Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,4,6-Tris(4-fluorophenyl)-2-(1-pyridyl)-boroxine

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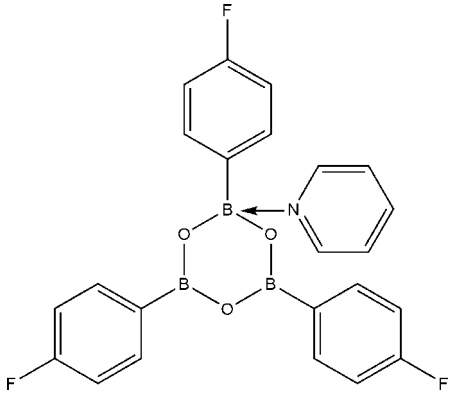
Received 15 November 2007; accepted 29 November 2007

Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.038; wR factor = 0.103; data-to-parameter ratio = 12.2.

Crystals of the title compound, $C_{23}H_{17}B_3F_3NO_3$, were obtained unintentionally by slow evaporation of a chloroform solution of the preformed boroxine–pyridine adduct. The molecule contains three fluoro-substituted benzene rings, each bonded to one of the three B atoms of a six-membered boroxine ring. A pyridyl ring is also bound to one of the B atoms through a Lewis acid–base interaction. The binding of the pyridyl substituent causes the otherwise planar boroxine ring to twist, resulting in a maximum torsion angle within the ring of 17.6 (2)°.

Related literature

For related literature, see: Beckett *et al.* (1997, 1998); Beckmann *et al.* (2001); Frost *et al.* (2006); Hall (2005); Iovine *et al.* (2006); Kua *et al.* (2006); Perttu *et al.* (2005); Sánchez *et al.* (2004); Wu *et al.* (1999).



Experimental

Crystal data

$C_{23}H_{17}B_3F_3NO_3$
M_r = 444.81
Monoclinic, $P2_1/n$
a = 11.6333 (5) Å
b = 14.0230 (7) Å
c = 14.1181 (7) Å
β = 109.337 (3)°
V = 2173.21 (18) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.88 mm^{-1}
T = 173 (1) K
0.21 × 0.17 × 0.09 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.627, T_{max} = 0.925
14062 measured reflections
3644 independent reflections
2938 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.103
S = 1.05
3644 reflections
298 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Selected torsion angles (°).

B3—O3—B1—O1	6.2 (2)	B1—O1—B2—O2	−3.7 (2)
B3—O3—B1—C1	−172.23 (14)	B1—O3—B3—O2	−16.6 (2)
B2—O1—B1—O3	4.7 (2)	B2—O2—B3—O3	17.6 (2)
B3—O2—B2—O1	−8.1 (2)		

Data collection: *APEX2* (Bruker, 2007); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This research was supported by Cottrell College Science Awards from Research Corporation (to SL and PMI).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LN2002).

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supporting information

Acta Cryst. (2008). E**64**, o235 [https://doi.org/10.1107/S1600536807064367]

2,4,6-Tris(4-fluorophenyl)-2-(1-pyridyl)-boroxine

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S1. Comment

Boroxines are cyclic trimers of organoboronic acids produced by dehydration of the acids (Hall, 2005). Arylboroxines have recently found applications in the areas of covalent organic frameworks, nanoscale molecular scaffolds, and noncovalent polymer functionalization (Iovine *et al.*, 2006). The Lewis acidic boroxines are known to form 1:1 adducts with a variety of nitrogenous Lewis bases such as amines, pyridines, azaindoles, and salen-type ligands (Kua *et al.*, 2006).

The structure of the title molecule (Fig. 1) contains features that are consistent with similar boroxine compounds (Beckett *et al.*, 1997, 1998; Beckmann *et al.*, 2001; Frost *et al.*, 2006; Sánchez *et al.*, 2004; Wu *et al.*, 1999). Two of the boron atoms, B1 and B2, are centered in a trigonal planar geometry, while B3 is part of a tetrahedral geometry. The boron-oxygen bonds involving B3 are elongated, by just over 0.10 Å, compared to the other boron-oxygen bonds. As expected, the boron-carbon bonds involving the sp^2 hybridized B1 and B2 are shorter than the B3—C13 bond involving the sp^3 hybridized boron atom. The four-coordinate bonding of B3 causes considerable distortion in the boroxine ring. Torsion angles involving B3 average 12.1 (2)° while the torsion angles that do not contain B3 average 4.2 (2)°. The approximate Td symmetry of the molecule results in a rather open packing arrangement, as seen by viewing down the unit cell *a* axis (Fig. 2).

