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## Structure Reports

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## 5-Fluoroisophthalic acid

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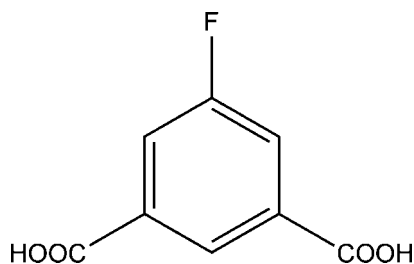
Received 18 January 2011; accepted 1 February 2011

Key indicators: single-crystal X-ray study;  $T = 297$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  
R factor = 0.041; wR factor = 0.161; data-to-parameter ratio = 11.6.

In the crystal structure of the title compound,  $\text{C}_8\text{H}_5\text{FO}_4$ , the complete molecule is generated by crystallographic twofold symmetry with two C atoms and the F atom lying on the axis. The molecule is almost planar with the carboxyl group twisted with respect to the mean plane of the benzene ring by a dihedral angle of  $2.01(1)^\circ$ . In the crystal, intermolecular O—H...O hydrogen bonds and C—H...F interactions connect the molecules into a two-dimensional supramolecular array.

## Related literature

For isophthalic acid, see: Bhogala *et al.* (2005); Derissen (1974). For the use of the title compound in crystal engineering, see: Zhang *et al.* (2010).



## Experimental

## Crystal data

 $\text{C}_8\text{H}_5\text{FO}_4$  $M_r = 184.12$ 

Monoclinic,  $P2_1/m$   
 $a = 3.7736(8)$  Å  
 $b = 16.292(4)$  Å  
 $c = 6.2753(14)$  Å  
 $\beta = 91.871(5)^\circ$   
 $V = 385.60(14)$  Å<sup>3</sup>

$Z = 2$   
Mo  $K\alpha$  radiation  
 $\mu = 0.14$  mm<sup>-1</sup>  
 $T = 297$  K  
 $0.22 \times 0.20 \times 0.15$  mm

## Data collection

Bruker APEXII CCD  
diffractometer  
Absorption correction: multi-scan  
(SADABS; Sheldrick, 2003)  
 $T_{\min} = 0.969$ ,  $T_{\max} = 0.979$

2201 measured reflections  
743 independent reflections  
603 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.018$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$   
 $wR(F^2) = 0.161$   
 $S = 1.04$   
743 reflections

64 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.16$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.15$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1}\cdots\text{O2}^{\text{i}}$	0.82	1.81	2.625 (2)	174
$\text{C5}-\text{H5}\cdots\text{F1}^{\text{ii}}$	0.93	2.52	3.404 (2)	160

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

Data collection: APEX2 (Bruker, 2003); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008) and DIAMOND (Brandenburg, 2005); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GO2002).

## References

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## supporting information

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## 5-Fluoroisophthalic acid

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### S1. Comment

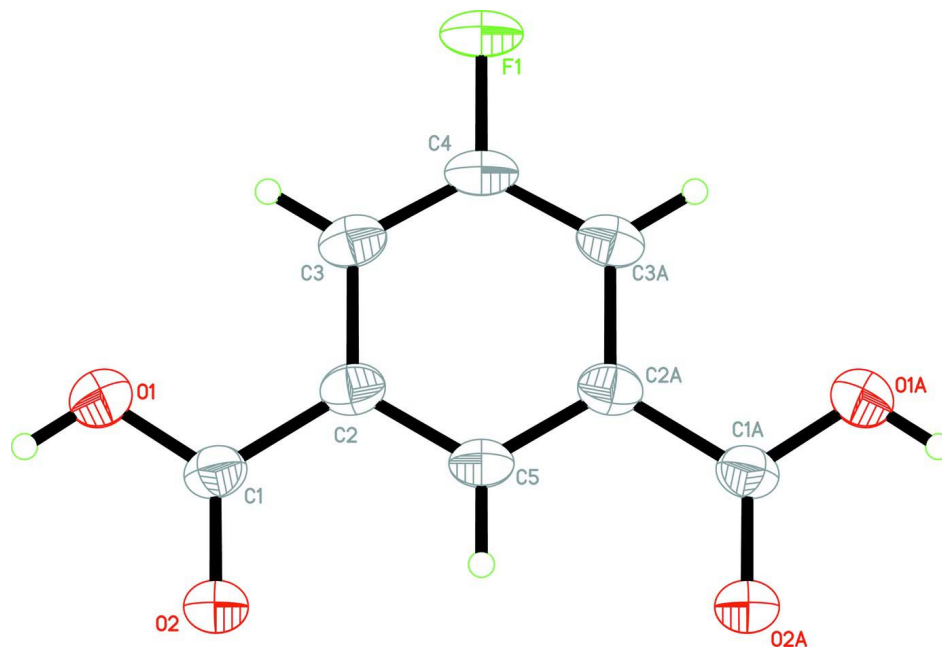
As an analogue of isophthalic acid (Bhogala *et al.* 2005; Derissen, 1974), 5-fluoroisophthalic acid has been seldom used in the crystal engineering of organic or inorganic-organic systems (Zhang *et al.* 2010). The fluorinated group may participate in hydrogen-bonding and may also induce luminescence properties. Herein we report the crystal structure of the title compound, C<sub>8</sub>H<sub>5</sub>FO<sub>4</sub>, to further investigate the supramolecular interactions involving the fluorine atom. The structure of the title compound, is shown below. The molecule presents C<sub>2</sub> symmetry with the fundamental unit lying on a C<sub>2</sub>-axis at [x, 3/4, z]. Intermolecular O—H···O interactions between adjoining centrosymmetry-related carboxylic groups form a hydrogen-bonded ribbon running along the [010] direction. C—H···F interactions connect the ribbons into a two-dimensional supramolecular array.

