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3-Fluoro-4-methylbenzoic acid

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.054
wR factor = 0.157
Data-to-parameter ratio = 15.9

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

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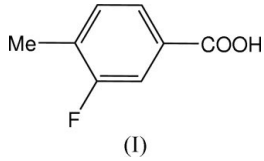
The title compound, $C_8H_7FO_2$, shows a nearly planar molecular structure, with a dihedral angle between the benzene ring and the carboxyl group of 6.2 (1)°. Pairs of molecules are linked *via* O—H···O hydrogen bonding into dimers, which are located around centres of inversion.

Comment

The molecule of the title compound, (I), has been determined to provide a reference point for the study of ^{19}F–^{13}C–^{1}H coupling in NMR spectra of solids and liquid crystals (Antonioli, 2004). The molecule is nearly planar (Fig. 1 and Table 1). The dihedral angle between the benzene ring and the carboxyl group of 6.2 (1)° is somewhat larger than that in the parent 4-methylbenzoic (*p*-toluic) acid, (II), of 2.9° (Takwale & Pant, 1971). In the crystal structure of (I), pairs of molecules are linked into dimers by O—H···O hydrogen bonding, with an O···H distance of 1.70 (4) Å and an O···O distance of 2.612 (2) Å. The O—H···O angle of 176 (3)° indicates strong hydrogen bonding and the dimers are located around centres of inversion. Dimers are also found in (II) but the crystal packing is completely different from that in (I). In contrast to the structure determination of (II), in the present determination the carboxy H atom was located in a difference map.



(I)

Experimental

Compound (I) was commercially available from Acros Organics (Loughborough, England). It was recrystallized from an aqueous solution.

Crystal data

$C_8H_7FO_2$
M_r = 154.14
Monoclinic, $P2_1/c$
a = 3.8132 (5) Å
b = 6.0226 (8) Å
c = 30.378 (4) Å
β = 92.50 (2)°
V = 696.98 (16) Å^3
Z = 4
D_x = 1.469 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 979 reflections
θ = 10.3–26.0°
μ = 0.12 mm^{-1}
T = 120 (2) K
Prism, colourless
0.55 × 0.19 × 0.16 mm

Data collection

SMART 6000 CCD area-detector diffractometer
ω scans
Absorption correction: none
9290 measured reflections
2036 independent reflections
1773 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 30.0°
$h = -5 \rightarrow 5$
$k = -8 \rightarrow 8$
$l = -42 \rightarrow 42$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0713P)^2 + 0.4137P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.054$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.157$	$\Delta\rho_{max} = 0.49$ e Å^{-3}
$S = 1.12$	$\Delta\rho_{min} = -0.25$ e Å^{-3}
2036 reflections	
128 parameters	
All H-atom parameters refined	

Table 1
Selected geometric parameters (Å, °).

F—C3	1.3595 (17)	C2—C3	1.379 (2)
O1—C7	1.3076 (18)	C3—C4	1.389 (2)
O2—C7	1.2354 (18)	C4—C5	1.396 (2)
C1—C6	1.389 (2)	C4—C8	1.505 (2)
C1—C2	1.395 (2)	C5—C6	1.393 (2)
C1—C7	1.481 (2)		
C6—C1—C2	120.18 (13)	C3—C4—C5	116.56 (14)
C3—C2—C1	117.86 (14)	C3—C4—C8	121.47 (14)
F—C3—C2	117.88 (14)	C5—C4—C8	121.97 (15)
F—C3—C4	117.96 (13)	C6—C5—C4	121.15 (14)
C2—C3—C4	124.15 (14)	C1—C6—C5	120.10 (14)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H01···O2^{i}	0.92 (4)	1.70 (4)	2.6117 (17)	176 (3)

Symmetry code: (i) $-x, 2-y, 1-z$.

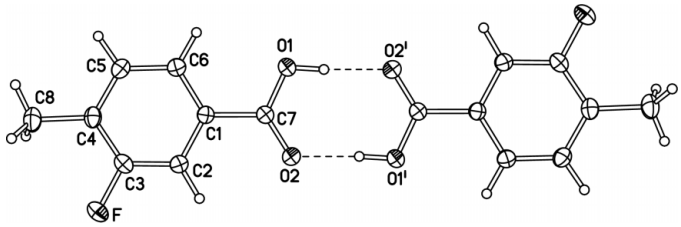


Figure 1
The crystal structure of the title compound, showing a hydrogen-bonded dimer with labelling and displacement ellipsoids drawn at the 50% probability level. Hydrogen bonding is indicated by dashed lines. [Symmetry code: (i) $-x, 2-y, 1-z$.]

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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supporting information

Acta Cryst. (2004). E**60**, o1948–o1949 [https://doi.org/10.1107/S1600536804024389]

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$M_r = 154.14$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 3.8132$ (5) Å
$b = 6.0226$ (8) Å
$c = 30.378$ (4) Å
$\beta = 92.50$ (2)°
$V = 696.98$ (16) Å^3
$Z = 4$
$F(000) = 320$
$D_x = 1.469$ Mg m^{-3}
Melting point = 442–444 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 979 reflections
$\theta = 10.3$–$26.0°$
$\mu = 0.12$ mm^{-1}
$T = 120$ K
Prism, colourless
0.55 × 0.19 × 0.16 mm

Data collection

SMART 6000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8 pixels mm^{-1}
ω scans
9290 measured reflections
2036 independent reflections
1773 reflections with $I > 2\sigma(I)$
$R_{int} = 0.067$
$\theta_{max} = 30.0°$, $\theta_{min} = 1.3°$
$h = -5 \rightarrow 5$
$k = -8 \rightarrow 8$
$l = -42 \rightarrow 42$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.157$
$S = 1.12$
2036 reflections
128 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0713P)^2 + 0.4137P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Special details

Experimental. The data collection nominally covered full sphere of reciprocal space, by a combination of 4 sets of ω scans; each set at different φ and/or 2θ angles and each scan (10 sec exposure) covering 0.3° in ω. Crystal to detector distance 4.85 cm.

