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9-[(Z)-2-(4,4,5,5-Tetramethyl-1,3,2-dioxaborolan-2-yl)ethenyl]-9H-carbazole

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The title compound, $C_{20}H_{22}BNO_2$, has a polarized π-system due to resonance between N—C(H)=C(H)—B and ionic N^+=C(H)—C(H)=B^- canonical structures. The dihedral angles between the ethenyl plane (r.m.s. deviation for C_2H_2 = 0.0333 Å) with the ethenyl-$C(NC_2$-pyrrole) plane (r.m.s. deviation CNC_2 0.0423 Å) and the ethenyl-C(BO_2-1,3,2-dioxaborolane) plane (r.m.s. deviation BCO_2 0.0082 Å) are 45.86 (8) and 37.47 (8)°, respectively, and are greater than those found for the previously reported E-isomer [Hatayama & Okuno (2012) Acta Cryst. E**68**, o84]. In comparison with the E-isomer, the reduced planarity of Z-isomer results in a decrease of the contribution of the N^+=C(H)—C(H)=B^- canonical structure.

3D view
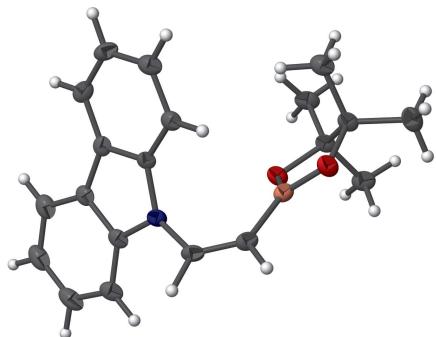
Chemical scheme
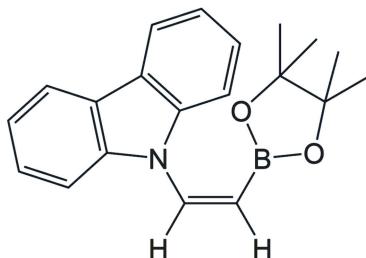
Structure description

The title compound, $C_{20}H_{22}BNO_2$, has a hybrid π-conjugated system comprising an N—C(H)=C(H)—B unit (Fig. 1). The insertion of a π-conjugated system in the N—B bond can give a highly polarized π-system as a result of the contribution of an ionic canonical structure, N^+=C(H)—C(H)=B^-. However, the contribution of the ionic canonical structure is very small when p-phenylene is inserted into the N—B bond (Yuan et al., 2006). By contrast, there is a significant contribution of the ionic canonical structure when a C≡C bond is inserted into the N—B bond (Onuma et al., 2015). The crystal structure of one isomer of the C=C bond-inserted system, namely 9-[(E)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethenyl]-9H-carbazole has been reported (Hatayama & Okuno, 2012), which is an E-isomer of the title compound. In this work, the preparation of the Z-isomer is reported as is a comparison of the crystal structures of the isomers.

The dihedral angles between the C13/C14/H13/H14 plane (r.m.s. deviation 0.0333 Å) and the N1/C1/C12/C13 plane (r.m.s. deviation 0.0423 Å) and B1/O1/O2/C14 plane (r.m.s. deviation 0.0082 Å) are 45.86 (8) and 37.47 (8)°, respectively. The relatively large angles
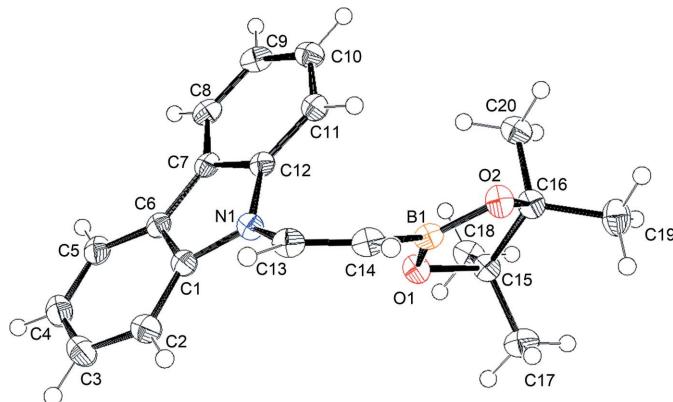
Figure 1
The molecular structure of the title compound showing the atom-numbering scheme with displacement ellipsoids drawn at the 50% probability level and H atoms shown as arbitrary spheres.

