Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,4-Diacetylquinoline

Ray J. Butcher,[a] Jerry P. Jasinski,[b]* B. Narayana,[c] Anil. N. Mayekar[d] and H. S. Yathirajan[d]

[a]Department of Chemistry, Howard University, 525 College Street NW, Washington, DC 20059, USA, [b]Department of Chemistry, Keene State College, 229 Main Street, Keene, NH 03435-2001, USA, [c]Department of Studies in Chemistry, Mangalore University, Mangalagangotri 574 199, India, and [d]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India
Correspondence e-mail: jjasinski@keene.edu

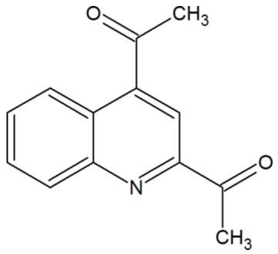
Received 13 July 2007; accepted 16 July 2007

Key indicators: single-crystal X-ray study; T = 203 K; mean σ(C–C) = 0.002 Å; R factor = 0.049; wR factor = 0.114; data-to-parameter ratio = 24.0.

In the title molecule, $C_{13}H_{11}NO_2$, one of the acetyl groups is coplanar with the quinoline ring system, whereas the other is slightly twisted from it. Intermolecular C—H⋯O hydrogen bonding between methyl H atoms and both of the acetyl O atoms links the molecules into a ribbon. The crystal packing is further stabilized by π–π stacking interactions between the pyridine rings of inversion-related molecules, with the ring centroids separated by 3.5246 (9) Å.

Related literature

For related structures, see: Lynch & McClenaghan (2001); Firley *et al.* (2005); Yathirajan *et al.* (2007). For related literature, see: Robert & Meunier (1998); Padwa *et al.* (1999); Franck *et al.* (2004).



Experimental

Crystal data

$C_{13}H_{11}NO_2$
M_r = 213.23
Monoclinic, $P2_1/n$
a = 7.5285 (6) Å
b = 15.0366 (12) Å
c = 9.7202 (7) Å
β = 105.704 (9)°
V = 1059.28 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 203 K
0.57 × 0.43 × 0.41 mm

Data collection

Oxford Diffraction Gemini R diffractometer
Absorption correction: none
9975 measured reflections
3533 independent reflections
1078 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.058

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.114
S = 0.75
3533 reflections
147 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max}$ = 0.29 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.20 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C13—H13A⋯O1$^{\rm i}$	0.97	2.57	3.531 (2)	173
C13—H13B⋯O2$^{\rm ii}$	0.97	2.51	3.392 (2)	151

Symmetry codes: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

ANM thanks Sequent Scientific Ltd, Mangalore, India, for the gift of a sample of the title compound. RJB acknowledges the NSF MRI program (grant No. CHE-0619278) for funds to purchase the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2417).

References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Firley, D., Fraisse, B., Zouhiri, F., Spasojević-de Biré, A., Desmaële, D., d'Angelo, J. & Ghermani, N. E. (2005). *Acta Cryst.* C**61**, o154–o157.
Franck, X., Fournet, A., Prina, E., Mahieuxe, R., Hocquemiller, R. & Fiqadere, B. (2004). *Bioorg. Med. Chem. Lett.* **14**, 3635–3638.
Lynch, D. E. & McClenaghan, I. (2001). *Acta Cryst.* E**57**, o54–o55.
Oxford Diffraction (2007). *CrysAlisPro*. Version 171.31.8. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Padwa, A., Brodney, M. A., Liu, B., Satake, K. & Wu, T. (1999). *J. Org. Chem.* **64**, 3595–3607.
Robert, A. & Meunier, B. (1998). *Chem. Soc. Rev.* **27**, 273–279.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Yathirajan, H. S., Sreevidya, T. V., Prathap, M., Narayana, B. & Bolte, M. (2007). *Acta Cryst.* E**63**, o763–o765.

doi:10.1107/S1600536807034769

supplementary materials

Acta Cryst. (2007). E**63**, o3557 [**doi:10.1107/S1600536807034769**]

2,4-Diacetylquinoline

R. J. Butcher, J. P. Jasinski, B. Narayana, A. N. Mayekar and **H. S. Yathirajan**

Comment

Quinolines have been interesting to researchers for many years because a large number of natural products contain these heterocycles. They are found in numerous commercial products, including pharmaceuticals, fragrances and dyes. Quinoline alkaloids such as quinine, chloroquin, mefloquine and amodiaquine are used as efficient drugs for the treatment of malaria. Several quinoline derivatives have been evaluated *in vitro* against several parasites and HTLV-1 transformed cells. Prompted by the varied biological activities, the crystal structure of the title compound is reported (Fig. 1).

