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2-Chloro-7-methylquinoline-3-carbaldehyde

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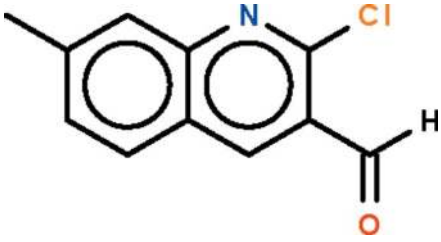
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.005 Å; R factor = 0.078; wR factor = 0.209; data-to-parameter ratio = 14.0.

The quinoline fused-ring system of the title compound, $C_{11}H_8ClNO$, is planar (r.m.s. deviation = 0.007 Å); the formyl group is bent slightly out of the plane [C—C—C—O torsion angles = −9.6 (5) and 170.4 (3)°].

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
Monoclinic, $P2_1/n$
a = 15.458 (3) Å
b = 3.9382 (8) Å
c = 16.923 (3) Å
β = 112.854 (3)°
V = 949.3 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 290 K
0.24 × 0.18 × 0.06 mm

Data collection

Bruker SMART area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.918, T_{max} = 0.979
6484 measured reflections
1796 independent reflections
1356 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.078
$wR(F^2)$ = 0.209
S = 1.13
1796 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.78 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 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: XU2629).

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supporting information

Acta Cryst. (2009). E**65**, o2721 [https://doi.org/10.1107/S1600536809040823]

2-Chloro-7-methylquinoline-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 *N*-(3-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 1.2–1.5*U*(C).

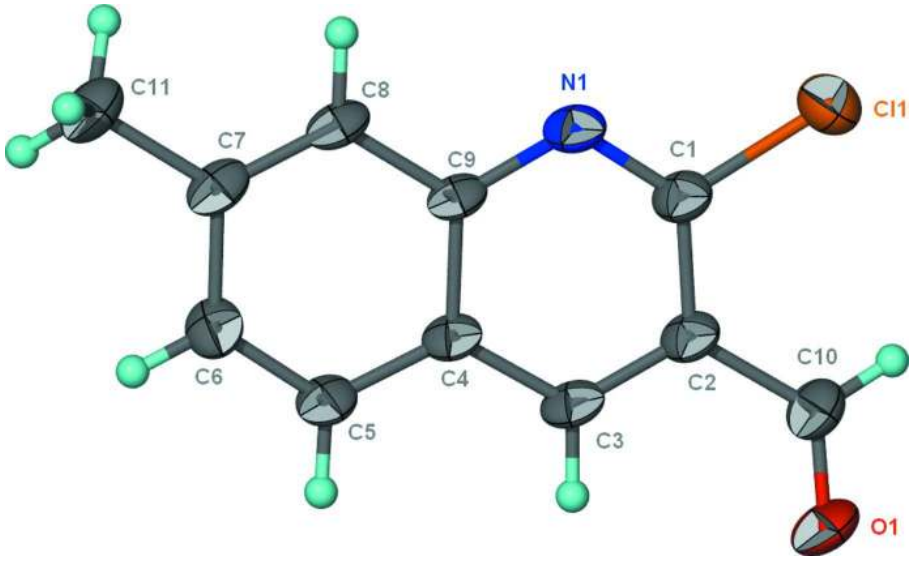

Figure 1

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-7-methylquinoline-3-carbaldehyde

Crystal data

$C_{11}H_8ClNO$
$M_r = 205.63$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 15.458$ (3) Å
$b = 3.9382$ (8) Å
$c = 16.923$ (3) Å
$\beta = 112.854$ (3)°
$V = 949.3$ (3) Å^3
$Z = 4$

