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4-[(*E*)-(2,3-Dichlorobenzylidene)amino]-phenol

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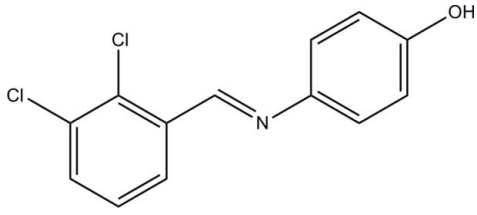
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.030; wR factor = 0.072; data-to-parameter ratio = 14.0.

In the title compound, $C_{13}H_9Cl_2NO$, the dihedral angle between the benzene rings is 54.22 (10)°. In the crystal, molecules are linked by O—H···N intermolecular hydrogen bonds, forming a zigzag $C(7)$ chain along the a axis.

Related literature

For the biological properties of Schiff base ligands, see: Bedia *et al.* (2006). For related structures, see: Fun *et al.* (2008); Alhadi *et al.* (2008); Nie (2008). For reference bond-length values, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{13}H_9Cl_2NO$
M_r = 266.11
Orthorhombic, $P2_12_12_1$
a = 6.049 (4) Å
b = 10.038 (6) Å
c = 19.645 (12) Å
V = 1192.8 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.52 mm^{-1}
T = 296 K
0.25 × 0.23 × 0.21 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.880, T_{max} = 0.898
4853 measured reflections
2184 independent reflections
1998 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.072
S = 1.17
2184 reflections
156 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Absolute structure: Flack (1983), 869 Friedel pairs
Flack parameter: 0.04 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.82	1.99	2.811 (3)	174

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5895).

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supplementary materials

Acta Cryst. (2011). E**67**, o1564 [**doi:10.1107/S1600536811019933**]

4-[(*E*)-(2,3-Dichlorobenzylidene)amino]phenol

L.-X. Sun, Y.-D. Yu and G.-Y. Wei

Comment

Schiff base ligands have received considerable attention during the last decades, mainly because of their structures or for their biological properties (Bedia *et al.*, 2006). We report here the crystal structure of the title new Schiff base compound, (I). In (I) (Fig. 1), the bond lengths and angles are normal and comparable to the values observed in similar compounds (Nie *et al.*, 2008; Fun *et al.*, 2008; Alhadi *et al.*, 2008). The dihedral angle between the two aromatic rings in the Schiff base molecule is 54.22 (10) °, indicating that two these rings are not coplanar. Intermolecular O—H···N hydrogen bonds (Table 1) link the molecules along *a* axis (Fig. 2).

Experimental

A mixture of 2,3-dichlorobenzaldehyde (5 mmol), 4-aminophenol (5 mmol) and methanol (40 ml) was refluxed for 2 h. It was then allowed to cool and filtered. Recrystallization of the crude product from methanol yielded yellow blocks of (I).

Refinement

H atoms were positioned geometrically and refined using the riding-model approximation, with C—H = 0.93–0.97 Å, O—H = 0.82 Å, and U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(O).

Figures

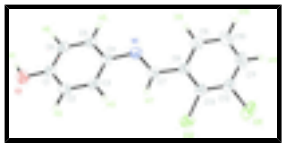

Fig. 1. The molecular structure of the title compounds with 50% probability displacement ellipsoids for non-hydrogen atoms.

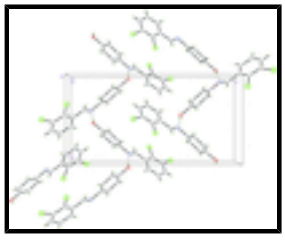

Fig. 2. Molecular packing of the title compound, viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

