

7-Chloro-8-methylcarbostyryl*

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Abstract. C₁₀H₈ClNO, monoclinic, $P2_1/c$, $a = 14.343(4)$, $b = 4.175(1)$, $c = 16.023(4)$ Å, $\beta = 114.963(8)^\circ$, $V = 869.85$ Å³, $Z = 4$, $D_m = 1.469$, $D_c = 1.477$ Mg m⁻³, $M_r = 193.6$. The structure was solved by direct methods and refined to an R of 0.052 for 1388 reflections. The entire molecule is nearly planar. The N—H...O hydrogen-bond distance is 2.878(4) Å.

Introduction. The structure analysis of the title compound (Fig. 1) was undertaken as a part of the study on the packing characteristics of naphthalene, quinoline and carbostyryl derivatives. A sample of 7-chloro-8-methylcarbostyryl was kindly supplied by Dr T. Manimaran, Department of Medicinal Chemistry, University of Illinois, Chicago. Crystals were obtained by slow evaporation from a mixture of benzene and chloroform. The cell parameters were derived from a least-squares refinement (Main & Woolfson, 1963) of 24 reflections. Intensity data for 1389 reflections were collected using a Picker four-circle diffractometer with $\theta/2\theta$ scan, Ni-filtered Cu $K\alpha$ radiation ($\lambda = 1.5418$ Å)

* IUPAC name: 7-chloro-8-methyl-2(1H)-quinolinone.

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Table 1. Fractional positional parameters ($\times 10^4$) and equivalent isotropic temperature factors for the non-H atoms with e.s.d.'s in parentheses

$$B_{eq} = \frac{1}{3}(\beta_{11}a^2 + \beta_{22}b^2 + \beta_{33}c^2 + 2\beta_{13}ac \cos \beta).$$

	x	y	z	B_{eq} (Å ²)
N(1)	1137 (2)	7153 (7)	818 (2)	2.77 (8)
C(2)	561 (3)	7863 (9)	1293 (2)	2.91 (10)
C(3)	926 (3)	6583 (10)	2216 (2)	3.35 (11)
C(4)	1784 (3)	4826 (10)	2578 (2)	3.58 (11)
C(5)	3293 (3)	2361 (10)	2448 (3)	4.27 (11)
C(6)	3842 (3)	1812 (10)	1943 (3)	4.73 (12)
C(7)	3501 (3)	3093 (10)	1067 (3)	3.48 (11)
C(8)	2600 (2)	4872 (9)	644 (2)	2.84 (9)
C(9)	2043 (2)	5369 (8)	1177 (2)	2.76 (9)
C(10)	2382 (3)	4172 (9)	2073 (2)	3.28 (10)
C(11)	2230 (3)	6193 (10)	-310 (2)	3.30 (11)
O(1)	-231 (2)	9508 (8)	928 (2)	3.73 (9)
Cl(1)	4264 (1)	2384 (3)	475 (1)	4.78 (4)

* Hamilton (1959).

and a 2° min⁻¹ scan speed. The scan range was 2° and the background was measured on either side of the peak for 10s. The data were not corrected for absorption.

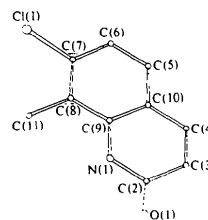


Fig. 1. Perspective view of the molecule with the atom-numbering scheme.

Table 2. Fractional positional ($\times 10^3$) and isotropic thermal parameters of the H atoms with e.s.d.'s in parentheses

	x	y	z	B (Å ²)
H(N1)	80 (3)	827 (12)	15 (3)	3.95
H(C3)	55 (3)	710 (11)	261 (3)	3.89
H(C4)	206 (3)	385 (9)	326 (2)	1.55
H(C5)	353 (3)	165 (10)	311 (2)	2.84
H(C6)	446 (3)	39 (11)	220 (3)	4.67
H(C111)	160 (4)	487 (13)	-70 (3)	2.92
H(C112)	207 (3)	840 (12)	-36 (3)	5.47
H(C113)	266 (3)	587 (12)	-59 (3)	3.41