S2. Experimental

The title compound was synthesized by stirring 4-fluorophenylboronic acid with pyridine in CH_2Cl_2 in the presence of activated 4 Å molecular sieves. After decanting the reaction solution away from the sieves, the solvent was removed *in vacuo* and the resulting solid was dried at 323 K at atmospheric pressure (Perttu *et al.*, 2005). Crystals of the title compound were obtained unintentionally by slow evaporation of a chloroform solution of the pre-formed boroxine:pyridine adduct (m.p. 513 decomp.).

S3. Refinement

Although all of the aromatic H atoms were located in difference maps, H-atoms were placed at idealized positions with C—H = 0.93 Å and refined with a riding model with U_{iso}(H) = 1.2U_{eq}(C).

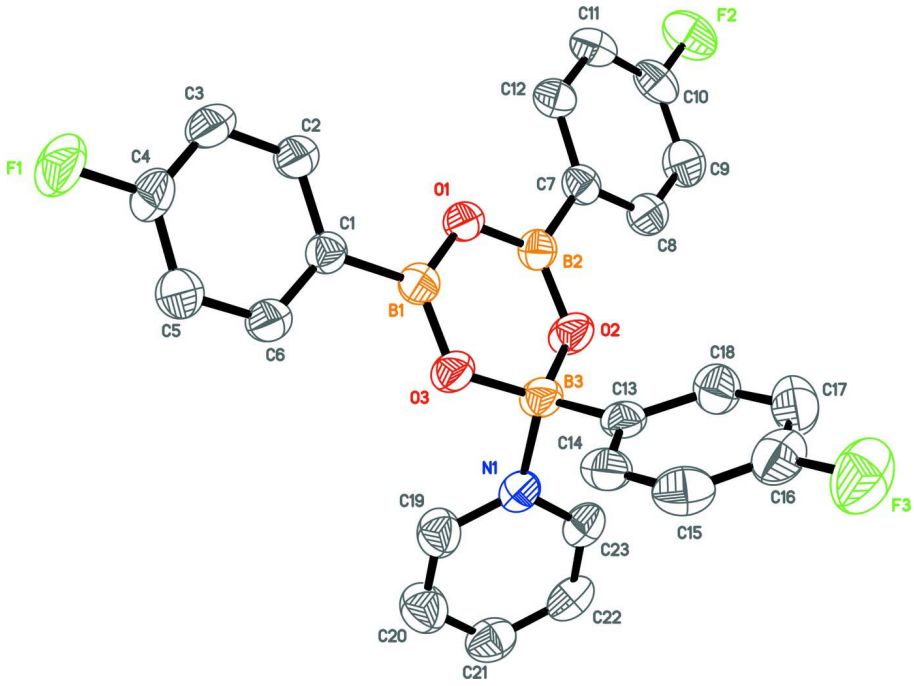

Figure 1

The molecular structure of the title compound, with atom labels and 50% probability displacement ellipsoids for non-H atoms.

