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Key indicators

Single-crystal X-ray study
$T = 290$ K
Mean σ(C–C) = 0.005 Å
R factor = 0.069
wR factor = 0.159
Data-to-parameter ratio = 12.3

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

4-Fluoro-3-phenoxybenzoic acid

In the title compound, $C_{13}H_9FO_3$, the dihedral angle between the benzene rings is 82.1 (1)°. The crystal structure is mainly stabilized by carboxylic acid dimers involving O—H···O hydrogen bonds, along with the formation of weak but highly directional intermolecular C—H···O and C—H···F interactions.

Comment

Pesticides are widely used as pyrethroids (insecticides) in agriculture, forestry, horticulture and homes (Heudork & Angerer, 2001, and references therein). The title compound, (I), is one such compound.
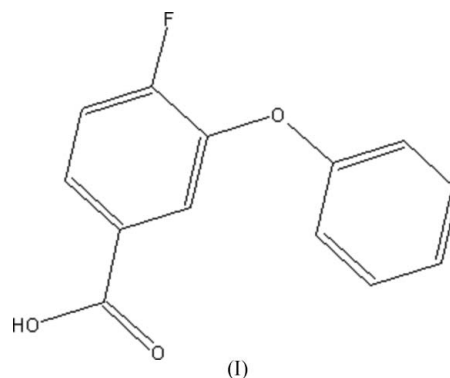

(I)

Fig. 1 shows the asymmetric unit of (I). The C5—O4—C7 bond angle is considerably widened and this eliminates the possibility of formation of an intramolecular C—H···π interaction with the H atom bonded to C6. The molecules pack *via* the formation of classical carboxylic acid dimers involving O—H···O hydrogen bonds (Table 2). In addition, molecules are linked *via* C—H···O and C—H···F interactions, forming a sheet-like structure (Fig. 2).

Experimental

The compound (I) was supplied by Rallis India Limited. Crystals of suitable size and quality were grown by slow evaporation of a solution in acetone at 298 K.

Crystal data

$C_{13}H_9FO_3$	$D_x = 1.412$ Mg m^{-3}
$M_r = 232.20$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 565
$a = 16.659$ (3) Å	reflections
$b = 5.1494$ (9) Å	$\theta = 1.4$–25.8°
$c = 13.916$ (2) Å	$\mu = 0.11$ mm^{-1}
$\beta = 113.821$ (3)°	$T = 290$ (2) K
$V = 1092.0$ (3) Å^3	Plate, colorless
$Z = 4$	$0.30 \times 0.20 \times 0.10$ mm
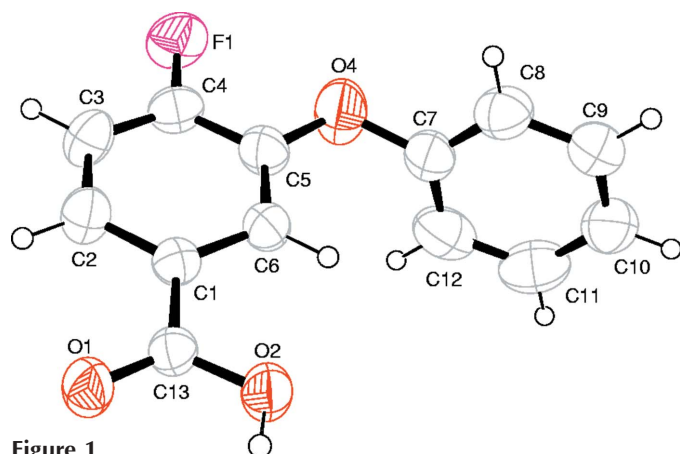
Figure 1
Molecular structure of (I), showing 50% probability displacement ellipsoids.

Figure 2
Packing diagram of (I), highlighting O—H···O hydrogen bonds forming dimers, and C—H···O interactions and C—H···F interactions forming molecular sheets. H atoms have been omitted for clarity, except for those involved in hydrogen bonds. Intermolecular interactions are shown as dotted lines.

Data collection

Bruker SMART CCD area-detector diffractometer	1914 independent reflections
φ and ω scans	1695 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.022$
	$\theta_{max} = 25.0°$
$T_{min} = 0.940$, $T_{max} = 0.989$	$h = -19 \rightarrow 19$
7407 measured reflections	$k = -6 \rightarrow 6$
	$l = -15 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0566P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.069$	$+ 0.4402P]$
$wR(F^2) = 0.159$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.25$	$(\Delta/\sigma)_{max} < 0.001$
1914 reflections	$\Delta\rho_{max} = 0.28$ e Å^{-3}
155 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

O2—C13	1.308 (3)	F1—C4	1.345 (3)
O1—C13	1.218 (3)	C5—O4	1.364 (3)
C5—O4—C7	119.8 (2)		
C2—C1—C13—O1	1.7 (4)	C5—O4—C7—C12	78.0 (4)
C6—C5—O4—C7	11.2 (5)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1[i]	0.82	1.85	2.667 (3)	178
C3—H3A···O1[ii]	0.93	2.56	3.224 (3)	129
C9—H9···F1[iii]	0.93	2.55	3.216 (4)	129

Symmetry codes: (i) $-x+1, -y-1, -z+1$; (ii) $-x+1, +y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $x, -y+\frac{3}{2}, +z-\frac{1}{2}$.
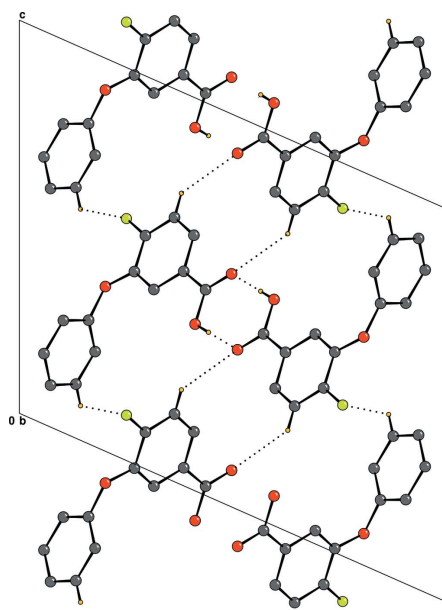
The H atom of the carboxylic group was positioned assuming an intermolecular hydrogen bond and constrained geometrically [O—H = 0.82 Å and U_{iso}(H) = 1.5U_{eq}(O)]. The C-bound H atoms were placed in idealized position (C—H= 0.93 Å) and constrained to ride on their parent atom, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

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