

# 2-[4-(Dimethylamino)phenyl]-3,3-difluoro-3*H*-naphtho[1,2-*e*][1,3,2]oxazaborinin-2-ium-3-uide

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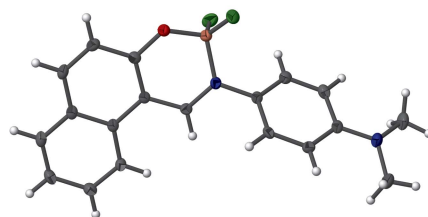
Keywords: crystal structure; BODIPY dyes; fluorophores.

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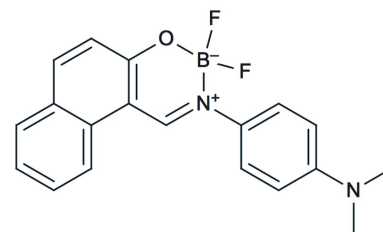
Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

In the title compound, C<sub>19</sub>H<sub>17</sub>BF<sub>2</sub>N<sub>2</sub>O, a twist about the N–C single bond is observed, making the cross conjugation not as efficient as in the case of a planar structure. The borone complex has tetrahedral geometry. In the crystal, molecules are connected by weak C–H···F hydrogen bonds.

## 3D view



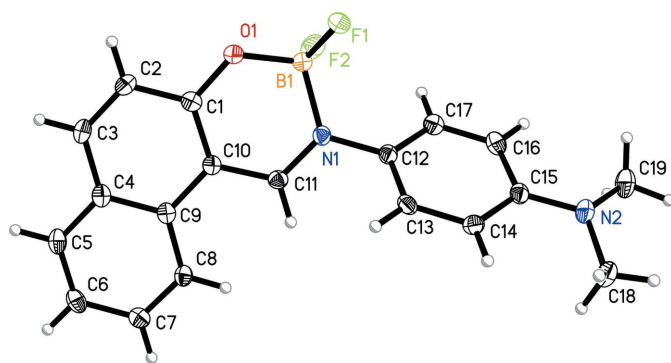
## Chemical scheme



## Structure description

The organic fluorophores commonly known as BODIPY dyes are a class of compounds that are characterized by intense fluorescence, high stability and relatively small Stokes shifts. On the other hand, the difluoroborates that are hydroxy Schiff base derivatives are also important fluorophores. It is known that benzannulation and the presence of a strong electron-donating group shift the maxima of absorption and emission towards the red part of the spectrum (Fabian & Hartmann, 1980). On the other hand, elongation of the molecule by a  $\pi$ -conjugated spacer also gives similar effect. In such a case, the presence of single bonds gives an opportunity for rotation while the presence of the  $-\text{CH}=\text{CH}-$  moiety introduces the possibility of photoisomerization. The last two features cause the fluorescence to be less intensive than in rigid compounds. The rigidification of the molecular skeleton may be realized by benzannulation, which is seen in the vibrationally resolved absorption spectra (Grabarz *et al.*, 2016; Ośmiałowski *et al.*, 2015). In any case, the geometry of molecules in their ground state is the most fundamental property that should be considered.

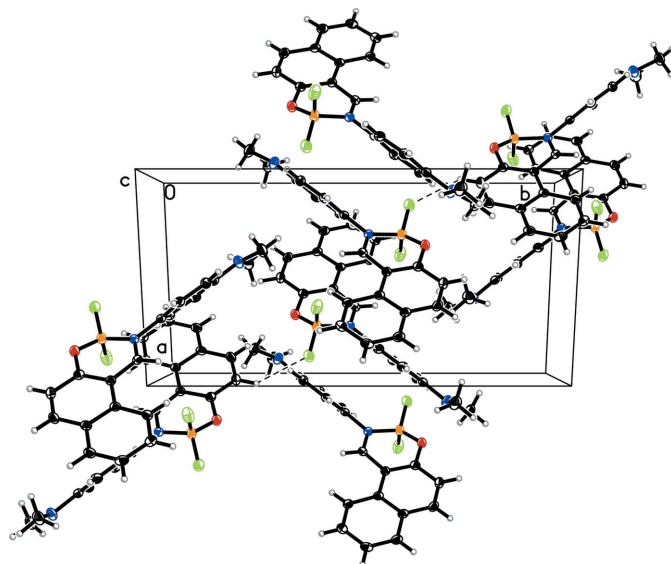
There is one independent molecule in the asymmetric unit of the title compound. Its molecular structure is shown in Fig. 1. In the crystal, there is only one classical intermolecular hydrogen bond (Table 1), which connects molecules into zigzag chains along



**Figure 1**  
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level.

the [101] direction (see Fig. 2). The chains are connected to each other by weak van der Waals interactions.

