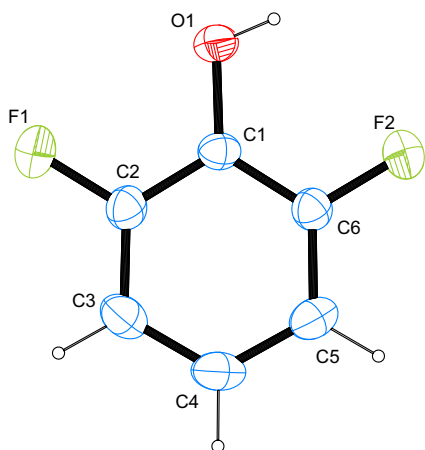


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The crystal structure of 2,6-difluorophenol, $C_6H_4F_2O$



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Abstract

$C_6H_4F_2O$, orthorhombic, $P2_12_12_1$ (no. 19), $a = 4.9287(5)$ Å, $b = 10.1752(8)$ Å, $c = 10.9156(10)$ Å, $V = 547.42(9)$ Å³, $Z = 4$, $R_{gt}(F) = 0.0248$, $wR_{ref}(F^2) = 0.0705$, $T = 200$ K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of material

The compound was obtained commercially (fluorochem). Crystals suitable for the diffraction studies were obtained

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Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.54 × 0.52 × 0.48 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.15 mm ⁻¹
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max} , completeness:	28.4°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int} :	5425, 1357, 0.014
Criterion for I_{obs} , $N(hkl)_{gt}$:	$I_{obs} > 2 \sigma(I_{obs})$, 1290
$N(param)_{refined}$:	98
Programs:	Bruker [1, 6], SHELX [2], WinGX/ORTEP [3], Mercury [4], PLATON [5]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	x	y	z	U_{iso}^*/U_{eq}
F1	0.2083 (2)	0.49910 (11)	0.54795 (10)	0.0461 (3)
F2	0.9445 (2)	0.63057 (11)	0.30789 (10)	0.0438 (3)
O1	0.5649 (2)	0.68580 (11)	0.48661 (11)	0.0350 (3)
H1	0.711 (6)	0.723 (3)	0.484 (2)	0.059 (7)*
C1	0.5775 (3)	0.56673 (14)	0.42963 (12)	0.0263 (3)
C2	0.3940 (3)	0.46969 (15)	0.46046 (13)	0.0306 (3)
C3	0.3923 (4)	0.34802 (15)	0.40540 (16)	0.0371 (4)
H3	0.267 (5)	0.286 (2)	0.428 (2)	0.051 (6)*
C4	0.5833 (4)	0.32147 (16)	0.31579 (16)	0.0389 (4)
H4	0.591 (5)	0.235 (2)	0.271 (2)	0.052 (6)*
C5	0.7712 (4)	0.41559 (16)	0.28131 (14)	0.0355 (3)
H5	0.901 (5)	0.401 (2)	0.223 (2)	0.049 (6)*
C6	0.7636 (3)	0.53635 (13)	0.33867 (13)	0.0291 (3)

by repeated melting and freezing of the compound in a fridge around 0 °C.

Experimental details

All H atoms were located on a difference map and refined freely.

Comment

Phenol and derivatives are interesting bonding partners for a variety of transition metals and elements from the *p*-block.

They can act as neutral or – upon deprotonation – as anionic ligands. Upon variation of the substituents on the aromatic system, a seemingly endless series of symmetric as well as asymmetric phenol derivatives featuring different steric pretenses and acidities of the hydroxyl-group are available. For phenol and phenolate, all bonding modes from monodentate (e.g. towards beryllium [7]) *via* bidentate (e.g. towards tin [8]) and tridentate (e.g. towards zinc [9, 10]) to tetradentate (e.g. towards sodium [11]) have been observed and secured on grounds of structural studies. Elucidating the coordination behaviour of various phenol in dependence of pH-value and substitution pattern it seemed of interest to determine the crystal structure of the title compound to enable comparisons with metric parameters in envisioned coordination compounds. Recently, the molecular and crystal structures of 2-hydroxy-5-methylisophthalaldehyde [12], 3,5-dimethylphenol [13], 2,3,4,5,6-pentabromophenol [14] and 4-ethylphenol [15] have been determined. The structures of 2,6-dichlorophenol [16] and 2,6-diiodophenol in a co-crystal [17] are apparent in the literature next to the structure of the title compound co-crystallized with a 4-alkoxystilbazole [18].

The title compound is the difluorinated derivative of phenol bearing the two fluoro substituents in the two *ortho* positions to the hydroxyl group. The two C–F bond lengths vary slightly with values of 1.3514(17) Å and 1.3634(16) Å. Both values are in good agreement with compounds featuring fluorinated phenyl groups whose metrical parameters have been deposited with the Cambridge Structural Database [19]. C–C–C angles cover a range of 116.65(12)–122.75(14)° and 122.78(14)° with the smallest angle found on the carbon atom bearing the hydroxyl group and the largest two values invariably found on the carbon atoms bonded to the fluorine atoms.

In the crystal structure, the molecules are connected by means of cooperative hydrogen bonds. In terms of graph-set analysis [20], the descriptor for these hydrogen bonds – on the unary level – is $C_1^1(2)$. The molecules are connected to infinite chains along the crystallographic *a* axis. π stacking is not a prominent feature in the title structure with the shortest distance between two centers of gravity of 4.9287(11) Å being in line with the length of the *a* axis of the unit cell.

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