

## (*E,E*)-*N*<sup>1</sup>,*N*<sup>4</sup>-Bis(2,6-difluorobenzylidene)butane-1,4-diamine

Mohammad Khaledi,<sup>a\*</sup> Reza Kia,<sup>b</sup> William Clegg<sup>c</sup> and Ross W. Harrington<sup>c</sup>

<sup>a</sup>Department of Chemistry, Faculty of Science, Islamic Azad University, Shahrekord Branch, Box 166, Tehran, Iran, <sup>b</sup>Department of Chemistry, Science and Research Branch, Islamic Azad University, Tehran, Iran, and <sup>c</sup>School of Chemistry, Newcastle University, Newcastle upon Tyne NE1 7RU, England

Correspondence e-mail: khaledi1974@yahoo.com

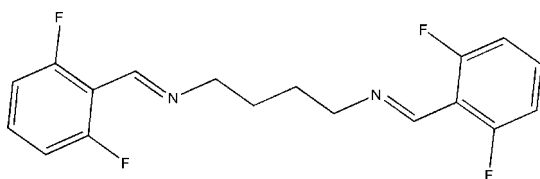
Received 24 October 2011; accepted 26 October 2011

Key indicators: single-crystal X-ray study; *T* = 150 K; mean  $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$ ; *R* factor = 0.037; *wR* factor = 0.100; data-to-parameter ratio = 12.9.

The asymmetric unit of the title compound,  $\text{C}_{18}\text{H}_{16}\text{F}_4\text{N}_2$ , comprises two half crystallographically independent potentially bidentate Schiff base ligands, with an inversion centre located at the mid-point of the central C—C bond. The crystal packing is stabilized by intermolecular C—H...F and  $\pi$ – $\pi$  interactions [centroid–centroid distance =  $3.8283(11) \text{ \AA}$ ].

### Related literature

For background to the synthesis and structural variations of Schiff base ligands and their complexes, see: Granovski *et al.* (1993); Elmali *et al.* (2000).



### Experimental

#### Crystal data

$\text{C}_{18}\text{H}_{16}\text{F}_4\text{N}_2$   
 $M_r = 336.33$   
 Triclinic,  $P\bar{1}$

$a = 6.4672(8) \text{ \AA}$   
 $b = 8.9296(12) \text{ \AA}$   
 $c = 14.4939(19) \text{ \AA}$

$\alpha = 104.956(2)^\circ$   
 $\beta = 94.474(2)^\circ$   
 $\gamma = 93.679(2)^\circ$   
 $V = 803.10(18) \text{ \AA}^3$   
 $Z = 2$

Mo  $K\alpha$  radiation  
 $\mu = 0.12 \text{ mm}^{-1}$   
 $T = 150 \text{ K}$   
 $0.34 \times 0.30 \times 0.20 \text{ mm}$

#### Data collection

Bruker SMART 1K CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2005)  
 $T_{\min} = 0.962$ ,  $T_{\max} = 0.977$

5828 measured reflections  
 2819 independent reflections  
 2394 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.019$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.037$   
 $wR(F^2) = 0.100$   
 $S = 1.11$   
 2819 reflections

218 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.25 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.17 \text{ e \AA}^{-3}$

**Table 1**

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

<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>
C3—H3...F3 <sup>i</sup>	0.95	2.43	3.137 (2)	131
C7—H7...F1 <sup>ii</sup>	0.95	2.54	3.378 (2)	148
C12—H12...F2	0.95	2.42	3.192 (2)	138

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

Data collection: SMART (Bruker, 2005); cell refinement: SAINT (Bruker, 2005); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL and PLATON (Spek, 2009).

MK thanks the Islamic Azad University, Shahrkord Branch, for the support of this work. WC and RWH thank the EPSRC (UK) for equipment funding.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2336).

