

Aqua{1-[(2-oxidophenyl)iminomethyl]-
naphthalen-2-olato}pyridinecopper(II)Xiu-Lian Zhang,^a Chun-Xia Ren,^a
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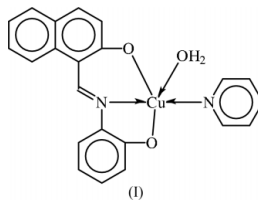
Key indicators

Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$
Disorder in main residue
 R factor = 0.041
 wR factor = 0.117
Data-to-parameter ratio = 15.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

In the title compound, $[\text{Cu}(\text{C}_{17}\text{H}_{11}\text{NO}_2)(\text{C}_5\text{H}_5\text{N})(\text{H}_2\text{O})]$, the anionic naphthalen-2-olate group chelates to the Cu atom through its O, O' and N atoms, and the N atom of the heterocycle completes the square-planar coordination of the Cu atom. The apical site of the square-pyramidal environment is occupied by the water ligand. Adjacent molecules are linked by hydrogen bonds into a linear chain running along the b axis of the monoclinic unit cell.

Comment

We have reported several copper complexes of Schiff bases having an imidazole entity, and have concluded that hydrogen bonding involving this group influences the geometry around the metal atom and the crystallization mechanism (Long *et al.*, 2001). This study has been extended to Schiff bases derived from the condensation of aromatic aldehydes and amino-substituted phenols, as such Schiff bases can function as O,N,O -chelates. The copper derivative of 2-hydroxyphenyl-salicylaldehyde, $\text{HOC}_6\text{H}_4\text{-N-CH-C}_6\text{H}_4\text{OH}$, forms an adduct with pyridine in which the metal atom shows square-planar coordination (Emali *et al.*, 1993). The change from the salicylaldehyde unit to the 2-hydroxynaphthaldehyde probably renders the metal center more Lewis acidic, so that it is able to accept a water molecule into its coordination sphere. In the title aqua complex, (I) (Fig. 1), the Cu atom shows square-pyramidal coordination, with the O, O' and N atoms of the dianion occupying three positions of the square. The fourth is occupied by the pyridine molecule, and the coordination geometry is completed by the apical water ligand. Hydrogen bonds link adjacent molecules into a linear chain (Table 2 and Fig. 2).



Experimental

The Schiff base $\text{C}_{17}\text{H}_{13}\text{NO}_2$ was synthesized by condensing equimolar quantities of 2-hydroxynaphthalenaldehyde and 2-aminophenol in a methanol medium. Copper dichloride dihydrate (0.03 g, 0.2 mmol) and the Schiff base (0.05 g, 0.2 mmol) were dissolved in pyridine (8 ml). The dark-brown solution was stirred for an hour and then filtered. Evaporation of the solvent yielded dark-green crystals of the pyridine adduct. Analysis found: C 62.87, H 4.33, N 6.38%; calculated for $\text{C}_{22}\text{H}_{18}\text{N}_2\text{O}_3\text{Cu}$: C 62.62, H 4.30, N 6.64%.

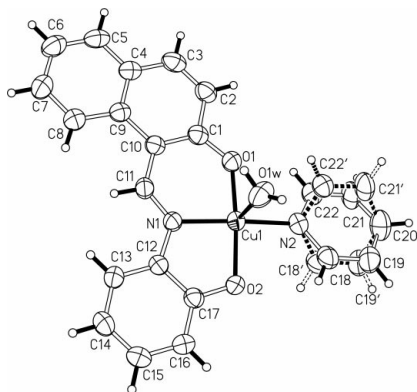


Figure 1
ORTEPII (Johnson, 1976) plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. The pyridine molecule is disordered.

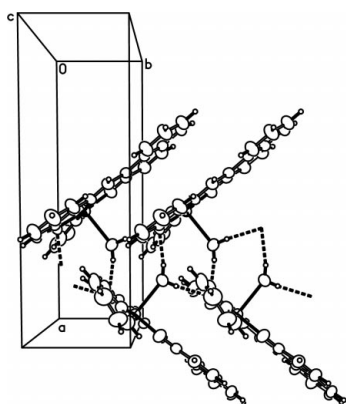


Figure 2
ORTEPII (Johnson, 1976) plot depicting the hydrogen-bonded chain structure.

Crystal data

[Cu(C₁₇H₁₁NO₂)(C₅H₅N)(H₂O)]
M_r = 421.92
 Monoclinic, *P*₂₁/*n*
a = 16.947 (1) Å
b = 5.5645 (4) Å
c = 19.462 (2) Å
 β = 95.803 (1)°
V = 1825.9 (2) Å³
Z = 4

D_x = 1.535 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 2530 reflections
 θ = 2.4–24.1°
 μ = 1.22 mm⁻¹
T = 298 (2) K
 Plate, green
 0.24 × 0.17 × 0.03 mm

Data collection

Bruker APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.651, *T_{max}* = 0.888
 10 709 measured reflections

4087 independent reflections
 2683 reflections with *I* > 2σ(*I*)
R_{int} = 0.035
 θ_{\max} = 27.5°
h = -17 → 21
k = -6 → 7
l = -25 → 25

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.041
wR(*F*²) = 0.117
S = 0.90
 4087 reflections
 273 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0671P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.43 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.43 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Cu1—O1	1.915 (2)	Cu1—N1	1.941 (2)
Cu1—O2	1.953 (2)	Cu1—N2	2.030 (2)
Cu1—O1w	2.389 (2)		
O1—Cu1—O2	174.1 (1)	O2—Cu1—N2	93.6 (1)
O1—Cu1—O1w	91.0 (1)	O2—Cu1—O1w	93.9 (1)
O1—Cu1—N2	89.5 (1)	O1w—Cu1—N1	92.7 (1)
O1—Cu1—N1	91.7 (1)	O1w—Cu1—N2	93.0 (1)
O2—Cu1—N1	84.7 (1)	N1—Cu1—N2	174.2 (1)

Table 2

Hydrogen-bonding geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1w—H1w1...O2 ⁱ	0.84 (3)	2.02 (2)	2.860 (3)	173 (4)
O1w—H1w2...O2 ⁱⁱ	0.84 (3)	2.03 (2)	2.858 (3)	168 (3)

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

H atoms, excluding water H, were placed at calculated positions in the riding-model approximation (C—H = 0.93 Å), with their displacement parameters set to 1.2 times *U_{eq}* of the parent atoms. The water H atoms were located in a difference map and their positional parameters were refined, with distance restraints of O—H = 0.85 (1) Å and H...H = 1.39 (1) Å. The pyridine molecule is disordered by rotation about the N—C_{para} axis; as the occupancy refined to nearly 50:50, the occupancies were fixed to exactly 0.5. Distance restraints of C—C and C—N = 1.390 (5) Å, and C...C and C...N = 2.780 (5) Å, were applied to the molecule; the displacement parameters of the unprimed and primed atoms were made equal to one another. The two rings are twisted from each other by about 45°.

Data collection: SMART (Bruker, 2001); cell refinement: SMART; data reduction: SAINT (Bruker, 2001); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97 (Sheldrick, 1997).

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