Crystal structure of 7-iodo-8-hydroxyquinoline, C₉H₆INO

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Fig. 1. The molecular structure showing 50% probability displacement ellipsoids.

Monoiodo-8-quinolinol, mp 400 K–401 K, was reported in 1927. Although no proof of structure was acknowledged, the iodine was assigned to the 5 position by analogy with the corresponding chloro and bromo analogues (see ref. 1). The product became commercially available from Aldrich, and a number of articles was published using this compound in physical chemical, analytical, and biological studies. In 1995, a material identified as 7-iodo-8-quinolinol, mp 308 K, was prepared (see ref. 2) using essentially the same method as for the reported 5-iodo-8-quinolinol. The structure was assigned primarily based on the C-13 NMR spectrum. An X-ray crystal structure determination was undertaken to determine whether the compound melting at 400 K–401 K is the 5- or 7-iodo-8-quinolinol.

The existence of bifurcated hydrogen bonds in the derivatives of 8-hydroxyquinoline had been reported (see refs. 3–4). There is no evidence of bifurcated H bonds in the title compound, perhaps due to the sterically hindered iodine in position C7. The hydroxyl hydrogen forms only a cyclic intramolecular hydrogen bond. The H1–N1 bond distance is 1.91(6) Å and O1–H1–N1 bond angle 145.2(8)°.

C₉H₆INO, monoclinic, *P*12₁/*n*1 (No. 14), *a* = 7.8780(8) Å, *b* = 13.095(1) Å, *c* = 8.8957(9) Å, β = 107.66(1)°, *V* = 874.5 Å³, *Z* = 4, *R*(*F*) = 0.038, *R*_w(*F*) = 0.041.

Fig. 2. Packing of the molecules viewed down the *c* axis. The hydrogen atoms have been omitted.

Table 1. Parameters used for the X-ray data collection

Crystal:	colorless prism, size 0.3 x 0.3 x 0.4 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	36.1 cm ⁻¹
Diffractometer:	Enraf-Nonius CAD4
Scan mode:	$\omega/2\theta$
<i>T</i> _{measurement} :	293 K
2 θ _{max} :	53°
<i>N</i> (<i>hkl</i>) _{unique} :	1363
Criterion for <i>F</i> _o :	<i>F</i> _o > 3 σ (<i>F</i> _o)
<i>N</i> (<i>param</i>) _{refined} :	133
Program:	Xtal3.4

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(6)	4e	0.420(8)	0.738(4)	−0.082(6)	0.04(2)
H(5)	4e	0.699(9)	0.670(6)	−0.039(8)	0.07(3)
H(4)	4e	0.923(7)	0.532(5)	0.113(7)	0.05(2)
H(3)	4e	1.002(6)	0.410(5)	0.310(8)	0.05(2)
H(1)	4e	0.422(7)	0.550(6)	0.372(8)	0.07(3)
H(2)	4e	0.81(1)	0.393(6)	0.478(7)	0.09(3)

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
I(1)	4e	0.1328(1)	0.7551(1)	0.0783(1)	0.0630(3)	0.0591(3)	0.0638(3)	0.0140(3)	0.0182(2)	0.0181(3)
N(1)	4e	0.6336(8)	0.4820(4)	0.3638(7)	0.046(4)	0.045(3)	0.040(3)	0.005(3)	0.019(3)	0.004(3)
O(1)	4e	0.3180(7)	0.5812(4)	0.3140(6)	0.048(3)	0.065(3)	0.051(3)	0.011(3)	0.026(3)	0.021(3)
C(4)	4e	0.845(1)	0.5156(7)	0.169(1)	0.060(5)	0.060(5)	0.058(5)	−0.008(4)	0.038(4)	−0.010(4)
C(5)	4e	0.623(1)	0.6414(6)	0.0168(9)	0.071(6)	0.051(4)	0.050(4)	−0.013(4)	0.034(4)	−0.001(4)
C(6)	4e	0.467(1)	0.6918(6)	−0.0007(9)	0.072(5)	0.046(4)	0.040(4)	−0.007(4)	0.020(4)	0.008(3)
C(7)	4e	0.3644(9)	0.6727(5)	0.1040(8)	0.048(4)	0.038(3)	0.039(4)	−0.004(3)	0.011(3)	0.003(3)
C(8)	4e	0.4196(9)	0.6016(5)	0.2187(8)	0.045(4)	0.040(4)	0.036(3)	−0.005(3)	0.015(3)	−0.001(3)
C(9)	4e	0.5822(9)	0.5491(5)	0.2423(8)	0.042(4)	0.036(3)	0.035(4)	−0.006(3)	0.013(3)	−0.005(3)
C(10)	4e	0.686(1)	0.5696(5)	0.1398(9)	0.051(4)	0.042(4)	0.042(4)	−0.010(3)	0.023(4)	−0.008(3)
C(3)	4e	0.895(1)	0.4477(7)	0.288(1)	0.052(5)	0.063(5)	0.065(6)	0.014(4)	0.024(4)	−0.009(4)
C(2)	4e	0.786(1)	0.4334(6)	0.384(1)	0.057(5)	0.056(5)	0.049(5)	0.009(4)	0.019(4)	0.002(4)

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