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2-Formylquinolin-8-yl acetate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.134
Data-to-parameter ratio = 15.7

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

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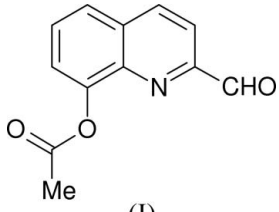
In the crystal structure of the title compound, $C_{12}H_9NO_3$, the molecules are linked through weak intermolecular C—H···O hydrogen bonds, forming a two-dimensional network.

Comment

The title compound, (I), is a derivative of 2-pyridaldehyde, which readily forms Schiff base compounds by condensation with amines.



(I)

In (I), all the bond lengths are within normal ranges (Allen *et al.*, 1987). The dihedral angle between the plane of atoms O2/C11/O3 and the quinoline ring system is 82.9 (2)° (Fig. 1). The conformation of the acetoxy group is described by the torsion angle of −169.42 (17)° for C9—O2—C11—C12.

In the crystal structure, molecules are linked *via* weak intermolecular C—H···O hydrogen bonds to form a two-dimensional sheet perpendicular to the *c* axis (Table 1).

Experimental

One drop of concentrated sulfuric acid was added to a mixture of 2-methyl-8-hydroxyquinoline (15.9 g, 0.1 mol) and acetic anhydride (10.2 g, 9.4 ml, 0.1 mol) in a 250 ml Erlenmeyer flask. The mixture was warmed rapidly and stirred gently by hand. After 5 min, the clear solution was poured on to crushed ice (about 200 ml). The solid was

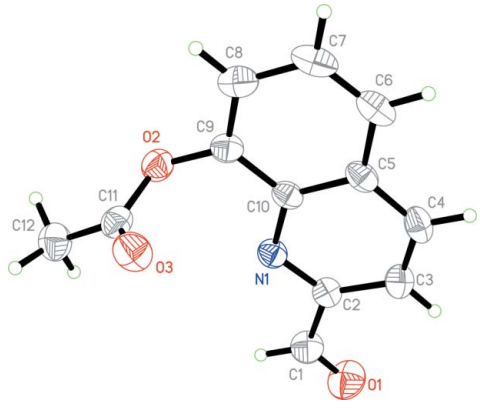


Figure 1
The structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

filtered off and washed with water (200 ml). The compound obtained was 2-methyl-8-acetoxyquinoline (18.6 g, 93%; m.p. 394–395 K). To a dioxane supension (40 ml) of freshly sublimed selenium dioxide (5.8 g), a dioxane solution (50 ml) of 2-methyl-8-acetoxyquinoline (11.4 g) was added with stirring over a water bath at 323–328 K for 3 h. The mixture was filtered after being allowed to stand for 2 h. The dioxane was distilled off to give light-yellow crystals of (I) (9.0 g; m.p. 367–368 K).

Crystal data

$C_{12}H_9NO_3$
M_r = 215.20
Monoclinic, $C2/c$
a = 19.743 (3) Å
b = 7.863 (1) Å
c = 14.771 (2) Å
β = 111.66 (2)°
V = 2131.1 (6) Å^3
Z = 8
D_x = 1.341 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3212 reflections
θ = 2.3–24.9°
μ = 0.10 mm^{-1}
T = 298 (2) K
Block, light-yellow
0.53 × 0.46 × 0.41 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.950, T_{max} = 0.961
6309 measured reflections
2315 independent reflections
1225 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 27.0°
$h = -24 \rightarrow 25$
$k = -8 \rightarrow 10$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.134
S = 1.00
2315 reflections
147 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 0.2105P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997*a*)
Extinction coefficient: 0.0073 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O1^{i}	0.93	2.57	3.486 (3)	168
C12—H12C···O1^{ii}	0.96	2.59	3.447 (3)	149

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

H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.96 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl}).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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