Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Bis(2-{[5-fluoro-2-(trifluoromethyl)phenyl]iminomethyl}phenolato-κ^2N,O)copper(II)

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Received 31 December 2006
Accepted 2 January 2007

In the mononuclear title complex, $[Cu(C_{14}H_8F_4NO)_2]$, the Cu atom, which lies on a center of inversion, exists in a square planar environment defined by two N atoms and two O atoms from the Schiff base ligands.

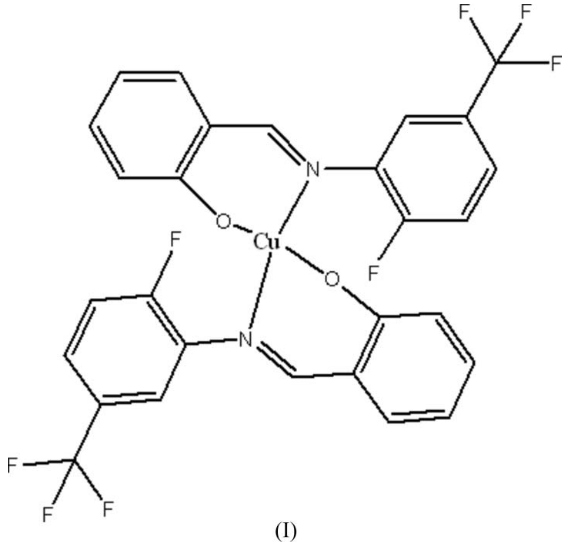
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.005 Å
R factor = 0.035
wR factor = 0.089
Data-to-parameter ratio = 12.8

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

Comment

There has been continuing interest in bis-bidentate Schiff base Cu(II) complexes because the ligands display a wide range of geometric arrangements in the solid state, from ideal *trans*-square-planar to deformed tetrahedral (Bluhm *et al.*, 2003; (Lacroix *et al.*, 2004). In investigations of these complexes based on bis-bidentate Schiff base ligands, both electronic effects (Maslen *et al.*, 1975) and crystal packing (Panova *et al.*, 1980) have been invoked as the driving forces responsible for the distortion. In this paper, we report the synthesis and crystal structure of the title complex, (I).



(I)

The Cu atom is located on an inversion center, and its coordinated atoms, two oxygen and two nitrogen, are coplanar (Fig. 1).

Experimental

The title compound was prepared by the addition of $Cu(OAc)_2$ (0.5 mmol), 5-fluoro-2-(trifluoromethyl)aniline (2.3 g,10 mmol) and salicylaldehyde (1.5 g,8 mmol) to a hot ethanol solution (50%, 30 ml). The mixture was stirred for 10 h and then filtered. The filtrate was added to a mixed solution ($EtOH:CH_2Cl_2$ 1:1, 10 ml), and dark-blue single crystals were obtained at room temperature over a period of days.

Crystal data

$[Cu(C_{14}H_8F_4NO)_2]$
$M_r = 627.97$
Monoclinic, $P2_1/c$
$a = 12.805\ (3)$ Å
$b = 7.0850\ (14)$ Å
$c = 13.893\ (3)$ Å
$\beta = 96.481\ (3)^\circ$
$V = 1252.3\ (4)$ Å^3
$Z = 2$
$D_x = 1.665$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.96$ mm^{-1}
$T = 296\ (2)$ K
Block, blue
0.20 × 0.15 × 0.15 mm

Data collection

Bruker APEX-II area-detector diffractometer
φ and ω scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\rm min} = 0.831$, $T_{\rm max} = 0.869$
7797 measured reflections
2401 independent reflections
1405 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.040$
$\theta_{\rm max} = 26.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.089$
$S = 0.85$
2401 reflections
187 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.53$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.28$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cu1—O1	1.871 (2)	Cu1—N1	1.996 (2)
O1$^{\rm i}$—Cu1—O1	180	O1—Cu1—N1	91.50 (9)
O1$^{\rm i}$—Cu1—N1	88.50 (9)	N1—Cu1—N1$^{\rm i}$	180

Symmetry code: (i) $-x + 1, -y, -z + 1$.

H atoms were placed in calculated positions with C—H = 0.93 Å and refined in riding mode, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

Data collection: *SMART* (Bruker,1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

The authors are grateful to the Natural Science Foundation of Zhejiang Province (No. M203052) and the Research Foundation of Lishui University (No. FC06002) for financial support.

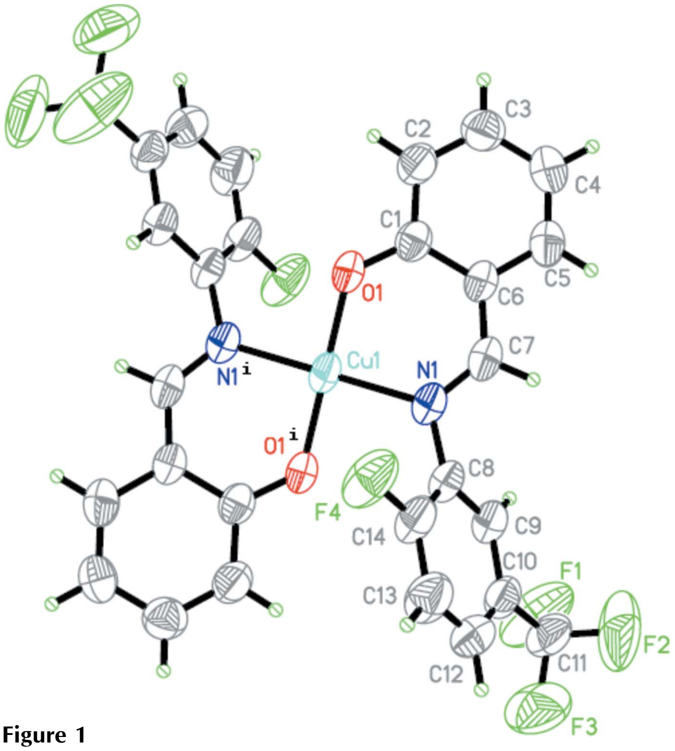


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids. [Symmetry code: (i) $1 - x, -y, 1 - z$.]

References

Bluhm, M. E., Ciesielski, M., Görls, H., Walter, O. & Döring, M. (2003). *Inorg. Chem.* **42**, 8878–8885.
Bruker (1998). *SMART* (Version 5.0) and *SHELXTL* (Version 6.12). Bruker AXS Inc, Madison, Wisconsin, USA.
Bruker (1999). *SAINT*. Version 6.12. Bruker AXS Inc., Madison, Wisconsis, USA.
Lacroix, P. G., Averseng, F., Malfant, I. & Nakatani, K. (2004). *Inorg. Chim. Acta*, **357**, 3825–3835.
Maslen, H. S. & Waters, T. N. (1975). *Coord. Chem. Rev.* **17**, 137–176.
Panova, G. V., Vikulova, V. M. & Potapov, V. M. (1980). *Russ. Chem. Rev.* **49**, 655–667.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.