

# 2,2-Difluoro-3-(4-fluorophenyl)-2*H*-benzo[*e*]-[1,3,2]oxazaborinin-3-ium-2-uide

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Received 26 July 2017

Accepted 27 July 2017

Edited by M. Bolte, Goethe-Universität Frankfurt, Germany

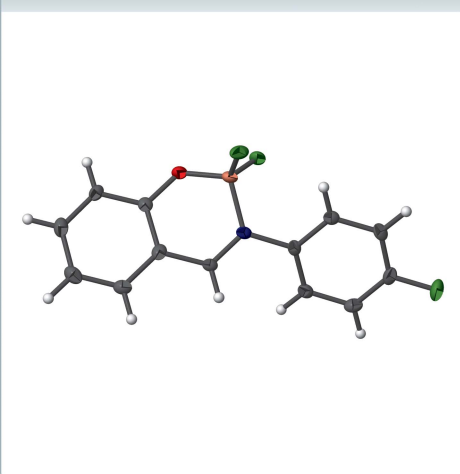
Keywords: crystal structure; BF<sub>2</sub><sup>-</sup>salicylates; BF<sub>2</sub> complexes.

CCDC reference: 1565160

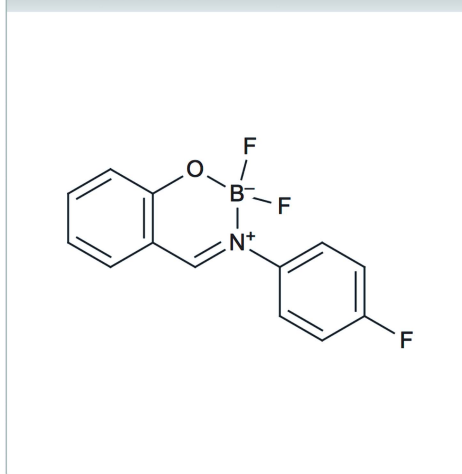
Structural data: full structural data are available from iucrdata.iucr.org

There is one independent molecule in the asymmetric unit of the title compound, C<sub>13</sub>H<sub>9</sub>BF<sub>3</sub>NO, which crystallizes in the non-centrosymmetric space group *Cc*. In the molecular structure, the BF<sub>2</sub>-carrying ring is distorted from planarity and its mean plane makes a dihedral angle of 42.3 (1)° with the 4-fluorophenyl ring. F atoms are involved in all of the short intermolecular contacts of the crystal structure, which link molecules to form chains along [001] and [010].

## 3D view

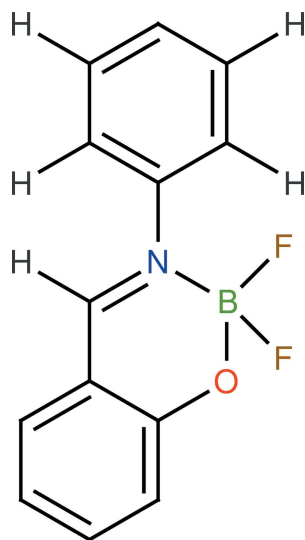


## Chemical scheme



## Structure description

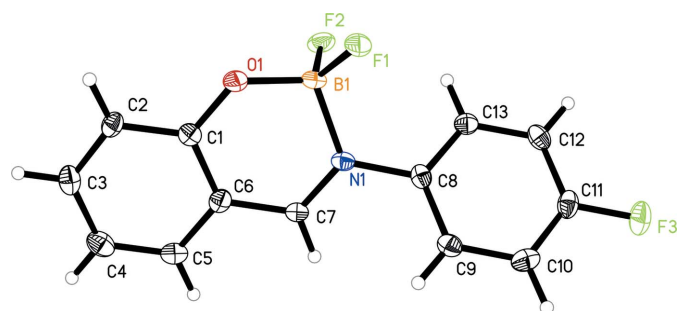
Schiff bases containing a 2-OH group are molecules that are stabilized by intramolecular hydrogen bonding. These molecules act as chelating agents for many cations (Chohan *et al.*, 2001; Topal *et al.*, 2007). The exchange of the OH proton with a cationic species is relatively easy. The same is realised for the exchange of a proton by a strong Lewis acid (BF<sub>2</sub> group). In such a case, the N/BF<sub>2</sub> interaction is much stronger than hydrogen bonding due to the high mobility of the proton. As a consequence, the BF<sub>2</sub><sup>-</sup> derivatives do not lose excitation energy by vibration but fluoresce very intensively. Thus, salicylaldehyde has been used several times to develop BF<sub>2</sub>-carrying fluorophores. These were reviewed by Ziessel and co-workers (Frath *et al.*, 2014). From the structural point of view, the geometry is a molecular property that can be used in both experimental and theoretical studies of the properties of compounds and hence knowledge about the spatial arrangement of parts of the molecule is crucial. The introduction of various substituents causes changes in the properties of molecules. However, for BF<sub>2</sub>-carrying molecules, this field is still to be explored. It is important to note that up to now the structures of only five molecules containing the fragment shown in Fig. 1 have been crystallographically



