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(2-Chloro-6-methylquinolin-3-yl)-methanol

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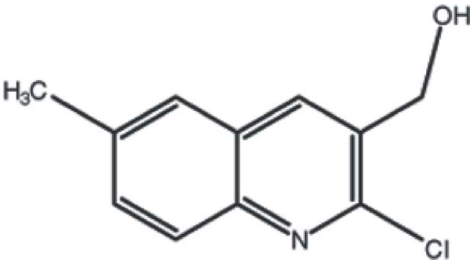
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; R factor = 0.085; wR factor = 0.222; data-to-parameter ratio = 13.1.

The title compound, $C_{11}H_{10}ClNO$, is close to being planar (r.m.s deviation for the non-H atoms = 0.026 Å). In the crystal, molecules are linked by O—H⋯O hydrogen bonds, generating $C(2)$ chains, and weak C—H⋯π interactions and aromatic π–π stacking interactions [centroid–centroid distance = 3.713 (3) Å] help to consolidate the sturcture.

Related literature

For a related structure and background references, see: Roopan *et al.* (2010). For the structure of the starting material, see: Khan *et al.* (2009). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{11}H_{10}ClNO$
M_r = 207.65
Monoclinic, $P2_1/c$
a = 14.8091 (17) Å
b = 4.6387 (5) Å
c = 14.5098 (11) Å
β = 96.594 (9)°
V = 990.16 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 295 K
0.35 × 0.15 × 0.08 mm

Data collection

Oxford Xcalibur Eos(Nova) CCD diffractometer
Absorption correction: multi-scan *CrysAlis PRO* RED (Oxford Diffraction, 2009)
T_{min} = 0.888, T_{max} = 0.973
15485 measured reflections
1721 independent reflections
913 reflections with $I > 2\sigma(I)$
R_{int} = 0.136

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.085
$wR(F^2)$ = 0.222
S = 0.94
1721 reflections
131 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

$Cg1$ is the centroid of the N1/C1/C6–C9 ring.

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1—H1O⋯O1^{i}	0.79 (6)	1.93 (6)	2.716 (5)	177 (7)
C10—H10A⋯$Cg1^{ii}$	0.97	2.73	3.526 (5)	139

Symmetry codes: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, y+1, z$.

Data collection: *CrysAlis PRO CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO CCD*; data reduction: *CrysAlis PRO RED* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We thank the Department of Science and Technology, India, for use of the CCD facility set up under the FIST–DST program at SSCU, IISc. We also thank Professor T. N. Guru Row, IISc, Bangalore, for his help with the data collection. FNK thanks the DST for Fast Track Proposal funding.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5471).

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supplementary materials

Acta Cryst. (2010). E**66**, o1544 [**doi:10.1107/S1600536810020507**]

(2-Chloro-6-methylquinolin-3-yl)methanol

F. N. Khan, S. M. Roopan, A. K. Kushwaha, V. R. Hathwar and **M. Akkurt**

Comment

The importance and general background of the title compound is given in our earler paper (Roopan *et al.*, 2010).

The molecule of the title compound, (I), (Fig. 1), except the hydroxyl and methyl H atoms, is close to planar (r.m.s deviation 0.026 Å).

An intramolecular C—H···O hydrogen bond generates an S(5) ring motif (Bernstein *et al.*, 1995). Molecules of (I) are linked *via* O—H···O hydrogen bonds (Table 1, Fig. 2), an intermolecular C–H···π interactions between the aromatic H atoms of the ethenol substituent and the pyridine (N1/C1/C6–C9) ring of an adjacent molecule (Table 1), and π-π stacking interactions helping to stabilize the crystal structure [$Cg1\cdots Cg2(x, 1+y, z)$ = 3.713 (3) Å, where *Cg*1 and *Cg*2 are centroids of the N1/C1/C6–C9 and C1–C6 rings, respectively].

Experimental

2-Chloro-6-methylquinoline-3-carbaldehyde (206 mg, 1 mmol), sodium borohydride (38 mg, 1 mmol) and catalytic amount of montmorillonite K-10 were taken in an open vessel and the resulting mixture was irradiating at 500 W for 5 min. Ethylacetate was poured into the reaction mixture and filtered off. The filtrated after removal of solvent was subjected to column chromatography packed with silica and ethyl acetate/petroleum ether was used as the eluant. Colourless plates of (I) were grown by solvent evaporation from a solution of the compound in chloroform.