One acetyl group is coplanar with the quinoline ring system, with a N—C1—C10—O1 torsion angle of −178.24 (14) Å, while the second is slightly twisted out of the plane, with a C2—C3—C12—C13 torsion angle of −20.9 (2)°.

Intermolecular C—H···O hydrogen bonding interactions involving the H13A and H13B methyl hydrogen atoms and acetyl oxygen atoms O1 and O2 link the molecules into a ribbon (Fig. 2). In addition, the crystal structure is stabilized by π-π stacking interactions between the pyridine rings of the inversion-related molecules at (x, y, z) and ($-x$, $-y$, $-z$), with the ring centroids separated by 3.5246 (9) Å.

Experimental

The title compound was obtained as a gift sample from Sequent Scientific Ltd, Mangalore, India. The sample was crystallized from methanol (m.p. 341–343 K).

Refinement

The H atoms were included in the riding model approximation with C—H = 0.94 or 0.97 Å, and with $U_{\rm iso}$(H) = 1.18–1.49$U_{\rm eq}$(C). Owing to the poor diffraction quality of the crystal, the ratio of observed to unique reflections is low (31%).

Figures

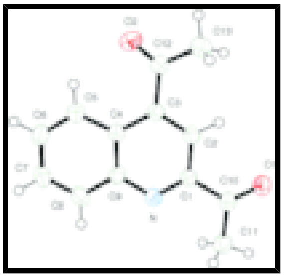


Fig. 1. Molecular structure of the title compound, showing atom labelling and 50% probability displacement ellipsoids.

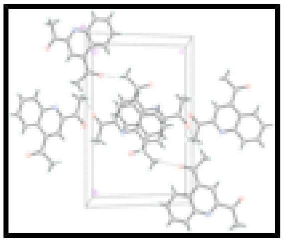


Fig. 2. Part of the crystal structure of the title compound, showing the formation of C—H···O hydrogen-bonded (dashed lines) ribbons.

2,4-Diacetylquinoline

Crystal data

$C_{13}H_{11}NO_2$

$M_r = 213.23$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 7.5285$ (6) Å

$b = 15.0366$ (12) Å

$c = 9.7202$ (7) Å

$\beta = 105.704$ (9)°

$V = 1059.28$ (14) Å^3

$Z = 4$

$F_{000} = 448$

$D_x = 1.337$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 1840 reflections

$\theta = 4.6$–32.5°

$\mu = 0.09$ mm^{-1}

$T = 203$ K

Prism, pale yellow

0.57 × 0.43 × 0.41 mm

Data collection

Oxford Diffraction Gemini R diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 203$ K

φ and ω scans

Absorption correction: none

9975 measured reflections

3533 independent reflections

1078 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.058$

$\theta_{\rm max} = 32.6$°

$\theta_{\rm min} = 4.6$°

$h = -11\rightarrow11$

$k = -22\rightarrow19$

$l = -14\rightarrow14$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.049$

$wR(F^2) = 0.114$

$S = 0.75$

3533 reflections

147 parameters

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0508P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\rm max} = 0.001$