### References

- Bruker (2005). *SADABS*, *SMART* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Elmali, A., Zeyrek, C. T., Elerman, Y. & Svoboda, I. (2000). *Acta Cryst.* **C56**, 1302–1304.
- Granovski, A. D., Nivorozhkin, A. L. & Minkin, V. I. (1993). *Coord. Chem. Rev.* **126**, 1–69.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

**supplementary materials**

*Acta Cryst.* (2011). E67, o3108 [ doi:10.1107/S1600536811044801 ]

## (*E,E*)-*N*<sup>1</sup>,*N*<sup>4</sup>-Bis(2,6-difluorobenzylidene)butane-1,4-diamine

M. Khaledi, R. Kia, W. Clegg and R. W. Harrington

### Comment

Schiff base ligands are among the most prevalent ligands in the field of coordination chemistry. Metal derivatives of Schiff bases have been studied extensively, and Ni<sup>II</sup> and Cu<sup>II</sup> complexes play a major role in both synthetic and structural research (Elmali *et al.*, 2000; Granovski *et al.*, 1993).

The asymmetric unit of the title compound comprises two half crystallographically independent Schiff base molecules; A (including N1) and B (including N2), see Fig. 1. Each molecule lies about an inversion centre, which is located in the middle of the central C—C bond (Fig. 1). In both molecules the aromatic ring and the imine segment (C=N=C) are approximately coplanar [dihedral angle 14.9 (2)° for molecule A and 3.4 (2)° for molecule B]. These two essentially planar units are linked by a step formed by the four CH<sub>2</sub> groups, so that they are strictly parallel by inversion symmetry but not coplanar.

The crystal packing is stabilized by intermolecular C—H...F interactions (Fig. 2 and Table 1), and by ring stacking of the benzene rings of the two independent molecules [centroid...centroid distance 3.8283 (11) Å, dihedral angle 2.33 (8)°].

### Experimental

The title compound was synthesized by mixing 2,4-difluorobenzaldehyde (4 mmol) and butylenediamine (2 mmol) in chloroform (20 ml). After stirring for 2 h, the solution was filtered and the resulting yellow solid was crystallized from ethanol, giving single crystals suitable for X-ray diffraction.

### Refinement

All H atoms were positioned geometrically and constrained to ride on the parent atoms: C—H = 0.95 and 0.99 %A for CH and CH<sub>2</sub> H atoms, respectively, with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ .

### Figures

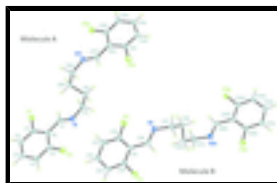


Fig. 1. The molecular structure of the two independent molecules of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering scheme [Symmetry codes for suffix A:  $-x, -y + 1, -z + 1$  for molecule A, and  $-x, -y, -z + 2$  for molecule B].

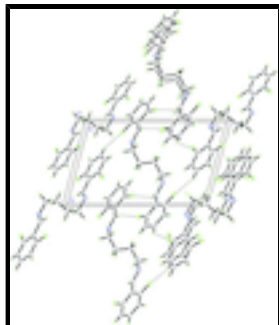


Fig. 2. The crystal packing, viewed down the *a* axis, showing the intermolecular C—H...F hydrogen bonds (dashed lines), which link the molecules to form a three-dimensional network.

**(*E,E*)-*N*<sup>1</sup>,*N*<sup>4</sup>-Bis(2,6-difluorobenzylidene)butane-1,4-diamine**

*Crystal data*

$C_{18}H_{16}F_4N_2$	$Z = 2$
$M_r = 336.33$	$F(000) = 348$
Triclinic, <i>P</i> $\bar{1}$	$D_x = 1.391 \text{ Mg m}^{-3}$
Hall symbol: - <i>P</i> 1	Mo <i>K</i> $\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 6.4672 (8) \text{ \AA}$	Cell parameters from 4637 reflections
$b = 8.9296 (12) \text{ \AA}$	$\theta = 2.9\text{--}28.3^\circ$
$c = 14.4939 (19) \text{ \AA}$	$\mu = 0.12 \text{ mm}^{-1}$
$\alpha = 104.956 (2)^\circ$	$T = 150 \text{ K}$
$\beta = 94.474 (2)^\circ$	Block, colourless
$\gamma = 93.679 (2)^\circ$	$0.34 \times 0.30 \times 0.20 \text{ mm}$
$V = 803.10 (18) \text{ \AA}^3$	

