

2-[(2-Aminophenylimino)(phenyl)methyl]-4-chlorophenol

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Key indicators

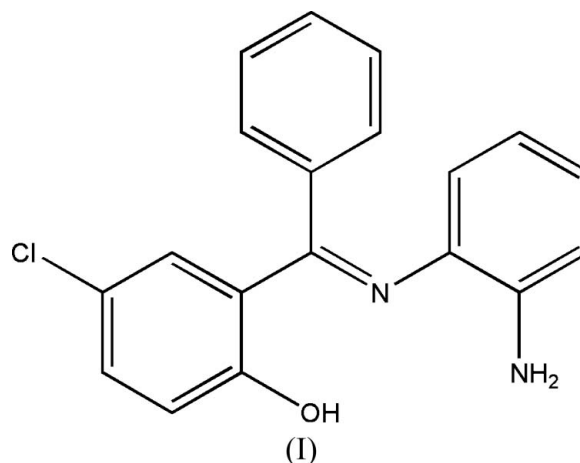
Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.044
 wR factor = 0.134
Data-to-parameter ratio = 16.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The title compound, $\text{C}_{19}\text{H}_{15}\text{ClN}_2\text{O}$, a tridentate Schiff base, has been synthesized and structurally characterized by IR spectroscopy and X-ray structure analysis. The hydroxy and imino groups are involved in a resonance-assisted $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond with $\text{O}\cdots\text{N} = 2.517(2)$ Å. Intermolecular $\text{O}-\text{H}\cdots\text{N}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds create centrosymmetric dimers in the crystal packing.

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Comment

2-[(2-Aminophenylimino)(phenyl)methyl]-4-chlorophenol has been widely investigated as a useful unsymmetrical tetradentate Schiff base ligand for the preparation of metal complexes (Bi & Fan, 2004; Zhu *et al.*, 2004; Kong & Ding, 1999; Atkins *et al.*, 1985). In the course of the synthesis of such a complex, single crystals of the compound, (I), were obtained. The crystal structure of (I) is reported here (Fig. 1).



In the molecular structure of (I), the hydroxy group is involved in an intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond (Fig. 1, Table 1), through which atoms O1, H1, N2, C7, C14 and C15 form a six-membered ring. The $\text{C7}=\text{N2}$ [1.298(2) Å], $\text{C7}-\text{C14}$ [1.480(2) Å] and $\text{O1}-\text{C15}$ [1.348(2) Å] bond lengths are shorter than normal $\text{C}=\text{N}$ (1.32 Å), $\text{C}-\text{C}$ (1.54 Å) and $\text{O}-\text{C}$ (1.44 Å) bonds; Allen *et al.*, 1987). The $\text{C14}=\text{C15}$ bond length [1.419(2) Å] is longer than a normal $\text{C}=\text{C}$ bond (1.40 Å in benzene). These differences in bond lengths are related to a resonance-assisted hydrogen bond (RAHB) acting between molecules with conjugated multiple π bonds (Gilli *et al.*, 2000).

In the crystal packing of (I), there are centrosymmetric dimers generated by $\text{O}-\text{H}\cdots\text{N}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds (Fig. 2 and Table 1).

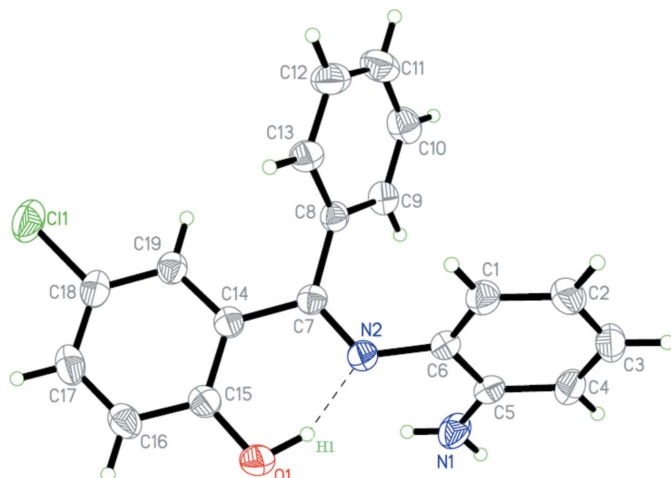


Figure 1
The structure of the title compound, with 30% probability displacement ellipsoids and the atom-numbering scheme. The intramolecular hydrogen bond is shown as a dashed line.

