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2′-(3,5-Dichloro-2-hydroxybenzylidene)-2-hydroxybenzohydrazide

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The molecule of the title compound, $C_{14}H_{10}Cl_2N_2O_3$, has a *trans* configuration with respect to the C=N and C—N bonds. The dihedral angle between the two benzene rings is 2.0 (2)°. In the crystal structure, molecules are linked through O—H···O and weak C—H···O intermolecular hydrogen bonds, forming chains running along the [001] axis.

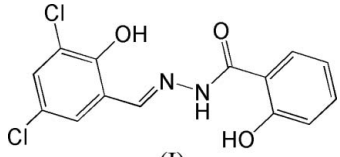
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.106
Data-to-parameter ratio = 13.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The condensation reaction of aromatic aldehydes with primary amines has been shown to offer an easy and inexpensive way of forming a variety of Schiff bases. These Schiff bases exhibit a wide range of biological activities and applications (Bernardo *et al.*, 1996; Tarafder *et al.*, 2002; Çukurovali *et al.*, 2002; Ali *et al.*, 2002). We recently reported a Schiff base–Ni^{II} complex (Hu *et al.*, 2005). As an extension of the work on the crystal structures of Schiff base compounds, the the crystal structure of the title compound, (I), is reported here.



(I)

All bond lengths in (I) are within normal ranges (Allen *et al.*, 1987), including the central C7=N1 bond length of 1.273 (3) Å. The whole molecule is nearly planar (Fig. 1), with a dihedral angle of 2.0 (2)° between the two benzene rings. The C8—N2 bond length of 1.337 (3) Å is intermediate between that of a single and a double bond, suggesting some degree of delocalization in the acetohydrazide system. The molecule displays a *trans* configuration about the C=N and C—N bonds.

In the crystal structure, molecules are linked through intermolecular O—H···O and weak C—H···O hydrogen bonds (Table 1), forming chains running along the [001] axis (Fig. 2).

Experimental

3,5-Dichlorosalicylaldehyde (0.1 mmol, 19.1 mg) and 2-hydroxybenzoic acid hydrazide (0.1 mmol, 15.2 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for 10 min, giving a clear yellow solution. Crystals of (I) were formed by gradual evaporation of the solvent over a week at room temperature (yield 83.7%). Analysis found: C 51.40, H 3.15, N 8.71%; calculated for $C_{14}H_{10}Cl_2N_2O_3$: C 51.72, H 3.10, N 8.62%.

Crystal data

$C_{14}H_{10}Cl_2N_2O_3$
M_r = 325.14
Monoclinic, $P2_1/c$
a = 16.003 (2) Å
b = 7.080 (1) Å
c = 13.269 (2) Å
β = 108.723 (2)°
V = 1423.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.47 mm^{-1}
T = 298 (2) K
0.20 × 0.13 × 0.11 mm

Data collection

Bruker SMART APEX 1K area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.913, T_{max} = 0.951
7101 measured reflections
2625 independent reflections
1704 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.106
S = 1.02
2625 reflections
199 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.853 (10)	1.907 (17)	2.654 (2)	145 (2)
O3—H3···O2^{i}	0.852 (10)	1.737 (11)	2.584 (2)	173 (3)
N2—H2···O3	0.895 (10)	1.874 (18)	2.600 (2)	137 (2)
C11—H11···O2^{i}	0.93	2.51	3.167 (2)	128 (2)
C14—H14···O2	0.93	2.42	2.744 (2)	100

Symmetry code: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

Atoms H1, H2 and H3 were located in a difference map and refined with an O—H distance restraint of 0.85 (1) Å and an N—H distance restraint of 0.90 (1) Å. Isotropic displacement parameters for these H atoms were fixed at 0.08 Å^2. Other H atoms were positioned geometrically and refined as riding (C—H = 0.93 Å), with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2002); software used to prepare material for publication: *SHELXTL*.

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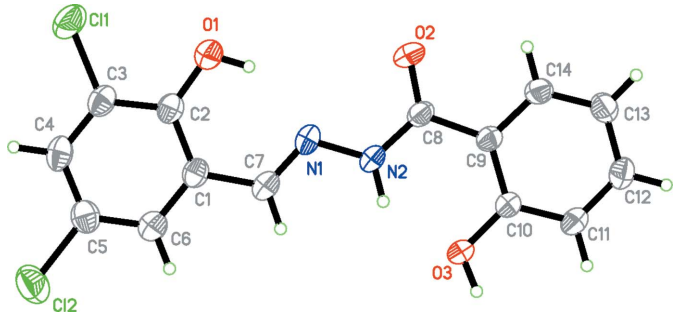

Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids for non-H atoms.

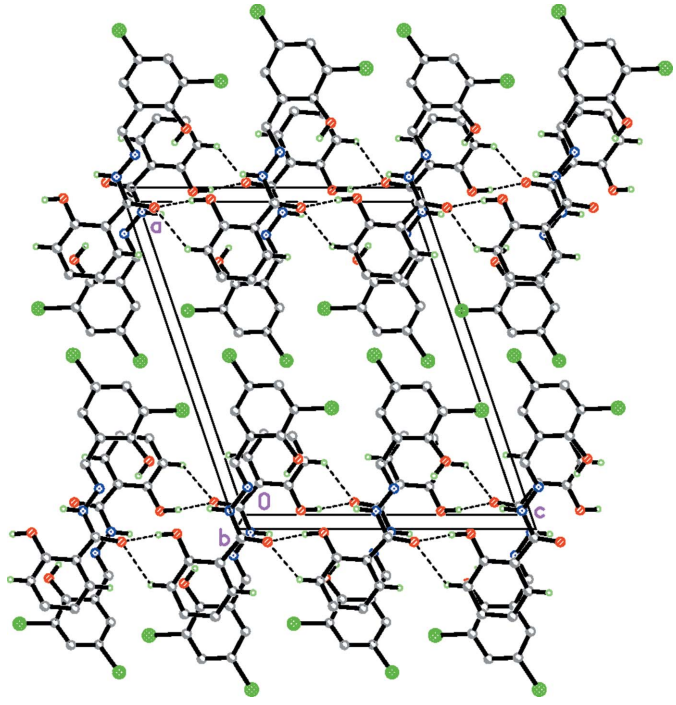

Figure 2
Packing of (I), viewed along the [010] axis. Intermolecular hydrogen bonds are shown as dashed lines.

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