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2-Chloro-6-methylquinoline-3-carbaldehyde

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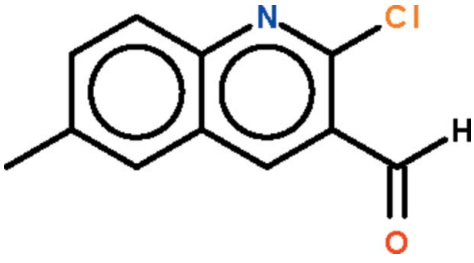
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.003 Å; R factor = 0.034; wR factor = 0.089; data-to-parameter ratio = 16.0.

The quinolinyl fused-ring of the title compound, $C_{11}H_8ClNO$, is almost planar (r.m.s. deviation = 0.013 Å); the formyl group is slightly bent out of the plane of the fused ring system [C—C—C—O torsion angle = 13.5 (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
Monoclinic, Pc
a = 5.944 (1) Å
b = 3.9210 (19) Å
c = 20.390 (2) Å
β = 101.377 (15)°
V = 465.9 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 290 K
0.25 × 0.15 × 0.15 mm

Data collection

Oxford Diffraction Excalibur diffractometer
Absorption correction: multi-scan (*CrysAlis Pro*; Oxford Diffraction, 2009)
T_{min} = 0.913, T_{max} = 0.947
5980 measured reflections
2052 independent reflections
1831 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.089
S = 1.00
2052 reflections
128 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Absolute structure: Flack (1983), 990 Friedel pairs
Flack parameter: 0.02 (6)

Data collection: *CrysAlis Pro* (Oxford Diffraction, 2009); cell refinement: *CrysAlis Pro*; data reduction: *CrysAlis Pro*; 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: TK2550).

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supplementary materials

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2-Chloro-6-methylquinoline-3-carbaldehyde

F. N. Khan, R. Subashini, S. M. Roopan, 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 to *N*-(4-tolyl)acetamide (1.49 g, 10 mmol), and heated at 353 K for 15 h. The mixture was then poured onto ice, and 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_{iso}(H) set to 1.2–1.5U_{eq}(C).

Figures

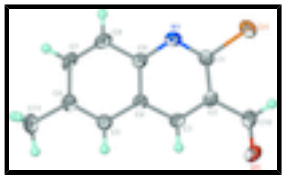

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $C_{11}H_8ClNO$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-Chloro-6-methylquinoline-3-carbaldehyde

Crystal data

$C_{11}H_8ClNO$	F_{000} = 212
M_r = 205.63	D_x = 1.466 Mg m^{-3}
Monoclinic, *Pc*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: P -2yc	Cell parameters from 1352 reflections
a = 5.944 (1) Å	θ = 2.0–20.7º
b = 3.9210 (19) Å	μ = 0.37 mm^{-1}
c = 20.390 (2) Å	*T* = 290 K
β = 101.377 (15)º	Block, colorless
V = 465.9 (2) Å^3	0.25 × 0.15 × 0.15 mm
Z = 2	

Data collection

Oxford Diffraction Excalibur diffractometer	2052 independent reflections
Radiation source: fine-focus sealed tube	1831 reflections with $I > 2\sigma(I)$

Monochromator: graphite	R_{int} = 0.028
T = 290 K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.5º
Absorption correction: Multi-scan (CrysAlis Pro; Oxford Diffraction, 2009)	h = −7→7
T_{min} = 0.913, T_{max} = 0.947	k = −5→5
5980 measured reflections	l = −26→25

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$w = 1/[\sigma^2(F_o^2) + (0.0584P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.089	$(\Delta/\sigma)_{max} < 0.001$
S = 1.00	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
2052 reflections	$\Delta\rho_{min}$ = −0.17 e Å^{-3}
128 parameters	Extinction correction: none
2 restraints	Absolute structure: Flack (1983), 990 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.02 (6)
Secondary atom site location: difference Fourier map	

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

	x	y	z	U_{iso}*/U_{eq}
Cl1	1.00002 (8)	1.11653 (14)	0.50000 (3)	0.04862 (17)
O1	0.4626 (4)	0.5444 (6)	0.55814 (8)	0.0676 (6)
N1	0.7865 (3)	0.9885 (5)	0.37983 (9)	0.0382 (4)
C1	0.7703 (3)	0.9492 (5)	0.44201 (10)	0.0351 (5)
C2	0.5905 (3)	0.7858 (5)	0.46557 (10)	0.0340 (4)
C3	0.4137 (4)	0.6644 (5)	0.41837 (10)	0.0341 (4)
H3	0.2906	0.5561	0.4315	0.041*
C4	0.4163 (3)	0.7021 (5)	0.34984 (10)	0.0320 (4)
C5	0.2378 (4)	0.5831 (5)	0.29839 (10)	0.0366 (4)
H5	0.1096	0.4792	0.3094	0.044*
C6	0.2519 (4)	0.6196 (5)	0.23214 (10)	0.0383 (5)
C7	0.4490 (4)	0.7786 (6)	0.21674 (10)	0.0454 (5)
H7	0.4598	0.8019	0.1721	0.054*
C8	0.6212 (4)	0.8971 (6)	0.26419 (11)	0.0441 (5)
H8	0.7474	1.0015	0.2521	0.053*
C9	0.6099 (4)	0.8627 (5)	0.33289 (10)	0.0335 (4)
C10	0.5895 (4)	0.7365 (7)	0.53783 (11)	0.0470 (5)
H10	0.6930	0.8615	0.5688	0.056*
C11	0.0664 (4)	0.4932 (7)	0.17678 (10)	0.0501 (6)
H11A	−0.0398	0.3562	0.1952	0.075*
H11B	0.1332	0.3584	0.1463	0.075*