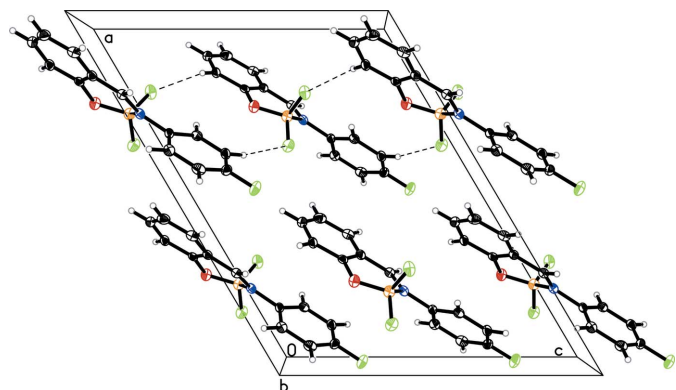
**Figure 1**  
Molecular fragment.

determined. Thus, any progress in this topic may be valuable to explore the effect of the substituents on the properties.

The title compound crystallizes in the non-centrosymmetric space group *Cc* with one independent molecule in the asymmetric unit. The molecular structure of (I) is shown in Fig. 2. The mean plane of the  $\text{BF}_2$ -carrying ring makes a dihedral



**Figure 2**  
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.



**Figure 3**  
The crystal packing of the title compound, viewed along the *b* axis. The strongest  $\text{C—H}\cdots\text{F}$  interactions are displayed.

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

<i>D—H</i> ⋯ <i>A</i>	<i>D—H</i>	<i>H</i> ⋯ <i>A</i>	<i>D</i> ⋯ <i>A</i>	<i>D—H</i> ⋯ <i>A</i>
$\text{C2—H2A}\cdots\text{F2}^i$	0.93	2.49	3.328 (3)	150
$\text{C7—H7A}\cdots\text{F2}^{ii}$	0.93	2.32	3.209 (2)	159
$\text{C9—H9A}\cdots\text{F1}^{ii}$	0.93	2.47	3.369 (3)	162
$\text{C12—H12A}\cdots\text{F1}^{iii}$	0.93	2.37	3.286 (3)	167
$\text{C13—H13A}\cdots\text{F2}$	0.93	2.47	3.114 (3)	127

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

angle of  $42.3 (1)^\circ$  with the 4-fluorophenyl ring. It seems that the twist about the single  $\text{N1—C8}$  bond is caused by the intramolecular  $\text{C13—H13A}\cdots\text{F2}$  hydrogen bond (Table 1), which is the strongest one [based on the  $\text{D}\cdots\text{A}$  distance of  $3.114 (3) \text{\AA}$ ] among the remaining rather weak  $\text{C—H}\cdots\text{F}$  interactions. The twist makes the cross conjugation between the 4-fluorophenyl and the boronic complex not as efficient as it could be for a planar conformation. The geometry around the boron atom is tetrahedral and the  $\text{BF}_2$ -carrying ring is distorted from planarity. Nevertheless, it exhibits normal bond distances and angles (Lugo & Richards, 2010; Dziuk *et al.*, 2017). The  $\text{B—N}$  distance [ $1.586 (3) \text{\AA}$ ] is notably longer than a normal  $\text{B1—N1}$  single bond (*ca*  $1.52 \text{\AA}$ ; Singh *et al.*, 1986; Lugo & Richards, 2010), indicating weak bonding. On the other hand, the  $\text{B1—O1}$  bond is slightly shortened [ $1.445 (3) \text{\AA}$  *versus*  $1.48 \text{\AA}$ ] (Singh *et al.*, 1986; Lugo & Richards, 2010). Fluorine atoms are involved in all of the short intermolecular

