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2-Chloro-8-methylquinoline-3-carbaldehyde

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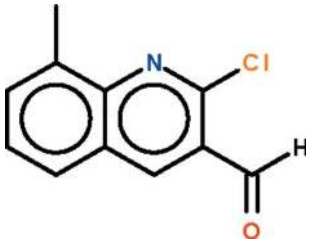
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.136; data-to-parameter ratio = 16.9.

The quinoline fused-ring system of the title compound, $C_{11}H_8ClNO$, is planar (r.m.s. deviation = 0.005 Å); the formyl group is slightly bent out of the plane [C—C—C–O1 torsion angles = 8.8 (7) and −172.8 (4)°].

Related literature

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



Experimental

Crystal data

$C_{11}H_8ClNO$
M_r = 205.63
Orthorhombic, $P2_12_12_1$
a = 6.8576 (5) Å
b = 7.4936 (6) Å
c = 18.5003 (14) Å
V = 950.70 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 290 K
0.26 × 0.22 × 0.17 mm

Data collection

Bruker SMART area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.912, T_{max} = 0.941
8224 measured reflections
2174 independent reflections
1734 reflections with $I > 2\sigma(I)$
R_{int} = 0.043

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.136
S = 1.00
2174 reflections
129 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Absolute structure: Flack (1983), 838 Friedel pairs
Flack parameter: 0.2 (2)

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: BT5085).

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supporting information

Acta Cryst. (2009). E**65**, o2722 [https://doi.org/10.1107/S1600536809040859]

2-Chloro-8-methylquinoline-3-carbaldehyde

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S1. Experimental

The Vilsmeier-Haack reagent 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-tolyl)acetamide (1.49 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

Carbon-bound 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 1.2–1.5U(C).

The crystal had two domains related by a translation of (1/2, 0, 0) so that all reflections with $h = 2n$ are affected. A scale factor was added for all reflections with $h = 2n$. The *hkl* file had a scale factor of 1 for $h = 2n + 1$ and a scale factor of 2 for the $h = 2n$ reflections.

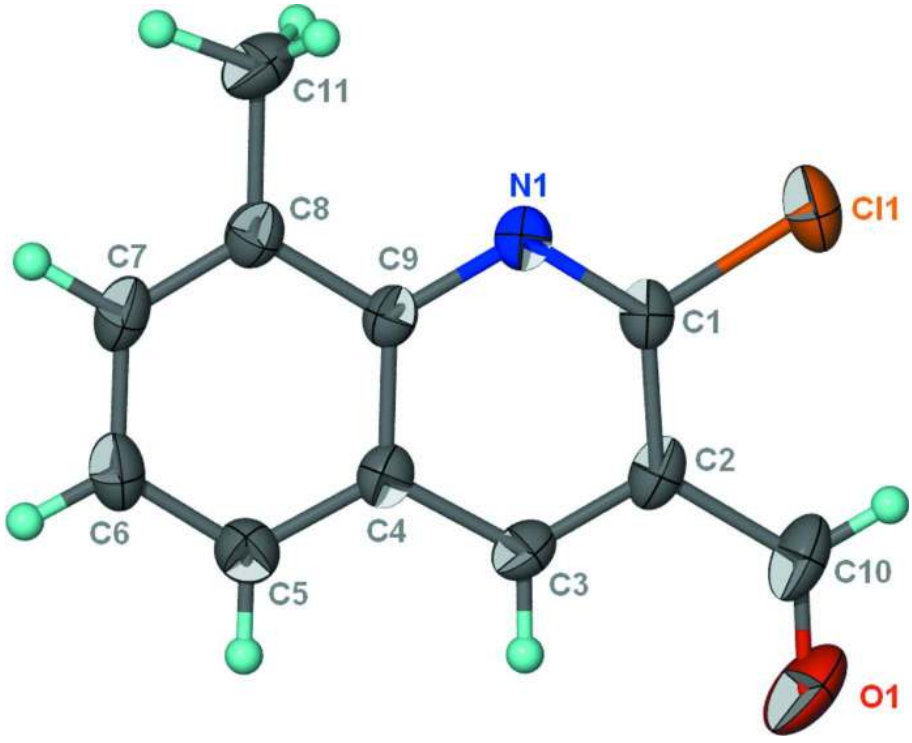

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{11}H_8ClNO$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-Chloro-8-methylquinoline-3-carbaldehyde

