

# Crystal structure and Hirshfeld surface analysis of bis[hydrazinium(1+)] hexafluoridosilicate: $(\text{N}_2\text{H}_5)_2\text{SiF}_6$

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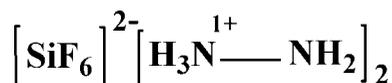
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In the title inorganic molecular salt,  $(\text{N}_2\text{H}_5)_2\text{SiF}_6$ , the silicon atom at the centre of the slightly distorted  $\text{SiF}_6$  octahedron [range of Si—F distances = 1.6777 (4)–1.7101 (4) Å] lies on a crystallographic inversion centre. In the crystal, the ions are connected by N—H $\cdots$ N and N—H $\cdots$ F hydrogen bonds; the former link the cations into [010] chains and the latter (some of which are bifurcated or trifurcated) link the ions into a three-dimensional network. The two-dimensional fingerprint plots show that F $\cdots$ H/H $\cdots$ F interactions dominate the Hirshfeld surface (75.5%) followed by H $\cdots$ H (13.6%) and N $\cdots$ H/H $\cdots$ N (8.4%) whereas F $\cdots$ F (1.9%) and F $\cdots$ N/N $\cdots$ F (0.6%) have negligible percentages. The title compound is isostructural with its germanium-containing analogue.

## 1. Chemical context

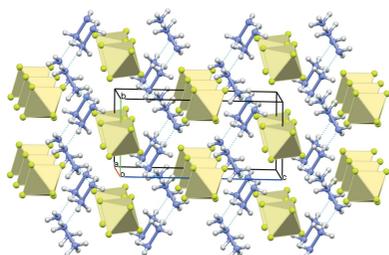
Hydrazinium hexafluoridometalate compounds have been studied by X-ray diffraction, vibrational spectroscopy and thermal analyses: they have been found to exist with two different formulae:  $\text{N}_2\text{H}_6\text{MF}_6$  (Kojić-Prodić *et al.*, 1971a,b; Frlec *et al.*, 1980; Golič *et al.*, 1980; Cameron *et al.*, 1983; Knop *et al.*, 1983; Ouasri *et al.*, 2002) and  $(\text{N}_2\text{H}_5)_2\text{MF}_6$  (Gantar & Rahten, 1988; Leban *et al.*, 1994) where  $M = \text{Ga}, \text{Si}, \text{Ti}, \text{Zr}$  and  $\text{Hf}$ . The name ‘hydrazinium hexafluoridosilicate’ has been applied to both compounds:  $\text{N}_2\text{H}_6\text{SiF}_6$  and  $(\text{N}_2\text{H}_5)_2\text{SiF}_6$ .

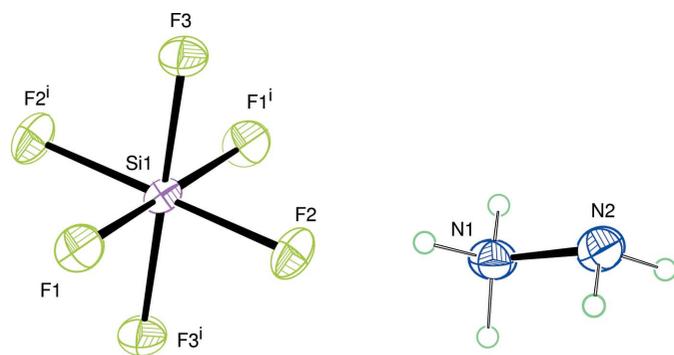


The crystal structure of  $\text{N}_2\text{H}_6\text{SiF}_6$  is well described by Frlec *et al.* (1980) and by Cameron *et al.* (1983), whereas that of  $(\text{N}_2\text{H}_5)_2\text{SiF}_6$  has not previously been reported to our best knowledge. However, this compound was characterized by chemical analysis, vibrational spectroscopy and X-ray powder photography by Gantar & Rahten (1986), who determined the unit-cell parameters and the space group. We now describe the synthesis, single crystal structure and Hirshfeld surface analysis of the title compound, (I), at room temperature.

