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Crystal structure of (*E*)-2-(1-((2-aminophenyl)imino)ethyl)-4,6-dichlorophenol, C₁₄H₁₂Cl₂N₂O

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.26 × 0.21 × 0.13 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.49 mm ⁻¹
Diffractometer, scan mode:	Bruker Apex-II, φ and ω
$\theta_{\max}$, completeness:	27.6°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	20571, 3006, 0.114
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1607
$N(\text{param})_{\text{refined}}$:	175
Programs:	Bruker [1], SHELX [2], Olex2 [3]

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Abstract

C₁₄H₁₂Cl₂N₂O, monoclinic, $P2_1/c$ (no. 14), $a = 3.9631(3)$ Å, $b = 24.119(2)$ Å, $c = 13.6138(11)$ Å, $\beta = 91.185(3)^\circ$, $V = 1301.01(18)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0586$, $wR_{\text{ref}}(F^2) = 0.1171$, $T = 293(2)$ K.

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The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

1,2-Diaminobenzene (1 mmol, 0.108 g) and 1-(3,5-dichloro-2-hydroxyphenyl)ethan-1-one (1 mmol, 0.205 g) were added to ethanol (10 mL). The obtained mixture was refluxed for almost 2 h. The solution was evaporated slowly at room temperature to obtain colourless prismatic crystals suitable for crystal structure determination.

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1935(8)	0.38738(12)	0.3802(2)	0.0430(8)
H1C	0.307858	0.370598	0.432623	0.052*
C2	0.1321(8)	0.44361(13)	0.3824(2)	0.0498(9)
H2	0.202167	0.464686	0.436267	0.060*
C3	−0.0339(8)	0.46825(13)	0.3040(3)	0.0516(9)
H3	−0.075740	0.506185	0.305100	0.062*
C4	−0.1382(8)	0.43744(12)	0.2245(2)	0.0446(8)
H4	−0.248592	0.454779	0.171966	0.053*
C5	−0.0810(7)	0.38044(12)	0.2213(2)	0.0352(7)
C6	0.0861(7)	0.35548(11)	0.3004(2)	0.0327(7)
C7	0.1254(6)	0.26066(11)	0.35901(19)	0.0283(7)
C8	−0.0406(8)	0.27219(11)	0.45439(19)	0.0381(7)
H8A	0.128367	0.275215	0.505670	0.057*
H8B	−0.192230	0.242463	0.469289	0.057*
H8C	−0.164493	0.306315	0.449509	0.057*
C9	0.2493(6)	0.20496(11)	0.33714(19)	0.0271(6)
C10	0.2214(6)	0.16238(11)	0.40696(19)	0.0309(7)
H10	0.124936	0.169927	0.467202	0.037*
C11	0.3338(7)	0.11013(11)	0.3876(2)	0.0315(7)
C12	0.4820(7)	0.09762(11)	0.2995(2)	0.0322(7)
H12	0.559124	0.061912	0.287213	0.039*
C13	0.5143(7)	0.13848(11)	0.23021(19)	0.0314(7)
C26	0.4013(7)	0.19298(11)	0.24609(19)	0.0293(7)
Cl1	0.2816(2)	0.05783(3)	0.47352(6)	0.0518(3)
Cl2	0.6959(2)	0.12236(3)	0.11905(5)	0.0469(3)
N1	−0.1777(6)	0.34886(10)	0.13921(17)	0.0470(7)
H1A	−0.244649	0.316698	0.158195	0.056*
H1B	−0.340991	0.365468	0.108605	0.056*
N2	0.1679(6)	0.29818(9)	0.29166(16)	0.0337(6)
O1	0.4361(5)	0.23097(8)	0.17695(13)	0.0409(5)
H1	0.352596	0.260240	0.195092	0.061*

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Experimental details

The H atoms were positioned geometrically with $d(\text{C}–\text{H}) = 0.93–0.98$ Å and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{carrier})$ or $1.5 U_{\text{eq}}(\text{methyl})$. Solving, refining and finishing of the crystal structure were finished by SHELXS [2] and

OLEX2 [3]. The data completeness is 1.00 up to the maximum diffraction angle of 55.16°.

Comment

Schiff bases are a class of important synthetic intermediates and are used as ligands to form coordination complexes. Their complexes can be used for catalysis and some other applications [4]. Mono-imine is one key intermediate for the synthesis of unsymmetrical tetradentate Schiff base ligands [5].

There is one title molecule in the asymmetric unit (*cf.* the figure). The dihedral angle between the two benzene rings (C1–C2–C3–C4–C5–C6 and C9–C10–C11–C12–C13–C26) is 49.10°, which is larger than that of similar crystal structure [6]. The intramolecular O–H···N hydrogen bond is able to stabilise the conformation of one part of the title molecule. The packing of crystal structure is *via* van der Waals forces.

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