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The crystal structure of (5-chloro-2-hydroxy-*N*-(4-methoxy-2-oxidobenzylidene)benzohydrazonato- $\kappa^3 N, O, O'$)-(pyridine- $\kappa^1 N$)copper(II), $C_{20}H_{16}ClCuN_3O_4$

Table 1: Data collection and handling.

Crystal:	Yellow block
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	1.33 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω -scans
$\theta_{\max}$, completeness:	27.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	27248, 4325, 0.022
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 4033
$N(\text{param})_{\text{refined}}$:	264
Programs:	Bruker programs [1], SHELX [2, 3]

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Abstract

$C_{20}H_{16}ClCuN_3O_4$, triclinic, $P\bar{1}$ (no. 2), $a = 7.629(4)$ Å, $b = 8.893(5)$ Å, $c = 14.193(8)$ Å, $\alpha = 88.603(6)^\circ$, $\beta = 81.093(6)^\circ$, $\gamma = 83.715(6)^\circ$, $V = 945.6(9)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0245$, $wR_{\text{ref}}(F^2) = 0.0709$, $T = 296(2)$ K.

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The crystal 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.

Source of material

2-Hydroxy-4-methoxybenzaldehyde 5-chlorosalicylhydrazide (0.32 g, 1 mmol) in 10 mL methanol and 1 mL pyridine was stirred at room temperature for 1 h. The mixture was filtered, and left at room temperature. After a few days, colourless block crystals formed. Yield (0.22 g, 50%).

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

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cu1	0.19265(2)	0.48068(2)	0.54625(2)	0.03257(7)
N1	0.33452(17)	0.62957(14)	0.48025(9)	0.0322(3)
O1	0.5673(2)	0.94101(15)	0.59279(9)	0.0531(3)
H1	0.5345	0.8853	0.5553	0.080*
Cl1	0.25167(10)	0.82672(8)	0.98876(4)	0.07745(19)
C1	0.3469(3)	0.8565(2)	0.87016(12)	0.0448(4)
C2	0.4604(3)	0.9683(2)	0.84987(13)	0.0464(4)
H2	0.4872	1.0259	0.8986	0.056*
O2	0.24477(15)	0.58381(13)	0.65634(8)	0.0372(2)
N2	0.12065(17)	0.29834(14)	0.62477(9)	0.0336(3)
O3	0.13323(15)	0.40800(13)	0.43103(8)	0.0371(2)
N3	0.39653(18)	0.72729(15)	0.54005(9)	0.0362(3)
C3	0.5333(2)	0.99298(19)	0.75623(13)	0.0438(4)
H3	0.6096	1.0679	0.7421	0.053*
C4	0.4945(2)	0.90753(18)	0.68250(12)	0.0368(3)
O4	0.1675(2)	0.3031(2)	0.10903(10)	0.0660(4)
C5	0.3828(2)	0.79102(17)	0.70432(11)	0.0328(3)
C6	0.3092(2)	0.76768(19)	0.79939(11)	0.0387(3)
H6	0.2346	0.6919	0.8148	0.046*
C7	0.33859(19)	0.69396(17)	0.62998(11)	0.0320(3)
C8	0.3831(2)	0.64364(17)	0.38936(11)	0.0339(3)
H8	0.4587	0.7166	0.3679	0.041*
C9	0.3267(2)	0.55272(17)	0.31959(10)	0.0329(3)
C10	0.3919(2)	0.5777(2)	0.22270(11)	0.0413(4)
H10	0.4705	0.6506	0.2072	0.050*
C11	0.3443(3)	0.4992(2)	0.14997(12)	0.0465(4)
H11	0.3885	0.5191	0.0866	0.056*
C12	0.2279(2)	0.3887(2)	0.17393(12)	0.0435(4)
C13	0.1631(2)	0.35871(19)	0.26819(11)	0.0391(3)
H13	0.0877	0.2831	0.2823	0.047*

Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
C14	0.20797(19)	0.43926(17)	0.34310(10)	0.0324(3)
C15	0.2294(4)	0.3250(4)	0.01095(16)	0.0907(10)
H15A	0.1890	0.4258	−0.0077	0.136*
H15B	0.1836	0.2533	−0.0258	0.136*
H15C	0.3574	0.3108	−0.0002	0.136*
C16	0.1098(2)	0.2974(2)	0.72013(12)	0.0425(4)
H16	0.1429	0.3801	0.7493	0.051*
C17	0.0515(3)	0.1789(2)	0.77645(13)	0.0476(4)
H17	0.0455	0.1824	0.8423	0.057*
C18	0.0024(3)	0.0560(2)	0.73497(14)	0.0489(4)
H18	−0.0375	−0.0250	0.7717	0.059*
C19	0.0137(3)	0.0558(2)	0.63768(15)	0.0628(6)
H19	−0.0187	−0.0262	0.6074	0.075*
C20	0.0731(3)	0.1774(2)	0.58478(13)	0.0503(4)
H20	0.0805	0.1752	0.5188	0.060*

Experimental details

The C-bound H atoms were geometrically placed (C–H = 0.95–0.98 Å) and refined as riding with $U_{iso}(H) = 1.2$ – $1.5 U_{eq}(C)$. The N-bound H atoms were located in a difference Fourier map but were refined with a distance restraint of N–H = 0.88 ± 0.01 Å, and with $U_{iso}(H)$ set to $1.2 U_{equiv}(N)$ [1–3].

Discussion

Polydentate Schiff base ligands are important for the development of the coordination chemistry [4, 5]. Aroylhydrazone Schiff bases are one type of a polydentate ligand, which are known for a variety of molecular architectures and coordination polyhedra [6–8]. The metal complexes of such Schiff bases have several applications in biological probes [9], DNA cleaving agents [10], catalysts [11], sensing materials [12] and corrosion inhibitors [13]. The Schiff base ligand has been synthesized by our group. The figure shows the title compound. The complex consists of one ligand, one pyridine molecule and one Cu atom. A similar complex has been reported [14]. The Cu atom is in a slightly distorted square coordination environment, with two oxygen atoms and one nitrogen atom from the chelate ligand, one nitrogen atom from the pyridine molecule. The bond lengths of Cu1–O2, Cu1–O3, Cu1–N1 and Cu–N2 are 1.945, 1.909, 1.934 and 2.022 Å, respectively, which are as expected [15].

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