## 2. Structural commentary

Compound (I) is an inorganic molecular salt built up from  $\text{N}_2\text{H}_5^+$  cations and  $\text{SiF}_6^{2-}$  anions, as shown in Fig. 1. In this





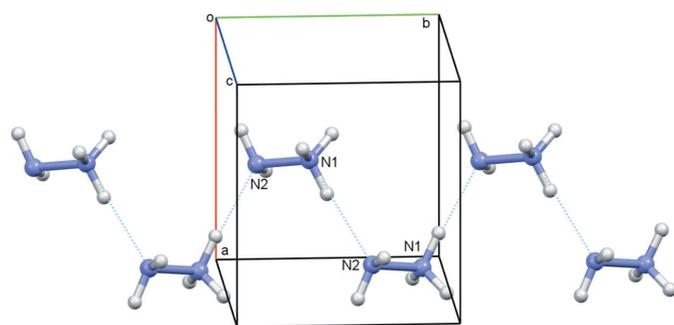
**Figure 1**  
Molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level.

structure, all atoms are in general positions except for the silicon atom, which is located at the Wyckoff position  $2d$  on the inversion centre  $\bar{1}$  of the space group  $P2_1/n$ . Thus, the silicon atom is connected to three unique fluorine atoms and their symmetry equivalents, forming a slightly elongated octahedron with Si–F distances in the range of 1.6777 (4) to 1.7101 (4) Å. The minimum and maximum *cis* F–S–F angles are 89.26 (2) and 90.74 (2)°, respectively. The N–N separation in the cation is 1.4416 (8) Å.

### 3. Supramolecular features and Hirshfeld surface analysis

In the extended structure of (I), the hydrazinium cations are linked by strong N–H···N hydrogen bonds (Table 1), building an infinite zigzag chain propagating along the [010] direction as shown in Fig. 2. The  $[\text{SiF}_6]^{2-}$  anion interacts with the  $(\text{N}_2\text{H}_5)^+$  cations through electrostatic attraction and accepts no fewer than ten simple, bifurcated or trifurcated N–H···F hydrogen bonds (Fig. 3, Table 1). This results in a three-dimensional network in which the hydrazinium cations build zigzag chains parallel to the *b*-axis direction and the  $[\text{SiF}_6]^{2-}$  anions are stacked along the [100] direction (Fig. 4).

The packing of (I) was further investigated and quantified with a Hirshfeld surface analysis (McKinnon *et al.*, 2004;



**Figure 2**  
A view of the hydrazinium (1+) cations building an [010] chain through N–H···F hydrogen bonds (dashed blue lines).

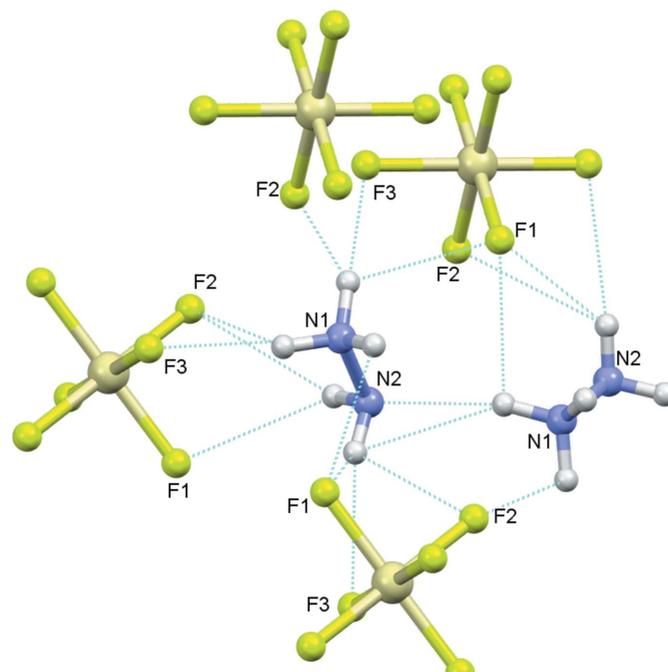
**Table 1**  
Hydrogen-bond geometry (Å, °).

