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## Hydrogen-Bonding Patterns in 8-Hydroxyquinoline Derivatives: (I) Structure of 5-Chloro-8-hydroxyquinoline and (II) Refinement of the Structure of 8-Hydroxyquinoline

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**Abstract.** (I): C<sub>9</sub>H<sub>6</sub>ClNO,  $M_r = 179.6$ , orthorhombic, space group *Fdd2*,  $a = 29.807$  (9),  $b = 27.495$  (4),  $c = 3.814$  (4) Å,  $V = 3126$  (3) Å<sup>3</sup>,  $Z = 16$ ,  $D_m = 1.55$ ,  $D_x = 1.53$  Mg m<sup>-3</sup>,  $\lambda(\text{Cu } K\alpha) = 1.5418$  Å,  $\mu = 3.92$  mm<sup>-1</sup>,  $F(000) = 1472$ ,  $T = 297$  K,  $R = 0.049$  for 469 'observed' reflections. (II): C<sub>9</sub>H<sub>7</sub>NO,  $M_r = 145.2$ , orthorhombic, space group *Fdd2*,  $a = 28.770$  (7),  $b = 25.055$  (12),  $c = 3.857$  (5) Å,  $V = 2780$  (4) Å<sup>3</sup>,  $Z = 16$ ,  $D_m = 1.41$ ,  $D_x = 1.39$  Mg m<sup>-3</sup>,  $\lambda(\text{Cu } K\alpha) = 1.5418$  Å,  $\mu = 0.703$  mm<sup>-1</sup>,  $F(000) = 1216$ ,  $T = 297$  K,  $R = 0.056$  for 474 'observed' reflections. In both structures the hydroxyl hydrogens are involved in bifurcated O–H...N hydrogen bonds, simultaneously leading to the formation of five-membered hydrogen-bonded chelate rings and the dimerization of the molecules. The stronger intramolecular hydrogen bond in the 5-chloro derivative is consistent with IR spectroscopic studies in solution.

**Introduction.** 8-Hydroxyquinoline and its derivatives are well known for their antifungal, antibacterial and antiamebic activities (Bambury, 1979). The biological activities of 8-hydroxyquinoline derivatives have been correlated with their capacity to chelate metal ions (Martell & Calvin, 1959). Structural analyses of 5-chloro-8-hydroxyquinoline (I) and 8-hydroxyquinoline (II) were undertaken in continuation of our programme of studying the hydrogen-bonding patterns in crystal structures of 8-hydroxyquinoline derivatives (Banerjee, Basak, Mazumdar & Chaudhuri, 1984). The structure of 8-hydroxyquinoline, reported earlier (Roychowdhury, Das & Basak, 1978), was based on photographic data; it has been refined by us with diffractometric data in order to locate the hydrogen atoms and to make more quantitative comparisons with other similar structures.

**Experimental.** Both compounds crystallized as colourless needles (elongated along the *c* axis) from benzene; density by flotation (KI solution); preliminary cell parameters and symmetry information for (I) from oscillation and Weissenberg photographs (systematic absences: *hkl*:  $h + k, k + l \neq 2n$ , *okl*:  $k + l \neq 4n$ , *h0l*:  $h + l \neq 4n$ ), for (II) from published data; crystal size: (I) 1.00 × 0.08 × 0.05 mm, (II) 0.65 × 0.45 × 0.15 mm; both crystals sealed in Lindemann-glass capillaries to avoid deterioration; accurate cell parameters from 25 selected reflections [in ranges (I)  $25 \leq \theta \leq 30^\circ$  and (II)  $23 \leq \theta \leq 30^\circ$ ] centred on an Enraf–Nonius CAD-4 diffractometer, graphite-monochromatized Cu *K*α radiation; 'needle option', with crystal needle axes normal to incident beam, adopted to minimize absorption; three 'orientation control' reflections monitored after every 50 reflections and three 'intensity control' reflections monitored after every hour of X-ray exposure; number of unique reflections measured: 599 ( $0 \leq h \leq 28, 0 \leq k \leq 28, 0 \leq l \leq 4, 2 \leq \theta \leq 55^\circ$ ) for (I) and 539 ( $0 \leq h \leq 30, 0 \leq k \leq 26, 0 \leq l \leq 3, 2 \leq \theta \leq 55^\circ$ ) for (II), number of unobserved reflections [ $I < 3\sigma(I)$ ]: 130 for (I) and 65 for (II); data corrected for Lp and for variations in intensity (*ca* 3%) of control reflections, absorption corrections ignored; structure (I) solved by *MULTAN* (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978); initial coordinates for structure (II) from published data (Roychowdhury, Das & Basak, 1978); H from  $\Delta F$  synthesis; anisotropic full-matrix least-squares refinement based on *F* (*ORFLS*, Busing, Martin & Levy, 1962); 133 parameters refined for (I) and 128 for (II);  $R = 0.049$  (I),  $0.056$  (II),  $wR = 0.057$  (I),  $0.068$  (II),  $S = 1.42$  (I),  $1.37$  (II),  $\Delta/\sigma < 0.05$  (I),  $< 0.03$  (II); residual  $\Delta\rho = -0.21$  to  $0.29$  e Å<sup>-3</sup> (I),  $-0.24$  to  $0.28$  e Å<sup>-3</sup> (II), weights  $w = 1/\sigma^2(|F_o|)$ ;

