

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

1,4-Bis(fluoromethyl)benzene

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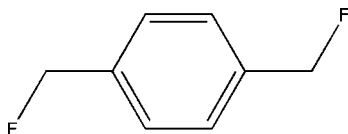
Received 16 January 2009; accepted 30 January 2009

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; disorder in main residue; R factor = 0.074; wR factor = 0.251; data-to-parameter ratio = 24.9.

The title compound, $\text{C}_8\text{H}_8\text{F}_2$, lies across a crystallographic inversion centre. The structure features short $\text{C}\cdots\text{F}$ [2.8515 (18) Å] and $\text{F}\cdots\text{F}$ [2.490 (4) Å] contacts, which are significantly shorter than the sum of the van der Waals radii of these atoms. The F atom and methylene H atoms are disordered over two positions with a site-occupancy ratio of 0.633 (3):0.367 (3). In the crystal structure, intermolecular $\text{C}-\text{H}\cdots\text{F}$ interactions link neighboring molecules into infinite chains along the b axis. In addition, $\text{C}-\text{H}\cdots\pi$ interactions link these molecules along [101], forming a two-dimensional network parallel to (101).

Related literature

For the structures of compounds with non-linear properties, see, for example: Chantrapromma *et al.* (2006); Fun *et al.* (2008); Patil *et al.* (2007).



Experimental

Crystal data

$\text{C}_8\text{H}_8\text{F}_2$
 $M_r = 143.15$
 Monoclinic, $P2_1/n$
 $a = 6.1886$ (2) Å

$b = 5.0152$ (2) Å
 $c = 10.4750$ (4) Å
 $\beta = 95.107$ (2)°
 $V = 323.82$ (2) Å³

$Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.12$ mm⁻¹

$T = 100.0$ (1) K
 $0.55 \times 0.24 \times 0.14$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2005)
 $T_{\min} = 0.935$, $T_{\max} = 0.982$

11592 measured reflections
 1591 independent reflections
 1343 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.074$
 $wR(F^2) = 0.251$
 $S = 1.18$
 1591 reflections
 64 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.67$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.59$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C4}-\text{H4D}\cdots\text{F1A}^i$	0.96	2.04	2.8515 (18)	141
$\text{C4}-\text{H4B}\cdots\text{Cg1}^{ii}$	0.97	2.84	3.5148 (12)	128
$\text{C4}-\text{H4C}\cdots\text{Cg1}^{ii}$	0.96	2.64	3.5148 (12)	144

Symmetry codes: (i) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$; (ii) $x, y + 1, z$. Cg1 is the centroid of the C1-C3/C1A-C3A benzene ring.

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2003).

HKF and RK thank the Malaysian Government and Universiti Sains Malaysia for the Science Fund grant No. 305/PFIZIK/613312. RK thanks Universiti Sains Malaysia for a post-doctoral research fellowship. HKF also thanks Universiti Sains Malaysia for the Research University Golden Goose grant No. 1001/PFIZIK/811012.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2122).

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supplementary materials

Acta Cryst. (2009). E65, o459 [doi:10.1107/S1600536809003730]

1,4-Bis(fluoromethyl)benzene

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Comment

As part of an ongoing investigation into compounds with non-linear optical properties (Chantrapromma *et al.*, 2006; Fun *et al.*, 2008; Patil *et al.*, 2007), the crystal structure of the title compound is presented here.

The title compound, (I), lies across a crystallographic inversion centre (Fig. 1). The interesting features of the crystal structure are the short C4A \cdots F1Aⁱ [2.8515 (18)Å; (i) 3/2-x, 1/2+y, 3/2-z] and F1B \cdots F1Bⁱⁱ [2.490 (4)Å; (ii) 1-x, 1-y, 1-z] contacts which are significantly shorter than the sum of the van der Waals radii of these atoms. The fluorine atom and methylene hydrogens are disordered over two positions with a site-occupancy ratio of 0.633 (3):0.367 (3). In the crystal structure, intermolecular C—H \cdots F interactions link neighboring molecules into one-dimensional infinite chains along the *b* axis (Table 1 and Fig. 2). In addition, C—H \cdots π interactions [C4—H4B \cdots Cg1ⁱⁱⁱ; (iii) *x*, 1+y, *z* and C4—H4C \cdots Cg1ⁱⁱⁱ; Cg1 is the centroid of the C1—C3/C1A—C3A benzene ring] link these molecules along the [10 $\bar{1}$] direction, thus forming a two-dimensional network which is parallel to the (101) plane.

Experimental

Commercially available 1,4-bis(difluoromethyl) benzene was further purified by repeated recrystallization from acetone. Single crystals suitable for X-ray analysis were grown by slow evaporation of an acetone solution at room temperature.

Refinement

The hydrogen atoms bound to C1 and C3 were located from the difference Fourier map and refined freely. Hydrogen atoms of the methylene groups were positioned geometrically and constrained to refine with a riding model approximation with C—H = 0.96–0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$.

