Crystal structure of bis[*N*-cyclopropyl-5-nitrosalicylaldiminato]copper(II), $Cu[(C_3H_5NCH)(O)C_6H_3(NO_2)]_2$

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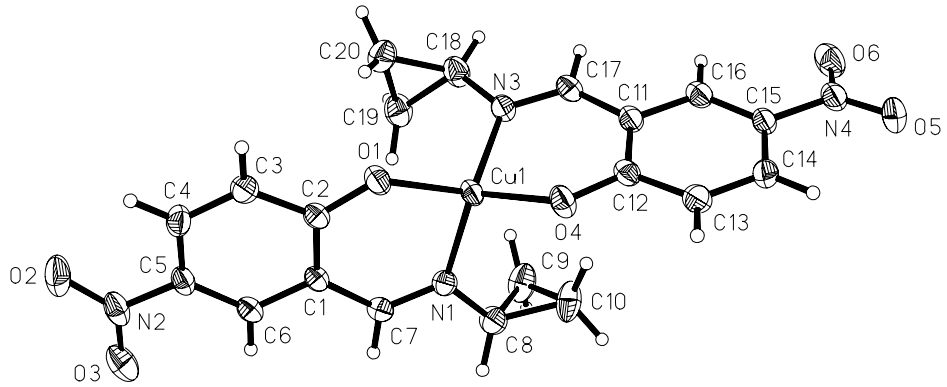

Abstract

$C_{20}H_{18}CuN_4O_6$, monoclinic, $P12_1/c1$ (no. 14), a = 11.365(1) Å, b = 16.863(2) Å, c = 11.257(1) Å, β = 113.223(1)°, V = 1982.6 Å^3, Z = 4, $R_{gt}(F)$ = 0.035, $wR_{ref}(F^2)$ = 0.083, T = 298 K.

Source of material

Reagents and solvents used were of commercially available quality. 5-Nitro-2-hydroxybenzaldehyde (33.5 mg, 0.2 mmol), cyclopropylamine (11.3 mg, 0.2 mmol) and $Cu(CH_3COO)_2 \cdot H_2O$ (19.9 mg, 0.1 mmol) were refluxed in MeOH at about 338 K for 30 min. The mixture was cooled to room temperature and filtered. After keeping the filtrate in dark for 21 d, blue block crystals were formed (yield 72.1 %, based on the 5-nitro-2-hydroxybenzaldehyde).

Elemental analysis: found – C, 50.50 %; H, 3.91 %; N, 11.73 %; calc. for $C_{20}H_{18}CuN_4O_6$ – C, 50.69 %; H, 3.83 %; N, 11.82 %.

Discussion

The chemical properties of Schiff bases and their complexes with some transition metal ions have been widely studied in several research areas because of their chelating capability and pharmacological applications [1-5]. The copper(II) complexes have shown to be more significantly in the biologically active species. Owing to the biological interest in these types of chelate systems, a great deal of structural studies have been carried out on their copper(II) complexes with Schiff bases [6-8]. In this study, we report a new copper(II) complex derived from the Schiff base 2-(cyclopropyliminomethyl)-4-nitrophenol.

In the title mononuclear copper(II) complex, the Cu1 atom is four-coordinated in a tetrahedral environment by two Schiff bases, as evidenced by the bond angles around the Cu1 atom (∠O1–Cu1–N1 = 96.54(6)°, ∠O4–Cu1–N3 = 96.95(6)°, ∠O4–Cu1–N1 = 114.54(7)°, ∠O1–Cu1–N3 = 115.11(7)°, ∠N3–Cu1–N1 = 116.47(7)°, ∠O1–Cu1–O4 = 118.63(6)°). The Schiff base acts as a bidentate ligand and ligates to the metal ion through the O and N atom. All the bond lengths related to the Cu1 atom are comparable to the values observed in other complexes [9,10].

Table 1. Data collection and handling.

