

1,2,3-Trifluorobenzene

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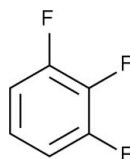
Received 12 August 2009; accepted 25 September 2009

Key indicators: single-crystal X-ray study; $T = 233$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.061; wR factor = 0.226; data-to-parameter ratio = 14.4.

In the title compound, $\text{C}_6\text{H}_3\text{F}_3$, weak electrostatic and dispersive forces between $\text{C}(\delta^+)-\text{F}(\delta^-)$ and $\text{H}(\delta^+)-\text{C}(\delta^-)$ groups are at the borderline of the hydrogen-bond phenomenon and are poorly directional and further deformed in the presence of $\pi-\pi$ stacking interactions. The molecule lies on a twofold rotation axis. In the crystal structure, one-dimensional tapes are formed *via* two antidromic $\text{C}-\text{H}\cdots\text{F}$ hydrogen bonds. These tapes are, in turn, connected into corrugated two-dimensional sheets by bifurcated $\text{C}-\text{H}\cdots\text{F}$ hydrogen bonds. Packing in the third dimension is furnished by $\pi-\pi$ stacking interactions with a centroid-centroid distance of 3.6362 (14) Å.

Related literature

For $\text{C}-\text{H}\cdots\text{F}$ interactions, see: Althoff *et al.* (2006); Bats *et al.* (2000); Choudhury *et al.* (2004); D'Oría & Novoa (2008); Dunitz & Taylor (1997); Howard *et al.* (1996); Müller *et al.* (2007); O'Hagan (2008); Reichenbacher *et al.* (2005); Weiss *et al.* (1997). For related crystal structures of several polyfluorinated benzenes, see: Thalladi *et al.* (1998). For crystallization techniques, see: Boese & Nussbaumer (1994).



Experimental

Crystal data

$\text{C}_6\text{H}_3\text{F}_3$	$V = 559.1$ (2) Å ³
$M_r = 132.08$	$Z = 4$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 7.4238$ (19) Å	$\mu = 0.16$ mm ⁻¹
$b = 11.590$ (3) Å	$T = 233$ K
$c = 7.0473$ (17) Å	$0.30 \times 0.30 \times 0.30$ mm
$\beta = 112.783$ (4)°	

Data collection

Siemens SMART three-axis goniometer with an APEXII area-detector system diffractometer	1074 measured reflections
Absorption correction: multi-scan (SADABS; Bruker; 2004)	634 independent reflections
$T_{\min} = 0.820$, $T_{\max} = 0.953$	413 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.013$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.061$	44 parameters
$wR(F^2) = 0.226$	H-atom parameters constrained
$S = 1.04$	$\Delta\rho_{\max} = 0.20$ e Å ⁻³
634 reflections	$\Delta\rho_{\min} = -0.18$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C3}-\text{H3}\cdots\text{F2}^{\text{i}}$	1.10	2.77	3.560 (3)	129
$\text{C3}-\text{H3}\cdots\text{F1}^{\text{ii}}$	1.10	2.59	3.528 (4)	144
$\text{C4}-\text{H4}\cdots\text{F2}^{\text{iii}}$	1.00	2.60	3.440 (4)	142

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

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINTE (Bruker, 2008); data reduction: SAINTE; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: Mercury (Macrae *et al.*, 2008) and GIMP2 (The GIMP team, 2008); software used to prepare material for publication: publCIF (Westrip, 2009).

MTK and RB thank the DFG FOR-618. GRD thanks the DST for the award of a J.C. Bose fellowship. TST thanks the UGC for an SRF.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2880).

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supplementary materials

Acta Cryst. (2009). E65, o2670 [doi:10.1107/S1600536809038975]

1,2,3-Trifluorobenzene

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Comment

Despite the high electronegativity difference between carbon and fluorine, the C–F bond acts as a poor hydrogen bond acceptor due to the hardness of the F-atom (Dunitz & Taylor, 1997; O'Hagan, 2008). The resultant weak C–H \cdots F–C interactions (Howard *et al.*, 1996; Reichenbacher *et al.*, 2005) arise mainly due to electrostatic and dispersive forces between the C(δ^+)–F(δ^-) and the H(δ^+)–C(δ^-) fragments. These interactions, at the borderline of the hydrogen bond phenomenon, are also poorly directional and are deformed by other dominant interactions (Weiss, *et al.*, 1997; D'Oria & Novoa, 2008; Müller *et al.*, 2007). In the absence of other interactions these weak interactions can play a role in the overall crystal packing of the molecule (Bats *et al.* 2000; Choudhury *et al.* 2004; Althoff *et al.* 2006). In activated systems such as polyfluorobenzenes, C–H \cdots F–C interactions may be of significance, and in connection there are some reports of the crystal structures of several polyfluorinated benzene compounds (Thalladi *et al.*, 1998). As a continuation of this work, we report here the crystal structure of 1,2,3-trifluorobenzene (1). The comparison crystal structures of 1,2- and 1,4-difluorobenzene and 1,3,5-trifluorobenzene have been reported in this earlier work.