<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
N1–H1A···F1 <sup>i</sup>	0.89	2.36	2.8436 (7)	114
N1–H1A···F3 <sup>ii</sup>	0.89	2.04	2.9174 (7)	170
N1–H1B···N2 <sup>iii</sup>	0.89	2.03	2.8963 (8)	165
N1–H1C···F3 <sup>iv</sup>	0.89	2.02	2.9025 (7)	170
N1–H1C···F2 <sup>v</sup>	0.89	2.49	2.9078 (7)	109
N2–H2A···F1 <sup>vi</sup>	0.83	2.52	3.0952 (7)	127
N2–H2A···F2 <sup>vi</sup>	0.83	2.64	3.0725 (7)	114
N2–H2A···F3 <sup>vi</sup>	0.83	2.43	3.2373 (7)	167
N2–H2B···F3 <sup>vii</sup>	0.86	2.49	3.2683 (7)	150
N2–H2B···F2 <sup>v</sup>	0.86	2.51	3.1036 (7)	127
N2–H2B···F1 <sup>iv</sup>	0.86	2.60	3.0124 (7)	110

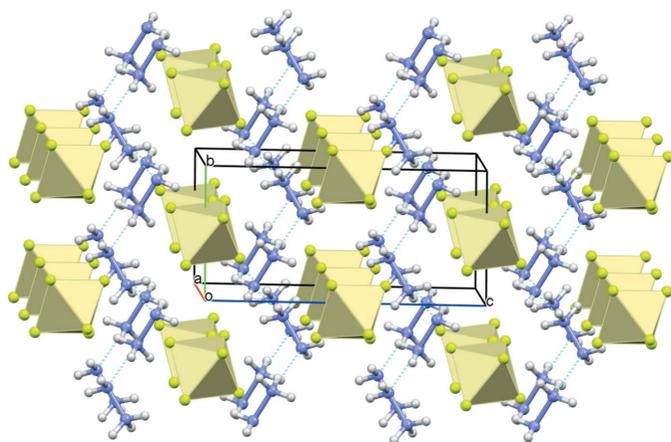
Symmetry codes: (i)  $x, y + 1, z$ ; (ii)  $-x + 1, -y + 1, -z + 1$ ; (iii)  $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$ ; (iv)  $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$ ; (v)  $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$ ; (vi)  $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$ ; (vii)  $x + \frac{1}{2}, -y + \frac{3}{2}, z + \frac{1}{2}$ .

Spackman & Jayatilaka, 2009) and two-dimensional fingerprint plots generated using the *CrystalExplorer* package (Turner *et al.*, 2017).

The acceptor atoms in the interactions are shown with negative electrostatic potentials (red regions), and donor atoms are shown with positive electrostatic potentials (blue regions). The N–H···F interactions in the structure are apparent from the relatively bright red-spots on the Hirshfeld surface of (I) mapped over  $d_{\text{norm}}$  (Fig. S1 in the supporting information). In order to provide quantitative information on the contribution of the intermolecular interactions to the crystal packing, the three-dimensional  $d_{\text{norm}}$  surface is resolved into two-dimensional fingerprint plots, generated based on  $d_e$  and  $d_i$  distance scales and illustrated in Fig. 5(a)–(f) The F···H/H···F interactions appear as distinct spikes in the fingerprint plot, and occupy the majority of the total



**Figure 3**  
Details of the hydrogen bonds between the hydrazinium (1+) cations and  $[\text{SiF}_6]^{2-}$  anions in (I).

