Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Chloro-4-methylquinoline

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Received 27 November 2000
Accepted 4 December 2000
Online 14 December 2000

Key indicators

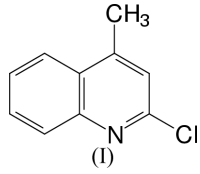
Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.115
Data-to-parameter ratio = 17.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The structure of the title compound, $C_{10}H_8ClN$, comprises planar molecules that form stacked columns parallel to the b cell direction. Two symmetry-related molecules associate *via* C—H···N interactions to form a non-planar $R_2^2(8)$ dimer.

Experimental

The title compound, (I), was prepared by Spa Contract Synthesis. Crystals of (I) were grown from a methanol solution.



(I)

Crystal data

$C_{10}H_8ClN$
M_r = 177.62
Orthorhombic, *Pbca*
a = 12.721 (3) Å
b = 7.8961 (16) Å
c = 16.617 (3) Å
V = 1669.1 (6) Å^3
Z = 8
D_x = 1.414 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3728 reflections
θ = 2.9–27.5°
μ = 0.39 mm^{-1}
T = 150 (2) K
Plate, colourless
0.20 × 0.15 × 0.07 mm

Data collection

Enraf–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.926, T_{max} = 0.973
7671 measured reflections
1892 independent reflections
1466 reflections with $I > 2\sigma(I)$
R_{int} = 0.074
θ_{max} = 27.5°
$h = -16 \rightarrow 16$
$k = -10 \rightarrow 10$
$l = -21 \rightarrow 17$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.115
S = 1.02
1892 reflections
110 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0699P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···N1^{i}	0.95	2.61	3.517 (2)	160

Symmetry code: (i) $1-x, -y, 1-z$.

All H atoms were included in the refinement at calculated positions as riding models, with C—H set to 0.95 (Ar–H) and 0.98 Å (CH_3).

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

The authors thank the EPSRC National Crystallography Service (Southampton).

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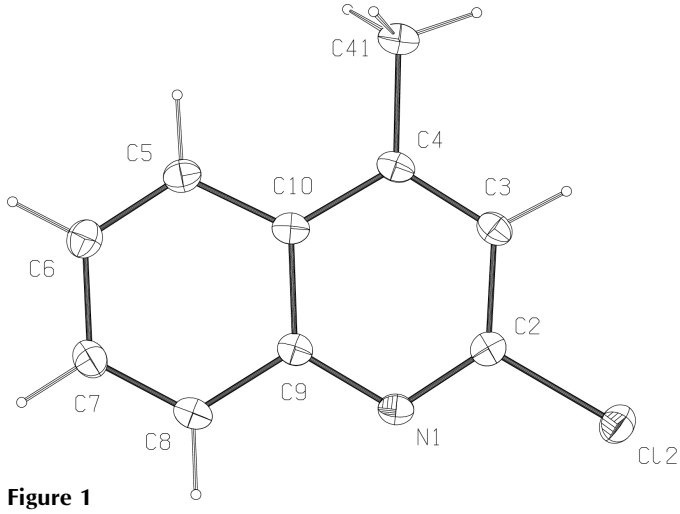

Figure 1
The molecular configuration and atom-numbering scheme for (I), showing 30% probability displacement ellipsoids.