Refinement

The H atom of the OH group were located in difference map and its positional parameters were refined freely [O1—H1O = 0.79 (6) Å]. The other H atoms were positioned geometrically, with C—H = 0.93–0.97 Å, and refined as riding with $U_{iso}(H)$ = 1.2 or 1.5 $U_{eq}(C)$. The value of R_{int} [0.136] is greater than 0.12. Since the overall quality of the data may be poor due to the crystal quality.

Figures

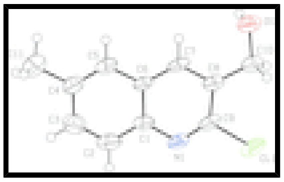

Fig. 1. View of the molecular structure of (I), showing 50% probability displacement ellipsoids.

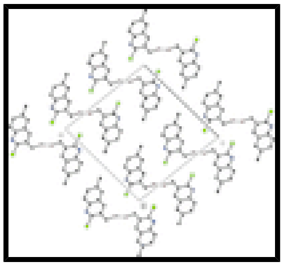

Fig. 2. Molecular packing and the hydrogen bonding of (I) viewed down *b* axis. The H atoms not involved in hydrogen bonds have been omitted for clarity.

(2-Chloro-6-methylquinolin-3-yl)methanol

Crystal data

$C_{11}H_{10}ClNO$

$M_r = 207.65$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 14.8091\ (17)$ Å

$b = 4.6387\ (5)$ Å

$c = 14.5098\ (11)$ Å

$\beta = 96.594\ (9)°$

$V = 990.16\ (17)$ Å^3

$Z = 4$

$F(000) = 432$

$D_x = 1.393$ Mg m^{-3}

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 865 reflections

$\theta = 2.7$–$21.4°$

$\mu = 0.35$ mm^{-1}

$T = 295$ K

Plate, colourless

0.35 × 0.15 × 0.08 mm

Data collection

Oxford Xcalibur Eos(Nova) CCD diffractometer

Radiation source: Enhance (Mo) X-ray Source

graphite

ω scans

Absorption correction: multi-scan *CrysAlis PRO* RED (Oxford Diffraction, 2009)

$T_{min} = 0.888$, $T_{max} = 0.973$

15485 measured reflections

1721 independent reflections

913 reflections with $I > 2\sigma(I)$

$R_{int} = 0.136$

$\theta_{max} = 25.0°$, $\theta_{min} = 3.0°$

$h = -17 \rightarrow 17$

$k = -5 \rightarrow 5$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.085$

$wR(F^2) = 0.222$

$S = 0.94$

1721 reflections

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.1359P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

131 parameters	$\Delta\rho_{max}$ = 0.41 e Å^{-3}
0 restraints	$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.13152 (10)	0.6780 (3)	−0.04947 (8)	0.0717 (6)
O1	0.0334 (3)	0.9035 (7)	0.2189 (2)	0.0580 (14)
N1	0.2440 (3)	0.3573 (8)	0.0535 (2)	0.0448 (14)
C1	0.2832 (3)	0.2406 (10)	0.1357 (3)	0.0409 (16)
C2	0.3535 (3)	0.0442 (11)	0.1360 (3)	0.0554 (19)
C3	0.3939 (3)	−0.0710 (12)	0.2179 (4)	0.0583 (19)
C4	0.3645 (3)	0.0074 (11)	0.3034 (3)	0.0529 (19)
C5	0.2963 (3)	0.1980 (10)	0.3040 (3)	0.0454 (16)
C6	0.2534 (3)	0.3238 (9)	0.2222 (3)	0.0369 (16)
C7	0.1817 (3)	0.5231 (9)	0.2194 (3)	0.0438 (16)
C8	0.1412 (3)	0.6383 (9)	0.1376 (3)	0.0414 (16)
C9	0.1799 (3)	0.5394 (10)	0.0572 (3)	0.0454 (16)
C10	0.0641 (3)	0.8449 (9)	0.1312 (3)	0.0465 (17)
C11	0.4114 (4)	−0.1220 (14)	0.3929 (4)	0.078 (2)
H1O	0.014 (4)	0.756 (13)	0.235 (4)	0.0870*
H2	0.37380	−0.01050	0.08020	0.0670*
H3	0.44130	−0.20220	0.21680	0.0700*
H5	0.27670	0.24850	0.36050	0.0550*
H7	0.16080	0.57900	0.27480	0.0520*
H10A	0.08270	1.02420	0.10460	0.0560*
H10B	0.01400	0.76690	0.08970	0.0560*
H11A	0.37370	−0.09620	0.44180	0.1170*
H11B	0.46870	−0.02720	0.40930	0.1170*
H11C	0.42160	−0.32400	0.38410	0.1170*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0999 (12)	0.0913 (12)	0.0243 (7)	0.0084 (8)	0.0089 (6)	0.0093 (6)
O1	0.085 (3)	0.051 (2)	0.043 (2)	0.0031 (19)	0.0292 (17)	−0.0008 (17)