The geometry of the 4-(dimethylamino)phenyl and naphthalene groups is typical (Allen, 2002). The groups are not coplanar, the dihedral angle between them being 55.12 (3)°. A twist about the N1—C12 single bond is observed, making the cross conjugation not as efficient as in the case of a planar structure. The geometry around B1 atom is tetrahedral and exhibits normal bond distances and angles (Lugo & Richards, 2010). The B—N distance [1.589 (2) Å] is notably longer than a normal B1—N1 single bond (*ca* 1.52 Å; Singh *et al.*, 1986; Lugo & Richards, 2010), indicating weak bonding, and the B1—O1 bond is slightly shorter [1.460 (2) *versus* 1.48 Å]. This pattern of bond lengths is contrary to the model of Itoh and co-workers where the B—O bond is shorter and B—N bond is markedly longer (Itoh *et al.*, 1998), indicating that the complex adopts a structure close to an enol tautomer.



**Figure 2**  
The crystal packing of the title compound, viewed along the *c* axis.

**Table 1**  
Hydrogen-bond geometry (Å, °) [The intramolecular H bond does not appear to be mentioned in the text].

D—H...A	D—H	H...A	D...A	D—H...A
C2—H2...F1 <sup>1</sup>	0.93	2.61	3.3138 (13)	133
C17—H17...F2	0.93	2.56	3.1938 (13)	125

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	C <sub>19</sub> H <sub>17</sub> BF <sub>2</sub> N <sub>2</sub> O
<i>M<sub>r</sub></i>	338.15
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>n</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.6529 (4), 17.7072 (5), 10.4833 (4)
$\beta$ (°)	114.106 (4)
<i>V</i> (Å <sup>3</sup> )	1635.60 (11)
<i>Z</i>	4
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	0.10
Crystal size (mm)	0.25 × 0.23 × 0.15
Data collection	
Diffractometer	Oxford Diffraction Xcalibur
Absorption correction	—
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	10886, 3196, 2485
<i>R</i> <sub>int</sub>	0.022
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.617
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.031, 0.080, 0.98
No. of reflections	3196
No. of parameters	228
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$ , $\Delta\rho_{min}$ (e Å <sup>-3</sup> )	0.18, -0.20

Computer programs: *CrysAlis CCD* and *CrysAlis RED* (Oxford Diffraction, 2008), *SHELXT* (Sheldrick, 2015a), *SHELXL2014* (Sheldrick, 2015b) and *SHELXTL* (Sheldrick, 2008).

## Synthesis and crystallization

The synthesis of 2-[4-(dimethylamino)phenyl]-3,3-difluoro-3*H*-naphtho[1,2-*e*][1,3,2]oxazaborinin-2-ium-3-uide was performed by the condensation of 2-hydroxy-1-naphtaldehyde (1 g) with *N,N*-dimethyl-*p*-phenylenediamine (0.79 g) in anhydrous methanol (10 ml) as a solvent by heating the mixture at boiling point for 12 h. The resulting precipitate was re-crystallized from methanol (m.p. 168.9–171.2°C). The resulting Schiff base (0.67 g, 85%) was treated with BF<sub>3</sub> etherate (1 ml) in chloroform (10 ml) and DIEA (1 ml). The reaction mixture was heated at 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 three portions of chloroform. The combined chloroform fractions were evaporated to dryness and next under vacuum to remove DIEA. The remaining solid was purified by flash chromatography on SiO<sub>2</sub> with chloroform as eluent. NMR spectra were recorded using CDCl<sub>3</sub> as a solvent. Crystals of good quality (m.p. 208–209.3°C) were obtained by slow evaporation of a CDCl<sub>3</sub> solution in the NMR tube.

