

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

2-Methoxyquinoline-3-carbaldehyde

K. Chandraprakash,^a P. Ramesh,^b K. Ravichandran,^b
P. S. Mohan^a and M. N. Ponnuswamy^{b*}

^aDepartment of Chemistry, School of Chemical Sciences, Bharathiar University, Coimbatore 641 046, India, and ^bCentre of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India
Correspondence e-mail: mnpsy2004@yahoo.com

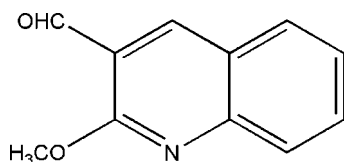
Received 18 August 2010; accepted 28 August 2010

Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.044; wR factor = 0.130; data-to-parameter ratio = 18.0.

In the title compound, $\text{C}_{11}\text{H}_9\text{NO}_2$, the quinoline ring system is essentially planar (r.m.s. deviation = 0.005 Å) and the methoxy and aldehyde groups are almost coplanar with it [$\text{N}-\text{C}-\text{O}-\text{C} = 6.24$ (19) and $\text{O}-\text{C}-\text{C}-\text{C} = 0.3$ (2)°]. In the crystal, molecules are linked by pairs of $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds, forming centrosymmetric $R_2^2(10)$ dimers. The dimers are linked via $\pi-\pi$ interactions involving the pyridine and benzene rings [centroid-centroid distance = 3.639 (1) Å].

Related literature

For general background to quinoline derivatives, see: Mali *et al.* (2010); Kuethe *et al.* (2003). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$\text{C}_{11}\text{H}_9\text{NO}_2$
 $M_r = 187.19$
Monoclinic, $P2_1/c$

$a = 8.8206$ (6) Å
 $b = 4.8446$ (3) Å
 $c = 21.6828$ (14) Å

$\beta = 90.612$ (4)°
 $V = 926.50$ (10) Å³
 $Z = 4$
Mo $K\alpha$ radiation

$\mu = 0.09$ mm⁻¹
 $T = 293$ K
 $0.20 \times 0.20 \times 0.18$ mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2008)
 $T_{\min} = 0.981$, $T_{\max} = 0.983$

8812 measured reflections
2305 independent reflections
1658 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.130$
 $S = 1.05$
2305 reflections

128 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.16$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.19$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C4}-\text{H4}\cdots\text{O2}^i$	0.93	2.56	3.4157 (16)	152

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2009).

The authors thank TBI consultancy, University of Madras, India, for the data collection

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5162).

References

- Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2008). APEX2, SAINT and SADABS. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Kuethe, J. T., Wong, A. & Davies, I. W. (2003). *Org. Lett.* **5**, 3975–3978.
Mali, J. R., Bhosle, M. R., Mahalle, S. R. & Mane, R. A. (2010). *Bull. Korean Chem. Soc.* **31**, 1859–1863.
Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

supporting information

Acta Cryst. (2010). E66, o2510 [doi:10.1107/S1600536810034744]

2-Methoxyquinoline-3-carbaldehyde

K. Chandraprakash, P. Ramesh, K. Ravichandran, P. S. Mohan and M. N. Ponnuswamy

S1. Comment

Quinolines have gained importance in medicinal and natural product chemistry due to their interesting biological and pharmacological activities. They possess anti-malarial, anti-tuberculosis, anti-inflammatory and anti-cancer properties (Mali *et al.*, 2010). Methoxy substituted quinolines are used as synthetic intermediates in the construction of novel class of KDR kinase inhibitors (Kuethe *et al.*, 2003). Against this background and to ascertain the structure of title compound, the crystallographic studies have been carried out.

In the title molecule (Fig.1), the quinoline ring system (N1/C2–C10) is essentially planar with a maximum deviation of 0.007 (1) Å for atom C3. The methoxy and carbaldehyde groups are almost coplanar with the quinoline ring system, which is evidenced from torsion angles C3—C2—O1—C11 and C2—C3—C12—O2 of 173.6 (1)° and 178.5 (2)°, respectively.