### S2. Experimental

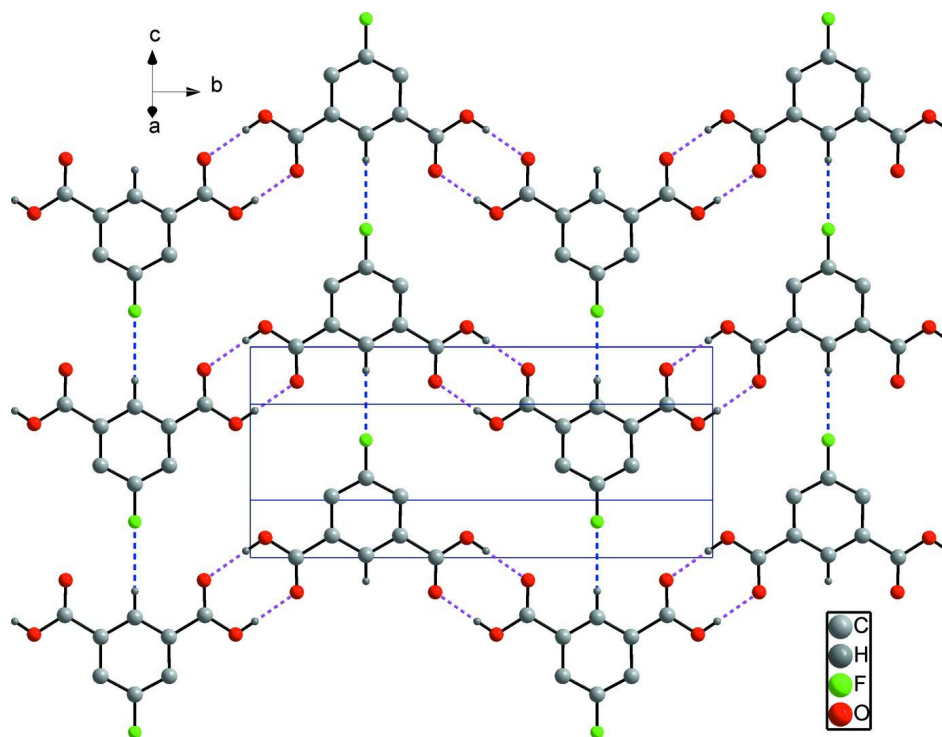
5-Fluoroisophthalic acid and solvents for synthesis and analysis were commercially available and used as received. Single crystals suitable for X-ray diffraction were obtained by slow evaporation of the methanol solution of the title compound.

### S3. Refinement

Benzene H atoms were assigned to calculated positions with C—H = 0.93 Å, and refined using a riding model, with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ . H atoms bound to carboxylic O atoms were located in difference maps and refined as riding with  $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$ .

**Figure 1**

The molecular structure of the title compound drawn with 30% probability ellipsoids.

**Figure 2**

Two-dimensional hydrogen-bonded layer of the title compound. Hydrogen bonds are indicated as dashed lines.

## 5-fluorobenzene-1,3-dicarboxylic acid

## Crystal data

C<sub>8</sub>H<sub>5</sub>FO<sub>4</sub> $M_r = 184.12$ Monoclinic,  $P2_1/m$ 

Hall symbol: -P 2yb

 $a = 3.7736$  (8) Å $b = 16.292$  (4) Å $c = 6.2753$  (14) Å $\beta = 91.871$  (5)° $V = 385.60$  (14) Å<sup>3</sup> $Z = 2$  $F(000) = 188$  $D_x = 1.586$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 1020 reflections

 $\theta = 2.5$ – $28.0$ ° $\mu = 0.14$  mm<sup>-1</sup> $T = 297$  K

Block, colourless

 $0.22 \times 0.20 \times 0.15$  mm

## Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 $\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 2003)

