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N,*N*′-Bis(5-chloro-2-hydroxybenzylidene)-ethane-1,2-diamine

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The title compound, $C_{16}H_{14}Cl_2N_2O_2$, is a Schiff base compound, derived from the condensation of 5-chlorosalicylaldehyde and ethane-1,2-diamine in MeOH. The molecule lies about an inversion centre at the mid-point of the C—C bond of the ethylenediamine unit. Intramolecular O—H···N hydrogen bonds contribute to the planarity of the aromatic imide units of the molecule.

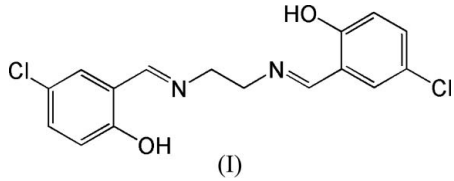
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.009 Å
R factor = 0.092
wR factor = 0.196
Data-to-parameter ratio = 13.8

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

Comment

As an extension of our work on the structural characterization of Schiff base compounds (Li & Zhang, 2004*a*,*b*, 2005; Zhang & Li, 2005), the crystal structure of the title compound, (I), is reported here.



(I)

Compound (I) is a Schiff base compound with crystallographically imposed inversion symmetry (Fig. 1). All the bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987) and are comparable to those observed in a similar Schiff base compound (Kennedy & Reglinski, 2001). The two symmetry-related benzene rings are strictly parallel and the planarity of the C1–C6/C7/N1/C8 segments of the molecule [r.m.s. deviation = 0.017 (6) Å] is supported by intramolecular O—H···N hydrogen bonds (Table 1). The C7═N1 bond length [1.271 (7) Å] confirms it to be a double bond. As expected, the molecule adopts *trans* configurations about the C═N bonds.

Experimental

5-Chlorosalicylaldehyde (0.1 mmol, 15.7 mg) and ethane-1,2-diamine (0.2 mmol, 12.1 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for about 30 min to give a clear yellow solution. After leaving the solution to stand in air for 12 d, yellow plate-like crystals formed.

Crystal data

$C_{16}H_{14}Cl_2N_2O_2$
M_r = 337.19
Monoclinic, $P2_1/c$
a = 17.790 (3) Å
b = 7.253 (6) Å
c = 6.137 (5) Å
β = 92.653 (7)°
V = 791.0 (9) Å^3
Z = 2
D_x = 1.416 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.42 mm^{-1}
T = 298 (2) K
Plate, yellow
0.34 × 0.13 × 0.06 mm

Data collection

Bruker SMART CCD area detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.871, T_{max} = 0.975
3620 measured reflections
1394 independent reflections
688 reflections with $I > 2\sigma(I)$
R_{int} = 0.110
θ_{max} = 25.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.092
$wR(F^2)$ = 0.196
S = 1.07
1394 reflections
101 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + 2.3249P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.92	2.639 (7)	146

All H atoms were placed in geometrically idealized positions and allowed to ride on their parent atoms, with C—H = 0.93–0.97 Å, O—H = 0.82 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O). The crystals were very weakly diffracting so that the ratio of observed to unique reflections is low (49%), and the value of R_{int} is 0.11.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

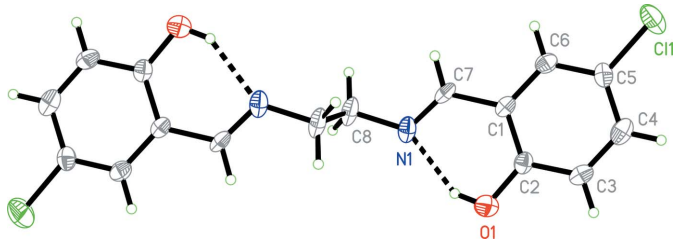


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Unlabelled atoms are at the symmetry positions (1 − x, 1 − y, 1 − z). Intramolecular O—H···N hydrogen bonds are shown as dashed lines.

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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.
Bruker (1998). *SMART* (Version 5.628) and *SAINT* (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
Kennedy, A. R. & Reglinski, J. (2001). *Acta Cryst.* E**57**, o1027–o1028.
Li, Z.-X. & Zhang, X.-L. (2004*a*). *Acta Cryst.* E**60**, m958–m959.
Li, Z.-X. & Zhang, X.-L. (2004*b*). *Acta Cryst.* E**60**, o2199–o2200.
Li, Z.-X. & Zhang, X.-L. (2005). *Acta Cryst.* E**61**, o875–o876.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97* and *SHELXS97*, University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Zhang, X.-L. & Li, Z.-X. (2005). *Acta Cryst.* E**61**, o266–o268.