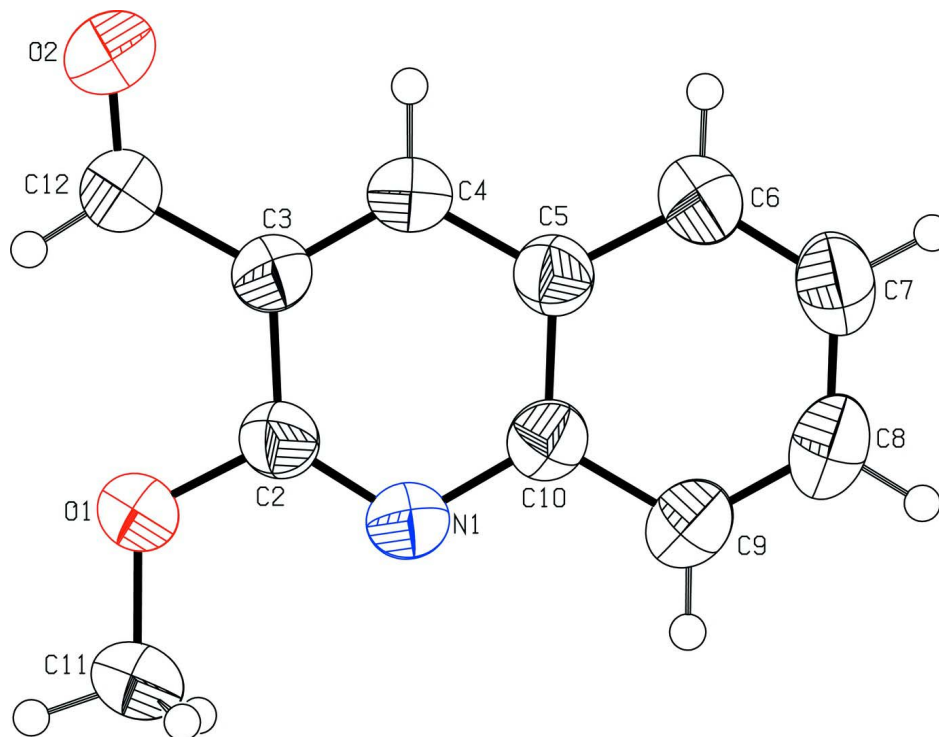
The packing of the molecules in the crystal is stabilized by C—H···O, and π – π types of intermolecular interactions. The molecules at (x, y, z) and (1-x, 1-y, 1-z) are linked by a pair of intermolecular C4—H4···O2 hydrogen bonds to form a centrosymmetric dimer containing $R_2^2(10)$ ring motif (Fig. 2) (Bernstein *et al.*, 1995). The π – π interaction between the pyridine ring (N1/C2–C10) of the quinoline ring system at (x, y, z) and the benzene ring (C5—C10) at (x, y-1, z) further stabilize the structure, with a centroid-centroid distance of 3.639 (1) Å.

S2. Experimental

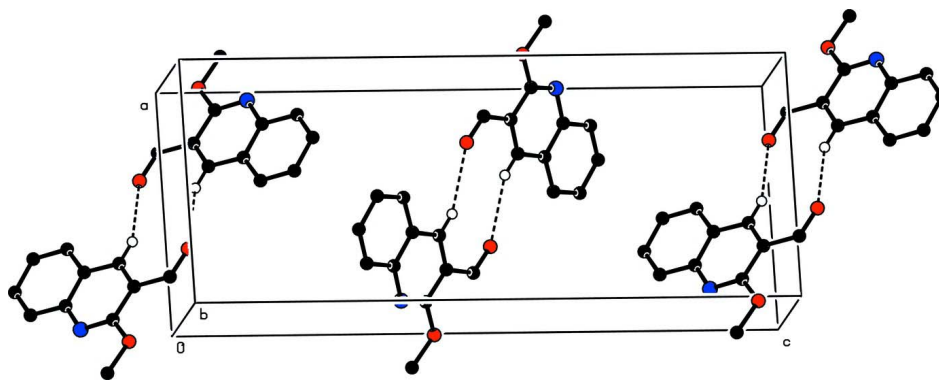
To a solution of 1 g (17.8 mmol) of KOH in 50 ml of MeOH was added 2.5 g (13.1 mmol) of 2-chloro-3-quinoline-carboxaldehyde. The mixture was heated at 373 K for 2.5 h and then cooled to room temperature, and poured into 200 g of crushed ice. The precipitate thus obtained was recuperated by filtration. The obtained product was a colourless solid. The product was purified by recrystallization from petroleum ether-ethyl acetate mixture.

S3. Refinement

H atoms were positioned geometrically (C–H = 0.93–0.96 Å) and allowed to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H and $1.2U_{\text{eq}}(\text{C})$ for other H atoms.

**Figure 1**

The molecular structure of the title compound, showing the atomic numbering and displacement ellipsoids drawn at the 50% probability level.

