Crystal Structure of 1-[*N*-(6-Methyl-2-pyridyl)aminomethylidene] 2(1*H*)-naphthalenone

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Two types of intramolecular hydrogen bonds (either N–H···O or N···H–O), found in aldimine Schiff-base ligands derived from aldehydes having a hydroxyl group, depend on the kind of aldehyde used. In aldimine ligands made from 2-hydroxy-1-naphthaldehyde, both types of hydrogen bonds were found.[1,2] However, the Schiff bases derived from salicylaldehyde always form the N···H–O type of hydrogen bonding regardless of the *N*-substituent (aryl or alkyl).[3]

The title ligand was prepared from mixtures of 6-methyl-2-aminopyridine (0.94 g, 0.01 mol) and 2-hydroxy-1-naphthaldehyde (1.72 g, 0.01 mol) in boiling methanol (50 mL). After filtration, the residue was dissolved in heptane and set aside for crystallization. The results of an X-ray structure

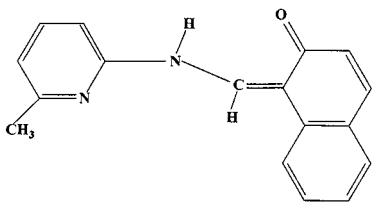

Fig. 1 Chemical structure.

Table 1 Crystal and experimental data

Formula: $C_{17}H_{14}N_2O$
Formula weight = 262.31
Crystal system: orthorhombic
Space group: Pbca $Z = 8$
a = 5.629(1)Å
b = 29.299(1)Å
c = 16.259(2)Å
V = 2681.3(2)Å
D_x = 1.30 g/cm^3
R = 0.042 wR = 0.053
$(\Delta/\sigma)_{max}$ = 0.01
$(\Delta\rho)_{max}$ = 0.16 eÅ^{-3}
$(\Delta\rho)_{min}$ =–0.12 eÅ^{-3}
No. of reflections used = 1014
Measurements: Enraf-Nonius CAD-4 diffractometer
Program system: CAD-4-EXPRESS Software
Structure determination: SHELXS86
Refinement: Full-matrix least-squares

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Table 2 Final atomic coordinates and equivalent isotropic thermal parameters

Atom	x	y	z	B_{eq}/Å
O1	1.0861(4)	0.05822(7)	0.4251(1)	6.63(6)
N1	0.7256(4)	0.08172(8)	0.5139(2)	4.65(6)
N2	0.3987(4)	0.10405(8)	0.5918(1)	4.37(6)
C1	1.1095(6)	0.0996(1)	0.4053(2)	5.44(8)
C2	1.3037(6)	0.1140(1)	0.3502(2)	6.46(9)
C3	1.3350(6)	0.1574(1)	0.3299(2)	6.52(9)
C4	1.1835(6)	0.1933(1)	0.3582(2)	5.36(8)
C5	1.2243(7)	0.2387(1)	0.3352(2)	6.58(9)
C6	1.0766(6)	0.2729(1)	0.3598(2)	6.67(9)
C7	0.8827(7)	0.2621(1)	0.4080(2)	6.25(9)
C8	0.8385(6)	0.2181(1)	0.4314(2)	5.44(8)
C9	0.9868(5)	0.1824(1)	0.4082(2)	4.58(7)
C10	0.9511(5)	0.1352(1)	0.4326(2)	4.34(7)
C11	0.7652(6)	0.1234(1)	0.4848(2)	4.44(7)
C12	0.5415(6)	0.07028(9)	0.5680(2)	4.12(7)
C13	0.5187(6)	0.0252(1)	0.5935(2)	5.09(8)
C14	0.3296(7)	0.0147(1)	0.6422(2)	5.68(9)
C15	0.1758(6)	0.0490(1)	0.6660(2)	5.54(8)
C16	0.2167(6)	0.0931(1)	0.6418(2)	4.57(7)
C17	0.0607(6)	0.1310(1)	0.6696(2)	6.08(9)

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

Table 3 Bond distances (Å) and angles (°)

