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2-Chloro-6-methoxyquinoline-3-carbaldehyde

 R. Subashini,^a F. Nawaz Khan,^a Machhindra Gund,^a
 Venkatesha R. Hathwar^b and Seik Weng Ng^{c*}

^aChemistry Division, School of Science and Humanities, VIT University, Vellore 632 014, Tamil Nadu, India, ^bSolid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore 560 012, Karnataka, India, and ^cDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
 Correspondence e-mail: seikweng@um.edu.my

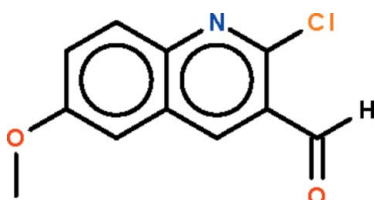
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 Key indicators: single-crystal X-ray study; $T = 290$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.038; wR factor = 0.115; data-to-parameter ratio = 16.2.

The quinoline fused-ring system of the title compound, $\text{C}_{11}\text{H}_8\text{ClNO}_2$, is planar (r.m.s. deviation = 0.0095 Å); the formyl group is slightly bent out of this plane [$\text{C}-\text{C}-\text{C}-\text{O}$ torsion angles = -2.4 (3) and 175.9 (2)°].

Related literature

For a review of the synthesis of quinolines by the Vilsmeier–Haack reaction, see: Meth-Cohn (1993).



Experimental

Crystal data

 $\text{C}_{11}\text{H}_8\text{ClNO}_2$
 $M_r = 221.63$

Monoclinic, $P2_1/c$
 $a = 7.7072$ (9) Å
 $b = 14.3474$ (13) Å
 $c = 9.3487$ (10) Å
 $\beta = 109.415$ (2)°
 $V = 974.98$ (18) Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.37$ mm⁻¹
 $T = 290$ K
 $0.24 \times 0.21 \times 0.18$ mm

Data collection

Bruker SMART area-detector
 diffractometer
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.917$, $T_{\max} = 0.937$

6533 measured reflections
 2221 independent reflections
 1702 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.115$
 $S = 1.03$
 2221 reflections

137 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.21$ e Å⁻³
 $\Delta\rho_{\min} = -0.24$ e Å⁻³

Data collection: SMART (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: publCIF (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5087).

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supporting information

Acta Cryst. (2009). E65, o2723 [https://doi.org/10.1107/S1600536809040847]

2-Chloro-6-methoxyquinoline-3-carbaldehyde

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S1. Experimental

A Vilsmeier-Haack adduct prepared from phosphorus oxytrichloride (6.5 ml, 70 mmol) and *N,N*-dimethylformamide (2.3 ml, 30 mmol) at 273 K was added to *N*-(4-anisyl)acetamide (1.65 g, 10 mmol). The mixture was heated at 353 K for 15 h. The mixture was poured onto ice; the white product was collected and dried. The compound was purified by recrystallization from a petroleum ether/ethyl acetate mixture.

S2. Refinement

H-atoms were placed in calculated positions (C–H 0.93–0.96 Å) and were included in the refinement in the riding model approximation, with $U(\text{H})$ set to 1.2–1.5 $U(\text{C})$.

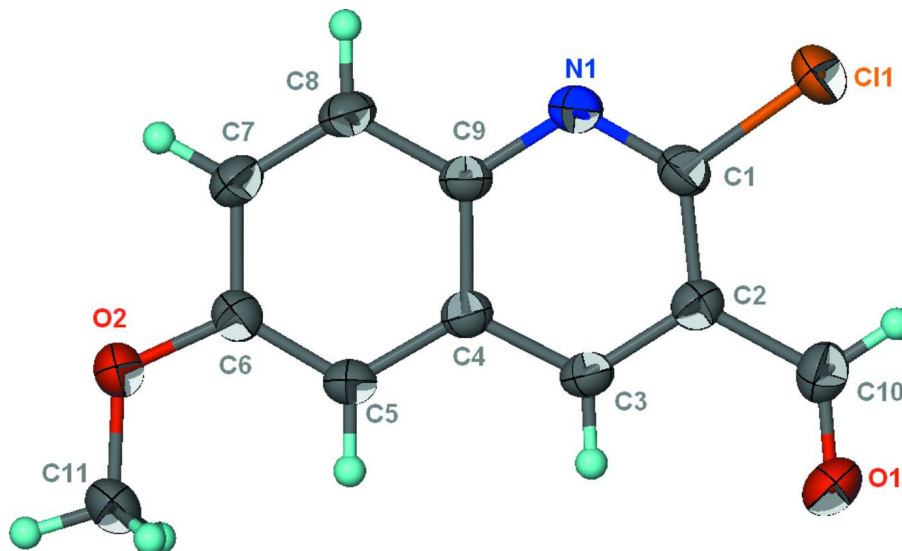


Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of the title compound at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-Chloro-6-methoxyquinoline-3-carbaldehyde