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	$\text{C}_{13}\text{H}_9\text{BF}_3\text{NO}$
$M_r$	263.02
Crystal system, space group	Monoclinic, <i>Cc</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> ( $\text{\AA}$ )	16.4374 (9), 6.2657 (2), 12.5689 (6)
$\beta$ ( $^\circ$ )	120.523 (7)
<i>V</i> ( $\text{\AA}^3$ )	1115.11 (11)
<i>Z</i>	4
Radiation type	$\text{Mo K}\alpha$
$\mu$ ( $\text{mm}^{-1}$ )	0.13
Crystal size (mm)	$0.30 \times 0.27 \times 0.20$
Data collection	
Diffractometer	Oxford Diffraction Xcalibur
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	3617, 2009, 1893
$R_{\text{int}}$	0.012
$(\sin \theta/\lambda)_{\text{max}}$ ( $\text{\AA}^{-1}$ )	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , <i>S</i>	0.027, 0.068, 1.01
No. of reflections	2009
No. of parameters	172
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$ , $\Delta\rho_{\text{min}}$ ( $\text{e \AA}^{-3}$ )	0.32, $-0.16$
Absolute structure	Flack <i>x</i> determined using 822 quotients $[(I^+) - (I^-)] / [(I^+) + (I^-)]$ (Parsons <i>et al.</i> , 2013)
Absolute structure parameter	0.4 (2)

Computer programs: *CrysAlis CCD* (Oxford Diffraction, 2008), *SHELXS2014* and *SHELXTL* (Sheldrick, 2008) and *SHELXL2014* (Sheldrick, 2015).

contacts and thus the presence of fluorine may be important for crystal engineering by weak C—H...F intermolecular forces. In the crystal, these intermolecular interactions link the molecules, forming chains propagating along [001] and [010]; see Table 1 and Fig. 3.

### Synthesis and crystallization

The synthesis of 2,2-Difluoro-3-(4-fluorophenyl)-2*H*-benzo[*e*]-[1,3,2]oxazaborinin-3-ium-2-uide was performed by the condensation of salicylaldehyde (1.2 g) with 4-fluoroaniline (1.09 g) in anhydrous ethanol (20 ml) as a solvent by heating the mixture at the boiling point for 12 h. The resulting precipitate was recrystallized from ethanol solution, m.p. 86.7–87.5° C (lit. 86–87° C; Gooden, 1965). The obtained Schiff base (1.81 g of pure compound, 70%) was treated with BF<sub>3</sub> etherate (1 ml) in dry chloroform (10 ml) and DIEA (1 ml). The reaction mixture was heated at the boiling point for 5 h and 5 ml of Na<sub>2</sub>CO<sub>3</sub> (saturated) was added to decompose the excess of BF<sub>3</sub> and neutralize HF. The organic layer was separated and the remaining water layer was extracted with DCM (50 ml). The joined organic fractions were evaporated to dryness and purified by column chromatography (SiO<sub>2</sub>, DCM as eluent). Crystals of good quality characterized by the melting point of 256.6–258.0° C were obtained by slow evaporation of the eluent.

### Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

### References

- Chohan, Z. H., Munawar, A. & Supuran, C. T. (2001). *Met.-Based Drugs*, **8**, 137–143.
- Dziuk, B., Ośmiałowski, B., Skotnicka, A., Ejsmont, K. & Zarychta, B. (2017). *IUCrData*, Submitted.
- Frath, D., Massue, J., Ulrich, G. & Ziesel, R. (2014). *Angew. Chem. Int. Ed.* **53**, 2290–2310.
- Gooden, E. W. (1965). *Aust. J. Chem.* **18**, 637–650.
- Lugo née Gushwa, A. F. & Richards, A. F. (2010). *Eur. J. Inorg. Chem.* **2010**, 2025–2035.
- Oxford Diffraction (2008). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Oxfordshire, England.
- Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* **B69**, 249–259.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Singh, Y. P., Rupani, P., Singh, A., Rai, A. K., Mehrotra, R. C., Rogers, R. D. & Atwood, J. L. (1986). *Inorg. Chem.* **25**, 3076–3081.
- Topal, G., Tümerdem, R., Basaran, I., Gümüş, A. & Cakir, U. (2007). *Int. J. Mol. Sci.* **8**, 933–942.