Figures

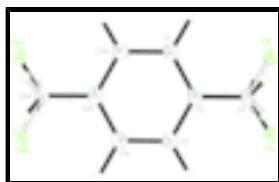


Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering. Open bonds indicate the minor disordered component.

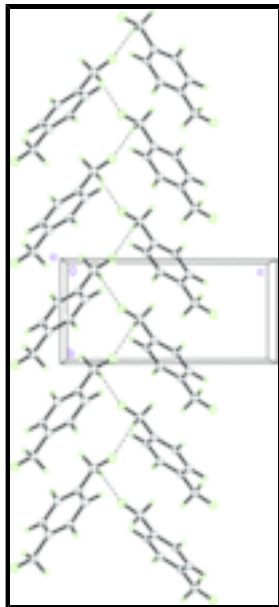


Fig. 2. The crystal packing of the major component of (I), viewed down the *a*-axis, showing a one-dimensional infinite chain of molecules along the *b*-axis. Intramolecular and intermolecular interactions are drawn as dashed lines.

1,4-Bis(fluoromethyl)benzene

Crystal data

$C_8H_8F_2$

$M_r = 143.15$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1/n$

$a = 6.1886\ (2)\ \text{\AA}$

$b = 5.0152\ (2)\ \text{\AA}$

$c = 10.4750\ (4)\ \text{\AA}$

$\beta = 95.107\ (2)^\circ$

$V = 323.82\ (2)\ \text{\AA}^3$

$Z = 2$

$F_{000} = 148$

$D_x = 1.458\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3653 reflections

$\theta = 2.5\text{--}34.7^\circ$

$\mu = 0.12\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Needle, colourless

$0.55 \times 0.24 \times 0.14\ \text{mm}$

Data collection

Bruker APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 100\ \text{K}$

φ and ω scans

Absorption correction: multi-scan (*SADABS*; Bruker, 2005)

$T_{\min} = 0.935$, $T_{\max} = 0.982$

11592 measured reflections

1591 independent reflections

1343 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.029$

$\theta_{\max} = 36.6^\circ$

$\theta_{\min} = 3.7^\circ$

$h = -10 \rightarrow 10$

$k = -7 \rightarrow 8$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.074$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.251$	$w = 1/[\sigma^2(F_o^2) + (0.1441P)^2 + 0.1329P]$
$S = 1.18$	where $P = (F_o^2 + 2F_c^2)/3$
1591 reflections	$(\Delta/\sigma)_{\max} < 0.001$
64 parameters	$\Delta\rho_{\max} = 0.67 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.59 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

Special details

Experimental. The low-temperature data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
F1A	0.9163 (2)	0.5267 (3)	0.72717 (12)	0.0219 (3)	0.633 (3)
F1B	0.6221 (4)	0.4849 (5)	0.6008 (3)	0.0260 (6)	0.367 (3)
C4	0.8122 (2)	0.4155 (2)	0.63866 (12)	0.0204 (3)	
H4C	0.7640	0.5505	0.5776	0.025*	0.633 (3)
H4D	0.6847	0.3437	0.6718	0.025*	0.633 (3)
H4A	0.8129	0.3600	0.7274	0.025*	0.367 (3)
H4B	0.9052	0.5709	0.6369	0.025*	0.367 (3)
C1	0.7876 (2)	0.0844 (3)	0.46363 (13)	0.0222 (3)	
C2	0.9095 (2)	0.1998 (2)	0.56704 (11)	0.0194 (3)	
C3	1.1209 (2)	0.1184 (3)	0.60446 (12)	0.0217 (3)	
H1	0.620 (4)	0.159 (6)	0.431 (2)	0.037 (6)*	
H3	1.207 (4)	0.205 (5)	0.682 (2)	0.026 (5)*	

Atomic displacement parameters (\AA^2)

U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
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supplementary materials

F1A	0.0227 (6)	0.0216 (6)	0.0215 (6)	0.0012 (4)	0.0030 (4)	-0.0057 (4)
F1B	0.0216 (10)	0.0244 (11)	0.0324 (12)	0.0115 (8)	0.0045 (8)	-0.0018 (8)
C4	0.0224 (5)	0.0170 (5)	0.0227 (5)	0.0024 (4)	0.0064 (4)	0.0013 (4)
C1	0.0204 (5)	0.0220 (5)	0.0243 (5)	0.0030 (4)	0.0023 (4)	0.0001 (4)
C2	0.0208 (5)	0.0176 (5)	0.0204 (5)	0.0020 (3)	0.0048 (4)	0.0013 (4)
C3	0.0207 (5)	0.0217 (6)	0.0226 (5)	0.0016 (4)	0.0007 (4)	-0.0006 (4)

Geometric parameters (Å, °)

