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2-Chloro-4-{(*E*)-[(4-chlorophenyl)imino]-methyl}phenol

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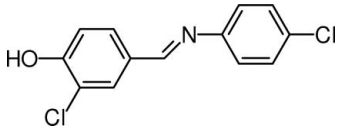
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.064; data-to-parameter ratio = 15.1.

In the title Schiff base compound, $C_{13}H_9Cl_2NO$, the dihedral angle between the mean planes of the benzene rings is 10.20 (10)°. The crystal structure is stabilized by O—H···N hydrogen bonds and weak π–π stacking interactions [centroid–centroid distance = 3.757 (1) Å].

Related literature

For Schiff bases related to coordination chemistry, see: Calligaris *et al.* (1972); Cozzi (2004); Curini *et al.* (2002). For the antibacterial, anticancer, antiinflammatory and antitoxic properties, see: Williams (1972); Karia & Parsania (1999); Desai *et al.* (2001). For the industrial and biological properties of Schiff bases, see: Lozier *et al.* (1975); Aydogan *et al.* (2001). For structural studies of Schiff bases, see: Gül *et al.* (2007); Şahin *et al.* (2005); Şahin, Ağar *et al.* (2009); Şahin, Erşahin *et al.* (2009); Şahin, Işık *et al.* (2009). For the classification of hydrogen-bonding patterns, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{13}H_9Cl_2NO$
M_r = 266.11
Orthorhombic, $P2_12_12$
a = 9.7438 (6) Å
b = 9.9953 (5) Å
c = 12.1342 (6) Å
V = 1181.78 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.53 mm^{-1}
T = 296 K
0.42 × 0.34 × 0.24 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.807, T_{max} = 0.901
11473 measured reflections
2325 independent reflections
1960 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.064
S = 0.96
2325 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Absolute structure: Flack (1983), 968 Friedel pairs
Flack parameter: 0.02 (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	1.96	2.778 (2)	176

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors acknowledge the Faculty of Arts and Sciences of Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDSII diffractometer (purchased under grant No. F279 of the University Research Grant of Ondokuz Mayıs University).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JJ2120).

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supplementary materials

Acta Cryst. (2012). E**68**, o678 [doi:10.1107/S1600536812005193]

2-Chloro-4-{(*E*)-[(4-chlorophenyl)imino]methyl}phenol

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Comment

Schiff bases are important in diverse fields of chemistry and biochemistry owing to their biological activites (Calligaris *et al.*, 1972; Lozier *et al.*, 1975). Most Schiff bases have antibacterial, anticancer, antinflammatory and antioxic properties (Williams, 1972). The present work is part of our structral study of Schiff bases (Gül *et al.*, 2007; Şahin, Ağar *et al.*, 2009; Şahin, Işık *et al.*, 2009; Şahin, Erşahin *et al.*, 2009) and we report here the structure of the title compound, $C_{13}H_9Cl_2NO$, (I).

The dihedral angle between the mean planes of the two aromatic rings is 10.20° and the C12—C13—N1—C3 torsion angle is 175.96 (17)° (Fig. 1). All bond lenghs are within normal values. The N1—C13 double bond length (1.268 (2)Å) is similar to the corresponding bond lengths in *E*-2-Methoxy-6-[(2-trifluoromethylphenylimino) methyl]phenol (1.270 (5) Å) (Şahin *et al.*, 2005) and *E*-4-Methyl-2-[3-(trifluoromethyl)-phenyliminomethyl]phenol (1.270 (3) Å] (Gül *et al.*, 2007).

In the crystal, the molecules are linked into sheets by O—H···N hydrogen bonds (Table 1) generating C(8) chains (Bernstein *et al.*,1995) along (011)(Fig. 2). Weak, symmetry independent π–π stacking interactions are observed which may influence crystal stability . The perpendicular distance from *Cg*1 to *Cg*1^{ii} [symmetry code: (ii) = -*x*, 1 - *y*, *z*] is 3.62 (0)Å. The centroid-to-centroid distance is 3.757 (1)Å.

Experimental

The title compound, (I), was prepared by refluxing a solution mixture containing 3-chloro-4-hydroxybenzaldehyde (0.008 g 0.051 mmol) in 20 ml ethanol and 4-chloroaniline (0.007 g 0.051 mmol) in 20 ml ethanol for 1 h. Crystals of (I) suitable for X-ray analysis were obtained from ethyl alcohol by slow evaporation (yield %54; m.p 441–442 K).

