Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

2-[(2-Chlorophenyl)iminomethyl]-4,6-dimethylquinoline

Sema Öztürk,[a]* Mehmet Akkurt,[a] Muhíttín Aygün[b] and Feray Aydoğan[c]

[a]Department of Physics, Faculty of Arts and Sciences, Erciyes University, 38039 Kayseri, Turkey, [b]Department of Physics, Faculty of Arts and Sciences, Dokuz Eylül University, 33150, Buca İzmir, Turkey, and [c]Department of Chemistry, Faculty of Arts and Sciences, Yıldız Technical University, 80270 İstanbul, Turkey

Correspondence e-mail: ozturk@erciyes.edu.tr

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.071
wR factor = 0.217
Data-to-parameter ratio = 17.4

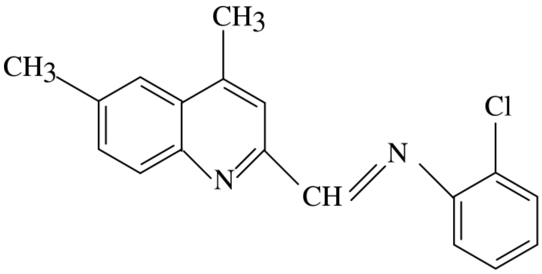
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 5 July 2001
Accepted 11 July 2001
Online 20 July 2001

The molecule of the title compound, $C_{18}H_{15}ClN_2$, is not planar. The dihedral angle between the quinoline and phenyl rings is 116.2 (1)°. Bond lengths and angles are normal.

Comment

Schiff bases, occupying an important place in medicine and industry, are generally useful compounds as starting materials in the preparation of textiles, dyestuffs, pesticides and pharmaceuticals, and of compounds that serve as stabilizers and inhibitors in photography (Sommes, 1976). Great attention has recently begun to concentrate on the compounds obtained from heterocyclic carbaldehydes for the therapy of cancer, the disease of our age (Kouznetsov *et al.*, 1998; Öcal & Kaban, 1998). Hence, in our research, new Schiff bases containing different functional groups have been synthesized for the purpose of making some contributions to that class of substances which are now being tested as anticancer reagents.



(I)

The structure of the title compound, 4,6-dimethylquinoline-2-[*N*-(*o*-chlorophenyl)formimidoyl], (I), is isomorphous with 4,6-dimethylquinoline-2-[*N*-(*o*-tolyl)formimidoyl], (II) (Akkurt *et al.*, 2001). The quinoline and phenyl rings are planar. In the quinoline ring, the C3—C4—C5 angle is larger than 120° [124.0 (3)°] and the N1—C9—C8 angle is smaller than 120° [118.4 (3)°]. Corresponding values are almost comparable with those in 3-(*p*-chlorophenyl)-5-methyl-2-(8-quinolinyl)-4-thiazolidinone (Öztürk *et al.*, 2000) [for molecule *A* of two independent molecules in the asymmetric unit, 122.8 (6) and 120.3 (5)°, respectively, and for molecule *B*, 124.4 (7) and 117.4 (4)°, respectively] and in (II) [123.4 (2) and 118.2 (2)°, respectively]. The dihedral angles between the least-squares planes of the quinoline and phenyl rings are 116.2 (1) and 118.5 (1)° in (II) and 61.8 (1)° in *N*-8-azanaphtylmethylene-4-chloroaniline (Öztürk *et al.*, 2001). This large deviation is possibly due to the steric factors which occur for the different positions of the Cl atom in the phenyl ring. There are non-bonded contacts greater than 3.3 Å between non-H atoms.

DOI: 10.1107/S1600536801011771

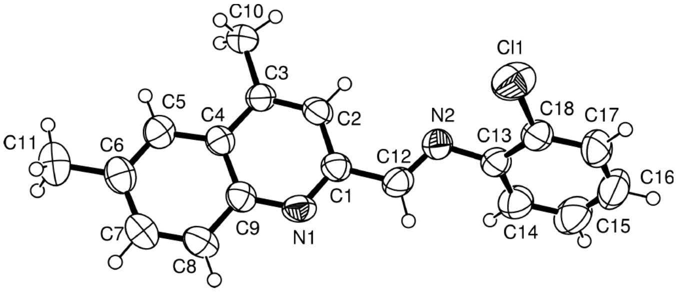


Figure 1
An *ORTEP*II (Johnson, 1976) drawing of the title compound showing the labelling of the non-H atoms. Displacement ellipsoids are shown at the 50% probability level.

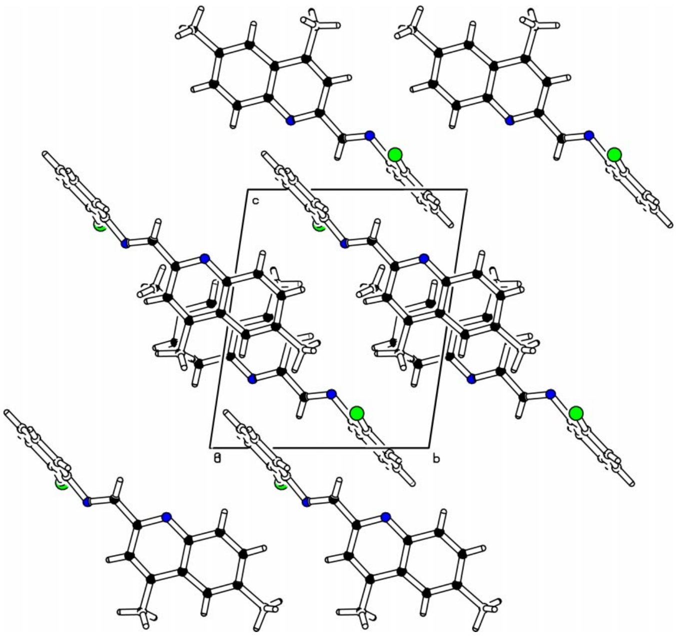


Figure 2
A view of the unit cell along the *a* axis.