$\sigma(|F_o|)$  based on counting statistics; H (from  $\Delta F$  syntheses) isotropic; scattering factors for non-H from Cromer & Waber (1965), for H from Stewart, Davidson & Simpson (1965); anomalous-dispersion corrections for all non-H atoms from *International Tables for X-ray Crystallography* (1974).

**Discussion.** The final atomic coordinates, together with the net charges on the atoms calculated by the CNDO/2 method (Pople & Beveridge, 1970), are listed in Table 1. Tables 2 and 3 list the molecular dimensions and the geometries of the hydrogen bonds respectively. Fig. 1 shows the molecular packing arrangements together with the atom labelling schemes.\*

The existence of bifurcated hydrogen bonds in the crystal structures of molecular complexes and derivatives of 8-hydroxyquinoline had been pointed out by Prout & Wheeler (1967), Castellano & Prout (1971) and Polyakova, Starikova, Trunov, Parusnikov & Krasavin (1980). In both the present structures, the O—H...N contacts (Table 3) and the charge densities on the atoms concerned (Table 1) establish the formation of a pair of bifurcated hydrogen bonds, one intramolecular and the other intermolecular; this appears to be a common feature of 8-hydroxyquinoline derivatives. A five-membered chelate ring [N, C(9), C(8), O, H(8)] results from the intramolecular bond, while twofold-related molecules dimerize through a pair of intermolecular bonds. Similar dimerization has also been observed in related structures (Kashino & Haisa, 1973; Stankovic, Ribar, Janic, Lazar, Andreotti & Sgarabotto, 1976).

Spectroscopic studies indicate that both intramolecular and intermolecular H-bonding patterns are also maintained in 8-hydroxyquinoline solutions (Badger & Moritz, 1958). This is significant in view of the fact that biologically active molecules manifest their

\* Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and least-squares planes and deviations have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 43017 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Fractional atomic coordinates with e.s.d.'s in parentheses, equivalent isotropic thermal parameters (Hamilton, 1959) and the net charges on the atoms of (I) and (II)*