## full crystallographic data

*IUCrData* (2017). 2, x171109 [https://doi.org/10.1107/S2414314617011099]

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2,2-Difluoro-3-(4-fluorophenyl)-2*H*-benzo[e][1,3,2]oxazaborinin-3-ium-2-uide*Crystal data*

$C_{13}H_9BF_3NO$

$M_r = 263.02$

Monoclinic, *Cc*

$a = 16.4374$  (9) Å

$b = 6.2657$  (2) Å

$c = 12.5689$  (6) Å

$\beta = 120.523$  (7)°

$V = 1115.11$  (11) Å<sup>3</sup>

$Z = 4$

$F(000) = 536$

$D_x = 1.567$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 3617 reflections

$\theta = 3.6$ – $26.0$ °

$\mu = 0.13$  mm<sup>-1</sup>

$T = 100$  K

Irregular, colourless

$0.30 \times 0.27 \times 0.20$  mm

*Data collection*

Oxford Diffraction Xcalibur  
diffractometer

Radiation source: fine-focus sealed tube

Detector resolution: 1024 x 1024 with blocks 2  
x 2 pixels mm<sup>-1</sup>

$\omega$  scan

3617 measured reflections

2009 independent reflections

1893 reflections with  $I > 2\sigma(I)$

$R_{int} = 0.012$

$\theta_{max} = 26.0$ °,  $\theta_{min} = 3.6$ °

$h = -20 \rightarrow 20$

$k = -7 \rightarrow 6$

$l = -15 \rightarrow 14$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.068$

$S = 1.01$

2009 reflections

172 parameters

2 restraints

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0483P)^2]$

where  $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.32$  e Å<sup>-3</sup>

$\Delta\rho_{min} = -0.16$  e Å<sup>-3</sup>

Absolute structure: Flack  $x$  determined using

822 quotients  $[(I^-)-(I)]/[(I^+)+(I)]$  (Parsons *et al.*,  
2013)

Absolute structure parameter: 0.4 (2)

*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.

**Refinement.** All H atoms were found in a difference map but set to idealized positions and treated as riding with C—H = 0.93 Å and  $U_{iso}(H) = 1.2U_{eq}(C)$ .

