O_2)_2(C_5H_5NO)_2]$
$M_r = 371.83$
Triclinic, $P\overline{1}$
$a = 8.9725\ (18)$ Å
$b = 10.138\ (2)$ Å
$c = 10.247\ (2)$ Å
$\alpha = 114.92\ (3)°$
$\beta = 100.20\ (3)°$
$\gamma = 100.07\ (3)°$
$V = 798.8\ (4)$ Å^3
$Z = 2$
$D_x = 1.546$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6857 reflections
$\theta = 3.4–27.5°$
$\mu = 1.40$ mm^{-1}
$T = 293\ (2)$ K
Prism, blue
0.39 × 0.28 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.631$, $T_{max} = 0.778$
7445 measured reflections
3601 independent reflections
2890 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 27.5°$
$h = -11 \rightarrow 10$
$k = -13 \rightarrow 13$
$l = -12 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.108$
$S = 1.06$
3601 reflections
219 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 0.1657P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.53$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.979 (2)	Cu2—N2	2.014 (2)
Cu1—N1	1.997 (2)	O1—C2	1.272 (3)
Cu1—O2	2.586 (2)	O2—C2	1.249 (3)
Cu2—O4	1.975 (2)	O4—C9	1.275 (3)
Cu2—O5	2.614 (2)	O5—C9	1.244 (3)
O1—Cu1—O2	55.76 (7)	O4—Cu2—O5	55.23 (7)
O1—Cu1—N1	89.89 (8)	O4—Cu2—N2	90.02 (8)
O2—Cu1—N1	93.72 (8)	N2—Cu2—O5	89.87 (8)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H15···O5	0.85 (3)	1.78 (3)	2.632 (3)	175 (4)
O6—H16···O2	0.85 (3)	1.78 (1)	2.618 (3)	171 (4)

H atoms on C atoms were placed in calculated positions [C—H = 0.93 (aromatic) or 0.96 Å (methyl), and $U_{iso}(H) = 1.2U_{eq}$(aromatic C) and $1.5U_{eq}$(methyl C)] using the riding-model approximation. The

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hydroxyl H atoms were located in a difference map and refined with O—H distance restraints of 0.85 (1) Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(O).

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); 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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