Refinement

All H atoms were placed in calculated positions and constrained to ride on their parents atoms, with CH = 0.93Å and OH (hydroxyl) = 0.82Å with U_{iso}(H)=1.2U_{eq}(C, O).

Computing details

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

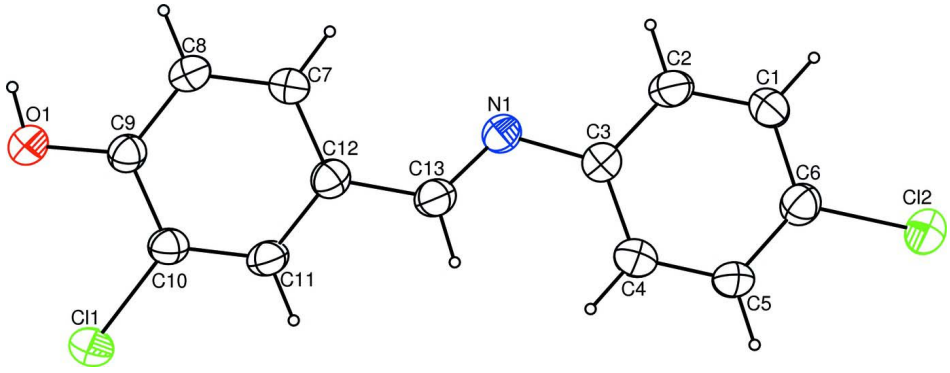

Figure 1

The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability.

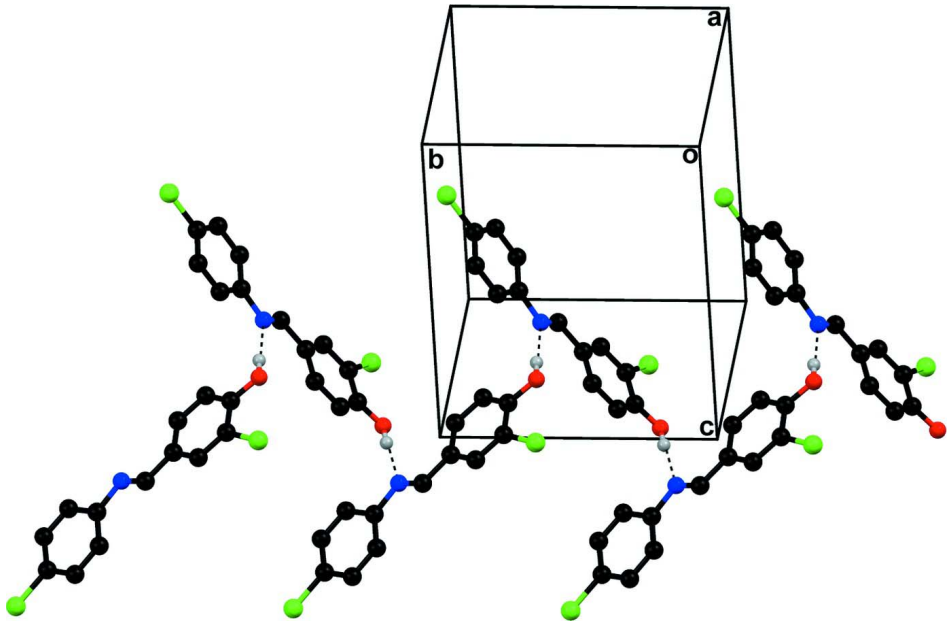

Figure 2

Molecular packing of the title compound, viewed along the *b* axis. O—H···N hydrogen bonds are shown as dashed lines. H atoms not involved in these interactions have been omitted for clarity.

2-Chloro-4-{(*E*)-[(4-chlorophenyl)imino]methyl}phenol

Crystal data

$C_{13}H_9Cl_2NO$
$M_r = 266.11$
Orthorhombic, $P2_12_12$
Hall symbol: P 2 2ab
$a = 9.7438\ (6)$ Å
$b = 9.9953\ (5)$ Å
$c = 12.1342\ (6)$ Å
$V = 1181.78\ (11)$ Å^3
$Z = 4$
$F(000) = 544$
$D_x = 1.496$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 20026 reflections
$\theta = 1.7$–$27.3°$
$\mu = 0.53$ mm^{-1}
$T = 296$ K
Prism, yellow
0.42 × 0.34 × 0.24 mm

