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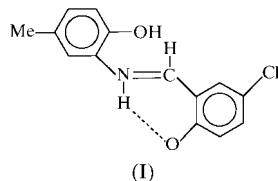
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The title compound, *N*-(5-chloro-2-oxidobenzylidene)-2-hydroxy-5-methylanilinium, C₁₄H₁₂ClNO₂, is a tridentate Schiff base with almost planar molecules. Each molecule contains a strong intramolecular N—H···O hydrogen bond [2.576 (2) Å]. There is also an intermolecular O—H···O hydrogen bond [2.695 (2) Å] linking neighbouring molecules into infinite chains along the [101] direction.

Comment

Although many structures of transition metal complexes with Schiff bases have been determined, a relatively small number of free Schiff bases have been structurally characterized (Garnovskii *et al.*, 1993). Schiff bases are of interest because they have long been known to show photochromism and thermochromism in the solid state which may involve reversible proton transfer from the amino N atom to the hydroxyl O atom (Cohen *et al.*, 1964; Moustakali *et al.*, 1978; Hadjoudis *et al.*, 1987). On the basis of some thermochromic and photochromic Schiff base compounds, it was proposed that molecules exhibiting thermochromism are planar, while those exhibiting photochromism are non-planar (Moustakali *et al.*, 1978), and that planarity of the molecule facilitates proton



transfer through the hydrogen bond in the ground state (Bregman, Leiserowitz & Schmidt, 1964; Bregman, Leiserowitz & Osaki, 1964). In the course of a systematic structural investigation of Schiff bases (Elmali & Elerman, 1998; Elmali, Elerman & Zeyrek, 1998; Elmali, Elerman, Svoboda & Fuess,

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1998; Elmali *et al.*, 1999a,b; Elerman, Elmali *et al.*, 1999), the structure of the title compound, (I), was determined.

The title molecule is almost planar; moieties *A* (C1–C7, O1, Cl1) and *B* (C8–C14, N1, O2) [both nearly planar with a maximum deviation of 0.0406 (10) Å] are inclined at an angle of 9.51 (6)° with respect to one another, reflecting mainly the twist about C8–N1 [C9–C8–N1–C7 = –8.7 (2)°].

Two types of intramolecular hydrogen bonds (either N—H···O or N···H—O) can exist in Schiff bases (Garnovskii *et al.*, 1993). The Schiff bases derived from salicylaldehyde always form the N···H—O type of hydrogen bonding regardless of the nature of the N substituent (alkyl or aryl) (Gavranić *et al.*, 1996, and references therein). In the aldimine compounds derived from 2-hydroxy-1-naphthaldehyde, both

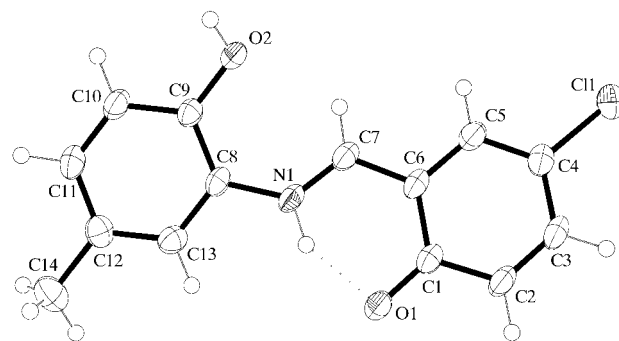


Figure 1

The molecular structure (ORTEP-3; Farrugia, 1997) of the title compound showing the atom-labelling scheme and 50% probability level displacement ellipsoids.

