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Bisaquabis(8-hydroxyquinolinato-*N*,*O*)copper(II)

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Key indicators

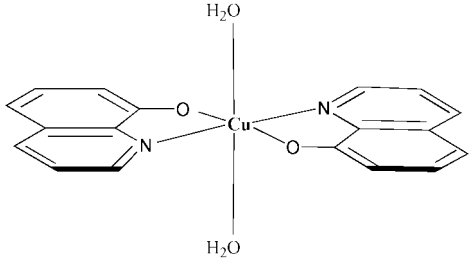
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.033
wR factor = 0.111
Data-to-parameter ratio = 13.2

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

The title compound, $[Cu(C_9H_6NO)_2(H_2O)_2]$, has a distorted octahedral geometry. The two N,O-bidentate ligand molecules lie in a *trans* geometry, in which the six-coordinate Cu^{II} ion lies on an inversion center.

Comment

8-Hydroxyquinoline (8-quinolinol, oxine) is a well known analytical reagent for forming chelate complexes with metal ions. Its metal complexes with copper(II), zinc(II) or nickel(II) have remarkable antimicrobial or fungicidal activity (Okide *et al.*, 2000; Patel *et al.*, 1999). The bismuth(III) complex has antitumor activity against leukaemia (Smith *et al.*, 1998). These results indicate that the metal complex of 8-hydroxyquinoline may be useful as a chemotherapeutic agent. Although the molecular mechanisms of the above activities are not yet clear, it is clear that the coordination geometry of these compounds plays an important role in their biological function. Although crystal structures of two types of copper(II) complexes of 8-hydroxyquinoline have been determined previously (Palenik, 1964; Hoy & Morriss, 1967), we have determined the structure of a different copper(II) complex, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. The Cu^{II} ion is bonded to two N and two O atoms of the bidentate ligand molecules, forming two five-membered rings including the C7 and C8 atoms of the ligand molecule. The molecule has a distorted octahedral geometry. The two ligand molecules are centrosymmetrically related and the six-coordinate Cu^{II} ion lies on an inversion center of six-coordination. The Cu^{II} ion is bonded to two N atoms and two deprotonated O atoms of two ligand molecules which are located in a *trans* configuration with respect to each other, and also to two water O atoms in axial positions.

The Cu1—O1 distance of 1.966 (2) Å is slightly shorter than the Cu1—N1 distance of 2.013 (2) Å. This difference corresponds well to the difference of the Pauling's covalent radii

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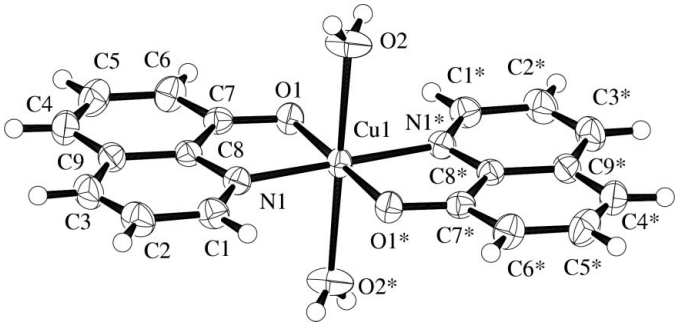

Figure 1
*ORTEP*II (Johnson, 1976) drawing of the title compound with the atomic numbering scheme. Ellipsoids for non-H atoms corresponding to 50% probability.

r(N) = 0.70 Å and r(O) = 0.66 Å. The values found correspond well to the averages given by Orpen *et al.* (1989). The Cu1—O1 distance is somewhat longer than 1.930 Å of the five-coordinate anhydrous copper(II) complex (Palenik, 1964) and 1.939 Å of the six-coordinate anhydrous copper(II) complex (Hoy & Morriss, 1967). The Cu1—N1 distance is also longer than 1.972 Å of the five-coordinate complex and 1.984 Å of the six-coordinate one. On the other hand, the distance between Cu1 and the water O atom O2, 2.41 (2) Å is shorter than the corresponding Cu—O distances of the five-coordinate complex, 2.830 Å (Palenik, 1964), and the six-coordinate one, 3.324 Å (Hoy & Morriss, 1967).

Experimental

The light-blue plate crystal was obtained by slow evapolation from a solution in ethanol–water (9:1) of a mixture containing 8-hydroxyquinoline and copper(II) chloride in a 5:1 molar ratio at room temperature.

Crystal data

$[Cu(C_9H_6NO)_2(H_2O)_2]$
M_r = 387.88
Monoclinic, $P2_1/a$
a = 11.425 (3) Å
b = 5.542 (3) Å
c = 12.950 (4) Å
β = 106.39 (2)°
V = 786.7 (5) Å^3
Z = 2
D_x = 1.637 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 24 reflections
θ = 14.9–15.0°
μ = 1.42 mm^{-1}
T = 296.2 K
Plate, light blue
0.50 × 0.40 × 0.30 mm

Data collection

Rigaku AFC-5*R* diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.512, T_{max} = 0.654
2094 measured reflections
1813 independent reflections
1516 reflections with $I > 2\sigma(I)$
R_{int} = 0.011
θ_{max} = 27.5°
$h = 0 \rightarrow 14$
$k = -7 \rightarrow 0$
$l = -16 \rightarrow 16$
3 standard reflections every 150 reflections intensity decay: 0.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.111
S = 0.91
1516 reflections
115 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ < 0.001
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.966 (2)	O1—C7	1.318 (2)
Cu1—O2	2.451 (2)	N1—C1	1.321 (3)
Cu1—N1	2.013 (2)	N1—C8	1.357 (3)
O1—Cu1—O2	90.88 (6)	C4—C5—C6	122.1 (2)
O1—Cu1—N1	83.70 (6)	C5—C6—C7	121.0 (2)
O2—Cu1—N1	93.67 (6)	O1—C7—C6	124.5 (2)
Cu1—O1—C7	112.0 (1)	O1—C7—C8	118.1 (2)
Cu1—N1—C1	130.7 (2)	C6—C7—C8	117.4 (2)
Cu1—N1—C8	110.1 (1)	N1—C8—C7	116.1 (2)
C1—N1—C8	119.2 (2)	N1—C8—C9	122.8 (2)
N1—C1—C2	121.9 (2)	C7—C8—C9	121.1 (2)
C1—C2—C3	119.8 (2)	C3—C9—C4	125.1 (2)
C2—C3—C9	120.2 (2)	C3—C9—C8	116.0 (2)
C5—C4—C9	119.5 (2)	C4—C9—C8	118.9 (2)
O1—Cu1—N1—C1	178.4 (2)	O2—Cu1—N1—C1	−91.2 (2)
O2—Cu1—O1—C7	−92.9 (1)	O2—Cu1—N1—C8	89.3 (1)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H7···O1^{i}	0.89	1.94	2.829 (2)	171
O2—H8···O1^{ii}	0.77	2.07	2.839 (2)	175

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

All H atoms were located from difference Fourier maps and were not refined.

Data collection and cell refinement: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation and Rigaku Corporation, 1999*a*); data reduction: *TEXSAN* (Molecular Structure Corporation and Rigaku Corporation, 1999*b*); program(s) used to solve structure: *SAPI*91 (Fan, 1991); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *TEXSAN*.

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