result in steric repulsion between carbazolyl and Bpin (pin = pinacolato) residues. The equivalent dihedral angles for the two independent molecules in the *E*-isomer are 19.37 (3) and 10.74 (6)° and 5.70 (11) and 9.74 (9)°, respectively (Hatayama & Okuno, 2012). In comparison with the *Z*-isomer, the *E*-isomer has a more planar conformation. The C=C bond length of the olefinic unit in the *Z*-isomer is *ca* 0.01 Å shorter than those of the *E*-isomer in spite of the steric repulsion. This is presumably because the reduced planarity of the *Z*-isomer decreases the contribution of the N^+=C(H)—C(H)=B^- canonical structure.

In conclusion, structural analyses of both isomers of the hybrid π-system afford an important insight showing the discussed dihedral angles play a crucial role for contribution of the ionic canonical structure.

Synthesis and crystallization

A solution of [Rh(cod)Cl]₂ (0.024 g, 0.050 mmol), tricyclo-hexylphosphane (0.056 g, 0.198 mmol) and 4,4,5,5-tetra-methyl-1,3,2-dioxaborolane (0.478 ml, 3.30 mmol) in a mixture of cyclohexane (10 ml) and triethylamine (2.3 ml, 17 mmol) was stirred for 3 h under an Ar atmosphere. Powdered 9-ethynyl-9*H*-carbazole (0.78 g, 4.1 mmol) was added to the solution followed by stirring for 4 h, also under Ar. After a filtration, the filtrate was concentrated under reduced pressure. The residue was extracted with CHCl₃, and the solvent was removed *via* a rotary evaporator. The crude product was purified by gel permeation chromatography (GPC) (0.020 g, 1.5%). ¹H NMR (400 MHz, CDCl₃): δ 1.05 (*s*, 12H); 5.64 (*d*, *J* = 11.0 Hz, 1H); 7.25 (*t*, *J* = 7.2 Hz, 2H); 7.41 (*t*, *J* = 8.2 Hz, 2H);

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{22}BNO_2$
M_r	319.21
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	93
a, b, c (Å)	8.204 (3), 9.700 (5), 11.330 (5)
α, β, γ (°)	80.975 (15), 81.242 (17), 78.726 (17)
V (Å³)	866.4 (7)
Z	2
Radiation type	Mo $K\alpha$
μ (mm⁻¹)	0.08
Crystal size (mm)	$0.20 \times 0.10 \times 0.04$
Data collection	
Diffractometer	Rigaku Saturn724+
Absorption correction	Numerical (*NUMABS*; Rigaku, 1999)
T_{min}, T_{max}	0.990, 0.997
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	5921, 3005, 2462
R_{int}	0.041
$(\sin \theta/\lambda)_{max}$ (Å⁻¹)	0.594
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.148, 1.04
No. of reflections	3005
No. of parameters	217
H-atom treatment	H-atom parameters not refined
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å⁻³)	0.24, −0.30

Computer programs: *CrystalClear* (Rigaku, 2008), *SHELXD* and *SHELXL* (Sheldrick, 2008), *OPTEP-3 for Windows* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

7.45 (*d*, *J* = 11.0 Hz, 1H); 7.47 (*d*, *J* = 8.2 Hz, 2H); 8.04 (*d*, *J* = 7.7 Hz, 2H).

Single crystals of the title compound suitable for X-ray crystallographic analysis were prepared by recrystallization from its hexane solution.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

References

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full crystallographic data

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Crystal data

$C_{20}H_{22}BNO_2$	$Z = 2$
$M_r = 319.21$	$F(000) = 340.00$
Triclinic, $P\bar{1}$	$D_x = 1.224$ Mg m^{-3}
$a = 8.204$ (3) Å	Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
$b = 9.700$ (5) Å	Cell parameters from 2244 reflections
$c = 11.330$ (5) Å	$\theta = 1.8$–25.0°
$\alpha = 80.975$ (15)°	$\mu = 0.08$ mm^{-1}
$\beta = 81.242$ (17)°	$T = 93$ K
$\gamma = 78.726$ (17)°	Chip, colorless
$V = 866.4$ (7) Å^3	$0.20 \times 0.10 \times 0.04$ mm

