Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

[(4-Chlorophenyl)iminomethyl]phenol

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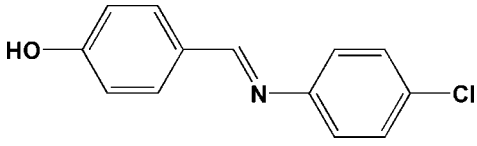
Received 14 November 2007; accepted 15 November 2007

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.036; wR factor = 0.099; data-to-parameter ratio = 11.1.

In the molecular structure of the title Schiff base, $C_{13}H_{10}ClNO$, the dihedral angle between the mean planes through the two benzene rings is 48.98 (8)°. The crystal structure is stabilized by intermolecular O—H···N hydrogen bonds, which lead to the formation of one-dimensional zigzag chains running parallel to the c axis.

Related literature

For related literature, see: Kazak *et al.* (2000, 2004); Sekikawa *et al.* (1997); Vijayalakshmi *et al.* (1997); Williams (1972).



Experimental

Crystal data

$C_{13}H_{10}ClNO$
M_r = 231.67
Orthorhombic, *Pbcn*
a = 21.3211 (18) Å
b = 11.0697 (10) Å
c = 9.2754 (10) Å
V = 2189.2 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 173 (2) K
0.45 × 0.40 × 0.20 mm

Data collection

Stoe IPDS2 diffractometer
Absorption correction: none
14167 measured reflections
2070 independent reflections
1662 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.099
S = 1.05
2070 reflections
186 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O*···N1^{i}	0.98 (3)	1.76 (3)	2.7294 (18)	176 (2)

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

Data collection: *X-AREA* (Stoe & Cie, 2006); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2006); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

LS and KR gratefully acknowledge the financial support of the University Grants Commission, Government of India [File No. 3237/2006(SR)], and Mr Mothi Mohamed, School of Chemistry, Bharathidasan University, Tiruchirappalli, for fruitful discussions.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LW2045).

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supplementary materials

Acta Cryst. (2007). E**63**, o4805 [**doi:10.1107/S1600536807059326**]

[(4-Chlorophenyl)iminomethyl]phenol

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Comment

Schiff bases have attracted much attention not only due to their versatile coordination chemistry but also due to their antibacterial, anticancer, anti-inflammatory and antitoxic properties (Williams, 1972). Further, the thermochromism, photochromism and non-linear optical properties of this class of compounds has found numerous applications in modern technologies (Sekikawa *et al.*, 1997). As a part of our reseach in assessing the second harmonic generation (SHG) efficiency of Schiff base compounds, we have undertaken the crystallographic analysis of the title compound, (I).

Compound (I) exists in the solid state in a non-planar conformation arising mainly from the rotation of the benzylidene moiety about the N1—C8 bond with a C7—N1—C8—C13 torsion angle of −34.8 (2)°. The dihedral angle between the planes of the chlorophenyl and hydroxyphenyl rings is 48.98 (8)°. The N1═C7 bond distance of 1.283 (2) Å is characteristic of a double bond [1.282 (2) A°; Kazak *et al.*, 2000]. The Cl1—C11 bond distance of 1.7375 (19) Å and the O1—C1 bond distance of 1.349 (2) Å are similar to the corresponding distances in 4-[(4-chlorobenzylidene)amino]phenol [1.741 (2) Å; Kazak *et al.*, 2004] and *N*-(*p*-hydroxybenzylidene)phenylamine N–oxide [1.353 (3) Å; Vijayalakshmi *et al.*, 1997], respectively. Other selected bond distances and angles are listed in Table 1.

The crystal structure of (I) is stabilized by intermolecular O—H···N hydrogen bonds formed between the phenol group and the imine nitrogen atom. This interaction leads to the formation of one-dimensional zigzag chains, which propagate along the *c* axis (Fig. 2 and Table 2).

Experimental

The title compound, (I), was prepared by the reaction of 4-hydroxybenzaldehyde with 4-chloroaniline (molar ratio 1:1) in absolute ethanol. The reaction mixture was heated under refluxed for 4 h. The resulting solution was filtered and the filtrated allowed to stand in air for about 2 days giving a yellow solid. Good quality crystals were obtained by recrystallized from methanol.

Refinement

The H-atoms were located from difference Fourier maps and freely refined: C—H = 0.934 (19) − 1.001 (19) Å.

