IUCrData

ISSN 2414-3146

N-Phenyl-*N*-[(*E*)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethenyl]aniline

Yuki Hatayama, Kazuto Akagi and Tsunehisa Okuno*

Department of Systems Engineering, Wakayama University, Sakaedani, Wakayama, 640-8510, Japan. *Correspondence e-mail: okuno@wakayama-u.ac.jp

Received 18 January 2022
Accepted 24 January 2022

Edited by E. R. T. Tiekink, Sunway University, Malaysia

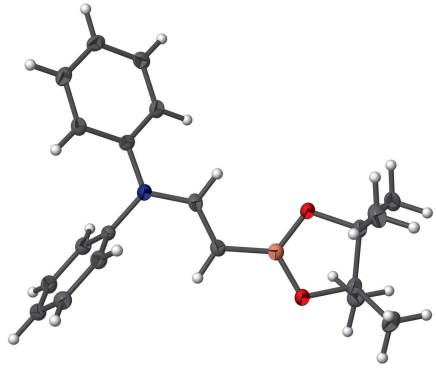
Keywords: crystal structure; dioxaborolan-2-yl; resonance.

CCDC reference: 2129837

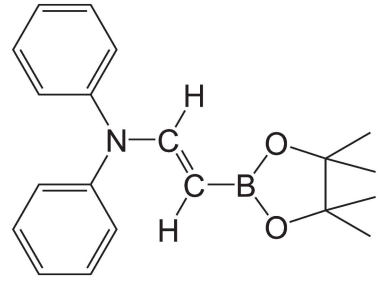
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{20}H_{24}BNO_2$, has a polarized π-system due to significant resonance between the N—C(H)═C(H)—B and ionic N^+═C(H)—C(H)═B^- canonical forms. The dihedral angles between the NC_2B plane (r.m.s. deviation 0.0223 Å) and the C_3N (r.m.s. deviation 0.0025 Å) and BCO_2 (r.m.s. deviation 0.0044 Å) planes are 2.51 (12) and 3.09 (19)°, respectively. This indicates the lone pair of the nitrogen atom and a vacant *p* orbital of the boron atom are conjugated with the central C═C bond. In comparison with the carbazole analogue [Hatayama & Okuno (2012). *Acta Cryst.* E**68**, o84], the C—N and C—B bonds are shorter. The results are well explained by the increase in the contribution of the N^+═C(H)—C(H)═B^- canonical form in the title compound.

3D view



Chemical scheme



Structure description

The title compound, $C_{20}H_{24}BNO_2$, has a hybrid π-conjugated system within the N—C(H)═C(H)—B fragment. The insertion of a π-conjugated system in the N—B bond affords a highly polarized π-system owing to the contribution of an ionic canonical structure, *i.e.* N^+═C(H)—C(H)═B^-. The contribution of the ionic canonical structure is small when *p*-phenylene is inserted into the N—B bond (Yuan *et al.*, 2006). However, when a C≡C bond is inserted into the N—B bond (Onuma *et al.*, 2015), a relatively large contribution of the ionic canonical structure is apparent. The structure of the C═C bond inserted system, namely 9-[(*E*)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethenyl]-9*H*-carbazole has been reported (Hatayama & Okuno, 2012). In the title compound, the carbazole unit of the former is replaced by a diphenylamino residue (Fig. 1).

The dihedral angles between the C13/C14/B1/N1 plane (r.m.s. deviation 0.0223 Å) and the N1/C1/C7/C13 (r.m.s. deviation 0.0025 Å) and B1/O1/O2/C14 (r.m.s. deviation 0.0044 Å) planes are 2.51 (12) and 3.09 (19)°, respectively, indicating the lone pair of the

