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4,6-Dimethyl-2-(2,4-dimethylphenyliminomethyl)-quinoline

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Key indicators

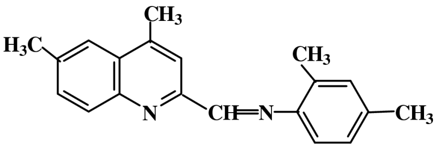
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.063
wR factor = 0.190
Data-to-parameter ratio = 15.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The molecule of the title compound, $C_{20}H_{20}N_2$, is not planar. The dihedral angle between the planes of the quinoline and phenyl rings is 64.6 (1)°, and these two planes make angles of 17.7 (2) and 47.7 (3)°, respectively, with the plane of the central iminomethyl moiety.

Comment

Imine derivatives have long found great use in analytical chemistry and are now being actively investigated in medicinal and polymer chemistry. 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 reactions of amines (Sandler & Karo, 1986). Schiff base compounds can be classified by their photochromic and thermochromic characteristics (Cohen *et al.*, 1964; Moustakali *et al.*, 1978). Most Schiff bases possess antibacterial, anticancer and antitoxic activities (Williams, 1972). The structure of the title compound, (I), has been determined and is presented here.



(I)

The molecular structure of (I) is shown in Fig. 1, together with the atomic numbering scheme. The C12=N2 bond length of 1.259 (3) Å is typical of the double bond observed in similar structures, *viz*. 1.265 (4) (Öztürk *et al.*, 2001) and 1.267 (3) Å (Akkurt *et al.*, 2001). In the quinoline ring, the angle C3—C4—C5 is greater than 120° [123.6 (2)°] and C8—C9—N1 is smaller than 120° [118.2 (2)°] (Aygün *et al.*, 1999; Öztürk *et al.*, 2000). Other relevant bond lengths and angles are listed in Table 1.

The quinoline and phenyl rings are planar; the dihedral angle between their planes is 64.6 (1)°, and the two planes make angles of 17.7 (2) and 47.7 (3)°, respectively, with the plane of the central iminomethyl moiety. There are no unusual short contacts between the molecules and the crystal structure is stabilized by van der Waals interactions.

Experimental

4,6-Dimethylquinoline-2-carbaldehyde (0.54 mmol) was dissolved in absolute ethanol (10 ml) and an equimolar amount of 2,4-dimethylaniline dissolved in absolute ethanol (5 ml) was added. The reaction

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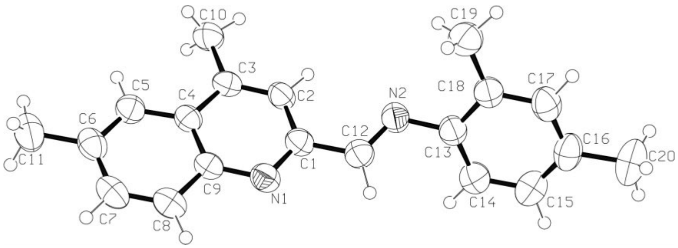

Figure 1
An *ORTEP*III (Burnett & Johnson, 1996) drawing of the molecular structure of (I) showing the labelling of the non-H atoms. Anisotropic displacement ellipsoids are shown at the 50% probability level.

mixture was refluxed for 3 h. The crude product which precipitated on cooling was recrystallized from ethanol. Yield: 92%; m.p.: 417 K; IR (KBr): 3060, 3000, 2780, 1605, 1585, 1480, 1430, 880, 830 and 810 cm^{-1}. ^{1}H NMR (CDCl$_3$, δ, 200 MHz): 2.36 (*s, o*-CH$_3$, 3H), 2.45 (*s, p*-CH$_3$, 3H), 2.59 (*s*, 6-CH$_3$, 3H), 2.75 (*s*, 4–CH$_3$, 3H) 7.03–8.65 (*m*, ArH and CH, 8H) p.p.m.

Crystal data

$C_{20}H_{20}N_2$
M_r = 288.38
Triclinic, $P\overline{1}$
a = 7.4939 (6) Å
b = 9.6449 (8) Å
c = 12.1632 (9) Å
α = 84.559 (2)°
β = 84.522 (2)°
γ = 68.944 (2)°
V = 814.95 (11) Å^3
Z = 2
D_x = 1.175 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2189 reflections
θ = 2.7–27.5°
μ = 0.07 mm^{-1}
T = 293 (2) K
Plate, colourless
0.42 × 0.30 × 0.08 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: none
5288 measured reflections
3600 independent reflections
2078 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.026
$\theta_{\rm max}$ = 27.5°
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -10 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.190
S = 1.03
3600 reflections
235 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0792P)^2 + 0.1802P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max}$ = 0.003
$\Delta\rho_{\rm max}$ = 0.17 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.16 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.320 (3)	C3—C10	1.503 (3)
N1—C9	1.373 (3)	C4—C9	1.421 (3)
N2—C12	1.259 (3)	C6—C11	1.515 (3)
N2—C13	1.423 (3)	C16—C20	1.514 (3)
C1—C12	1.473 (3)	C18—C19	1.504 (3)
C1—N1—C9	117.2 (2)	C5—C4—C3	123.6 (2)
C12—N2—C13	119.4 (2)	N1—C9—C8	118.2 (2)
N1—C1—C12	115.4 (2)	N2—C12—C1	121.6 (2)
C2—C3—C10	121.4 (2)		

The methyl groups were allowed to rotate about their local threefold axes.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL*97.

References

Akkurt, M., Öztürk, S., Aygün, M. & Aydoğan, F. (2001). *Acta Cryst.* E**57**, o454–o455.
Aygün, M., Işık, Ş., Turgut, Z., Özbey, S. & Kendi, E. (1999). *Acta Cryst.* C**55**, 1689–1690.
Burnett, M. N. & Johnson, C. K. (1996). *ORTEP*III. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.
Cohen, M. D., Schmidt, G. M. J. & Flavian, S. (1964). *J. Chem. Soc.* pp. 2041–2051.
Moustakali, I., Mavridis, I. & Hadjoudis, E. (1978). *Acta Cryst.* B**34**, 3709–3715.
Öztürk, S., Aygün, M., Öcal, N., Yolaçan, Ç. & Fun, H.-K. (2001). *Anal. Sci.* **17**, 797–798.
Öztürk, S., Aygün, M., Öcal, N., Yolaçan, Ç. & Fun, H.-K. (2000). *Z. Kristallogr. New Cryst. Struct.* **215**, 526.
Sandler, S. R. & Karo, W. (1986). *Organic Functional Group Preparations*, Vol. 11, 2nd ed., pp. 291–319. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Siemens (1996). *SMART* and *SAINT* (Version 4). Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Williams, D. R. (1972). *Chem. Rev.* **72**, 203–213.