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
F	0.1213 (3)	0.71029 (19)	0.29337 (3)	0.0340 (3)
O1	0.2296 (4)	0.7513 (2)	0.48864 (4)	0.0310 (3)
H01	0.167 (9)	0.843 (6)	0.5110 (11)	0.069 (9)*
O2	−0.0547 (3)	0.9999 (2)	0.44542 (4)	0.0273 (3)
C1	0.2068 (4)	0.6875 (2)	0.41215 (5)	0.0194 (3)
C2	0.1227 (4)	0.7663 (3)	0.36981 (5)	0.0211 (3)
H2	−0.001 (6)	0.911 (4)	0.3651 (7)	0.028 (5)*
C3	0.2043 (4)	0.6340 (3)	0.33464 (5)	0.0227 (3)
C4	0.3647 (4)	0.4276 (3)	0.33872 (5)	0.0222 (3)
C5	0.4442 (4)	0.3533 (3)	0.38153 (5)	0.0232 (3)
H5	0.565 (6)	0.209 (4)	0.3840 (7)	0.026 (5)*
C6	0.3668 (4)	0.4818 (3)	0.41798 (5)	0.0220 (3)
H6	0.423 (6)	0.428 (4)	0.4486 (7)	0.030 (5)*
C7	0.1160 (4)	0.8265 (2)	0.45024 (5)	0.0206 (3)
C8	0.4497 (5)	0.2923 (3)	0.29891 (6)	0.0305 (4)
H81	0.597 (7)	0.368 (5)	0.2804 (9)	0.049 (7)*
H82	0.592 (8)	0.165 (5)	0.3067 (9)	0.052 (8)*
H83	0.247 (8)	0.252 (5)	0.2817 (10)	0.049 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F	0.0460 (6)	0.0376 (6)	0.0181 (5)	0.0058 (5)	−0.0011 (4)	0.0025 (4)
O1	0.0440 (7)	0.0308 (6)	0.0179 (5)	0.0139 (5)	−0.0005 (5)	−0.0008 (4)
O2	0.0357 (6)	0.0240 (6)	0.0219 (5)	0.0085 (5)	0.0003 (4)	−0.0002 (4)
C1	0.0196 (6)	0.0198 (6)	0.0191 (6)	0.0008 (5)	0.0015 (5)	−0.0002 (5)
C2	0.0216 (6)	0.0207 (7)	0.0211 (7)	0.0017 (5)	0.0008 (5)	0.0007 (5)
C3	0.0240 (7)	0.0265 (7)	0.0176 (6)	−0.0024 (6)	0.0002 (5)	0.0007 (5)
C4	0.0177 (6)	0.0258 (7)	0.0231 (7)	−0.0013 (5)	0.0025 (5)	−0.0048 (5)
C5	0.0214 (6)	0.0216 (7)	0.0267 (7)	0.0023 (5)	0.0014 (5)	−0.0017 (5)
C6	0.0220 (6)	0.0222 (7)	0.0218 (7)	0.0018 (5)	0.0003 (5)	0.0002 (5)
C7	0.0223 (6)	0.0209 (7)	0.0186 (6)	0.0011 (5)	0.0013 (5)	0.0003 (5)
C8	0.0293 (8)	0.0356 (9)	0.0268 (8)	0.0023 (7)	0.0031 (6)	−0.0099 (7)

Geometric parameters (Å, º)

F—C3	1.3595 (17)	C3—C4	1.389 (2)
O1—C7	1.3076 (18)	C4—C5	1.396 (2)
O1—H01	0.92 (4)	C4—C8	1.505 (2)
O2—C7	1.2354 (18)	C5—C6	1.393 (2)
C1—C6	1.389 (2)	C5—H5	0.98 (2)

C1—C2	1.395 (2)	C6—H6	1.00 (2)
C1—C7	1.481 (2)	C8—H81	0.93 (3)
C2—C3	1.379 (2)	C8—H82	0.96 (3)
C2—H2	1.00 (2)	C8—H83	0.95 (3)
C7—O1—H01	111 (2)	C6—C5—H5	123.0 (13)
C6—C1—C2	120.18 (13)	C4—C5—H5	115.8 (13)
C6—C1—C7	121.39 (13)	C1—C6—C5	120.10 (14)
C2—C1—C7	118.42 (13)	C1—C6—H6	118.9 (14)
C3—C2—C1	117.86 (14)	C5—C6—H6	121.0 (14)
C3—C2—H2	120.9 (13)	O2—C7—O1	123.44 (14)
C1—C2—H2	121.2 (13)	O2—C7—C1	121.65 (13)
F—C3—C2	117.88 (14)	O1—C7—C1	114.91 (13)
F—C3—C4	117.96 (13)	C4—C8—H81	112.2 (18)
C2—C3—C4	124.15 (14)	C4—C8—H82	111.8 (17)
C3—C4—C5	116.56 (14)	H81—C8—H82	101 (2)
C3—C4—C8	121.47 (14)	C4—C8—H83	112.7 (18)
C5—C4—C8	121.97 (15)	H81—C8—H83	107 (2)
C6—C5—C4	121.15 (14)	H82—C8—H83	112 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H01···O2^{i}	0.92 (4)	1.70 (4)	2.6117 (17)	176 (3)

Symmetry code: (i) −*x*, −*y*+2, −*z*+1.