organic papers

2,6-Dimethylquinolin-4(1*H*)-one

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The structure of 2,6-dimethylquinolin-4(1*H*)-one, $C_{11}H_{11}NO$, has been determined as part of our study on the synthesis and crystallography of quinoline and quinazoline derivatives. It crystallizes in the monoclinic space group $P2_1/c$. The molecule is planar, with the dihedral angle between the planes of the two rings being 2 (1)°.

Comment

Compounds containing a quinoline moiety are of considerable interest due to their biological properties (Zacharias & Glusker, 1988; Hua & Chen, 1997; Newell *et al.*, 1998); these include high antibacterial, antiarrhythmic and anti-hypertensive activities (Yates, 1984; Jones, 1977). The crystal structures of related compounds have been reported previously (Rajnikant *et al.*, 2000, 2001; Rajnikant, Gupta, Suri & Lal, 2002; Rajnikant, Gupta, Deshmukh & Varghese, 2002).

(I)
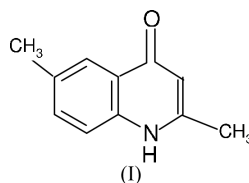
Bond distances and angles in the quinoline ring system of the title compound, (I), are normal (Sudha, Subramanian, Sivaraman, Ramakrishnan *et al.*, 1995; Sudha, Subramanian, Sivaraman, Sriraghavan & Steiner, 1995; Sudha *et al.*, 1997; Rajnikant, Gupta, Deshmukh & Varghese, 2002). The double-bond character of C4=O1 is confirmed by its length [1.262 (2) Å]. The angle between the planes of the two rings is 2 (1)°, confirming that the molecule is planar. There is a strong intermolecular hydrogen bond N1—H1···O1[i], with H···*A* = 1.89 Å, *D*—H···*A* = 174° and D···*A* = 2.743 (1) Å [symmetry code: (i) $x, \frac{1}{2} - y, z + \frac{1}{2}$].
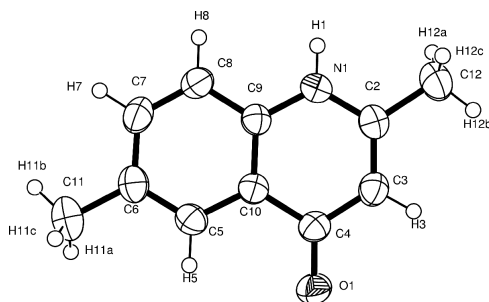

Figure 1
An view of the title molecule, with displacement ellipsoids drawn at the 50% probability level.

Experimental

A mixture of *p*-toluidine (0.01 mol) and ethyl acetoacetate (0.01 mol) in ethanol (20 ml) was stirred for 2–3 h and allowed to stand for 36 h. The mixture was then concentrated, giving a viscous oily liquid which was vacuum distilled to afford 2-(*p*-methylbenzylidene)ethyl butyrate in 60% yield. This latter compound (0.1 mol) and H_2SO_4 (75 ml) were heated on an oil bath at 323 K for 0.5 h, at 373 K for a further 3 h, cooled and poured on to crushed ice, giving the title compound (yield 50%), which was then recrystallized from ethanol.

Crystal data

$C_{11}H_{11}NO$	$D_x = 1.243$ Mg m^{-3}
$M_r = 173.21$	Mo Kα radiation
Monoclinic, $P2_1/c$	Cell parameters from 25
$a = 9.068\ (7)$ Å	reflections
$b = 8.352\ (3)$ Å	$\theta = 6.2–11.5°$
$c = 12.253\ (5)$ Å	$\mu = 0.08$ mm^{-1}
$\beta = 94.15\ (4)°$	$T = 293\ (2)$ K
$V = 925.6\ (9)$ Å^3	Plate, yellow
$Z = 4$	$0.4 \times 0.3 \times 0.1$ mm