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
B1	0.77468 (19)	0.1468 (4)	0.5089 (2)	0.0181 (6)
N1	0.77972 (13)	0.3792 (3)	0.46252 (16)	0.0156 (4)
O1	0.74538 (11)	0.1567 (2)	0.59940 (15)	0.0198 (4)
F1	0.86187 (10)	0.0523 (2)	0.56040 (12)	0.0238 (3)
F2	0.70869 (10)	0.03147 (19)	0.40483 (13)	0.0238 (3)
F3	0.98722 (11)	0.5268 (2)	0.23374 (14)	0.0305 (4)
C1	0.68820 (15)	0.3108 (3)	0.59781 (19)	0.0154 (5)
C2	0.64062 (16)	0.2866 (4)	0.66190 (19)	0.0181 (5)
H2A	0.6467	0.1614	0.7050	0.022*
C3	0.58407 (17)	0.4510 (4)	0.6609 (2)	0.0218 (5)
H3A	0.5516	0.4334	0.7030	0.026*
C4	0.57420 (17)	0.6424 (4)	0.5989 (2)	0.0237 (5)
H4A	0.5360	0.7508	0.5999	0.028*
C5	0.62172 (16)	0.6682 (4)	0.5364 (2)	0.0200 (5)
H5A	0.6161	0.7956	0.4952	0.024*
C6	0.67883 (16)	0.5040 (3)	0.5339 (2)	0.0173 (5)
C7	0.73105 (16)	0.5331 (3)	0.4728 (2)	0.0156 (5)
H7A	0.7303	0.6659	0.4392	0.019*
C8	0.83503 (15)	0.4185 (4)	0.40454 (19)	0.0161 (5)
C9	0.88431 (16)	0.6091 (4)	0.4256 (2)	0.0190 (5)
H9A	0.8829	0.7109	0.4785	0.023*
C10	0.93566 (17)	0.6471 (4)	0.3674 (2)	0.0217 (5)
H10A	0.9683	0.7746	0.3799	0.026*
C11	0.93716 (17)	0.4909 (4)	0.2905 (2)	0.0205 (5)
C12	0.88997 (16)	0.2993 (4)	0.2704 (2)	0.0194 (5)
H12A	0.8927	0.1961	0.2192	0.023*
C13	0.83857 (17)	0.2640 (3)	0.3283 (2)	0.0174 (5)
H13A	0.8063	0.1360	0.3158	0.021*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
B1	0.0223 (13)	0.0108 (11)	0.0220 (14)	0.0011 (10)	0.0117 (12)	0.0001 (10)
N1	0.0181 (9)	0.0121 (8)	0.0143 (9)	-0.0008 (8)	0.0066 (8)	-0.0015 (7)
O1	0.0261 (9)	0.0143 (8)	0.0216 (8)	0.0034 (7)	0.0140 (7)	0.0039 (6)
F1	0.0296 (8)	0.0170 (7)	0.0295 (8)	0.0092 (6)	0.0185 (7)	0.0086 (6)
F2	0.0357 (8)	0.0142 (7)	0.0229 (7)	-0.0078 (6)	0.0160 (7)	-0.0047 (5)
F3	0.0319 (8)	0.0403 (9)	0.0308 (8)	-0.0023 (7)	0.0243 (8)	0.0007 (7)
C1	0.0125 (10)	0.0170 (11)	0.0128 (11)	-0.0020 (8)	0.0037 (9)	-0.0027 (8)
C2	0.0193 (11)	0.0213 (11)	0.0138 (12)	-0.0028 (9)	0.0084 (10)	0.0012 (9)
C3	0.0182 (12)	0.0304 (13)	0.0177 (12)	-0.0018 (10)	0.0098 (10)	-0.0033 (10)
C4	0.0179 (12)	0.0234 (11)	0.0255 (13)	0.0031 (10)	0.0079 (11)	-0.0037 (10)
C5	0.0181 (12)	0.0161 (11)	0.0203 (12)	-0.0002 (9)	0.0058 (10)	0.0003 (9)
C6	0.0160 (11)	0.0200 (11)	0.0138 (10)	-0.0054 (9)	0.0062 (10)	-0.0033 (8)
C7	0.0164 (11)	0.0126 (10)	0.0160 (11)	-0.0002 (8)	0.0069 (10)	-0.0004 (8)

C8	0.0160 (11)	0.0198 (11)	0.0124 (11)	0.0035 (9)	0.0071 (9)	0.0018 (9)
C9	0.0205 (12)	0.0166 (11)	0.0187 (11)	0.0030 (9)	0.0092 (10)	0.0006 (9)
C10	0.0202 (12)	0.0173 (11)	0.0226 (13)	-0.0027 (9)	0.0071 (11)	0.0010 (9)
C11	0.0178 (12)	0.0271 (13)	0.0185 (11)	0.0033 (10)	0.0106 (10)	0.0064 (10)
C12	0.0204 (11)	0.0227 (11)	0.0145 (11)	0.0033 (10)	0.0085 (10)	-0.0027 (9)
C13	0.0170 (11)	0.0159 (10)	0.0165 (11)	0.0013 (9)	0.0066 (10)	0.0016 (9)

