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## Structure Reports

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## 1,3-Difluorobenzene

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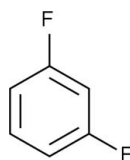
Received 12 August 2009; accepted 25 September 2009

Key indicators: single-crystal X-ray study;  $T = 153$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  
R factor = 0.032; wR factor = 0.100; data-to-parameter ratio = 14.4.

The weak electrostatic and dispersive forces between  $\text{C}(\delta+)-\text{F}(\delta-)$  and  $\text{H}(\delta+)-\text{C}(\delta-)$  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.  $\text{C}-\text{H}\cdots\pi$ . The title compound,  $\text{C}_6\text{H}_4\text{F}_2$ ,  $Z' = 2$ , forms one-dimensional tapes along two homodromic  $\text{C}-\text{H}\cdots\text{F}$  hydrogen bonds. The one-dimensional tapes are connected into corrugated two-dimensional sheets by further bi- or trifurcated  $\text{C}-\text{H}\cdots\text{F}$  hydrogen bonds. Packing in the third dimension is controlled by  $\text{C}-\text{H}\cdots\pi$  interactions.

## 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'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

$\text{C}_6\text{H}_4\text{F}_2$	$V = 2097.55$ (18) Å <sup>3</sup>
$M_r = 114.09$	$Z = 16$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 24.6618$ (13) Å	$\mu = 0.13$ mm <sup>-1</sup>
$b = 12.2849$ (5) Å	$T = 153$ K
$c = 7.2336$ (4) Å	$0.30 \times 0.30 \times 0.30$ mm
$\beta = 106.842$ (3)°	

## Data collection

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

## Refinement

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

Table 1

Hydrogen-bond geometry (Å, °).

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

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## 1,3-Difluorobenzene

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### S1. Comment

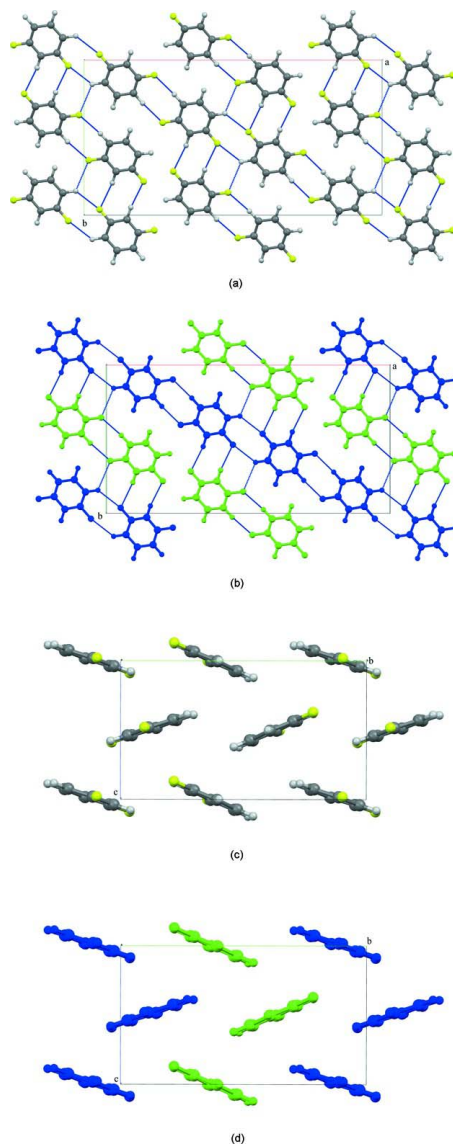
Despite the high electronegativity difference between carbon and fluorine, the C—F bond acts as a poor hydrogen bond acceptor due to the hardness of the F-atom (Dunitz & Taylor, 1997; O'Hagan, 2008). The resultant weak C—H $\cdots$ F—C interactions (Howard *et al.*, 1996; Reichenbacher *et al.*, 2005) arise mainly due to electrostatic and dispersive forces between the C $\delta^{\pm}$ -F $\delta^-$  and the H $\delta^{\pm}$ -C $\delta^-$  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 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.