4-[(*E*)-(2,3-Dichlorobenzylidene)amino]phenol

Crystal data

$C_{13}H_9Cl_2NO$	$F(000) = 544$
$M_r = 266.11$	$D_x = 1.482$ Mg m^{-3}

Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 2869 reflections
$a = 6.049$ (4) Å	$\theta = 2.3–27.2°$
$b = 10.038$ (6) Å	$\mu = 0.52$ mm^{-1}
$c = 19.645$ (12) Å	$T = 296$ K
$V = 1192.8$ (13) Å^3	Block, yellow
$Z = 4$	0.25 × 0.23 × 0.21 mm

Data collection

Bruker APEXII CCD diffractometer	2184 independent reflections
Radiation source: fine-focus sealed tube	1998 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.037$
φ and ω scans	$\theta_{max} = 25.5°$, $\theta_{min} = 2.3°$
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)	$h = -7\rightarrow7$
$T_{min} = 0.880$, $T_{max} = 0.898$	$k = -8\rightarrow12$
4853 measured reflections	$l = -23\rightarrow21$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.030$	$w = 1/[\sigma^2(F_o^2) + (0.0269P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.072$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.17$	$\Delta\rho_{max} = 0.15$ e Å^{-3}
2184 reflections	$\Delta\rho_{min} = -0.14$ e Å^{-3}
156 parameters	Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
0 restraints	Extinction coefficient: 0.073 (4)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 869 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.04 (6)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.6782 (4)	0.13161 (18)	0.30064 (9)	0.0315 (5)
C2	0.8717 (4)	0.2032 (2)	0.29247 (10)	0.0380 (5)
H2	0.9883	0.1903	0.3226	0.046*
C3	0.8932 (4)	0.2937 (2)	0.23991 (10)	0.0353 (5)
H3	1.0241	0.3413	0.2347	0.042*
C4	0.7192 (3)	0.31355 (18)	0.19496 (10)	0.0305 (5)
C5	0.5261 (4)	0.2441 (2)	0.20450 (11)	0.0389 (5)
H5	0.4074	0.2593	0.1754	0.047*
C6	0.5046 (4)	0.1522 (2)	0.25642 (11)	0.0380 (5)
H6	0.3739	0.1045	0.2615	0.046*
C7	0.9040 (4)	0.3995 (2)	0.10174 (10)	0.0305 (5)
H7	1.0160	0.3406	0.1138	0.037*
C8	0.9356 (3)	0.48183 (19)	0.04113 (10)	0.0302 (5)
C9	0.7862 (4)	0.5815 (2)	0.02412 (11)	0.0404 (5)
H9	0.6685	0.5997	0.0531	0.049*
C10	0.8097 (4)	0.6539 (2)	−0.03507 (13)	0.0528 (6)
H10	0.7081	0.7203	−0.0457	0.063*
C11	0.9837 (5)	0.6281 (2)	−0.07860 (12)	0.0502 (6)
H11	0.9987	0.6761	−0.1188	0.060*
C12	1.1338 (4)	0.5315 (2)	−0.06226 (10)	0.0392 (5)
C13	1.1149 (4)	0.45927 (17)	−0.00259 (10)	0.0317 (5)
Cl1	1.35264 (12)	0.50375 (7)	−0.11774 (3)	0.0628 (2)
Cl2	1.31056 (9)	0.33967 (5)	0.01639 (3)	0.04412 (18)
N1	0.7322 (3)	0.40395 (17)	0.13882 (8)	0.0321 (4)
O1	0.6681 (3)	0.04560 (15)	0.35434 (8)	0.0447 (4)
H1	0.5510	0.0045	0.3531	0.067*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0295 (12)	0.0359 (10)	0.0290 (10)	−0.0003 (9)	0.0016 (9)	0.0003 (8)
C2	0.0288 (12)	0.0525 (12)	0.0326 (11)	−0.0050 (10)	−0.0052 (9)	0.0053 (9)
C3	0.0249 (12)	0.0454 (12)	0.0355 (11)	−0.0058 (10)	0.0016 (9)	0.0011 (9)
C4	0.0271 (12)	0.0343 (10)	0.0302 (10)	0.0027 (9)	0.0046 (8)	0.0020 (8)
C5	0.0230 (12)	0.0556 (14)	0.0382 (12)	0.0002 (10)	−0.0027 (10)	0.0068 (10)
C6	0.0241 (11)	0.0480 (12)	0.0419 (12)	−0.0102 (11)	0.0010 (9)	0.0070 (10)
C7	0.0270 (11)	0.0325 (10)	0.0319 (11)	0.0014 (9)	−0.0015 (9)	0.0009 (8)
C8	0.0271 (11)	0.0311 (10)	0.0323 (10)	−0.0043 (9)	−0.0019 (8)	−0.0004 (8)
C9	0.0368 (13)	0.0421 (11)	0.0424 (12)	0.0024 (10)	0.0006 (11)	0.0075 (10)
C10	0.0516 (16)	0.0468 (13)	0.0601 (15)	0.0043 (13)	−0.0085 (13)	0.0184 (12)
C11	0.0582 (17)	0.0521 (14)	0.0403 (13)	−0.0114 (13)	−0.0060 (12)	0.0166 (11)
C12	0.0396 (14)	0.0467 (12)	0.0312 (11)	−0.0145 (11)	0.0007 (10)	−0.0038 (9)
C13	0.0323 (12)	0.0321 (10)	0.0309 (11)	−0.0072 (8)	−0.0015 (9)	−0.0021 (8)
Cl1	0.0631 (5)	0.0830 (5)	0.0424 (4)	−0.0188 (4)	0.0200 (3)	−0.0021 (3)