*Data collection*

Bruker SMART 1K CCD area-detector diffractometer	2819 independent reflections
Radiation source: fine-focus sealed tube graphite	2394 reflections with $I > 2\sigma(I)$
Detector resolution: $8.33 \text{ pixels mm}^{-1}$	$R_{\text{int}} = 0.019$
$\omega$ scans	$\theta_{\text{max}} = 25.0^\circ$ , $\theta_{\text{min}} = 2.4^\circ$
Absorption correction: multi-scan ( <i>SADABS</i> ; Bruker, 2005)	$h = -7 \rightarrow 7$
$T_{\text{min}} = 0.962$ , $T_{\text{max}} = 0.977$	$k = -10 \rightarrow 10$
5828 measured reflections	$l = -16 \rightarrow 17$

*Refinement*

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.037$	H-atom parameters constrained
$wR(F^2) = 0.100$	$w = 1/[\sigma^2(F_o^2) + (0.0437P)^2 + 0.2616P]$
	where $P = (F_o^2 + 2F_c^2)/3$

$S = 1.11$	$(\Delta/\sigma)_{\max} < 0.001$
2819 reflections	$\Delta\rho_{\max} = 0.25 \text{ e } \text{\AA}^{-3}$
218 parameters	$\Delta\rho_{\min} = -0.17 \text{ e } \text{\AA}^{-3}$
0 restraints	Extinction correction: <i>SHELXL97</i> (Sheldrick, 2008), $F_c^* = kF_c[1+0.001xF_c^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0064 (19)

### Special details

**Experimental.** The low-temperature data were collected with the Oxford Cyrosystems Cryostream 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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.1808 (2)	0.73556 (16)	0.64201 (10)	0.0304 (3)
N2	0.1964 (2)	0.08666 (15)	0.86448 (9)	0.0280 (3)
F1	0.19530 (16)	1.11574 (12)	0.54522 (8)	0.0423 (3)
F2	0.57474 (16)	0.85519 (11)	0.73666 (7)	0.0392 (3)
F3	0.14208 (16)	0.33304 (13)	0.78309 (9)	0.0486 (3)
F4	0.76402 (16)	0.30222 (12)	0.96638 (8)	0.0424 (3)
C1	0.3727 (2)	1.10083 (19)	0.59734 (11)	0.0274 (4)
C2	0.5378 (3)	1.21002 (19)	0.60645 (12)	0.0327 (4)
H2	0.5284	1.2924	0.5764	0.039*
C3	0.7184 (3)	1.1967 (2)	0.66064 (12)	0.0323 (4)
H3	0.8348	1.2707	0.6677	0.039*
C4	0.7309 (2)	1.07689 (19)	0.70447 (12)	0.0290 (4)
H4	0.8539	1.0686	0.7425	0.035*
C5	0.5610 (2)	0.96960 (18)	0.69179 (11)	0.0260 (4)
C6	0.3742 (2)	0.97517 (17)	0.63782 (10)	0.0236 (3)
C7	0.1858 (2)	0.86668 (18)	0.62385 (11)	0.0262 (4)
H7	0.0593	0.8975	0.5995	0.031*
C8	-0.0223 (3)	0.6452 (2)	0.62406 (12)	0.0353 (4)
H8A	-0.1286	0.7057	0.6011	0.042*
H8B	-0.0627	0.6257	0.6847	0.042*
C9	-0.0163 (3)	0.49050 (19)	0.54960 (12)	0.0324 (4)
H9A	0.0978	0.4343	0.5706	0.039*
H9B	-0.1488	0.4263	0.5459	0.039*
C10	0.3370 (2)	0.38982 (19)	0.82192 (12)	0.0285 (4)