Experimental

The title compound was synthesized by the condensation of 4,6-dimethylquinoline-2-carbaldehyde with *o*-chloroaniline in dry benzene over a period of 11 h. Light-yellow crystals were obtained after crystallization from petroleum ether (313–333 K). Yield: 81%; m.p.: 405 K; IR (KBr): γ = 3030, 2900, 1580 cm^{-1}; ^{1}H NMR (CDCl$_3$, δ, 200 MHz): 2.58 (3H, *s*, 6-CH$_3$), 2.74 (3H, *s*, 4-CH$_3$), 7.12–8.65 (9H, *m*, ArH and CH) p.p.m.; UV (CHCl$_3$): $\lambda_{\max}$ = 262.3, 314.4 nm. Elemental analysis, $C_{18}H_{15}N_2$ requires: C 73.34, H 5.13, N 9.50%; found: C 73.18, H 5.07, N 9.43% (Aydoğan, 1993).

Crystal data

$C_{18}H_{15}ClN_2$
$M_r = 294.77$
Triclinic, $P\bar{1}$
$a = 7.4962$ (7) Å
$b = 9.5511$ (9) Å
$c = 11.4013$ (11) Å
$\alpha = 79.039$ (2)°
$\beta = 76.866$ (2)°
$\gamma = 76.886$ (2)°
$V = 765.90$ (13) Å^3
$Z = 2$
$D_x = 1.278$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1530 reflections
$\theta = 2.8$–27.5°
$\mu = 0.24$ mm^{-1}
$T = 293$ (2) K
Needle, light yellow
0.34 × 0.22 × 0.10 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.922$, $T_{\max} = 0.976$
4930 measured reflections
3363 independent reflections
1573 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.040$
$\theta_{\max} = 27.5°$
$h = -8 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -12 \rightarrow 14$
Intensity decay: <2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.071$
$wR(F^2) = 0.217$
$S = 0.98$
3363 reflections
193 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0995P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.006$
$\Delta\rho_{\max} = 0.24$ e Å^{-3}
$\Delta\rho_{\min} = -0.29$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.012 (6)

Table 1
Selected geometric parameters (Å, °).

Cl1—C18	1.738 (4)	C2—C3	1.355 (5)
N1—C1	1.321 (4)	C3—C10	1.505 (5)
N1—C9	1.361 (4)	C6—C11	1.512 (5)
N2—C12	1.260 (4)	C7—C8	1.357 (5)
N2—C13	1.413 (4)	C13—C14	1.382 (5)
C1—C2	1.416 (5)	C13—C18	1.389 (5)
C1—C12	1.466 (5)		
C1—N1—C9	117.8 (3)	C7—C6—C11	120.3 (4)
C12—N2—C13	119.0 (3)	N1—C9—C8	118.4 (3)
N1—C1—C2	122.5 (3)	N1—C9—C4	122.7 (3)
N1—C1—C12	115.9 (3)	N2—C12—C1	122.5 (3)
C2—C1—C12	121.6 (3)	C14—C13—C18	117.6 (4)
C2—C3—C10	120.7 (3)	C14—C13—N2	122.9 (3)
C4—C3—C10	121.7 (3)	C18—C13—N2	119.5 (3)
C5—C4—C3	124.0 (3)	C17—C18—Cl1	119.1 (3)
C5—C6—C11	121.2 (4)	C13—C18—Cl1	119.0 (3)
C1—C2—C3—C10	−179.1 (3)	C2—C1—C12—N2	9.5 (5)
C4—C5—C6—C11	178.6 (3)	C12—N2—C13—C14	54.7 (5)
C13—N2—C12—C1	−178.9 (3)	C12—N2—C13—C18	−129.3 (4)
N1—C1—C12—N2	−169.1 (3)	N2—C13—C18—Cl1	4.1 (4)

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, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976).

References

Akkurt, M., Öztürk, S., Aygün, M. & Yolaçan, Ç. (2001). *Acta Cryst.* E**57**, o454–o455.
Aydoğan, F. (1993). MSc Thesis, Yıldız Technical University, İstanbul, Turkey.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Kouznetsov, V., Öcal, N., Turgut, Z., Zubkov, F., Kaban, Ş. & Varlamov, A. V. (1998). *Monatsh. Chem.* **129**, 671–675.
Öcal, N. & Kaban, Ş. (1998). *Indian J. Chem.* **37**, 1051–1056.
Öztürk, S., Aygün, M., Öcal, N., Yolaçan, Ç. & Fun, H. K. (2000). *Z. Kristallogr. New Cryst. Struct.* **215**, 526–528.

Öztürk, S., Aygün, M., Öcal, N., Yolaçan, Ç. & Fun, H. K. (2001). *Anal. Sci.* **17**, 797–780.

Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467– 473.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. Release 97–2. University of Göttingen, Germany.

Siemens (1996). *SMART* and *SAINT* (Version 4). Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Sommes, P. G. (1976). *Chem. Rev.* **76**, 113–117.