F1A—C4	1.2162 (18)	C4—H4A	0.9699
F1A—H4A	1.0529	C4—H4B	0.9700
F1A—H4B	0.9681	C1—C2	1.3900 (18)
F1B—C4	1.257 (3)	C1—C3 ⁱ	1.3916 (19)
F1B—H4C	0.9881	C1—H1	1.13 (3)
F1B—H4D	1.0739	C2—C3	1.3927 (18)
C4—C2	1.4754 (17)	C3—C1 ⁱ	1.3916 (19)
C4—H4C	0.9600	C3—H3	1.02 (2)
C4—H4D	0.9600		
C4—F1A—H4A	50.0	C2—C4—H4A	108.0
C4—F1A—H4B	51.2	H4C—C4—H4A	144.6
H4A—F1A—H4B	101.2	H4D—C4—H4A	58.7
C4—F1B—H4C	48.9	F1A—C4—H4B	51.1
C4—F1B—H4D	47.9	F1B—C4—H4B	108.2
H4C—F1B—H4D	96.7	C2—C4—H4B	108.0
F1A—C4—F1B	122.09 (16)	H4C—C4—H4B	64.6
F1A—C4—C2	120.74 (12)	H4D—C4—H4B	144.8
F1B—C4—C2	117.11 (16)	H4A—C4—H4B	107.3
F1A—C4—H4C	107.2	C2—C1—C3 ⁱ	119.09 (12)
F1B—C4—H4C	50.8	C2—C1—H1	121.3 (14)
C2—C4—H4C	107.2	C3 ⁱ —C1—H1	119.6 (14)
F1A—C4—H4D	107.0	C1—C2—C3	121.91 (12)
F1B—C4—H4D	56.0	C1—C2—C4	118.92 (11)
C2—C4—H4D	107.1	C3—C2—C4	119.17 (12)
H4C—C4—H4D	106.8	C1 ⁱ —C3—C2	119.00 (12)
F1A—C4—H4A	56.2	C1 ⁱ —C3—H3	120.6 (14)
F1B—C4—H4A	107.9	C2—C3—H3	120.4 (14)
C3 ⁱ —C1—C2—C3	0.1 (2)	F1A—C4—C2—C3	1.96 (19)
C3 ⁱ —C1—C2—C4	179.75 (11)	F1B—C4—C2—C3	179.18 (17)
F1A—C4—C2—C1	-177.73 (13)	C1—C2—C3—C1 ⁱ	-0.1 (2)
F1B—C4—C2—C1	-0.5 (2)	C4—C2—C3—C1 ⁱ	-179.75 (11)

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

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C4—H4D \cdots F1A ⁱⁱ	0.96	2.04	2.8515 (18)	141

C4—H4B···Cg1 ⁱⁱⁱ	0.97	2.84	3.5148 (12)	128
C4—H4C···Cg1 ⁱⁱⁱ	0.96	2.64	3.5148 (12)	144

Symmetry codes: (ii) $-x+3/2, y-1/2, -z+3/2$; (iii) $x, y+1, z$.

Fig. 1

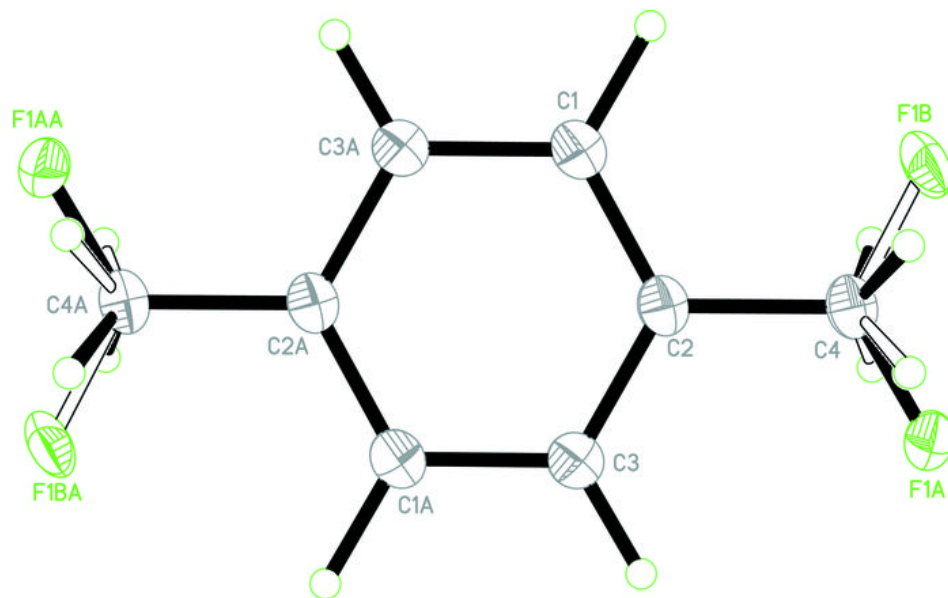


Fig. 2