Experimental

The title compound, (I), was prepared according to the literature procedure of Bi & Fan (2004). A mixture of 2-[[[(2-aminophenyl)imino]phenylmethyl]-4-chlorophenol (1.29 g) dissolved in heated *n*-butanol (25 ml) and cadmium acetate dihydrate (1.07 g) dissolved in methanol (25 ml) was heated under reflux for 4 h. After cooling, the resulting solution was filtered and kept in air. After slow evaporation of the solvent over several weeks, large orange-red crystals of (I) formed at the bottom of the vessel. Single crystals suitable for X-ray analysis were isolated, washed twice with methanol and dried in air.

Crystal data

$C_{19}H_{15}ClN_2O$	$V = 820.7 (3) \text{ \AA}^3$
$M_r = 322.78$	$Z = 2$
Triclinic, $P1$	$D_x = 1.306 \text{ Mg m}^{-3}$
$a = 8.5630 (17) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 9.4940 (19) \text{ \AA}$	$\mu = 0.24 \text{ mm}^{-1}$
$c = 11.069 (2) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\alpha = 68.96 (3)^\circ$	Block, orange-red
$\beta = 84.84 (3)^\circ$	$0.25 \times 0.20 \times 0.18 \text{ mm}$
$\gamma = 77.75 (3)^\circ$	

Data collection

Enraf–Nonius CAD-4 diffractometer	2455 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.012$
Absorption correction: none	$\theta_{\text{max}} = 27.0^\circ$
3790 measured reflections	3 standard reflections
3549 independent reflections	every 100 reflections
	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0738P)^2 + 0.1224P]$
$R[F^2 > 2\sigma(F^2)] = 0.044$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.134$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.26 \text{ e \AA}^{-3}$
3549 reflections	$\Delta\rho_{\text{min}} = -0.28 \text{ e \AA}^{-3}$
213 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	(Sheldrick, 1997)
	Extinction coefficient: 0.025 (5)

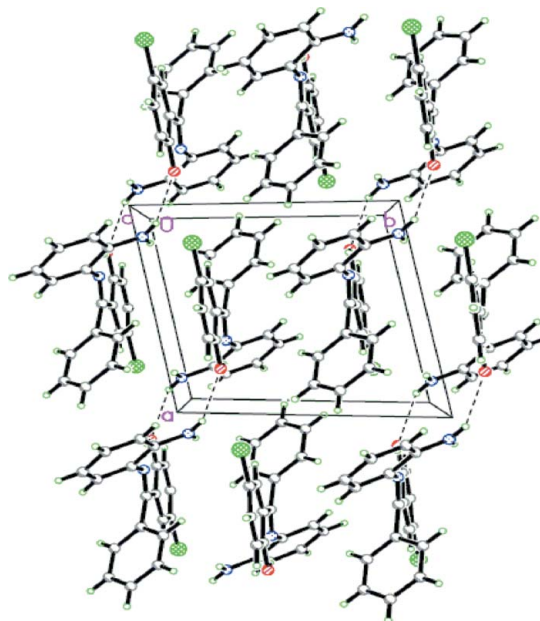


Figure 2
The crystal packing of (I), viewed along the *c* axis. Intermolecular hydrogen bonds are shown as dashed lines.

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1A\cdots O1^i$	0.86	2.31	3.035 (2)	142
$O1-H1\cdots N2$	0.95 (3)	1.64 (3)	2.517 (2)	153 (3)

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

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with $N-H = 0.86 \text{ \AA}$, $C-H = 0.93 \text{ \AA}$ and $O-H = 0.95 (3) \text{ \AA}$, and with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$ for the aromatic H atoms or $1.2U_{\text{eq}}(\text{parent})$ for the other atoms.

Data collection and cell refinement: *CAD-4 Software* (Enraf–Nonius, 1989); data reduction: *NRCVAX* (Gabe *et al.*, 1989); structure solution: *SHELXS97* (Sheldrick, 1997); structure refinement: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL/PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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