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Crystal structure of (*E*)-4,4,4-trifluoro-3-phenylbut-2-enoic acid

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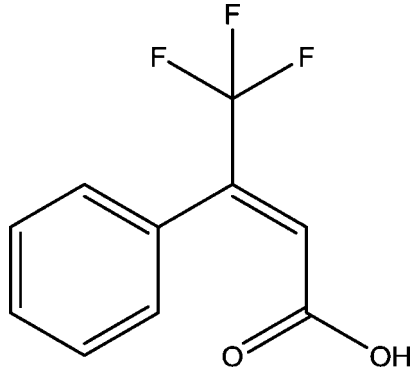
In the title compound, $C_{10}H_7F_3O_2$, the dihedral angle between the benzene ring and the ethylene plane is 76.34 (11)°. In the crystal, O—H···O hydrogen bonds link the molecules into *C*(4) chains propagating in [010].

Keywords: crystal structure; trifluoromethyl acid; hydrogen bonding.

CCDC reference: 1441578

1. Scheme



2. Experimental

2.1. Crystal data

$C_{10}H_7F_3O_2$ M_r = 216.16

Monoclinic, $P2_1/c$
a = 11.4093 (9) Å
b = 5.7749 (4) Å
c = 14.7469 (8) Å
β = 96.300 (6)°
V = 965.77 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.14 mm^{-1}
T = 295 K
0.25 × 0.12 × 0.03 mm

2.2. Data collection

Agilent Xcalibur, Eos diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
T_{min} = 0.835, T_{max} = 1.000
3799 measured reflections
1960 independent reflections
1252 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.171
S = 1.02
1960 reflections
140 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 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}	0.97 (3)	1.77 (3)	2.715 (2)	166 (3)

Symmetry code: (i) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2013); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SUPERFLIP* (Palatinus & Chapuis, 2007); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7527).

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supporting information

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S1. Refinement

The OH H atom was freely refined. C-bound H atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C).

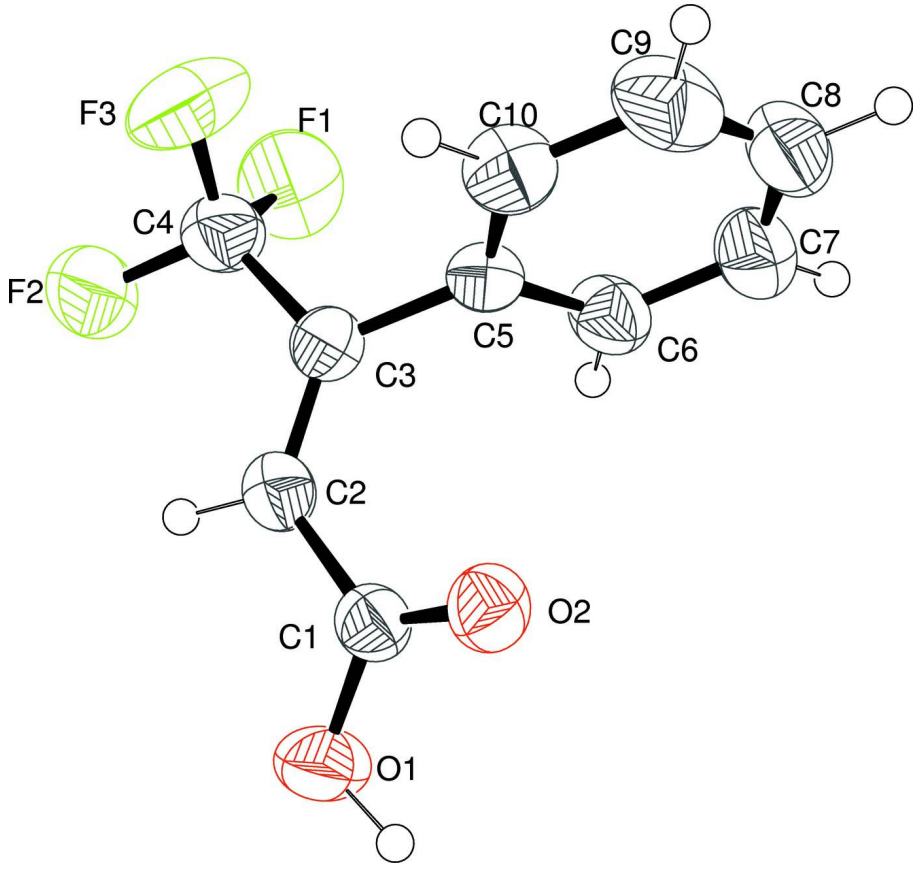

Figure 1

Ellipsoid plot.

