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2-Chloroquinoline-3-carbaldehyde

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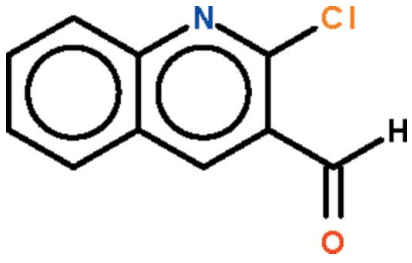
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.002 Å; R factor = 0.033; wR factor = 0.145; data-to-parameter ratio = 16.0.

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).

References

Ali, M. M., Sana, S., Tasneem, Rajanna, K. C. & Saiprakash, P. K. (2002). *Synth. Commun.* **32**, 1351–1356.
Ali, M. M., Tasneem, Rajanna, K. C. & Prakash, P. K. S. (2001). *Synlett*, pp. 251–253.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2004). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Meth-Cohn, O. (1993). *Heterocycles*, **35**, 539–557.
Mogilaiah, K., Reddy, N. V. & Rao, R. B. (2002). *Indian J. Heterocycl. Chem.* **11**, 253–254. .
Pawar, R. A., Bajare, P. B. & Mundade, S. B. (1990). *J. Indian Chem. Soc.* **67**, 685-686.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Srivastava, A. & Singh, R. M. (2005). *Indian J. Chem. Sect. B*, **44**, 1868–1875.
Westrip, S. P. (2009). *publCIF*. In preparation.

supplementary materials

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2-Chloroquinoline-3-carbaldehyde

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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.

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).

Figures

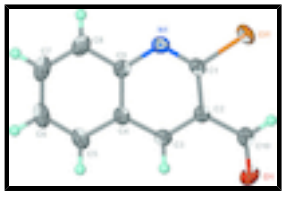

Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $C_{10}H_6ClNO$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-Chloroquinoline-3-carbaldehyde

Crystal data

$C_{10}H_6ClNO$	F_{000} = 392
M_r = 191.61	D_x = 1.536 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 781 reflections
a = 11.8784 (9) Å	θ = 2.1–24.3º
b = 3.9235 (3) Å	μ = 0.41 mm^{-1}
c = 18.1375 (12) Å	T = 290 K
β = 101.365 (4)º	Block, colorless
V = 828.72 (10) Å^3	0.24 × 0.18 × 0.14 mm
Z = 4	

Data collection

Bruker SMART area-detector diffractometer	1889 independent reflections

Radiation source: fine-focus sealed tube	1626 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.021$
$T = 290$ K	$\theta_{max} = 27.5^o$
φ and ω scans	$\theta_{min} = 1.9^o$
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	$h = -15\rightarrow15$
$T_{min} = 0.908$, $T_{max} = 0.945$	$k = -3\rightarrow5$
6886 measured reflections	$l = -23\rightarrow23$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.033$	H-atom parameters constrained
$wR(F^2) = 0.145$	$w = 1/[\sigma^2(F_o^2) + (0.0923P)^2 + 0.077P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.19$	$(\Delta/\sigma)_{max} = 0.001$
1889 reflections	$\Delta\rho_{max} = 0.36$ e Å^{-3}
118 parameters	$\Delta\rho_{min} = -0.29$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 (Å^2)

	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, °)

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)		

Fig. 1