Cl2	0.0381 (3)	0.0505 (3)	0.0437 (3)	0.0092 (3)	0.0070 (3)	−0.0034 (2)
N1	0.0269 (10)	0.0360 (9)	0.0334 (9)	0.0021 (7)	0.0006 (8)	0.0007 (7)
O1	0.0372 (10)	0.0563 (9)	0.0407 (8)	−0.0109 (8)	−0.0033 (7)	0.0166 (7)

Geometric parameters (Å, °)

C1—O1	1.365 (2)	C7—H7	0.9300
C1—C6	1.379 (3)	C8—C9	1.390 (3)
C1—C2	1.382 (3)	C8—C13	1.402 (3)
C2—C3	1.382 (3)	C9—C10	1.378 (3)
C2—H2	0.9300	C9—H9	0.9300
C3—C4	1.388 (3)	C10—C11	1.381 (4)
C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.373 (3)	C11—C12	1.366 (3)
C4—N1	1.430 (2)	C11—H11	0.9300
C5—C6	1.381 (3)	C12—C13	1.383 (3)
C5—H5	0.9300	C12—Cl1	1.737 (2)
C6—H6	0.9300	C13—Cl2	1.727 (2)
C7—N1	1.270 (3)	O1—H1	0.8200
C7—C8	1.462 (3)		
O1—C1—C6	123.22 (19)	C9—C8—C13	118.18 (19)
O1—C1—C2	117.18 (18)	C9—C8—C7	121.20 (19)
C6—C1—C2	119.58 (18)	C13—C8—C7	120.60 (18)
C3—C2—C1	120.57 (19)	C10—C9—C8	121.0 (2)
C3—C2—H2	119.7	C10—C9—H9	119.5
C1—C2—H2	119.7	C8—C9—H9	119.5
C2—C3—C4	119.86 (19)	C9—C10—C11	120.1 (2)
C2—C3—H3	120.1	C9—C10—H10	119.9
C4—C3—H3	120.1	C11—C10—H10	119.9
C5—C4—C3	119.06 (18)	C12—C11—C10	119.6 (2)
C5—C4—N1	118.29 (18)	C12—C11—H11	120.2
C3—C4—N1	122.66 (17)	C10—C11—H11	120.2
C4—C5—C6	121.3 (2)	C11—C12—C13	121.1 (2)
C4—C5—H5	119.3	C11—C12—Cl1	118.21 (17)
C6—C5—H5	119.3	C13—C12—Cl1	120.71 (18)
C1—C6—C5	119.6 (2)	C12—C13—C8	119.9 (2)
C1—C6—H6	120.2	C12—C13—Cl2	119.40 (17)
C5—C6—H6	120.2	C8—C13—Cl2	120.68 (15)
N1—C7—C8	123.66 (19)	C7—N1—C4	117.70 (17)
N1—C7—H7	118.2	C1—O1—H1	109.5
C8—C7—H7	118.2		
O1—C1—C2—C3	−179.00 (19)	C9—C10—C11—C12	−0.8 (4)
C6—C1—C2—C3	−0.8 (3)	C10—C11—C12—C13	−0.2 (3)
C1—C2—C3—C4	0.2 (3)	C10—C11—C12—Cl1	−179.07 (19)
C2—C3—C4—C5	1.3 (3)	C11—C12—C13—C8	2.0 (3)
C2—C3—C4—N1	−178.85 (18)	Cl1—C12—C13—C8	−179.16 (15)
C3—C4—C5—C6	−2.1 (3)	C11—C12—C13—Cl2	−179.20 (17)
N1—C4—C5—C6	177.97 (19)	Cl1—C12—C13—Cl2	−0.4 (2)
O1—C1—C6—C5	178.0 (2)	C9—C8—C13—C12	−2.8 (3)