Data collection

Rigaku Saturn724+ diffractometer	3005 independent reflections
Detector resolution: 28.445 pixels mm^{-1}	2462 reflections with $F^2 > 2.0\sigma(F^2)$
ω scans	$R_{int} = 0.041$
Absorption correction: numerical (NUMABS; Rigaku, 1999)	$\theta_{max} = 25.0°$, $\theta_{min} = 3.0°$
$T_{min} = 0.990$, $T_{max} = 0.997$	$h = -9 \rightarrow 9$
5921 measured reflections	$k = -11 \rightarrow 10$
	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.054$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.148$	
$S = 1.04$	H-atom parameters not refined
3005 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0817P)^2 + 0.3242P]$ where $P = (F_o^2 + 2F_c^2)/3$
217 parameters	
0 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.24$ e Å^{-3}
	$\Delta\rho_{min} = -0.30$ e Å^{-3}

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. Refinement was performed using all reflections. The weighted R-factor (wR) and goodness of fit (S) are based on F^2. R-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating R-factor (gt).

The C-bound H atoms were placed at ideal positions and were refined as riding on their parent C atoms. U_{iso}(H) values of the H atoms were set at $1.2U_{eq}$(parent atom for C_{sp2}) and $1.5\ U_{eq}$(parent atom for C_{sp3}).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	y	z	$U_{iso}*/U_{eq}$
O1	0.20319 (15)	0.34856 (14)	1.00915 (12)	0.0230 (3)
O2	0.38376 (15)	0.17377 (14)	1.10767 (12)	0.0239 (3)
N1	0.41036 (19)	0.40247 (16)	0.74648 (14)	0.0205 (4)
C1	0.3703 (2)	0.5164 (2)	0.65803 (17)	0.0216 (4)
C2	0.4130 (2)	0.6510 (2)	0.64047 (19)	0.0270 (5)
C3	0.3585 (3)	0.7445 (2)	0.5436 (2)	0.0326 (5)
C4	0.2609 (3)	0.7075 (2)	0.46672 (19)	0.0323 (5)
C5	0.2164 (2)	0.5748 (2)	0.48530 (18)	0.0281 (5)
C6	0.2716 (2)	0.4769 (2)	0.58157 (17)	0.0216 (4)
C7	0.2548 (2)	0.3314 (2)	0.62426 (16)	0.0204 (4)
C8	0.1799 (2)	0.2338 (2)	0.58267 (18)	0.0252 (5)
C9	0.1991 (2)	0.0959 (2)	0.63799 (19)	0.0272 (5)
C10	0.2929 (2)	0.0528 (2)	0.73549 (19)	0.0267 (5)
C11	0.3653 (2)	0.1483 (2)	0.78009 (17)	0.0223 (4)
C12	0.3436 (2)	0.28763 (19)	0.72443 (16)	0.0190 (4)
C13	0.5305 (2)	0.3982 (2)	0.82481 (18)	0.0236 (4)
C14	0.5195 (2)	0.3395 (2)	0.93873 (17)	0.0228 (4)
C15	0.1022 (2)	0.2904 (2)	1.11685 (17)	0.0222 (4)
C16	0.2149 (2)	0.1462 (2)	1.15663 (18)	0.0226 (4)
C17	0.0748 (3)	0.3957 (2)	1.2068 (2)	0.0312 (5)
C18	−0.0659 (2)	0.2788 (2)	1.0809 (2)	0.0291 (5)
C19	0.2125 (3)	0.1056 (2)	1.29157 (19)	0.0326 (5)
C20	0.1851 (2)	0.0232 (2)	1.09897 (19)	0.0285 (5)
B1	0.3668 (3)	0.2849 (2)	1.0180 (2)	0.0212 (5)
H2	0.4774	0.6774	0.6934	0.032*
H3	0.3882	0.8361	0.5289	0.039*
H4	0.2249	0.7744	0.4010	0.039*
H5	0.1489	0.5503	0.4333	0.034*
H8	0.1165	0.2624	0.5168	0.030*
H9	0.1486	0.0291	0.6100	0.033*
H10	0.3067	−0.0434	0.7715	0.032*
H11	0.4278	0.1194	0.8465	0.027*
H13	0.6280	0.4470	0.7822	0.028*
H14	0.6200	0.3320	0.9790	0.037*
H17A	0.0075	0.3607	1.2804	0.037*
H17B	0.1834	0.4073	1.2262	0.037*
H17C	0.0159	0.4874	1.1718	0.037*
H18A	−0.1358	0.2401	1.1515	0.035*
H18B	−0.1225	0.3730	1.0494	0.035*