N1	0.066 (3)	0.048 (2)	0.0223 (19)	−0.001 (2)	0.0139 (17)	−0.0045 (16)
C1	0.048 (3)	0.051 (3)	0.025 (2)	−0.003 (2)	0.0102 (18)	−0.007 (2)
C2	0.061 (3)	0.073 (4)	0.035 (3)	−0.005 (3)	0.018 (2)	−0.007 (2)
C3	0.056 (3)	0.069 (4)	0.051 (3)	0.004 (3)	0.011 (2)	−0.009 (3)
C4	0.056 (3)	0.070 (4)	0.033 (3)	−0.001 (3)	0.007 (2)	0.006 (2)
C5	0.056 (3)	0.056 (3)	0.025 (2)	−0.005 (2)	0.008 (2)	−0.004 (2)
C6	0.050 (3)	0.041 (3)	0.021 (2)	−0.001 (2)	0.0102 (18)	−0.0049 (18)
C7	0.063 (3)	0.053 (3)	0.017 (2)	−0.009 (3)	0.0118 (19)	−0.0055 (19)
C8	0.056 (3)	0.042 (3)	0.028 (2)	−0.007 (2)	0.0125 (19)	−0.003 (2)
C9	0.068 (3)	0.049 (3)	0.020 (2)	−0.005 (3)	0.009 (2)	0.000 (2)
C10	0.070 (3)	0.037 (3)	0.035 (3)	−0.003 (2)	0.017 (2)	−0.003 (2)
C11	0.087 (4)	0.105 (5)	0.041 (3)	0.009 (3)	0.001 (3)	0.006 (3)

Geometric parameters (Å, °)

Cl1—C9	1.751 (5)	C7—C8	1.375 (6)
O1—C10	1.426 (5)	C8—C9	1.433 (6)
O1—H1O	0.79 (6)	C8—C10	1.485 (6)
N1—C9	1.276 (6)	C2—H2	0.9300
N1—C1	1.376 (5)	C3—H3	0.9300
C1—C2	1.383 (7)	C5—H5	0.9300
C1—C6	1.431 (6)	C7—H7	0.9300
C2—C3	1.376 (7)	C10—H10A	0.9700
C3—C4	1.409 (7)	C10—H10B	0.9700
C4—C11	1.524 (7)	C11—H11A	0.9600
C4—C5	1.343 (7)	C11—H11B	0.9600
C5—C6	1.407 (6)	C11—H11C	0.9600
C6—C7	1.405 (6)		

C10—O1—H1O	105 (4)	O1—C10—C8	112.9 (4)
C1—N1—C9	117.8 (4)	C1—C2—H2	120.00
N1—C1—C2	120.3 (4)	C3—C2—H2	120.00
N1—C1—C6	120.8 (4)	C2—C3—H3	120.00
C2—C1—C6	118.9 (4)	C4—C3—H3	120.00
C1—C2—C3	120.7 (4)	C4—C5—H5	119.00
C2—C3—C4	120.8 (4)	C6—C5—H5	119.00
C3—C4—C11	119.5 (4)	C6—C7—H7	119.00
C5—C4—C11	121.6 (4)	C8—C7—H7	119.00
C3—C4—C5	119.0 (4)	O1—C10—H10A	109.00
C4—C5—C6	122.3 (4)	O1—C10—H10B	109.00
C1—C6—C5	118.3 (4)	C8—C10—H10A	109.00
C5—C6—C7	124.3 (4)	C8—C10—H10B	109.00
C1—C6—C7	117.4 (4)	H10A—C10—H10B	108.00
C6—C7—C8	122.3 (4)	C4—C11—H11A	110.00
C7—C8—C10	124.1 (4)	C4—C11—H11B	110.00
C9—C8—C10	122.2 (4)	C4—C11—H11C	110.00
C7—C8—C9	113.8 (4)	H11A—C11—H11B	109.00
Cl1—C9—N1	115.9 (3)	H11A—C11—H11C	110.00
N1—C9—C8	128.0 (4)	H11B—C11—H11C	109.00
Cl1—C9—C8	116.2 (3)		