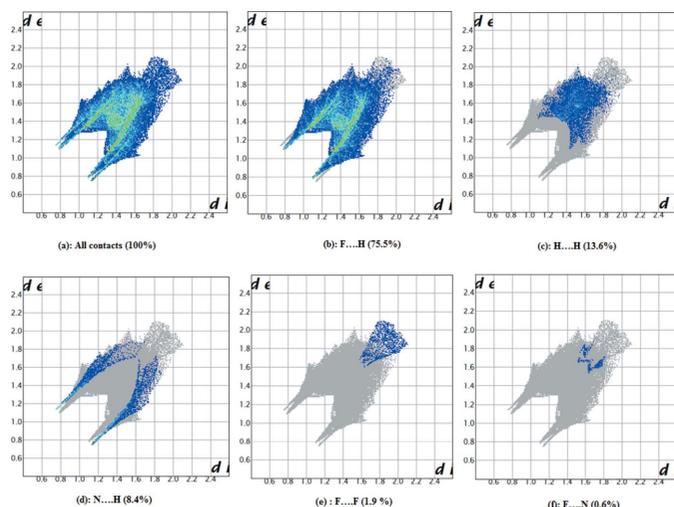


**Figure 4**  
The crystal structure of (I) with the anions shown as polyhedra.

Hirshfeld surface (75.5%) as illustrated in Fig. 5(a); the characteristic ‘wingtip’ features indicate the N—H···F hydrogen bonds. The H···F interaction are represented by a spike ( $d_i = 0.8$ ,  $d_e = 1.1$  Å) at the bottom left (donor), whereas the F···H interactions are represented by a spike ( $d_i = 1.1$ ,  $d_e = 0.8$  Å) at the bottom right (acceptor) of the fingerprint plot. The H···H contacts appear in the middle of the scattered points; these contacts comprise 13.6% of the total Hirshfeld surface [Fig. 5(c)]. The N···H contacts cover 8.4% of the total surface, as the third important contributor in the crystal packing, Fig. 5(d) while the F···F and F···N/N···F contacts make negligible contributions of 1.9% [Fig. 5(e)] and 0.6% [Fig. 5(f)], respectively.

#### 4. Database survey

Hydrazinium (2+) hexafluorosilicate,  $N_2H_6SiF_6$ , at room temperature, crystallizes in a pseudo-tetragonal orthorhombic



**Figure 5**  
Fingerprint plots for the interactions present in the crystal packing of (I) showing (a) all contacts and those delineated into (b) F···H, (c) H···H, (d) N···H, (e) F···F and (f) F···N. The outline of the full fingerprint is shown in grey.

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	$F_6H_{10}N_4Si$
$M_r$	208.21
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
$a$ , $b$ , $c$ (Å)	5.9496 (3), 5.2484 (2), 11.0029 (5)
$\beta$ (°)	100.245 (1)
$V$ (Å <sup>3</sup> )	338.10 (3)
$Z$	2
Radiation type	Mo $K\alpha$
$\mu$ (mm <sup>-1</sup> )	0.42
Crystal size (mm)	0.31 × 0.24 × 0.16
Data collection	
Diffractometer	Bruker D8 VENTURE Super DUO
Absorption correction	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)
$T_{min}$ , $T_{max}$	0.638, 0.746
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	19683, 1488, 1379
$R_{int}$	0.027
$(\sin \theta/\lambda)_{max}$ (Å <sup>-1</sup> )	0.806
Refinement	
$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , $S$	0.021, 0.059, 1.06
No. of reflections	1488
No. of parameters	54
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$ , $\Delta\rho_{min}$ (e Å <sup>-3</sup> )	0.27, -0.22

Computer programs: *APEX3* and *SAINT-Plus* (Bruker, 2016), *SHELXT2014/7* (Sheldrick, 2015a), *SHELXL2014/7* (Sheldrick, 2015b), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *pubCIF* (Westrip, 2010).

space group ( $Pbca$ ,  $Z = 4$ ), with  $a = 7.605$  (1) Å,  $b = 7.586$  (2) Å and  $c = 8.543$  (1) Å (Frlec *et al.*, 1980; Cameron *et al.*, 1983). Its structure consists of centrosymmetric  $N_2H_6^{2+}$  and  $SiF_6^{2-}$  ions arranged in a NaCl-type packing and connected by N—H···F hydrogen bonds, forming layers of cations and anions lying parallel to (001) plane.

Hydrazinium (1+) hexahalogenometallates were studied by Gantar and co-workers (Gantar *et al.*, 1985; Gantar & Rahten, 1986) who showed that  $(N_2H_5)_2GeF_6$  crystallizes in the monoclinic system, space group  $P2_1/n$  ( $Z = 2$ ), with cell parameters  $a = 6.015$  (2) Å,  $b = 5.249$  (1) Å,  $c = 11.181$  (2) Å and  $\beta = 100.15$  (2)° and is clearly isostructural with (I).