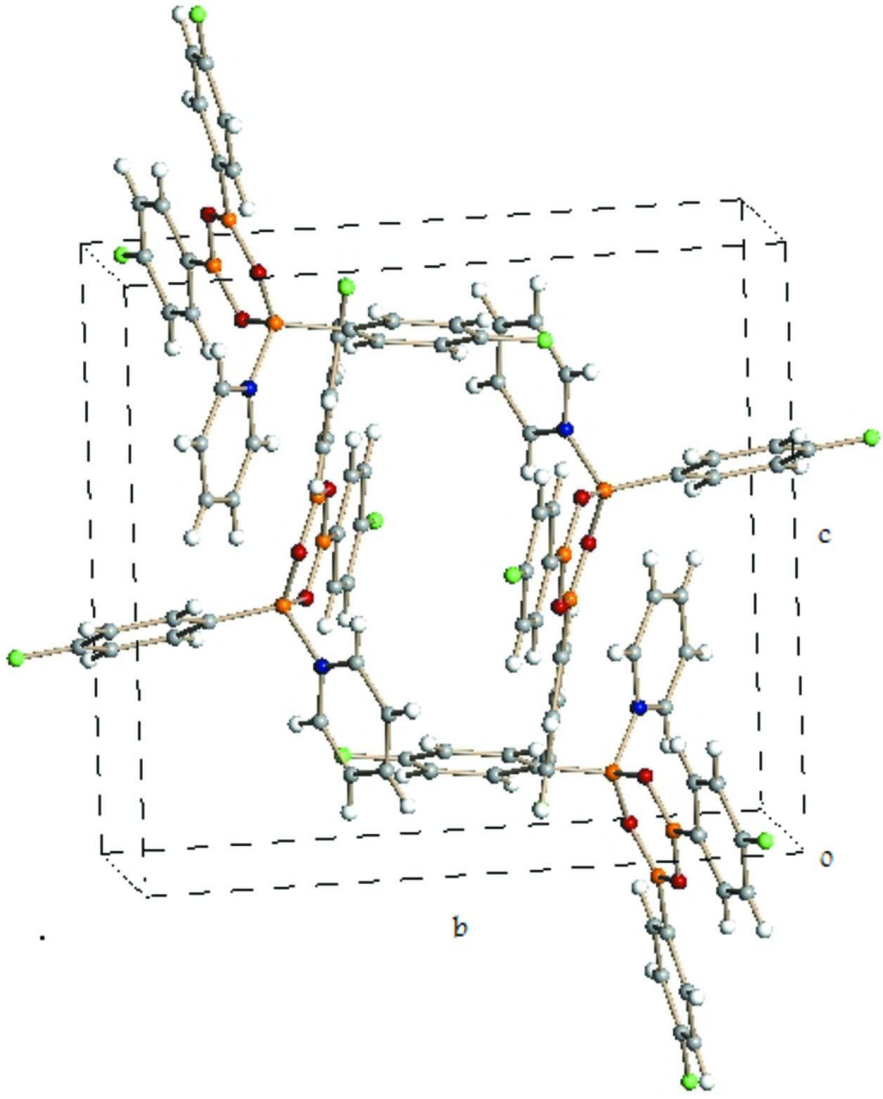

Figure 2

The packing in the unit cell, viewed along the *a* axis.

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Crystal data

$C_{23}H_{17}B_3F_3NO_3$
$M_r = 444.81$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 11.6333\ (5)$ Å
$b = 14.0230\ (7)$ Å
$c = 14.1181\ (7)$ Å
$\beta = 109.337\ (3)°$
$V = 2173.21\ (18)$ Å^3
$Z = 4$
$F(000) = 912$

$D_x = 1.359$ Mg m^{-3}
$D_m = 1.337\ (1)$ Mg m^{-3}
D_m measured by flotation
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 3658 reflections
$\theta = 4.4–65.8°$
$\mu = 0.88$ mm^{-1}
$T = 173$ K
Regular parallelpiped, colorless
0.21 × 0.17 × 0.09 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Multi-layer optics monochromator
Detector resolution: 512 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.627, T_{max} = 0.925

14062 measured reflections
3644 independent reflections
2938 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 65.8°, θ_{min} = 4.3°
h = −13→13
k = −14→15
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.103
S = 1.05
3644 reflections
298 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 0.2495P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.18 e $Å^{-3}$

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 ($Å^2$)

	x	y	z	U_{iso}*/U_{eq}
B1	0.21425 (16)	0.82584 (13)	1.08171 (13)	0.0359 (4)
B2	0.36099 (16)	0.84177 (13)	0.99727 (13)	0.0363 (4)
B3	0.16567 (16)	0.76504 (15)	0.91115 (13)	0.0401 (4)
C1	0.17805 (14)	0.83897 (11)	1.17787 (11)	0.0358 (3)
C2	0.26454 (15)	0.86102 (13)	1.27032 (11)	0.0441 (4)
C3	0.23264 (17)	0.87064 (14)	1.35604 (12)	0.0513 (4)
C4	0.11304 (17)	0.85978 (13)	1.34796 (12)	0.0472 (4)
C5	0.02435 (16)	0.83801 (13)	1.25904 (12)	0.0498 (4)
C6	0.05796 (15)	0.82702 (13)	1.17446 (12)	0.0435 (4)
C7	0.49109 (14)	0.87074 (11)	0.99830 (12)	0.0373 (3)
C8	0.51903 (15)	0.86678 (13)	0.90953 (13)	0.0459 (4)
C9	0.63189 (16)	0.89261 (14)	0.90573 (14)	0.0530 (5)
C10	0.71823 (15)	0.92310 (13)	0.99324 (14)	0.0494 (4)
C11	0.69654 (15)	0.92824 (13)	1.08238 (13)	0.0476 (4)
C12	0.58232 (14)	0.90218 (12)	1.08448 (12)	0.0409 (4)
C13	0.16258 (13)	0.65162 (12)	0.89309 (10)	0.0382 (4)