Table 3. Bond lengths (Å) and bond angles (°) with e.s.d.'s in parentheses

N(1)—C(2)	1.371 (5)	C(5)—C(10)	1.405 (5)
N(1)—C(9)	1.394 (4)	C(6)—C(7)	1.384 (6)
C(2)—C(3)	1.446 (5)	C(7)—C(8)	1.394 (5)
C(2)—O(1)	1.243 (4)	C(7)—Cl(1)	1.749 (5)
C(3)—C(4)	1.335 (5)	C(8)—C(9)	1.410 (6)
C(4)—C(10)	1.432 (6)	C(8)—C(11)	1.495 (5)
C(5)—C(6)	1.366 (7)	C(9)—C(10)	1.399 (5)
N(1)—C(2)—C(3)	116.4 (3)	C(5)—C(6)—C(7)	119.4 (3)
N(1)—C(2)—O(1)	120.2 (3)	C(6)—C(5)—C(10)	120.1 (3)
C(2)—N(1)—C(9)	124.1 (2)	C(5)—C(10)—C(9)	119.3 (3)
N(1)—C(9)—C(8)	119.7 (3)	C(6)—C(7)—C(8)	123.9 (3)
N(1)—C(9)—C(10)	118.3 (3)	C(6)—C(7)—Cl(1)	116.8 (3)
C(2)—C(3)—C(4)	121.1 (3)	C(7)—C(8)—C(9)	115.5 (3)
C(3)—C(2)—O(1)	123.4 (3)	C(7)—C(8)—C(11)	123.3 (3)
C(3)—C(4)—C(10)	121.4 (3)	C(8)—C(7)—Cl(1)	119.4 (3)
C(4)—C(10)—C(5)	122.1 (3)	C(8)—C(9)—C(10)	121.9 (3)
C(4)—C(10)—C(9)	118.6 (3)	C(9)—C(8)—C(11)	121.2 (3)

The structure was solved by symbolic addition (Karle & Karle, 1963). 168 reflections with $|E| \geq 1.4$ were used and the phase propagation was carried out by hand using the Σ_2 formula (Hauptman & Karle, 1953). An E map with 148 reflections clearly revealed all the 13 non-H atoms ($R = 0.45$). Successive block-diagonal least-squares refinement (Shiono, 1968) with isotropic temperature factors reduced R to 0.15. A difference Fourier map revealed all the eight H atoms. Full-matrix least-squares refinement (Gantzel, Sparks & Trueblood, 1961) was carried out with isotropic temperature factors for the H atoms, anisotropic temperature factors for the non-H atoms and unit weights for all the observed reflections giving a final R of 0.052. Scattering factors for C, H, N, O and Cl were taken from *International Tables for X-ray Crystallography* (1962). The final positional parameters of the non-H atoms are listed in Table 1* and those of the H atoms in Table 2.

Discussion. The bond lengths and angles are given in Table 3 and are close to the normal values. The entire molecule is nearly planar. The equation of the least-squares plane through all atoms in the molecule is given in Table 4 along with the deviations of individual atoms from the plane; the maximum deviation [0.048 (1) Å] is for Cl(1).

A stereoscopic view of the packing of the molecule obtained using a computer program developed by one of the authors (RR) is depicted in Fig. 2. There is a N—H...O hydrogen bond of 2.878 (4) Å; the angle at H is 176 (3)°.

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36249 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 4. Equation of least-squares plane through the entire molecule and deviations (Å) of atoms from the plane

$$0.4073X + 0.8348Y + 0.3705Z = 3.3982$$

N(1)	0.025 (3)	C(8)	0.013 (3)
C(2)	-0.010 (4)	C(9)	0.024 (3)
C(3)	-0.019 (4)	C(10)	0.008 (3)
C(4)	-0.003 (4)	C(11)	0.019 (4)
C(5)	0.009 (4)	O(1)	-0.024 (3)
C(6)	0.012 (4)	Cl(1)	-0.048 (1)
C(7)	-0.005 (4)		

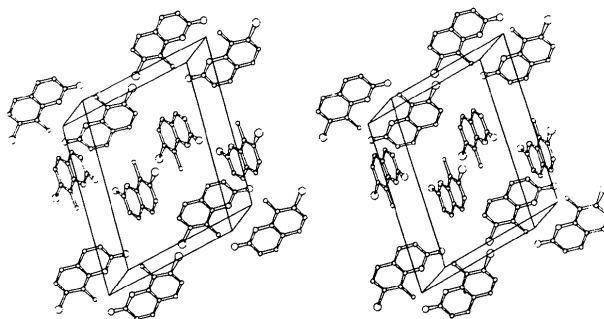


Fig. 2. Stereoscopic view of the packing of the molecules.

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