Fluoride complexes of titanium (IV) with ammonium cation derivatives include two hydrazinium hexafluoridotitanates (IV),  $(N_2H_5)_2TiF_6$  (Leban *et al.*, 1994) and  $N_2H_6TiF_6$  (Kojić-Prodić *et al.*, 1971a,b). The monoclinic crystals of  $(N_2H_5)_2TiF_6$  [ $P2_1$ ;  $Z = 4$ ;  $a = 7.815$  (1) Å,  $b = 10.019$  (1) Å,  $c = 9.338$  (1) Å;  $\beta = 93.58$  (1)°] exhibit racemic twinning but are not isostructural with (I). The crystal structure of  $(N_2H_5)_2TiF_6$  consists of  $N_2H_5^+$  cations and two types of slightly distorted octahedral  $(TiF_6)^{2-}$  anions. The  $N_2H_5^+$  cations and  $(TiF_6)^{2-}$  anions are linked via N—H···F and N—H···N hydrogen bonds, building a three-dimensional network. Two other isostructural hydrazinium (1+) hexafluorido complexes,  $(N_2H_5)_2ZrF_6$  and  $(N_2H_5)_2HfF_6$ , were prepared and characterized by chemical analysis, vibrational spectroscopy and X-ray powder diffraction (Gantar & Rahten, 1988). The infrared spectrum analysis of the title compound at room temperature confirms the obtained results

by Gantar & Rahten with the exception of the assignments of two infrared bands (see supporting information).

## 5. Synthesis and Infrared measurement technique.

Hydrazinium (1+) hexafluorosilicate  $(\text{N}_2\text{H}_5)_2\text{SiF}_6$  crystals in the form of colourless blocks were obtained by slow evaporation, at room temperature, of an aqueous solution containing stoichiometric amounts of hydrazine  $\text{NH}_2\text{NH}_2$  and  $\text{H}_2\text{SiF}_6$ . The infrared spectrum was recorded in the range 450–4000  $\text{cm}^{-1}$  with a Vertex 70 FTIR spectrometer.

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were located in a difference-Fourier map and refined using a riding model with  $\text{N}-\text{H} = 0.86 \text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$ . The highest peak and the deepest hole in the final Fourier map are at 0.67  $\text{Å}$  from F3 and 0.0  $\text{Å}$  from Si1.

## Acknowledgements

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## References

Bruker (2016). *APEX3* and *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.

- Cameron, T. S., Knop, O. & MacDonald, L. A. (1983). *Can. J. Chem.* **61**, 184–188.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Frlec, B., Gantar, D., Golič, L. & Leban, I. (1980). *Acta Cryst.* **B36**, 1917–1918.
- Gantar, D., Golic, L., Leban, I. & Rahten, A. (1985). *J. Fluor. Chem.* **30**, 19–28.
- Gantar, D. & Rahten, A. (1986). *Thermochim. Acta*, **108**, 149–155.
- Gantar, D., Rahten, A. & Volavsek, B. (1988). *J. Fluor. Chem.* **41**, 335–344.
- Golič, L., Kaučič, V. & Kojić-Prodić, B. (1980). *Acta Cryst.* **B36**, 659–661.
- Knop, O., Cameron, T. S., James, M. A. & Falk, M. (1983). *Can. J. Chem.* **61**, 1620–1646.
- Kojić-Prodić, B., Matković, B. & Šćavničar, S. (1971a). *Acta Cryst.* **B27**, 635–637.
- Kojić-Prodić, B., Šćavničar, S. & Matković, B. (1971b). *Acta Cryst.* **B27**, 638–644.
- Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
- Leban, I., Jesih, A. & Rahten, A. (1994). *Acta Cryst.* **C50**, 842–843.
- Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
- McKinnon, J. J., Spackman, M. A. & Mitchell, A. S. (2004). *Acta Cryst.* **B60**, 627–668.
- Ouasri, A., Rhandour, A., Dhamelincourt, M.-C., Dhamelincourt, P. & Mazzah, A. (2002). *J. Raman Spectrosc.* **33**, 726–729.
- Sheldrick, G. M. (2015a). *Acta Cryst.* **A71**, 3–8.
- Sheldrick, G. M. (2015b). *Acta Cryst.* **C71**, 3–8.
- Spackman, M. A. & Jayatilaka, D. (2009). *CrystEngComm*, **11**, 19–32.
- Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Spackman, P. R., Jayatilaka, D. & Spackman, M. A. (2017). *CrystalExplorer17*. The University of Western Australia.
- Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