Figures

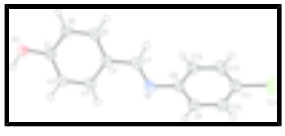

Fig. 1. View of the molecular structure of compound (I), showing the atom labelling scheme and displacement ellipsoids drawn at the 50% probability level.

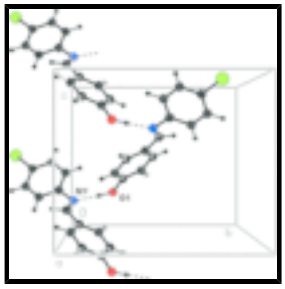

Fig. 2. View, along the *a* axis, of the crystal packing in compound (I). The intermolecular O—H···N hydrogen bonds are shown as dashed lines [symmetry operator (i) = −*x* + 1/2, −*y* + 1/2, *z* − 1/2].

[(4-Chlorophenyl)iminomethyl]phenol

Crystal data

$C_{13}H_{10}ClNO$	F_{000} = 960
M_r = 231.67	D_x = 1.406 Mg m^{-3}
Orthorhombic, *Pbcn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2n 2ab	Cell parameters from 11010 reflections
a = 21.3211 (18) Å	θ = 1.9–26.1º
b = 11.0697 (10) Å	μ = 0.32 mm^{-1}
c = 9.2754 (10) Å	*T* = 173 (2) K
V = 2189.2 (4) Å^3	Plate, pale-yellow
Z = 8	0.45 × 0.40 × 0.20 mm

Data collection

Stoe IPDS2 diffractometer	2070 independent reflections
Radiation source: fine-focus sealed tube	1662 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.049
Detector resolution: 6.67 pixels mm^{-1}	θ_{max} = 25.7º
T = 173(2) K	θ_{min} = 1.9º
φ & ω scans	*h* = −25→23
Absorption correction: none	*k* = −13→13
14167 measured reflections	*l* = −11→11

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	All H-atom parameters refined
$R[F^2 > 2\sigma(F^2)]$ = 0.036	$w = 1/[\sigma^2(F_o^2) + (0.0603P)^2 + 0.2783P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.099	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.05	$\Delta\rho_{max}$ = 0.38 e Å^{-3}
2070 reflections	$\Delta\rho_{min}$ = −0.49 e Å^{-3}