Data collection

Stoe IPDS II diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.807, T_{max} = 0.901
11473 measured reflections
2325 independent reflections
1960 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 26.0°, θ_{min} = 1.7°
h = −11→12
k = −12→12
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.064
S = 0.96
2325 reflections
154 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0363P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Absolute structure: Flack (1983), 968 Friedel pairs
Flack parameter: 0.02 (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}
Cl1	−0.02767 (6)	0.22741 (7)	0.73432 (4)	0.06816 (19)
Cl2	0.78712 (7)	1.02829 (7)	0.54617 (5)	0.0792 (2)
O1	0.01370 (14)	0.20491 (15)	0.96945 (11)	0.0596 (4)
H1	0.0307	0.1983	1.0354	0.089*
N1	0.42961 (15)	0.66841 (17)	0.80818 (13)	0.0474 (4)
C12	0.25372 (18)	0.4980 (2)	0.82414 (15)	0.0491 (5)
C9	0.09145 (18)	0.3021 (2)	0.92525 (15)	0.0475 (5)
C11	0.16101 (18)	0.4218 (2)	0.76339 (16)	0.0532 (5)
H11	0.1528	0.4365	0.6880	0.064*
C6	0.6818 (2)	0.9216 (2)	0.62138 (17)	0.0562 (5)
C8	0.1838 (2)	0.3779 (2)	0.98593 (16)	0.0568 (5)
H8	0.1924	0.3631	1.0613	0.068*
C13	0.33844 (19)	0.5943 (2)	0.76529 (17)	0.0541 (5)
H13	0.3245	0.6022	0.6897	0.065*
C1	0.68403 (19)	0.9260 (2)	0.73602 (17)	0.0562 (5)

H1A	0.7417	0.9850	0.7730	0.067*
C10	0.08170 (19)	0.3259 (2)	0.81251 (15)	0.0487 (5)
C2	0.5999 (2)	0.8419 (2)	0.79293 (17)	0.0596 (6)
H2	0.6014	0.8442	0.8695	0.072*
C4	0.5127 (2)	0.7514 (2)	0.62570 (17)	0.0675 (6)
H4	0.4552	0.6925	0.5885	0.081*
C5	0.5955 (2)	0.8342 (2)	0.56650 (18)	0.0685 (6)
H5	0.5940	0.8320	0.4899	0.082*
C7	0.2623 (2)	0.4739 (2)	0.93676 (16)	0.0527 (5)
H7	0.3227	0.5241	0.9794	0.063*
C3	0.51177 (17)	0.75259 (19)	0.74034 (15)	0.0469 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0696 (3)	0.0808 (4)	0.0541 (3)	−0.0187 (3)	−0.0139 (2)	−0.0002 (3)
Cl2	0.0909 (4)	0.0874 (4)	0.0592 (3)	−0.0312 (3)	0.0115 (3)	0.0010 (3)
O1	0.0660 (8)	0.0659 (9)	0.0468 (7)	−0.0123 (7)	0.0010 (6)	0.0061 (7)
N1	0.0488 (9)	0.0486 (10)	0.0448 (9)	0.0033 (8)	0.0035 (7)	0.0006 (8)
C12	0.0462 (10)	0.0534 (12)	0.0477 (11)	0.0029 (9)	0.0022 (8)	0.0021 (9)
C9	0.0450 (9)	0.0526 (12)	0.0447 (10)	−0.0002 (9)	0.0026 (8)	0.0009 (9)
C11	0.0550 (10)	0.0667 (13)	0.0379 (10)	−0.0020 (10)	−0.0040 (9)	0.0050 (10)
C6	0.0606 (12)	0.0551 (13)	0.0528 (12)	−0.0015 (11)	0.0068 (9)	−0.0004 (10)
C8	0.0636 (12)	0.0680 (14)	0.0387 (11)	−0.0075 (11)	−0.0017 (9)	0.0044 (9)
C13	0.0536 (11)	0.0650 (13)	0.0438 (11)	0.0004 (10)	−0.0004 (9)	0.0027 (10)
C1	0.0545 (11)	0.0591 (13)	0.0549 (12)	−0.0096 (10)	−0.0027 (10)	−0.0073 (10)
C10	0.0464 (10)	0.0563 (13)	0.0433 (10)	0.0008 (9)	−0.0038 (8)	−0.0006 (9)
C2	0.0635 (12)	0.0741 (16)	0.0413 (11)	−0.0017 (12)	−0.0010 (9)	−0.0027 (10)
C4	0.0827 (14)	0.0689 (16)	0.0510 (12)	−0.0199 (13)	−0.0014 (11)	−0.0100 (12)
C5	0.0920 (15)	0.0728 (16)	0.0406 (11)	−0.0281 (13)	0.0017 (11)	−0.0082 (11)
C7	0.0552 (10)	0.0596 (13)	0.0432 (10)	−0.0070 (10)	−0.0054 (9)	−0.0026 (10)
C3	0.0482 (9)	0.0446 (11)	0.0480 (10)	0.0051 (8)	0.0021 (8)	−0.0001 (9)