Data collection

Enraf–Nonius CAD-4 diffractometer	$\theta_{max} = 25.0°$
$\omega/2\theta$ scans	$h = 0 \rightarrow 10$
Absorption correction: none	$k = 0 \rightarrow 9$
1737 measured reflections	$l = -14 \rightarrow 14$
1629 independent reflections	2 standard reflections
1306 reflections with $I > 2\sigma(I)$	frequency: 60 min
$R_{int} = 0.009$	intensity decay: <2%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0684P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.043$	$+ 0.2584P]$
$wR(F^2) = 0.135$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} < 0.001$
1629 reflections	$\Delta\rho_{max} = 0.24$ e Å^{-3}
121 parameters	$\Delta\rho_{min} = -0.15$ e Å^{-3}
H-atom parameters constrained	Extinction correction: *SHELXL*97
	Extinction coefficient: 0.020 (5)

Table 1
Selected geometric parameters (Å, °).

O1—C4	1.2618 (19)	C5—C6	1.371 (2)
N1—C2	1.351 (2)	C5—C10	1.406 (2)
N1—C9	1.379 (2)	C6—C7	1.405 (3)
C2—C3	1.366 (2)	C6—C11	1.505 (3)
C2—C12	1.502 (3)	C7—C8	1.366 (3)
C3—C4	1.418 (2)	C8—C9	1.406 (2)
C4—C10	1.461 (2)	C9—C10	1.400 (2)
C2—N1—C9	121.81 (14)	C5—C6—C11	121.09 (17)
N1—C2—C3	120.48 (15)	C7—C6—C11	121.36 (17)
N1—C2—C12	116.38 (16)	C8—C7—C6	122.37 (16)
C3—C2—C12	123.13 (17)	C7—C8—C9	119.38 (16)
C2—C3—C4	122.37 (16)	N1—C9—C10	119.86 (14)
O1—C4—C3	122.82 (15)	N1—C9—C8	120.34 (15)
O1—C4—C10	121.44 (15)	C10—C9—C8	119.80 (15)
C3—C4—C10	115.74 (15)	C9—C10—C5	118.58 (15)
C6—C5—C10	122.28 (16)	C9—C10—C4	119.69 (15)
C5—C6—C7	117.55 (16)	C5—C10—C4	121.73 (15)

All H atoms were included in the final cycles of refinement; they were constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}$(parent), where $x = 1.5$ for methyl and 1.2 for all others. The constrained distances were N—H = 0.86 Å, C—H = 0.96 Å for methyl H and 0.93 Å for all other C—H H atoms.
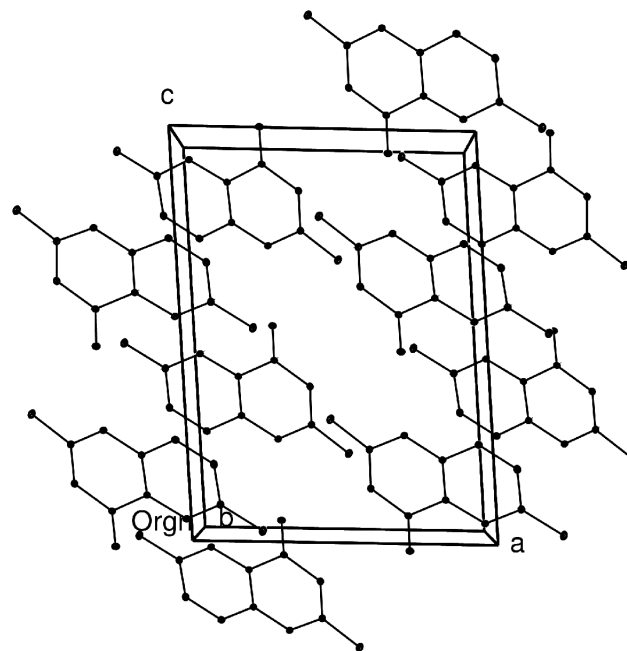

Figure 2
A packing diagram, viewed down the *b* axis.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *CAD-4 Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *PARST*95 (Nardelli, 1995).

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