$$B_{eq} = \frac{4}{3} \sum_i \sum_j \beta_{ij} a_i \cdot a_j$$

	x	y	z	$B_{eq}(\text{\AA}^2)$	Net charge
<b>Compound (I)</b>					
Cl	0.42060 (6)	0.27705 (6)	0.25	4.6	-0.1853
O	0.5395 (1)	0.4439 (2)	0.015 (2)	4.6	-0.2702
N	0.4567 (2)	0.4605 (2)	0.308 (2)	3.1	-0.1506
C(2)	0.4172 (2)	0.4678 (2)	0.458 (3)	3.1	0.1047
C(3)	0.3871 (2)	0.4304 (3)	0.534 (3)	3.1	-0.0192
C(4)	0.3982 (2)	0.3839 (2)	0.450 (3)	3.2	0.0167
C(5)	0.4544 (2)	0.3272 (2)	0.193 (3)	3.3	0.0535
C(6)	0.4957 (2)	0.3207 (2)	0.036 (3)	3.2	0.0111
C(7)	0.5238 (2)	0.3607 (3)	-0.027 (3)	3.5	-0.0527
C(8)	0.5113 (2)	0.4065 (2)	0.073 (2)	2.8	0.1737
C(9)	0.4682 (2)	0.4141 (2)	0.225 (3)	2.8	0.0572
C(10)	0.4395 (2)	0.3737 (2)	0.292 (2)	2.4	0.0254
<b>Compound (II)</b>					
O	0.2182 (1)	0.31655 (9)	0.501 (1)	5.0	-0.2574
N	0.2997 (1)	0.2837 (1)	0.200 (1)	4.0	-0.1547
C(2)	0.3392 (1)	0.2695 (2)	0.046 (1)	4.2	0.0961
C(3)	0.3747 (1)	0.3050 (2)	-0.034 (2)	4.4	-0.0278
C(4)	0.3699 (2)	0.3575 (2)	0.045 (2)	4.4	0.0278
C(5)	0.3215 (2)	0.4289 (1)	0.303 (1)	4.5	-0.0380
C(6)	0.2809 (2)	0.4432 (1)	0.461 (2)	4.6	0.0164
C(7)	0.2455 (1)	0.4049 (2)	0.533 (2)	4.6	-0.0671
C(8)	0.2527 (1)	0.3528 (2)	0.438 (1)	4.1	0.1718
C(9)	0.2940 (1)	0.3367 (1)	0.281 (1)	3.5	0.0546
C(10)	0.3292 (1)	0.3753 (2)	0.208 (2)	3.7	0.0167

Table 2. *Bond lengths (\AA) and bond angles ( $^\circ$ ), with e.s.d.'s in parentheses, of (I) and (II)*

	(I)	(II)	(I)	(II)
N—C(2)	1.324 (10)	1.331 (4)	C(7)—C(8)	1.367 (10) 1.371 (7)
C(2)—C(3)	1.395 (10)	1.389 (6)	C(8)—O	1.346 (7) 1.367 (5)
C(3)—C(4)	1.359 (10)	1.357 (7)	C(8)—C(9)	1.425 (9) 1.393 (4)
C(4)—C(10)	1.399 (10)	1.402 (8)	C(9)—N	1.358 (8) 1.374 (4)
C(10)—C(5)	1.405 (8)	1.410 (6)	C(9)—C(10)	1.425 (8) 1.428 (5)
C(5)—C(6)	1.381 (10)	1.365 (8)	C(5)—Cl	1.721 (6)
C(6)—C(7)	1.403 (10)	1.427 (6)		
C(2)—N—C(9)	117.9 (6)	117.5 (3)	C(8)—C(9)—C(10)	120.0 (5) 119.6 (3)
N—C(2)—C(3)	123.3 (6)	123.8 (4)	C(9)—C(8)—O	121.2 (5) 120.3 (4)
C(2)—C(3)—C(4)	119.2 (6)	119.7 (4)	O—C(8)—C(7)	119.2 (5) 118.4 (3)
C(3)—C(4)—C(10)	120.3 (5)	119.6 (4)	C(7)—C(8)—C(9)	119.6 (5) 121.4 (4)
C(4)—C(10)—C(5)	125.2 (5)	123.4 (3)	C(8)—C(7)—C(6)	120.8 (6) 118.7 (3)
C(4)—C(10)—C(9)	116.7 (5)	117.7 (4)	C(7)—C(6)—C(5)	120.3 (6) 121.4 (3)
C(9)—C(10)—C(5)	118.1 (5)	118.8 (4)	C(6)—C(5)—C(10)	121.1 (5) 120.0 (4)
N—C(9)—C(10)	122.6 (6)	121.6 (3)	C(6)—C(5)—Cl	118.2 (4)
N—C(9)—C(8)	117.4 (5)	118.7 (3)	C(10)—C(5)—Cl	120.6 (5)

Table 3. *Geometric characteristics of hydrogen bonds in (I) and (II)*

Compound	D—H...A	D...A (\AA)	D—H (\AA)	H...A (\AA)	D—H...A ( $^\circ$ )	A(1)...H...A(2)* ( $^\circ$ )
5-Chloro-8-hydroxyquinoline (I)	O—H(8)...N <sup>i</sup>	2.747 (7)	0.77 (6)	2.35 (6)	113 (5)	97 (2)
	O—H(8)...N <sup>ii</sup>	2.858 (8)	0.77 (6)	2.16 (6)	150 (6)	
8-Hydroxyquinoline (II)	O—H(8)...N <sup>i</sup>	2.742 (4)	1.00 (3)	2.42 (3)	98 (2)	101 (1)
	O—H(8)...N <sup>ii</sup>	2.815 (4)	1.00 (3)	1.86 (3)	159 (3)	

