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Aquabis(1-formyl-2-naphtholato-κ^2O,O')copper(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.049
wR factor = 0.102
Data-to-parameter ratio = 13.6

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

In the title complex, $[Cu(C_{11}H_7O_2)_2(H_2O)]$, the Cu^{II} atom exists in a square-pyramidal environment, coordinated by four O atoms from two formylnaphtholate ligands and one water O atom. Molecules are linked by weak Cu···O interactions and hydrogen bonding into a two-dimensional network.

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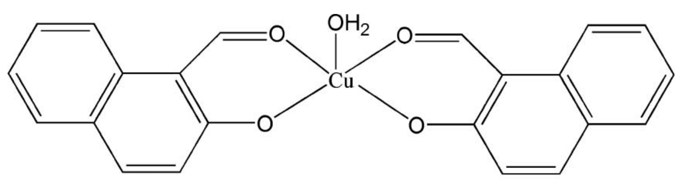
Comment

Aldehydes are one of the most important ligands found in numerous transition metal complexes (Janzen *et al.*, 2004). They are also used extensively as starting materials for the synthesis of new ligands (Vigato & Tamburini, 2004; Collinson & Fenton, 1996; Tsuchida & Oyaizu, 2003; Yamada, 1999). In this paper, we describe the title mononuclear bis Cu^{II} complex, (I), with 2-oxy-1-naphthaldehyde and apically coordinated water.



(I)

The Cu^{II} atom adopts a (4+1) distorted square-pyramidal geometry, with four donor O atoms of two 2-hydroxy-1-naphthaldehyde ligands in the basal plane. The mean Cu—O distance is 1.928 (3) Å. Examination of the metal–ligand distances shows that the Cu—O(oxy group) distances are shorter than the Cu—O(aldehyde group) distances, as observed in (2,2′-bipyridine)(2-oxy-1-naphthaldehyde-O,O')-(perchlorate-O)copper(II) (Bu *et al.*, 2002; Elmali & Elerman, 2002). One water O atom (O5) completes the coordination environment in the apical site (Fig. 1). The apical Cu—O bond [2.364 (4) Å] is longer than those of the basal O atoms. The Cu atom is displaced 0.0815 (2) Å from its basal plane towards the apical atom O5. The value of τ is equal to 0.007, where τ =

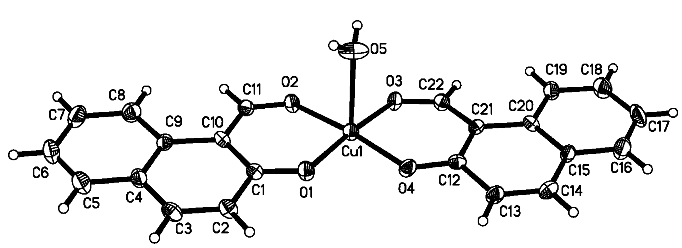


Figure 1
A view of the molecular structure of (I), with the atom-numbering scheme and 30% probability displacement ellipsoids.

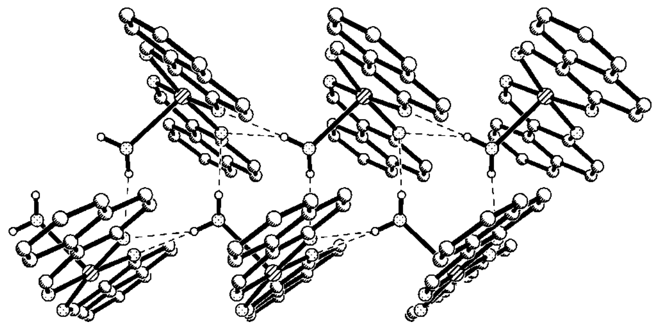


Figure 2
View of the one-dimensional chain built by the mononuclear units *via* hydrogen bonding (dashed lines). H atoms not involved in hydrogen bonding have been omitted.

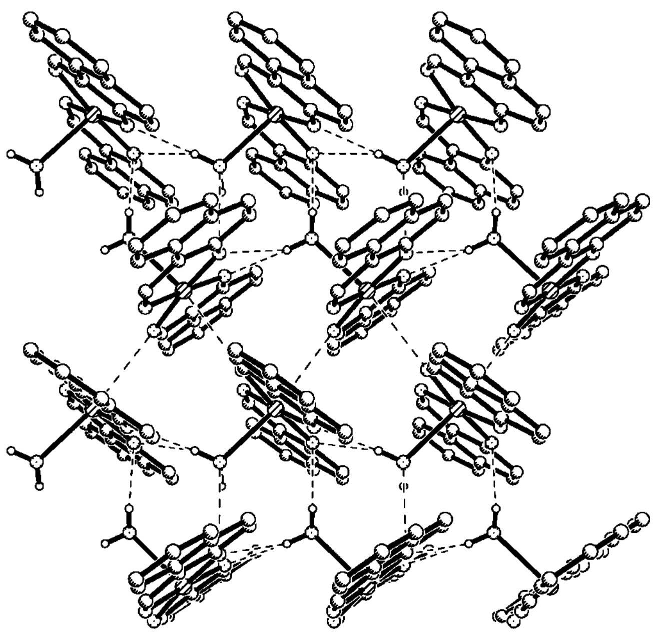


Figure 3
The two-dimensional sheet structure formed by weak interactions (hydrogen bonding and weak Cu···O interactions, shown as dashed lines). H atoms not involved in hydrogen bonding have been omitted.

