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4-Ethoxy-*N*-(6-methylquinolin-2-ylmethylene)aniline

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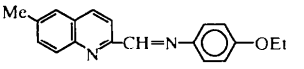
Abstract

The crystal structure of the title Schiff base, $C_{19}H_{18}N_2O$, has been determined. The 6-methylquinoline group and formimidoyl moiety are almost planar, and the dihedral angle between the planes of ethoxyphenyl and 6-methylquinoline is 44.02 (8)°. The crystal structure is stabilized by intramolecular and intermolecular hydrogen bonds of the C—H···N type forming a chain extending in the *a* direction.

Comment

It is interesting to note that several Schiff bases have physical properties which impart to them liquid-crystal behaviour (Gray, 1962; Arora *et al.*, 1970). The formation of Schiff bases may proceed readily in many cases under relatively mild conditions. It is therefore not surprising that biochemistry, biomedical research, immunochemistry *etc.* have found uses for the reaction of amines (Sandler & Karo, 1986). In this paper we report the structure of 4-ethoxy-*N*-(6-methylquinolin-2-ylmethylene)aniline, (I).



(I)

Fig. 1 shows a view of the title compound with the atom-numbering scheme. The C9=N1 bond length of 1.268 (2) Å is typical of a double bond as has been observed in a similar structure [1.270 (3) and 1.276 (3) Å; Cannadine *et al.*, 1996]. The bond lengths and angles in the title compound are in agreement with related structures reported earlier (Abu-Surrah *et al.*, 1997; Işık *et al.*, 1998).

The formimidoyl and methyl groups are almost coplanar with the quinoline moiety, the maximum

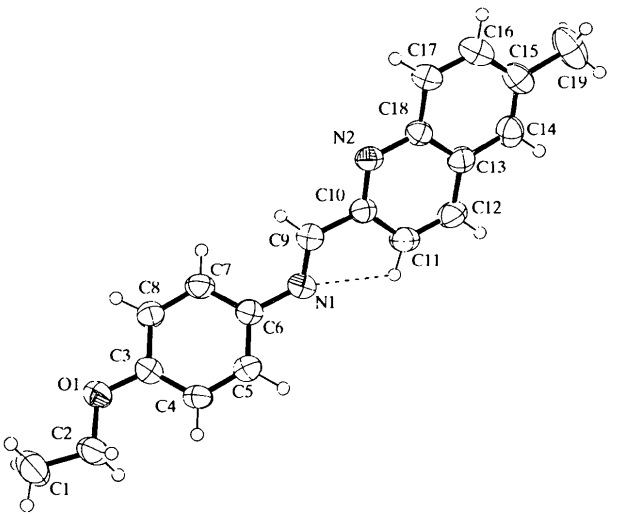


Fig. 1. An *ORTEP*III (Burnett & Johnson, 1996) drawing of the title compound showing the atomic numbering scheme. Displacement ellipsoids of non-H atoms are shown at the 50% probability level; H atoms are shown as small spheres of arbitrary size. The intramolecular hydrogen bond is shown as a dashed line.

deviation from the quinoline plane being 0.021 (2) Å for C9. The ethoxy group is not coplanar with the phenyl ring. The O1, C2 and C1 atoms of the ethoxy group deviate by −0.019 (1), −0.132 (3) and −0.238 (4) Å, respectively, from the plane of the phenyl ring. The dihedral angle between the plane of the phenyl ring and the plane of the 6-methylquinoline formimidoyl moiety is 44.02 (8)°.

The crystal structure is stabilized by one intramolecular hydrogen bond between C11 and N1 [C11···N1 2.812 (3), C11—H11 0.95 (3) Å and C11—H11···N1 105 (1)°] and one intermolecular hydrogen bond between C5···N2^{i} [C5···N2^{i} 3.549 (3), C5—H5 1.00 (2) Å and C5—H5···N2^{i} 161.4 (18)°; symmetry code: (i) $-1+x, y, z$]. The molecules in the crystal structure are thus linked by hydrogen bonds to form a chain in the a direction.

Experimental

The synthesis of the title compound and ^{1}H NMR, IR and MS spectroscopy characterizations have been described (Kaban & Fidaner, 1990). Pale brown–yellow crystals suitable for X-ray diffraction were obtained from ethanol.

Crystal data

$C_{19}H_{18}N_2O$
$M_r = 290.35$
Triclinic
$P\bar{1}$
$a = 7.4127\ (8)$ Å
$b = 10.1982\ (17)$ Å
$c = 10.8971\ (11)$ Å
$\alpha = 85.969\ (11)°$
$\beta = 74.899\ (8)°$
$\gamma = 78.473\ (12)°$
$V = 779.15\ (17)$ Å^3
$Z = 2$
$D_x = 1.238$ Mg m^{-3}
D_m not measured

Mo $K\alpha$ radiation
$\lambda = 0.71070$ Å
Cell parameters from 25 reflections
$\theta = 11.12–18.64°$
$\mu = 0.077$ mm^{-1}
$T = 293\ (2)$ K
Prismatic
0.48 × 0.48 × 0.30 mm
Pale yellow

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
2769 measured reflections
2769 independent reflections
1919 reflections with $I > 2\sigma(I)$

$\theta_{max} = 26.29°$
$h = 0 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -12 \rightarrow 13$
3 standard reflections
frequency: 120 min
intensity decay: 0.3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.116$
$S = 0.933$
2769 reflections
272 parameters
H atoms refined

$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997*a*)
Extinction coefficient: 0.010 (2)

$w = 1/[\sigma^2(F_o^2) + (0.0436P)^2 + 0.3468P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

Scattering factors from *International Tables for Crystallography* (Vol. C)

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

N1—C9	1.268 (2)	O1—C3	1.366 (2)
N1—C6	1.415 (2)	O1—C2	1.431 (2)
N2—C10	1.326 (2)	C1—C2	1.479 (4)
N2—C18	1.371 (2)	C9—C10	1.466 (3)
C9—N1—C6	121.10 (17)	C7—C6—N1	123.90 (17)
C10—N2—C18	117.19 (16)	N1—C9—C10	120.21 (19)
C3—O1—C2	117.10 (16)	C14—C13—C12	123.39 (19)
O1—C2—C1	108.5 (2)	N2—C18—C17	118.45 (18)
O1—C3—C4	125.14 (17)		

The H atoms were located from difference maps and refined isotropically. The C—H bond distances range from 0.89 (3) to 1.05 (3) Å, while U_{iso} values for H atoms are in the range 0.051 (5)–0.18 (2) Å^2.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1993). Cell refinement: *CAD*-4 *EXPRESS*. Data reduction: *MolEN* (Fair, 1990). Program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*b*). Program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*) in *WINGX* (Farrugia, 1997). Molecular graphics: *ORTEP*III (Burnett & Johnson, 1996). Software used to prepare material for publication: *SHELXL*97.

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