Symmetry code: (I) (i) x, y, z; (ii) 1 - x, 1 - y, z  
(II) (i) x, y, z; (ii)  $\frac{1}{2} - x, \frac{1}{2} - y, z$

\* Angle subtended at H by two acceptors in a bifurcated hydrogen bond (Jeffrey & Maluszynska, 1982).

activities in the solution state. 8-Hydroxyquinoline can form complexes with metal ions as a neutral molecule (Hughes & Truter, 1979) and, in most cases, as a deprotonated anion with the loss of the hydroxyl hydrogen (Palenik, 1964; Camerman & Taylor, 1968). However, an example of a metal complex where one of the three coordinating ligands is a zwitterion with the hydroxyl hydrogen transferred to the quinoline nitrogen can be found in the crystal structure of the dioxido-(8-quinolinolato)(8-quinolino)uranium(VI) (Hall, Rae & Waters, 1967). In forming the metal complexes the quinoline nitrogen and the hydroxyl oxygen act as electron donors to the metal ion resulting in the formation of five-membered rings. The bite distances between the nitrogen and the oxygen atoms in different metal complexes [2.653 (5) Å (Palenik, 1964); 2.611 (4) Å (Raston, Skelton & White, 1978); 2.862 (6) Å and 2.766 (5) Å (Hall *et al.* 1967)] are close to the N...O distance [2.742 (4) Å] in the

intramolecular hydrogen-bonded ring in the uncoordinated 8-hydroxyquinoline molecule. Metal chelation through deprotonation of one of the donor atoms which remain intramolecularly hydrogen-bonded to the other donor in the free molecule has also been observed in the crystal structure of [chloro{2-(*N*-ethyleneamine)-amino-cyclopentene-1-(*S*-methyl)-dithiocarboxylato}-nickel(II)] (Chaudhuri, 1986).

The distributions of the aromatic bond lengths in both compounds are in good agreement with that calculated for quinoline (Dewar & Gleicher, 1966), and with those observed in different derivatives of quinoline (Stankovic *et al.* 1976; Kashino & Haisa, 1973; Polyakova *et al.* 1980; Banerjee *et al.* 1984) and other N-heterocyclic compounds like the acridines (Achari & Neidle, 1977; Courseille, Leroy, Hospital & Barbet, 1977). The endocyclic bond angles of the present molecules are also close to the values observed in similar structures (Stankovic *et al.* 1976; Kashino & Haisa, 1973; Prout & Wheeler, 1967; Castellano & Prout, 1971; Banerjee *et al.* 1984). In (I), the C—Cl bond length and the angle *ipso* to Cl indicate that the Cl atom acts as an electron-withdrawing group and has no conjugative effect (Domenicano, Vaciago & Coulson, 1975).

The C—O(hydroxyl) bond distances in (I) and (II) are close to the average value of 1.364 (6) Å for neutral 8-hydroxyquinolines (Hughes & Truter, 1979). The endocyclic angle at C(8) is smaller in (I) than in (II). This observation indicates conjugation between the benzene ring and the hydroxyl group in (I) (Domenicano *et al.*, 1975). We observe that similar conjugation also occurs in other 8-hydroxyquinoline derivatives having electron-withdrawing substituents at the *para* positions (Kashino & Haisa, 1973; Stankovic *et al.* 1976; Merrit & Duffin, 1970) and in the metal complexes of 8-hydroxyquinolines (Palenik, 1964; Camerman & Taylor, 1968; Raston, Skelton & White, 1978).

The shorter hydrogen acceptor distances in the case of the intermolecular hydrogen bonds (Table 3) indicate that these members of the bifurcated pairs are stronger than the intramolecular ones (Ceccarelli, Jeffrey & Taylor, 1981). It is also evident that the intramolecular hydrogen bond in 5-chloro-8-hydroxyquinoline is stronger than that in 8-hydroxyquinoline; this is consistent with the results of the IR spectral study in solution which showed that electron-withdrawing substituents *para* to the hydroxyl group in 8-hydroxyquinoline result in the formation of stronger intramolecular hydrogen bonds (Badger & Moritz, 1958).