OPEN ACCESS

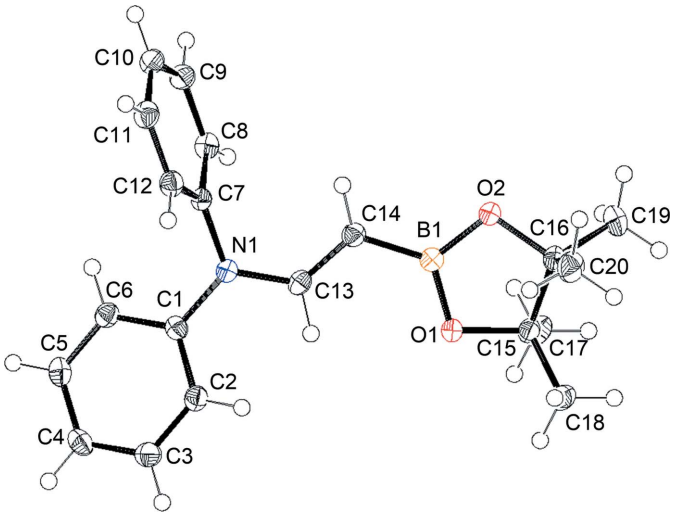


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level; H are atoms shown as small spheres.

nitrogen atom and a vacant *p* orbital of the boron are conjugated with the central C═C bond. The C13—N1 [1.3824 (19) Å] and C14—B1 [1.532 (2) Å] bonds are shortened, compared with those in the carbazole analogue of 1.396 (3) Å and 1.537 (3) Å, respectively; the central C═C bond at 1.341 (2) Å is experimentally equivalent to that of 1.336 (4) Å in the carbazolyl derivative. The results are well explained by the increase in the contribution of the N^{+}═C(H)—C(H)═B^{-} canonical structure in the title compound. This is presumably because the nitrogen atom of diphenylamino group donates its lone pair to the π-system more effectively compared to that of the carbazolyl group, which leads to a decrease in the contribution of the N^{+}═C(H)—C(H)═B^{-} canonical structure in the latter.

Synthesis and crystallization

The title compound was obtained by hydroboration of *N*-ethynyl-*N*-phenylaniline (Tokutome & Okuno, 2013) with 4,4,5,5-tetramethyl-1,3,2-dioxaborolane in 16% yield. ^{1}H NMR ($CDCl_3$): δ 1.25 (*s*, 12H), 4.17 (*d*, *J* = 15.6 Hz, 1H), 7.07 (*d*, *J* = 7.7 Hz, 4H), 7.12 (*t*, *J* = 7.7 Hz, 2H), 7.31 (*t*, *J* = 7.7 Hz, 4H), 7.64 (*d*, *J* = 15.6 Hz, 1H).

Single crystals were obtained by recrystallization from hexane solution.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{20}H_{24}BNO_2$
M_r	321.23
Crystal system, space group	Monoclinic, *C*2/*c*
Temperature (K)	93
a, *b*, *c* (Å)	32.071 (11), 6.011 (2), 22.219 (8)
β (°)	122.590 (4)
V (Å^3)	3609 (2)
Z	8
Radiation type	Mo *K*α
μ (mm^{-1})	0.07
Crystal size (mm)	0.13 × 0.11 × 0.05
Data collection	
Diffractometer	Rigaku Saturn724+
Absorption correction	Numerical (*NUMABS*; Rigaku, 1999)
T_{min}, T_{max}	0.991, 0.996
No. of measured, independent and observed [$F^2 > 2.0\sigma(F^2)$] reflections	13892, 3869, 3041
R_{int}	0.084
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.639
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.052, 0.147, 1.09
No. of reflections	3869
No. of parameters	217
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.27

Computer programs: *CrystalClear* (Rigaku, 2008), *CrystalStructure* (Rigaku, 2019), *SHELXS* and *SHELXL* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *publCIF* (Westrip, 2010).

Refinement

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

References

Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Hatayama, Y. & Okuno, T. (2012). *Acta Cryst.* E**68**, o84.
Onuma, K., Suzuki, K. & Yamashita, M. (2015). *Chem. Lett.* **44**, 405–407.
Rigaku (1999). *NUMABS*. Rigaku Corporation, Tokyo, Japan.
Rigaku (2008). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Rigaku (2019). *CrystalStructure*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Tokutome, Y. & Okuno, T. (2013). *J. Mol. Struct.* **1047**, 136–142.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Yuan, Z., Entwistle, C. D., Collings, J. C., Albesa-Jové, D., Batsanov, A. S., Howard, J. A. K., Taylor, N. J., Kaiser, H. M., Kaufmann, D. E., Poon, S. Y., Wong, W. Y., Jardin, C., Fathallah, S., Boucekkine, A., Halet, J. F. & Marder, T. B. (2006). *Chem. Eur. J.* **12**, 2758–2771.