$\Delta\rho_{\rm max} = 0.29$ e Å^{-3}

$\Delta\rho_{\rm min} = -0.19$ e Å^{-3}

Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\mathrm{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.19345 (15)	0.03032 (8)	−0.46646 (11)	0.0490 (3)
O2	0.25235 (18)	0.21491 (9)	0.09646 (12)	0.0755 (5)
N	0.09472 (16)	−0.07751 (9)	−0.17029 (12)	0.0350 (3)
C1	0.0180 (2)	−0.00917 (10)	−0.24815 (15)	0.0327 (4)
C2	0.05337 (19)	0.07988 (11)	−0.20552 (15)	0.0337 (4)
H2	−0.0049	0.1260	−0.2664	0.040*
C3	0.17264 (19)	0.09967 (10)	−0.07536 (15)	0.0322 (4)
C4	0.26019 (19)	0.02745 (11)	0.01274 (15)	0.0313 (4)
C5	0.3888 (2)	0.03630 (11)	0.14916 (16)	0.0384 (4)
H5	0.4245	0.0934	0.1858	0.046*
C6	0.4609 (2)	−0.03655 (12)	0.22760 (17)	0.0432 (4)
H6	0.5448	−0.0290	0.3180	0.052*
C7	0.4124 (2)	−0.12220 (12)	0.17607 (17)	0.0444 (5)
H7	0.4613	−0.1718	0.2324	0.053*
C8	0.2942 (2)	−0.13380 (11)	0.04399 (17)	0.0408 (4)
H8	0.2644	−0.1916	0.0085	0.049*
C9	0.21614 (19)	−0.06001 (10)	−0.03993 (15)	0.0327 (4)
C10	−0.1207 (2)	−0.02998 (11)	−0.38780 (16)	0.0375 (4)
C11	−0.1623 (2)	−0.12551 (11)	−0.42487 (18)	0.0516 (5)
H11A	−0.2681	−0.1296	−0.5079	0.077*
H11B	−0.1896	−0.1557	−0.3448	0.077*
H11C	−0.0564	−0.1532	−0.4460	0.077*
C12	0.1988 (2)	0.19507 (11)	−0.02893 (17)	0.0424 (4)
C13	0.1504 (2)	0.26635 (12)	−0.13877 (18)	0.0595 (5)
H13A	0.1814	0.3238	−0.0933	0.089*
H13B	0.0192	0.2642	−0.1856	0.089*
H13C	0.2190	0.2576	−0.2090	0.089*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

O1	0.0586 (8)	0.0419 (8)	0.0376 (7)	0.0030 (6)	−0.0023 (6)	0.0038 (6)
O2	0.1174 (11)	0.0434 (9)	0.0470 (8)	0.0042 (8)	−0.0099 (7)	−0.0099 (7)
N	0.0388 (7)	0.0316 (8)	0.0335 (7)	−0.0013 (6)	0.0077 (6)	0.0007 (6)
C1	0.0387 (9)	0.0292 (9)	0.0292 (9)	−0.0001 (7)	0.0075 (7)	0.0021 (7)
C2	0.0374 (9)	0.0323 (9)	0.0308 (9)	0.0025 (7)	0.0084 (7)	0.0042 (7)
C3	0.0362 (9)	0.0290 (9)	0.0308 (9)	−0.0004 (7)	0.0081 (7)	0.0002 (8)
C4	0.0308 (8)	0.0328 (10)	0.0298 (8)	0.0004 (7)	0.0074 (7)	0.0007 (7)
C5	0.0380 (9)	0.0378 (11)	0.0364 (9)	0.0029 (8)	0.0048 (7)	−0.0012 (8)
C6	0.0391 (9)	0.0534 (13)	0.0324 (9)	0.0031 (9)	0.0015 (7)	0.0007 (9)
C7	0.0452 (10)	0.0426 (12)	0.0414 (10)	0.0091 (8)	0.0048 (8)	0.0102 (9)
C8	0.0447 (10)	0.0316 (10)	0.0443 (10)	0.0047 (8)	0.0087 (8)	0.0061 (8)
C9	0.0329 (8)	0.0339 (10)	0.0303 (8)	−0.0012 (7)	0.0071 (7)	0.0024 (8)
C10	0.0420 (9)	0.0369 (10)	0.0315 (9)	0.0013 (8)	0.0062 (7)	0.0015 (8)
C11	0.0627 (11)	0.0378 (11)	0.0434 (10)	−0.0064 (9)	−0.0041 (9)	−0.0031 (9)
C12	0.0435 (10)	0.0356 (11)	0.0415 (10)	0.0010 (8)	0.0002 (8)	−0.0023 (9)
C13	0.0752 (13)	0.0351 (11)	0.0554 (11)	−0.0019 (10)	−0.0045 (10)	0.0005 (9)