(*E*)-4,4,4-Trifluoro-3-phenylbut-2-enoic acid

Crystal data

$C_{10}H_7F_3O_2$
M_r = 216.16
Monoclinic, $P2_1/c$
a = 11.4093 (9) Å
b = 5.7749 (4) Å
c = 14.7469 (8) Å
β = 96.300 (6)°
V = 965.77 (11) Å^3

$Z = 4$
$F(000) = 440$
$D_x = 1.487$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.7107$ Å
Cell parameters from 816 reflections
$\theta = 2.8$–$24.2°$
$\mu = 0.14$ mm^{-1}
$T = 295$ K
Plate, colourless
0.25 × 0.12 × 0.03 mm

Data collection

Agilent Xcalibur, Eos diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
Detector resolution: 15.9555 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2013)
$T_{min} = 0.835$, $T_{max} = 1.000$
3799 measured reflections
1960 independent reflections
1252 reflections with $I > 2\sigma(I)$
$R_{int} = 0.022$
$\theta_{max} = 26.4°$, $\theta_{min} = 1.8°$
$h = -14 \rightarrow 11$
$k = -7 \rightarrow 6$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.171$
$S = 1.02$
1960 reflections
140 parameters
0 restraints
Primary atom site location: iterative
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}

Special details

Experimental. Absorption correction: CrysAlisPro, Agilent Technologies, Version 1.171.36.32 (release 02-08-2013 CrysAlis171 .NET) (compiled Aug 2 2013,16:46:58) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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. 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^2)

	x	y	z	U_{iso}*/U_{eq}
F1	0.33889 (15)	0.9642 (4)	0.53424 (11)	0.0878 (6)
F2	0.16331 (17)	1.0064 (3)	0.47259 (11)	0.0956 (7)
F3	0.23597 (19)	1.2390 (3)	0.57582 (12)	0.0938 (6)
O1	−0.01828 (17)	0.4089 (3)	0.62622 (12)	0.0651 (6)
H1	−0.042 (3)	0.311 (6)	0.674 (2)	0.101 (11)*
O2	0.06645 (14)	0.5790 (3)	0.75208 (10)	0.0510 (5)
C1	0.04817 (19)	0.5707 (4)	0.66953 (15)	0.0439 (6)

