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5-Fluorosalicylic acid

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.111
Data-to-parameter ratio = 10.0

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

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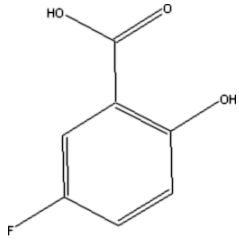
The title compound, $C_7H_5FO_3$, is nearly planar, and the dihedral angle between the phenyl and carboxyl groups is 4.0 (1)°. There are intramolecular O—H···O and intermolecular O—H···O and O—H···F hydrogen bonds, forming ribbons along the *c* axis.

Comment

The study of interactions involving fluorine has been a major theme in crystal engineering in recent years (Thalladi *et al.*, 1998; Shimoni & Glusker, 1994; Prasanna & Guru Row, 2000*a*,*b*,*c*, 2001; Choudhury *et al.*, 2002, 2003; Choudhury & Guru Row, 2004; Choudhury, Nagarajan & Guru Row, 2004*a*,*b*; Banerjee *et al.*, 2004; Kui *et al.*, 2003). It has been demonstrated that the intermolecular interactions involving the F atom play a major role in structures of small organic molecules in the absence of any other significant interactions (Choudhury *et al.*, 2002; Choudhury & Guru Row, 2004). It has also been observed that, in some cases, interactions involving fluorine gets preference over those involving other halogens (Prasanna & Guru Row, 2001; Choudhury *et al.*, 2003). We report here the crystal and molecular structure of the title compound, (I).



(I)

In (I), the OH group forms a strong intramolecular hydrogen bond (Table 1) with the C=O of the carboxyl group thus forming a pseudo-six-membered ring (Fig. 1). The molecule is very close to planar, the dihedral angle between the phenyl ring (C1–C6) and the carboxyl group (O1/C7/O2) is 4.0 (1)°. The molecules pack *via* strong centrosymmetric O—H···O hydrogen bond forming a dimer (Fig. 2). The packing is reinforced by another significant hydrogen bond *via* O—H···F involving the hydroxyl group. Also, a significantly short intermolecular C7—O2···F1^{ii} contact have been identified in the structure [symmetry code: (ii) *x*, *y*, *z* + 1], with an O2···F1^{ii} distance of 2.844 (2) Å and a C7—O2···F1^{ii} angle of 158.8 (1)°.

The structure of salicylic acid (Sundaralingam & Jensen, 1965) differs significantly from that of (I). The molecule is planar with a dihedral angle between the phenyl ring and the carboxyl group of 0.98 (1)°. Even though the molecules pack *via* O—H···O dimers, there are significant C—H···O

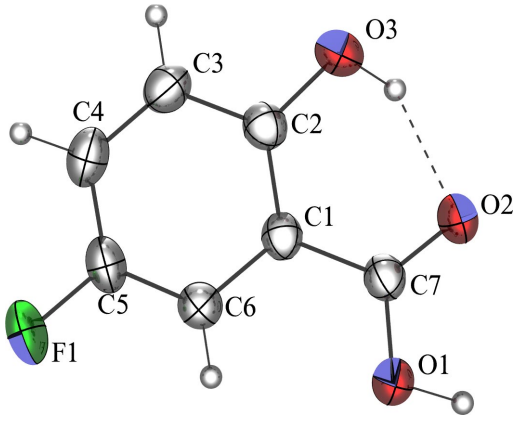


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids. H atoms represented by small spheres of arbitrary radius. A dashed line indicates the hydrogen bond.

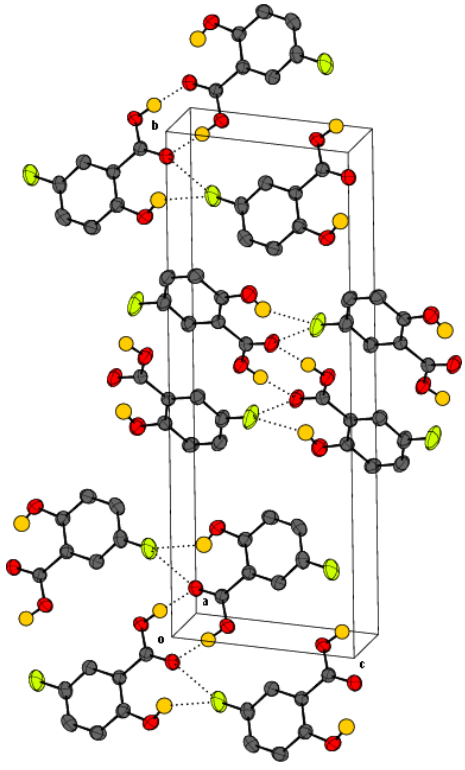


Figure 2
The packing diagram of (I). Dashed lines indicate hydrogen bonding.

hydrogen-bonded chains in the packing. This feature is absent in (I). 5-Bromosalicylic acid (Liu *et al.*, 2004) also shows a deviation between the plane of the phenyl ring and the carboxyl group. The bromo derivative has two molecules in the asymmetric unit and in one the carboxyl group deviates by 1.64 (1)° while in the other it deviates by 0.60 (1)° from the plane of the phenyl ring. A short C—O···Br contact has been identified in 5-bromosalicylic acid. A significantly short C—H···O hydrogen bond holds the neighbouring O—H···O dimers together.

In conclusion, it can be mentioned that the F atom does change the packing modes of small organic molecules even in the presence of strong hydrogen bonds like O—H···O.

Experimental

The tile compound, (I), was purchased from Sigma Aldrich and recrystallized from a 1:1 mixture of dichloromethane and hexane by slow evaporation at 263 K.

Crystal data

$C_7H_5FO_3$
M_r = 156.11
Monoclinic, $P2_1/n$
a = 3.8184 (8) Å
b = 21.219 (4) Å
c = 8.2107 (17) Å
β = 101.172 (4)°
V = 652.7 (2) Å^3
Z = 4
D_x = 1.589 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2543 reflections
θ = 2.6–24.1°
μ = 0.14 mm^{-1}
T = 293 (2) K
Rod, colourless
0.30 × 0.10 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.949, T_{max} = 0.986
4794 measured reflections
1201 independent reflections
990 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.3°
$h = -4 \rightarrow 4$
$k = -25 \rightarrow 25$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.111
S = 1.12
1201 reflections
120 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.046P)^2 + 0.2148P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1O···O2^{i}	0.96 (3)	1.72 (3)	2.676 (2)	177 (2)
O3—H3O···F1^{ii}	0.87 (3)	2.47 (3)	3.107 (2)	130 (3)
O3—H3O···O2	0.87 (3)	1.83 (3)	2.615 (2)	149 (3)

Symmetry codes: (i) $1-x, 2-y, 2-z$; (ii) $x, y, 1+z$.

All the H atoms were located from a difference Fourier map and refined isotropically. The C—H and O—H bond lengths are in the ranges 0.91 (2)–0.94 (3) and 0.87 (3)–0.95 (3) Å, respectively.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-32 *for Windows* (Farrugia, 1997), *POV-Ray for Windows* (The POV-Ray Team, 2004) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

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