Geometric parameters (Å, °)

O1—C10	1.2164 (17)	C6—C7	1.394 (2)
O2—C12	1.2128 (17)	C6—H6	0.94
N—C1	1.3137 (18)	C7—C8	1.361 (2)
N—C9	1.3723 (17)	C7—H7	0.94
C1—C2	1.406 (2)	C8—C9	1.408 (2)
C1—C10	1.505 (2)	C8—H8	0.94
C2—C3	1.3713 (19)	C10—C11	1.493 (2)
C2—H2	0.94	C11—H11A	0.97
C3—C4	1.429 (2)	C11—H11B	0.97
C3—C12	1.501 (2)	C11—H11C	0.97
C4—C9	1.418 (2)	C12—C13	1.487 (2)
C4—C5	1.4206 (19)	C13—H13A	0.97
C5—C6	1.361 (2)	C13—H13B	0.97
C5—H5	0.94	C13—H13C	0.97
C1—N—C9	117.46 (13)	C7—C8—H8	119.7
N—C1—C2	123.82 (13)	C9—C8—H8	119.7
N—C1—C10	116.53 (14)	N—C9—C8	116.95 (14)
C2—C1—C10	119.60 (13)	N—C9—C4	122.92 (13)
C3—C2—C1	120.21 (14)	C8—C9—C4	120.10 (13)
C3—C2—H2	119.9	O1—C10—C11	122.41 (14)
C1—C2—H2	119.9	O1—C10—C1	119.76 (15)
C2—C3—C4	117.95 (14)	C11—C10—C1	117.82 (14)
C2—C3—C12	118.99 (13)	C10—C11—H11A	109.5
C4—C3—C12	122.99 (13)	C10—C11—H11B	109.5
C9—C4—C5	117.24 (14)	H11A—C11—H11B	109.5
C9—C4—C3	117.63 (13)	C10—C11—H11C	109.5
C5—C4—C3	125.13 (15)	H11A—C11—H11C	109.5
C6—C5—C4	121.02 (16)	H11B—C11—H11C	109.5
C6—C5—H5	119.5	O2—C12—C13	119.64 (16)
C4—C5—H5	119.5	O2—C12—C3	121.21 (15)

C5—C6—C7	121.08 (15)	C13—C12—C3	119.10 (13)
C5—C6—H6	119.5	C12—C13—H13A	109.5
C7—C6—H6	119.5	C12—C13—H13B	109.5
C8—C7—C6	119.87 (16)	H13A—C13—H13B	109.5
C8—C7—H7	120.1	C12—C13—H13C	109.5
C6—C7—H7	120.1	H13A—C13—H13C	109.5
C7—C8—C9	120.63 (16)	H13B—C13—H13C	109.5

C9—N—C1—C2	0.0 (2)	C1—N—C9—C4	0.2 (2)
C9—N—C1—C10	−177.46 (12)	C7—C8—C9—N	−178.39 (14)
N—C1—C2—C3	−0.6 (2)	C7—C8—C9—C4	0.0 (2)
C10—C1—C2—C3	176.78 (13)	C5—C4—C9—N	−179.72 (12)
C1—C2—C3—C4	0.9 (2)	C3—C4—C9—N	0.1 (2)
C1—C2—C3—C12	−176.29 (14)	C5—C4—C9—C8	2.0 (2)
C2—C3—C4—C9	−0.7 (2)	C3—C4—C9—C8	−178.20 (13)
C12—C3—C4—C9	176.44 (13)	N—C1—C10—O1	−178.24 (14)
C2—C3—C4—C5	179.12 (13)	C2—C1—C10—O1	4.2 (2)
C12—C3—C4—C5	−3.8 (2)	N—C1—C10—C11	1.2 (2)
C9—C4—C5—C6	−2.3 (2)	C2—C1—C10—C11	−176.43 (15)
C3—C4—C5—C6	177.91 (15)	C2—C3—C12—O2	156.46 (15)
C4—C5—C6—C7	0.6 (2)	C4—C3—C12—O2	−20.6 (2)
C5—C6—C7—C8	1.5 (3)	C2—C3—C12—C13	−20.9 (2)
C6—C7—C8—C9	−1.7 (2)	C4—C3—C12—C13	162.01 (14)
C1—N—C9—C8	178.57 (13)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C13—H13A···O1^{i}	0.97	2.57	3.531 (2)	173
C13—H13B···O2^{ii}	0.97	2.51	3.392 (2)	151

Symmetry codes: (i) *x*+1/2, −*y*+1/2, *z*+1/2; (ii) *x*−1/2, −*y*+1/2, *z*−1/2.