## Refinement

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

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## full crystallographic data

*IUCrData* (2017). 2, x171141 [https://doi.org/10.1107/S2414314617011415]

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(I)

### Crystal data

C<sub>19</sub>H<sub>17</sub>BF<sub>2</sub>N<sub>2</sub>O

*M<sub>r</sub>* = 338.15

Monoclinic, *P*2<sub>1</sub>/*n*

*a* = 9.6529 (4) Å

*b* = 17.7072 (5) Å

*c* = 10.4833 (4) Å

β = 114.106 (4)°

*V* = 1635.60 (11) Å<sup>3</sup>

*Z* = 4

*F*(000) = 704

*D<sub>x</sub>* = 1.373 Mg m<sup>-3</sup>

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 10886 reflections

θ = 3.3–26.0°

μ = 0.10 mm<sup>-1</sup>

*T* = 100 K

Irregular, colourless

0.25 × 0.23 × 0.15 mm

### Data collection

Oxford Diffraction Xcalibur  
diffractometer

Radiation source: fine-focus sealed tube

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

ω scan

10886 measured reflections

3196 independent reflections

2485 reflections with *I* > 2σ(*I*)

*R*<sub>int</sub> = 0.022

θ<sub>max</sub> = 26.0°, θ<sub>min</sub> = 3.3°

*h* = -11 → 11

*k* = -21 → 17

*l* = -12 → 12

### Refinement

Refinement on *F*<sup>2</sup>

Least-squares matrix: full

*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.031

*wR*(*F*<sup>2</sup>) = 0.080

*S* = 0.98

3196 reflections

228 parameters

0 restraints

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

*w* = 1/[σ<sup>2</sup>(*F*<sub>o</sub><sup>2</sup>) + (0.0519*P*)<sup>2</sup>]

where *P* = (*F*<sub>o</sub><sup>2</sup> + 2*F*<sub>c</sub><sup>2</sup>)/3

(Δ/σ)<sub>max</sub> = 0.001

Δρ<sub>max</sub> = 0.18 e Å<sup>-3</sup>

Δρ<sub>min</sub> = -0.20 e Å<sup>-3</sup>

### 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<sub>Ar</sub>—H = 0.93 Å and *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C) for C—H and with C—H<sub>3</sub> = 0.96 Å and *U*<sub>iso</sub>(H) = 1.5*U*<sub>eq</sub>(C).