## supporting information

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### Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINTE-Plus* (Bruker, 2016); data reduction: *SAINTE-Plus* (Bruker, 2016); program(s) used to solve structure: *SHELXT2014/7* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014/7* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *Mercury* (Macrae *et al.*, 2008) and *publCIF* (Westrip, 2010).

### Bis[hydrazinium(1+)] hexafluoridosilicate

#### Crystal data

$\text{F}_6\text{H}_{10}\text{N}_4\text{Si}$	$F(000) = 212$
$M_r = 208.21$	$D_x = 2.045 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 5.9496 (3) \text{ \AA}$	Cell parameters from 1488 reflections
$b = 5.2484 (2) \text{ \AA}$	$\theta = 3.7\text{--}35.0^\circ$
$c = 11.0029 (5) \text{ \AA}$	$\mu = 0.42 \text{ mm}^{-1}$
$\beta = 100.245 (1)^\circ$	$T = 296 \text{ K}$
$V = 338.10 (3) \text{ \AA}^3$	Block, colourless
$Z = 2$	$0.31 \times 0.24 \times 0.16 \text{ mm}$

#### Data collection

Bruker D8 VENTURE Super DUO diffractometer	$T_{\min} = 0.638, T_{\max} = 0.746$
Radiation source: INCOATEC $I\mu\text{S}$ micro-focus source	19683 measured reflections
HELIOS mirror optics monochromator	1488 independent reflections
Detector resolution: $10.4167 \text{ pixels mm}^{-1}$	1379 reflections with $I > 2\sigma(I)$
$\varphi$ and $\omega$ scans	$R_{\text{int}} = 0.027$
Absorption correction: multi-scan (SADABS; Krause <i>et al.</i> , 2015)	$\theta_{\max} = 35.0^\circ, \theta_{\min} = 3.7^\circ$
	$h = -9 \rightarrow 9$
	$k = -8 \rightarrow 8$
	$l = -17 \rightarrow 17$

#### Refinement

Refinement on $F^2$	Hydrogen site location: mixed
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.021$	$w = 1/[\sigma^2(F_o^2) + (0.0348P)^2 + 0.036P]$
$wR(F^2) = 0.059$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{\max} = 0.001$
1488 reflections	$\Delta\rho_{\max} = 0.27 \text{ e \AA}^{-3}$
54 parameters	$\Delta\rho_{\min} = -0.22 \text{ e \AA}^{-3}$
0 restraints	

Extinction correction: SHELXL-2018/3  
 (Sheldrick 2015b),  
 $F_c^* = kF_c [1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$   
 Extinction coefficient: 0.093 (10)