C2—C1—C6—C5	0.0 (3)	C7—C8—C13—C12	175.34 (18)
C4—C5—C6—C1	1.5 (3)	C9—C8—C13—Cl2	178.46 (15)
N1—C7—C8—C9	6.8 (3)	C7—C8—C13—Cl2	−3.4 (3)
N1—C7—C8—C13	−171.26 (19)	C8—C7—N1—C4	177.33 (18)
C13—C8—C9—C10	1.8 (3)	C5—C4—N1—C7	−133.5 (2)
C7—C8—C9—C10	−176.3 (2)	C3—C4—N1—C7	46.7 (3)
C8—C9—C10—C11	−0.1 (4)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.82	1.99	2.811 (3)	174

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2.

Fig. 1

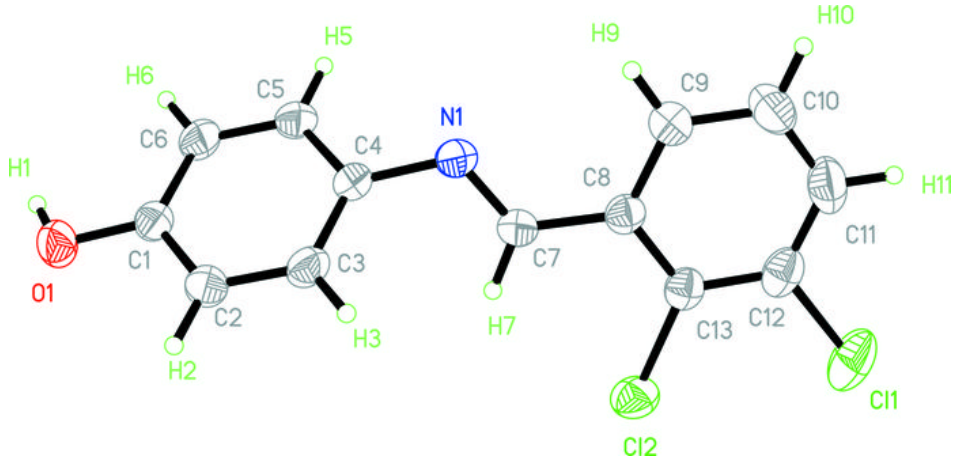
H5
H6
C5
C6
N1
C4
H1
C8
H9
C9
H10
C10
H11
C11
C1
C3
C7
O1
C2
H3
H7
C13
C12
H2
Cl1
Cl2

Fig. 2