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4-[(4-Chlorobenzylidene)amino]phenol

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.063
wR factor = 0.193
Data-to-parameter ratio = 17.6

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

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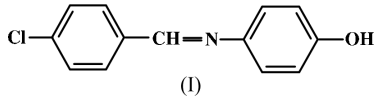
In the molecular structure of the title Schiff base, $C_{13}H_{10}ClNO$, the chlorophenyl ring and formimidoyl moiety are almost coplanar, and the dihedral angle between the planes of the phenol and chlorophenyl ring is 34.57 (9)°. The crystal structure is stabilized by intermolecular O—H···N hydrogen bonds, forming an infinite one-dimensional chain extending in the **b** direction, with an O···N distance of 2.846 (2) Å.

Comment

Schiff bases have been used widely as ligands in the formation of transition metal complexes. Many such complexes have been structurally characterized, but only a relatively small number of free Schiff bases have been characterized (Calligaris & Randaccio, 1987). Schiff base compounds can be classified by their photochromic and thermochromic characteristics (Cohen *et al.*, 1964). Most Schiff bases possess antibacterial, anticancer and antitoxic activities (Williams, 1972). Interesting photochromic compounds have been increasing in number ever since the potential applications of photochromic materials were realised in various areas, such as the control and measurement of radiation intensity, optical computers and display systems (Dürr, 1989; Dürr & Bouas-Laurent, 1990). The aim of our study was to synthesize and examine the characteristics of new derivatives of cyclotriphosphazenes containing an imino group, which were used in the above-mentioned fields (Odabaşoğlu *et al.*, 1999). In this paper, we report the structure of 4-[(4-chlorobenzylidene)-amino]phenol, (I) (Fig. 1).



(I)

The Cl1—C11 bond distance is 1.741 (2) Å, which is similar to the corresponding bond length in 1-(4-chlorobenzoyloxy)-2-methoxy-4-(2-propenyl)benzene [1.754 (3) Å; Aygün *et al.*, 1997]. The O1—C1 bond distance is 1.360 (2) Å, which is similar to the corresponding bond distances in *N*-(*p*-hydroxybenzylidene)phenylamine *N*-oxide [1.353 (3) Å; Vijayalakshmi, *et al.*, 1997] and the N1=C7 bond distance of 1.275 (2) Å is typical of a double bond [1.282 (2) Å; Kazak *et al.*, 2000]. Other relevant bond distances and bond angles are listed in Table 1. The formimidoyl group is almost coplanar with the chlorophenyl ring,d atoms Cl1, C7 and N1 deviating by −0.048 (1), −0.064 (2) and 0.134 (2) Å, respectively, from the plane of the chlorophenyl ring. The dihedral angle between the planes of the phenol and chlorophenyl rings is 34.57 (9)°. The crystal structure is stabilized by intermolecular

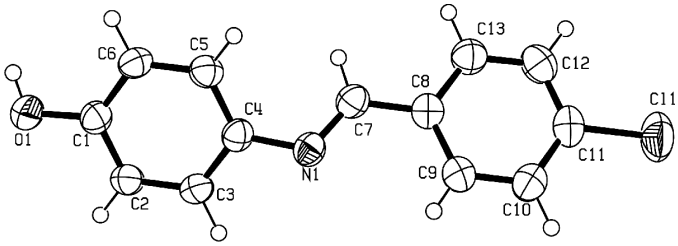


Figure 1
An *ORTEP*III drawing (Burnett & Johnson, 1997) of the title compound, showing the atomic numbering scheme. Displacement ellipsoids of non-H atoms are shown at the 50% probability level and H atoms are shown as small spheres of arbitrary size.

