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The crystal structure of (*E*)-2-((*tert*-butylimino)methyl)-4-chlorophenol, C₁₁H₁₄ClNO

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Abstract

C₁₁H₁₄ClNO, monoclinic, *P*₂/c (no. 14), *a* = 9.072(3) Å, *b* = 5.882(2) Å, *c* = 21.258(7) Å, β = 100.351°, *V* = 1115.9(7) Å³, *Z* = 4, *R*_{gt}(*F*) = 0.0391, *wR*_{ref}(*F*²) = 0.1167, *T* = 296(2) 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.

Source of material

5-Chlorosalicylaldehyde (0.78 g, 5 mmol), *tert*-butylamine (0.40 g, 5.5 mmol) and ethanol (20 mL) were heated and stirred at 373 K for 6 h, then cooled to room temperature,

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Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.40 × 0.36 × 0.32 mm
Wavelength:	MoKα radiation (0.71073 Å)
μ:	0.31 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ _{max} , completeness:	25.0°, >99%
<i>N</i> (<i>hkl</i>) _{measured} , <i>N</i> (<i>hkl</i>) _{unique} , <i>R</i> _{int} :	10,033, 1951, 0.023
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 1663
<i>N</i> (<i>param</i>) _{refined} :	134
Programs:	Bruker [1], SHELX [2, 3]

filter and the product was recrystallized from ethanol to afford yellow crystals (0.95 g, yield 90%).

Experimental details

All hydrogen atoms were identified in difference Fourier syntheses. The *U*_{iso} values of the hydrogen atoms of methyl groups were set to 1.5*U*_{eq}(C) and the *U*_{iso} values of all other hydrogen atoms were set to 1.2*U*_{eq}(C).

Comment

O-hydroxy Schiff bases are an important class of organic compounds [4–6]. Because of the hydrogen bonds in the

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
Cl1	0.19184 (6)	0.51912 (10)	0.26871 (2)	0.0772 (2)
O1	0.47557 (17)	1.0449 (2)	0.08837 (8)	0.0739 (4)
N1	0.66082 (14)	0.7152 (2)	0.08808 (6)	0.0497 (3)
C1	0.47057 (16)	0.7084 (3)	0.15192 (7)	0.0453 (4)
C2	0.41302 (19)	0.9225 (3)	0.13020 (8)	0.0529 (4)
C3	0.2888 (2)	1.0081 (3)	0.15245 (10)	0.0616 (5)
H3	0.250500	1.149413	0.138316	0.074*
C4	0.22181 (19)	0.8871 (3)	0.19497 (9)	0.0602 (5)
H4	0.139075	0.946261	0.209583	0.072*
C5	0.27871 (18)	0.6759 (3)	0.21588 (8)	0.0533 (4)
C6	0.40190 (18)	0.5877 (3)	0.19522 (7)	0.0495 (4)
H6	0.439690	0.446943	0.210179	0.059*
C7	0.59859 (17)	0.6114 (3)	0.12877 (7)	0.0473 (4)
H7	0.635550	0.470585	0.144086	0.057*

Table 2: (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
C8	0.78748 (18)	0.6178 (3)	0.06182 (8)	0.0508 (4)
C9	0.7200 (2)	0.4827 (4)	0.00233 (10)	0.0720 (6)
H9A	0.665110	0.355407	0.014490	0.108*
H9B	0.798782	0.429047	−0.018553	0.108*
H9C	0.653604	0.578636	−0.026389	0.108*
C10	0.8744 (2)	0.8199 (4)	0.04281 (13)	0.0831 (7)
H10A	0.808548	0.914088	0.013326	0.125*
H10B	0.954806	0.766582	0.022874	0.125*
H10C	0.914593	0.906666	0.080212	0.125*
C11	0.8897 (2)	0.4695 (4)	0.10950 (11)	0.0798 (6)
H11A	0.924668	0.554994	0.147734	0.120*
H11B	0.973729	0.421092	0.091153	0.120*
H11C	0.835149	0.338803	0.119713	0.120*
H1	0.558 (3)	0.948 (4)	0.0806 (13)	0.102 (8)*

molecule, *o*-hydroxy Schiff base compounds have two possible tautomeric forms of phenol imine and ketoamine, which makes researchers very interested in the structure of the *o*-hydroxy Schiff base [7–11].

In the title structure, it can be clearly observed that the intra-molecular hydrogen bond is formed between the nitrogen atom of the imine and the hydrogen atom of the phenolic hydroxyl group [12]. The molecule is in the *E*-configuration at the C(7)–N(1) double bond (1.271(2) Å) and has a C(1)–C(7)–N(1)–C(8) torsion angle 177.73(13). The bond angle of C(7)–N(1)–C(8) is 122.73(14).

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