C14	0.07361 (14)	0.59365 (13)	0.90899 (12)	0.0444 (4)
C15	0.07124 (17)	0.49535 (14)	0.89499 (13)	0.0541 (5)
C16	0.16146 (19)	0.45509 (14)	0.86634 (13)	0.0561 (5)
C17	0.2526 (2)	0.50777 (15)	0.85120 (14)	0.0601 (5)
C18	0.25204 (17)	0.60527 (14)	0.86471 (12)	0.0496 (4)
C19	−0.03505 (17)	0.86020 (14)	0.82476 (13)	0.0509 (4)
C20	−0.12200 (18)	0.90124 (15)	0.74360 (14)	0.0587 (5)
C21	−0.10989 (18)	0.89522 (13)	0.65028 (13)	0.0529 (4)
C22	−0.01015 (17)	0.84869 (13)	0.64049 (12)	0.0488 (4)
C23	0.07340 (16)	0.80916 (12)	0.72425 (11)	0.0440 (4)
F1	0.08044 (11)	0.87144 (9)	1.43108 (7)	0.0677 (3)
F2	0.82939 (9)	0.95033 (9)	0.98983 (9)	0.0696 (3)
F3	0.16178 (14)	0.35866 (8)	0.85394 (9)	0.0824 (4)
N1	0.06137 (12)	0.81444 (9)	0.81514 (9)	0.0386 (3)
O1	0.33071 (9)	0.84911 (8)	1.08391 (7)	0.0375 (3)
O2	0.28014 (10)	0.80708 (9)	0.91196 (8)	0.0452 (3)
O3	0.13168 (10)	0.78966 (8)	0.99819 (7)	0.0421 (3)
H2	0.3454	0.8695	1.2746	0.053*
H3	0.2912	0.8842	1.4177	0.062*
H5	−0.0564	0.8308	1.2556	0.060*
H6	−0.0011	0.8112	1.1138	0.052*
H8	0.4597	0.8461	0.8511	0.055*
H9	0.6491	0.8895	0.8460	0.064*
H11	0.7569	0.9487	1.1404	0.057*
H12	0.5662	0.9058	1.1447	0.049*
H14	0.0135	0.6216	0.9298	0.053*
H15	0.0100	0.4582	0.9049	0.065*
H17	0.3135	0.4787	0.8323	0.072*
H18	0.3139	0.6415	0.8545	0.060*
H19	−0.0436	0.8644	0.8878	0.061*
H20	−0.1883	0.9328	0.7520	0.070*
H21	−0.1680	0.9221	0.5946	0.063*
H22	0.0005	0.8441	0.5782	0.059*
H23	0.1406	0.7777	0.7175	0.053*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
B1	0.0377 (9)	0.0344 (10)	0.0351 (9)	0.0012 (7)	0.0115 (7)	0.0014 (7)
B2	0.0382 (9)	0.0332 (9)	0.0379 (9)	0.0002 (7)	0.0131 (7)	−0.0012 (7)
B3	0.0352 (9)	0.0529 (12)	0.0333 (9)	−0.0059 (8)	0.0128 (7)	−0.0055 (8)
C1	0.0381 (8)	0.0357 (8)	0.0331 (8)	0.0019 (6)	0.0111 (6)	0.0004 (6)
C2	0.0379 (8)	0.0573 (11)	0.0366 (8)	−0.0016 (8)	0.0117 (7)	−0.0043 (7)
C3	0.0482 (10)	0.0710 (13)	0.0315 (8)	−0.0040 (9)	0.0088 (7)	−0.0072 (8)
C4	0.0570 (10)	0.0548 (11)	0.0357 (8)	−0.0021 (8)	0.0233 (7)	−0.0041 (7)
C5	0.0426 (9)	0.0658 (12)	0.0449 (10)	−0.0041 (8)	0.0199 (7)	−0.0031 (8)
C6	0.0385 (8)	0.0557 (11)	0.0352 (8)	−0.0025 (7)	0.0105 (6)	−0.0038 (7)
C7	0.0373 (8)	0.0323 (8)	0.0423 (8)	0.0027 (6)	0.0130 (6)	0.0026 (6)

