metal-organic compounds

Bis(N-octylsalicylideniminato-N,O)-copper(II)

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In the title compound, $[Cu(C_{15}H_{22}NO)_2]$, the Cu^{II} cation lies on a centre of symmetry. The coordination geometry about the Cu^{II} ion is a parallelogram, formed by the N_2O_2 donor set of the two bidentate long alkane chain Schiff base imine–phenol ligands. The Cu—N and Cu—O distances are 2.009 (3) and 1.888 (3) Å, respectively.

Comment

In enzyme systems, metal ions play an important role in terms of both structure and function. Hard cations are not only involved in the structural properties of proteins, but also show catalytic activity. Over the past few decades, metal–Schiff base complexes have been extensively investigated with regard to their function as model compounds for biological enzymes (Espinet *et al.*, 1992; Giroud-Godquin & Maitlis, 1991). Some N,O-containing metal–Schiff base complexes possessing high catalytic activity show potential application in the fields of catalysis and medicine (Jacobsen *et al.*, 1991; Schmidt *et al.*, 1996). Copper–Schiff base complexes play an important role

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in both synthetic and structural research because they are useful stereochemical models in catalytic chemistry as a result of their preparative accessibility and structural variety (Garnovskii *et al.*, 1993). Tetracoordinated copper–Schiff base complexes may form *trans*- or *cis*-planar, or tetrahedral structures. A strictly planar or slightly distorted coordination is characteristic of transition metal complexes of Cu^{II} with a CuN_2O_2 coordination sphere (Elerman, Elmali, Kabak & Svoboda, 1998; Elerman, Elmali & Özbey, 1998; Elmali *et al.*, 2000; Kabak *et al.*, 1999). Often, the geometry of a *trans*-planar copper complex is a parallelogram. Here, we report the results of the reaction of Cu^{II} with a long alkane chain ligand, namely N-octylsalicylidenimine, which forms a monomeric copper–Schiff base complex, (I), in a *trans*-planar parallelogram coordination geometry, with the Cu^{II} ion on a crystallographic centre of symmetry (Fig. 1).

(I)
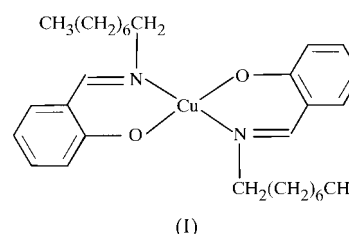
The bond lengths and angles around the Cu^{II} ion in (I) are in good agreement with the values found in similar copper complexes (Akhtar & Drew, 1982; Labisbal *et al.*, 1994) and in long alkane chain metal–Schiff base complexes (Asada *et al.*, 2000). The Cu—N distance is longer than the Cu—O distance. No unusual bond lengths and angles are observed in the salen ligands of (I). The long alkane chain C—C distances are in the range 1.473 (7)–1.528 (9) Å, the phenyl C—C distances are in the range 1.371 (6)–1.415 (5) Å, C—O is 1.304 (4) Å, C—N is 1.470 (4) Å and C=N is 1.288 (5) Å. These values are within the expected ranges for related salen derivatives (Blake *et al.*, 1995; Zamian *et al.*, 1995).

