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Bis[2-(phenethyliminomethyl)phenolato-κ^2N,O]-copper(II)

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Key indicators

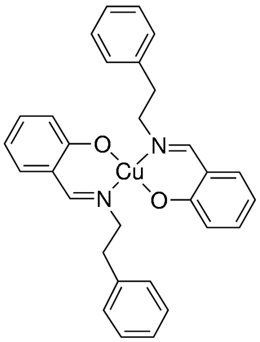
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.033
wR factor = 0.104
Data-to-parameter ratio = 13.2

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

The title compound, $[Cu(C_{15}H_{14}NO)_2]$, adopts a stepped conformation and displays a square-planar *trans*-$[CuN_2O_2]$ coordination geometry. The asymmetric unit contains two independent half molecules and each Cu atom is located on a center of symmetry. For one molecule, the Cu—N and Cu—O bond distances are 2.013 (2) and 1.893 (2) Å, respectively, while for the other molecule, these distances are 2.008 (2) and 1.896 (2) Å. The extended conformation of the phenethylimine pendant groups results in crystal packing formed by weakly aggregated planar molecules.

Comment

Schiff base complexes have been widely investigated in the field of coordination chemistry (Yamada, 1999). For instance, interest has focused on catalysts for Co^{II} (Akitsu *et al.*, 2004), thermally induced structural phase transition for Cu^{II} (Akitsu & Einaga, 2004), and so on. Planar–tetrahedral distortion isomerism on temperature change can potentially be applied for supramolecular switching materials of co-operating crystalline systems. However, the correlation between steric factors of ligands and molecular or crystal structures has been unclear. Hence, systematic studies on various substituents of ligands is necessary. For example, the 1-phenylethylamine moiety is employed for chiral homogeneous catalysts (Li *et al.*, 1987), while the 2-phenylethylamine moiety is employed not only in Werner-type complexes but also in organometallic complexes such as Pd^{II} complexes (Albert *et al.*, 1990; Lopez *et al.*, 1992; Bosque *et al.*, 1994) We report here the result of the crystal structure analysis of the title compound, (I), having a 2-phenylethylamine moiety.



(I)

There are two half molecules in the asymmetric unit of (I), generating molecule 1 (Cu1 complex) and molecule 2 (Cu2 complex). Each Cu atom is located on a center of symmetry. Each complex of (I) affords a square-planar *trans*-$[CuN_2O_2]$

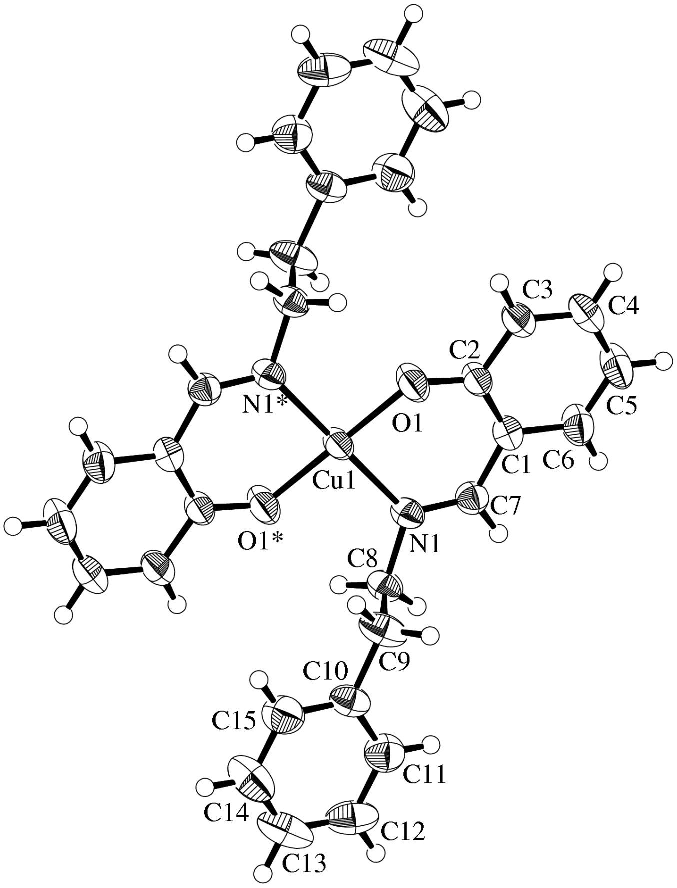


Figure 1
The molecular structure of (I) (molecule 1), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. Atoms marked with an asterisk (*) are at the symmetry-generated position (−*x*, −*y*, −*z*).

