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2-Chloro-8-methoxyquinoline-3-carbaldehyde

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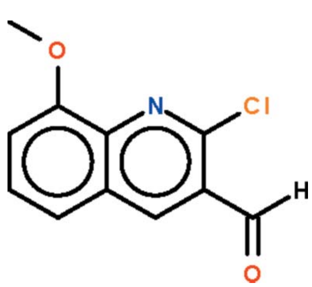
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.003 Å; R factor = 0.037; wR factor = 0.149; data-to-parameter ratio = 16.1.

In the title compound, $C_{11}H_8ClNO_2$, the quinoline fused-ring system is almost planar (r.m.s. deviation = 0.020 Å). The formyl group is slightly bent out of the quinoline plane [deviation of the O atom = 0.371 (2) Å].

Related literature

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



Experimental

Crystal data

$C_{11}H_8ClNO_2$	V = 968.36 (9) Å^3
M_r = 221.63	Z = 4
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
a = 14.4763 (8) Å	μ = 0.37 mm^{-1}
b = 3.9246 (2) Å	T = 290 K
c = 17.6295 (9) Å	0.30 × 0.18 × 0.11 mm
β = 104.802 (3)°	

Data collection

Bruker SMART area-detector diffractometer	8150 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2212 independent reflections
T_{min} = 0.897, T_{max} = 0.961	1769 reflections with $I > 2\sigma(I)$
	R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037	137 parameters
$wR(F^2)$ = 0.149	H-atom parameters constrained
S = 1.18	$\Delta\rho_{max}$ = 0.30 e Å^{-3}
2212 reflections	$\Delta\rho_{min}$ = −0.38 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: HB5131).

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supplementary materials

Acta Cryst. (2009). E**65**, o2720 [**doi:10.1107/S1600536809040835**]

2-Chloro-8-methoxyquinoline-3-carbaldehyde

R. Subashini, F. N. Khan, M. Gund, V. R. Hathwar and S. W. Ng

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 *N*-(2-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 to yield colourless blocks of (I).

Refinement

The 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).

Figures

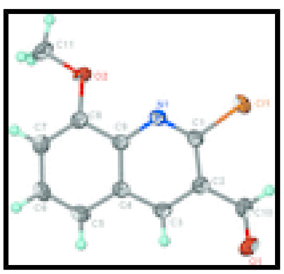

Fig. 1. The molecular structure of (I) at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-Chloro-8-methoxyquinoline-3-carbaldehyde

Crystal data

$C_{11}H_8ClNO_2$	F_{000} = 456
M_r = 221.63	D_x = 1.520 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 943 reflections
a = 14.4763 (8) Å	θ = 1.9–24.6º
b = 3.9246 (2) Å	μ = 0.37 mm^{-1}
c = 17.6295 (9) Å	*T* = 290 K
β = 104.802 (3)º	Block, colourless
V = 968.36 (9) Å^3	0.30 × 0.18 × 0.11 mm
Z = 4	

Data collection

Bruker SMART area-detector diffractometer	2212 independent reflections
Radiation source: fine-focus sealed tube	1769 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.026$
$T = 290$ K	$\theta_{max} = 27.5°$
φ and ω scans	$\theta_{min} = 2.1°$
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	$h = -18 \rightarrow 18$
$T_{min} = 0.897$, $T_{max} = 0.961$	$k = -4 \rightarrow 5$
8150 measured reflections	$l = -22 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.149$	$w = 1/[\sigma^2(F_o^2) + (0.0883P)^2 + 0.0632P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.18$	$(\Delta/\sigma)_{max} = 0.001$
2212 reflections	$\Delta\rho_{max} = 0.30$ e Å^{-3}
137 parameters	$\Delta\rho_{min} = -0.38$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.80902 (4)	0.23452 (14)	0.68475 (3)	0.0499 (2)
N1	0.71583 (11)	0.3286 (4)	0.54057 (8)	0.0338 (4)
O1	1.02603 (11)	0.8263 (5)	0.61921 (10)	0.0627 (5)
O2	0.54659 (9)	0.2331 (4)	0.44173 (8)	0.0450 (4)
C1	0.79779 (12)	0.3856 (5)	0.58921 (9)	0.0333 (4)
C2	0.87625 (12)	0.5588 (5)	0.57179 (10)	0.0347 (4)
C3	0.86350 (13)	0.6661 (5)	0.49563 (10)	0.0344 (4)
H3	0.9129	0.7785	0.4811	0.041*
C4	0.77669 (12)	0.6081 (5)	0.43926 (10)	0.0320 (4)
C5	0.75979 (14)	0.7149 (5)	0.36018 (11)	0.0377 (4)
H5	0.8080	0.8205	0.3426	0.045*
C6	0.67289 (14)	0.6619 (5)	0.31039 (10)	0.0395 (4)
H6	0.6620	0.7325	0.2585	0.047*
C7	0.59819 (13)	0.5015 (5)	0.33542 (10)	0.0381 (4)
H7	0.5390	0.4710	0.3001	0.046*
C8	0.61230 (12)	0.3907 (5)	0.41126 (10)	0.0339 (4)
C9	0.70294 (11)	0.4414 (4)	0.46533 (9)	0.0304 (4)