Crystal data

$\text{C}_{11}\text{H}_8\text{ClNO}_2$

$M_r = 221.63$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1bc$

$a = 7.7072(9)\ \text{\AA}$

$b = 14.3474(13)\ \text{\AA}$

$c = 9.3487(10)\ \text{\AA}$

$\beta = 109.415(2)^\circ$

$V = 974.98(18)\ \text{\AA}^3$

$Z = 4$

$F(000) = 456$
 $D_x = 1.510 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 842 reflections
 $\theta = 2.0\text{--}24.7^\circ$

$\mu = 0.37 \text{ mm}^{-1}$
 $T = 290 \text{ K}$
 Block, colorless
 $0.24 \times 0.21 \times 0.18 \text{ mm}$

Data collection

Bruker SMART area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.917$, $T_{\max} = 0.937$

6533 measured reflections
 2221 independent reflections
 1702 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$
 $\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 2.7^\circ$
 $h = -10 \rightarrow 9$
 $k = -18 \rightarrow 10$
 $l = -12 \rightarrow 12$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.115$
 $S = 1.03$
 2221 reflections
 137 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
 $w = 1/[\sigma^2(F_o^2) + (0.068P)^2 + 0.0419P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.24 \text{ e \AA}^{-3}$

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.12213 (7)	0.04921 (3)	0.68956 (6)	0.05816 (19)
O1	0.02629 (18)	0.34429 (9)	0.71932 (16)	0.0563 (4)
O2	0.77125 (17)	0.34949 (8)	0.35759 (14)	0.0480 (3)
N1	0.35512 (19)	0.10458 (9)	0.56310 (15)	0.0399 (3)
C1	0.2333 (2)	0.13533 (11)	0.62026 (18)	0.0386 (4)
C2	0.1913 (2)	0.23022 (11)	0.63341 (17)	0.0365 (4)
C3	0.2892 (2)	0.29435 (11)	0.58240 (18)	0.0366 (3)
H3	0.2659	0.3576	0.5885	0.044*
C4	0.4244 (2)	0.26584 (10)	0.52104 (16)	0.0340 (3)
C5	0.5323 (2)	0.32923 (11)	0.47029 (18)	0.0372 (4)
H5	0.5165	0.3931	0.4772	0.045*
C6	0.6601 (2)	0.29554 (11)	0.41088 (18)	0.0375 (4)
C7	0.6864 (2)	0.19874 (12)	0.40126 (18)	0.0406 (4)
H7	0.7733	0.1771	0.3600	0.049*
C8	0.5865 (2)	0.13662 (11)	0.45142 (18)	0.0403 (4)
H8	0.6067	0.0730	0.4456	0.048*
C9	0.4520 (2)	0.16836 (10)	0.51239 (17)	0.0342 (3)
C10	0.0534 (2)	0.26334 (14)	0.70166 (19)	0.0446 (4)
H10	-0.0153	0.2191	0.7322	0.054*
C11	0.7544 (3)	0.44805 (12)	0.3677 (2)	0.0542 (5)
H11A	0.8378	0.4783	0.3259	0.081*

H11B	0.7835	0.4657	0.4721	0.081*
H11C	0.6306	0.4665	0.3120	0.081*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C11	0.0724 (4)	0.0424 (3)	0.0754 (4)	−0.0099 (2)	0.0455 (3)	0.0028 (2)
O1	0.0572 (8)	0.0491 (9)	0.0728 (9)	0.0069 (6)	0.0355 (7)	−0.0077 (6)
O2	0.0529 (7)	0.0395 (7)	0.0631 (8)	−0.0047 (5)	0.0347 (6)	−0.0021 (5)
N1	0.0497 (8)	0.0302 (8)	0.0442 (7)	0.0003 (6)	0.0216 (6)	−0.0002 (5)
C1	0.0455 (9)	0.0337 (8)	0.0394 (8)	−0.0033 (7)	0.0176 (7)	0.0014 (6)
C2	0.0376 (8)	0.0358 (8)	0.0369 (8)	0.0018 (6)	0.0136 (7)	−0.0017 (6)
C3	0.0423 (8)	0.0285 (8)	0.0411 (8)	0.0043 (6)	0.0168 (7)	−0.0013 (6)
C4	0.0379 (8)	0.0307 (8)	0.0346 (8)	0.0030 (6)	0.0135 (6)	0.0001 (6)
C5	0.0425 (8)	0.0278 (8)	0.0435 (8)	0.0003 (6)	0.0174 (7)	−0.0018 (6)
C6	0.0393 (8)	0.0353 (9)	0.0397 (8)	−0.0029 (6)	0.0157 (7)	−0.0001 (6)
C7	0.0437 (9)	0.0385 (9)	0.0442 (9)	0.0056 (7)	0.0209 (7)	−0.0032 (7)
C8	0.0493 (9)	0.0303 (9)	0.0448 (9)	0.0069 (7)	0.0205 (7)	−0.0013 (6)
C9	0.0406 (8)	0.0278 (8)	0.0350 (8)	0.0019 (6)	0.0138 (6)	−0.0001 (6)
C10	0.0431 (9)	0.0510 (11)	0.0445 (9)	0.0002 (8)	0.0208 (7)	−0.0024 (8)
C11	0.0605 (12)	0.0381 (10)	0.0751 (13)	−0.0109 (8)	0.0373 (10)	−0.0039 (8)

