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Instrumental Achievements

Crystal Structure of 1-[*N*-(4-Fluorophenyl)]naphthaldimine

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(Received December 19, 2000; Accepted May 21, 2001)

Schiff bases have been extensively used as ligands in the field of coordination chemistry. The Schiff-base compounds can be classified by their photochromic and thermochromic characteristics.[1] Photochromism is produced by an intramolecular proton transfer associated with a change in the π-electron configuration. Studies on photochromic compounds have been increasing ever since the potential applications of photochromic materials were realized in various areas, such as the control and measurement of radiation intensity, optical computers and display systems. Two types of intramolecular hydrogen bonds [either N–H···O (*keto* form) or N···H–O (*enol* form)] can exist in Schiff bases. 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).[2] In aldimine compounds derived from 2-hydroxy-1-naphthaldehyde, both types of hydrogen bonds were found.[3]

Suitable crystals were obtained directly from the synthesis of the compound. A solution of 0.01 mol 2-hydroxy-1-naphthaldehyde in 100 ml pure ethanol and 0.01 mol of 4-fluoroaniline in 50 ml hot ethanol were prepared and heated to the boiling temperature. The mixture of the two solutions was then refluxed for 5 h. Yellow color crystals were formed during the reflux (mp 129˚C).

The title molecule is not planar. The angle between moieties **A** (C1–C11, O1) and **B** (C12–C17, F1, N1) [both planar with a maximum deviation of 0.002(2)Å] is 20.5(1). There is an intramolecular hydrogen bond between the N1 and O1 atoms [2.547(3)Å]. The O1···N1 distance is comparable to those observed for *N*-*n*-propyl-2-oxo-1-naphthylidenemethylamine[2] [2.578(2)Å], *N*-(α-naphtyl)-2-oxo-1-naphthaldimine[3] [N···O 2.536(3)Å], and *N*-(2-bromo-4-methylphenyl)naphthaldimine[4] [2.553(4)Å]. X-ray structure determinations reveal that the *enol*

Table 1 Crystal and experimental data

Formula: $C_{17}H_{12}NOF$	
Formula weight = 265.28	
Crystal system: monoclinic	
Space group: *P*21/*a*	*Z* = 4
a = 6.988(3)Å	
b = 13.998(4)Å	β(˚) = 92.850(1)
c = 13.050(4)Å	
V = 1275.0(4)Å^3	
D_x = 1.382 g/cm^3	
μ (Mo K$_\alpha$) = 0.96 mm^{-1}	
T = 293 K	
F (0 0 0) = 552	
Crystal size: 0.20×0.15×0.10	
λ (Mo K$_\alpha$) = 0.71069 Å	
$2\theta_{max}$: 59.98	
Final value of *R*: 0.048, *Rw*: 0.089	
Number of reflections measured = 3754	
Number of reflections used = 3703	
Number of parameters = 185	
Goodness-of-fit = 1.113	
$(\Delta/\sigma)_{max}$ = 0.002	
$(\Delta\rho)_{max}$ = 0.310 eÅ^{-3}	
$(\Delta\rho)_{min}$ = –0.240 eÅ^{-3}	
Measurements: RIGAKU MSC/AFC7-S diffractometer	
Program system: TEXSAN	
Structure determination: SHELXS97	
Refinement: full matrix least-squares (SHELXL97)	
Treatment of hydrogen atoms: all the H atoms except the one bonded to O1 were located geometrically.	

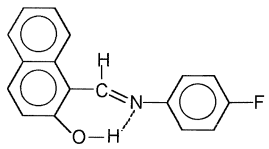


Fig. 1 Chemical structure.

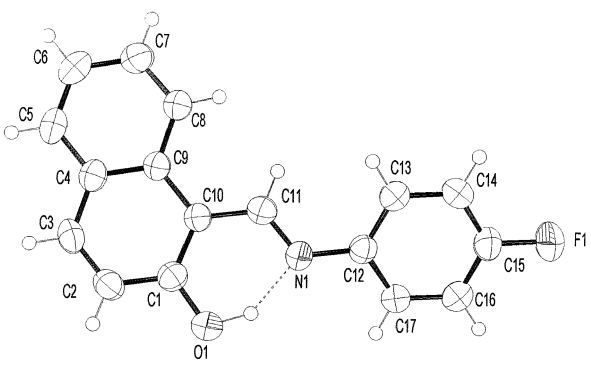


Fig. 2 Molecular structure of the compound. The displacement ellipsoids are plotted at the 50% probability level.

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Table 2 Final atomic coordinates and equivalent isotropic thermal parameters for non-hydrogen atoms

Atom	*x*	*y*	*z*	B_{eq}/Å^2
C1	0.1417(3)	0.6961(2)	0.9341(2)	3.63(5)
C2	0.1624(3)	0.7754(2)	0.9998(2)	4.12(6)
C3	0.1534(3)	0.8647(2)	0.9614(2)	4.14(5)
C4	0.1237(3)	0.8828(1)	0.8547(2)	3.54(5)
C5	0.1178(3)	0.9764(2)	0.8162(2)	4.22(5)
C6	0.0921(4)	0.9930(2)	0.7133(2)	4.70(4)
C7	0.0701(4)	0.9162(2)	0.6464(2)	4.67(5)
C8	0.0756(4)	0.8242(1)	0.6815(2)	4.08(5)
C9	0.1033(3)	0.8038(1)	0.7871(1)	3.18(4)
C10	0.1122(3)	0.7079(1)	0.8278(1)	3.18(6)
C11	0.0924(3)	0.6255(2)	0.7640(2)	3.58(6)
C12	0.0859(3)	0.4580(1)	0.7352(2)	3.39(4)
C13	0.1193(4)	0.4582(2)	0.6310(2)	4.17(4)
C14	0.1021(4)	0.3750(2)	0.5746(2)	4.47(4)
C15	0.0548(4)	0.2926(2)	0.6225(2)	4.46(5)
C16	0.0206(5)	0.2899(2)	0.7250(2)	4.62(6)
C17	0.0368(3)	0.3728(2)	0.7809(2)	3.94(5)
N1	0.1016(3)	0.5404(1)	0.7981(1)	3.56(5)
O1	0.1507(3)	0.6097(1)	0.9777(1)	4.58(4)
F1	0.0437(4)	0.2106(1)	0.5671(2)	6.57(5)

$B_{eq} = (8\pi^2/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* (\boldsymbol{a}_i \cdot \boldsymbol{a}_j)$.

Table 3 Selected bond lengths (Å), bond angles (˚) and torsion angle (˚)

C1-O1	1.337(4)
C11-N1	1.273(4)
C12-N1	1.415(4)
O1-HO1	1.130
N1LHO1	1.534
C10-C1-O1	121.9(3)
C1-O1-HO1	107.3
O1-HO1-N1	145.0
C11-N1-HO1	102.7
C12-N1-HO1	133.2
C10-C1-O1-HO1	-1.0

tautomer is favored over the *keto* tautomer. This is evident from the observed O1–C1 bond distance of 1.337(4)Å, which is consistent with the O–C single bond; similarly, the N1–C11 distance of 1.273(4)Å is also consistent with the N=C double bonding. The HO1 atom was located from a difference Fourier map at the end of the refinement process as a small positive electron density.

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