C10	0.96654 (14)	0.6382 (6)	0.63092 (11)	0.0451 (5)
H10	0.9774	0.5355	0.6799	0.054*
C11	0.45218 (13)	0.1914 (6)	0.39243 (13)	0.0477 (5)
H11A	0.4134	0.0738	0.4208	0.072*
H11B	0.4548	0.0613	0.3469	0.072*
H11C	0.4249	0.4110	0.3764	0.072*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0550 (4)	0.0636 (4)	0.0312 (3)	−0.0071 (2)	0.0116 (2)	0.00723 (19)
N1	0.0347 (8)	0.0368 (8)	0.0325 (7)	−0.0019 (6)	0.0132 (6)	−0.0004 (6)
O1	0.0409 (8)	0.0860 (13)	0.0560 (10)	−0.0244 (8)	0.0028 (7)	0.0043 (9)
O2	0.0321 (7)	0.0598 (10)	0.0421 (8)	−0.0124 (6)	0.0078 (6)	0.0026 (6)
C1	0.0373 (9)	0.0355 (9)	0.0288 (8)	−0.0012 (7)	0.0115 (6)	−0.0005 (7)
C2	0.0315 (9)	0.0369 (10)	0.0360 (9)	−0.0019 (7)	0.0088 (7)	−0.0028 (7)
C3	0.0311 (9)	0.0372 (9)	0.0377 (9)	−0.0035 (7)	0.0138 (7)	−0.0011 (7)
C4	0.0338 (9)	0.0318 (9)	0.0326 (8)	0.0006 (7)	0.0127 (7)	−0.0016 (7)
C5	0.0399 (10)	0.0411 (11)	0.0353 (10)	−0.0009 (8)	0.0157 (8)	0.0031 (7)
C6	0.0451 (10)	0.0443 (11)	0.0297 (9)	0.0047 (8)	0.0110 (7)	0.0032 (7)
C7	0.0359 (9)	0.0411 (10)	0.0358 (9)	0.0021 (8)	0.0062 (7)	−0.0036 (7)
C8	0.0312 (9)	0.0344 (10)	0.0372 (9)	−0.0005 (7)	0.0109 (7)	−0.0034 (7)
C9	0.0310 (8)	0.0310 (9)	0.0315 (8)	−0.0002 (7)	0.0121 (6)	−0.0024 (6)
C10	0.0403 (11)	0.0549 (12)	0.0376 (10)	−0.0038 (9)	0.0053 (8)	0.0011 (9)
C11	0.0304 (10)	0.0542 (13)	0.0553 (13)	−0.0076 (8)	0.0053 (8)	−0.0010 (9)

Geometric parameters (Å, °)

Cl1—C1	1.7536 (17)	C4—C9	1.425 (2)
N1—C1	1.294 (2)	C5—C6	1.354 (3)
N1—C9	1.365 (2)	C5—H5	0.9300
O1—C10	1.192 (3)	C6—C7	1.416 (3)
O2—C8	1.355 (2)	C6—H6	0.9300
O2—C11	1.429 (2)	C7—C8	1.371 (2)
C1—C2	1.423 (3)	C7—H7	0.9300
C2—C3	1.374 (2)	C8—C9	1.425 (2)
C2—C10	1.482 (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
C1—N1—C9	117.55 (15)	C7—C6—H6	119.2
C8—O2—C11	118.05 (15)	C8—C7—C6	120.64 (16)
N1—C1—C2	125.95 (16)	C8—C7—H7	119.7
N1—C1—Cl1	114.99 (13)	C6—C7—H7	119.7
C2—C1—Cl1	119.05 (13)	O2—C8—C7	125.91 (16)
C3—C2—C1	116.23 (15)	O2—C8—C9	114.72 (15)
C3—C2—C10	119.81 (16)	C7—C8—C9	119.37 (16)
C1—C2—C10	123.91 (16)	N1—C9—C8	118.58 (15)

C2—C3—C4	120.89 (16)	N1—C9—C4	122.33 (15)
C2—C3—H3	119.6	C8—C9—C4	119.09 (16)
C4—C3—H3	119.6	O1—C10—C2	123.71 (19)
C3—C4—C5	123.09 (16)	O1—C10—H10	118.1
C3—C4—C9	117.00 (16)	C2—C10—H10	118.1
C5—C4—C9	119.89 (16)	O2—C11—H11A	109.5
C6—C5—C4	119.43 (17)	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
C5—C6—C7	121.57 (17)	H11A—C11—H11C	109.5
C5—C6—H6	119.2	H11B—C11—H11C	109.5

C9—N1—C1—C2	0.5 (3)	C11—O2—C8—C9	176.32 (16)
C9—N1—C1—Cl1	179.85 (12)	C6—C7—C8—O2	−179.69 (18)
N1—C1—C2—C3	−1.7 (3)	C6—C7—C8—C9	0.6 (3)
Cl1—C1—C2—C3	179.00 (14)	C1—N1—C9—C8	−178.13 (16)
N1—C1—C2—C10	175.74 (18)	C1—N1—C9—C4	1.7 (3)
Cl1—C1—C2—C10	−3.6 (3)	O2—C8—C9—N1	0.5 (2)
C1—C2—C3—C4	0.6 (3)	C7—C8—C9—N1	−179.81 (16)
C10—C2—C3—C4	−176.92 (17)	O2—C8—C9—C4	−179.36 (16)
C2—C3—C4—C5	179.70 (17)	C7—C8—C9—C4	0.3 (3)
C2—C3—C4—C9	1.3 (3)	C3—C4—C9—N1	−2.6 (3)
C3—C4—C5—C6	−177.25 (17)	C5—C4—C9—N1	178.97 (16)
C9—C4—C5—C6	1.1 (3)	C3—C4—C9—C8	177.22 (16)
C4—C5—C6—C7	−0.1 (3)	C5—C4—C9—C8	−1.2 (3)
C5—C6—C7—C8	−0.8 (3)	C3—C2—C10—O1	9.2 (3)
C11—O2—C8—C7	−3.4 (3)	C1—C2—C10—O1	−168.2 (2)

Fig. 1