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2-Methyl-4-trifluoromethyl-1,3-thiazole-5-carboxylic acid

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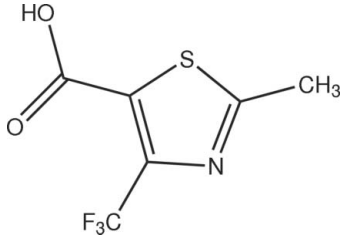
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.048; wR factor = 0.158; data-to-parameter ratio = 12.6.

In crystal of the title compound, $C_6H_4F_3NO_2S$, molecules are linked by O—H···N and C—H···O hydrogen bonds, forming chains.

Related literature

For a related compound, see: Liu (2004). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_6H_4F_3NO_2S$
M_r = 211.16
Monoclinic, $P2_1/c$
a = 4.961 (1) Å
b = 15.682 (3) Å
c = 10.632 (2) Å
β = 90.35 (3)°
V = 827.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.41 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.888, T_{max} = 0.960
1672 measured reflections
1494 independent reflections
1209 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
3 standard reflections
every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.158
S = 1.15
1494 reflections
119 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 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
O2—H2A···N^{i}	0.82	2.02	2.820 (3)	166
C1—H1A···O1^{ii}	0.96	2.34	3.277 (4)	166

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5094).

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supporting information

Acta Cryst. (2009). E**65**, o2500 [doi:10.1107/S1600536809037325]

2-Methyl-4-trifluoromethyl-1,3-thiazole-5-carboxylic acid

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S1. Experimental

To a cooled solution of methyl 2-methyl-4-(trifluoromethyl)thiazole-5-carboxylate (0.12 mol) in ethyl alcohol (200 ml) was added a solution of sodium hydroxide (9.62 g) in 200ml of water. The solution was heated at 358 K for 1.5 h. After evaporation of the ethyl alcohol, the aqueous solution was diluted with 200 ml of water and acidified to pH = 1 with concentrated aqueous hydrochloric acid. The solid material was filtered and washed twice with 100 ml of water and 100 ml of dichloromethane. After drying in a vacuum oven,the title compound was obtained (yield; 85%). Colourless blocks of (I) were obtained by slow evaporation of an ethyl acetate solution.

S2. Refinement

The H atoms were positioned geometrically (C—H = 0.93–0.96 Å, O—H = 0.82Å) and refined as with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C, O).

