Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Chloro-8-methylquinoline-3-carbaldehyde

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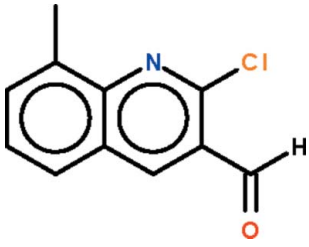
Received 6 October 2009; accepted 6 October 2009

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).

We thank the Department of Science and Technology, India, for use of the diffraction facility at IISc under the IRHPA–DST program. FNK thanks the DST for Fast Track Proposal funding. We also thank VIT University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5085).

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supplementary materials

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

2-Chloro-8-methylquinoline-3-carbaldehyde

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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.

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 1.2–1.5*U*(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.

Figures

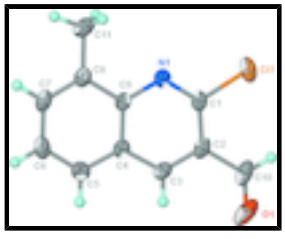

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $C_{11}H_8ClNO$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-Chloro-8-methylquinoline-3-carbaldehyde

Crystal data

$C_{11}H_8ClNO$	$F_{000} = 424$
$M_r = 205.63$	$D_x = 1.437$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 867 reflections
$a = 6.8576$ (5) Å	$\theta = 2.0$–$24.4°$
$b = 7.4936$ (6) Å	$\mu = 0.36$ mm^{-1}
$c = 18.5003$ (14) Å	$T = 290$ K
$V = 950.70$ (13) Å^3	Block, colorless
$Z = 4$	0.26 × 0.22 × 0.17 mm

Data collection

Bruker SMART area-detector diffractometer	2174 independent reflections
Radiation source: fine-focus sealed tube	1734 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.043$
$T = 290$ K	$\theta_{max} = 27.5^{o}$
φ and ω scans	$\theta_{min} = 2.2^{o}$
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	$h = -8\rightarrow8$
$T_{min} = 0.912$, $T_{max} = 0.941$	$k = -9\rightarrow9$
8224 measured reflections	$l = -22\rightarrow24$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.048$	$w = 1/[\sigma^2(F_o^2) + (0.0861P)^2 + 0.0263P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.136$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.00$	$\Delta\rho_{max} = 0.25$ e Å^{-3}
2174 reflections	$\Delta\rho_{min} = -0.32$ e Å^{-3}
129 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 838 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.2 (2)

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

	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 (Å^2)

	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, °)

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)

Fig. 1