Geometric parameters (Å, º)

Cl1—C10	1.733 (2)	C6—C1	1.392 (3)
Cl2—C6	1.738 (2)	C8—C7	1.364 (3)
O1—C9	1.344 (2)	C8—H8	0.9300
O1—H1	0.8200	C13—H13	0.9300
N1—C13	1.268 (2)	C1—C2	1.362 (3)
N1—C3	1.424 (2)	C1—H1A	0.9300
C12—C7	1.390 (3)	C2—C3	1.394 (3)
C12—C11	1.392 (3)	C2—H2	0.9300
C12—C13	1.456 (3)	C4—C5	1.360 (3)
C9—C8	1.388 (3)	C4—C3	1.391 (3)
C9—C10	1.392 (3)	C4—H4	0.9300
C11—C10	1.368 (3)	C5—H5	0.9300
C11—H11	0.9300	C7—H7	0.9300
C6—C5	1.384 (3)		

C9—O1—H1	109.5	C2—C1—H1A	120.7
C13—N1—C3	120.11 (16)	C6—C1—H1A	120.7
C7—C12—C11	117.68 (18)	C11—C10—C9	120.60 (18)
C7—C12—C13	124.26 (18)	C11—C10—Cl1	120.45 (15)
C11—C12—C13	118.02 (17)	C9—C10—Cl1	118.90 (16)
O1—C9—C8	123.27 (17)	C1—C2—C3	122.28 (19)
O1—C9—C10	118.49 (17)	C1—C2—H2	118.9
C8—C9—C10	118.21 (18)	C3—C2—H2	118.9
C10—C11—C12	121.26 (18)	C5—C4—C3	121.8 (2)
C10—C11—H11	119.4	C5—C4—H4	119.1
C12—C11—H11	119.4	C3—C4—H4	119.1
C5—C6—C1	120.6 (2)	C4—C5—C6	119.4 (2)
C5—C6—Cl2	119.58 (16)	C4—C5—H5	120.3
C1—C6—Cl2	119.77 (16)	C6—C5—H5	120.3
C7—C8—C9	121.02 (19)	C8—C7—C12	121.22 (19)
C7—C8—H8	119.5	C8—C7—H7	119.4
C9—C8—H8	119.5	C12—C7—H7	119.4
N1—C13—C12	125.60 (19)	C4—C3—C2	117.33 (18)
N1—C13—H13	117.2	C4—C3—N1	125.25 (18)
C12—C13—H13	117.2	C2—C3—N1	117.42 (16)
C2—C1—C6	118.58 (19)		

C7—C12—C11—C10	−0.5 (3)	C8—C9—C10—Cl1	177.26 (15)
C13—C12—C11—C10	177.53 (18)	C6—C1—C2—C3	−0.3 (3)
O1—C9—C8—C7	178.76 (19)	C3—C4—C5—C6	0.4 (4)
C10—C9—C8—C7	0.5 (3)	C1—C6—C5—C4	−0.3 (4)
C3—N1—C13—C12	175.96 (17)	Cl2—C6—C5—C4	−179.65 (19)
C7—C12—C13—N1	−0.3 (3)	C9—C8—C7—C12	−0.8 (3)
C11—C12—C13—N1	−178.15 (18)	C11—C12—C7—C8	0.7 (3)
C5—C6—C1—C2	0.3 (3)	C13—C12—C7—C8	−177.13 (19)
Cl2—C6—C1—C2	179.62 (16)	C5—C4—C3—C2	−0.3 (3)
C12—C11—C10—C9	0.2 (3)	C5—C4—C3—N1	−179.3 (2)
C12—C11—C10—Cl1	−177.24 (16)	C1—C2—C3—C4	0.3 (3)
O1—C9—C10—C11	−178.58 (17)	C1—C2—C3—N1	179.32 (18)
C8—C9—C10—C11	−0.2 (3)	C13—N1—C3—C4	−7.7 (3)
O1—C9—C10—Cl1	−1.1 (3)	C13—N1—C3—C2	173.35 (18)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.82	1.96	2.778 (2)	176

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