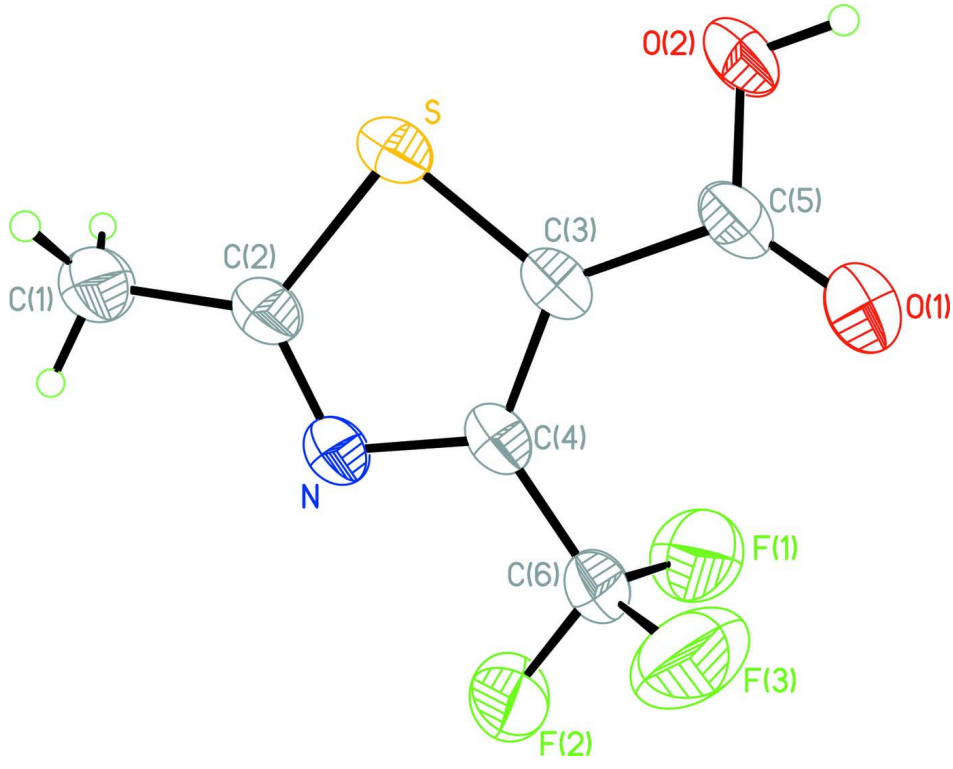

Figure 1

The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

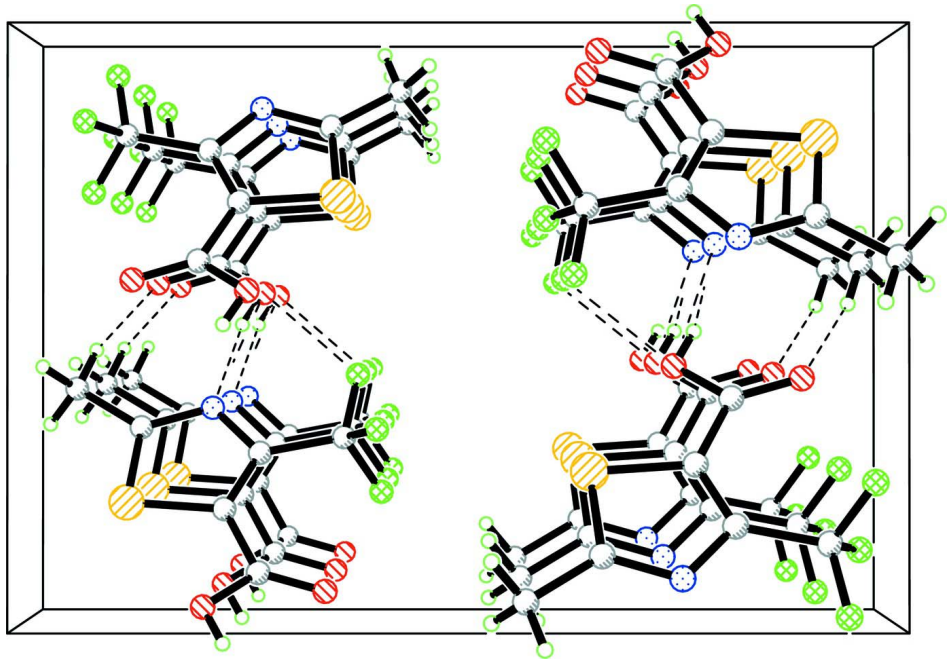

Figure 2

A packing diagram for (I). C—H···O hydrogen bonds are shown by dashed lines.

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Crystal data

$C_6H_4F_3NO_2S$
$M_r = 211.16$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 4.961$ (1) Å
$b = 15.682$ (3) Å
$c = 10.632$ (2) Å
$\beta = 90.35$ (3)°
$V = 827.1$ (3) Å^3
$Z = 4$
$F(000) = 424$
$D_x = 1.696$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10$–14°
$\mu = 0.41$ mm^{-1}
$T = 293$ K
Block, colourless
0.30 × 0.20 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.888$, $T_{max} = 0.960$
1672 measured reflections
1494 independent reflections
1209 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 25.3°$, $\theta_{min} = 2.3°$
$h = 0 \rightarrow 5$
$k = 0 \rightarrow 18$
$l = -12 \rightarrow 12$
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.158$
$S = 1.15$
1494 reflections
119 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
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.25$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.050 (8)

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S	1.03912 (15)	0.13345 (4)	0.21544 (7)	0.0482 (4)
N	0.7571 (4)	0.22213 (14)	0.3665 (2)	0.0406 (6)
F1	1.1047 (4)	0.41020 (12)	0.3353 (2)	0.0813 (7)
F2	0.7272 (5)	0.38613 (12)	0.4214 (2)	0.0844 (8)
F3	0.7499 (4)	0.41298 (12)	0.2261 (2)	0.0816 (7)
O1	1.2183 (5)	0.35504 (14)	0.0770 (2)	0.0683 (7)
O2	1.4044 (4)	0.22652 (13)	0.0592 (2)	0.0647 (7)
H2A	1.4972	0.2497	0.0056	0.097*
C1	0.6926 (6)	0.06626 (19)	0.3979 (3)	0.0569 (8)
H1A	0.5699	0.0842	0.4621	0.085*
H1B	0.8346	0.0330	0.4351	0.085*
H1C	0.5978	0.0324	0.3368	0.085*
C2	0.8109 (6)	0.14311 (16)	0.3348 (3)	0.0426 (7)
C3	1.0636 (5)	0.24181 (18)	0.2054 (2)	0.0401 (7)
C4	0.8996 (5)	0.27820 (16)	0.2937 (2)	0.0381 (6)
C5	1.2368 (5)	0.28263 (18)	0.1076 (2)	0.0431 (7)
C6	0.8700 (6)	0.37191 (17)	0.3191 (3)	0.0465 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S	0.0564 (5)	0.0417 (5)	0.0467 (5)	0.0035 (3)	0.0250 (4)	−0.0018 (3)
N	0.0444 (13)	0.0400 (12)	0.0374 (12)	0.0008 (9)	0.0163 (10)	0.0033 (9)