Experimental

The crystals were prepared from commercial samples by zone melting in a quartz capillary at 235 K (1) according to the procedure outlined by (Boese & Nussbaumer, 1994).

Refinement

Treatment of hydrogen atoms: Riding model with the 1.2 fold isotropic displacement parameters of the equivalent U^{ij} of the corresponding carbon atom.

Figures

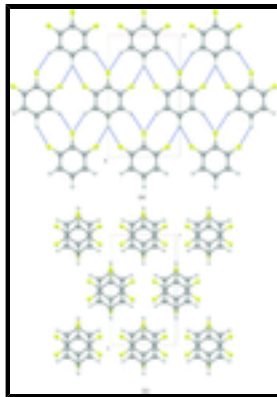


Fig. 1. Part of the crystal structure of 1 (a) 2D network of C–H \cdots F–C interactions viewed along the c-axis (b) π – π stacking of molecules viewed along the c-axis.

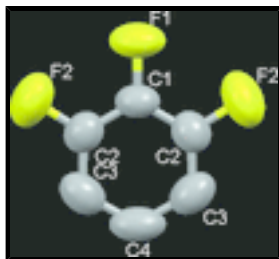


Fig. 2. The molecular structure of (1) with displacement ellipsoids drawn at the 50% probability level. The identically labelled atoms are related to each other by the symmetry operator $(2-x, y, -z+1/2)$.

1,2,3-Trifluorobenzene

Crystal data

$C_6H_3F_3$

$M_r = 132.08$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 7.4238$ (19) Å

$b = 11.590$ (3) Å

$c = 7.0473$ (17) Å

$\beta = 112.783$ (4)°

$V = 559.1$ (2) Å³

$Z = 4$

$F_{000} = 264$

$D_x = 1.569$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 376 reflections

$\theta = 3.8$ – 22.7 °

$\mu = 0.16$ mm⁻¹

$T = 233$ K

Cylindric, colourless

$0.30 \times 0.30 \times 0.30$ mm

Data collection

Siemens SMART three-axis goniometer with an APEXII area-detector system diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 512 pixels mm⁻¹

$T = 233$ K

in ω at 0.3° scan width one run with 740 frames, $\phi = 0^\circ$, $\chi = 0^\circ$

Absorption correction: multi-scan (SADABS; Bruker, 2004)

$T_{\min} = 0.820$, $T_{\max} = 0.953$

1074 measured reflections

634 independent reflections

413 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.013$

$\theta_{\max} = 28.2^\circ$

$\theta_{\min} = 3.5^\circ$

$h = -9 \rightarrow 9$

$k = -14 \rightarrow 10$

$l = -9 \rightarrow 4$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.061$

$wR(F^2) = 0.226$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1501P)^2 + 0.039P]$,

where $P = (F_o^2 + 2F_c^2)/3$

$S = 1.04$	$(\Delta/\sigma)_{\max} = 0.017$
634 reflections	$\Delta\rho_{\max} = 0.20 \text{ e } \text{\AA}^{-3}$
44 parameters	$\Delta\rho_{\min} = -0.18 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	1.0000	0.30558 (17)	0.2500	0.1156 (10)
F2	0.6666 (2)	0.4183 (2)	0.1576 (3)	0.1354 (10)
C1	1.0000	0.4213 (3)	0.2500	0.0769 (9)
C2	0.8308 (3)	0.4803 (2)	0.2036 (3)	0.0824 (8)
C3	0.8265 (4)	0.5973 (3)	0.2023 (3)	0.0942 (9)
H3	0.6833	0.6388	0.1585	0.113*
C4	1.0000	0.6558 (3)	0.2500	0.1006 (13)
H4	1.0000	0.7422	0.2500	0.121*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.161 (2)	0.0623 (13)	0.1249 (16)	0.000	0.0563 (14)	0.000
F2	0.0959 (12)	0.157 (2)	0.1484 (16)	-0.0341 (10)	0.0415 (10)	0.0067 (12)
C1	0.1030 (19)	0.0573 (16)	0.0725 (15)	0.000	0.0364 (13)	0.000
C2	0.0830 (14)	0.0890 (17)	0.0770 (13)	-0.0101 (9)	0.0327 (10)	0.0013 (9)
C3	0.1073 (17)	0.0935 (18)	0.0858 (15)	0.0277 (12)	0.0419 (12)	0.0094 (10)
C4	0.163 (4)	0.0605 (17)	0.0848 (19)	0.000	0.056 (2)	0.000

Geometric parameters (\AA , $^\circ$)