C2	0.0965 (2)	0.7311 (4)	0.60493 (15)	0.0484 (6)
H2	0.0581	0.7394	0.5460	0.058*
C3	0.19045 (19)	0.8642 (4)	0.62488 (14)	0.0435 (5)
C4	0.2304 (2)	1.0167 (5)	0.55131 (17)	0.0565 (7)
C5	0.26860 (18)	0.8691 (4)	0.71297 (14)	0.0408 (5)
C6	0.3474 (2)	0.6892 (4)	0.73361 (17)	0.0536 (6)
H6	0.3493	0.5657	0.6933	0.064*
C7	0.4226 (2)	0.6914 (5)	0.81282 (19)	0.0683 (8)
H7	0.4753	0.5699	0.8258	0.082*
C8	0.4205 (3)	0.8706 (6)	0.87260 (18)	0.0703 (8)
H8	0.4713	0.8706	0.9264	0.084*
C9	0.3438 (3)	1.0505 (5)	0.85370 (18)	0.0719 (8)
H9	0.3428	1.1728	0.8947	0.086*
C10	0.2672 (2)	1.0519 (4)	0.77358 (17)	0.0555 (7)
H10	0.2153	1.1748	0.7608	0.067*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0745 (12)	0.1200 (16)	0.0741 (11)	−0.0052 (10)	0.0318 (9)	0.0103 (10)
F2	0.1015 (14)	0.1180 (16)	0.0611 (10)	−0.0450 (11)	−0.0194 (9)	0.0354 (10)
F3	0.1397 (17)	0.0535 (10)	0.0926 (13)	−0.0185 (10)	0.0318 (11)	0.0081 (10)
O1	0.0751 (13)	0.0738 (13)	0.0452 (9)	−0.0342 (10)	0.0011 (8)	0.0002 (9)
O2	0.0586 (11)	0.0528 (10)	0.0413 (9)	−0.0007 (7)	0.0039 (7)	−0.0017 (7)
C1	0.0409 (13)	0.0449 (13)	0.0454 (12)	0.0004 (9)	0.0022 (9)	−0.0006 (10)
C2	0.0481 (14)	0.0533 (14)	0.0424 (11)	−0.0035 (11)	−0.0016 (9)	0.0031 (11)
C3	0.0436 (13)	0.0414 (12)	0.0452 (12)	0.0013 (10)	0.0039 (9)	0.0006 (10)
C4	0.0573 (16)	0.0594 (16)	0.0526 (14)	−0.0103 (12)	0.0050 (11)	0.0034 (12)
C5	0.0394 (12)	0.0399 (12)	0.0435 (11)	−0.0034 (9)	0.0068 (9)	−0.0021 (10)
C6	0.0513 (14)	0.0470 (14)	0.0605 (14)	0.0025 (11)	−0.0030 (11)	−0.0087 (12)
C7	0.0594 (17)	0.0656 (18)	0.0750 (18)	0.0028 (13)	−0.0138 (13)	0.0047 (16)
C8	0.0666 (19)	0.087 (2)	0.0536 (15)	−0.0150 (17)	−0.0080 (13)	0.0038 (16)
C9	0.084 (2)	0.077 (2)	0.0546 (15)	−0.0144 (17)	0.0094 (14)	−0.0261 (15)
C10	0.0611 (16)	0.0498 (14)	0.0566 (14)	0.0052 (12)	0.0114 (11)	−0.0091 (12)

Geometric parameters (Å, º)

F1—C4	1.326 (3)	C5—C6	1.386 (3)
F2—C4	1.320 (3)	C5—C10	1.385 (3)
F3—C4	1.333 (3)	C6—H6	0.9300
O1—H1	0.96 (3)	C6—C7	1.371 (3)
O1—C1	1.323 (3)	C7—H7	0.9300
O2—C1	1.213 (2)	C7—C8	1.361 (4)
C1—C2	1.478 (3)	C8—H8	0.9300
C2—H2	0.9300	C8—C9	1.367 (4)
C2—C3	1.326 (3)	C9—H9	0.9300
C3—C4	1.506 (3)	C9—C10	1.390 (4)
C3—C5	1.493 (3)	C10—H10	0.9300

C1—O1—H1	105.0 (18)	C10—C5—C3	121.9 (2)
O1—C1—C2	111.47 (19)	C10—C5—C6	118.9 (2)
O2—C1—O1	122.6 (2)	C5—C6—H6	119.7
O2—C1—C2	125.9 (2)	C7—C6—C5	120.7 (2)
C1—C2—H2	117.6	C7—C6—H6	119.7
C3—C2—C1	124.7 (2)	C6—C7—H7	119.8
C3—C2—H2	117.6	C8—C7—C6	120.3 (3)
C2—C3—C4	118.7 (2)	C8—C7—H7	119.8
C2—C3—C5	126.5 (2)	C7—C8—H8	119.9
C5—C3—C4	114.63 (19)	C7—C8—C9	120.1 (3)
F1—C4—F3	104.7 (2)	C9—C8—H8	119.9
F1—C4—C3	111.4 (2)	C8—C9—H9	119.8
F2—C4—F1	106.6 (2)	C8—C9—C10	120.4 (2)
F2—C4—F3	106.7 (2)	C10—C9—H9	119.8
F2—C4—C3	114.5 (2)	C5—C10—C9	119.6 (2)
F3—C4—C3	112.2 (2)	C5—C10—H10	120.2
C6—C5—C3	119.22 (19)	C9—C10—H10	120.2

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{i}	0.97 (3)	1.77 (3)	2.715 (2)	166 (3)

Symmetry code: (i) −*x*, *y*−1/2, −*z*+3/2.