Crystal:	blue block, size 0.11 × 0.13 × 0.32 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	11.49 cm^{-1}
Diffractometer, scan mode:	Siemens P4, ω
$2\theta_{max}$:	55°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	16810, 4524
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 3463
$N(param)_{refined}$:	280
Program:	SHELXTL [11]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(3)	4*e*	0.3582	0.9246	1.0956	0.055
H(4)	4*e*	0.5196	0.8643	1.2627	0.058
H(6)	4*e*	0.7189	0.8361	1.0421	0.047
H(7)	4*e*	0.6452	0.8743	0.8309	0.045
H(8)	4*e*	0.6110	0.8921	0.6280	0.062
H(9A)	4*e*	0.5066	0.7952	0.4719	0.078
H(9B)	4*e*	0.3832	0.7971	0.5121	0.078
H(10A)	4*e*	0.3532	0.9334	0.4581	0.077
H(10B)	4*e*	0.4766	0.9315	0.4179	0.077
H(13)	4*e*	0.1983	1.1374	0.4215	0.055
H(14)	4*e*	0.0650	1.1396	0.2073	0.056
H(16)	4*e*	–0.0586	0.9211	0.2352	0.052
H(17)	4*e*	0.0095	0.8511	0.4237	0.051
H(18)	4*e*	0.0615	0.7553	0.5593	0.064
H(19A)	4*e*	0.2412	0.6809	0.6927	0.070
H(19B)	4*e*	0.3286	0.7613	0.7323	0.070
H(20A)	4*e*	0.1866	0.8167	0.8190	0.075
H(20B)	4*e*	0.0992	0.7363	0.7794	0.075