full crystallographic data

IUCrData (2022). **7**, x220083 [https://doi.org/10.1107/S2414314622000839]

N-Phenyl-*N*-[(*E*)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethenyl]aniline

Yuki Hatayama, Kazuto Akagi and Tsunehisa Okuno

_N_-Phenyl-_N_-[(_E_)-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)ethenyl]aniline

Crystal data

$C_{20}H_{24}BNO_2$
M_r = 321.23
Monoclinic, $C2/c$
a = 32.071 (11) Å
b = 6.011 (2) Å
c = 22.219 (8) Å
β = 122.590 (4)°
V = 3609 (2) Å^3
Z = 8
$F(000)$ = 1376.00
D_x = 1.182 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71075 Å
Cell parameters from 5341 reflections
θ = 1.5–31.1°
μ = 0.07 mm^{-1}
T = 93 K
Prism, colourless
0.13 × 0.11 × 0.05 mm

Data collection

Rigaku Saturn724+ diffractometer
Detector resolution: 7.111 pixels mm^{-1}
ω scans
Absorption correction: numerical (NUMABS; Rigaku, 1999)
T_{min} = 0.991, T_{max} = 0.996
13892 measured reflections
3869 independent reflections
3041 reflections with $F^2 > 2.0\sigma(F^2)$
R_{int} = 0.084
θ_{max} = 27.0°, θ_{min} = 1.5°
h = −33→40
k = −7→7
l = −28→26

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.147
S = 1.09
3869 reflections
217 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
$w = 1/[\sigma^2(F_o^2) + (0.0758P)^2 + 0.8943P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 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. The U_{iso}(H) values were set at 1.2U_{eq}(C_{sp2}) and 1.5 U_{eq}(C_{sp3}).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.34742 (4)	0.98270 (18)	0.51068 (5)	0.0221 (3)
O2	0.41736 (4)	0.82168 (18)	0.60407 (5)	0.0218 (3)
N1	0.36028 (5)	0.6152 (2)	0.35305 (7)	0.0199 (3)
C1	0.32337 (5)	0.6584 (3)	0.28043 (8)	0.0190 (3)
C2	0.29881 (6)	0.8631 (3)	0.25973 (8)	0.0218 (3)
H2	0.3090	0.9801	0.2936	0.026*
C3	0.25961 (6)	0.8955 (3)	0.18984 (8)	0.0242 (4)
H3	0.2427	1.0342	0.1764	0.029*
C4	0.24475 (6)	0.7281 (3)	0.13936 (8)	0.0242 (4)
H4	0.2173	0.7497	0.0919	0.029*
C5	0.27059 (6)	0.5283 (3)	0.15912 (8)	0.0239 (4)
H5	0.2613	0.4146	0.1244	0.029*
C6	0.30963 (6)	0.4925 (3)	0.22861 (8)	0.0217 (3)
H6	0.3271	0.3555	0.2412	0.026*
C7	0.39973 (5)	0.4638 (2)	0.36945 (8)	0.0186 (3)
C8	0.40344 (6)	0.2606 (3)	0.40195 (8)	0.0220 (3)
H8	0.3798	0.2207	0.4133	0.026*
C9	0.44182 (6)	0.1166 (3)	0.41769 (8)	0.0237 (3)
H9	0.4446	−0.0221	0.4401	0.028*
C10	0.47629 (6)	0.1748 (3)	0.40080 (8)	0.0246 (4)
H10	0.5025	0.0757	0.4115	0.030*
C11	0.47247 (6)	0.3772 (3)	0.36832 (8)	0.0248 (4)
H11	0.4960	0.4166	0.3567	0.030*
C12	0.43426 (6)	0.5225 (3)	0.35273 (8)	0.0226 (3)
H12	0.4317	0.6617	0.3307	0.027*
C13	0.35865 (6)	0.7131 (2)	0.40803 (8)	0.0194 (3)
H13	0.3305	0.8029	0.3942	0.023*
C14	0.39193 (6)	0.6968 (3)	0.47847 (8)	0.0206 (3)
H14	0.4197	0.6011	0.4957	0.025*
C15	0.34973 (6)	1.0522 (3)	0.57530 (8)	0.0210 (3)
C16	0.40496 (6)	1.0063 (3)	0.63455 (8)	0.0226 (3)
C17	0.31353 (6)	0.9064 (3)	0.58176 (10)	0.0296 (4)
H17A	0.3140	0.9481	0.6247	0.036*
H17B	0.2801	0.9272	0.5396	0.036*
H17C	0.3232	0.7500	0.5851	0.036*
C18	0.33465 (6)	1.2945 (3)	0.56815 (9)	0.0261 (4)
H18A	0.3361	1.3421	0.6115	0.031*
H18B	0.3573	1.3857	0.5616	0.031*
H18C	0.3008	1.3124	0.5267	0.031*