$(\beta - \alpha)/60$, β(O1—Cu1—O3) = 174.47 (16)° and α(O4—Cu1—O2) = 174.05 (16)° (Addison *et al.*, 1984), which indicates that the coordination environment of the Cu^{II} atom is square-pyramidal. In addition, the distance of 3.098 (6) Å between Cu1 and O3($1 - x, \frac{1}{2} + y, -z$) indicates some weak interaction, which may be viewed as a weak coordination mode (Fu *et al.*, 1997). Thus, the environment of the Cu^{II} atom can also be described as a distorted octahedron. The equatorial plane contains atoms O1, O2, O3 and O4, while the axial positions are filled by atoms O5 and O3 from another molecule.

In the crystal structure, atom H5*A* of O5 is involved in one intermolecular hydrogen bond with O1($-x, y - \frac{1}{2}, -z$). The water molecule, in addition to being a double donor, also interacts with the H atom (H5*B*) bonded to two O atoms, O1 and O4($x, y - 1, z$), of one mononuclear unit. The individual units assemble *via* O—H···O hydrogen bonds, resulting in one-dimensional chains (Fig. 2), which thereby yield two-dimensional sheets through the weak Cu···O interactions (Fig. 3).

Experimental

2-Hydroxy-1-naphthaldehyde (1 mmol) was dissolved in methanol (15 ml), and $CuCl_2\cdot 2H_2O$ (1 mmol) in distilled water (5 ml) was added dropwise. The mixture was stirred and refluxed for 2 h and then filtered. The filtrate was allowed to stand in air at room temperature for several weeks, yielding dark-green single crystals suitable for analysis. The complex is air-stable at room temperature and soluble in EtOH and MeOH.

Crystal data

$[Cu(C_{11}H_7O_2)_2(H_2O)]$	D_x = 1.594 Mg m^{-3}
M_r = 423.89	Mo $K\alpha$ radiation
Monoclinic, $P2_1$	Cell parameters from 838 reflections
a = 9.037 (4) Å	θ = 3.2–23.4°
b = 5.590 (3) Å	μ = 1.27 mm^{-1}
c = 17.484 (8) Å	T = 293 (2) K
β = 90.248 (8)°	Prism, dark green
V = 883.3 (7) Å^3	0.22 × 0.18 × 0.12 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	3452 independent reflections
φ and ω scans	2625 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.034
T_{min} = 0.768, T_{max} = 0.863	θ_{max} = 26.5°
5096 measured reflections	$h = -11 \rightarrow 11$
	$k = -7 \rightarrow 7$
	$l = -11 \rightarrow 21$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0411P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.049	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.102	$\Delta\rho_{max}$ = 0.66 e Å^{-3}
S = 0.98	$\Delta\rho_{min}$ = −0.43 e Å^{-3}
3452 reflections	Absolute structure: Flack (1983), 1431 Friedel pairs
254 parameters	Flack parameter: 0.00 (2)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Cu1—O4	1.906 (3)	Cu1—O2	1.945 (3)
Cu1—O1	1.923 (3)	Cu1—O5	2.364 (4)
Cu1—O3	1.938 (3)		
O4—Cu1—O1	84.95 (14)	O3—Cu1—O2	90.83 (13)
O4—Cu1—O3	92.77 (14)	O4—Cu1—O5	98.88 (14)
O1—Cu1—O3	174.47 (16)	O1—Cu1—O5	96.96 (15)
O4—Cu1—O2	174.05 (16)	O3—Cu1—O5	88.36 (14)
O1—Cu1—O2	91.04 (14)	O2—Cu1—O5	85.95 (14)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5*A*···O1^{i}	0.87	2.45	2.919 (5)	114
O5—H5*B*···O1^{ii}	0.84	2.55	3.165 (5)	131
O5—H5*B*···O4^{ii}	0.84	2.31	3.126 (5)	163

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

H atoms of the water molecules were located in a difference Fourier map and refined as riding in their as-found positions. H atoms of 2-hydroxy-1-naphthaldehyde were positioned geometrically and refined using a riding model, with C—H = 0.93 Å. U_{iso}(H) values were set at $1.2U_{eq}$(C,O).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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