186 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0094 (17)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.48652 (3)	0.83860 (5)	1.00582 (6)	0.0538 (2)
O1	0.12979 (6)	0.25164 (11)	0.25210 (13)	0.0345 (4)
N1	0.33136 (7)	0.47845 (12)	0.69545 (14)	0.0274 (4)
C1	0.16661 (8)	0.30820 (14)	0.34915 (17)	0.0272 (5)
C2	0.22508 (8)	0.26384 (15)	0.39185 (17)	0.0273 (5)
C3	0.26144 (8)	0.32800 (15)	0.48853 (17)	0.0274 (5)
C4	0.24065 (8)	0.43796 (15)	0.54534 (17)	0.0271 (5)
C5	0.18169 (8)	0.48131 (15)	0.50178 (18)	0.0304 (5)
C6	0.14498 (8)	0.41745 (15)	0.40608 (19)	0.0303 (5)
C7	0.27980 (8)	0.51329 (15)	0.63758 (17)	0.0282 (5)
C8	0.36938 (8)	0.56623 (15)	0.76578 (17)	0.0275 (5)
C9	0.40427 (8)	0.53086 (16)	0.88569 (18)	0.0323 (5)
C10	0.44020 (9)	0.61442 (18)	0.9602 (2)	0.0363 (6)
C11	0.44232 (8)	0.73248 (17)	0.9124 (2)	0.0362 (6)
C12	0.41060 (9)	0.76778 (17)	0.7893 (2)	0.0363 (5)
C13	0.37430 (8)	0.68476 (16)	0.71684 (19)	0.0325 (5)
H1O	0.1452 (13)	0.171 (3)	0.229 (3)	0.078 (8)*
H2	0.2404 (9)	0.188 (2)	0.352 (2)	0.036 (5)*
H3	0.3029 (9)	0.2982 (17)	0.5113 (19)	0.032 (5)*
H5	0.1673 (9)	0.5574 (18)	0.538 (2)	0.032 (5)*
H6	0.1032 (9)	0.4479 (18)	0.373 (2)	0.037 (5)*
H7	0.2644 (9)	0.5966 (19)	0.648 (2)	0.034 (5)*
H9	0.4030 (9)	0.4458 (18)	0.920 (2)	0.033 (5)*
H10	0.4615 (9)	0.5918 (18)	1.044 (2)	0.036 (5)*
H12	0.4148 (11)	0.852 (2)	0.757 (2)	0.057 (6)*
H13	0.3539 (10)	0.7085 (19)	0.629 (2)	0.042 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0487 (4)	0.0569 (4)	0.0558 (3)	−0.0189 (2)	−0.0028 (2)	−0.0194 (2)
O1	0.0378 (7)	0.0292 (7)	0.0365 (7)	−0.0010 (5)	−0.0084 (5)	−0.0047 (5)
N1	0.0336 (8)	0.0238 (7)	0.0248 (6)	−0.0035 (6)	0.0030 (6)	−0.0005 (5)
C1	0.0320 (9)	0.0239 (8)	0.0257 (8)	−0.0045 (7)	−0.0003 (7)	0.0024 (6)
C2	0.0330 (9)	0.0225 (8)	0.0265 (8)	0.0002 (7)	0.0025 (7)	−0.0008 (6)
C3	0.0297 (9)	0.0248 (8)	0.0277 (8)	0.0003 (7)	0.0026 (7)	0.0028 (6)
C4	0.0318 (9)	0.0235 (8)	0.0261 (8)	−0.0031 (7)	0.0027 (6)	0.0011 (6)
C5	0.0347 (9)	0.0224 (9)	0.0340 (9)	0.0003 (7)	0.0045 (7)	−0.0014 (7)
C6	0.0298 (9)	0.0259 (9)	0.0353 (9)	0.0011 (7)	−0.0003 (7)	0.0019 (7)
C7	0.0337 (9)	0.0232 (8)	0.0276 (8)	−0.0012 (7)	0.0044 (7)	−0.0011 (6)
C8	0.0304 (8)	0.0272 (9)	0.0250 (8)	−0.0008 (7)	0.0044 (7)	−0.0022 (6)
C9	0.0341 (9)	0.0309 (10)	0.0320 (9)	0.0017 (7)	0.0001 (7)	0.0006 (7)
C10	0.0325 (9)	0.0427 (10)	0.0338 (10)	0.0024 (8)	−0.0039 (8)	−0.0037 (8)
C11	0.0307 (9)	0.0396 (10)	0.0382 (10)	−0.0062 (8)	0.0032 (7)	−0.0106 (8)
C12	0.0411 (10)	0.0289 (9)	0.0388 (9)	−0.0069 (8)	0.0052 (8)	−0.0017 (7)
C13	0.0381 (9)	0.0293 (9)	0.0301 (9)	−0.0023 (7)	0.0000 (7)	0.0018 (7)

Geometric parameters (Å, °)

Cl1—C11	1.7375 (19)	C9—C10	1.386 (3)
O1—C1	1.349 (2)	C10—C11	1.381 (3)
O1—H1O	0.98 (3)	C11—C12	1.383 (3)
N1—C8	1.424 (2)	C12—C13	1.377 (3)
N1—C7	1.283 (2)	C2—H2	0.97 (2)
C1—C6	1.398 (2)	C3—H3	0.967 (19)
C1—C2	1.397 (2)	C5—H5	0.96 (2)
C2—C3	1.382 (2)	C6—H6	1.001 (19)
C3—C4	1.399 (2)	C7—H7	0.98 (2)
C4—C5	1.405 (2)	C9—H9	0.99 (2)
C4—C7	1.457 (2)	C10—H10	0.934 (19)
C5—C6	1.379 (2)	C12—H12	0.98 (2)
C8—C13	1.392 (2)	C13—H13	0.960 (19)
C8—C9	1.394 (2)		
Cl1···C12^{i}	3.594 (2)	C9···H3^{x}	3.100 (19)
Cl1···Cl1^{ii}	3.6209 (9)	C9···H1O^{v}	2.87 (3)
Cl1···C6^{iii}	3.5839 (19)	C10···H10^{xi}	3.10 (2)
Cl1···H6^{iii}	2.986 (19)	C13···H7	2.617 (19)
O1···N1^{iv}	2.7294 (18)	H1O···H2	2.34 (3)
O1···H3^{iv}	2.712 (18)	H1O···N1^{iv}	1.76 (3)
O1···H9^{iv}	2.773 (19)	H1O···C3^{iv}	2.99 (3)
N1···O1^{v}	2.7294 (18)	H1O···C7^{iv}	2.73 (3)
N1···C10^{vi}	3.347 (2)	H1O···C8^{iv}	2.67 (3)
N1···C9^{vi}	3.268 (2)	H1O···C9^{iv}	2.87 (3)

