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Bis{*N*-(2-hydroxybenzoyl)-*N*′-[1-(2-pyridyl)-ethylidene}hydrazinato]copper(II)

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The title complex, $[Cu(C_{14}H_{12}N_3O_2)_2]$, consists of two deprotonated 2-acetylpyridine salicylhydrazone ligands coordinated to the copper as *N*,*N*,*O*-tridentate ligands, forming a neutral complex. The Cu atom lies on a twofold rotation axis. The structure is stabilized by intramolecular O—H···N hydrogen bonding, and π–π stacking interactions between the pyridyl and benzene rings lead to a two-dimensional network in the crystal structure.

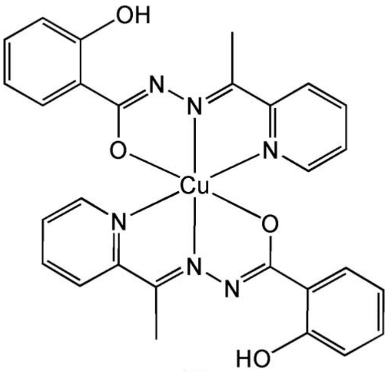
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.036
wR factor = 0.077
Data-to-parameter ratio = 11.0

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

Comment

Diazine Schiff base ligands with two coordination compartments linked by a single N—N bridge have received considerable attention due to the diversity of their structural and functional properties (Grove *et al.*, 2004; Bai *et al.*, 2006). This type of polydentate ligand usually generates a variety of different structural forms (Bai *et al.*, 2005; Song *et al.*, 2004). Transition-metal-directed self-assembly has also become a powerful methodology for the construction of different coordination complexes with different geometries and spectroscopic characteristics and can give rise to extended solids with a variety of structures and physical properties (Leininger *et al.*, 2000).



(I)

The title copper(II) complex, (I), was obtained by the reaction of $CuCl_2{\cdot}2H_2O$ with the pentadentate Schiff base ligand 2-acetylpyridine salicylhydrazone (H_2L). The X-ray structure determination shows that the molecule consists of two HL^- ligands coordinated to the copper as *N*,*N*,*O*-tridentate ligands, forming a neutral complex (Fig. 1). A feature of the structure is that the copper atom lies on a twofold rotation axis. The ligands bond to the copper in the *mer* configuration (with pairs of carbonyl O atoms and pyridyl N atoms each bearing a *cis* relationship, whereas the imino N atoms are *trans* to each other). The intramolecular O—H···N hydrogen bond

(Table 2) is an important factor in the stabilization of the molecule. In the crystal structure, molecules interact with each other, forming a two-dimensional network through π–π stacking interactions between the benzene and pyridine rings.

Experimental

2-Acetylpyridine salicylhydrazone (H_2L) was obtained in high yield by the direct combination of 1:1 molar equivalents of salicylaldehyde and 2-acetylpyridine in methanol. A solution of the H_2L ligand (0.025 g, 0.1 mmol) and Et_3N (0.011 g, 0.1 mmol) in methanol (6 ml) was layered on to a solution of DMF (6 ml) containing $CuCl_2\cdot 2H_2O$ (0.017 g, 0.1 mmol) at the bottom. The solutions were left for few weeks at room temperature in darkness to give X-ray quality crystals (84% yield).

Crystal data

$[Cu(C_{14}H_{12}N_3O_2)_2]$
$M_r = 572.07$
Orthorhombic, *Aba*2
$a = 12.570$ (2) Å
$b = 18.731$ (4) Å
$c = 10.6482$ (19) Å
$V = 2507.1$ (8) Å^3
$Z = 4$
$D_x = 1.516$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.92$ mm^{-1}
$T = 293$ (2) K
Block, green
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
6226 measured reflections
1968 independent reflections
1628 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.041$
$\theta_{\rm max} = 25.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.077$
$S = 1.02$
1968 reflections
179 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.035P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.52$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.16$ e Å^{-3}
Absolute structure: Flack (1983), 738 Friedel pairs
Flack parameter: −0.018 (19)

Table 1
Selected geometric parameters (Å, °).

Cu1—N2	1.966 (3)	Cu1—O1	2.158 (3)
Cu1—N1	2.156 (3)		
N2—Cu1—N2^i	172.1 (2)	N1—Cu1—O1^i	93.46 (10)
N2—Cu1—N1^i	108.75 (13)	N2—Cu1—O1	76.59 (12)
N2—Cu1—N1	77.11 (13)	N1—Cu1—O1	152.95 (10)
N1^i—Cu1—N1	89.07 (16)	O1^i—Cu1—O1	96.32 (15)
N2—Cu1—O1^i	98.04 (11)		

Symmetry code: (i) −*x*, −*y*, *z*.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N3	0.82	1.82	2.550 (4)	148

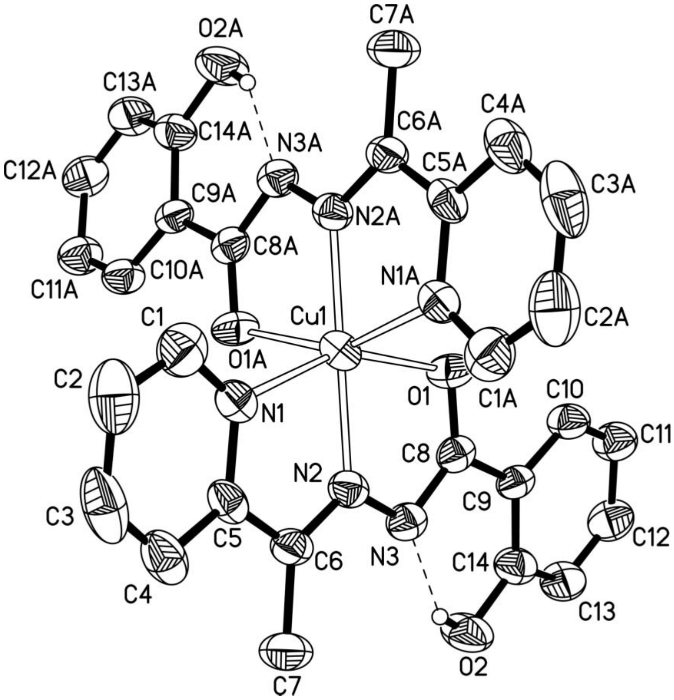


Figure 1
The molecular structure of the title complex, with displacement ellipsoids drawn at the 30% probability level. H atoms other than those of hydroxyl have been omitted for clarity. Hydrogen bonds are indicated by dashed lines. [Symmetry code: (A) −*x*, −*y*, *z*.]

The H atoms bonded to C and O atoms were constrained to ride on their parent atoms, with distances of 0.97 and 0.89 Å, respectively, and $U_{\rm iso}(H) = 1.2U_{\rm eq}(C)$ and $1.5U_{\rm eq}(O)$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2000); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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