The molecules of the title copper–Schiff base complex exist as monomers, with Cu···Cu separations of 6.804 Å, leading to no dimeric interaction (Fig. 2). The long alkane chain mol-
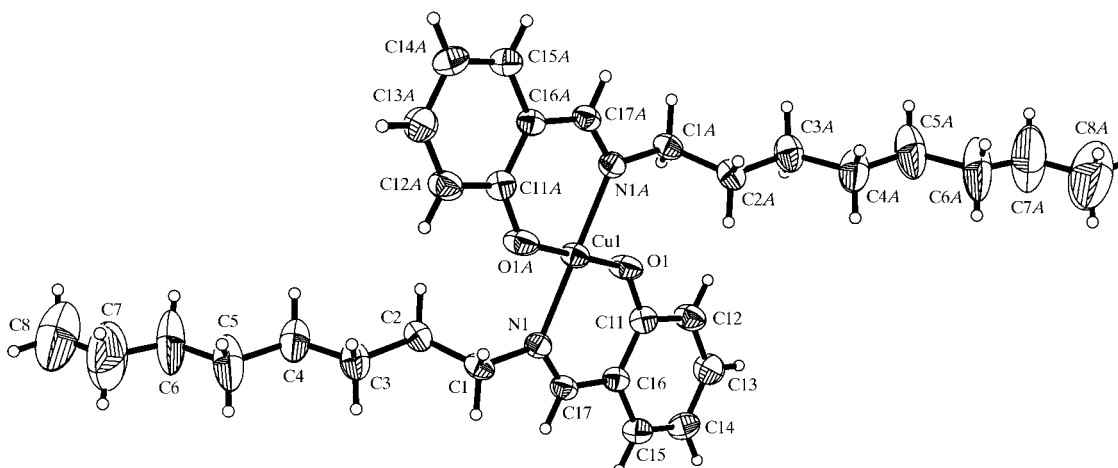
Figure 1
The molecular structure and atom-labelling scheme of (I). Displacement ellipsoids are plotted at the 30% probability level and H atoms are drawn as small spheres of arbitrary radii. The suffix *A* denotes symmetry-related atoms at $(-x, -y, 2 - z)$.

ecules are stacked in columns along the *a* axis, while no connections are formed between the chain ends of two adjacent copper complexes. The alkane chains are reasonably linear, but the entire molecule is not as planar as some other copper–Schiff base complexes (Elmali *et al.*, 2000; Kabak *et al.*, 1999). No overlap between the aromatic rings of two adjacent
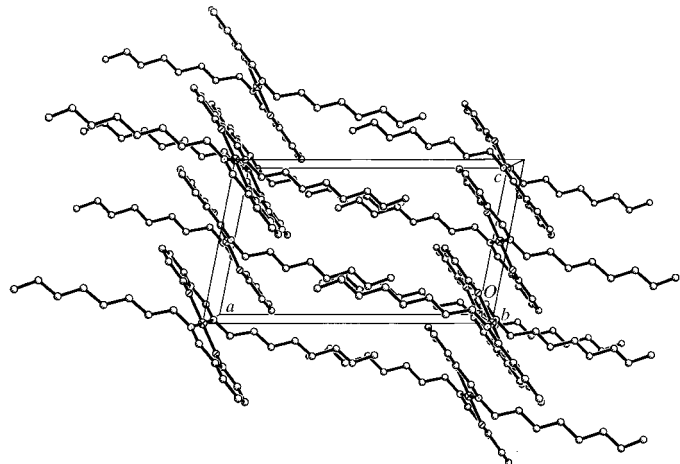
Figure 2
A perspective view of the unit cell of (I). H atoms have been omitted for clarity.

$[Cu(C_{15}H_{22}NO)_2]$ units is seen, which is in contrast with the cases of π-stacking of aromatic rings that have been reported recently by Amoroso *et al.* (1995) and Muñoz *et al.* (1998).

Experimental

n-Octylamine (2.0 mmol) was added dropwise to a solution of salicylaldehyde (2.0 mmol) in boiling absolute ethanol (10 ml). After stirring for a few minutes, a solution containing $[Cu(O_2CCH_3)_2]\cdot H_2O$ (1.0 mmol) and $CH_3CO_2Na\cdot 3H_2O$ (1.5 mmol) in hot water (6 ml) was added slowly to the boiling mixture. During this addition, a large amount of brown powder precipitated. The reaction mixture was refluxed for half an hour and then cooled to room temperature. The crystalline precipitate was filtered off (yield 80%). Brown single crystals of (I) (m.p. 337 K) suitable for X-ray diffraction were grown by slow evaporation over a period of a few weeks. The product was soluble in organic solvents, *e.g.* chloroform. IR (KBr), ν (C=N): 1618 and 1597 cm^{-1}.