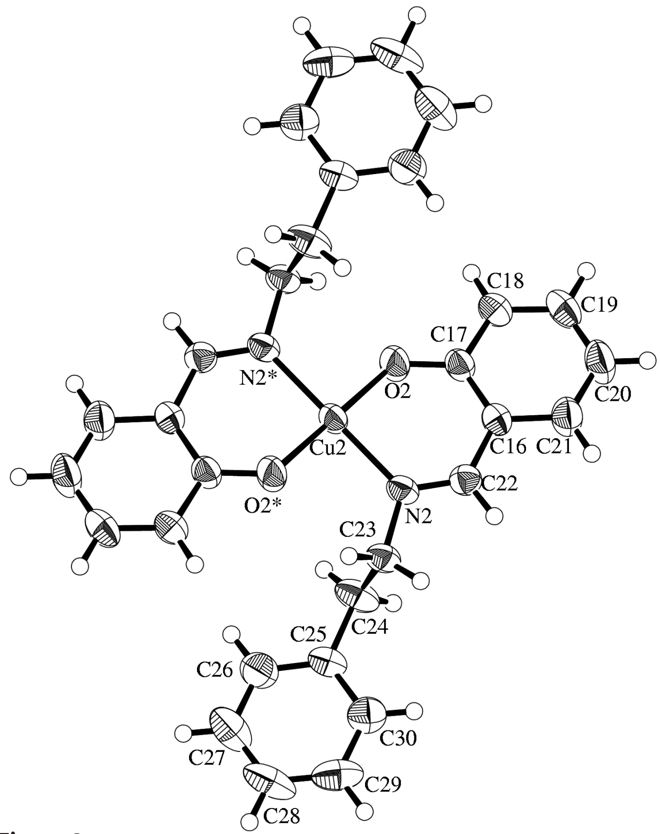


Figure 2
The molecular structure of (I) (molecule 2), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. Atoms marked with an asterisk (*) are at the symmetry-generated position (−*x*, 1 − *y*, 1 − *z*).

coordination geometry (Table 1) and adopts a stepped conformation. For molecule 1 (Fig. 1), the Cu1—O1 and Cu1—N1 bond distances are 1.893 (2) and 2.013 (2) Å, respectively. The *cis*–O1—Cu1—N1 and *cis*-O1—Cu1—N1$^{\rm i}$ bond angles are 90.68 (7) and 89.32 (7)°, respectively [symmetry code: (i) −*x*, −*y*, −*z*]. On the other hand, for molecule 2 (Fig. 2), the Cu2—O2 and Cu2—N2 bond distances are 1.896 (2) and 2.008 (2) Å, respectively. The *cis*-O2—Cu2—N2 and *cis*-O2—Cu2—N2$^{\rm ii}$ bond angles are 90.66 (7) and 89.34 (7)°, respectively [symmetry code: (ii) −*x*, 1 − *y*, 1 − *z*].

The bond lengths and angles around the imine groups are N1═C7 = 1.283 (3) Å, C1—C7 = 1.441 (3) Å and N1—C7—C1 = 126.7 (2)° for molecule 1, and N2═C22 = 1.286 (2) Å, C16—C22 = 1.442 (3) Å and N2—C22—C16 = 126.6 (2)° for molecule 2. Because of the typical square-planar environment, these values are comparable to those of related Schiff base copper(II) complexes (Nepveu *et al.*, 1983; Kirchner *et al.*, 1973).

In contrast to a 1-phenylethylamine complex (Li *et al.*, 1987), bulky phenyl groups are on the outside of the molecule, reducing steric repulsion with no remarkable interactions. Indeed, the torsion angles of the 2-phenylethylamine moiety are N1—C8—C9—C10 = 171.6 (2)° for molecule 1 and N2—C23—C24—C25 = −171.7 (2)° for molecule 2.

There are no significant intermolecular hydrogen bonds or other interactions within van der Waals radii (Bondi, 1964) in the crystal structure of (I) (Fig. 3). Hence, crystal packing is formed by weak van der Waals forces. Despite five-coordination, the chlorobis(*N*-2-phenylethylsalicylideniminato)-iron(III) complex (Magurany & Strouse, 1982) adopts a similar conformation and takes a similar overall molecular shape. On the other hand, bis(*N*-2-phenyethylsalicylideniminato)nickel(II) (Ravikumar & Rajan, 1986) adopts a more bent shape and exhibits different crystal-packing features.