**Figure 2**

The crystal packing of the title compound. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

2-Methoxyquinoline-3-carbaldehyde

Crystal data

$C_{11}H_9NO_2$

$M_r = 187.19$

Monoclinic, $P2_1/c$

Hall symbol: $-P 2_1/c$

$a = 8.8206 (6) \text{ \AA}$

$b = 4.8446 (3) \text{ \AA}$

$c = 21.6828 (14) \text{ \AA}$

$\beta = 90.612 (4)^\circ$

$V = 926.50 (10) \text{ \AA}^3$

$Z = 4$

$F(000) = 392$

$D_x = 1.342 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 1216 reflections
 $\theta = 1.9\text{--}28.4^\circ$
 $\mu = 0.09 \text{ mm}^{-1}$

$T = 293 \text{ K}$
 Block, colourless
 $0.20 \times 0.20 \times 0.18 \text{ mm}$

Data collection

Bruker SMART APEXII area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 ω and ϕ scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2008)
 $T_{\min} = 0.981$, $T_{\max} = 0.983$

8812 measured reflections
 2305 independent reflections
 1658 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$
 $\theta_{\max} = 28.4^\circ$, $\theta_{\min} = 1.9^\circ$
 $h = -9 \rightarrow 11$
 $k = -6 \rightarrow 6$
 $l = -27 \rightarrow 28$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.044$
 $wR(F^2) = 0.130$
 $S = 1.05$
 2305 reflections
 128 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods

Secondary atom site location: difference Fourier
 map
 Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0622P)^2 + 0.1045P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.16 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.19 \text{ e \AA}^{-3}$

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 $F^2 > \sigma(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	-0.04660 (11)	0.2962 (2)	0.42027 (4)	0.0664 (3)
O2	0.32252 (12)	0.2311 (3)	0.52502 (5)	0.0860 (4)
N1	0.05048 (11)	0.6258 (2)	0.35559 (5)	0.0522 (3)
C2	0.06704 (13)	0.4656 (3)	0.40308 (5)	0.0498 (3)
C3	0.20052 (14)	0.4490 (3)	0.44096 (5)	0.0505 (3)
C4	0.31810 (14)	0.6144 (3)	0.42593 (6)	0.0546 (3)
H4	0.4064	0.6107	0.4497	0.066*
C5	0.30810 (14)	0.7921 (3)	0.37465 (6)	0.0502 (3)
C6	0.42741 (16)	0.9652 (3)	0.35643 (7)	0.0639 (4)
H6	0.5179	0.9658	0.3789	0.077*
C7	0.41177 (18)	1.1312 (3)	0.30644 (7)	0.0682 (4)
H7	0.4913	1.2450	0.2947	0.082*

C8	0.27587 (18)	1.1311 (3)	0.27260 (6)	0.0656 (4)
H8	0.2658	1.2462	0.2385	0.079*
C9	0.15831 (16)	0.9657 (3)	0.28878 (6)	0.0594 (3)
H9	0.0691	0.9678	0.2655	0.071*
C10	0.17083 (14)	0.7915 (2)	0.34040 (5)	0.0476 (3)
C11	-0.17739 (17)	0.2814 (4)	0.38058 (7)	0.0822 (5)
H11A	-0.2189	0.4630	0.3750	0.123*
H11B	-0.2521	0.1638	0.3989	0.123*
H11C	-0.1487	0.2076	0.3413	0.123*
C12	0.21226 (17)	0.2551 (3)	0.49311 (6)	0.0634 (4)
H12	0.1288	0.1449	0.5017	0.076*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0566 (5)	0.0821 (7)	0.0603 (6)	-0.0219 (5)	-0.0105 (4)	0.0149 (5)
O2	0.0747 (7)	0.1034 (9)	0.0792 (7)	-0.0159 (6)	-0.0249 (6)	0.0365 (7)
N1	0.0530 (6)	0.0557 (6)	0.0476 (5)	-0.0036 (5)	-0.0056 (4)	0.0005 (5)
C2	0.0503 (7)	0.0530 (7)	0.0460 (6)	-0.0067 (5)	-0.0017 (5)	-0.0021 (5)
C3	0.0527 (7)	0.0535 (7)	0.0453 (6)	-0.0035 (5)	-0.0034 (5)	0.0014 (5)
C4	0.0504 (7)	0.0603 (8)	0.0529 (7)	-0.0056 (6)	-0.0084 (5)	0.0023 (6)
C5	0.0532 (7)	0.0488 (7)	0.0486 (6)	-0.0042 (5)	0.0001 (5)	-0.0024 (5)
C6	0.0608 (8)	0.0660 (9)	0.0648 (8)	-0.0129 (7)	-0.0002 (6)	0.0044 (7)
C7	0.0759 (9)	0.0609 (8)	0.0679 (9)	-0.0156 (7)	0.0118 (7)	0.0043 (7)
C8	0.0894 (10)	0.0541 (8)	0.0536 (7)	0.0015 (7)	0.0092 (7)	0.0081 (6)
C9	0.0694 (8)	0.0574 (8)	0.0512 (7)	0.0043 (6)	-0.0030 (6)	0.0039 (6)
C10	0.0555 (7)	0.0441 (6)	0.0432 (6)	0.0010 (5)	0.0002 (5)	-0.0039 (5)
C11	0.0647 (9)	0.1064 (13)	0.0750 (10)	-0.0338 (9)	-0.0203 (8)	0.0167 (9)
C12	0.0607 (8)	0.0698 (9)	0.0595 (8)	-0.0115 (7)	-0.0078 (6)	0.0136 (7)