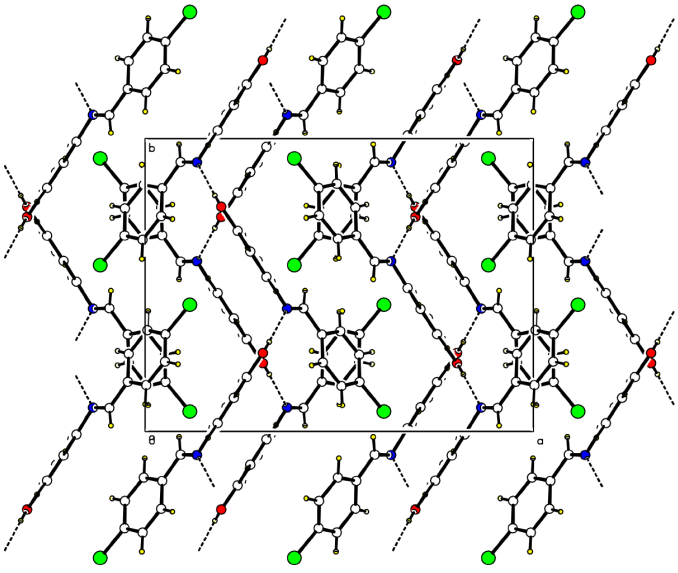


Figure 2
A view of the unit cell along the *c* axis. Hydrogen bonds are drawn as dashed lines

O—H···N hydrogen bonds, forming an infinite one-dimensional zigzag chain extending in the **b** direction (Fig. 2). The distances O1···N1^{i}, N1^{i}···H1 and O1—H1 are 2.846 (2), 2.03 (4) and 0.83 (3) Å, respectively, and the O1—H1···N1^{i} angle is 168 (3)° [symmetry code: (i) $\frac{3}{2}-x, y-\frac{1}{2}, z$].

Experimental

The title compound, (I), was prepared by reaction of 4-chlorobenzaldehyde with 4-aminophenol by modifying published procedures (Kamonuah *et al.*, 1992; Rao *et al.*, 1985). The Schiff base crystallized out on cooling the hot reaction mixture and was recrystallized from ethanol several times for purification. Crystals suitable for X-ray diffraction were obtained by slowly cooling a saturated solution in hot tetrahydrofuran–$CHCl_3$ (2:1) to room temperature.

Crystal data

$C_{13}H_{10}ClNO$
M_r = 231.67
Orthorhombic, *Pbca*
a = 16.866 (3) Å
b = 12.704 (5) Å
c = 10.410 (2) Å
V = 2230.6 (10) Å^3
Z = 8
D_x = 1.380 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 25 reflections
θ = 20.6–24.2°
μ = 0.32 mm^{-1}
T = 293 (2) K
Prism, yellow
0.40 × 0.38 × 0.30 mm

Data collection

Rigaku AFC-7*S* diffractometer
ω/2θ scans
3250 measured reflections
3250 independent reflections
2209 reflections with $I > 2\sigma(I)$
θ_{max} = 30.0°
$h = 0 \rightarrow 23$
$k = 0 \rightarrow 17$
$l = 0 \rightarrow 14$
3 standard reflections
every 150 reflections
intensity decay: 0.5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.193
S = 1.11
3250 reflections
185 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0975P)^2 + 0.6308P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—C11	1.741 (2)	O1—C1	1.360 (2)
N1—C7	1.275 (2)	O1—H1	0.83 (4)
N1—C4	1.422 (2)	C7—C8	1.467 (2)
C7—N1—C4	119.4 (2)	C5—C4—N1	124.3 (2)
C1—O1—H1	110 (2)	N1—C7—C8	123.6 (2)
O1—C1—C6	123.2 (2)	C9—C8—C7	122.3 (2)
O1—C1—C2	117.2 (2)	C12—C11—Cl1	119.4 (2)

H atoms were located in difference maps and refined isotropically. The C—H bond distances range from 0.91 (3) to 1.00 (2) Å, while U_{iso} values for H atoms are in the range 0.045 (6)–0.089 (10) Å^2.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1994); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996).

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