Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

3,4-Dichlorobenzaldehyde (2-hydroxybenzoyl)-hydrazone

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Received 29 March 2005
Accepted 9 May 2005
Online 14 May 2005

Key indicators

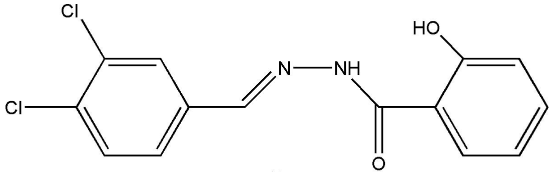
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.039
wR factor = 0.102
Data-to-parameter ratio = 10.7

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

The molecule of the title compound, $C_{14}H_{10}Cl_2N_2O_2$, is roughly planar and displays a *trans* configuration with respect to the C═N double bond. The dihedral angle between the two benzene rings is 14.5 (2)°. The compound adopts a chain structure which is stabilized by intermolecular O—H···O hydrogen bonds.

Comment

Schiff base compounds have been of great interest for many years. These compounds play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism, and molecular architectures. The deprotonated hydroxyl group of salicylhydrazone will sometimes cause the N atom of the hydrazone to become more electron-rich as a result of conjugation effects, and the N atom can thus coordinate more strongly (Bansse *et al.*, 1998). As an extension of work on the structural characterization of salicylhydrazone Schiff base compounds, we report here the crystal structure of the title compound, (I), a new salicylhydrazone with 3,4-dichlorobenzaldehyde.



(I)

In the molecule of (I), the C8═N2 bond length of 1.272 (3) Å and the C1—N1 bond length of 1.339 (3) Å are both less than normal values because of conjugation effects, while all other bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The dihedral angle between the two benzene rings is 14.5 (2)°.

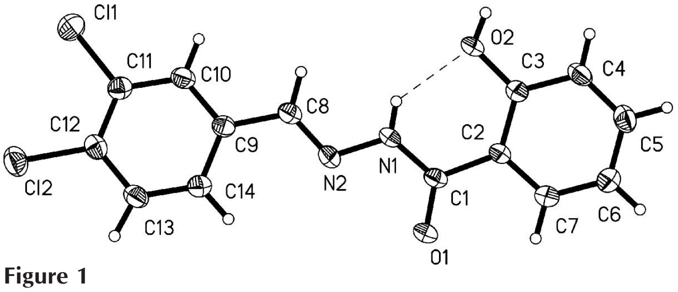


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. The dashed line indicates the intramolecular hydrogen bond.

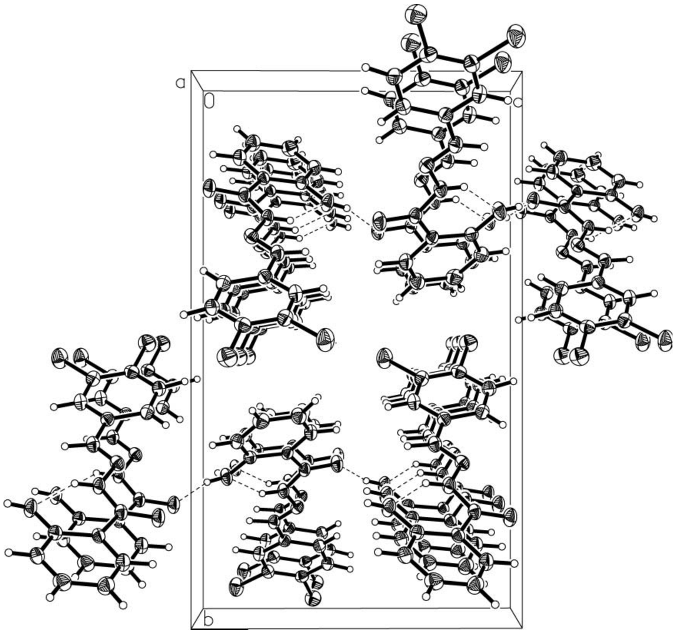


Figure 2
The crystal packing of (I), viewed along the *a* axis. Dashed lines show intra- and intermolecular hydrogen bonds.

In the molecule of (I), there is an intramolecular N1—H1···O2 hydrogen bond which facilitates the formation of another six-membered ring (C1/C2/C3/O2/H1/N1). The crystal structure is stabilized by intermolecular O—H···O hydrogen bonds (Table 1 and Fig. 2).

Experimental

All reagents were commercial products and were used without further purification. 3,4-Dichlorobenzaldehyde (0.2 mmol, 35 mg) and 2-hydroxybenzoic acid hydrazine (0.2 mmol, 30.4 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. The solution was set aside for 8 d to allow slow evaporation of the solvent. Large colourless block-shaped crystals of (I) precipitated from the solution at the bottom of the vessel; these were collected and washed three times with water.

Crystal data

$C_{14}H_{10}Cl_2N_2O_2$
$M_r = 309.14$
Monoclinic, $P2_1/n$
$a = 6.0466$ (18) Å
$b = 19.314$ (6) Å
$c = 11.452$ (3) Å
$\beta = 91.034$ (4)°
$V = 1337.2$ (7) Å^3
$Z = 4$
$D_x = 1.536$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2023 reflections
$\theta = 2.76$–25.18°
$\mu = 0.49$ mm^{-1}
$T = 298$ (2) K
Block, colourless
0.43 × 0.32 × 0.21 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\min} = 0.818$, $T_{\max} = 0.905$
6948 measured reflections
2363 independent reflections
1580 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.031$
$\theta_{\max} = 25.0°$
$h = -7 \rightarrow 7$
$k = -17 \rightarrow 22$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.102$
$S = 1.03$
2363 reflections
221 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0388P)^2 + 0.6353P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.21$ e Å^{-3}
$\Delta\rho_{\min} = -0.23$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—C11	1.729 (3)	N1—C1	1.339 (3)
Cl2—C12	1.723 (3)	N1—N2	1.373 (3)
O1—C1	1.236 (3)	N2—C8	1.272 (3)
O2—C3	1.360 (3)		
O1—C1—C2—C7	−3.7 (4)	C7—C2—C3—O2	179.1 (2)
N1—C1—C2—C7	175.9 (2)	C1—C2—C3—O2	−3.0 (4)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.79 (3)	1.99 (3)	2.724 (3)	155 (3)
N1—H1···O2	0.79 (2)	2.02 (2)	2.641 (3)	135 (2)

Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{3}{2}, z - \frac{1}{2}$.

All H atoms were initially located in a difference Fourier map and their positions were refined freely along with an isotropic displacement parameter, giving distances O—H = 0.79 (3), N—H = 0.79 (2) and C—H = 0.89 (3)–0.95 (3) Å.

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*.

The authors thank the Education Office of Anhui Province, China, for research grant No. 2005kj137.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bansse, W., Fliegner, J., Sawusch, S., Schilde, U. & Uhlemann, E. (1998). *Z. Naturforsch. Teil B*, **53**, 689–695.
Bruker (2002). *SADABS*, *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

o1748 Ma *et al.* • $C_{14}H_{10}Cl_2N_2O_2$ *Acta Cryst.* (2005). E**61**, o1747–o1748