C8	0.0413 (9)	0.0516 (10)	0.0463 (9)	−0.0015 (8)	0.0165 (7)	−0.0039 (7)
C9	0.0487 (10)	0.0624 (12)	0.0557 (11)	−0.0008 (9)	0.0278 (8)	−0.0003 (9)
C10	0.0326 (8)	0.0518 (11)	0.0670 (11)	0.0018 (8)	0.0207 (8)	0.0092 (8)
C11	0.0341 (8)	0.0497 (11)	0.0532 (10)	0.0008 (7)	0.0069 (7)	0.0059 (8)
C12	0.0388 (8)	0.0407 (9)	0.0409 (9)	0.0018 (7)	0.0101 (7)	0.0045 (7)
C13	0.0330 (8)	0.0525 (10)	0.0261 (7)	−0.0010 (7)	0.0059 (6)	−0.0006 (6)
C14	0.0361 (8)	0.0536 (11)	0.0396 (9)	−0.0005 (7)	0.0073 (7)	0.0014 (7)
C15	0.0519 (11)	0.0556 (12)	0.0475 (10)	−0.0066 (9)	0.0068 (8)	0.0070 (8)
C16	0.0768 (13)	0.0442 (11)	0.0401 (10)	0.0067 (9)	0.0095 (9)	0.0036 (7)
C17	0.0695 (13)	0.0623 (13)	0.0520 (11)	0.0206 (10)	0.0250 (9)	0.0043 (9)
C18	0.0492 (10)	0.0592 (12)	0.0445 (9)	0.0028 (9)	0.0210 (8)	0.0005 (8)
C19	0.0549 (10)	0.0566 (11)	0.0452 (10)	0.0053 (9)	0.0219 (8)	0.0004 (8)
C20	0.0568 (11)	0.0645 (13)	0.0548 (11)	0.0121 (10)	0.0186 (9)	0.0064 (9)
C21	0.0602 (11)	0.0459 (11)	0.0454 (10)	−0.0024 (9)	0.0079 (8)	0.0023 (8)
C22	0.0645 (11)	0.0457 (10)	0.0347 (9)	−0.0103 (9)	0.0143 (8)	−0.0045 (7)
C23	0.0520 (10)	0.0451 (10)	0.0377 (8)	−0.0067 (8)	0.0185 (7)	−0.0058 (7)
F1	0.0732 (7)	0.0978 (9)	0.0428 (6)	−0.0116 (7)	0.0336 (5)	−0.0133 (6)
F2	0.0372 (6)	0.0859 (9)	0.0901 (8)	−0.0050 (6)	0.0269 (6)	0.0086 (7)
F3	0.1228 (12)	0.0477 (8)	0.0700 (8)	0.0105 (7)	0.0230 (7)	0.0021 (6)
N1	0.0419 (7)	0.0398 (8)	0.0353 (7)	−0.0067 (6)	0.0145 (6)	−0.0049 (5)
O1	0.0352 (5)	0.0430 (6)	0.0341 (6)	−0.0018 (5)	0.0110 (4)	−0.0021 (4)
O2	0.0411 (6)	0.0601 (8)	0.0371 (6)	−0.0141 (5)	0.0168 (5)	−0.0105 (5)
O3	0.0377 (6)	0.0569 (7)	0.0330 (6)	−0.0074 (5)	0.0136 (5)	−0.0086 (5)

Geometric parameters (Å, º)