$F(000) = 424$
$D_x = 1.439$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 973 reflections
$\theta = 1.3$–$24.9°$
$\mu = 0.36$ mm^{-1}
$T = 290$ K
Block, colorless
0.24 × 0.18 × 0.06 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)
$T_{min} = 0.918$, $T_{max} = 0.979$
6484 measured reflections
1796 independent reflections
1356 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 25.7°$, $\theta_{min} = 2.3°$
$h = -18 \rightarrow 18$
$k = -4 \rightarrow 4$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.078$
$wR(F^2) = 0.209$
$S = 1.13$
1796 reflections
128 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
$w = 1/[\sigma^2(F_o^2) + (0.1371P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.78$ e Å^{-3}
$\Delta\rho_{min} = -0.49$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.37647 (6)	0.6903 (3)	0.18658 (6)	0.0603 (4)
O1	0.36833 (17)	0.1214 (8)	0.39875 (18)	0.0705 (9)
N1	0.55664 (19)	0.6719 (7)	0.27097 (16)	0.0402 (7)
C1	0.4781 (2)	0.5835 (8)	0.27548 (19)	0.0393 (7)
C2	0.4683 (2)	0.4068 (8)	0.34482 (19)	0.0383 (7)
C3	0.5497 (2)	0.3312 (8)	0.4129 (2)	0.0387 (7)
H3	0.5468	0.2182	0.4601	0.046*
C4	0.6373 (2)	0.4210 (7)	0.41281 (18)	0.0347 (7)
C5	0.7243 (2)	0.3490 (8)	0.48060 (19)	0.0407 (8)
H5	0.7253	0.2376	0.5294	0.049*
C6	0.8064 (2)	0.4414 (8)	0.47489 (19)	0.0424 (8)
H6	0.8628	0.3923	0.5201	0.051*
C7	0.8080 (2)	0.6125 (7)	0.4009 (2)	0.0394 (8)
C8	0.7248 (2)	0.6851 (8)	0.3354 (2)	0.0391 (7)
H8	0.7252	0.7978	0.2872	0.047*
C9	0.6379 (2)	0.5927 (7)	0.33897 (18)	0.0341 (7)
C10	0.3769 (2)	0.3059 (9)	0.3458 (2)	0.0503 (9)
H10	0.3228	0.3900	0.3029	0.060*
C11	0.9001 (3)	0.7114 (9)	0.3968 (2)	0.0523 (9)
H11A	0.8906	0.9001	0.3584	0.078*
H11B	0.9248	0.5226	0.3764	0.078*

H11C	0.9436	0.7746	0.4530	0.078*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0499 (6)	0.0826 (8)	0.0457 (6)	0.0050 (4)	0.0157 (4)	0.0154 (4)
O1	0.0512 (17)	0.103 (2)	0.0731 (18)	−0.0030 (14)	0.0416 (15)	0.0286 (15)
N1	0.0478 (16)	0.0474 (15)	0.0341 (14)	0.0010 (12)	0.0252 (13)	0.0033 (10)
C1	0.0427 (18)	0.0452 (17)	0.0380 (16)	0.0017 (13)	0.0245 (14)	0.0012 (13)
C2	0.0407 (18)	0.0452 (17)	0.0395 (17)	0.0026 (12)	0.0272 (14)	0.0014 (12)
C3	0.0476 (19)	0.0439 (17)	0.0383 (16)	0.0018 (13)	0.0316 (15)	0.0017 (12)
C4	0.0424 (17)	0.0396 (15)	0.0323 (15)	0.0025 (12)	0.0257 (13)	−0.0005 (11)
C5	0.0439 (18)	0.0549 (19)	0.0338 (16)	0.0035 (14)	0.0267 (14)	0.0011 (13)
C6	0.0390 (17)	0.0560 (19)	0.0386 (17)	0.0053 (14)	0.0221 (14)	−0.0053 (14)
C7	0.0467 (19)	0.0403 (16)	0.0449 (18)	−0.0047 (13)	0.0328 (16)	−0.0095 (12)
C8	0.0477 (19)	0.0440 (17)	0.0400 (17)	−0.0032 (13)	0.0327 (15)	−0.0016 (12)
C9	0.0423 (17)	0.0391 (15)	0.0322 (15)	−0.0007 (12)	0.0268 (13)	−0.0019 (11)
C10	0.0388 (19)	0.065 (2)	0.055 (2)	0.0019 (15)	0.0272 (17)	0.0066 (17)
C11	0.0469 (19)	0.060 (2)	0.063 (2)	−0.0075 (15)	0.0351 (17)	−0.0042 (16)