 $T_{\min} = 0.969$ ,  $T_{\max} = 0.979$ 

2201 measured reflections

743 independent reflections

603 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.018$  $\theta_{\text{max}} = 25.5$ °,  $\theta_{\text{min}} = 2.5$ ° $h = -4 \rightarrow 4$  $k = -17 \rightarrow 19$  $l = -7 \rightarrow 5$ 

## Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.041$  $wR(F^2) = 0.161$  $S = 1.04$ 

743 reflections

64 parameters

0 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.1244P)^2]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\text{max}} < 0.001$  $\Delta\rho_{\text{max}} = 0.16$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.15$  e Å<sup>-3</sup>

## Special details

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted R-factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional R-factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and R-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å<sup>2</sup>)

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6268 (4)	0.59855 (9)	0.8588 (3)	0.0524 (5)
C2	0.7105 (4)	0.67633 (9)	0.7484 (2)	0.0487 (5)
C3	0.8602 (4)	0.67563 (10)	0.5486 (3)	0.0529 (5)
H3	0.9107	0.6265	0.4806	0.063*

C4	0.9312 (5)	0.7500	0.4549 (3)	0.0540 (6)
C5	0.6370 (5)	0.7500	0.8476 (3)	0.0477 (6)
H5	0.5379	0.7500	0.9813	0.057*
F1	1.0787 (4)	0.7500	0.2629 (2)	0.0744 (6)
O1	0.7073 (4)	0.53205 (8)	0.7622 (2)	0.0775 (6)
H1	0.6348	0.4905	0.8205	0.116*
O2	0.4837 (4)	0.60037 (7)	1.0328 (2)	0.0722 (6)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0490 (9)	0.0612 (10)	0.0474 (10)	-0.0023 (6)	0.0088 (7)	-0.0080 (7)
C2	0.0385 (8)	0.0652 (11)	0.0424 (9)	-0.0012 (6)	0.0022 (6)	-0.0051 (6)
C3	0.0420 (9)	0.0726 (12)	0.0441 (10)	-0.0006 (6)	0.0027 (7)	-0.0087 (7)
C4	0.0426 (11)	0.0852 (16)	0.0346 (11)	0.000	0.0069 (9)	0.000
C5	0.0400 (10)	0.0642 (14)	0.0395 (11)	0.000	0.0072 (8)	0.000
F1	0.0745 (10)	0.1105 (12)	0.0393 (8)	0.000	0.0190 (7)	0.000
O1	0.1022 (11)	0.0610 (8)	0.0715 (10)	-0.0050 (6)	0.0359 (8)	-0.0121 (6)
O2	0.0938 (10)	0.0622 (9)	0.0628 (9)	-0.0038 (6)	0.0355 (7)	-0.0032 (5)

*Geometric parameters (Å, °)*

C1—O2	1.235 (2)	C3—H3	0.9300
C1—O1	1.2826 (19)	C4—F1	1.343 (2)
C1—C2	1.483 (2)	C4—C3 <sup>i</sup>	1.377 (2)
C2—C5	1.3841 (18)	C5—C2 <sup>i</sup>	1.3841 (19)
C2—C3	1.392 (2)	C5—H5	0.9300
C3—C4	1.377 (2)	O1—H1	0.8201
O2—C1—O1	123.73 (15)	C2—C3—H3	121.1
O2—C1—C2	119.91 (13)	F1—C4—C3	118.37 (11)
O1—C1—C2	116.35 (15)	F1—C4—C3 <sup>i</sup>	118.36 (11)
C5—C2—C3	120.34 (15)	C3—C4—C3 <sup>i</sup>	123.3 (2)
C5—C2—C1	118.83 (15)	C2—C5—C2 <sup>i</sup>	120.3 (2)
C3—C2—C1	120.83 (14)	C2—C5—H5	119.9
C4—C3—C2	117.89 (16)	C2 <sup>i</sup> —C5—H5	119.9
C4—C3—H3	121.1	C1—O1—H1	113.5
O2—C1—C2—C5	2.3 (3)	C1—C2—C3—C4	179.97 (14)
O1—C1—C2—C5	-178.51 (16)	C2—C3—C4—F1	179.40 (14)
O2—C1—C2—C3	-177.68 (14)	C2—C3—C4—C3 <sup>i</sup>	-0.3 (3)
O1—C1—C2—C3	1.5 (3)	C3—C2—C5—C2 <sup>i</sup>	0.3 (3)
C5—C2—C3—C4	0.0 (3)	C1—C2—C5—C2 <sup>i</sup>	-179.72 (12)

Symmetry code: (i)  $x, -y+3/2, z$ .

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
O1—H1···O2 <sup>ii</sup>	0.82	1.81	2.625 (2)	174
C5—H5···F1 <sup>iii</sup>	0.93	2.52	3.404 (2)	160

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