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4,4,4-Trifluoro-*trans*-2-butenoic acid

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The title compound, $C_4H_3O_2F_3$, crystallizes with two molecules in the asymmetric unit. These two molecules form a dimer *via* a pair of hydrogen-bonding interactions between the carboxylic acid groups of the two molecules. The correspondences of H···O distances and O—H···O angles are 1.77 (3) Å and 179 (3)°, and 1.59 (4) Å and 175 (4)°. The uncertainty in their position indicates disorder in the carboxylic acid H atoms.

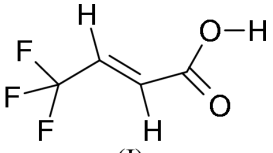
Key indicators

Single-crystal X-ray study
T = 190 K
Mean σ(C–C) = 0.002 Å
R factor = 0.039
wR factor = 0.100
Data-to-parameter ratio = 13.0

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

Comment

The structure of the title compound, (I), was determined as part of a study into the polymorphic forms of the related compound tetrolic acid, and an investigation into the structures preferentially formed by small compounds with a single carboxylic acid moiety. Compounds with a double bond α to the C atom of the carboxylic acid group have a strong tendency to form dimers. This compound is no exception, crystallizing in the space group $P2_1/c$. The two molecules forming the dimer have a non-crystallographic centre of symmetry between the carboxylic acid groups [at x = 0.586 (3), y = 0.360 (3) z = 0.696 (3)]. This can be contrasted with the structure of crotonic acid (Shimizu *et al.*, 1974), which utilizes a crystallographic centre of symmetry to form the dimer. The hydrogen-bonded dimers form ribbons through close contacts involving the F atoms (F···F distances of 3.0, 3.3 and 3.4 Å), and the ribbons lie side-by-side to form sheets.



(I)

Experimental

A crystal of suitable quality for single-crystal X-ray diffraction was obtained from the sample supplied by Fluorochem. The synthesis of the title compound has been described by Haszeldine (1957).

Crystal data

$C_4H_3F_3O_2$
M_r = 140.06
Monoclinic, $P2_1/c$
a = 10.8280 (2) Å
b = 9.8064 (2) Å
c = 10.1768 (2) Å
β = 94.307 (1)°
V = 1077.56 (4) Å^3
Z = 8

D_x = 1.727 Mg m^{-3}
Mo Kα radiation
Cell parameters from 2437 reflections
θ = 5–27°
μ = 0.20 mm^{-1}
T = 190 K
Plate, colourless
0.30 × 0.30 × 0.15 mm

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Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: multi-scan (*DENZO* and *SCALEPACK*; Otwinowski & Minor, 1997)
$T_{\min} = 0.94$, $T_{\max} = 0.97$
4700 measured reflections

2429 independent reflections
1961 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.01$
$\theta_{\max} = 27.5°$
$h = -14 \rightarrow 14$
$k = -12 \rightarrow 12$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.100$
$S = 0.99$
2429 reflections
187 parameters

All H-atom parameters refined
$w = 1/[\sigma^2(F^*) + (0.0388p)^2 + 0.474p]$ where $p = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.35$ e Å^{-3}
$\Delta\rho_{\min} = -0.31$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O101—C103	1.282 (2)	O1—C3	1.281 (2)
O102—C103	1.239 (2)	O2—C3	1.249 (2)
C103—C104	1.485 (2)	C3—C4	1.482 (2)
C104—C105	1.308 (2)	C4—C5	1.312 (2)
C105—C106	1.487 (2)	C5—C6	1.488 (2)
C106—F107	1.327 (2)	C6—F7	1.329 (2)
C106—F108	1.338 (2)	C6—F8	1.331 (2)
C106—F109	1.323 (2)	C6—F9	1.330 (2)
O101—C103—O102	124.4 (1)	O1—C3—O2	124.5 (1)
O101—C103—C104	115.0 (1)	O1—C3—C4	114.6 (1)
O102—C103—C104	120.6 (1)	O2—C3—C4	120.9 (1)
C103—C104—C105	121.4 (1)	C3—C4—C5	122.4 (1)
C104—C105—C106	123.1 (1)	C4—C5—C6	122.7 (2)
C105—C106—F107	111.7 (1)	C5—C6—F7	111.7 (1)
C105—C106—F108	111.0 (1)	C5—C6—F8	111.7 (1)
F107—C106—F108	105.5 (1)	F7—C6—F8	106.1 (1)
C105—C106—F109	113.5 (1)	C5—C6—F9	113.1 (1)
F107—C106—F109	107.3 (1)	F7—C6—F9	106.4 (1)
F108—C106—F109	107.4 (1)	F8—C6—F9	107.4 (1)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O102	0.92 (3)	1.76 (3)	2.676 (2)	179 (3)
O101—H101···O2	1.07 (4)	1.59 (4)	2.654 (2)	175 (4)

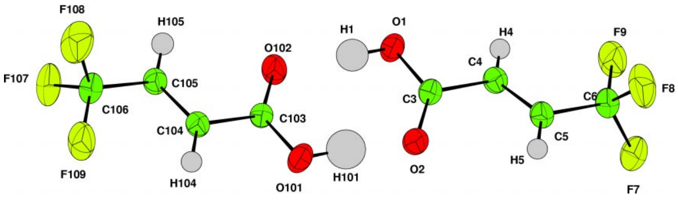

Figure 1
Crystallographic diagram of the asymmetric unit, with atomic numbering. Displacement ellipsoids are drawn at the 50% probability level.

H atoms were refined isotropically; C—H distances were in the range 0.88 (2)–0.92 (2) Å and O—H distances were 0.91 (3) and 1.07 (4) Å.

Data collection: *COLLECT* (Nonius, 1997–2001); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Watkin *et al.*, 2001); molecular graphics: *CAMERON* (Watkin *et al.*, 1996); software used to prepare material for publication: *CRYSTALS*.

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