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1,3-Difluorobenzene

Michael T. Kirchner,[a] Dieter Bläser,[a] Roland Boese,[a]* Tejender S. Thakur[b] and Gautam R. Desiraju[b]*

[a]Institut für Anorganische Chemie der Universität, 45117 Essen, Germany, and [b]Indian Institute of Science, Bangalore 560 012, India
Correspondence e-mail: roland.boese@uni-due.de, gautam_desiraju@yahoo.com

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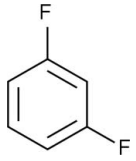
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.100; data-to-parameter ratio = 14.4.

The weak electrostatic and dispersive forces between C(δ+)—F(δ−) and H(δ+)—C(δ−) are at the borderline of the hydrogen-bond phenomenon and are poorly directional and further deformed in the presence of other dominant interactions, *e.g.* C—H$\cdots\pi$. The title compound, $C_6H_4F_2$, Z' = 2, forms one-dimensional tapes along two homodromic C—H$\cdots$F hydrogen bonds. The one-dimensional tapes are connected into corrugated two-dimensional sheets by further bi- or trifurcated C—H$\cdots$F hydrogen bonds. Packing in the third dimension is controlled by C—H$\cdots\pi$ interactions.

Related literature

For C—H$\cdots$F interactions, see: Althoff *et al.* (2006); Bats *et al.* (2000); Choudhury *et al.* (2004); D'Oria & 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 the crystal structures of polyfluorinated benzenes, see: Thalladi *et al.* (1998). For crystallization techniques, see: Boese & Nussbaumer (1994).



Experimental

Crystal data

$C_6H_4F_2$
M_r = 114.09
Monoclinic, $C2/c$
a = 24.6618 (13) Å
b = 12.2849 (5) Å
c = 7.2336 (4) Å
β = 106.842 (3)°
V = 2097.55 (18) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 153 K
0.30 × 0.30 × 0.30 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.876, T_{max} = 0.961
7831 measured reflections
2099 independent reflections
1578 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.100
S = 1.01
2099 reflections
146 parameters
H-atom parameters not refined
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C2—H2$\cdots$F12^{i}	0.96	2.72	3.3750 (14)	126
C4—H4$\cdots$F2^{ii}	0.96	2.76	3.5386 (16)	139
C5—H5$\cdots$F11^{iii}	0.95	2.71	3.2948 (16)	121
C6—H6$\cdots$F11^{iii}	0.96	2.66	3.2644 (15)	121
C6—H6$\cdots$F1^{iv}	0.96	2.82	3.5789 (17)	137
C12—H12$\cdots$F1^{v}	0.96	2.70	3.3919 (14)	130
C14—H14$\cdots$F2^{vi}	0.96	2.72	3.3442 (16)	123
C14—H14$\cdots$F12^{vii}	0.96	2.73	3.5075 (18)	138
C15—H15$\cdots$F2^{vi}	0.96	2.81	3.3995 (17)	120
C16—H16$\cdots$F11^{viii}	0.96	2.75	3.5591 (16)	142
C2—H2$\cdots Cg2^{ix}$	0.96	2.96	3.6653 (13)	131
C12—H12$\cdots Cg2^{v}$	0.96	2.99	3.6547 (13)	127
C5—H5$\cdots Cg1^{x}$	0.95	2.83	3.5153 (12)	130
C15—H15$\cdots Cg1$	0.96	2.87	3.5283 (13)	127

Symmetry codes: (i) $x, -y, z+\frac{1}{2}$; (ii) $-x, -y+1, -z+1$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z+1$; (v) $x, -y, z-\frac{1}{2}$; (vi) $-x, y, -z+\frac{1}{2}$; (vii) $-x, -y, -z$; (viii) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z$; (ix) $x, y, z+1$; (x) $x, -y+1, z-\frac{1}{2}$. $Cg1$ and $Cg2$ are the centroids of the C1–C6 and C11–C16 rings, respectively.

