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Crystal structure of (*E*)-3-chloro-2-(((4-nitrophenyl)imino)methyl)phenol, C₁₃H₉ClN₂O₃

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Abstract

C₁₃H₉ClN₂O₃, orthorhombic, *P*₂₁₂₁₂₁ (no. 19), *a* = 7.401(3) Å, *b* = 12.005(5) Å, *c* = 13.808(5) Å, *V* = 1226.8(8) Å³, *Z* = 4, *R*_{gt}(*F*) = 0.0673, *wR*_{ref}(*F*²) = 0.1473, *T* = 293(2) K.

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The asymmetric unit of 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

4-Nitroaniline (1 mmol, 138.1 mg) and 2-chloro-6-hydroxybenzaldehyde (1 mmol, 156.6 mg) were added to the solution of ethanol (20 mL) containing a few drops of glacial acetic acid, then the mixture was refluxed for 6 h. The title compound was obtained after the evaporation of the solvent. The solid product was dissolved in acetone and the solution was evaporated slowly at room temperature. Yellow needle crystals suitable for X-ray diffraction determination were obtained after 4 d.

Experimental details

All H atoms were positioned geometrically and refined as riding atoms, with C–H = 0.93 Å and O–H = 0.82 Å. The *U*_{iso}

Table 1: Data collection and handling.

Crystal:	Yellow needle
Size:	0.22 × 0.16 × 0.12 mm
Wavelength:	Mo Kα radiation (0.71073 Å)
μ:	0.32 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} :	6049, 2133, 0.081
Criterion for <i>I</i> _{obs} , <i>N</i> (<i>hkl</i>) _{gt} :	<i>I</i> _{obs} > 2 σ(<i>I</i> _{obs}), 1408
<i>N</i> (<i>param</i>) _{refined} :	173
Programs:	Bruker [1], SHELX [2]

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}
C1	0.6012(8)	0.3132(5)	0.6511(4)	0.0294(14)
C2	0.5397(8)	0.2335(5)	0.7155(4)	0.0377(16)
H2	0.490050	0.167737	0.691938	0.045*
C3	0.5508(8)	0.2500(6)	0.8133(4)	0.0414(16)
H3	0.508172	0.196186	0.856093	0.050*
C4	0.6261(8)	0.3473(6)	0.8477(4)	0.0419(17)
C5	0.6832(8)	0.4293(6)	0.7854(4)	0.0419(17)
H5	0.730911	0.495311	0.809611	0.050*
C6	0.6695(7)	0.4133(5)	0.6875(4)	0.0362(15)
H6	0.705672	0.469268	0.645102	0.043*
C7	0.6296(7)	0.2042(5)	0.5125(4)	0.0327(15)
H7	0.660422	0.145641	0.553450	0.039*
C8	0.6236(7)	0.1844(5)	0.4096(4)	0.0313(14)
C9	0.5690(8)	0.2683(5)	0.3442(4)	0.0348(15)
C10	0.5667(8)	0.2495(6)	0.2464(4)	0.0426(17)
H10	0.533403	0.306334	0.204329	0.051*
C11	0.6136(9)	0.1466(7)	0.2103(5)	0.0519(19)
H11	0.608477	0.134019	0.143918	0.062*
C12	0.6683(8)	0.0618(6)	0.2715(5)	0.0465(17)
H12	0.701216	−0.007314	0.246636	0.056*
C13	0.6730(8)	0.0812(5)	0.3689(4)	0.0385(16)
Cl1	0.7461(3)	−0.02596(13)	0.44412(12)	0.0605(6)
N1	0.5938(6)	0.3000(4)	0.5499(3)	0.0322(11)
N2	0.6464(9)	0.3631(8)	0.9518(5)	0.0684(19)
O1	0.5216(6)	0.3709(3)	0.3766(3)	0.0454(12)
H1	0.537398	0.374190	0.435314	0.068*
O2	0.6006(11)	0.2873(6)	1.0059(4)	0.106(3)
O3	0.7025(11)	0.4513(8)	0.9804(4)	0.132(3)

values were refined with *U*_{iso}(H) = 1.2 *U*_{eq}(C) and 1.5 *U*_{eq}(O). The absolute structure was established by refinement of the Flack parameter (0.14(8) from 422 selected quotients) using Parsons' method [3].

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Comment

For decades Schiff-bases and their derivative chemistry have gained increasingly more and more attention due to their simple synthetic and wide applications in the fields of coordination chemistry, biochemistry, and analytical chemistry [4–9]. In order to expand the research of Schiff bases, the title compound was synthesized and its crystal structure determined.

The asymmetric unit of the title compound consists of one formula unit (*cf.* the figure). The molecule displays an *E* configuration. In the crystal structure of the title compound, the C=N double bond length is 1.289(7) Å (C7=N1), exhibiting the double bond character. The title compound is a non-planar molecule. The dihedral angle between the two aromatic ring systems is 42.46(1)°. The nitro group is nearly co-planar with its aryl ring making a dihedral angle of 3.2°. In the crystal structure, molecules are linked into one-dimensional chains by weak C—H···O hydrogen bonds. One intramolecular O—H···N hydrogen bond exists, which stabilizes the conformation of the title molecule (see the figure). Geometric parameters are similar to that of the parent structure [10].

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