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3-Chloro-2-methylquinolin-4(1*H*)-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.050
wR factor = 0.151
Data-to-parameter ratio = 13.8

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

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The title compound, $C_{10}H_8ClNO$, crystallizes in the centrosymmetric space group $C2/c$. The compound exists in the keto form in the crystalline state. The heterocyclic ring is not aromatic. The N atom is sp^2 hybridized. The structure is stabilized by N—H···O intermolecular hydrogen bonds.

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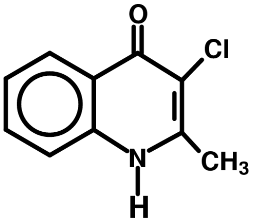
Comment

Quinolines are ligands which are used as complexing agents for different metals (Hensen *et al.*, 1999). The structure determination of the title compound, (I), was undertaken to study the effect of substitutions at the 2 and 3 positions on the quinolinone ring as well as the nature of the hydrogen bonding.



(I)

The torsion angles and the least-squares plane confirm that the quinolinone ring is planar with the largest out-of-plane displacement for C4 [0.051 (2) Å]. The exocyclic angles of C3—C2—C11 [124.4 (2)°] and C3—C4—O4 [124.4 (2)°] deviate significantly from the normal value of 120°. This may be due to the steric repulsion between the substituents at positions 2 and 3, and at 3 and 4 respectively. The C4═O4 bond length [1.255 (3) Å] indicates a typical double-bond character and keto form of the compound in the crystalline state. In the non-aromatic heterocyclic ring, due to conjugation in N1—C2═C3—C4═O4, C3—C4 [1.421 (3) Å] shows the characteristic shortening of the bond from the normal value of 1.478 Å (Allen *et al.*, 1987). In the absence of substituents at C2, the average bond distance of N1—C2 is 1.310 (3) Å in related structures (Dobson & Gerkin, 1999; Lokaj *et al.*, 1999). In the present structure, due to the substitution of the methyl group at C2, there is a significant increase in the bond length N1—C2 [1.342 (3) Å] from the average value. The N atom is sp^2 hybridized. The structure is stabilized by a linear intermolecular hydrogen bond N1—H1···O4^{i} [symmetry code: (i) $x, -y, z+\frac{1}{2}$]. The hydrogen-bond parameters are: N1—H1 = 0.89 Å, N1···O4^{i} = 2.712 (2) Å, H1···O4^{i} = 1.825 Å and N1—H1···O4^{i} = 174°. All the other intermolecular interactions are van der Waals in nature.

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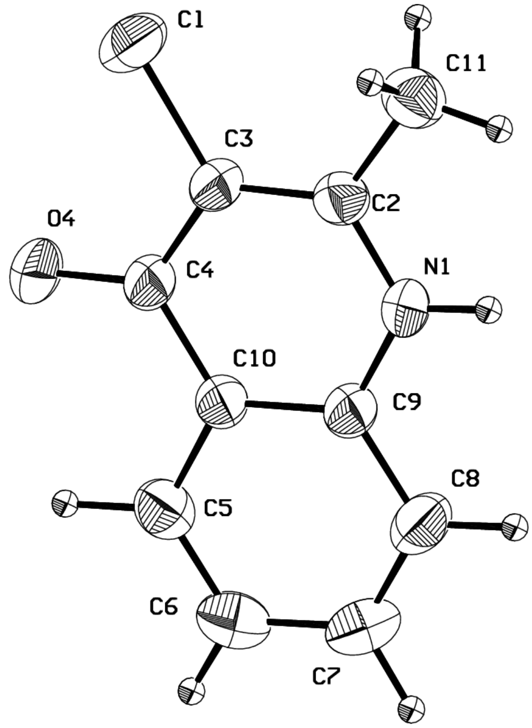

Figure 1
The molecular structure of (I) showing 50% probability displacement ellipsoids.

Experimental

2-Methyl-4-quinolone was treated with an equimolar amount of *N*-chlorosuccinimide in glacial acetic acid at 323–333 K for 30 min. The reaction mixture was poured over ice and the solid was filtered. It was washed with ice-cold water and dried over anhydrous calcium chloride (yield 75%). The compound was crystallized from ethanol by slow evaporation at 298–303 K.

Crystal data

$C_{10}H_8ClNO$
$M_r = 193.62$
Monoclinic, *C*2/*c*
$a = 24.493$ (4) Å
$b = 6.365$ (2) Å
$c = 12.859$ (8) Å
$\beta = 117.240$ (3)°
$V = 1782.2$ (13) Å^3
$Z = 8$
$D_x = 1.443$ Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 20$–30°
$\mu = 3.42$ mm^{-1}
$T = 293$ (2) K
Plate, yellow
0.35 × 0.20 × 0.15 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.320$, $T_{\max} = 0.603$
1661 measured reflections
1624 independent reflections
1440 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.050$
$\theta_{\max} = 68.0°$
$h = 0 \rightarrow 29$
$k = 0 \rightarrow 7$
$l = -15 \rightarrow 13$
2 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.151$
$S = 1.08$
1624 reflections
118 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0966P)^2 + 1.8554P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.002$
$\Delta\rho_{\max} = 0.43$ e Å^{-3}
$\Delta\rho_{\min} = -0.36$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C9	1.373 (3)	C5—C10	1.405 (3)
C5—C6	1.364 (4)	C9—C10	1.400 (3)
N1—C2—C3	119.1 (2)	N1—C9—C8	120.8 (2)
N1—C2—C11	116.5 (2)	N1—C9—C10	119.4 (2)
C2—C3—Cl	119.55 (18)	C9—C10—C5	119.0 (2)
O4—C4—C3	124.4 (2)	C9—C10—C4	120.1 (2)
C9—N1—C2—C3	−2.8 (3)	Cl—C3—C4—C10	−177.38 (16)
N1—C2—C3—C4	0.9 (3)	C7—C8—C9—C10	−2.2 (4)
C2—C3—C4—O4	−178.1 (2)	O4—C4—C10—C9	176.3 (2)

All H atoms, except the methyl H atoms, were located from difference Fourier maps and were included in the structure-factor calculations with isotropic displacement parameters equal to $1.1U_{\rm eq}$ of their respective carrier atom, but their parameters were not refined. The methyl H atoms were fixed with HFIX options of the *SHELX* program, using the riding model. $U_{\rm iso}$ of methyl H atoms were taken as $1.5U_{\rm eq}$(C11).

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ZORTEP* (Zsolnai, 1997); software used to prepare material for publication: *SHELXL*97.

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