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2886).

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supplementary materials

Acta Cryst. (2009). E**65**, o2668-o2669 [**doi:10.1107/S1600536809038987**]

1,3-Difluorobenzene

M. T. Kirchner, D. Bläser, R. Boese, T. S. Thakur and G. R. Desiraju

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···F—C interactions (Howard *et al.*, 1996; Reichenbacher *et al.*, 2005) arise mainly due to electrostatic and dispersive forces between the Cδ±-Fδ- and the Hδ±-Cδ- 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···F—C interactions may be of significance, and some of us had reported the crystal structures of several polyfluorinated benzenes in this connection (Thalladi *et al.*, 1998). As a continuation of this work, we report here the crystal structure of 1,3-difluorobenzene. The comparison crystal structures of 1,2- and 1,4-difluorobenzene and 1,3,5-trifluorobenzene have been reported in this earlier work.

Experimental

Single crystals of 1,3-difluorobenzene were grown from commerical samples by zone melting in a quartz capillary at 163 K according to the procedure outlined by Boese & Nussbaumer (1994).

Refinement

H atoms were positioned geoemtrically (C-H = 0.95 or 0.96 Å) and refined using a riding model, with their isotropic displacement parameters set equal to 1.2 times U^{eq} of the corresponding carbon atom.

Figures

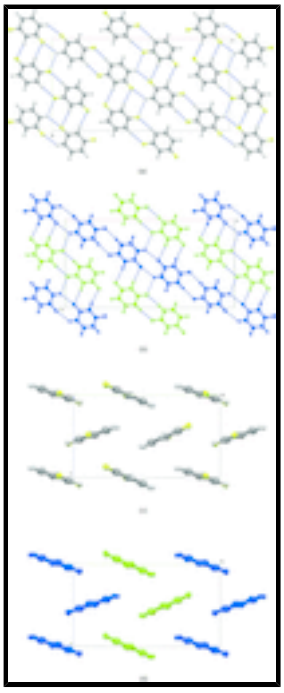

Fig. 1. Crystal structure of 1,3-difluorobenzene: (*a*) two-dimensional network of C—H···F—C interactions viewed along the *c* axis, (*b*) with independent molecules coloured blue and green, (*c*) Herringbone arrangement of molecules viewed along the *a* axis and (*d*) coloured as before.

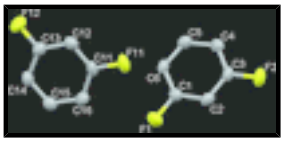

Fig. 2. Displacement ellipsoid plot of 1,3-difluorobenzene.

1,3-Difluorobenzene

Crystal data

$C_6H_4F_2$	F_{000} = 928
M_r = 114.09	D_x = 1.445 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 2977 reflections
a = 24.6618 (13) Å	θ = 2.9–28.2°
b = 12.2849 (5) Å	μ = 0.13 mm^{-1}
c = 7.2336 (4) Å	*T* = 153 K
β = 106.842 (3)°	Cylindric, colourless
V = 2097.55 (18) Å^3	0.30 × 0.30 × 0.30 mm
Z = 16	

Data collection

Bruker SMART APEXII area-detector diffractometer	2099 independent reflections
Radiation source: fine-focus sealed tube	1578 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.020

Detector resolution: 512 pixels mm^{-1}

T = 153 K

Data collection strategy APEX 2/COSMO with chi +/– 10° scans

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

T_{min} = 0.876, T_{max} = 0.961

7831 measured reflections

θ_{max} = 28.3º

θ_{min} = 1.9º

h = −27→29

k = −16→16

l = −9→8

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.032

$wR(F^2)$ = 0.100

S = 1.01

2099 reflections

146 parameters

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 not refined

$w = 1/[s^2(F_o^2) + (0.0494P)^2 + 0.6228P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.19 e $Å^{-3}$