Crystal data

$C_{11}H_8ClNO$
$M_r = 205.63$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 6.8576\ (5)$ Å
$b = 7.4936\ (6)$ Å
$c = 18.5003\ (14)$ Å
$V = 950.70\ (13)$ Å^3
$Z = 4$
$F(000) = 424$
$D_x = 1.437$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 867 reflections
$\theta = 2.0$–$24.4°$
$\mu = 0.36$ mm^{-1}
$T = 290$ K
Block, colorless
0.26 × 0.22 × 0.17 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)
$T_{min} = 0.912$, $T_{max} = 0.941$
8224 measured reflections
2174 independent reflections
1734 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.2°$
$h = -8 \rightarrow 8$
$k = -9 \rightarrow 9$
$l = -22 \rightarrow 24$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.136$
$S = 1.00$
2174 reflections
129 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
$w = 1/[\sigma^2(F_o^2) + (0.0861P)^2 + 0.0263P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.33$ e Å^{-3}
Absolute structure: Flack (1983), 838 Friedel pairs
Absolute structure parameter: 0.2 (2)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.87010 (13)	1.14505 (9)	0.37890 (4)	0.0579 (3)
O1	0.8672 (5)	0.6106 (3)	0.29577 (10)	0.0763 (6)
N1	0.8717 (4)	0.9871 (2)	0.50346 (10)	0.0366 (4)
C1	0.8734 (5)	0.9563 (3)	0.43459 (13)	0.0368 (5)
C2	0.8754 (5)	0.7858 (3)	0.40176 (11)	0.0398 (5)
C3	0.8734 (5)	0.6423 (4)	0.44734 (12)	0.0389 (5)
H3	0.8741	0.5276	0.4281	0.047*
C4	0.8705 (4)	0.6651 (3)	0.52293 (10)	0.0344 (5)
C5	0.8691 (5)	0.5212 (3)	0.57186 (14)	0.0443 (6)
H5	0.8707	0.4045	0.5547	0.053*
C6	0.8654 (6)	0.5531 (3)	0.64410 (13)	0.0468 (6)
H6	0.8633	0.4585	0.6766	0.056*
C7	0.8648 (5)	0.7301 (4)	0.66955 (13)	0.0443 (6)
H7	0.8614	0.7491	0.7192	0.053*
C8	0.8690 (4)	0.8754 (3)	0.62492 (11)	0.0372 (5)
C9	0.8702 (4)	0.8426 (3)	0.54918 (11)	0.0327 (4)
C10	0.8840 (6)	0.7545 (5)	0.32246 (14)	0.0551 (7)
H10	0.9034	0.8521	0.2922	0.066*
C11	0.8698 (7)	1.0624 (3)	0.65349 (14)	0.0547 (7)
H11A	0.8779	1.0598	0.7053	0.082*
H11B	0.7519	1.1218	0.6392	0.082*
H11C	0.9801	1.1255	0.6343	0.082*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0687 (4)	0.0591 (4)	0.0459 (4)	0.0008 (5)	0.0006 (4)	0.0218 (3)
O1	0.0887 (16)	0.1007 (17)	0.0394 (10)	−0.008 (2)	−0.0031 (13)	−0.0254 (11)
N1	0.0371 (10)	0.0403 (10)	0.0324 (10)	−0.0007 (12)	0.0005 (12)	0.0028 (7)
C1	0.0327 (11)	0.0459 (13)	0.0318 (12)	0.0001 (17)	−0.0007 (16)	0.0062 (10)
C2	0.0347 (11)	0.0576 (14)	0.0272 (10)	−0.0003 (15)	−0.0008 (12)	−0.0019 (10)
C3	0.0393 (11)	0.0427 (11)	0.0348 (12)	−0.002 (2)	−0.0005 (14)	−0.0084 (10)