Geometric parameters (Å, º)

Cl1—C1	1.753 (3)	C5—H5	0.9300
O1—C10	1.200 (4)	C6—C7	1.430 (4)
N1—C1	1.293 (4)	C6—H6	0.9300
N1—C9	1.370 (4)	C7—C8	1.363 (4)
C1—C2	1.422 (4)	C7—C11	1.502 (5)
C2—C3	1.369 (4)	C8—C9	1.416 (4)
C2—C10	1.473 (4)	C8—H8	0.9300
C3—C4	1.400 (4)	C10—H10	0.9300
C3—H3	0.9300	C11—H11A	0.9600
C4—C5	1.417 (4)	C11—H11B	0.9600
C4—C9	1.424 (4)	C11—H11C	0.9600
C5—C6	1.359 (4)		
C1—N1—C9	117.7 (3)	C8—C7—C6	118.6 (3)
N1—C1—C2	125.7 (3)	C8—C7—C11	121.3 (3)
N1—C1—Cl1	115.7 (2)	C6—C7—C11	120.1 (3)
C2—C1—Cl1	118.5 (2)	C7—C8—C9	121.5 (3)
C3—C2—C1	116.3 (3)	C7—C8—H8	119.3
C3—C2—C10	120.2 (3)	C9—C8—H8	119.3
C1—C2—C10	123.5 (3)	N1—C9—C8	118.8 (3)
C2—C3—C4	121.2 (3)	N1—C9—C4	121.9 (3)
C2—C3—H3	119.4	C8—C9—C4	119.3 (3)
C4—C3—H3	119.4	O1—C10—C2	123.8 (3)
C3—C4—C5	124.3 (3)	O1—C10—H10	118.1
C3—C4—C9	117.2 (3)	C2—C10—H10	118.1
C5—C4—C9	118.5 (3)	C7—C11—H11A	109.5

C6—C5—C4	120.5 (3)	C7—C11—H11B	109.5
C6—C5—H5	119.7	H11A—C11—H11B	109.5
C4—C5—H5	119.7	C7—C11—H11C	109.5
C5—C6—C7	121.5 (3)	H11A—C11—H11C	109.5
C5—C6—H6	119.3	H11B—C11—H11C	109.5
C7—C6—H6	119.3		

C9—N1—C1—C2	−0.7 (5)	C5—C6—C7—C11	179.9 (3)
C9—N1—C1—Cl1	−179.8 (2)	C6—C7—C8—C9	−0.5 (4)
N1—C1—C2—C3	1.3 (5)	C11—C7—C8—C9	−180.0 (3)
Cl1—C1—C2—C3	−179.6 (2)	C1—N1—C9—C8	179.6 (3)
N1—C1—C2—C10	−178.7 (3)	C1—N1—C9—C4	−0.4 (4)
Cl1—C1—C2—C10	0.5 (4)	C7—C8—C9—N1	−179.8 (3)
C1—C2—C3—C4	−0.8 (4)	C7—C8—C9—C4	0.2 (4)
C10—C2—C3—C4	179.2 (3)	C3—C4—C9—N1	0.8 (4)
C2—C3—C4—C5	−179.5 (3)	C5—C4—C9—N1	−179.8 (3)
C2—C3—C4—C9	−0.2 (4)	C3—C4—C9—C8	−179.2 (3)
C3—C4—C5—C6	179.1 (3)	C5—C4—C9—C8	0.1 (4)
C9—C4—C5—C6	−0.2 (4)	C3—C2—C10—O1	−9.6 (5)
C4—C5—C6—C7	−0.1 (5)	C1—C2—C10—O1	170.4 (3)
C5—C6—C7—C8	0.5 (5)		