N1···H3	2.696 (18)	H1O···H3^{iv}	2.33 (3)
N1···H2^{v}	2.80 (2)	H1O···H9^{iv}	2.42 (4)
N1···H1O^{v}	1.76 (3)	H2···H1O	2.34 (3)
C2···C7^{vii}	3.591 (2)	H2···N1^{iv}	2.80 (2)
C3···C9^{vi}	3.553 (2)	H2···C7^{iv}	3.02 (2)
C3···C13^{vi}	3.487 (2)	H3···N1	2.696 (18)
C3···C8^{vi}	3.307 (2)	H3···O1^{v}	2.712 (18)
C6···Cl1^{viii}	3.5839 (19)	H3···H1O^{v}	2.33 (3)
C7···C2^{ix}	3.591 (2)	H3···C8^{vi}	3.074 (18)
C7···C9^{vi}	3.569 (2)	H3···C9^{vi}	3.100 (19)
C8···C3^{x}	3.307 (2)	H5···H7	2.35 (3)
C9···N1^{x}	3.268 (2)	H6···H12^{xii}	2.49 (3)
C9···C3^{x}	3.553 (2)	H6···Cl1^{viii}	2.986 (19)
C9···C7^{x}	3.569 (2)	H7···C13	2.617 (19)
C10···N1^{x}	3.347 (2)	H7···H5	2.35 (3)
C12···Cl1^{i}	3.594 (2)	H7···H13	2.28 (3)
C13···C3^{x}	3.487 (2)	H7···C2^{ix}	3.02 (2)
C1···H13^{vii}	2.854 (19)	H7···C3^{ix}	3.01 (2)
C1···H7^{vi}	2.990 (19)	H7···C1^{x}	2.990 (19)
C2···H7^{vi}	2.865 (19)	H7···C2^{x}	2.865 (19)
C2···H7^{vii}	3.02 (2)	H9···O1^{v}	2.77 (2)
C2···H13^{vii}	2.84 (2)	H9···H1O^{v}	2.42 (3)
C3···H1O^{v}	2.99 (3)	H10···C10^{xi}	3.10 (2)
C3···H13^{vii}	3.08 (2)	H12···H6^{xiii}	2.49 (3)
C3···H7^{vii}	3.01 (2)	H13···C7	2.68 (2)
C7···H13	2.68 (2)	H13···H7	2.28 (3)
C7···H1O^{v}	2.73 (3)	H13···C1^{ix}	2.854 (19)
C7···H2^{v}	3.02 (2)	H13···C2^{ix}	2.84 (2)
C8···H1O^{v}	2.67 (3)	H13···C3^{ix}	3.08 (2)
C8···H3^{x}	3.074 (18)		
C1—O1—H1O	112.1 (16)	C11—C12—C13	119.29 (17)
C7—N1—C8	118.33 (14)	C8—C13—C12	120.81 (16)
O1—C1—C6	117.50 (15)	C1—C2—H2	119.7 (11)
C2—C1—C6	119.43 (15)	C3—C2—H2	120.1 (11)
O1—C1—C2	123.06 (14)	C2—C3—H3	118.6 (11)
C1—C2—C3	120.26 (15)	C4—C3—H3	120.3 (11)
C2—C3—C4	120.93 (16)	C4—C5—H5	119.1 (12)
C3—C4—C5	118.20 (15)	C6—C5—H5	119.7 (11)
C5—C4—C7	119.07 (15)	C1—C6—H6	118.0 (11)
C3—C4—C7	122.52 (15)	C5—C6—H6	122.0 (11)
C4—C5—C6	121.20 (15)	N1—C7—H7	121.8 (11)
C1—C6—C5	119.97 (16)	C4—C7—H7	113.8 (11)
N1—C7—C4	124.37 (15)	C8—C9—H9	120.5 (11)