## supplementary materials

---

C11	0.4160 (3)	0.52544 (19)	0.80426 (12)	0.0335 (4)
H11	0.3351	0.5768	0.7664	0.040*
C12	0.6160 (3)	0.58532 (19)	0.84294 (12)	0.0336 (4)
H12	0.6728	0.6790	0.8316	0.040*
C13	0.7339 (3)	0.51022 (19)	0.89783 (12)	0.0331 (4)
H13	0.8712	0.5509	0.9245	0.040*
C14	0.6470 (3)	0.37536 (18)	0.91265 (12)	0.0275 (4)
C15	0.4472 (2)	0.30737 (17)	0.87626 (11)	0.0245 (3)
C16	0.3732 (2)	0.15886 (18)	0.89413 (11)	0.0261 (4)
H16	0.4662	0.1137	0.9310	0.031*
C17	0.1558 (3)	-0.06100 (18)	0.88829 (12)	0.0298 (4)
H17A	0.2825	-0.0846	0.9229	0.036*
H17B	0.1225	-0.1454	0.8284	0.036*
C18	-0.0243 (2)	-0.05570 (17)	0.95036 (11)	0.0248 (3)
H18A	-0.1474	-0.0238	0.9176	0.030*
H18B	-0.0605	-0.1615	0.9571	0.030*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0337 (8)	0.0262 (7)	0.0285 (7)	-0.0040 (6)	0.0007 (6)	0.0044 (6)
N2	0.0307 (8)	0.0286 (7)	0.0266 (7)	-0.0016 (6)	0.0052 (6)	0.0109 (6)
F1	0.0344 (6)	0.0431 (6)	0.0530 (7)	-0.0030 (5)	-0.0134 (5)	0.0260 (5)
F2	0.0374 (6)	0.0374 (6)	0.0489 (6)	0.0016 (4)	-0.0052 (5)	0.0257 (5)
F3	0.0304 (6)	0.0456 (6)	0.0743 (8)	-0.0077 (5)	-0.0171 (5)	0.0333 (6)
F4	0.0352 (6)	0.0387 (6)	0.0568 (7)	-0.0022 (4)	-0.0143 (5)	0.0255 (5)
C1	0.0260 (8)	0.0301 (8)	0.0258 (8)	0.0033 (7)	-0.0027 (6)	0.0084 (7)
C2	0.0371 (10)	0.0287 (9)	0.0350 (9)	-0.0022 (7)	0.0009 (7)	0.0155 (7)
C3	0.0289 (9)	0.0348 (9)	0.0318 (9)	-0.0058 (7)	0.0035 (7)	0.0081 (7)
C4	0.0230 (8)	0.0350 (9)	0.0283 (8)	0.0023 (7)	0.0009 (7)	0.0075 (7)
C5	0.0308 (9)	0.0254 (8)	0.0241 (8)	0.0054 (7)	0.0048 (7)	0.0092 (6)
C6	0.0265 (8)	0.0231 (8)	0.0200 (7)	0.0018 (6)	0.0043 (6)	0.0029 (6)
C7	0.0260 (8)	0.0274 (8)	0.0242 (8)	0.0016 (6)	0.0019 (6)	0.0053 (6)
C8	0.0376 (10)	0.0330 (9)	0.0333 (9)	-0.0093 (8)	0.0081 (8)	0.0069 (7)
C9	0.0382 (10)	0.0260 (8)	0.0323 (9)	-0.0096 (7)	0.0027 (7)	0.0098 (7)
C10	0.0240 (8)	0.0277 (8)	0.0334 (9)	0.0004 (7)	-0.0009 (7)	0.0088 (7)
C11	0.0392 (10)	0.0287 (9)	0.0349 (9)	0.0038 (7)	-0.0034 (8)	0.0142 (7)
C12	0.0421 (10)	0.0228 (8)	0.0365 (9)	-0.0041 (7)	0.0004 (8)	0.0116 (7)
C13	0.0301 (9)	0.0285 (9)	0.0382 (10)	-0.0053 (7)	-0.0045 (7)	0.0087 (7)
C14	0.0278 (9)	0.0261 (8)	0.0297 (8)	0.0048 (7)	-0.0007 (7)	0.0100 (7)
C15	0.0262 (8)	0.0229 (8)	0.0250 (8)	0.0031 (6)	0.0055 (6)	0.0062 (6)
C16	0.0271 (9)	0.0269 (8)	0.0269 (8)	0.0058 (7)	0.0049 (7)	0.0101 (7)
C17	0.0370 (9)	0.0243 (8)	0.0284 (9)	-0.0009 (7)	0.0064 (7)	0.0076 (7)
C18	0.0281 (8)	0.0212 (7)	0.0246 (8)	-0.0053 (6)	-0.0003 (6)	0.0080 (6)