O3—B1	1.349 (2)	C11—C10	1.365 (2)
O3—B3	1.4517 (19)	C11—H11	0.9300
F1—C4	1.3574 (17)	C3—H3	0.9300
F2—C10	1.3645 (18)	C10—C9	1.377 (3)
F3—C16	1.364 (2)	C6—H6	0.9300
O1—B1	1.384 (2)	C9—H9	0.9300
O1—B2	1.3842 (19)	C14—C15	1.391 (3)
O2—B2	1.350 (2)	C14—C13	1.392 (2)
O2—B3	1.453 (2)	C14—H14	0.9300
B1—C1	1.560 (2)	C18—C17	1.381 (3)
B2—C7	1.563 (2)	C18—C13	1.394 (2)
B3—C13	1.609 (3)	C18—H18	0.9300
B3—N1	1.643 (2)	C16—C15	1.366 (3)
C1—C6	1.392 (2)	C16—C17	1.366 (3)
C1—C2	1.394 (2)	C17—H17	0.9300
C8—C9	1.380 (2)	C15—H15	0.9300
C8—C7	1.396 (2)	C23—N1	1.3382 (18)
C8—H8	0.9300	C23—C22	1.374 (2)
C12—C11	1.388 (2)	C23—H23	0.9300
C12—C7	1.395 (2)	C22—C21	1.377 (3)
C12—H12	0.9300	C22—H22	0.9300
C4—C3	1.366 (2)	C21—C20	1.373 (2)

C4—C5	1.370 (2)	C21—H21	0.9300
C5—C6	1.383 (2)	C19—N1	1.338 (2)
C5—H5	0.9300	C19—C20	1.378 (3)
C2—C3	1.385 (2)	C19—H19	0.9300
C2—H2	0.9300	C20—H20	0.9300

B1—O3—B3	120.97 (13)	C11—C10—C9	122.76 (16)
B1—O1—B2	119.75 (13)	C5—C6—C1	121.63 (15)
B2—O2—B3	121.28 (12)	C5—C6—H6	119.2
O3—B1—O1	121.11 (14)	C1—C6—H6	119.2
O3—B1—C1	119.07 (14)	C10—C9—C8	117.86 (16)
O1—B1—C1	119.81 (14)	C10—C9—H9	121.1
O2—B2—O1	120.62 (14)	C8—C9—H9	121.1
O2—B2—C7	119.24 (14)	C15—C14—C13	122.45 (17)
O1—B2—C7	120.11 (14)	C15—C14—H14	118.8
O3—B3—O2	113.75 (13)	C13—C14—H14	118.8
O3—B3—C13	111.78 (14)	C17—C18—C13	122.66 (18)
O2—B3—C13	111.99 (14)	C17—C18—H18	118.7
O3—B3—N1	105.32 (13)	C13—C18—H18	118.7
O2—B3—N1	105.07 (13)	F3—C16—C15	118.89 (19)
C13—B3—N1	108.32 (12)	F3—C16—C17	118.75 (18)
C6—C1—C2	117.65 (14)	C15—C16—C17	122.35 (19)
C6—C1—B1	120.85 (14)	C14—C13—C18	116.10 (17)
C2—C1—B1	121.48 (14)	C14—C13—B3	122.04 (14)
C9—C8—C7	122.12 (16)	C18—C13—B3	121.80 (15)
C9—C8—H8	118.9	C16—C17—C18	118.34 (18)
C7—C8—H8	118.9	C16—C17—H17	120.8
C11—C12—C7	121.45 (15)	C18—C17—H17	120.8
C11—C12—H12	119.3	C16—C15—C14	118.08 (18)
C7—C12—H12	119.3	C16—C15—H15	121.0
F1—C4—C3	118.86 (15)	C14—C15—H15	121.0
F1—C4—C5	118.55 (16)	N1—C23—C22	122.28 (16)
C3—C4—C5	122.59 (14)	N1—C23—H23	118.9
C4—C5—C6	118.28 (16)	C22—C23—H23	118.9
C4—C5—H5	120.9	C23—C22—C21	118.94 (15)
C6—C5—H5	120.9	C23—C22—H22	120.5
C12—C7—C8	117.36 (15)	C21—C22—H22	120.5
C12—C7—B2	123.03 (14)	C20—C21—C22	118.87 (17)
C8—C7—B2	119.61 (14)	C20—C21—H21	120.6
C3—C2—C1	121.39 (16)	C22—C21—H21	120.6
C3—C2—H2	119.3	N1—C19—C20	121.68 (16)
C1—C2—H2	119.3	N1—C19—H19	119.2
C10—C11—C12	118.45 (16)	C20—C19—H19	119.2
C10—C11—H11	120.8	C21—C20—C19	119.46 (18)
C12—C11—H11	120.8	C21—C20—H20	120.3
C4—C3—C2	118.44 (15)	C19—C20—H20	120.3
C4—C3—H3	120.8	C19—N1—C23	118.77 (15)
C2—C3—H3	120.8	C19—N1—B3	122.24 (13)