*Geometric parameters (Å, °)*

B1—F1	1.372 (3)	C4—H4A	0.9300
B1—F2	1.403 (3)	C5—C6	1.403 (3)
B1—O1	1.445 (3)	C5—H5A	0.9300
B1—N1	1.586 (3)	C6—C7	1.425 (3)
N1—C7	1.300 (3)	C7—H7A	0.9300
N1—C8	1.446 (3)	C8—C13	1.384 (3)
O1—C1	1.340 (3)	C8—C9	1.391 (3)
F3—C11	1.354 (3)	C9—C10	1.389 (3)
C1—C2	1.387 (3)	C9—H9A	0.9300
C1—C6	1.418 (3)	C10—C11	1.385 (3)
C2—C3	1.383 (3)	C10—H10A	0.9300
C2—H2A	0.9300	C11—C12	1.381 (3)
C3—C4	1.394 (4)	C12—C13	1.384 (3)
C3—H3A	0.9300	C12—H12A	0.9300
C4—C5	1.370 (3)	C13—H13A	0.9300
F1—B1—F2	110.23 (19)	C5—C6—C1	119.7 (2)
F1—B1—O1	109.4 (2)	C5—C6—C7	120.8 (2)
F2—B1—O1	110.31 (19)	C1—C6—C7	119.5 (2)
F1—B1—N1	109.44 (19)	N1—C7—C6	121.89 (19)
F2—B1—N1	106.89 (19)	N1—C7—H7A	119.1
O1—B1—N1	110.49 (17)	C6—C7—H7A	119.1
C7—N1—C8	119.98 (18)	C13—C8—C9	120.5 (2)
C7—N1—B1	119.66 (19)	C13—C8—N1	119.2 (2)
C8—N1—B1	120.32 (17)	C9—C8—N1	120.32 (19)
C1—O1—B1	122.08 (17)	C10—C9—C8	119.8 (2)
O1—C1—C2	120.73 (19)	C10—C9—H9A	120.1
O1—C1—C6	119.8 (2)	C8—C9—H9A	120.1
C2—C1—C6	119.42 (19)	C11—C10—C9	118.5 (2)
C3—C2—C1	119.2 (2)	C11—C10—H10A	120.7
C3—C2—H2A	120.4	C9—C10—H10A	120.7
C1—C2—H2A	120.4	F3—C11—C12	118.9 (2)
C2—C3—C4	122.1 (2)	F3—C11—C10	118.8 (2)
C2—C3—H3A	118.9	C12—C11—C10	122.3 (2)
C4—C3—H3A	118.9	C11—C12—C13	118.6 (2)
C5—C4—C3	119.0 (2)	C11—C12—H12A	120.7
C5—C4—H4A	120.5	C13—C12—H12A	120.7
C3—C4—H4A	120.5	C12—C13—C8	120.2 (2)
C4—C5—C6	120.6 (2)	C12—C13—H13A	119.9

C4—C5—H5A	119.7	C8—C13—H13A	119.9
C6—C5—H5A	119.7		
F1—B1—N1—C7	-143.2 (2)	O1—C1—C6—C7	-0.5 (3)
F2—B1—N1—C7	97.4 (2)	C2—C1—C6—C7	177.1 (2)
O1—B1—N1—C7	-22.6 (3)	C8—N1—C7—C6	-177.25 (19)
F1—B1—N1—C8	39.3 (3)	B1—N1—C7—C6	5.3 (3)
F2—B1—N1—C8	-80.1 (2)	C5—C6—C7—N1	-175.6 (2)
O1—B1—N1—C8	159.87 (18)	C1—C6—C7—N1	7.4 (3)
F1—B1—O1—C1	150.84 (18)	C7—N1—C8—C13	-141.0 (2)
F2—B1—O1—C1	-87.7 (2)	B1—N1—C8—C13	36.5 (3)
N1—B1—O1—C1	30.3 (3)	C7—N1—C8—C9	39.2 (3)
B1—O1—C1—C2	162.2 (2)	B1—N1—C8—C9	-143.3 (2)
B1—O1—C1—C6	-20.3 (3)	C13—C8—C9—C10	1.5 (3)
O1—C1—C2—C3	178.3 (2)	N1—C8—C9—C10	-178.7 (2)
C6—C1—C2—C3	0.7 (3)	C8—C9—C10—C11	-0.8 (3)
C1—C2—C3—C4	-0.9 (3)	C9—C10—C11—F3	-179.9 (2)
C2—C3—C4—C5	0.3 (3)	C9—C10—C11—C12	-0.4 (3)
C3—C4—C5—C6	0.5 (3)	F3—C11—C12—C13	-179.7 (2)
C4—C5—C6—C1	-0.7 (3)	C10—C11—C12—C13	0.8 (3)
C4—C5—C6—C7	-177.7 (2)	C11—C12—C13—C8	-0.1 (3)
O1—C1—C6—C5	-177.57 (19)	C9—C8—C13—C12	-1.1 (3)
C2—C1—C6—C5	0.1 (3)	N1—C8—C13—C12	179.11 (19)

*Hydrogen-bond geometry (Å, °)*

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
C2—H2A...F2 <sup>i</sup>	0.93	2.49	3.328 (3)	150
C7—H7A...F2 <sup>ii</sup>	0.93	2.32	3.209 (2)	159
C9—H9A...F1 <sup>ii</sup>	0.93	2.47	3.369 (3)	162
C12—H12A...F1 <sup>iii</sup>	0.93	2.37	3.286 (3)	167
C13—H13A...F2	0.93	2.47	3.114 (3)	127

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