H11C	−0.0131	0.6841	0.1534	0.075*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0366 (3)	0.0578 (3)	0.0488 (3)	−0.0066 (3)	0.00193 (19)	−0.0056 (3)
O1	0.0607 (12)	0.1037 (15)	0.0375 (9)	−0.0252 (12)	0.0074 (8)	0.0170 (10)
N1	0.0348 (9)	0.0388 (8)	0.0428 (10)	−0.0031 (7)	0.0118 (7)	−0.0002 (7)
C1	0.0309 (11)	0.0349 (11)	0.0389 (11)	0.0019 (8)	0.0056 (8)	−0.0021 (8)
C2	0.0325 (11)	0.0377 (10)	0.0325 (9)	0.0060 (9)	0.0083 (8)	0.0028 (8)
C3	0.0310 (10)	0.0375 (10)	0.0354 (11)	0.0007 (8)	0.0106 (8)	0.0031 (8)
C4	0.0327 (10)	0.0302 (10)	0.0337 (10)	0.0022 (8)	0.0077 (8)	0.0012 (8)
C5	0.0346 (11)	0.0376 (11)	0.0375 (10)	−0.0002 (8)	0.0067 (8)	0.0003 (8)
C6	0.0412 (12)	0.0384 (11)	0.0348 (10)	0.0030 (9)	0.0062 (9)	−0.0016 (8)
C7	0.0575 (15)	0.0519 (12)	0.0294 (10)	0.0032 (11)	0.0148 (10)	0.0014 (9)
C8	0.0480 (13)	0.0471 (12)	0.0421 (11)	−0.0048 (10)	0.0207 (10)	0.0018 (10)
C9	0.0355 (10)	0.0326 (10)	0.0337 (10)	0.0021 (8)	0.0099 (8)	0.0003 (8)
C10	0.0412 (13)	0.0631 (14)	0.0350 (10)	−0.0026 (11)	0.0035 (9)	0.0021 (11)
C11	0.0573 (15)	0.0555 (13)	0.0346 (11)	−0.0024 (12)	0.0019 (10)	−0.0041 (10)

Geometric parameters (Å, °)

Cl1—C1	1.748 (2)	C5—H5	0.9300
O1—C10	1.196 (3)	C6—C7	1.416 (3)
N1—C1	1.300 (2)	C6—C11	1.498 (3)
N1—C9	1.365 (3)	C7—C8	1.345 (3)
C1—C2	1.409 (3)	C7—H7	0.9300
C2—C3	1.363 (3)	C8—C9	1.422 (3)
C2—C10	1.487 (3)	C8—H8	0.9300
C3—C4	1.408 (3)	C10—H10	0.9300
C3—H3	0.9300	C11—H11A	0.9600
C4—C9	1.414 (3)	C11—H11B	0.9600
C4—C5	1.416 (3)	C11—H11C	0.9600
C5—C6	1.377 (3)		
C1—N1—C9	116.50 (17)	C8—C7—C6	122.5 (2)
N1—C1—C2	126.42 (19)	C8—C7—H7	118.7
N1—C1—Cl1	114.64 (15)	C6—C7—H7	118.7
C2—C1—Cl1	118.93 (14)	C7—C8—C9	119.9 (2)
C3—C2—C1	116.68 (17)	C7—C8—H8	120.0
C3—C2—C10	120.06 (19)	C9—C8—H8	120.0
C1—C2—C10	123.25 (19)	N1—C9—C4	122.69 (17)
C2—C3—C4	120.41 (18)	N1—C9—C8	118.51 (19)
C2—C3—H3	119.8	C4—C9—C8	118.81 (19)
C4—C3—H3	119.8	O1—C10—C2	123.4 (2)
C3—C4—C9	117.27 (17)	O1—C10—H10	118.3
C3—C4—C5	123.20 (18)	C2—C10—H10	118.3
C9—C4—C5	119.53 (17)	C6—C11—H11A	109.5
C6—C5—C4	120.73 (19)	C6—C11—H11B	109.5

C6—C5—H5	119.6	H11A—C11—H11B	109.5
C4—C5—H5	119.6	C6—C11—H11C	109.5
C5—C6—C7	118.4 (2)	H11A—C11—H11C	109.5
C5—C6—C11	121.8 (2)	H11B—C11—H11C	109.5
C7—C6—C11	119.78 (19)		
C9—N1—C1—C2	1.0 (3)	C5—C6—C7—C8	−0.6 (3)
C9—N1—C1—Cl1	−179.69 (15)	C11—C6—C7—C8	−180.0 (2)
N1—C1—C2—C3	−1.7 (3)	C6—C7—C8—C9	0.4 (3)
Cl1—C1—C2—C3	179.00 (15)	C1—N1—C9—C4	0.9 (3)
N1—C1—C2—C10	177.0 (2)	C1—N1—C9—C8	−179.45 (19)
Cl1—C1—C2—C10	−2.3 (3)	C3—C4—C9—N1	−2.0 (3)
C1—C2—C3—C4	0.5 (3)	C5—C4—C9—N1	178.91 (17)
C10—C2—C3—C4	−178.30 (18)	C3—C4—C9—C8	178.38 (18)
C2—C3—C4—C9	1.2 (3)	C5—C4—C9—C8	−0.7 (3)
C2—C3—C4—C5	−179.73 (19)	C7—C8—C9—N1	−179.4 (2)
C3—C4—C5—C6	−178.44 (18)	C7—C8—C9—C4	0.2 (3)
C9—C4—C5—C6	0.6 (3)	C3—C2—C10—O1	13.5 (4)
C4—C5—C6—C7	0.0 (3)	C1—C2—C10—O1	−165.1 (3)
C4—C5—C6—C11	179.4 (2)		

Fig. 1