Furthermore, complex (I) also exhibits a phase transition, which is confirmed by an endothermal peak of the DSC curve at 458 K. As with analogous Cu$^{\rm II}$ complexes (Yamada, 1999), this structural phase transition produced by heating leads to a distorted tetrahedral coordination environment.

Experimental

The reaction of copper(II) acetate (0.91 g, 5.00 mmol), salicylaldehyde (1.22 g, 10.0 mmol) and 2-phenylethylamine (1.21 g, 10.0 mmol) in ethanol (100 ml) at 318 K for 3 h gave a brown compound. Plate-shaped crystals were obtained by the slow evaporation of an acetone solution at 278 K; the yield was about 20%.

Analysis found: C 70.31, H 5.49, N 5.43%; calculated for $C_{30}H_{28}CuN_2O_2$: C 70.36, H 5.51, N 5.47%. IR (KBr): 1619 cm^{-1} (imine band); m.p. 598 K (decomposition).

Crystal data

$[Cu(C_{15}H_{14}NO)_2]$
$M_r = 512.09$
Triclinic, $P\overline{1}$
$a = 11.943$ (4) Å
$b = 11.944$ (5) Å
$c = 9.102$ (3) Å
$\alpha = 89.81$ (3)°
$\beta = 91.89$ (3)°
$\gamma = 75.43$ (3)°
$V = 1255.9$ (8) Å^3
$Z = 2$
$D_x = 1.354$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 11.0$–12.5°
$\mu = 0.90$ mm^{-1}
$T = 298$ (1) K
Plate, brown
0.20 × 0.20 × 0.15 mm

Data collection

Rigaku AFC-7*R* diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.835$, $T_{max} = 0.874$
6444 measured reflections
5773 independent reflections
4237 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$
$\theta_{max} = 27.5°$
$h = -15 \rightarrow 15$
$k = -15 \rightarrow 15$
$l = -11 \rightarrow 4$
3 standard reflections every 150 reflections intensity decay: 0.9%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.104$
$S = 1.01$
4237 reflections
320 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 0.2726P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.41$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.893 (2)	Cu2—O2	1.896 (2)
Cu1—N1	2.013 (2)	Cu2—N2	2.008 (2)
O1—Cu1—N1	90.68 (7)	O2—Cu2—N2	90.66 (7)
O1—Cu1—N1^{i}	89.32 (7)	O2—Cu2—N2^{ii}	89.34 (7)

Symmetry codes: (i) $-x, -y, -z$; (ii) $-x, 1-y, 1-z$.

H atoms were placed in calculated positions, with C—H = 0.95 Å, and included in the final cycles of refinement using a riding model, with $U_{iso}(H) = 1.2U_{eq}$(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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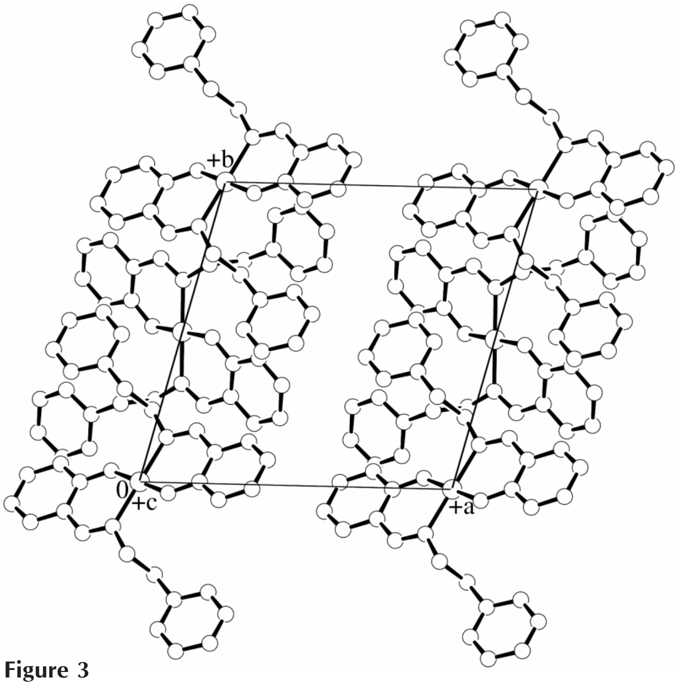

Figure 3
A molecular packing diagram of (I), viewed down the crystallographic *c* axis. H atoms have been omitted for clarity.

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