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2-Chloroquinoline-3-carbaldehyde

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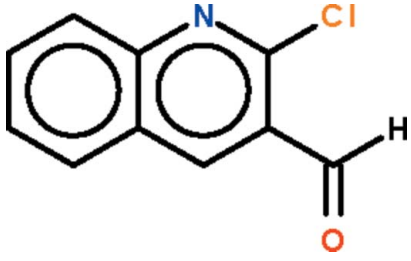
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.002 Å; R factor = 0.033; wR factor = 0.145; data-to-parameter ratio = 16.0.

The quinolinyl fused ring system of the title compound, $C_{10}H_6ClNO$, is planar (r.m.s. deviation = 0.018 Å); the formyl group is slightly bent out of the plane of the fused ring system [C—C—C—O torsion angle = 8.2 (3)°].

Related literature

For the synthesis of 2-chloroquinoline-3-carbaldehyde by Vilsmeier–Haack cyclization, see: Ali *et al.* (2001, 2002); Mogilaiah *et al.* (2002); Pawar *et al.* (1990); Srivastava & Singh (2005). For a review of the synthesis of quinolines by this reaction, see: Meth-Cohn (1993).



Experimental

Crystal data

$C_{10}H_6ClNO$ M_r = 191.61
Monoclinic, $P2_1/n$
a = 11.8784 (9) Å
b = 3.9235 (3) Å
c = 18.1375 (12) Å
β = 101.365 (4)°
V = 828.72 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.41 mm^{-1}
T = 290 K
0.24 × 0.18 × 0.14 mm

Data collection

Bruker SMART area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.908, T_{max} = 0.945
6886 measured reflections
1889 independent reflections
1626 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.145
S = 1.19
1889 reflections
118 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 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: TK2549).

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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 to *N*-phenylacetamide (1.35 g, 10 mmol), 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.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93 Å) and were included in the refinement in the riding model approximation with U_{iso}(H) set to 1.2U_{eq}(C).

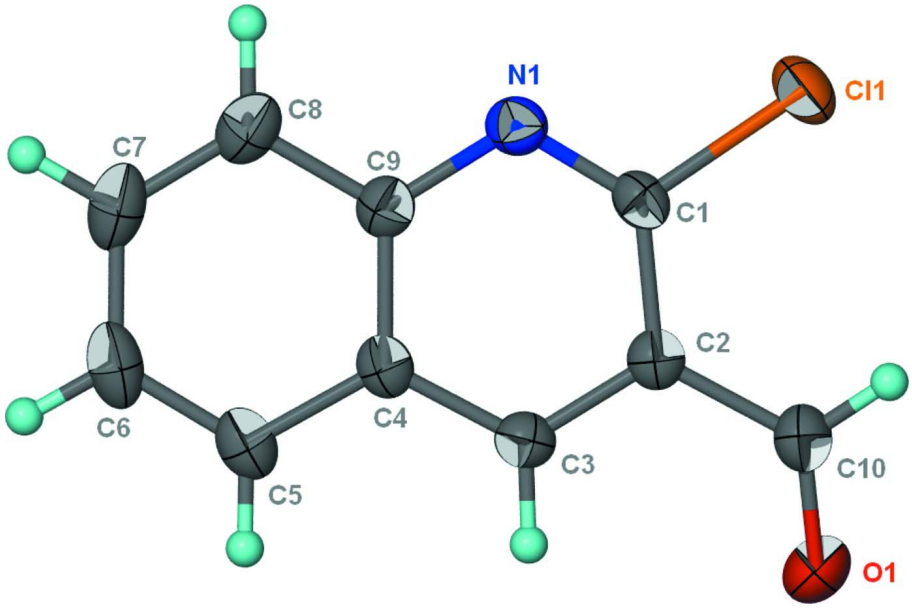

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{10}H_6ClNO$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-Chloroquinoline-3-carbaldehyde

Crystal data

$C_{10}H_6ClNO$
M_r = 191.61
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 11.8784 (9) Å
b = 3.9235 (3) Å

c = 18.1375 (12) Å
β = 101.365 (4)°
V = 828.72 (10) Å^3
Z = 4
F(000) = 392
D_x = 1.536 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 781 reflections
θ = 2.1–24.3°
μ = 0.41 mm^{-1}
T = 290 K
Block, colorless
0.24 × 0.18 × 0.14 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} = 0.908, T_{max} = 0.945

