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2-Fluoro-4-hydroxybenzonitrile

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In the title compound, C_7H_4FNO, the molecule is essentially planar. In the crystal structure, the molecules are linked *via* weak intermolecular O—H···N hydrogen bonds into linear chains. The packing is further stabilized by van der Waals forces.

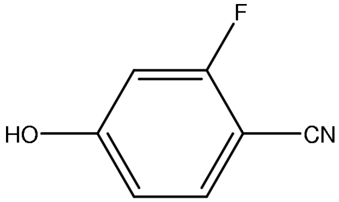
Key indicators

Single-crystal X-ray study
T = 293 K
Mean *σ*(C–C) = 0.002 Å
R factor = 0.034
wR factor = 0.098
Data-to-parameter ratio = 11.7

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

Comment

The synthesis of organofluorine compounds has attracted rapidly increasing interest in recent years, due to the anomalous physical properties and decreased availability of these compounds when used in physiologically active substances, liquid crystals and other materials (Itoh *et al.*, 2003). In syntheses in which one or three F atoms are introduced in specific absolute configurations, these organofluorine compounds exhibit particularly high physiological activity and remarkable physical properties (Schlesser, 1998). Liquid crystals substituted with F are a new type of liquid crystal, and their performance is excellent. Because the volume of an F atom is similar to that of an H atom, the ordered structures of liquid crystals are not influenced by steric effects, and the higher electronegativity of F atoms can guarantee the dipole moment which the structures of liquid crystals substituted with F possess. Here, we report the crystal structure of 2-fluoro-4-hydroxybenzonitrile, (I) (Fig. 1), an important intermediate for the synthesis of liquid crystals substituted with F.



(I)

The bond lengths and angles in (I) (Table 1) are within normal ranges (Allen *et al.*, 1987). The whole molecule is essentially planar, with a maximum deviation from the mean plane of 0.071 (8) Å for atom N1. In the crystal structure, the molecules are linked into chains *via* weak intermolecular O—H···N hydrogen bonds (Table 2, Fig. 2). The packing is further stabilized by van der Waals forces.

Experimental

To a solution of copper(I) cyanate (4.5 g, 0.05 mol) in dimethylformamide (60 ml) was added 3-fluoro-4-iodophenol (11.9 g, 0.05 mol) with stirring, and the mixture was refluxed for 5 h.

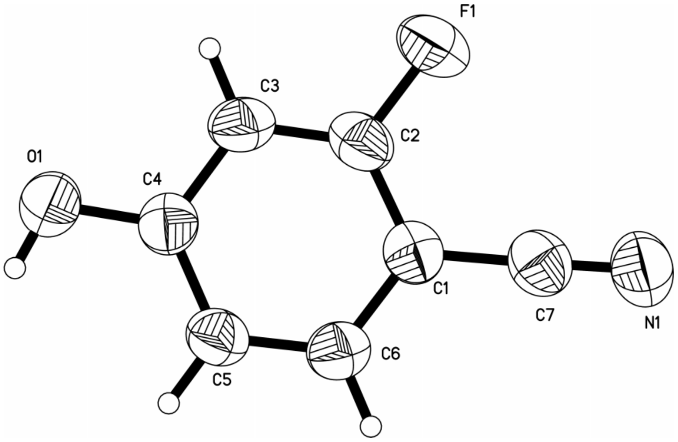


Figure 1
A view of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

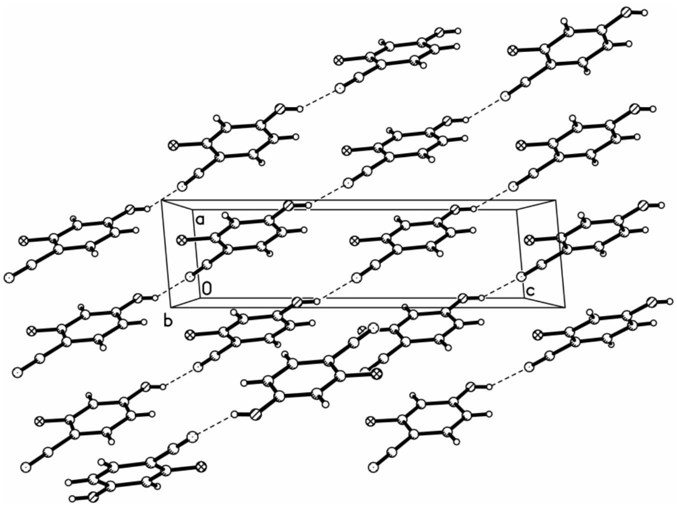


Figure 2
The crystal packing of (I), with the O—H···hydrogen bonds denoted by dashed lines.

Evaporation of the solvent afforded a residue to which a mixture of water and concentrated hydrochloric acid was added with stirring, followed by extraction with diethyl ether. The solid which appeared after evaporation of the solvent was recrystallized from toluene. Single crystals of (I) suitable for X-ray diffraction study were obtained by recrystallization from an ethanol solution at room temperature.

Crystal data

C_7H_4FNO
$M_r = 137.11$
Monoclinic, $P2_1/c$
$a = 3.8051$ (17) Å
$b = 11.852$ (5) Å
$c = 13.903$ (6) Å
$\beta = 95.035$ (7)°
$V = 624.5$ (5) Å^3
$Z = 4$
$D_x = 1.458$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1352 reflections
$\theta = 2.3$–25.0°
$\mu = 0.12$ mm^{-1}
$T = 293$ (2) K
Plate, colourless
0.25 × 0.22 × 0.09 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.971$, $T_{\max} = 0.989$
2477 measured reflections
1065 independent reflections
919 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.009$
$\theta_{\max} = 25.0°$
$h = -4 \rightarrow 4$
$k = -9 \rightarrow 14$
$l = -16 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.099$
$S = 1.08$
1065 reflections
91 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0517P)^2 + 0.0925P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.14$ e Å^{-3}
$\Delta\rho_{\min} = -0.17$ e Å^{-3}

Table 1
Selected bond lengths (Å).

C1—C7	1.430 (2)	C4—O1	1.3460 (17)
C2—F1	1.3544 (17)	C7—N1	1.1402 (19)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N1$^{\rm i}$	0.82	2.07	2.822 (2)	153

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

All H atoms were positioned geometrically and treated as riding, with C—H and O—H distances of 0.93 Å and 0.82 Å, respectively, and with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ and $1.5U_{\rm eq}({\rm O})$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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