H18C	−0.0474	0.2158	1.0186	0.035*
H19A	0.1013	0.0863	1.3272	0.039*
H19B	0.2966	0.0203	1.3079	0.039*
H19C	0.2382	0.1835	1.3270	0.039*
H20A	0.0733	0.0020	1.1298	0.034*
H20B	0.1935	0.0488	1.0113	0.034*
H20C	0.2697	−0.0606	1.1186	0.034*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0134 (7)	0.0253 (7)	0.0279 (8)	−0.0019 (5)	−0.0006 (5)	−0.0002 (6)
O2	0.0119 (7)	0.0310 (8)	0.0269 (8)	−0.0027 (5)	−0.0019 (5)	0.0002 (6)
N1	0.0150 (8)	0.0221 (9)	0.0245 (8)	−0.0050 (6)	−0.0014 (6)	−0.0022 (7)
C1	0.0137 (9)	0.0220 (10)	0.0256 (10)	−0.0010 (7)	0.0058 (7)	−0.0031 (8)
C2	0.0174 (10)	0.0248 (10)	0.0360 (12)	−0.0037 (8)	0.0065 (8)	−0.0052 (9)
C3	0.0241 (11)	0.0224 (11)	0.0421 (13)	0.0013 (8)	0.0108 (9)	0.0018 (9)
C4	0.0258 (11)	0.0287 (12)	0.0323 (12)	0.0058 (9)	0.0062 (9)	0.0035 (9)
C5	0.0209 (10)	0.0296 (11)	0.0270 (11)	0.0056 (8)	0.0032 (8)	−0.0019 (9)
C6	0.0144 (9)	0.0243 (10)	0.0223 (10)	0.0008 (7)	0.0048 (7)	−0.0041 (8)
C7	0.0114 (9)	0.0261 (10)	0.0214 (10)	0.0008 (7)	0.0022 (7)	−0.0058 (8)
C8	0.0157 (9)	0.0326 (11)	0.0277 (11)	−0.0001 (8)	−0.0023 (8)	−0.0105 (9)
C9	0.0185 (10)	0.0308 (11)	0.0362 (12)	−0.0062 (8)	−0.0028 (8)	−0.0141 (9)
C10	0.0204 (10)	0.0236 (10)	0.0343 (11)	−0.0036 (8)	0.0020 (8)	−0.0043 (8)
C11	0.0158 (9)	0.0252 (10)	0.0250 (10)	−0.0038 (8)	0.0010 (8)	−0.0032 (8)
C12	0.0120 (9)	0.0222 (10)	0.0222 (10)	−0.0038 (7)	0.0028 (7)	−0.0048 (7)
C13	0.0148 (9)	0.0257 (10)	0.0324 (11)	−0.0078 (8)	−0.0012 (8)	−0.0065 (8)
C14	0.0135 (9)	0.0266 (10)	0.0298 (11)	−0.0033 (8)	−0.0035 (8)	−0.0077 (8)
C15	0.0132 (9)	0.0257 (10)	0.0269 (10)	−0.0043 (7)	0.0002 (7)	−0.0024 (8)
C16	0.0131 (9)	0.0272 (10)	0.0265 (10)	−0.0045 (8)	−0.0002 (7)	−0.0013 (8)
C17	0.0217 (11)	0.0338 (12)	0.0388 (12)	−0.0069 (9)	0.0044 (9)	−0.0125 (10)
C18	0.0145 (10)	0.0297 (11)	0.0433 (13)	−0.0047 (8)	−0.0055 (8)	−0.0027 (9)
C19	0.0261 (11)	0.0415 (13)	0.0278 (11)	−0.0075 (9)	−0.0012 (9)	0.0026 (9)
C20	0.0217 (10)	0.0260 (11)	0.0360 (12)	−0.0038 (8)	−0.0003 (9)	−0.0023 (9)
B1	0.0150 (10)	0.0245 (11)	0.0249 (11)	−0.0018 (8)	−0.0027 (8)	−0.0073 (9)