$\Delta\rho_{min}$ = −0.13 e $Å^{-3}$

Extinction correction: SHELXTL (Bruker, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0034 (7)

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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.20034 (3)	0.21738 (6)	0.63089 (12)	0.0520 (3)
F2	0.01617 (3)	0.35397 (7)	0.49907 (14)	0.0587 (3)
C1	0.16251 (5)	0.29864 (9)	0.56491 (16)	0.0349 (3)
C2	0.10797 (6)	0.28273 (9)	0.56876 (17)	0.0372 (3)
H2	0.0966	0.2170	0.6188	0.045*
C3	0.07043 (6)	0.36645 (10)	0.49742 (18)	0.0370 (3)
C4	0.08585 (6)	0.46202 (9)	0.42616 (17)	0.0378 (3)
H4	0.0586	0.5187	0.3775	0.045*

C5	0.14156 (6)	0.47408 (9)	0.42727 (16)	0.0370 (3)
H5	0.1531	0.5394	0.3793	0.044*
C6	0.18102 (6)	0.39238 (9)	0.49720 (17)	0.0355 (3)
H6	0.2199	0.4008	0.4989	0.043*
F11	0.23615 (3)	0.09707 (6)	0.01979 (13)	0.0571 (3)
F12	0.05258 (4)	−0.03682 (6)	−0.08892 (13)	0.0625 (3)
C11	0.18189 (6)	0.11273 (10)	0.01807 (17)	0.0365 (3)
C12	0.14440 (6)	0.02770 (9)	−0.03976 (17)	0.0382 (3)
H12	0.1558	−0.0409	−0.0800	0.046*
C13	0.08994 (6)	0.04613 (9)	−0.03803 (18)	0.0385 (3)
C14	0.07131 (6)	0.14411 (9)	0.01511 (18)	0.0380 (3)
H14	0.0325	0.1545	0.0122	0.046*
C15	0.11075 (6)	0.22716 (9)	0.07194 (17)	0.0383 (3)
H15	0.0992	0.2961	0.1105	0.046*
C16	0.16634 (6)	0.21260 (9)	0.07456 (18)	0.0392 (3)
H16	0.1934	0.2705	0.1133	0.047*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0441 (6)	0.0416 (4)	0.0679 (5)	0.0105 (3)	0.0124 (4)	0.0059 (3)
F2	0.0295 (6)	0.0668 (5)	0.0841 (6)	−0.0076 (4)	0.0234 (5)	−0.0023 (4)
C1	0.0343 (9)	0.0338 (5)	0.0352 (6)	0.0013 (5)	0.0078 (6)	−0.0017 (4)
C2	0.0397 (9)	0.0341 (6)	0.0401 (6)	−0.0071 (5)	0.0153 (6)	−0.0012 (4)
C3	0.0257 (9)	0.0455 (6)	0.0411 (6)	−0.0062 (5)	0.0118 (6)	−0.0064 (5)
C4	0.0346 (9)	0.0382 (6)	0.0379 (6)	0.0027 (5)	0.0064 (6)	0.0002 (5)
C5	0.0405 (9)	0.0351 (6)	0.0362 (6)	−0.0046 (5)	0.0123 (6)	0.0017 (4)
C6	0.0267 (9)	0.0421 (6)	0.0395 (6)	−0.0053 (5)	0.0122 (6)	−0.0038 (5)
F11	0.0289 (6)	0.0654 (5)	0.0794 (6)	0.0116 (4)	0.0195 (5)	0.0076 (4)
F12	0.0502 (6)	0.0499 (5)	0.0894 (6)	−0.0173 (4)	0.0235 (5)	−0.0145 (4)
C11	0.0242 (9)	0.0468 (6)	0.0392 (6)	0.0077 (5)	0.0100 (6)	0.0073 (5)
C12	0.0425 (9)	0.0346 (6)	0.0402 (6)	0.0064 (5)	0.0161 (6)	0.0016 (5)
C13	0.0370 (9)	0.0375 (6)	0.0416 (6)	−0.0045 (5)	0.0122 (6)	−0.0014 (5)
C14	0.0283 (9)	0.0452 (6)	0.0433 (7)	0.0049 (5)	0.0149 (6)	0.0019 (5)
C15	0.0403 (9)	0.0357 (6)	0.0409 (6)	0.0049 (5)	0.0150 (6)	−0.0018 (4)
C16	0.0355 (9)	0.0381 (6)	0.0423 (7)	−0.0041 (5)	0.0086 (6)	−0.0017 (5)

