Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5,7-Diiodoquinolin-8-ol

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.006 Å
R factor = 0.031
wR factor = 0.077
Data-to-parameter ratio = 18.7

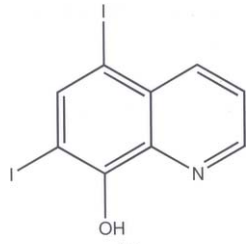
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_9H_5I_2NO$, features an almost planar molecule. Geometric parameters are in the usual ranges. The crystal packing shows that two hydrogen-bonded molecules are related by a twofold rotation axis.

Received 31 August 2006
Accepted 24 November 2006

Comment

5,7-Diiodoquinolin-8-ol, (I), is of therapeutic interest. Quinolin-8-ol and its derivatives have antibacterial activity and form chelate complexes with divalent metal ions (Rohde *et al.*, 1976). The importance of metallic oxinates in analytical chemistry is also well known. Oxine and its derivatives have found extensive application as analytical reagents (Guerreiro *et al.*, 2002) in absorption spectroscopy, fluorimetry, extraction with solvents and chromatography. In an attempt to prepare the manganese complex of 5,7-diiodo-8-hydroxyquinoline we obtained crystals of the ligand, (I). A perspective view of the title compound is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database; Version 5.27, November 2005, updated August 2006; Allen, 2002). The molecule is essentially planar (r.m.s. deviation for all non-H atoms is 0.058 Å). The packing diagram (Fig. 2) reveals that two molecules, which are related by a twofold rotation axis, are connected by an O—H···N hydrogen bonds (Table 1).



(I)

Experimental

An attempt was made to complex 5,7-diiodoquinolin-8-ol with manganese. Unfortunately, ligand (I) crystallized out in an attempt to recrystallize the complex (m.p. 471–473 K) from toluene.

Crystal data

$C_9H_5I_2NO$
M_r = 396.94
Monoclinic, $P2/c$
a = 14.1699 (13) Å
b = 4.2915 (4) Å
c = 16.1565 (13) Å
β = 96.801 (7)°
V = 975.57 (15) Å^3
Z = 4
D_x = 2.703 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 6.40 mm^{-1}
T = 173 (2) K
Rod, yellow
0.31 × 0.11 × 0.10 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.318, T_{max} = 0.527
7396 measured reflections
2244 independent reflections
2163 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.077
S = 1.17
2244 reflections
120 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0385P)^2 + 2.4632P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.25 e Å^{-3}
$\Delta\rho_{min}$ = −1.23 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0083 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N7^{i}	0.84	1.98	2.757 (5)	154

Symmetry code: (i) $-x+1, y, -z+\frac{3}{2}$.

H atoms were found in a difference Fourier map but they were constrained, with C—H = 0.95 Å and O—H = 0.84 Å, and were refined using a riding model; U_{iso}(H) = 1.2U_{eq}(C,O). The hydroxyl group was allowed to rotate but not to tip. The highest peak in the final difference Fourier map is located at 0.77 Å from I1 and the deepest hole is at 0.98 Å from I2.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS86* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON*.

The authors are grateful to the Department of Chemistry, Quaid-I-Azam University, Islamabad, Pakistan.

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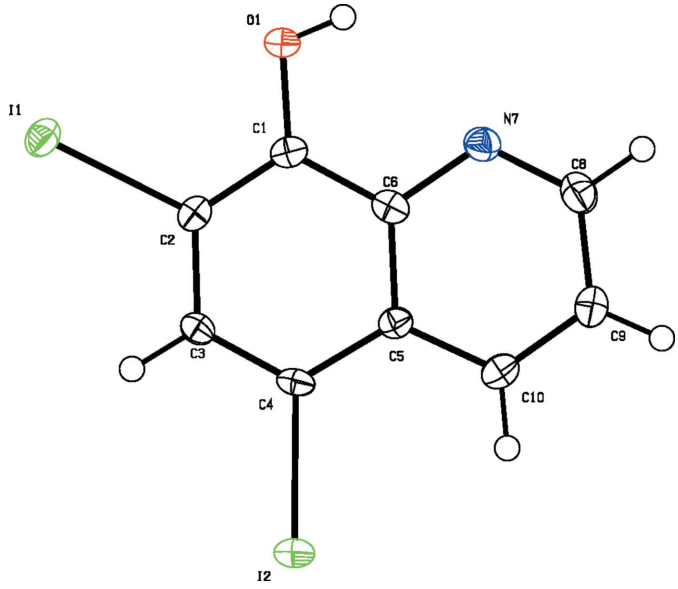

Figure 1
Molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level.

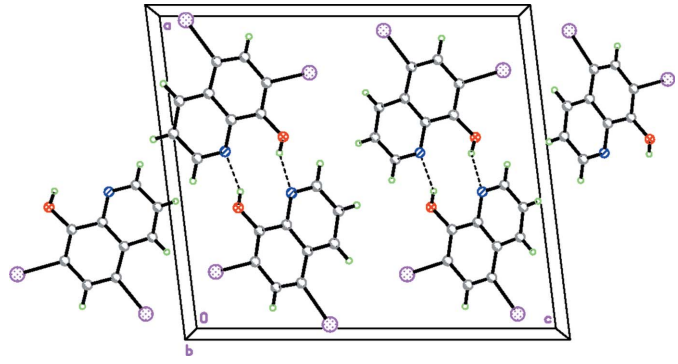

Figure 2
Packing diagram of (I) viewed along the *b* axis. Hydrogen bonds are shown as dashed lines.

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