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Table 3. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu(1)	4*e*	0.30027(2)	0.93379(2)	0.68613(2)	0.0321(2)	0.0434(2)	0.0288(1)	0.0021(1)	0.0052(1)	–0.0001(1)
O(1)	4*e*	0.3318(1)	0.94020(9)	0.8650(1)	0.0363(8)	0.061(1)	0.0338(8)	0.0089(7)	0.0093(6)	–0.0014(7)
O(2)	4*e*	0.7115(2)	0.7831(1)	1.3656(2)	0.096(1)	0.064(1)	0.0412(9)	–0.005(1)	0.0097(9)	0.0139(9)
O(3)	4*e*	0.8312(2)	0.7833(1)	1.2565(2)	0.055(1)	0.072(1)	0.063(1)	0.015(1)	–0.0015(9)	0.0053(9)
O(4)	4*e*	0.2425(1)	1.02646(9)	0.5820(1)	0.0474(9)	0.0449(9)	0.0382(8)	–0.0015(7)	0.0008(7)	0.0007(7)
O(5)	4*e*	–0.1047(2)	1.0943(1)	0.0070(2)	0.061(1)	0.096(1)	0.049(1)	0.011(1)	0.0114(9)	0.031(1)
O(6)	4*e*	–0.1491(2)	0.9710(1)	0.0147(2)	0.057(1)	0.087(1)	0.0409(9)	0.004(1)	0.0065(8)	–0.0056(9)
N(1)	4*e*	0.4776(2)	0.8972(1)	0.7101(2)	0.039(1)	0.044(1)	0.0337(9)	–0.0010(8)	0.0159(8)	–0.0039(7)
N(2)	4*e*	0.7314(2)	0.8009(1)	1.2697(2)	0.061(1)	0.040(1)	0.039(1)	–0.007(1)	–0.002(1)	–0.0003(8)
N(3)	4*e*	0.1541(2)	0.8629(1)	0.5809(2)	0.038(1)	0.040(1)	0.0377(9)	0.0008(8)	0.0088(8)	0.0018(8)
N(4)	4*e*	–0.0934(2)	1.0319(2)	0.0652(2)	0.039(1)	0.080(2)	0.037(1)	0.012(1)	0.0143(9)	0.009(1)
C(1)	4*e*	0.5441(2)	0.8847(1)	0.9440(2)	0.033(1)	0.036(1)	0.033(1)	–0.0012(8)	0.0083(8)	–0.0036(8)
C(2)	4*e*	0.4314(2)	0.9111(1)	0.9585(2)	0.035(1)	0.038(1)	0.035(1)	–0.0027(9)	0.0089(9)	–0.0047(8)
C(3)	4*e*	0.4283(2)	0.9046(1)	1.0823(2)	0.042(1)	0.060(1)	0.039(1)	–0.000(1)	0.018(1)	–0.005(1)
C(4)	4*e*	0.5255(2)	0.8698(1)	1.1830(2)	0.057(1)	0.057(1)	0.031(1)	–0.006(1)	0.015(1)	–0.001(1)
C(5)	4*e*	0.6327(2)	0.8429(1)	1.1662(2)	0.042(1)	0.038(1)	0.031(1)	–0.0037(9)	0.0033(9)	–0.0006(9)
C(6)	4*e*	0.6441(2)	0.8519(1)	1.0502(2)	0.035(1)	0.039(1)	0.038(1)	–0.0018(9)	0.0075(9)	–0.0048(9)
C(7)	4*e*	0.5626(2)	0.8846(1)	0.8246(2)	0.033(1)	0.040(1)	0.040(1)	–0.0007(9)	0.0135(9)	–0.0041(9)
C(8)	4*e*	0.5188(2)	0.8862(2)	0.6050(2)	0.046(1)	0.073(2)	0.040(1)	0.000(1)	0.021(1)	–0.006(1)
C(9)	4*e*	0.4543(3)	0.8259(2)	0.5055(2)	0.104(2)	0.052(2)	0.046(1)	0.007(1)	0.036(2)	–0.006(1)
C(10)	4*e*	0.4357(3)	0.9102(2)	0.4721(2)	0.096(2)	0.064(2)	0.041(1)	0.026(2)	0.036(1)	0.008(1)
C(11)	4*e*	0.0792(2)	0.9595(1)	0.4039(2)	0.034(1)	0.045(1)	0.035(1)	0.0038(9)	0.0094(9)	0.0015(9)
C(12)	4*e*	0.1595(2)	1.0253(1)	0.4616(2)	0.032(1)	0.045(1)	0.039(1)	0.0058(9)	0.0115(9)	0.0003(9)
C(13)	4*e*	0.1491(2)	1.0929(1)	0.3845(2)	0.041(1)	0.045(1)	0.050(1)	0.000(1)	0.014(1)	0.002(1)
C(14)	4*e*	0.0685(2)	1.0949(1)	0.2570(2)	0.042(1)	0.054(1)	0.046(1)	0.009(1)	0.018(1)	0.014(1)
C(15)	4*e*	–0.0080(2)	1.0298(1)	0.2021(2)	0.034(1)	0.060(1)	0.032(1)	0.008(1)	0.0113(9)	0.006(1)
C(16)	4*e*	–0.0048(2)	0.9636(1)	0.2733(2)	0.036(1)	0.051(1)	0.038(1)	0.002(1)	0.0104(9)	–0.002(1)
C(17)	4*e*	0.0759(2)	0.8858(1)	0.4686(2)	0.037(1)	0.045(1)	0.038(1)	–0.0021(9)	0.0064(9)	–0.0045(9)
C(18)	4*e*	0.1326(2)	0.7854(1)	0.6221(2)	0.053(1)	0.043(1)	0.049(1)	–0.007(1)	0.005(1)	0.004(1)
C(19)	4*e*	0.2442(3)	0.7378(1)	0.7064(2)	0.065(2)	0.043(1)	0.059(2)	0.008(1)	0.016(1)	0.007(1)
C(20)	4*e*	0.1561(2)	0.7722(2)	0.7602(2)	0.068(2)	0.060(2)	0.062(2)	0.001(1)	0.029(1)	0.017(1)

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