Geometric parameters (Å, °)

F1—C1	1.3553 (13)	F11—C11	1.3486 (14)
F2—C3	1.3506 (15)	F12—C13	1.3515 (14)
C1—C2	1.3673 (18)	C11—C12	1.3773 (17)
C1—C6	1.3797 (15)	C11—C16	1.3820 (16)
C2—C3	1.3800 (17)	C12—C13	1.3656 (18)
C2—H2	0.96	C12—H12	0.96
C3—C4	1.3793 (16)	C13—C14	1.3821 (16)
C4—C5	1.3794 (18)	C14—C15	1.3872 (17)
C4—H4	0.96	C14—H14	0.96
C5—C6	1.3874 (17)	C15—C16	1.3772 (18)

C5—H5	0.95	C15—H15	0.96
C6—H6	0.96	C16—H16	0.96
F1—C1—C2	117.92 (10)	F11—C11—C12	118.14 (11)
F1—C1—C6	118.36 (11)	F11—C11—C16	118.92 (11)
C2—C1—C6	123.71 (11)	C12—C11—C16	122.94 (12)
C1—C2—C3	116.30 (10)	C13—C12—C11	116.54 (11)
C1—C2—H2	121.7	C13—C12—H12	121.6
C3—C2—H2	122.0	C11—C12—H12	121.8
F2—C3—C2	118.12 (10)	F12—C13—C12	117.85 (10)
F2—C3—C4	118.76 (12)	F12—C13—C14	118.50 (11)
C2—C3—C4	123.12 (12)	C12—C13—C14	123.65 (11)
C3—C4—C5	118.11 (11)	C13—C14—C15	117.50 (12)
C3—C4—H4	121.0	C13—C14—H14	121.3
C5—C4—H4	120.9	C15—C14—H14	121.2
C4—C5—C6	121.10 (11)	C16—C15—C14	121.22 (11)
C4—C5—H5	119.5	C16—C15—H15	119.3
C6—C5—H5	119.4	C14—C15—H15	119.5
C1—C6—C5	117.64 (12)	C15—C16—C11	118.14 (11)
C1—C6—H6	121.2	C15—C16—H16	120.8
C5—C6—H6	121.2	C11—C16—H16	121.0

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···F12^{i}	0.96	2.72	3.3750 (14)	126
C4—H4···F2^{ii}	0.96	2.76	3.5386 (16)	139
C5—H5···F11^{iii}	0.95	2.71	3.2948 (16)	121
C6—H6···F11^{iii}	0.96	2.66	3.2644 (15)	121
C6—H6···F1^{iv}	0.96	2.82	3.5789 (17)	137
C12—H12···F1^{v}	0.96	2.70	3.3919 (14)	130
C14—H14···F2^{vi}	0.96	2.72	3.3442 (16)	123
C14—H14···F12^{vii}	0.96	2.73	3.5075 (18)	138
C15—H15···F2^{vi}	0.96	2.81	3.3995 (17)	120
C16—H16···F11^{viii}	0.96	2.75	3.5591 (16)	142
C2—H2···Cg2^{ix}	0.96	2.96	3.6653 (13)	131
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C5—H5···Cg1^{x}	0.95	2.83	3.5153 (12)	130
C15—H15···Cg1	0.96	2.87	3.5283 (13)	127