Crystal data

$[Cu(C_{15}H_{22}NO)_2]$	$D_x = 1.167$ Mg m^{-3}
$M_r = 528.21$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 37
$a = 16.571$ (4) Å	reflections
$b = 9.742$ (3) Å	$\theta = 2.4$–25.0°
$c = 9.500$ (3) Å	$\mu = 0.75$ mm^{-1}
$\beta = 101.507$ (5)°	$T = 298$ (2) K
$V = 1502.9$ (7) Å^3	Block, brown
$Z = 2$	$0.20 \times 0.20 \times 0.15$ mm

Data collection

Bruker SMART1000 CCD area-detector diffractometer	2656 independent reflections
	1414 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.056$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 25°$
	$h = -19 \rightarrow 18$
$T_{min} = 0.864$, $T_{max} = 0.896$	$k = -11 \rightarrow 10$
6066 measured reflections	$l = -6 \rightarrow 11$

Refinement

Refinement on F^2	H-atom parameters constrained
$R(F) = 0.048$	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$
$wR(F^2) = 0.126$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} = 0.017$
2656 reflections	$\Delta\rho_{max} = 0.27$ e Å^{-3}
160 parameters	$\Delta\rho_{min} = -0.23$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.888 (3)	Cu1—N1	2.009 (3)
O1^i—Cu1—N1	88.91 (13)	O1—Cu1—N1	91.09 (13)

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

All H atoms were placed at calculated positions and treated as riding, with C—H = 0.93–0.97 Å, and U_{iso}(H) = 1.5U_{eq}(C) for methyl H and 1.2U_{eq}(C) for other H atoms.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SHELXTL* (Bruker, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

References

Akhtar, F. & Drew, M. G. B. (1982). *Acta Cryst.* B**38**, 1149–1154.
Amoroso, A. J., Jeffery, J. C., Jones, P. L., McCleverty, J. A., Thornton, P. & Ward, M. D. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1443–1446.
Asada, H., Fujiwara, M. & Matsushita, T. (2000). *Polyhedron*, **19**, 2039–2048.
Blake, A. B., Chipperfield, J. R., Hussian, W., Paschke, R. & Sinn, E. (1995). *Inorg. Chem.* **34**, 1125–1129.
Bruker (1997). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SMART*. Version 5.624. Bruker AXS Inc., Madison, Wisconsin, USA.
Elerman, Y., Elmali, A., Kabak, M. & Svoboda, I. (1998). *Acta Cryst.* C**54**, 1701–1703.
Elerman, Y., Elmali, A. & Özbey, S. (1998). *Acta Cryst.* C**54**, 1072–1074.
Elmali, A., Elerman, Y. & Svoboda, I. (2000). *Acta Cryst.* C**56**, 423–424.
Espinet, P., Esteruelas, M. A., Oro, L. A., Serrano, J. L. & Sola, E. (1992). *Coord. Chem. Rev.* **117**, 215–274.
Garnovskii, A. D., Nivorozhkin, A. L. & Minkin, V. I. (1993). *Coord. Chem. Rev.* **126**, 1–69.
Giroud-Godquin, A.-M. & Maitlis, P. M. (1991). *Angew. Chem. Int. Ed. Engl.* **30**, 375–402.
Jacobsen, E. N., Zhang, W., Muci, A. R., Ecker, J. R. & Deng, L. (1991). *J. Am. Chem. Soc.* **113**, 7063–7064.
Kabak, M., Elmali, A., Kavlakoglu, E., Elerman, Y. & Durlu, T. N. (1999). *Acta Cryst.* C**55**, 1650–1652.
Labisbal, E., Romero, J., García-Vázquez, J. A., Sousa, A., Castellano, E. E. & Zukerman-Schpector, J. (1994). *Acta Cryst.* C**50**, 1043–1044.
Muñoz, M. C., Julve, M., Lloret, F., Faus, J. & Andruh, M. (1998). *J. Chem. Soc. Dalton Trans.* pp. 3125–3131.
Schmidt, H., Bashirpoor, M. & Rehder, D. (1996). *J. Chem. Soc. Dalton Trans.* pp. 3865–3870.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.
Zamian, J. R., Dockal, E. R., Castellan, G. & Oliva, G. (1995). *Polyhedron*, **14**, 2411–2418.