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Bis[2-(quinolin-3-yliminomethyl)phenolato-κ^2N,O]-copper(II)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.039
wR factor = 0.112
Data-to-parameter ratio = 10.0

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

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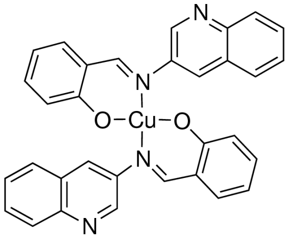
In the title complex, $[Cu(C_{16}H_{11}N_2O)_2]$, the Cu^{II} atom lies on a center of symmetry within a square-planar *trans*-N_2O_2 coordination geometry and adopts a stepped conformation with regard to the bulky Schiff base ligands.

Comment

Schiff base complexes have been studied extensively in the field of coordination chemistry. For instance, it is well known that introduction of bulky groups or electronically appropriate substituents to Ni^{II} or Cu^{II} complexes leads to square-planar–tetrahedral isomerism (Yamada, 1999); this property may be applied in supramolecular switching materials. However, the correlation between the steric or electronic factors of ligands and overall molecular structure remains unclear, thus demanding further investigation. In this context, it is important to investigate bulky ligands and, if possible, those that can form intermolecular interactions. Our studies in this field have focused on catalytic applications (Akitsu *et al.*, 2004) and a structural phase transition (Akitsu & Einaga, 2004). We describe here the crystal structure of bis[2-(quinolin-3-yliminomethyl)phenolato-κ^2N,O]copper(II), (I).



(I)

Complex (I) is centrosymmetric with the central Cu atom located on a center of inversion (Fig. 1 and Table 1). The structure features a square-planar *trans*–N_2O_2 coordination geometry. The distortions from the ideal square-planar geometry are minor, as seen in the Cu—N and Cu—O bond distances of 2.040 (2) and 1.898 (2) Å, respectively. Similarly, the O1—Cu1—N1 and O1—Cu1—N1^i bond angles are 90.46 (9) and 89.54 (9)°, respectively [symmetry code: (i) $2 - x, -y, 2 - z$]. The dihedral angle between the O1/Cu1/N1 and O1/C6/C1/C7/N1 planes is 26.79 (9)°, showing that there is a significant non-coplanarity of the CuN_2O_2 plane and the six-membered chelate ring. Thus, the molecule adopts a stepped conformation with respect to the arrangement of the ligands. In addition, there is a significant twist between the chelate ring and the pendant quinolin-3-ylimino group, as seen in the dihedral angle between the O1/C6/C1/C7/N1 and C9/C8/N2/C16/C11/C10 planes of 29.4 (1)°; the corresponding torsion

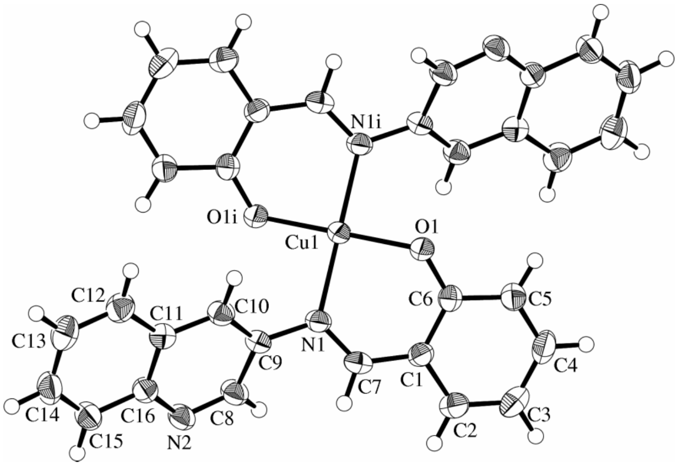


Figure 1
The molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are shown at the 50% prpbability level [symmetry code: (i) $2 - x, -y, 2 - z$].