Geometric parameters (Å, º)

O1—B1	1.375 (2)	C10—H10	0.9505
O1—C15	1.467 (2)	C11—C12	1.389 (3)
O2—B1	1.362 (3)	C11—H11	0.9501
O2—C16	1.471 (2)	C13—C14	1.324 (3)
N1—C1	1.395 (3)	C13—H13	1.0277
N1—C12	1.404 (3)	C14—B1	1.557 (3)
N1—C13	1.414 (3)	C14—H14	0.9869
C1—C2	1.393 (3)	C15—C17	1.517 (3)
C1—C6	1.412 (3)	C15—C18	1.525 (3)
C2—C3	1.380 (3)	C15—C16	1.561 (3)

C2—H2	0.9501	C16—C19	1.516 (3)
C3—C4	1.396 (3)	C16—C20	1.522 (3)
C3—H3	0.9502	C17—H17A	0.9797
C4—C5	1.383 (3)	C17—H17B	0.9805
C4—H4	0.9503	C17—H17C	0.9804
C5—C6	1.398 (3)	C18—H18A	0.9798
C5—H5	0.9509	C18—H18B	0.9799
C6—C7	1.445 (3)	C18—H18C	0.9805
C7—C8	1.397 (3)	C19—H19A	0.9804
C7—C12	1.407 (3)	C19—H19B	0.9808
C8—C9	1.375 (3)	C19—H19C	0.9800
C8—H8	0.9496	C20—H20A	0.9798
C9—C10	1.405 (3)	C20—H20B	0.9805
C9—H9	0.9497	C20—H20C	0.9807
C10—C11	1.386 (3)		
B1—O1—C15	106.68 (15)	N1—C13—H13	111.4
B1—O2—C16	107.55 (14)	C13—C14—B1	128.25 (18)
C1—N1—C12	108.46 (16)	C13—C14—H14	115.7
C1—N1—C13	123.14 (16)	B1—C14—H14	116.1
C12—N1—C13	126.85 (16)	O1—C15—C17	106.93 (15)
C2—C1—N1	129.49 (19)	O1—C15—C18	107.93 (16)
C2—C1—C6	121.62 (18)	C17—C15—C18	109.52 (16)
N1—C1—C6	108.89 (17)	O1—C15—C16	102.76 (14)
C3—C2—C1	117.8 (2)	C17—C15—C16	113.79 (17)
C3—C2—H2	121.1	C18—C15—C16	115.22 (16)
C1—C2—H2	121.1	O2—C16—C19	107.36 (15)
C2—C3—C4	121.6 (2)	O2—C16—C20	107.45 (15)
C2—C3—H3	119.2	C19—C16—C20	110.32 (17)
C4—C3—H3	119.3	O2—C16—C15	102.16 (14)
C5—C4—C3	120.7 (2)	C19—C16—C15	115.19 (17)
C5—C4—H4	119.7	C20—C16—C15	113.57 (17)
C3—C4—H4	119.6	C15—C17—H17A	109.5
C4—C5—C6	119.2 (2)	C15—C17—H17B	109.4
C4—C5—H5	120.5	H17A—C17—H17B	109.5
C6—C5—H5	120.4	C15—C17—H17C	109.4
C5—C6—C1	119.20 (18)	H17A—C17—H17C	109.5
C5—C6—C7	134.00 (19)	H17B—C17—H17C	109.4
C1—C6—C7	106.78 (16)	C15—C18—H18A	109.5
C8—C7—C12	119.23 (18)	C15—C18—H18B	109.5
C8—C7—C6	133.36 (18)	H18A—C18—H18B	109.5
C12—C7—C6	107.30 (16)	C15—C18—H18C	109.5
C9—C8—C7	119.36 (18)	H18A—C18—H18C	109.4
C9—C8—H8	120.4	H18B—C18—H18C	109.4
C7—C8—H8	120.3	C16—C19—H19A	109.5
C8—C9—C10	120.67 (18)	C16—C19—H19B	109.5
C8—C9—H9	119.7	H19A—C19—H19B	109.4
C10—C9—H9	119.6	C16—C19—H19C	109.5