C9—N1—C1—C2	−179.4 (4)	C11—C4—C5—C6	178.8 (5)
C9—N1—C1—C6	−0.6 (7)	C4—C5—C6—C1	1.0 (7)
C1—N1—C9—Cl1	−179.3 (3)	C4—C5—C6—C7	179.8 (5)
C1—N1—C9—C8	−1.1 (7)	C1—C6—C7—C8	−0.5 (6)
N1—C1—C2—C3	179.2 (5)	C5—C6—C7—C8	−179.3 (4)
C6—C1—C2—C3	0.4 (7)	C6—C7—C8—C9	−0.9 (6)
N1—C1—C6—C5	−179.8 (4)	C6—C7—C8—C10	178.7 (4)
N1—C1—C6—C7	1.4 (6)	C7—C8—C9—Cl1	−180.0 (3)
C2—C1—C6—C5	−1.0 (6)	C7—C8—C9—N1	1.8 (7)
C2—C1—C6—C7	−179.8 (4)	C10—C8—C9—Cl1	0.4 (6)
C1—C2—C3—C4	0.2 (8)	C10—C8—C9—N1	−177.8 (4)
C2—C3—C4—C5	−0.2 (7)	C7—C8—C10—O1	−2.5 (6)
C2—C3—C4—C11	−179.4 (5)	C9—C8—C10—O1	177.1 (4)
C3—C4—C5—C6	−0.4 (7)		

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the N1/C1/C6–C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1O···O1$^{\mathrm{i}}$	0.79 (6)	1.93 (6)	2.716 (5)	177 (7)
C10—H10A···Cg1$^{\mathrm{ii}}$	0.97	2.73	3.526 (5)	139

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+1/2; (ii) *x*, *y*+1, *z*.

Fig. 1

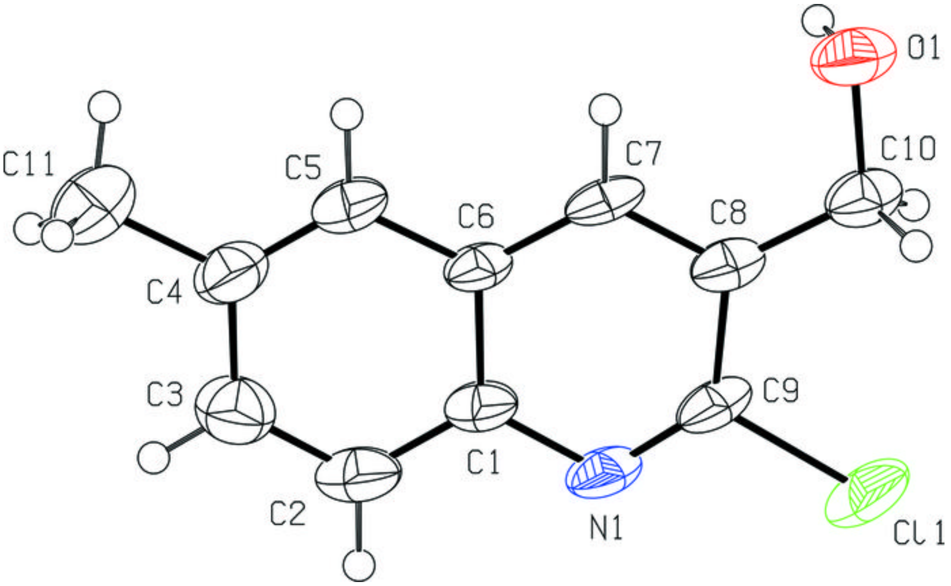

Fig. 2