O1 - C1	1.260(4)	C5 - C6	1.361(5)
N1 - C11	1.329(4)	C6 - C7	1.380(5)
N1 - C12	1.401(4)	C7 - C8	1.367(5)
N2 - C12	1.332(4)	C8 - C9	1.391(4)
N2- C16	1.347(4)	C9 - C10	1.452(4)
C1 - C2	1.476(5)	C10 - C11	1.390(4)
C1 - C10	1.442(4)	C12 - C13	1.390(4)
C2 - C3	1.327(5)	C13 - C14	1.363 (5)
C3 - C4	1.430(5)	C14 - C15	1.380(5)
C4 - C5	1.401(5)	C15 - C16	1.371(5)
C4 - C9	1.410(4)	C16 - C17	1.487(5)
C11 - N1 - C12	124.6(2)	C10 - C9 - C8	124.0(3)
C16 - N2 - C12	117.2(2)	C4 - C9 - C10	118.8(3)
C2 - C1 - O1	120.5(3)	C1 - C10 - C11	118.3(3)
C10 - C1 - O1	123.5(3)	C9 - C10 - C11	120.4(3)
C10 - C1 - C2	116.0(3)	C1 -C10 - C9	121.3(3)
C1 - C2 - C3	121.6(3)	C10 - C11 - N1	124.8(3)
C4 - C3- C2	123.1(3)	N1 - C12 - C13	118.9(3)
C5 - C4 - C3	121.0(3)	N2- C12 - C13	124.3(3)
C9 - C4 - C3	119.1(3)	N2 - C12 - N1	116.8(2)
C9 - C4 - C5	119.9(3)	C12 - C13 - C14	117.4(3)
C4 - C5 - C6	121.3(3)	C13 - C14 - C15	119.2(3)
C5 - C6 - C7	118.8(3)	C16 - C15 - C14	120.0(3)
C8 - C7 - C6	121.1(3)	N2 - C16 - C15	121.7(3)
C9 - C8 - C7	121.7(3)	N2 - C16 - C17	117.0(3)
C4 - C9 - C8	117.2(3)	C15 - C16 - C17	121.3(3)

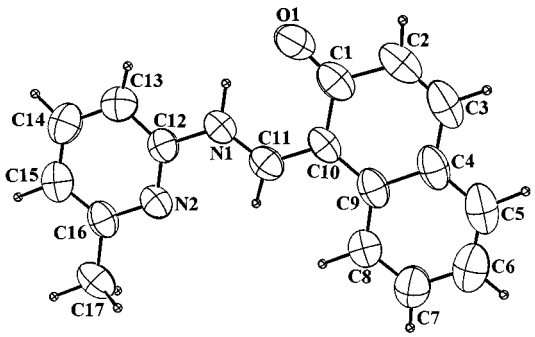

Fig. 2 Molecular structure of the title compound along with the atom-numbering scheme. The thermal ellipsoids are drawn at the 50% probability level.

determination are given in Tables 1 – 4.

The title molecule (Fig. 2) is approximately planar. There is a strong intramolecular N–H···O hydrogen bond [N1–H1 1.00(3), H1···O1 1.852(3), O1···N1 2.583(3)Å, N1–H1···O1 127.6(3)˚], which makes the *keto* amine form, as in *N*-*n*-propyl-2-oxo-1-naphthylidenemethylamine[4] [N···O 2.578(2), N–H 0.775, H···O 1.936 Å and *N*-(α-naphthyl)-2-oxo-1-naphthaldimine[5] [N···O 2.536, N–H 0.851 Å]. The H-atoms were found from a difference synthesis and refined isotropically, while the H31 and H61 positions were calculated geometrically, 0.95 Å from the corresponding atoms, and refined using a riding model.

Table 4 Torsion angles(˚)

C10-C11-N1-C12	178.4(3)	C13-C12-N1-C11	180.0(3)
N2-C12-N1-C11	0.0(4)	C1-C10-C11-N1	2.2(5)
C9-C10-C11-N1	-176.4(3)		

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