C19	0.41396 (7)	0.9327 (3)	0.70589 (9)	0.0344 (4)
H19A	0.4058	1.0548	0.7270	0.041*
H19B	0.3931	0.8038	0.6988	0.041*
H19C	0.4488	0.8920	0.7380	0.041*
C20	0.43914 (6)	1.1987 (3)	0.64438 (10)	0.0311 (4)
H20A	0.4321	1.3267	0.6648	0.037*
H20B	0.4737	1.1530	0.6767	0.037*
H20C	0.4336	1.2400	0.5980	0.037*
B1	0.38529 (6)	0.8323 (3)	0.53116 (9)	0.0188 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0242 (6)	0.0246 (6)	0.0168 (6)	0.0045 (4)	0.0105 (5)	−0.0009 (4)
O2	0.0246 (6)	0.0227 (6)	0.0180 (6)	0.0047 (4)	0.0114 (5)	−0.0001 (4)
N1	0.0220 (7)	0.0207 (6)	0.0176 (6)	0.0024 (5)	0.0110 (6)	−0.0006 (5)
C1	0.0176 (7)	0.0236 (8)	0.0171 (7)	−0.0014 (6)	0.0101 (6)	0.0001 (6)
C2	0.0258 (8)	0.0213 (8)	0.0214 (8)	−0.0001 (6)	0.0149 (7)	−0.0009 (6)
C3	0.0248 (8)	0.0283 (8)	0.0242 (8)	0.0046 (6)	0.0164 (7)	0.0051 (6)
C4	0.0211 (8)	0.0338 (9)	0.0172 (8)	−0.0005 (6)	0.0101 (7)	0.0024 (6)
C5	0.0247 (8)	0.0298 (8)	0.0201 (8)	−0.0048 (6)	0.0139 (7)	−0.0042 (6)
C6	0.0239 (8)	0.0219 (8)	0.0233 (8)	0.0005 (6)	0.0154 (7)	−0.0004 (6)
C7	0.0178 (7)	0.0201 (7)	0.0159 (7)	0.0012 (6)	0.0077 (6)	−0.0024 (6)
C8	0.0215 (8)	0.0241 (8)	0.0224 (8)	−0.0025 (6)	0.0132 (7)	−0.0023 (6)
C9	0.0256 (8)	0.0209 (8)	0.0231 (8)	0.0005 (6)	0.0121 (7)	−0.0002 (6)
C10	0.0215 (8)	0.0267 (8)	0.0226 (8)	0.0024 (6)	0.0099 (7)	−0.0038 (6)
C11	0.0216 (8)	0.0312 (9)	0.0244 (8)	−0.0018 (6)	0.0143 (7)	−0.0035 (7)
C12	0.0253 (8)	0.0236 (8)	0.0206 (8)	−0.0007 (6)	0.0135 (7)	−0.0002 (6)
C13	0.0210 (8)	0.0183 (7)	0.0241 (8)	−0.0015 (6)	0.0155 (7)	−0.0021 (6)
C14	0.0202 (8)	0.0212 (7)	0.0216 (8)	0.0012 (6)	0.0121 (7)	−0.0011 (6)
C15	0.0252 (8)	0.0207 (7)	0.0203 (8)	0.0021 (6)	0.0143 (7)	−0.0009 (6)
C16	0.0272 (8)	0.0227 (8)	0.0195 (8)	0.0014 (6)	0.0136 (7)	−0.0011 (6)
C17	0.0329 (9)	0.0244 (8)	0.0404 (10)	−0.0022 (7)	0.0256 (8)	−0.0032 (7)
C18	0.0313 (9)	0.0214 (8)	0.0286 (9)	0.0041 (6)	0.0182 (8)	0.0009 (6)
C19	0.0430 (10)	0.0406 (10)	0.0193 (8)	0.0060 (8)	0.0166 (8)	0.0008 (7)
C20	0.0280 (9)	0.0308 (9)	0.0300 (9)	−0.0045 (7)	0.0127 (8)	−0.0091 (7)
B1	0.0193 (8)	0.0187 (8)	0.0203 (9)	−0.0020 (6)	0.0118 (7)	−0.0007 (6)