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.67086 (9)	0.34092 (4)	0.45068 (8)	0.0198 (2)
F1	0.87188 (8)	0.37674 (4)	0.65386 (7)	0.0293 (2)
F2	0.63047 (8)	0.39784 (4)	0.63418 (7)	0.0302 (2)
B1	0.72560 (16)	0.39555 (7)	0.56491 (14)	0.0196 (3)
N1	0.72551 (10)	0.47697 (5)	0.50108 (9)	0.0161 (2)
N2	1.08863 (11)	0.71216 (5)	0.83259 (10)	0.0235 (2)
C1	0.56665 (13)	0.35922 (6)	0.32362 (12)	0.0175 (3)
C2	0.48595 (13)	0.30025 (6)	0.23360 (13)	0.0210 (3)
H2	0.5040	0.2504	0.2635	0.025*
C3	0.38129 (13)	0.31661 (7)	0.10243 (12)	0.0208 (3)
H3	0.3284	0.2773	0.0441	0.025*
C4	0.35069 (13)	0.39207 (6)	0.05228 (12)	0.0180 (3)
C5	0.23941 (13)	0.40864 (7)	-0.08298 (12)	0.0212 (3)
H5	0.1861	0.3694	-0.1413	0.025*
C6	0.20910 (13)	0.48159 (7)	-0.12919 (12)	0.0216 (3)
H6	0.1362	0.4917	-0.2184	0.026*
C7	0.28848 (13)	0.54113 (7)	-0.04138 (12)	0.0199 (3)
H7	0.2682	0.5906	-0.0732	0.024*
C8	0.39571 (12)	0.52711 (6)	0.09082 (12)	0.0177 (3)
H8	0.4461	0.5673	0.1480	0.021*
C9	0.43083 (12)	0.45235 (6)	0.14152 (12)	0.0160 (2)
C10	0.54181 (12)	0.43441 (6)	0.27937 (11)	0.0157 (2)
C11	0.63361 (12)	0.49104 (6)	0.37190 (12)	0.0164 (3)
H11	0.6278	0.5402	0.3388	0.020*
C12	0.82088 (12)	0.53630 (6)	0.58513 (11)	0.0164 (3)
C13	0.89989 (12)	0.58379 (6)	0.53311 (11)	0.0178 (3)
H13	0.8943	0.5761	0.4434	0.021*
C14	0.98708 (13)	0.64254 (6)	0.61356 (12)	0.0193 (3)
H14	1.0391	0.6739	0.5769	0.023*
C15	0.99802 (13)	0.65550 (6)	0.75010 (12)	0.0180 (3)
C16	0.91852 (13)	0.60575 (7)	0.80092 (12)	0.0202 (3)
H16	0.9238	0.6126	0.8907	0.024*
C17	0.83328 (13)	0.54721 (6)	0.72075 (12)	0.0187 (3)
H17	0.7835	0.5146	0.7576	0.022*
C18	1.14248 (15)	0.77096 (7)	0.76815 (13)	0.0293 (3)
H18A	1.2052	0.7490	0.7267	0.044*
H18B	1.2005	0.8071	0.8378	0.044*
H18C	1.0574	0.7958	0.6972	0.044*
C19	1.08519 (15)	0.72867 (7)	0.96778 (13)	0.0299 (3)
H19A	0.9841	0.7429	0.9542	0.045*
H19B	1.1537	0.7694	1.0119	0.045*
H19C	1.1154	0.6846	1.0261	0.045*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0213 (4)	0.0160 (4)	0.0181 (4)	0.0008 (3)	0.0041 (4)	0.0012 (3)
F1	0.0289 (4)	0.0209 (4)	0.0242 (4)	0.0021 (3)	-0.0032 (3)	0.0030 (3)
F2	0.0444 (5)	0.0246 (4)	0.0299 (4)	-0.0075 (3)	0.0235 (4)	-0.0028 (3)
B1	0.0229 (7)	0.0162 (7)	0.0172 (7)	-0.0006 (5)	0.0056 (6)	0.0008 (5)
N1	0.0144 (5)	0.0162 (5)	0.0161 (5)	0.0000 (4)	0.0046 (4)	-0.0010 (4)
N2	0.0272 (6)	0.0206 (5)	0.0202 (6)	-0.0052 (4)	0.0069 (5)	-0.0050 (4)
C1	0.0160 (6)	0.0193 (6)	0.0177 (6)	0.0008 (5)	0.0074 (5)	0.0012 (5)
C2	0.0237 (7)	0.0148 (6)	0.0244 (7)	-0.0006 (5)	0.0098 (5)	-0.0009 (5)
C3	0.0202 (6)	0.0193 (6)	0.0223 (6)	-0.0044 (5)	0.0080 (5)	-0.0066 (5)
C4	0.0142 (6)	0.0215 (6)	0.0191 (6)	-0.0017 (5)	0.0074 (5)	-0.0037 (5)
C5	0.0165 (6)	0.0252 (6)	0.0201 (6)	-0.0021 (5)	0.0057 (5)	-0.0068 (5)
C6	0.0163 (6)	0.0300 (7)	0.0158 (6)	0.0036 (5)	0.0038 (5)	-0.0013 (5)
C7	0.0194 (6)	0.0219 (6)	0.0191 (6)	0.0037 (5)	0.0085 (5)	0.0016 (5)
C8	0.0153 (6)	0.0185 (6)	0.0180 (6)	-0.0012 (5)	0.0055 (5)	-0.0026 (5)
C9	0.0131 (6)	0.0195 (6)	0.0169 (6)	-0.0007 (5)	0.0074 (5)	-0.0021 (5)
C10	0.0145 (6)	0.0166 (6)	0.0163 (6)	-0.0004 (5)	0.0067 (5)	-0.0007 (5)
C11	0.0150 (6)	0.0156 (6)	0.0178 (6)	0.0019 (4)	0.0059 (5)	0.0015 (5)
C12	0.0129 (6)	0.0157 (6)	0.0173 (6)	0.0019 (4)	0.0029 (5)	-0.0001 (5)
C13	0.0180 (6)	0.0192 (6)	0.0130 (6)	0.0028 (5)	0.0030 (5)	0.0010 (5)
C14	0.0190 (6)	0.0173 (6)	0.0200 (6)	-0.0004 (5)	0.0063 (5)	0.0023 (5)
C15	0.0148 (6)	0.0162 (6)	0.0189 (6)	0.0027 (4)	0.0026 (5)	-0.0011 (5)
C16	0.0175 (6)	0.0259 (7)	0.0170 (6)	0.0022 (5)	0.0068 (5)	-0.0023 (5)
C17	0.0159 (6)	0.0206 (6)	0.0199 (6)	0.0003 (5)	0.0077 (5)	0.0005 (5)
C18	0.0327 (8)	0.0199 (7)	0.0294 (7)	-0.0066 (6)	0.0067 (6)	-0.0041 (5)
C19	0.0323 (8)	0.0283 (7)	0.0269 (7)	-0.0050 (6)	0.0100 (6)	-0.0124 (6)