F1—C1	1.341 (4)	C3—C4	1.377 (3)
F2—C2	1.342 (3)	C3—H3	1.0973
C1—C2	1.354 (3)	C4—H4	1.0018
C2—C3	1.357 (4)		
F1—C1—C2	120.30 (15)	C2—C3—H3	117.3
C2 ⁱ —C1—C2	119.4 (3)	C4—C3—H3	124.4

supplementary materials

F2—C2—C3	121.1 (2)	C3—C4—C3 ⁱ	121.0 (3)
F2—C2—C1	117.3 (3)	C3—C4—H4	119.5
C3—C2—C1	121.5 (2)	C3 ⁱ —C4—H4	119.5
C2—C3—C4	118.3 (2)		

Symmetry codes: (i) $-x+2, y, -z+1/2$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3—H3 \cdots F2 ⁱⁱ	1.10	2.77	3.560 (3)	129
C3—H3 \cdots F1 ⁱⁱⁱ	1.10	2.59	3.528 (4)	144
C4—H4 \cdots F2 ^{iv}	1.00	2.60	3.440 (4)	142

Symmetry codes: (ii) $-x+1, -y+1, -z$; (iii) $x-1/2, y+1/2, z$; (iv) $x+1/2, y+1/2, z$.

Fig. 1

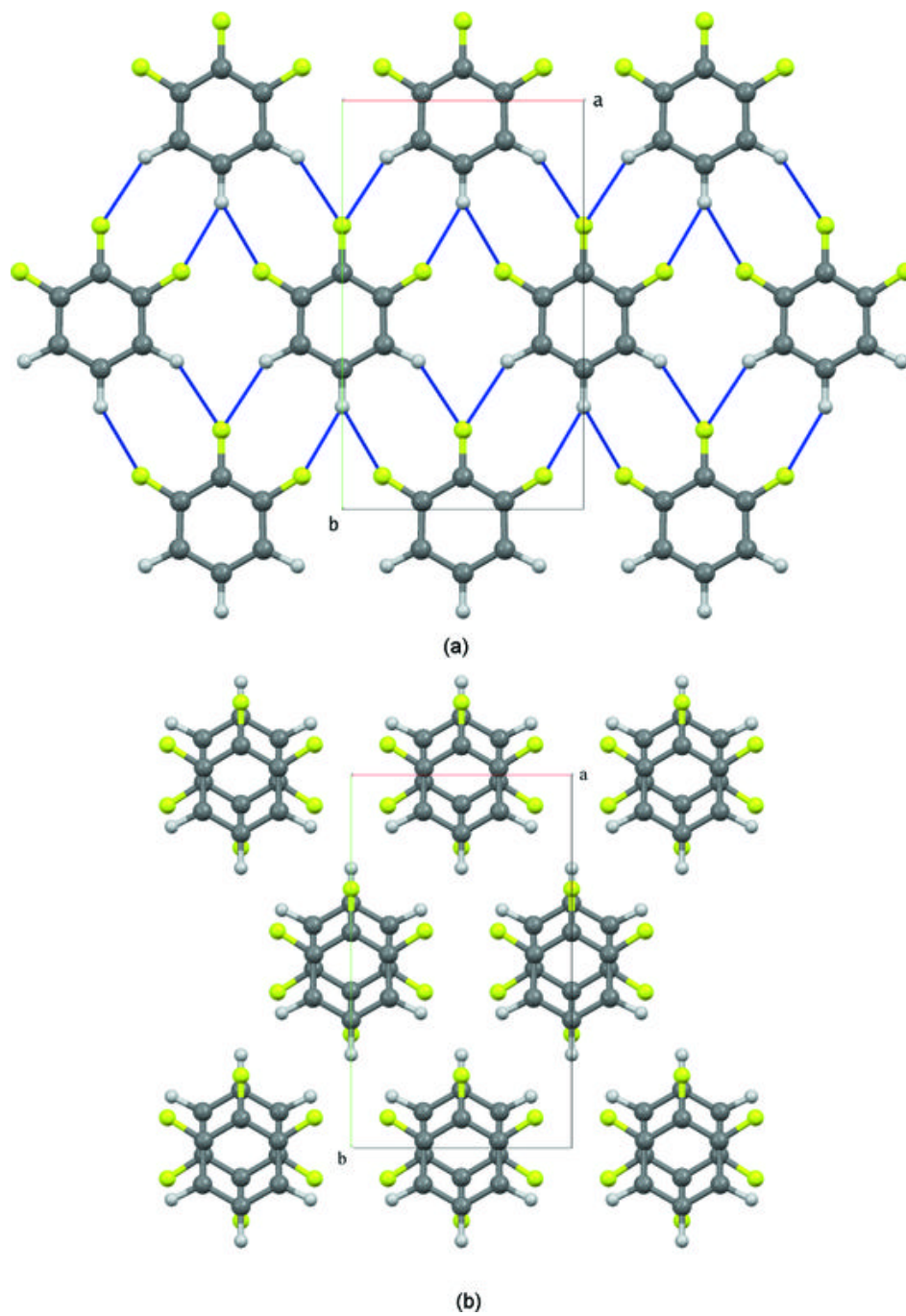


Fig. 2