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

N1—C7	1.264 (2)	C8—H8B	0.990
-------	-----------	--------	-------

N1—C8	1.465 (2)	C9—C9 <sup>i</sup>	1.520 (3)
N2—C16	1.262 (2)	C9—H9A	0.990
N2—C17	1.460 (2)	C9—H9B	0.990
F1—C1	1.3568 (18)	C10—C11	1.376 (2)
F2—C5	1.3492 (18)	C10—C15	1.396 (2)
F3—C10	1.3504 (19)	C11—C12	1.384 (2)
F4—C14	1.3562 (18)	C11—H11	0.950
C1—C2	1.373 (2)	C12—C13	1.382 (2)
C1—C6	1.394 (2)	C12—H12	0.950
C2—C3	1.385 (2)	C13—C14	1.370 (2)
C2—H2	0.950	C13—H13	0.950
C3—C4	1.382 (2)	C14—C15	1.394 (2)
C3—H3	0.950	C15—C16	1.473 (2)
C4—C5	1.379 (2)	C16—H16	0.950
C4—H4	0.950	C17—C18	1.522 (2)
C5—C6	1.398 (2)	C17—H17A	0.990
C6—C7	1.474 (2)	C17—H17B	0.990
C7—H7	0.950	C18—C18 <sup>ii</sup>	1.520 (3)
C8—C9	1.523 (2)	C18—H18A	0.990
C8—H8A	0.990	C18—H18B	0.990
C7—N1—C8	116.31 (15)	H9A—C9—H9B	107.8
C16—N2—C17	116.69 (14)	F3—C10—C11	117.55 (14)
F1—C1—C2	117.90 (14)	F3—C10—C15	118.52 (14)
F1—C1—C6	117.45 (14)	C11—C10—C15	123.92 (15)
C2—C1—C6	124.65 (15)	C10—C11—C12	118.54 (15)
C1—C2—C3	118.21 (15)	C10—C11—H11	120.7
C1—C2—H2	120.9	C12—C11—H11	120.7
C3—C2—H2	120.9	C13—C12—C11	120.70 (15)
C4—C3—C2	120.62 (16)	C13—C12—H12	119.7
C4—C3—H3	119.7	C11—C12—H12	119.7
C2—C3—H3	119.7	C14—C13—C12	118.07 (16)
C5—C4—C3	118.57 (15)	C14—C13—H13	121.0
C5—C4—H4	120.7	C12—C13—H13	121.0
C3—C4—H4	120.7	F4—C14—C13	117.68 (15)
F2—C5—C4	117.69 (14)	F4—C14—C15	117.52 (14)
F2—C5—C6	118.30 (14)	C13—C14—C15	124.80 (15)
C4—C5—C6	123.98 (15)	C14—C15—C10	113.96 (14)
C1—C6—C5	113.95 (14)	C14—C15—C16	119.93 (14)
C1—C6—C7	119.55 (14)	C10—C15—C16	126.07 (15)
C5—C6—C7	126.46 (14)	N2—C16—C15	125.39 (15)
N1—C7—C6	124.53 (15)	N2—C16—H16	117.3
N1—C7—H7	117.7	C15—C16—H16	117.3
C6—C7—H7	117.7	N2—C17—C18	111.32 (13)
N1—C8—C9	111.07 (14)	N2—C17—H17A	109.4
N1—C8—H8A	109.4	C18—C17—H17A	109.4
C9—C8—H8A	109.4	N2—C17—H17B	109.4
N1—C8—H8B	109.4	C18—C17—H17B	109.4
C9—C8—H8B	109.4	H17A—C17—H17B	108.0