Symmetry codes: (i) *x*, −*y*, *z*+1/2; (ii) −*x*, −*y*+1, −*z*+1; (iii) −*x*+1/2, *y*+1/2, −*z*+1/2; (iv) −*x*+1/2, −*y*+1/2, −*z*+1; (v) *x*, −*y*, *z*−1/2; (vi) −*x*, *y*, −*z*+1/2; (vii) −*x*, −*y*, −*z*; (viii) −*x*+1/2, −*y*+1/2, −*z*; (ix) *x*, *y*, *z*+1; (x) *x*, −*y*+1, *z*−1/2.

Fig. 1

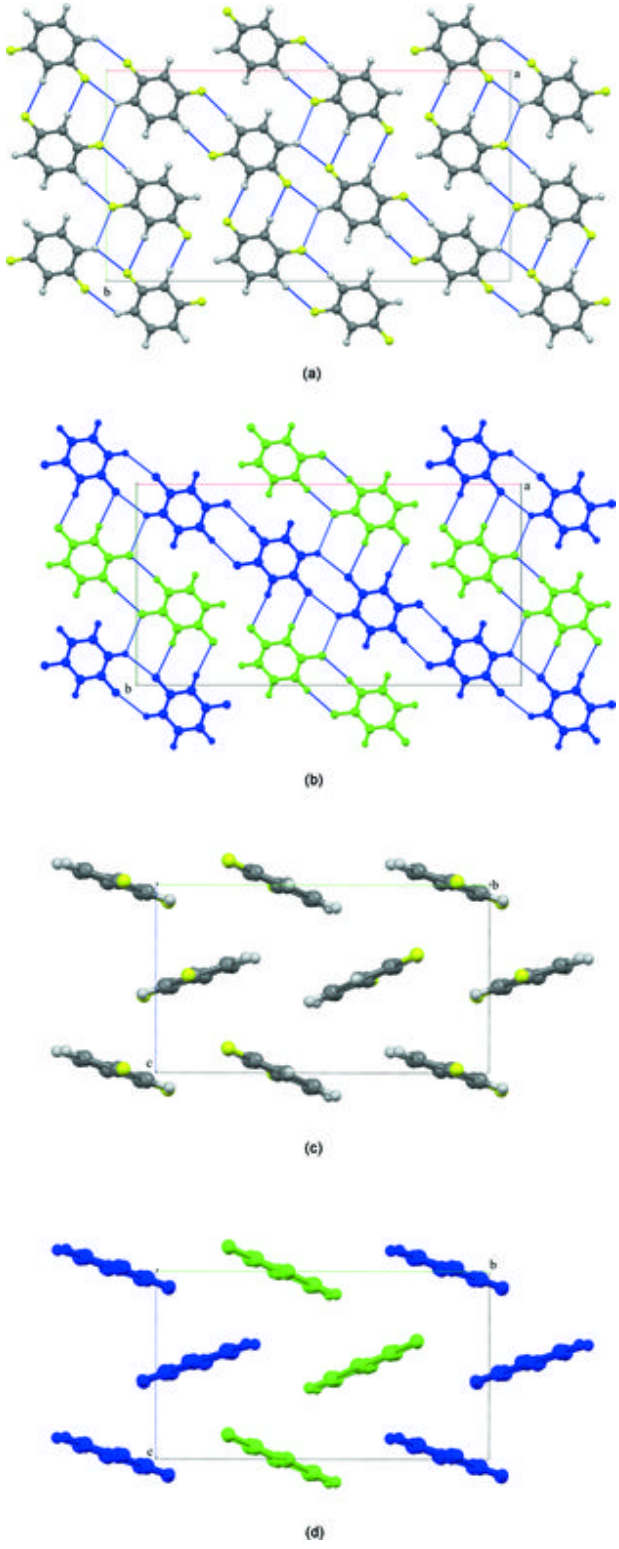

Fig. 2