6886 measured reflections
1889 independent reflections
1626 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 27.5°, θ_{min} = 1.9°
h = −15→15
k = −3→5
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.145
S = 1.19
1889 reflections
118 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
$w = 1/[\sigma^2(F_o^2) + (0.0923P)^2 + 0.077P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.24556 (4)	0.22180 (12)	0.67041 (2)	0.0464 (2)
O1	0.51095 (11)	0.8482 (4)	0.61287 (8)	0.0550 (4)
N1	0.15508 (12)	0.2731 (3)	0.52950 (9)	0.0353 (3)
C1	0.24476 (14)	0.3582 (4)	0.57833 (9)	0.0319 (4)
C2	0.34039 (13)	0.5468 (4)	0.56384 (9)	0.0323 (4)
C3	0.33695 (13)	0.6369 (4)	0.49061 (9)	0.0334 (4)
H3	0.3977	0.7585	0.4781	0.040*
C4	0.24263 (13)	0.5477 (4)	0.43407 (9)	0.0324 (4)
C5	0.23434 (16)	0.6341 (5)	0.35765 (10)	0.0419 (4)
H5	0.2944	0.7483	0.3424	0.050*
C6	0.13859 (17)	0.5504 (5)	0.30635 (10)	0.0481 (5)
H6	0.1334	0.6077	0.2560	0.058*
C7	0.04727 (17)	0.3774 (6)	0.32911 (11)	0.0493 (5)
H7	−0.0180	0.3243	0.2935	0.059*
C8	0.05247 (16)	0.2861 (5)	0.40222 (12)	0.0436 (4)
H8	−0.0082	0.1699	0.4162	0.052*
C9	0.15087 (13)	0.3697 (4)	0.45629 (9)	0.0325 (4)
C10	0.43810 (15)	0.6537 (5)	0.62315 (10)	0.0407 (4)
H10	0.4432	0.5645	0.6712	0.049*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0587 (3)	0.0522 (3)	0.0308 (3)	−0.00331 (19)	0.0147 (2)	0.00444 (16)
O1	0.0435 (8)	0.0681 (10)	0.0499 (8)	−0.0161 (6)	0.0004 (6)	0.0003 (7)
N1	0.0363 (7)	0.0355 (7)	0.0355 (8)	−0.0016 (5)	0.0107 (6)	−0.0029 (5)
C1	0.0381 (8)	0.0310 (8)	0.0283 (7)	0.0020 (6)	0.0107 (6)	0.0004 (6)
C2	0.0335 (8)	0.0312 (8)	0.0321 (8)	0.0024 (6)	0.0062 (6)	−0.0007 (6)
C3	0.0329 (8)	0.0332 (8)	0.0349 (8)	−0.0001 (6)	0.0089 (6)	0.0018 (7)
C4	0.0362 (8)	0.0317 (8)	0.0299 (8)	0.0056 (6)	0.0077 (6)	−0.0005 (6)
C5	0.0489 (10)	0.0444 (9)	0.0332 (9)	0.0076 (8)	0.0101 (7)	0.0039 (7)
C6	0.0591 (11)	0.0544 (11)	0.0289 (8)	0.0166 (9)	0.0039 (8)	−0.0021 (8)
C7	0.0454 (10)	0.0560 (11)	0.0407 (10)	0.0110 (8)	−0.0058 (8)	−0.0141 (9)
C8	0.0356 (9)	0.0467 (10)	0.0466 (11)	0.0012 (7)	0.0037 (8)	−0.0120 (8)
C9	0.0331 (8)	0.0320 (8)	0.0329 (8)	0.0032 (6)	0.0072 (6)	−0.0052 (6)
C10	0.0414 (9)	0.0459 (10)	0.0332 (9)	−0.0003 (7)	0.0031 (7)	0.0017 (7)

Geometric parameters (Å, º)

Cl1—C1	1.7519 (16)	C4—C9	1.418 (2)
O1—C10	1.196 (2)	C5—C6	1.360 (3)
N1—C1	1.288 (2)	C5—H5	0.9300
N1—C9	1.372 (2)	C6—C7	1.409 (3)
C1—C2	1.423 (2)	C6—H6	0.9300
C2—C3	1.367 (2)	C7—C8	1.363 (3)
C2—C10	1.479 (2)	C7—H7	0.9300
C3—C4	1.406 (2)	C8—C9	1.409 (2)
C3—H3	0.9300	C8—H8	0.9300
C4—C5	1.411 (2)	C10—H10	0.9300
C1—N1—C9	117.48 (14)	C5—C6—C7	120.28 (17)
N1—C1—C2	126.15 (15)	C5—C6—H6	119.9
N1—C1—Cl1	115.14 (12)	C7—C6—H6	119.9
C2—C1—Cl1	118.71 (12)	C8—C7—C6	121.46 (17)
C3—C2—C1	116.22 (14)	C8—C7—H7	119.3
C3—C2—C10	120.14 (15)	C6—C7—H7	119.3
C1—C2—C10	123.62 (15)	C7—C8—C9	119.23 (18)
C2—C3—C4	120.74 (14)	C7—C8—H8	120.4
C2—C3—H3	119.6	C9—C8—H8	120.4
C4—C3—H3	119.6	N1—C9—C8	118.45 (15)
C3—C4—C5	123.22 (15)	N1—C9—C4	121.83 (14)
C3—C4—C9	117.52 (14)	C8—C9—C4	119.71 (16)
C5—C4—C9	119.24 (15)	O1—C10—C2	123.76 (16)
C6—C5—C4	120.07 (17)	O1—C10—H10	118.1
C6—C5—H5	120.0	C2—C10—H10	118.1
C4—C5—H5	120.0		
C9—N1—C1—C2	0.6 (2)	C5—C6—C7—C8	−0.8 (3)

C9—N1—C1—Cl1	−179.13 (11)	C6—C7—C8—C9	0.7 (3)
N1—C1—C2—C3	−1.8 (2)	C1—N1—C9—C8	−178.61 (14)
Cl1—C1—C2—C3	177.90 (11)	C1—N1—C9—C4	1.8 (2)
N1—C1—C2—C10	176.39 (16)	C7—C8—C9—N1	−179.43 (15)
Cl1—C1—C2—C10	−3.9 (2)	C7—C8—C9—C4	0.1 (3)
C1—C2—C3—C4	0.6 (2)	C3—C4—C9—N1	−2.9 (2)
C10—C2—C3—C4	−177.67 (14)	C5—C4—C9—N1	178.69 (15)
C2—C3—C4—C5	179.92 (15)	C3—C4—C9—C8	177.57 (15)
C2—C3—C4—C9	1.5 (2)	C5—C4—C9—C8	−0.9 (2)
C3—C4—C5—C6	−177.55 (16)	C3—C2—C10—O1	8.2 (3)
C9—C4—C5—C6	0.8 (3)	C1—C2—C10—O1	−170.0 (2)
C4—C5—C6—C7	0.0 (3)		