*Geometric parameters (Å, °)*

O1—C1	1.3404 (14)	C7—H7	0.9300
O1—B1	1.4602 (15)	C8—C9	1.4152 (16)
F1—B1	1.3779 (15)	C8—H8	0.9300
F2—B1	1.3846 (15)	C9—C10	1.4396 (15)
B1—N1	1.5892 (16)	C10—C11	1.4246 (15)
N1—C11	1.3045 (14)	C11—H11	0.9300
N1—C12	1.4369 (14)	C12—C13	1.3878 (16)
N2—C15	1.3789 (14)	C12—C17	1.3907 (15)
N2—C18	1.4483 (15)	C13—C14	1.3863 (16)
N2—C19	1.4607 (15)	C13—H13	0.9300
C1—C10	1.3981 (15)	C14—C15	1.4105 (16)
C1—C2	1.4096 (16)	C14—H14	0.9300
C2—C3	1.3641 (17)	C15—C16	1.4081 (16)
C2—H2	0.9300	C16—C17	1.3759 (16)
C3—C4	1.4221 (16)	C16—H16	0.9300
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.4165 (16)	C18—H18A	0.9600

C4—C9	1.4218 (16)	C18—H18B	0.9600
C5—C6	1.3685 (17)	C18—H18C	0.9600
C5—H5	0.9300	C19—H19A	0.9600
C6—C7	1.4036 (16)	C19—H19B	0.9600
C6—H6	0.9300	C19—H19C	0.9600
C7—C8	1.3718 (16)		
C1—O1—B1	121.89 (9)	C8—C9—C10	123.32 (10)
F1—B1—F2	111.59 (10)	C4—C9—C10	118.47 (10)
F1—B1—O1	108.81 (10)	C1—C10—C11	118.02 (10)
F2—B1—O1	110.74 (10)	C1—C10—C9	119.98 (10)
F1—B1—N1	109.17 (10)	C11—C10—C9	121.95 (10)
F2—B1—N1	107.93 (9)	N1—C11—C10	122.86 (10)
O1—B1—N1	108.53 (9)	N1—C11—H11	118.6
C11—N1—C12	119.38 (9)	C10—C11—H11	118.6
C11—N1—B1	119.58 (9)	C13—C12—C17	119.07 (10)
C12—N1—B1	121.00 (9)	C13—C12—N1	121.29 (10)
C15—N2—C18	119.15 (10)	C17—C12—N1	119.64 (10)
C15—N2—C19	119.61 (10)	C14—C13—C12	120.68 (10)
C18—N2—C19	117.60 (9)	C14—C13—H13	119.7
O1—C1—C10	121.15 (10)	C12—C13—H13	119.7
O1—C1—C2	118.13 (10)	C13—C14—C15	120.98 (11)
C10—C1—C2	120.69 (11)	C13—C14—H14	119.5
C3—C2—C1	119.80 (11)	C15—C14—H14	119.5
C3—C2—H2	120.1	N2—C15—C16	121.47 (11)
C1—C2—H2	120.1	N2—C15—C14	121.35 (10)
C2—C3—C4	121.91 (11)	C16—C15—C14	117.11 (10)
C2—C3—H3	119.0	C17—C16—C15	121.51 (11)
C4—C3—H3	119.0	C17—C16—H16	119.2
C5—C4—C9	119.31 (11)	C15—C16—H16	119.2
C5—C4—C3	121.52 (10)	C16—C17—C12	120.63 (11)
C9—C4—C3	119.15 (11)	C16—C17—H17	119.7
C6—C5—C4	120.99 (11)	C12—C17—H17	119.7
C6—C5—H5	119.5	N2—C18—H18A	109.5
C4—C5—H5	119.5	N2—C18—H18B	109.5
C5—C6—C7	119.76 (11)	H18A—C18—H18B	109.5
C5—C6—H6	120.1	N2—C18—H18C	109.5
C7—C6—H6	120.1	H18A—C18—H18C	109.5
C8—C7—C6	120.74 (11)	H18B—C18—H18C	109.5
C8—C7—H7	119.6	N2—C19—H19A	109.5
C6—C7—H7	119.6	N2—C19—H19B	109.5
C7—C8—C9	120.99 (10)	H19A—C19—H19B	109.5
C7—C8—H8	119.5	N2—C19—H19C	109.5
C9—C8—H8	119.5	H19A—C19—H19C	109.5
C8—C9—C4	118.20 (10)	H19B—C19—H19C	109.5
C1—O1—B1—F1	-151.50 (10)	O1—C1—C10—C9	179.02 (10)
C1—O1—B1—F2	85.50 (13)	C2—C1—C10—C9	1.17 (16)