C11—C10—C9	121.08 (19)	H19A—C19—H19C	109.5
C11—C10—H10	119.5	H19B—C19—H19C	109.4
C9—C10—H10	119.5	C16—C20—H20A	109.6
C10—C11—C12	117.78 (18)	C16—C20—H20B	109.5
C10—C11—H11	121.1	H20A—C20—H20B	109.5
C12—C11—H11	121.1	C16—C20—H20C	109.5
C11—C12—N1	129.49 (18)	H20A—C20—H20C	109.4
C11—C12—C7	121.82 (18)	H20B—C20—H20C	109.4
N1—C12—C7	108.51 (16)	O2—B1—O1	113.61 (17)
C14—C13—N1	124.70 (17)	O2—B1—C14	122.75 (17)
C14—C13—H13	123.9	O1—B1—C14	123.54 (18)
C12—N1—C1—C2	−178.03 (18)	C13—N1—C12—C7	−168.45 (16)
C13—N1—C1—C2	−11.4 (3)	C8—C7—C12—C11	2.8 (3)
C12—N1—C1—C6	2.38 (19)	C6—C7—C12—C11	−173.95 (16)
C13—N1—C1—C6	169.01 (16)	C8—C7—C12—N1	178.38 (16)
N1—C1—C2—C3	179.05 (17)	C6—C7—C12—N1	1.58 (19)
C6—C1—C2—C3	−1.4 (3)	C1—N1—C13—C14	144.8 (2)
C1—C2—C3—C4	1.3 (3)	C12—N1—C13—C14	−51.1 (3)
C2—C3—C4—C5	−0.3 (3)	N1—C13—C14—B1	−10.5 (3)
C3—C4—C5—C6	−0.6 (3)	B1—O1—C15—C17	97.21 (18)
C4—C5—C6—C1	0.5 (3)	B1—O1—C15—C18	−145.05 (16)
C4—C5—C6—C7	−177.45 (19)	B1—O1—C15—C16	−22.88 (19)
C2—C1—C6—C5	0.5 (3)	B1—O2—C16—C19	−142.55 (17)
N1—C1—C6—C5	−179.86 (15)	B1—O2—C16—C20	98.79 (18)
C2—C1—C6—C7	178.99 (16)	B1—O2—C16—C15	−20.98 (19)
N1—C1—C6—C7	−1.38 (19)	O1—C15—C16—O2	26.31 (18)
C5—C6—C7—C8	1.9 (4)	C17—C15—C16—O2	−88.90 (18)
C1—C6—C7—C8	−176.28 (19)	C18—C15—C16—O2	143.41 (16)
C5—C6—C7—C12	178.03 (19)	O1—C15—C16—C19	142.33 (16)
C1—C6—C7—C12	−0.13 (19)	C17—C15—C16—C19	27.1 (2)
C12—C7—C8—C9	−2.1 (3)	C18—C15—C16—C19	−100.6 (2)
C6—C7—C8—C9	173.73 (18)	O1—C15—C16—C20	−89.07 (18)
C7—C8—C9—C10	0.0 (3)	C17—C15—C16—C20	155.71 (17)
C8—C9—C10—C11	1.4 (3)	C18—C15—C16—C20	28.0 (2)
C9—C10—C11—C12	−0.6 (3)	C16—O2—B1—O1	7.5 (2)
C10—C11—C12—N1	−175.98 (18)	C16—O2—B1—C14	−176.06 (17)
C10—C11—C12—C7	−1.5 (3)	C15—O1—B1—O2	10.7 (2)
C1—N1—C12—C11	172.61 (18)	C15—O1—B1—C14	−165.67 (17)
C13—N1—C12—C11	6.6 (3)	C13—C14—B1—O2	148.6 (2)
C1—N1—C12—C7	−2.46 (19)	C13—C14—B1—O1	−35.3 (3)