Geometric parameters (Å, °)

C11—C1	1.7461 (16)	C4—C9	1.421 (2)
O1—C10	1.201 (2)	C5—C6	1.370 (2)
O2—C6	1.3654 (18)	C5—H5	0.9300
O2—C11	1.426 (2)	C6—C7	1.411 (2)
N1—C1	1.302 (2)	C7—C8	1.359 (2)
N1—C9	1.362 (2)	C7—H7	0.9300
C1—C2	1.414 (2)	C8—C9	1.414 (2)
C2—C3	1.372 (2)	C8—H8	0.9300
C2—C10	1.487 (2)	C10—H10	0.9300
C3—C4	1.407 (2)	C11—H11A	0.9600
C3—H3	0.9300	C11—H11B	0.9600
C4—C5	1.416 (2)	C11—H11C	0.9600
C6—O2—C11	117.12 (13)	C5—C6—C7	120.73 (14)
C1—N1—C9	117.96 (13)	C8—C7—C6	120.92 (14)
N1—C1—C2	125.38 (14)	C8—C7—H7	119.5
N1—C1—C11	114.97 (12)	C6—C7—H7	119.5
C2—C1—C11	119.62 (12)	C7—C8—C9	120.21 (14)
C3—C2—C1	116.56 (14)	C7—C8—H8	119.9
C3—C2—C10	119.25 (15)	C9—C8—H8	119.9
C1—C2—C10	124.17 (15)	N1—C9—C8	118.96 (14)
C2—C3—C4	120.94 (14)	N1—C9—C4	122.11 (13)
C2—C3—H3	119.5	C8—C9—C4	118.93 (14)
C4—C3—H3	119.5	O1—C10—C2	123.35 (17)

C3—C4—C5	123.14 (14)	O1—C10—H10	118.3
C3—C4—C9	117.05 (14)	C2—C10—H10	118.3
C5—C4—C9	119.81 (13)	O2—C11—H11A	109.5
C6—C5—C4	119.40 (15)	O2—C11—H11B	109.5
C6—C5—H5	120.3	H11A—C11—H11B	109.5
C4—C5—H5	120.3	O2—C11—H11C	109.5
O2—C6—C5	124.81 (15)	H11A—C11—H11C	109.5
O2—C6—C7	114.46 (13)	H11B—C11—H11C	109.5
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C9—N1—C1—C2	0.5 (2)	C4—C5—C6—C7	-0.6 (2)
C9—N1—C1—C11	-177.49 (11)	O2—C6—C7—C8	179.38 (15)
N1—C1—C2—C3	-0.6 (2)	C5—C6—C7—C8	-0.4 (2)
C11—C1—C2—C3	177.35 (12)	C6—C7—C8—C9	0.9 (2)
N1—C1—C2—C10	-178.93 (16)	C1—N1—C9—C8	179.30 (15)
C11—C1—C2—C10	-1.0 (2)	C1—N1—C9—C4	0.3 (2)
C1—C2—C3—C4	-0.2 (2)	C7—C8—C9—N1	-179.39 (15)
C10—C2—C3—C4	178.22 (15)	C7—C8—C9—C4	-0.4 (2)
C2—C3—C4—C5	-178.40 (15)	C3—C4—C9—N1	-1.1 (2)
C2—C3—C4—C9	1.0 (2)	C5—C4—C9—N1	178.34 (14)
C3—C4—C5—C6	-179.51 (15)	C3—C4—C9—C8	179.98 (14)
C9—C4—C5—C6	1.1 (2)	C5—C4—C9—C8	-0.6 (2)
C11—O2—C6—C5	1.3 (2)	C3—C2—C10—O1	-2.4 (3)
C11—O2—C6—C7	-178.48 (16)	C1—C2—C10—O1	175.9 (2)
C4—C5—C6—O2	179.62 (15)		