Fig. 1

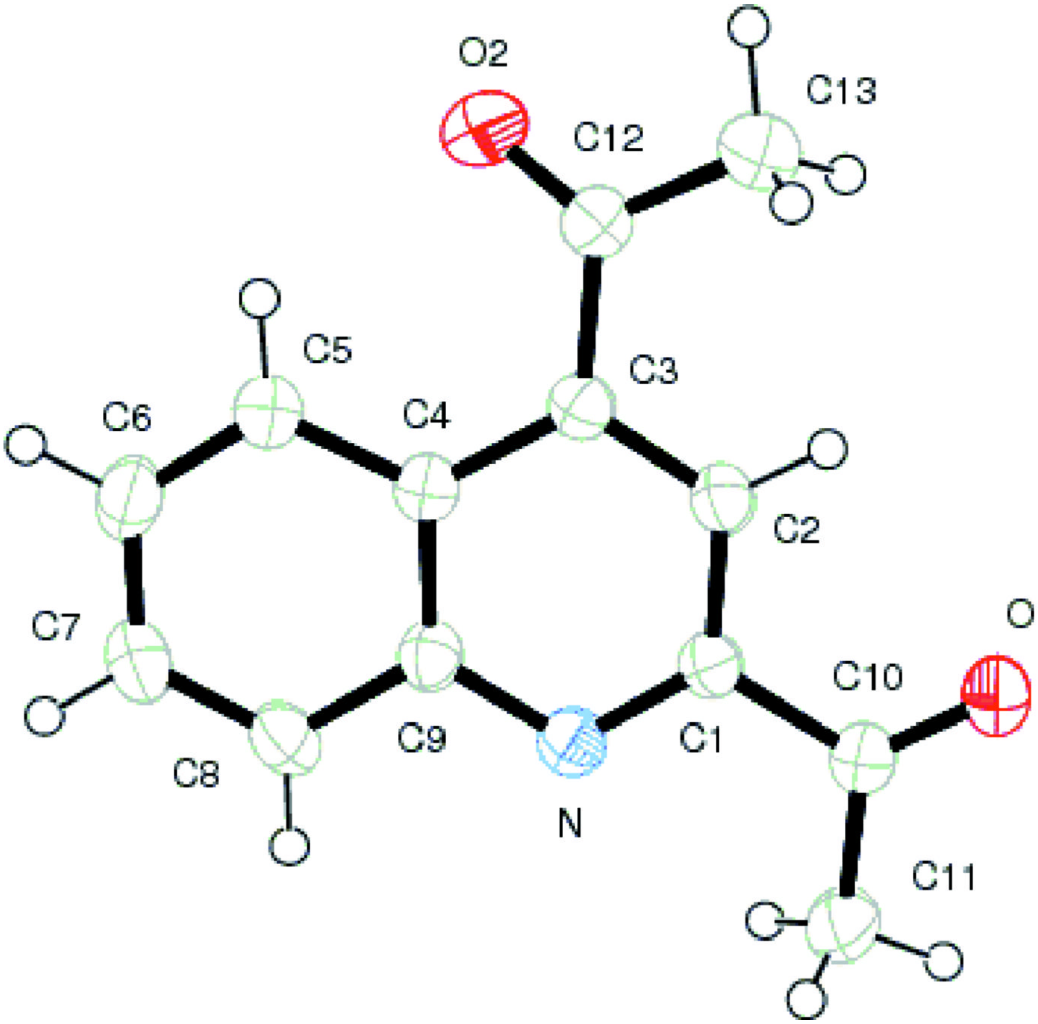


Fig. 2