N1—C8—C13	122.46 (15)	C10—C9—H9	119.2 (11)
C9—C8—C13	118.98 (16)	C9—C10—H10	120.3 (12)
N1—C8—C9	118.53 (15)	C11—C10—H10	120.3 (12)
C8—C9—C10	120.36 (16)	C11—C12—H12	118.3 (12)
C9—C10—C11	119.33 (17)	C13—C12—H12	122.4 (12)
Cl1—C11—C10	119.84 (14)	C8—C13—H13	120.0 (13)
Cl1—C11—C12	119.07 (15)	C12—C13—H13	119.1 (13)
C10—C11—C12	121.09 (17)		
C8—N1—C7—C4	171.05 (15)	C5—C4—C7—N1	172.70 (16)
C7—N1—C8—C9	147.05 (16)	C4—C5—C6—C1	−0.8 (3)
C7—N1—C8—C13	−34.8 (2)	N1—C8—C9—C10	−177.79 (16)
O1—C1—C2—C3	178.01 (15)	C13—C8—C9—C10	4.0 (3)
C6—C1—C2—C3	−0.6 (2)	N1—C8—C13—C12	178.74 (16)
O1—C1—C6—C5	−177.68 (15)	C9—C8—C13—C12	−3.1 (3)
C2—C1—C6—C5	1.0 (2)	C8—C9—C10—C11	−1.6 (3)
C1—C2—C3—C4	0.0 (2)	C9—C10—C11—Cl1	179.33 (14)
C2—C3—C4—C5	0.2 (2)	C9—C10—C11—C12	−1.8 (3)
C2—C3—C4—C7	−174.53 (15)	Cl1—C11—C12—C13	−178.45 (14)
C3—C4—C5—C6	0.2 (2)	C10—C11—C12—C13	2.7 (3)
C7—C4—C5—C6	175.13 (16)	C11—C12—C13—C8	−0.2 (3)
C3—C4—C7—N1	−12.6 (3)		

Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2; (ii) −*x*+1, −*y*+2, −*z*+2; (iii) *x*+1/2, *y*+1/2, −*z*+3/2; (iv) −*x*+1/2, −*y*+1/2, *z*−1/2; (v) −*x*+1/2, −*y*+1/2, *z*+1/2; (vi) *x*, −*y*+1, *z*−1/2; (vii) −*x*+1/2, *y*−1/2, *z*; (viii) *x*−1/2, *y*−1/2, −*z*+3/2; (ix) −*x*+1/2, *y*+1/2, *z*; (x) *x*, −*y*+1, *z*+1/2; (xi) −*x*+1, −*y*+1, −*z*+2; (xii) −*x*+1/2, −*y*+3/2, *z*−1/2; (xiii) −*x*+1/2, −*y*+3/2, *z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1O···N1^{iv}	0.98 (3)	1.76 (3)	2.7294 (18)	176 (2)

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

Fig. 1

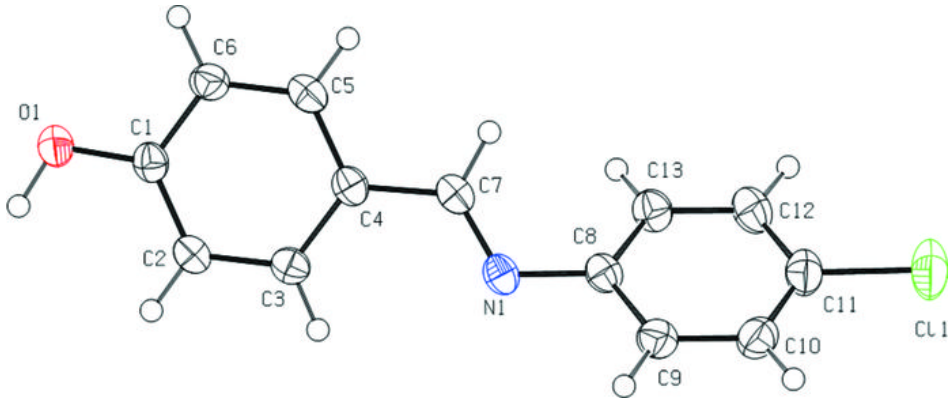

Fig. 2