F2—C10—C11	118.98 (16)	C23—N1—B3	118.99 (13)
F2—C10—C9	118.26 (16)		
B3—O3—B1—O1	6.2 (2)	C4—C5—C6—C1	−1.0 (3)
B3—O3—B1—C1	−172.23 (14)	C2—C1—C6—C5	1.0 (3)
B2—O1—B1—O3	4.7 (2)	B1—C1—C6—C5	179.74 (15)
B2—O1—B1—C1	−176.90 (14)	F2—C10—C9—C8	−178.89 (16)
B3—O2—B2—O1	−8.1 (2)	C11—C10—C9—C8	0.3 (3)
B3—O2—B2—C7	170.01 (15)	C7—C8—C9—C10	0.0 (3)
B1—O1—B2—O2	−3.7 (2)	C15—C14—C13—C18	−1.7 (2)
B1—O1—B2—C7	178.20 (14)	C15—C14—C13—B3	−179.04 (15)
B1—O3—B3—O2	−16.6 (2)	C17—C18—C13—C14	1.0 (2)
B1—O3—B3—C13	111.45 (16)	C17—C18—C13—B3	178.41 (16)
B1—O3—B3—N1	−131.13 (14)	O3—B3—C13—C14	38.0 (2)
B2—O2—B3—O3	17.6 (2)	O2—B3—C13—C14	167.00 (13)
B2—O2—B3—C13	−110.35 (16)	N1—B3—C13—C14	−77.59 (17)
B2—O2—B3—N1	132.28 (15)	O3—B3—C13—C18	−139.19 (15)
O3—B1—C1—C6	−9.3 (2)	O2—B3—C13—C18	−10.2 (2)
O1—B1—C1—C6	172.27 (15)	N1—B3—C13—C18	105.20 (16)
O3—B1—C1—C2	169.37 (15)	F3—C16—C17—C18	−179.49 (16)
O1—B1—C1—C2	−9.1 (2)	C15—C16—C17—C18	−0.6 (3)
F1—C4—C5—C6	179.47 (16)	C13—C18—C17—C16	0.0 (3)
C3—C4—C5—C6	−0.2 (3)	F3—C16—C15—C14	178.88 (15)
C11—C12—C7—C8	−0.2 (2)	C17—C16—C15—C14	0.0 (3)
C11—C12—C7—B2	−179.35 (15)	C13—C14—C15—C16	1.2 (3)
C9—C8—C7—C12	0.0 (3)	N1—C23—C22—C21	−0.1 (3)
C9—C8—C7—B2	179.20 (17)	C23—C22—C21—C20	0.5 (3)
O2—B2—C7—C12	−176.35 (15)	C22—C21—C20—C19	−0.5 (3)
O1—B2—C7—C12	1.8 (2)	N1—C19—C20—C21	0.0 (3)
O2—B2—C7—C8	4.5 (2)	C20—C19—N1—C23	0.4 (3)
O1—B2—C7—C8	−177.37 (15)	C20—C19—N1—B3	−179.92 (17)
C6—C1—C2—C3	0.1 (3)	C22—C23—N1—C19	−0.3 (2)
B1—C1—C2—C3	−178.59 (16)	C22—C23—N1—B3	179.95 (15)
C7—C12—C11—C10	0.4 (3)	O3—B3—N1—C19	−4.1 (2)
F1—C4—C3—C2	−178.37 (16)	O2—B3—N1—C19	−124.55 (16)
C5—C4—C3—C2	1.3 (3)	C13—B3—N1—C19	115.61 (16)
C1—C2—C3—C4	−1.2 (3)	O3—B3—N1—C23	175.57 (13)
C12—C11—C10—F2	178.71 (16)	O2—B3—N1—C23	55.15 (18)
C12—C11—C10—C9	−0.4 (3)	C13—B3—N1—C23	−64.69 (17)