Geometric parameters (Å, º)

O1—B1	1.380 (2)	C10—H10	0.9500
O1—C15	1.4585 (18)	C11—C12	1.388 (2)
O2—B1	1.375 (2)	C11—H11	0.9500
O2—C16	1.4623 (18)	C12—H12	0.9500
N1—C13	1.3824 (19)	C13—C14	1.341 (2)
N1—C1	1.419 (2)	C13—H13	0.9500
N1—C7	1.4369 (19)	C14—B1	1.532 (2)
C1—C2	1.398 (2)	C14—H14	0.9500

C1—C6	1.403 (2)	C15—C18	1.516 (2)
C2—C3	1.388 (2)	C15—C17	1.522 (2)
C2—H2	0.9500	C15—C16	1.560 (2)
C3—C4	1.386 (2)	C16—C19	1.516 (2)
C3—H3	0.9500	C16—C20	1.526 (2)
C4—C5	1.390 (2)	C17—H17A	0.9800
C4—H4	0.9500	C17—H17B	0.9800
C5—C6	1.384 (2)	C17—H17C	0.9800
C5—H5	0.9500	C18—H18A	0.9800
C6—H6	0.9500	C18—H18B	0.9800
C7—C12	1.390 (2)	C18—H18C	0.9800
C7—C8	1.391 (2)	C19—H19A	0.9800
C8—C9	1.387 (2)	C19—H19B	0.9800
C8—H8	0.9500	C19—H19C	0.9800
C9—C10	1.390 (2)	C20—H20A	0.9800
C9—H9	0.9500	C20—H20B	0.9800
C10—C11	1.386 (2)	C20—H20C	0.9800

B1—O1—C15	107.10 (11)	N1—C13—H13	116.0
B1—O2—C16	107.02 (12)	C13—C14—B1	120.13 (14)
C13—N1—C1	121.41 (13)	C13—C14—H14	119.9
C13—N1—C7	119.53 (13)	B1—C14—H14	119.9
C1—N1—C7	119.05 (12)	O1—C15—C18	109.14 (12)
C2—C1—C6	118.90 (14)	O1—C15—C17	106.93 (13)
C2—C1—N1	120.80 (14)	C18—C15—C17	110.29 (13)
C6—C1—N1	120.25 (14)	O1—C15—C16	102.26 (12)
C3—C2—C1	120.12 (15)	C18—C15—C16	114.30 (13)
C3—C2—H2	119.9	C17—C15—C16	113.29 (13)
C1—C2—H2	119.9	O2—C16—C19	108.47 (13)
C4—C3—C2	120.84 (15)	O2—C16—C20	106.72 (13)
C4—C3—H3	119.6	C19—C16—C20	110.72 (14)
C2—C3—H3	119.6	O2—C16—C15	102.24 (12)
C3—C4—C5	119.03 (15)	C19—C16—C15	115.10 (14)
C3—C4—H4	120.5	C20—C16—C15	112.83 (13)
C5—C4—H4	120.5	C15—C17—H17A	109.5
C6—C5—C4	120.93 (15)	C15—C17—H17B	109.5
C6—C5—H5	119.5	H17A—C17—H17B	109.5
C4—C5—H5	119.5	C15—C17—H17C	109.5
C5—C6—C1	120.06 (15)	H17A—C17—H17C	109.5
C5—C6—H6	120.0	H17B—C17—H17C	109.5
C1—C6—H6	120.0	C15—C18—H18A	109.5
C12—C7—C8	120.28 (14)	C15—C18—H18B	109.5
C12—C7—N1	119.38 (14)	H18A—C18—H18B	109.5
C8—C7—N1	120.34 (13)	C15—C18—H18C	109.5
C9—C8—C7	119.68 (14)	H18A—C18—H18C	109.5
C9—C8—H8	120.2	H18B—C18—H18C	109.5
C7—C8—H8	120.2	C16—C19—H19A	109.5
C8—C9—C10	120.11 (15)	C16—C19—H19B	109.5