Geometric parameters (Å, °)

O1—C2	1.3510 (15)	C6—C7	1.356 (2)
O1—C11	1.4336 (16)	C6—H6	0.93
O2—C12	1.1932 (16)	C7—C8	1.399 (2)
N1—C2	1.2964 (16)	C7—H7	0.93
N1—C10	1.3736 (16)	C8—C9	1.360 (2)
C2—C3	1.4307 (16)	C8—H8	0.93
C3—C4	1.3534 (17)	C9—C10	1.4050 (18)
C3—C12	1.4728 (18)	C9—H9	0.93
C4—C5	1.4081 (18)	C11—H11A	0.96
C4—H4	0.93	C11—H11B	0.96
C5—C6	1.4055 (18)	C11—H11C	0.96
C5—C10	1.4136 (17)	C12—H12	0.93
C2—O1—C11	117.35 (10)	C8—C7—H7	120.0
C2—N1—C10	117.35 (10)	C9—C8—C7	121.09 (13)
N1—C2—O1	120.34 (10)	C9—C8—H8	119.5

N1—C2—C3	125.09 (11)	C7—C8—H8	119.5
O1—C2—C3	114.57 (11)	C8—C9—C10	120.39 (13)
C4—C3—C2	117.15 (11)	C8—C9—H9	119.8
C4—C3—C12	120.99 (12)	C10—C9—H9	119.8
C2—C3—C12	121.83 (11)	N1—C10—C9	119.18 (12)
C3—C4—C5	120.70 (11)	N1—C10—C5	122.35 (11)
C3—C4—H4	119.7	C9—C10—C5	118.47 (12)
C5—C4—H4	119.7	O1—C11—H11A	109.5
C6—C5—C4	123.08 (12)	O1—C11—H11B	109.5
C6—C5—C10	119.56 (12)	H11A—C11—H11B	109.5
C4—C5—C10	117.36 (11)	O1—C11—H11C	109.5
C7—C6—C5	120.57 (13)	H11A—C11—H11C	109.5
C7—C6—H6	119.7	H11B—C11—H11C	109.5
C5—C6—H6	119.7	O2—C12—C3	123.89 (13)
C6—C7—C8	119.91 (13)	O2—C12—H12	118.1
C6—C7—H7	120.0	C3—C12—H12	118.1
C10—N1—C2—O1	-179.57 (11)	C5—C6—C7—C8	0.1 (2)
C10—N1—C2—C3	0.28 (19)	C6—C7—C8—C9	-0.3 (2)
C11—O1—C2—N1	6.24 (19)	C7—C8—C9—C10	0.4 (2)
C11—O1—C2—C3	-173.63 (13)	C2—N1—C10—C9	179.19 (11)
N1—C2—C3—C4	0.2 (2)	C2—N1—C10—C5	-0.34 (18)
O1—C2—C3—C4	-179.94 (11)	C8—C9—C10—N1	-179.80 (12)
N1—C2—C3—C12	-178.08 (13)	C8—C9—C10—C5	-0.25 (19)
O1—C2—C3—C12	1.78 (18)	C6—C5—C10—N1	179.55 (12)
C2—C3—C4—C5	-0.62 (19)	C4—C5—C10—N1	-0.06 (18)
C12—C3—C4—C5	177.68 (12)	C6—C5—C10—C9	0.02 (18)
C3—C4—C5—C6	-179.05 (13)	C4—C5—C10—C9	-179.60 (11)
C3—C4—C5—C10	0.56 (19)	C4—C3—C12—O2	0.3 (2)
C4—C5—C6—C7	179.67 (14)	C2—C3—C12—O2	178.47 (15)
C10—C5—C6—C7	0.1 (2)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C4—H4...O2 ⁱ	0.93	2.56	3.4157 (16)	152

Symmetry code: (i) $-x+1, -y+1, -z+1$.