F1	0.0727 (14)	0.0560 (12)	0.1153 (19)	−0.0172 (10)	0.0111 (12)	−0.0146 (11)
F2	0.1252 (18)	0.0513 (11)	0.0775 (15)	−0.0002 (10)	0.0667 (13)	−0.0088 (9)
F3	0.1088 (19)	0.0586 (12)	0.0774 (15)	0.0297 (11)	0.0010 (13)	0.0105 (10)
O1	0.0765 (17)	0.0537 (14)	0.0752 (17)	0.0031 (11)	0.0441 (13)	0.0126 (11)
O2	0.0737 (15)	0.0559 (13)	0.0651 (15)	0.0091 (10)	0.0492 (12)	0.0065 (10)
C1	0.068 (2)	0.0435 (16)	0.0600 (19)	−0.0010 (14)	0.0290 (16)	0.0046 (13)
C2	0.0462 (15)	0.0416 (15)	0.0403 (15)	0.0016 (11)	0.0174 (12)	0.0002 (11)
C3	0.0378 (14)	0.0461 (15)	0.0366 (14)	0.0000 (10)	0.0136 (11)	−0.0002 (11)
C4	0.0364 (13)	0.0431 (15)	0.0348 (14)	−0.0009 (10)	0.0110 (11)	0.0019 (10)
C5	0.0420 (15)	0.0515 (17)	0.0360 (14)	−0.0011 (12)	0.0153 (12)	−0.0004 (12)
C6	0.0533 (17)	0.0416 (14)	0.0447 (16)	−0.0004 (12)	0.0212 (14)	0.0030 (12)

Geometric parameters (Å, º)

S—C3	1.707 (3)	O2—H2A	0.8200
S—C2	1.712 (3)	C1—C2	1.501 (4)
N—C2	1.312 (3)	C1—H1A	0.9600
N—C4	1.371 (3)	C1—H1B	0.9600
F1—C6	1.320 (3)	C1—H1C	0.9600
F2—C6	1.321 (3)	C3—C4	1.371 (3)
F3—C6	1.319 (3)	C3—C5	1.496 (4)
O1—C5	1.185 (3)	C4—C6	1.501 (4)
O2—C5	1.317 (3)		
C3—S—C2	90.35 (12)	C5—C3—S	120.7 (2)
C2—N—C4	110.8 (2)	N—C4—C3	115.5 (3)
C5—O2—H2A	109.5	N—C4—C6	118.4 (2)
C2—C1—H1A	109.5	C3—C4—C6	126.1 (2)
C2—C1—H1B	109.5	O1—C5—O2	125.5 (2)
H1A—C1—H1B	109.5	O1—C5—C3	123.9 (2)
C2—C1—H1C	109.5	O2—C5—C3	110.6 (2)
H1A—C1—H1C	109.5	F3—C6—F1	105.6 (2)
H1B—C1—H1C	109.5	F3—C6—F2	107.0 (3)
N—C2—C1	124.3 (2)	F1—C6—F2	107.0 (3)
N—C2—S	114.24 (19)	F3—C6—C4	112.8 (2)
C1—C2—S	121.5 (2)	F1—C6—C4	112.4 (2)
C4—C3—C5	130.1 (3)	F2—C6—C4	111.5 (2)
C4—C3—S	109.18 (19)		
C4—N—C2—C1	178.7 (3)	S—C3—C4—C6	177.7 (2)
C4—N—C2—S	0.3 (3)	C4—C3—C5—O1	−14.8 (5)
C3—S—C2—N	−0.5 (2)	S—C3—C5—O1	162.6 (3)
C3—S—C2—C1	−179.0 (3)	C4—C3—C5—O2	166.9 (3)
C2—S—C3—C4	0.6 (2)	S—C3—C5—O2	−15.7 (3)
C2—S—C3—C5	−177.3 (2)	N—C4—C6—F3	−113.2 (3)
C2—N—C4—C3	0.1 (3)	C3—C4—C6—F3	68.6 (4)
C2—N—C4—C6	−178.2 (2)	N—C4—C6—F1	127.4 (3)
C5—C3—C4—N	177.1 (3)	C3—C4—C6—F1	−50.7 (4)

S—C3—C4—N	−0.5 (3)	N—C4—C6—F2	7.2 (4)
C5—C3—C4—C6	−4.7 (4)	C3—C4—C6—F2	−170.9 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···N^{i}	0.82	2.02	2.820 (3)	166
C1—H1*A*···O1^{ii}	0.96	2.34	3.277 (4)	166

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