C8—C9—H9	119.9	H19A—C19—H19B	109.5
C10—C9—H9	119.9	C16—C19—H19C	109.5
C11—C10—C9	120.09 (15)	H19A—C19—H19C	109.5
C11—C10—H10	120.0	H19B—C19—H19C	109.5
C9—C10—H10	120.0	C16—C20—H20A	109.5
C10—C11—C12	120.06 (15)	C16—C20—H20B	109.5
C10—C11—H11	120.0	H20A—C20—H20B	109.5
C12—C11—H11	120.0	C16—C20—H20C	109.5
C11—C12—C7	119.77 (15)	H20A—C20—H20C	109.5
C11—C12—H12	120.1	H20B—C20—H20C	109.5
C7—C12—H12	120.1	O2—B1—O1	112.71 (13)
C14—C13—N1	127.95 (14)	O2—B1—C14	123.48 (14)
C14—C13—H13	116.0	O1—B1—C14	123.79 (14)
C13—N1—C1—C2	30.2 (2)	C1—N1—C13—C14	−176.36 (15)
C7—N1—C1—C2	−150.72 (14)	C7—N1—C13—C14	4.5 (2)
C13—N1—C1—C6	−147.37 (14)	N1—C13—C14—B1	175.57 (14)
C7—N1—C1—C6	31.7 (2)	B1—O1—C15—C18	145.27 (13)
C6—C1—C2—C3	3.7 (2)	B1—O1—C15—C17	−95.43 (14)
N1—C1—C2—C3	−173.86 (13)	B1—O1—C15—C16	23.86 (15)
C1—C2—C3—C4	−1.1 (2)	B1—O2—C16—C19	146.11 (14)
C2—C3—C4—C5	−1.8 (2)	B1—O2—C16—C20	−94.56 (14)
C3—C4—C5—C6	2.1 (2)	B1—O2—C16—C15	24.11 (14)
C4—C5—C6—C1	0.6 (2)	O1—C15—C16—O2	−28.89 (14)
C2—C1—C6—C5	−3.4 (2)	C18—C15—C16—O2	−146.69 (13)
N1—C1—C6—C5	174.15 (13)	C17—C15—C16—O2	85.81 (15)
C13—N1—C7—C12	−113.40 (16)	O1—C15—C16—C19	−146.25 (14)
C1—N1—C7—C12	67.48 (19)	C18—C15—C16—C19	95.96 (17)
C13—N1—C7—C8	66.41 (19)	C17—C15—C16—C19	−31.54 (19)
C1—N1—C7—C8	−112.71 (16)	O1—C15—C16—C20	85.36 (15)
C12—C7—C8—C9	0.0 (2)	C18—C15—C16—C20	−32.44 (18)
N1—C7—C8—C9	−179.76 (14)	C17—C15—C16—C20	−159.93 (13)
C7—C8—C9—C10	−0.2 (2)	C16—O2—B1—O1	−10.22 (17)
C8—C9—C10—C11	0.2 (2)	C16—O2—B1—C14	168.01 (14)
C9—C10—C11—C12	0.1 (2)	C15—O1—B1—O2	−9.76 (17)
C10—C11—C12—C7	−0.3 (2)	C15—O1—B1—C14	172.01 (14)
C8—C7—C12—C11	0.3 (2)	C13—C14—B1—O2	178.88 (14)
N1—C7—C12—C11	−179.94 (13)	C13—C14—B1—O1	−3.1 (2)