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Crystal structure of bis{5-chloro-2-(((4-trifluoromethyl)imino)methyl)phenolato- $\kappa^2 N, O$ } copper(II), $C_{28}H_{16}Cl_2CuF_6N_2O_2$

Table 1: Data collection and handling.

Crystal:	Brown block
Size:	0.28 × 0.24 × 0.16 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.08 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$\theta_{\max}$, completeness:	26.0°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	9409, 2643, 0.030
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2127
$N(\text{param})_{\text{refined}}$:	187
Programs:	Bruker [1], SHELX [2], Olex2 [3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.500000	0.500000	0.500000	0.03283(16)
Cl1	0.02308(9)	0.61595(13)	0.83207(6)	0.0838(4)
F1	0.4436(3)	0.3164(3)	-0.00093(13)	0.0897(7)
F2	0.2325(2)	0.3016(3)	0.00824(15)	0.1068(10)
F3	0.3257(3)	0.4932(3)	-0.03235(14)	0.1034(10)
O1	0.39007(19)	0.4953(2)	0.60698(12)	0.0423(5)
N1	0.3386(2)	0.5246(2)	0.41516(14)	0.0354(5)
C1	0.2689(3)	0.5461(3)	0.61597(17)	0.0367(6)
C2	0.2123(3)	0.5512(3)	0.70646(19)	0.0457(7)
H2	0.260425	0.514686	0.757612	0.055*
C3	0.0880(3)	0.6092(3)	0.7190(2)	0.0519(8)
C4	0.0099(3)	0.6646(4)	0.6450(2)	0.0603(9)
H4	-0.073347	0.706685	0.655610	0.072*
C5	0.0599(3)	0.6549(3)	0.5573(2)	0.0526(8)
H5	0.007885	0.688513	0.507054	0.063*
C6	0.1880(3)	0.5958(3)	0.53931(18)	0.0399(6)
C7	0.2249(3)	0.5756(3)	0.44409(18)	0.0400(6)
H7	0.161282	0.601413	0.398191	0.048*
C8	0.3447(3)	0.4960(3)	0.31592(17)	0.0353(6)
C9	0.3175(3)	0.5966(3)	0.24975(19)	0.0469(7)
H9	0.300120	0.687123	0.268453	0.056*
C10	0.3161(3)	0.5629(4)	0.1550(2)	0.0510(7)
H10	0.296750	0.630692	0.110272	0.061*
C11	0.3434(3)	0.4294(3)	0.12746(17)	0.0436(7)
C12	0.3755(3)	0.3293(3)	0.19340(19)	0.0462(7)
H12	0.395688	0.239455	0.174387	0.055*
C13	0.3777(3)	0.3626(3)	0.28777(18)	0.0426(6)
H13	0.401240	0.295780	0.332294	0.051*
C14	0.3346(4)	0.3876(4)	0.0264(2)	0.0629(9)

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Abstract

$C_{28}H_{16}Cl_2CuF_6N_2O_2$, monoclinic, $P2_1/c$ (no. 14), $a = 9.850(3)$ Å, $b = 9.642(3)$ Å, $c = 14.249(4)$ Å, $\beta = 91.210(3)^\circ$, $V = 1352.9(6)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0377$, $wR_{\text{ref}}(F^2) = 0.1066$, $T = 296$ K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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Source of material

The Schiff base ligand 5-chloro-2-(((4-(trifluoromethyl)imino)methyl)phenol) was prepared according to the literature method [4]. The copper(II) acetate monohydrate (10 mmol) dissolved in ethanol solution (10 mL) was added dropwise to the ligand (20 mmol) dissolved in ethanol (10 mL) at room temperature. The mixture was kept being stirred for 1 h. The filtrate was allowed to stand for 35 days at quiet environment. Several brown crystal were obtained.

Experimental details

H atoms linked to N, C and O atoms were geometrically added and isotropically refined by the riding model.

Comment

Schiff bases ligands have been attracting much attention because of their excellent coordination ability to metal ions [5, 6], and their complexes exhibited magnetic properties and many other ones [7]. So far, we have synthesized a series of bidentate Schiff base copper complexes [8]. Particular attention has been paid to the structural and spectroscopic properties of Schiff base metal complexes [9, 10].

In the title crystal structure, the coordination sphere of Cu atom is found to be formed by two bidentate ligands. Each Cu atom in the complex is four-coordinated by two imino N and two phenolato O atoms of the corresponding Schiff base ligand, forming a square-planar coordination. The Cu1—N1 bond lengths are both 1.991(2), and the Cu1—O1 bond lengths are both 1.8889(18). The angles of N1—Cu1—O1 and N1—Cu1—O1' are 88.35(9) and 91.65(9), respectively.

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