### 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.

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Si1	0.500000	0.000000	0.500000	0.01562 (7)
F1	0.28419 (6)	-0.13785 (8)	0.55514 (4)	0.02516 (10)
F3	0.31234 (7)	0.21784 (8)	0.42375 (4)	0.02473 (10)
F2	0.55101 (7)	0.18926 (8)	0.62475 (4)	0.02576 (10)
N1	0.46840 (9)	0.60149 (11)	0.77712 (5)	0.02307 (11)
H1A	0.530893	0.639080	0.711612	0.035*
H1B	0.334122	0.525916	0.752445	0.035*
H1C	0.560407	0.497003	0.826736	0.035*
N2	0.43562 (9)	0.83227 (11)	0.84285 (5)	0.02447 (11)
H2A	0.390725	0.785787	0.906243	0.037*
H2B	0.567906	0.898565	0.869296	0.037*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Si1	0.01429 (10)	0.01983 (11)	0.01242 (10)	0.00065 (6)	0.00149 (6)	-0.00092 (6)
F1	0.02032 (17)	0.0332 (2)	0.02288 (17)	-0.00450 (14)	0.00636 (13)	0.00188 (14)
F3	0.02217 (17)	0.02512 (18)	0.02510 (18)	0.00506 (13)	-0.00071 (13)	0.00348 (13)
F2	0.02585 (18)	0.0309 (2)	0.01981 (17)	0.00025 (14)	0.00210 (13)	-0.01005 (14)
N1	0.0199 (2)	0.0245 (2)	0.0237 (2)	-0.00006 (16)	0.00101 (16)	0.00587 (18)
N2	0.0222 (2)	0.0289 (2)	0.0220 (2)	-0.00171 (18)	0.00320 (17)	0.00167 (18)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

Si1—F2 <sup>i</sup>	1.6777 (4)	N1—N2	1.4416 (8)
Si1—F2	1.6777 (4)	N1—H1A	0.8900
Si1—F1 <sup>i</sup>	1.6785 (4)	N1—H1B	0.8900
Si1—F1	1.6785 (4)	N1—H1C	0.8900
Si1—F3 <sup>i</sup>	1.7101 (4)	N2—H2A	0.8268
Si1—F3	1.7101 (4)	N2—H2B	0.8624
F2 <sup>i</sup> —Si1—F2	180.0	F1 <sup>i</sup> —Si1—F3	90.52 (2)
F2 <sup>i</sup> —Si1—F1 <sup>i</sup>	89.90 (2)	F1—Si1—F3	89.48 (2)
F2—Si1—F1 <sup>i</sup>	90.10 (2)	F3 <sup>i</sup> —Si1—F3	180.0
F2 <sup>i</sup> —Si1—F1	90.10 (2)	N2—N1—H1A	109.5

F2—Si1—F1	89.90 (2)	N2—N1—H1B	109.5
F1 <sup>i</sup> —Si1—F1	180.0	H1A—N1—H1B	109.5
F2 <sup>i</sup> —Si1—F3 <sup>i</sup>	90.74 (2)	N2—N1—H1C	109.5
F2—Si1—F3 <sup>i</sup>	89.26 (2)	H1A—N1—H1C	109.5
F1 <sup>i</sup> —Si1—F3 <sup>i</sup>	89.48 (2)	H1B—N1—H1C	109.5
F1—Si1—F3 <sup>i</sup>	90.52 (2)	N1—N2—H2A	105.6
F2 <sup>i</sup> —Si1—F3	89.26 (2)	N1—N2—H2B	108.1
F2—Si1—F3	90.74 (2)	H2A—N2—H2B	104.3

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

#### Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A $\cdots$ F1 <sup>ii</sup>	0.89	2.36	2.8436 (7)	114
N1—H1A $\cdots$ F3 <sup>iii</sup>	0.89	2.04	2.9174 (7)	170
N1—H1B $\cdots$ N2 <sup>iv</sup>	0.89	2.03	2.8963 (8)	165
N1—H1C $\cdots$ F3 <sup>v</sup>	0.89	2.02	2.9025 (7)	170
N1—H1C $\cdots$ F2 <sup>vi</sup>	0.89	2.49	2.9078 (7)	109
N2—H2A $\cdots$ F1 <sup>vii</sup>	0.83	2.52	3.0952 (7)	127
N2—H2A $\cdots$ F2 <sup>vii</sup>	0.83	2.64	3.0725 (7)	114
N2—H2A $\cdots$ F3 <sup>vii</sup>	0.83	2.43	3.2373 (7)	167
N2—H2B $\cdots$ F3 <sup>viii</sup>	0.86	2.49	3.2683 (7)	150
N2—H2B $\cdots$ F2 <sup>vi</sup>	0.86	2.51	3.1036 (7)	127
N2—H2B $\cdots$ F1 <sup>v</sup>	0.86	2.60	3.0124 (7)	110

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