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

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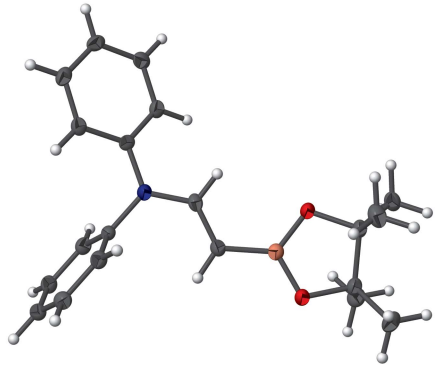
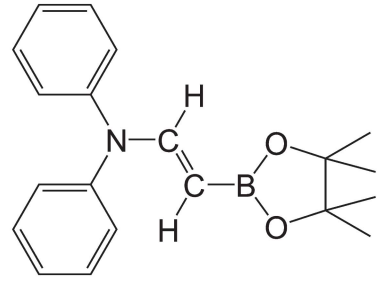
**Structural data**: full structural data are available from iucrdata.iucr.org

The title compound, $C_{20}H_{24}BNO_2$, has a polarized $\pi$-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 $\pi$-conjugated system within the N—C(H)═C(H)—B fragment. The insertion of a $\pi$-conjugated system in the N—B bond affords a highly polarized $\pi$-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

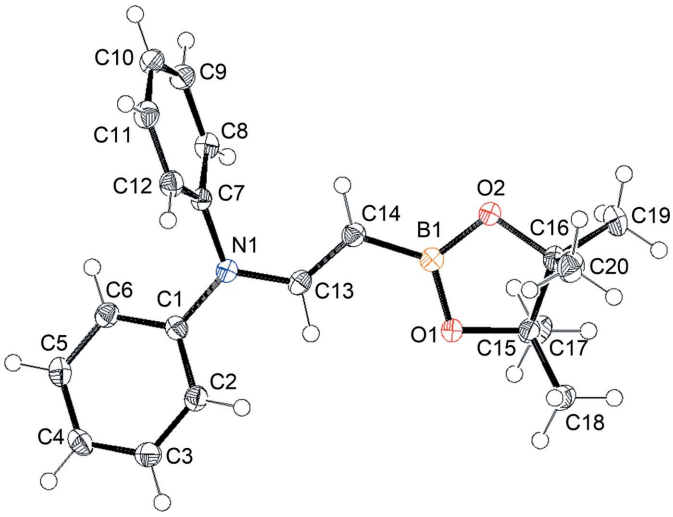



**Figure 1**
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level; H are atoms shown as small spheres.

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 $\pi$-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 ($CDCl_3$): $\delta$ 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) |
| $\beta$ (°) | 122.590 (4) |
| *V* (Å$^3$) | 3609 (2) |
| *Z* | 8 |
| Radiation type | Mo *K*$\alpha$ |
| $\mu$ (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.

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# full crystallographic data

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

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**_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
$\beta$ = 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, $\lambda$ = 0.71075 Å
Cell parameters from 5341 reflections
$\theta$ = 1.5–31.1°
$\mu$ = 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$^{-1}$
$\omega$ 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
$\theta_{max}$ = 27.0°, $\theta_{min}$ = 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 1.2$U_{eq}$($C_{sp2}$) 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 |

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| 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) |