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2-Chloro-6-methoxyquinoline-3-carbaldehyde

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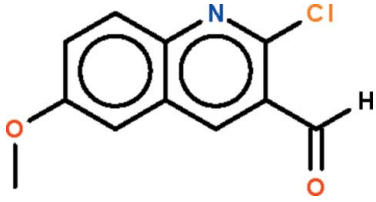
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.115; data-to-parameter ratio = 16.2.

The quinoline fused-ring system of the title compound, $C_{11}H_8ClNO_2$, is planar (r.m.s. deviation = 0.0095 Å); the formyl group is slightly bent out of this plane [C—C—C—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

$C_{11}H_8ClNO_2$ M_r = 221.63
Monoclinic, $P2_1/c$
a = 7.7072 (9) Å
b = 14.3474 (13) Å
c = 9.3487 (10) Å
β = 109.415 (2)°
V = 974.98 (18) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 290 K
0.24 × 0.21 × 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_{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). E**65**, 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*(H) set to 1.2–1.5*U*(C).

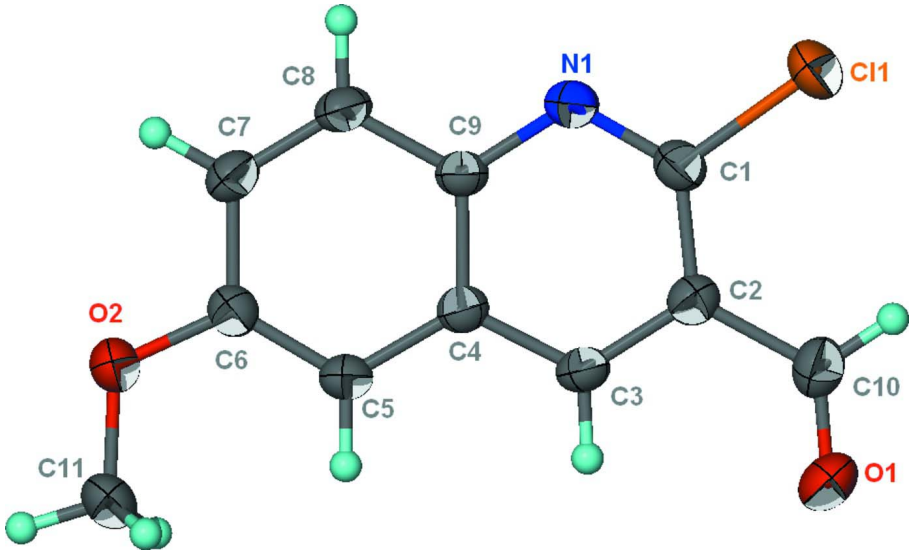

Figure 1

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

$C_{11}H_8ClNO_2$
$M_r = 221.63$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.7072$ (9) Å
$b = 14.3474$ (13) Å
$c = 9.3487$ (10) Å
$\beta = 109.415$ (2)°
$V = 974.98$ (18) Å^3
$Z = 4$

$F(000) = 456$
$D_x = 1.510$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 842 reflections
$\theta = 2.0$–$24.7°$
$\mu = 0.37$ mm^{-1}
$T = 290$ K
Block, colorless
0.24 × 0.21 × 0.18 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 $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.7°$
$h = -10 \rightarrow 9$
$k = -18 \rightarrow 10$
$l = -12 \rightarrow 12$

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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{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}
Cl1	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, º)

Cl1—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—Cl1	114.97 (12)	C6—C7—H7	119.5
C2—C1—Cl1	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
C9—N1—C1—C2	0.5 (2)	C4—C5—C6—C7	−0.6 (2)
C9—N1—C1—Cl1	−177.49 (11)	O2—C6—C7—C8	179.38 (15)
N1—C1—C2—C3	−0.6 (2)	C5—C6—C7—C8	−0.4 (2)
Cl1—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)
Cl1—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)		