## supplementary materials

H8A—C8—H8B	108.0	C18 <sup>ii</sup> —C18—C17	113.13 (16)
C9 <sup>i</sup> —C9—C8	112.91 (17)	C18 <sup>ii</sup> —C18—H18A	109.0
C9 <sup>i</sup> —C9—H9A	109.0	C17—C18—H18A	109.0
C8—C9—H9A	109.0	C18 <sup>ii</sup> —C18—H18B	109.0
C9 <sup>i</sup> —C9—H9B	109.0	C17—C18—H18B	109.0
C8—C9—H9B	109.0	H18A—C18—H18B	107.8
F1—C1—C2—C3	179.14 (15)	F3—C10—C11—C12	-179.66 (15)
C6—C1—C2—C3	-0.9 (3)	C15—C10—C11—C12	-0.5 (3)
C1—C2—C3—C4	-0.2 (3)	C10—C11—C12—C13	0.2 (3)
C2—C3—C4—C5	1.0 (2)	C11—C12—C13—C14	0.0 (3)
C3—C4—C5—F2	-178.75 (14)	C12—C13—C14—F4	179.83 (15)
C3—C4—C5—C6	-0.8 (2)	C12—C13—C14—C15	0.1 (3)
F1—C1—C6—C5	-178.90 (13)	F4—C14—C15—C10	179.92 (14)
C2—C1—C6—C5	1.2 (2)	C13—C14—C15—C10	-0.3 (2)
F1—C1—C6—C7	-0.8 (2)	F4—C14—C15—C16	-2.0 (2)
C2—C1—C6—C7	179.26 (15)	C13—C14—C15—C16	177.79 (16)
F2—C5—C6—C1	177.68 (13)	F3—C10—C15—C14	179.69 (14)
C4—C5—C6—C1	-0.3 (2)	C11—C10—C15—C14	0.5 (2)
F2—C5—C6—C7	-0.2 (2)	F3—C10—C15—C16	1.7 (2)
C4—C5—C6—C7	-178.22 (15)	C11—C10—C15—C16	-177.44 (16)
C8—N1—C7—C6	179.47 (14)	C17—N2—C16—C15	178.58 (14)
C1—C6—C7—N1	166.67 (15)	C14—C15—C16—N2	-179.69 (15)
C5—C6—C7—N1	-15.5 (2)	C10—C15—C16—N2	-1.8 (3)
C7—N1—C8—C9	119.39 (16)	C16—N2—C17—C18	118.07 (16)
N1—C8—C9—C9 <sup>i</sup>	-66.7 (2)	N2—C17—C18—C18 <sup>ii</sup>	-66.8 (2)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C3—H3 $\cdots$ F3 <sup>iii</sup>	0.95	2.43	3.137 (2)	131
C7—H7 $\cdots$ F1 <sup>iv</sup>	0.95	2.54	3.378 (2)	148
C12—H12 $\cdots$ F2	0.95	2.42	3.192 (2)	138

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



Fig. 1

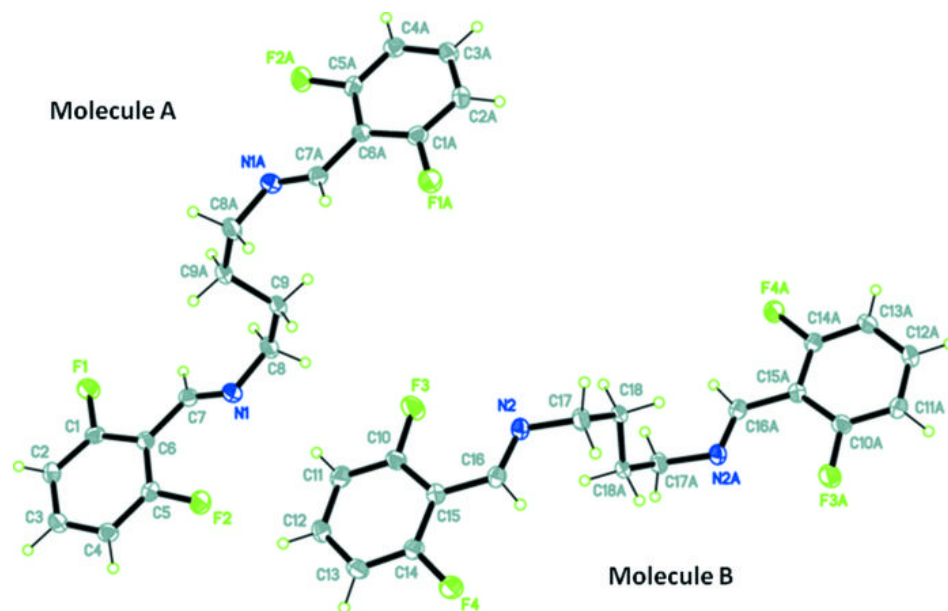


Fig. 2