### S2. Experimental

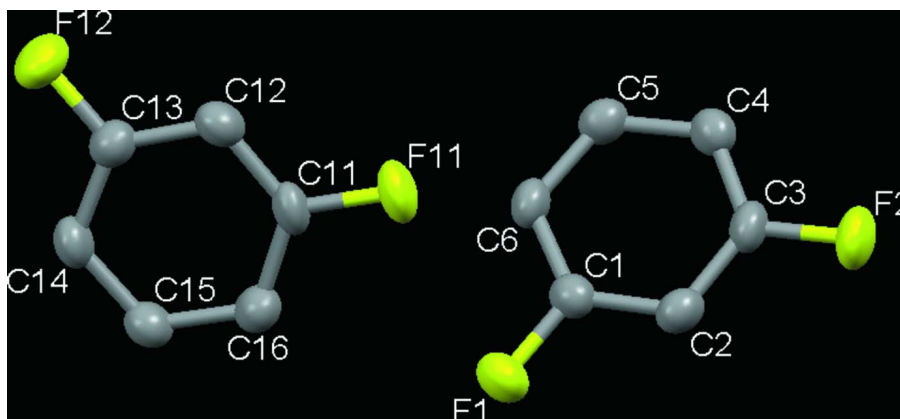
Single crystals of 1,3-difluorobenzene were grown from commercial samples by zone melting in a quartz capillary at 163 K according to the procedure outlined by Boese & Nussbaumer (1994).

### S3. Refinement

H atoms were positioned geometrically (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  $U^{\text{eq}}$  of the corresponding carbon atom.

**Figure 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.



**Figure 2**  
Displacement ellipsoid plot of 1,3-difluorobenzene.

### 1,3-Difluorobenzene

#### Crystal data

$C_6H_4F_2$   
 $M_r = 114.09$   
 Monoclinic,  $C2/c$   
 Hall symbol:  $-C\ 2yc$   
 $a = 24.6618\ (13)\ \text{\AA}$   
 $b = 12.2849\ (5)\ \text{\AA}$   
 $c = 7.2336\ (4)\ \text{\AA}$   
 $\beta = 106.842\ (3)^\circ$   
 $V = 2097.55\ (18)\ \text{\AA}^3$   
 $Z = 16$

#### Data collection

Bruker SMART APEXII area-detector  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 Detector resolution:  $512\ \text{pixels}\ \text{mm}^{-1}$   
 Data collection strategy APEX 2/COSMO with  
 $\chi\ +/-\ 10^\circ$  scans  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2004)

#### 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  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods  
 Secondary atom site location: difference Fourier  
 map

$F(000) = 928$   
 $D_x = 1.445\ \text{Mg}\ \text{m}^{-3}$   
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$   
 Cell parameters from 2977 reflections  
 $\theta = 2.9\text{--}28.2^\circ$   
 $\mu = 0.13\ \text{mm}^{-1}$   
 $T = 153\ \text{K}$   
 Cylindric, colourless  
 $0.30 \times 0.30 \times 0.30\ \text{mm}$

$T_{\min} = 0.876$ ,  $T_{\max} = 0.961$   
 7831 measured reflections  
 2099 independent reflections  
 1578 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.020$   
 $\theta_{\max} = 28.3^\circ$ ,  $\theta_{\min} = 1.9^\circ$   
 $h = -27 \rightarrow 29$   
 $k = -16 \rightarrow 16$   
 $l = -9 \rightarrow 8$

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  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.19\ \text{e}\ \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.13\ \text{e}\ \text{\AA}^{-3}$   
 Extinction correction: SHELXTL (Bruker,  
 2008),  $F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 \sin(2\theta)]^{-1/4}$   
 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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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 ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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, °)*

<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>
C2—H2 $\cdots$ F12 <sup>i</sup>	0.96	2.72	3.3750 (14)	126
C4—H4 $\cdots$ F2 <sup>ii</sup>	0.96	2.76	3.5386 (16)	139

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C5—H5…F11 <sup>iii</sup>	0.95	2.71	3.2948 (16)	121
C6—H6…F11 <sup>iii</sup>	0.96	2.66	3.2644 (15)	121
C6—H6…F1 <sup>iv</sup>	0.96	2.82	3.5789 (17)	137
C12—H12…F1 <sup>v</sup>	0.96	2.70	3.3919 (14)	130
C14—H14…F2 <sup>vi</sup>	0.96	2.72	3.3442 (16)	123
C14—H14…F12 <sup>vii</sup>	0.96	2.73	3.5075 (18)	138
C15—H15…F2 <sup>vi</sup>	0.96	2.81	3.3995 (17)	120
C16—H16…F11 <sup>viii</sup>	0.96	2.75	3.5591 (16)	142
C2—H2…Cg2 <sup>ix</sup>	0.96	2.96	3.6653 (13)	131
C12—H12…Cg2 <sup>v</sup>	0.96	2.99	3.6547 (13)	127
C5—H5…Cg1 <sup>x</sup>	0.95	2.83	3.5153 (12)	130
C15—H15…Cg1	0.96	2.87	3.5283 (13)	127

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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)  $x, -y+1, z-1/2$ .