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5-Fluoroisophthalic acid

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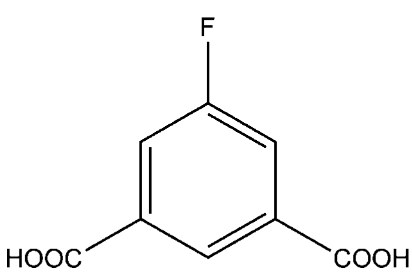
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.161; data-to-parameter ratio = 11.6.

In the crystal structure of the title compound, $C_8H_5FO_4$, 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)°. 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

$C_8H_5FO_4$
M_r = 184.12
Monoclinic, $P2_1/m$
a = 3.7736 (8) Å
b = 16.292 (4) Å
c = 6.2753 (14) Å
β = 91.871 (5)°
V = 385.60 (14) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 297 K
0.22 × 0.20 × 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_{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
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.82	1.81	2.625 (2)	174
C5—H5···F1^{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

Bhogala, B. R., Basavoju, S. & Nangia, A. (2005). *CrystEngComm*, **7**, 551–562.
Brandenburg, K. (2005). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2001). *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Derissen, J. L. (1974). *Acta Cryst.* B**30**, 2764–2765.
Sheldrick, G. M. (2003). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhang, Z.-H., Chen, S.-C., Mi, J.-L., He, M.-Y., Chen, Q., Wu, Z.-H. & Hu, Z.-J. (2010). *Inorg. Chem. Commun.* **13**, 1435–1438.

supplementary materials

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5-Fluoroisophthalic acid

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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, $C_8H_5FO_4$, to further investigate the supramolecular interactions involving the fluorine atom. The structure of the title compound, is shown below. The molecule presents C_2 symmetry with the fundamental unit lying on a C_2-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.

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.

Refinement

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

Figures

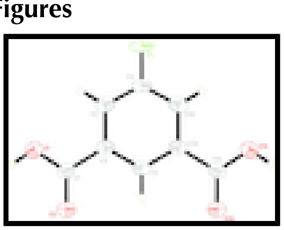

Fig. 1. The molecular structure of the title compound drawn with 30% probability ellipsoids.

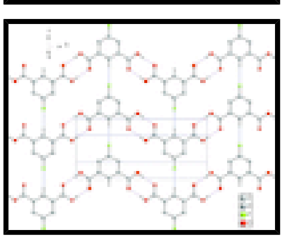

Fig. 2. Two-dimensional hydrogen-bonded layer of the title compound. Hydrogen bonds are indicated as dashed lines.

5-fluorobenzene-1,3-dicarboxylic acid

Crystal data

$C_8H_5FO_4$	$F(000) = 188$
$M_r = 184.12$	$D_x = 1.586$ Mg m^{-3}
Monoclinic, $P2_1/m$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yb	Cell parameters from 1020 reflections
$a = 3.7736$ (8) Å	$\theta = 2.5$–$28.0°$
$b = 16.292$ (4) Å	$\mu = 0.14$ mm^{-1}
$c = 6.2753$ (14) Å	$T = 297$ K
$\beta = 91.871$ (5)°	Block, colourless
$V = 385.60$ (14) Å^3	0.22 × 0.20 × 0.15 mm
$Z = 2$	

Data collection

Bruker APEXII CCD diffractometer	743 independent reflections
Radiation source: fine-focus sealed tube	603 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.018$
φ and ω scans	$\theta_{max} = 25.5°$, $\theta_{min} = 2.5°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	$h = -4 \rightarrow 4$
$T_{min} = 0.969$, $T_{max} = 0.979$	$k = -17 \rightarrow 19$
2201 measured reflections	$l = -7 \rightarrow 5$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.041$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.161$	H-atom parameters constrained
$S = 1.04$	$w = 1/[\sigma^2(F_o^2) + (0.1244P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
743 reflections	$(\Delta/\sigma)_{max} < 0.001$
64 parameters	$\Delta\rho_{max} = 0.16$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.15$ e Å^{-3}

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{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 (Å²)

	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^{i}	1.377 (2)
C2—C5	1.3841 (18)	C5—C2^{i}	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^{i}	118.36 (11)
C5—C2—C3	120.34 (15)	C3—C4—C3^{i}	123.3 (2)

C5—C2—C1	118.83 (15)	C2—C5—C2^{i}	120.3 (2)
C3—C2—C1	120.83 (14)	C2—C5—H5	119.9
C4—C3—C2	117.89 (16)	C2^{i}—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^{i}	−0.3 (3)
O1—C1—C2—C3	1.5 (3)	C3—C2—C5—C2^{i}	0.3 (3)
C5—C2—C3—C4	0.0 (3)	C1—C2—C5—C2^{i}	−179.72 (12)

Symmetry codes: (i) *x*, −*y*+3/2, *z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{ii}	0.82	1.81	2.625 (2)	174
C5—H5···F1^{iii}	0.93	2.52	3.404 (2)	160

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

Fig. 1

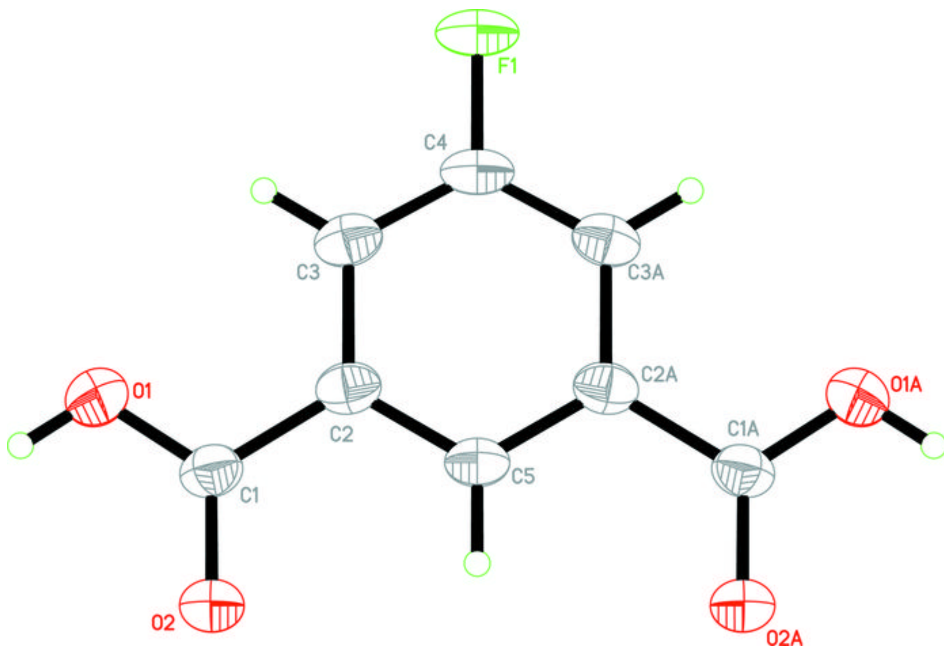

Fig. 2