types of hydrogen bonds were found (Kaitner & Pavlović, 1996; Elerman *et al.*, 1998). The crystal structure of the title compound is stabilized by intramolecular and intermolecular hydrogen bonds. In (I), the N1···O1 distance is 2.576 (2) Å. The position of the H atom was deduced from a small peak in a difference map, 0.910 (19) Å from N1, along with the angle N—H···O of 147 (2)°, which indicated the presence of an N—H···O intramolecular hydrogen bond. The bond lengths within the vicinity of the N and O atoms are consistent with this interpretation. The N1···O1 distance is comparable to those observed for *N*-(3,5-dichlorophenyl)naphthalimine [2.570 (3) Å; Elmali, Elerman, Svoboda & Fuess, 1998], 4-ethyl-2-(β-hydroxy-α-naphthylmethylidene)amino-5-methyl-3-thiophenecarbonitrile [2.575 (3) Å; Elerman *et al.*, 1997] and *N*-*n*-propyl-2-oxo-1-naphthylidenemethylamine [2.578 (2) Å; Kaitner & Pavlović, 1996]. There is an intermolecular O2—H···O1ⁱⁱⁱ hydrogen bond [2.695 (2) Å] linking neighbouring molecules into infinite chains along the [101] direction [symmetry code: (iii) $x - \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$].

Experimental

The title compound was obtained from the reaction of 2-hydroxy-5-methylaniline (0.01 mol) with a solution of 5-chlorosalicylaldehyde (0.01 mol) in ethanol (40 ml). The precipitate which separated from the solution was recrystallized for 1–2 d from 1.7 g of Schiff base in acetonitrile solution (70 ml).

Crystal data

$C_{14}H_{12}ClNO_2$	$D_x = 1.462 \text{ Mg m}^{-3}$
$M_r = 261.70$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 25 reflections
$a = 5.966 \text{ (3) \AA}$	$\theta = 3.03\text{--}15.16^\circ$
$b = 13.392 \text{ (2) \AA}$	$\mu = 0.313 \text{ mm}^{-1}$
$c = 14.898 \text{ (3) \AA}$	$T = 303 \text{ (2) K}$
$\beta = 93.01 \text{ (2)^\circ}$	Prism, orange
$V = 1188.6 \text{ (7) \AA}^3$	$0.55 \times 0.25 \times 0.23 \text{ mm}$
$Z = 4$	

Data collection

Nonius CAD-4 diffractometer	$h = -7 \rightarrow 7$
$\omega/2\theta$ scans	$k = -16 \rightarrow 0$
4649 measured reflections	$l = -18 \rightarrow 18$
2331 independent reflections	3 standard reflections
2069 reflections with $I > 2\sigma(I)$	frequency: 120 min
$R_{\text{int}} = 0.012$	intensity decay: 4.7%
$\theta_{\text{max}} = 25.99^\circ$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0630P)^2 + 0.4009P]$
$R[F^2 > 2\sigma(F^2)] = 0.037$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.106$	$(\Delta/\sigma)_{\text{max}} = 0.002$
$S = 1.069$	$\Delta\rho_{\text{max}} = 0.22 \text{ e \AA}^{-3}$
2331 reflections	$\Delta\rho_{\text{min}} = -0.40 \text{ e \AA}^{-3}$
197 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1

Selected geometric parameters (\AA , $^\circ$).

C1—O1	1.3033 (18)	C8—N1	1.4189 (18)
C4—Cl1	1.7479 (17)	C9—O2	1.3602 (18)
C7—N1	1.302 (2)		
O1—C1—C2	121.37 (13)	C9—C8—N1	124.37 (13)
O1—C1—C6	121.86 (12)	C13—C8—N1	115.96 (13)
C5—C4—Cl1	120.75 (13)	O2—C9—C8	120.61 (12)
C3—C4—Cl1	118.77 (12)	O2—C9—C10	121.34 (13)
N1—C7—C6	121.05 (14)	C7—N1—C8	129.67 (13)

H atoms were calculated geometrically and their positions, except that of the OH group, were refined. The H atoms H1N (on N1) and H₂O (on O2) were located in difference Fourier maps calculated near the end of the refinement as small positive electron density. The isotropic displacement parameters of the H atoms were fixed at

$1.2U_{\text{eq}}$ of their parent atoms. C—H distances ranged from 0.88 (2) to 0.98 (2) \AA .

Data collection: *CAD-4 Diffractometer Control Software* (Enraf-Nonius, 1993); cell refinement: *CAD-4 Diffractometer Control Software*; data reduction: *X-RED* (Stoe & Cie, 1991); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: FR1313). Services for accessing these data are described at the back of the journal.

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