C4	0.0323 (10)	0.0410 (11)	0.0300 (10)	−0.0007 (15)	0.0005 (11)	−0.0004 (8)
C5	0.0509 (14)	0.0398 (12)	0.0422 (14)	0.0026 (19)	0.0008 (19)	0.0040 (10)
C6	0.0509 (14)	0.0519 (14)	0.0375 (12)	0.0021 (17)	0.0007 (16)	0.0120 (10)
C7	0.0457 (14)	0.0596 (15)	0.0276 (11)	0.0043 (19)	−0.0022 (15)	0.0020 (11)
C8	0.0344 (10)	0.0461 (12)	0.0310 (11)	0.0029 (12)	−0.0009 (13)	−0.0014 (9)
C9	0.0292 (10)	0.0407 (11)	0.0280 (10)	−0.0001 (16)	0.0004 (12)	0.0002 (9)
C10	0.0538 (17)	0.084 (2)	0.0278 (12)	0.000 (2)	−0.0010 (17)	−0.0032 (13)
C11	0.0716 (17)	0.0543 (15)	0.0384 (13)	0.003 (2)	−0.0005 (19)	−0.0128 (11)

Geometric parameters (Å, º)

Cl1—C1	1.750 (2)	C5—H5	0.9300
O1—C10	1.191 (4)	C6—C7	1.407 (4)
N1—C1	1.295 (3)	C6—H6	0.9300
N1—C9	1.374 (3)	C7—C8	1.367 (3)
C1—C2	1.415 (3)	C7—H7	0.9300
C2—C3	1.367 (3)	C8—C9	1.423 (3)
C2—C10	1.487 (3)	C8—C11	1.498 (3)
C3—C4	1.409 (3)	C10—H10	0.9300
C3—H3	0.9300	C11—H11A	0.9600
C4—C5	1.408 (3)	C11—H11B	0.9600
C4—C9	1.416 (3)	C11—H11C	0.9600
C5—C6	1.358 (4)		
C1—N1—C9	117.73 (18)	C8—C7—C6	123.3 (2)
N1—C1—C2	125.68 (19)	C8—C7—H7	118.4
N1—C1—Cl1	115.80 (18)	C6—C7—H7	118.4
C2—C1—Cl1	118.52 (18)	C7—C8—C9	117.2 (2)
C3—C2—C1	116.47 (19)	C7—C8—C11	122.2 (2)
C3—C2—C10	119.0 (2)	C9—C8—C11	120.6 (2)
C1—C2—C10	124.5 (2)	N1—C9—C4	121.95 (19)
C2—C3—C4	121.1 (2)	N1—C9—C8	118.06 (19)
C2—C3—H3	119.4	C4—C9—C8	119.99 (19)
C4—C3—H3	119.4	O1—C10—C2	123.2 (3)
C5—C4—C3	123.0 (2)	O1—C10—H10	118.4
C5—C4—C9	119.9 (2)	C2—C10—H10	118.4
C3—C4—C9	117.0 (2)	C8—C11—H11A	109.5
C6—C5—C4	119.9 (2)	C8—C11—H11B	109.5
C6—C5—H5	120.1	H11A—C11—H11B	109.5
C4—C5—H5	120.1	C8—C11—H11C	109.5
C5—C6—C7	119.7 (2)	H11A—C11—H11C	109.5
C5—C6—H6	120.2	H11B—C11—H11C	109.5
C7—C6—H6	120.2		
C9—N1—C1—C2	−0.5 (5)	C6—C7—C8—C9	1.3 (5)
C9—N1—C1—Cl1	178.7 (2)	C6—C7—C8—C11	−179.5 (4)
N1—C1—C2—C3	0.6 (5)	C1—N1—C9—C4	0.0 (4)
Cl1—C1—C2—C3	−178.6 (3)	C1—N1—C9—C8	179.8 (3)

N1—C1—C2—C10	−177.9 (3)	C5—C4—C9—N1	179.9 (3)
Cl1—C1—C2—C10	2.9 (5)	C3—C4—C9—N1	0.3 (5)
C1—C2—C3—C4	−0.3 (5)	C5—C4—C9—C8	0.2 (4)
C10—C2—C3—C4	178.3 (3)	C3—C4—C9—C8	−179.4 (2)
C2—C3—C4—C5	−179.8 (3)	C7—C8—C9—N1	179.1 (3)
C2—C3—C4—C9	−0.1 (5)	C11—C8—C9—N1	−0.1 (5)
C3—C4—C5—C6	−179.7 (4)	C7—C8—C9—C4	−1.1 (4)
C9—C4—C5—C6	0.7 (5)	C11—C8—C9—C4	179.6 (3)
C4—C5—C6—C7	−0.6 (6)	C3—C2—C10—O1	8.8 (7)
C5—C6—C7—C8	−0.4 (6)	C1—C2—C10—O1	−172.8 (4)