C1—O1—B1—N1	-32.81 (14)	C8—C9—C10—C1	177.88 (10)
F1—B1—N1—C11	143.57 (10)	C4—C9—C10—C1	-1.18 (16)
F2—B1—N1—C11	-94.96 (12)	C8—C9—C10—C11	-4.96 (16)
O1—B1—N1—C11	25.11 (14)	C4—C9—C10—C11	175.99 (10)
F1—B1—N1—C12	-38.90 (14)	C12—N1—C11—C10	176.32 (10)
F2—B1—N1—C12	82.57 (12)	B1—N1—C11—C10	-6.11 (16)
O1—B1—N1—C12	-157.36 (9)	C1—C10—C11—N1	-8.74 (16)
B1—O1—C1—C10	21.42 (16)	C9—C10—C11—N1	174.03 (10)
B1—O1—C1—C2	-160.67 (11)	C11—N1—C12—C13	-44.76 (15)
O1—C1—C2—C3	-178.63 (10)	B1—N1—C12—C13	137.71 (11)
C10—C1—C2—C3	-0.71 (17)	C11—N1—C12—C17	134.44 (11)
C1—C2—C3—C4	0.29 (18)	B1—N1—C12—C17	-43.09 (15)
C2—C3—C4—C5	-178.58 (11)	C17—C12—C13—C14	-1.59 (16)
C2—C3—C4—C9	-0.32 (17)	N1—C12—C13—C14	177.62 (10)
C9—C4—C5—C6	0.60 (17)	C12—C13—C14—C15	0.10 (17)
C3—C4—C5—C6	178.85 (11)	C18—N2—C15—C16	-167.37 (11)
C4—C5—C6—C7	-0.39 (17)	C19—N2—C15—C16	-9.36 (17)
C5—C6—C7—C8	-0.38 (17)	C18—N2—C15—C14	15.88 (16)
C6—C7—C8—C9	0.94 (17)	C19—N2—C15—C14	173.89 (11)
C7—C8—C9—C4	-0.71 (16)	C13—C14—C15—N2	177.72 (10)
C7—C8—C9—C10	-179.77 (11)	C13—C14—C15—C16	0.83 (16)
C5—C4—C9—C8	-0.05 (15)	N2—C15—C16—C17	-177.17 (11)
C3—C4—C9—C8	-178.35 (10)	C14—C15—C16—C17	-0.28 (17)
C5—C4—C9—C10	179.05 (10)	C15—C16—C17—C12	-1.21 (17)
C3—C4—C9—C10	0.76 (15)	C13—C12—C17—C16	2.14 (17)
O1—C1—C10—C11	1.74 (16)	N1—C12—C17—C16	-177.08 (10)
C2—C1—C10—C11	-176.11 (10)		

*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—H2...F1 <sup>i</sup>	0.93	2.61	3.3138 (13)	133
C17—H17...F2	0.93	2.56	3.1938 (13)	125

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