Supplementary data for this paper are available from the IUCr electronic archives (Reference: BK1453). Services for accessing these data are described at the back of the journal.

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An N···H—O intramolecular strong hydrogen bond in *N*-(2-aminophenyl)-naphthaldimine

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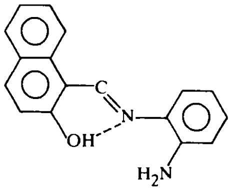
Abstract

The title compound, $C_{17}H_{14}N_2O$, contains a naphthaldimine and an *N*-(2-aminophenyl) group. There is a strong intramolecular N···H—O hydrogen bond between the imine and hydroxyl group [2.540 (2) Å].

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 (Calligaris & Randaccio, 1987). Schiff bases are of interest because they are known to show photochromism and thermochromism in the solid state; this may involve reversible proton transfer from the hydroxyl-O atom to the imine-N atom (Cohen *et al.*, 1964; Kevran *et al.*, 1996; Hadjoudis *et al.*, 1987). Photochromism is produced by intramolecular proton transfer associated with a change in the π-electron configuration (Barbara *et al.*, 1980; Hadjoudis, 1981; Higelin & Sixl, 1983). Thermochromism is also due to a change in the π-electron configuration induced by a proton transfer which can occur in the ground state (Cohen *et al.*, 1964). Interest in studies on photochromic compounds has been increasing ever since the potential application of photochromic materials was realised in various areas such as the control and measurement of radiation intensity, optical computers and display systems (Durr, 1989; Durr & Bouas-Laurent, 1990).

Fig. 1 shows the molecular structure and atomic labelling scheme of the title compound. The title molecule has two almost planar moieties *A* [O1, C7–C17; planar with a maximum deviation of 0.034 (2) Å for the O1 atom] and *B* [N1, N2, C1–C6; planar with a maximum deviation of 0.017 (1) Å for the C1 atom] which are inclined at an angle of 45.2 (1)° reflecting mainly the twist about C1—N2 [C2—C1—N2—C7 = 39.6 (3)°]. The conformation at the N2═C1 double bond is *trans* with the torsion angle C8—C7—N2—C1 = −174.9 (2)°.



(I)

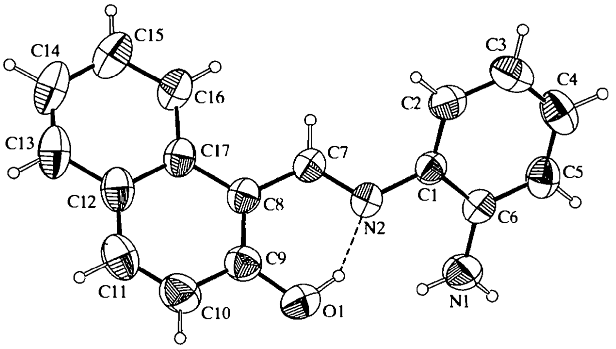


Fig. 1. The molecular structure showing 50% probability displacement ellipsoids with the atom-numbering scheme.

Two types of intramolecular hydrogen bond (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 bond regardless of the nature of the substituent on N (aryl or alkyl) (Gavranic *et al.*, 1996). Both types of hydrogen bond were found in aldimine compounds derived from 2-hydroxy-1-naphthaldehyde (Elerman *et al.*, 1998). In the title compound, the N···O distance [2.540 (2) Å] indicates a strong intramolecular hydrogen bond. The N2···H1 and O1—H1 bond distances are 1.70 (3) and 0.95 (3) Å, respectively, and the N2···H1—O1 angle is 146.3°. The N2···O1 distance is similar to those found in 1-[*N*-(4-methyl-2-pyridyl)aminomethylidene]-2(1*H*)-naphthalenone [2.532 (3) Å; Elerman *et al.*, 1998], *N*-(3,5-dichlorophenyl)naphthaldimine [2.570 (3) Å; Elmali *et al.*, 1998], *N*-*n*-propyl-2-oxo-1-naphthylidenemethylamine [2.578 (2) Å; Kaitner & Pavlovic, 1996], 4-ethyl-2-(2-hydroxynaphthylmethylidene)amino-5-methyl-3-thiophenecarbonitrile [2.275 (3) Å; Elerman *et al.*, 1997].

Experimental

The title compound was obtained from the reaction of 2-hydroxynaphthalene-1-carbaldehyde with a solution of 2-bromo-4-methylaniline in ethanol. The precipitate, which separated from the solution, was recrystallized over 1–3 d (2 g of the title Schiff base in 70 ml acetonitrile solution).

Crystal data

$C_{17}H_{14}N_2O$
$M_r = 262.30$
Monoclinic
$P2_1$
$a = 7.203$ (1) Å
$b = 7.670$ (2) Å
$c = 12.197$ (2) Å
$\beta = 99.10$ (3)°
$V = 665.4$ (2) Å^3
$Z = 2$
$D_x = 1.309$ Mg m^{-3}
D_m not measured

Cu $K\alpha$ radiation
$\lambda = 1.54178$ Å
Cell parameters from 25 reflections
$\theta = 3.67$–15.00°
$\mu = 0.658$ mm^{-1}
$T = 293$ (2) K
Prism
0.30 × 0.20 × 0.14 mm
Yellow

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
1465 measured reflections
1355 independent reflections
1273 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.052$

$\theta_{\rm max} = 69.89°$
$h = 0 \rightarrow 8$
$k = 0 \rightarrow 9$
$l = -14 \rightarrow 14$
3 standard reflections every 100 reflections frequency: 60 min intensity decay: <1.5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.107$
$S = 1.039$
1355 reflections
184 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.095P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.161$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.094$ e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.024 (4)
Scattering factors from *International Tables for Crystallography* (Vol. C)

Table 1. *Selected geometric parameters (Å, °)*

N1—C6	1.379 (2)	C10—C11	1.359 (4)
N2—C7	1.290 (2)	C12—C13	1.421 (3)
N2—C1	1.413 (2)	C12—C17	1.418 (3)
O1—C9	1.334 (2)	C13—C14	1.346 (4)
C7—C8	1.444 (3)	C14—C15	1.391 (4)
C8—C17	1.442 (2)		
C6—C1—N2	117.12 (15)	O1—C9—C8	122.11 (16)
O1—C9—C10	117.47 (18)		
C7—N2—C1—C2	39.6 (3)	N2—C7—C8—C9	4.3 (3)
C7—N2—C1—C6	−142.7 (2)	N2—C7—C8—C17	−177.3 (2)
C1—N2—C7—C8	−174.9 (2)		

The hydroxy-H atom was located in the difference Fourier synthesis and the positional coordinates were refined.

Data collection: *SDP* (Frenz, 1985). Cell refinement: *SDP*. Data reduction: *SDP*. Program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997). Molecular graphics: *ZORTEP* (Zsolnai, 1997). Software used to prepare material for publication: *SHELXL*97 and *PARST* (Nardelli, 1995).

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