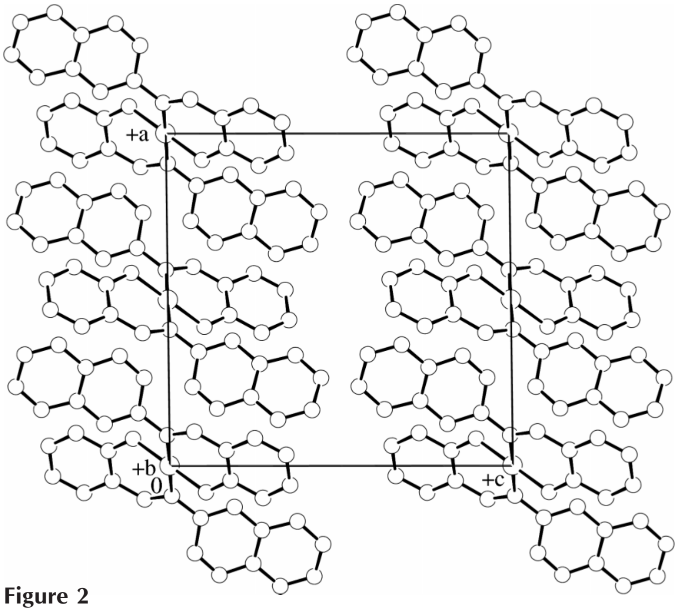


Figure 2
The packing of (I), viewed down the crystallographic *a* axis. H atoms have been omitted for clarity.

angles are C7—N1—C9—C8 = −38.2 (4)° and C7—N1—C9—C10 = 143.6 (3)°.

Recently, we reported the crystal structure of the related square-planar and stepped $\mathrm{Cu^{II}}$ complex bis(5-chloro-*N*-isopropylsalicyldenaminato-$\kappa^2 N,O$)copper(II) (Akitsu & Einaga, 2004). In general, the introduction of electron-withdrawing substituents into the salicylaldehyde ring moiety plays a role in reducing the electronic distribution of $d\pi$–$p\pi$ type coordination bonds through the π-conjugated system, which may cause a tetrahedral distortion and relatively long coordination bond distances.

The geometric parameters of the quinolin-3-ylimino moiety are comparable to those found in uncoordinated molecules (*e.g.* Leung & Nyburg, 1971; Laks *et al.*, 1986) and in ligands in metal complexes (*e.g.* Garralda *et al.*, 1999; Guo & Mayr, 1997).

Neither intermolecular hydrogen bonds nor π–π or weak C—H$\cdots\pi$ interactions within the sum of ionic radii (Bondi, 1964) were observed in the crystal structure of (I). In particular, atom N2 of the quinolin-3-ylimino rings is not involved in either coordination or intermolecular hydrogen bonds. In this way, the crystal packing of (I) is dominated by weak van der Waals forces (Fig. 2).

Experimental

Treatment of equimolar quantities of 3-aminoquinoline (1.44 g, 10.0 mmol), salicylaldehyde (1.22 g, 10.0 mmol) and copper(II) acetate (0.91 g, 5.00 mmol) in ethanol (100 ml) at 318 K for 2 h gave rise to the brown title compound, (I). Block-like crystals were grown from the resulting solution over a period of several days.

Crystal data

$[\mathrm{Cu(C_{16}H_{11}N_2O)_2}]$
$M_r = 558.09$
Monoclinic, $P2_1/a$
$a = 12.767$ (3) Å
$b = 7.346$ (2) Å
$c = 13.133$ (5) Å
$\beta = 90.66$ (3)°
$V = 1231.6$ (6) Å^3
$Z = 2$
$D_x = 1.505$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 10.0$–13.3°
$\mu = 0.93$ mm^{-1}
$T = 298$ (1) K
Block, brown
0.40 × 0.30 × 0.20 mm

Data collection

Rigaku AFC-7*R* diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.724$, $T_{\max} = 0.831$
3539 measured reflections
2832 independent reflections
1784 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.028$
$\theta_{\max} = 27.5$°
$h = -6 \rightarrow 16$
$k = -9 \rightarrow 3$
$l = -17 \rightarrow 17$
3 standard reflections every 150 reflections intensity decay: 0.2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.112$
$S = 1.00$
1784 reflections
179 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0388P)^2 + 0.6777P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.30$ e Å^{-3}
$\Delta\rho_{\min} = -0.32$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.898 (2)	N1—C7	1.296 (4)
Cu1—N1	2.040 (2)	N1—C9	1.429 (4)
O1—C6	1.306 (4)	C1—C7	1.427 (4)
O1—Cu1—N1	90.46 (9)	C7—N1—C9	115.9 (3)
O1—Cu1—N1$^{\rm i}$	89.54 (9)	O1—C6—C1	123.1 (3)
Cu1—O1—C6	125.6 (2)	O1—C6—C5	119.7 (3)
Cu1—N1—C7	120.6 (2)	N1—C9—C8	120.2 (3)
Cu1—N1—C9	122.9 (2)	N1—C9—C10	122.0 (3)

Symmetry code: (i) $2 - x, -y, 2 - z$.

H atoms were placed in calculated positions, with C—H = 0.95 Å, and refined using a riding model, with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(parent atom).

Data collection: *WinAFC Diffractometer Control Software* (Rigaku, 1999); cell refinement: *WinAFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 2001); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); 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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