In the molecular packing arrangements (Fig. 1) the dimers are separated by unit-cell translations along the *c* axes resulting in the characteristic stacking of the 8-hydroxyquinoline ring systems (Hughes & Truter, 1979). Van der Waals forces stabilize the crystal structures.

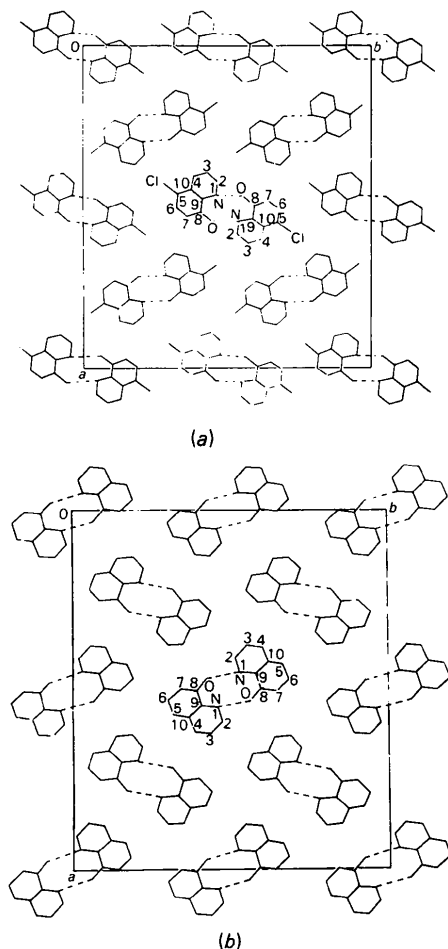


Fig. 1. The crystal structures of (a) 5-chloro-8-hydroxyquinoline and (b) 8-hydroxyquinoline viewed down the *c* axes; the hydrogen atoms have been omitted. Broken lines denote hydrogen bonds.

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## 2-Bromo-4'-phenylacetophenone\*

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**Abstract.** C<sub>14</sub>H<sub>11</sub>BrO,  $M_r = 275.15$ , orthorhombic, *Pcab* ( $a\bar{c}b$  orientation of *Pbca*),  $a = 7.794$  (1),  $b = 10.961$  (2),  $c = 27.106$  (3) Å,  $V = 2316$  (1) Å<sup>3</sup>,  $Z = 8$ ,  $D_x = 1.58$  Mg m<sup>-3</sup>, Cu  $K\alpha$ ,  $\lambda = 1.5418$  Å,  $\mu = 5.1$  mm<sup>-1</sup>,  $F(000) = 1104$ ,  $T = 293$  K,  $R = 0.050$  for 1600 reflections. The bromoacetyl group is tilted at 5.4 (1)° to the adjacent phenyl group and the two phenyl groups of the biphenyl are inclined at an angle of 33.9 (1)°. Bond lengths and angles fall within normal ranges.

**Introduction.** Although biphenyl is non-planar in the gas phase (Bastiansen & Trætteberg, 1962; Schmid &

Brosa, 1972), the phenyl rings are coplanar in the crystal (Trotter, 1961; Hargreaves & Rizvi, 1962; Charbonneau & Delugeard, 1976). In 4-nitrobiphenyl (Casalone, Gavezzotti & Simonetta, 1973) and 4,4'-dinitrobiphenyl (Boonstra, 1963) the phenyl rings are inclined at 33° and in 4,4'-bitolyl the angle of twist between the aromatic rings is *ca* 38° (Casalone, Mariani, Mugnoli & Simonetta, 1969). A halogen substituent at C(3) can be accommodated with little effect on the twist angle, which is 39° in 4-acetyl-3'-bromobiphenyl (Sutherland & Hoy, 1969). A halogen substituent at C(2) introduces greater steric interactions and several biphenyl derivatives of this type have interplanar angles of *ca* 48° (Young, Tollin & Sutherland, 1968; Sutherland & Hoy, 1968; Sutherland, 1969).

\* 4-Phenylphenacyl bromide; 4-bromoacetyl biphenyl.