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The crystal structure of (*E*)-5-chloro-2-hydroxy-*N'*-(2-hydroxy-4-methoxybenzylidene)benzohydrazide, C₁₅H₁₃ClN₂O₄

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Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.08 × 0.06 × 0.04 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.29 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω -scans
$\theta_{\max}$, completeness:	27.1°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	16118, 3329, 0.028
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2608
$N(\text{param})_{\text{refined}}$:	202
Programs:	Bruker programs [1], SHELX [2, 3]

Abstract

C₁₅H₁₃ClN₂O₄, monoclinic, $P2_1/c$ (no. 14), $a = 16.632(2)$ Å, $b = 7.2033(9)$ Å, $c = 12.9261(17)$ Å, $\beta = 112.87^\circ$, $V = 1427.0(3)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0409$, $wR_{\text{ref}}(F^2) = 0.1260$, $T = 296(2)$ 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

A mixture of 2-hydroxy-5-chlorobenzohydrazide (0.186 g, 1 mmol) and 2-hydroxy-4-methoxybenzaldehyde (0.152 g, 1 mmol) in 50 mL methanol was stirred at room temperature for 1 h. The mixture was filtered to remove impurities, and then left at room temperature. After a few days, colourless blocks of the title compound formed. Yield (0.25 g, 80%).

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.89078(7)	0.0820(2)	0.89053(10)	0.0556(3)
O2	0.58815(7)	0.2280(2)	0.73958(10)	0.0575(4)
H2	0.5472	0.2414	0.6790	0.086*
O3	0.35144(8)	0.36938(19)	0.49349(8)	0.0506(3)
O4	0.37832(7)	0.26592(19)	0.19203(9)	0.0493(3)
H4A	0.3720	0.2315	0.1289	0.074*
N1	0.44313(8)	0.28060(19)	0.41359(10)	0.0413(3)
H1	0.4514	0.2631	0.3527	0.050*
N2	0.51065(8)	0.25111(19)	0.51683(10)	0.0402(3)
Cl1	0.04256(3)	0.48559(9)	0.19785(4)	0.0736(2)
C1	0.89702(12)	0.1094(3)	1.00140(15)	0.0619(5)
H1A	0.8804	0.2344	1.0096	0.093*
H1B	0.9560	0.0882	1.0528	0.093*
H1C	0.8589	0.0243	1.0172	0.093*
C2	0.81249(10)	0.1099(2)	0.80400(13)	0.0414(3)
C3	0.81304(11)	0.0923(3)	0.69732(14)	0.0479(4)
H3	0.8643	0.0609	0.6885	0.057*
C4	0.73774(11)	0.1216(2)	0.60519(13)	0.0449(4)
H4	0.7389	0.1099	0.5341	0.054*
C5	0.65970(10)	0.1681(2)	0.61405(12)	0.0368(3)
C6	0.66038(9)	0.1833(2)	0.72224(12)	0.0386(3)
C7	0.73652(10)	0.1529(2)	0.81666(13)	0.0418(4)
H7	0.7358	0.1616	0.8881	0.050*
C8	0.58319(10)	0.2030(2)	0.51312(12)	0.0406(3)
H8	0.5871	0.1900	0.4436	0.049*
C9	0.36536(10)	0.3362(2)	0.40889(11)	0.0367(3)
C10	0.29387(9)	0.3547(2)	0.29488(11)	0.0344(3)
C11	0.30008(9)	0.3148(2)	0.19265(12)	0.0369(3)
C12	0.22591(11)	0.3265(2)	0.09316(12)	0.0429(4)

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} [*] / <i>U</i> _{eq}
H12	0.2304	0.2998	0.0252	0.052*
C13	0.14659(10)	0.3766(2)	0.09375(13)	0.0460(4)
H13	0.0973	0.3820	0.0272	0.055*
C14	0.14129(10)	0.4187(2)	0.19461(13)	0.0437(4)
C15	0.21367(10)	0.4080(2)	0.29366(12)	0.0405(3)
H15	0.2085	0.4372	0.3609	0.049*

Experimental details

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}(parent atom) [1–3].

Discussion

Schiff bases show interesting properties due to o-hydroxy group forming intra-molecular hydrogen bonds. The hydrazones may act as an efficient chelating ligand, which coordinate with various transition metals. Some complexes containing the hydrazones ligand have been reported [4–6]. Schiff base complexes are attracting considerable attention in several different fields ranging from bioinorganic chemistry to solid-state physics. Low-nuclearity species have been extensively studied as models for the water oxidizing complex in photosystem II, whereas nanometer-size clusters with high-spin ground states are currently being investigated as single-molecule magnets. However, to the best of our knowledge, the ligand has not been reported. The similar structure has been reported [7].

As shown in the figure, the title compound crystallizes in the monoclinic space group *P*2₁/*c* with one molecule in the asymmetric unit. The bond lengths of N2 = C8, N1–C9, C14–Cl1 and N2–N1 are 1.274, 1.333, 1.727 and 1.386 Å, respectively, which are similar with the directly related structures. The atoms O2, O3, N2, are the coordination atoms of the ligand, one ligand will coordinate with three metal atoms. The transition metal complexes have been reported, but the rare earth metal complexes have not been reported, our group will do this job in the future. This sentence was added after [7–16].

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