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Structure determination of a bis[4-(di-*n*-butylamino)-phenyl](pyridin-3-yl)borane tetramer highlighting a unique geometric conformation of the core 16-membered ring

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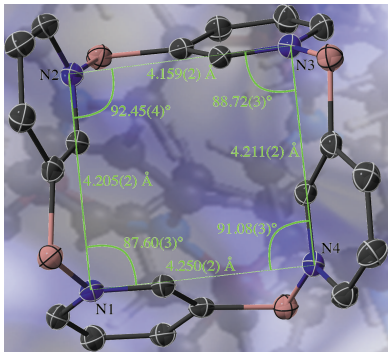
The tetramer of bis(4-di-*n*-butylaminophenyl)(pyridin-3-yl)borane [systematic name: $2\lambda^4,4\lambda^4,6\lambda^4,8\lambda^4$-tetrabora-1,3,5,7(1,3)-tetrapyridinacyclooctaphane-$1^1,3^1,5^1,7^1$-tetrakis(ylium)], $C_{132}H_{192}B_4N_{12}$, was synthesized unexpectedly and crystallized. Its structure contains an unusual 16-membered ring core made up of four (pyridin-3-yl)borane groups. The ring adopts a conformation with pseudo-S_4 symmetry that is very different from the two other reported examples of this ring system. Density functional theory (DFT) computations indicate that the stability of the three reported ring conformations is dependent on the substituents on the B atoms, and that the pseudo-S_4 geometry observed in the bis(4-dibutylamino-phenyl)(pyridin-3-yl)borane tetramer becomes significantly more stable when phenyl or 2,6-dimethylphenyl groups are attached to the boron centers.

1. Introduction

The field of organocatalysis has seen huge growth in recent decades as a greener alternative to the use of traditional metal-based catalysts (Krištofíková *et al.*, 2020). Previous work in our group has shown that the inclusion of charged sites in organocatalysts can significantly increase their catalytic activity (Samet *et al.*, 2015; Fan & Kass, 2016; Ma & Kass, 2016). An ongoing effort in our research has been the development of negatively charged Bronsted/Lewis base catalysts through the inclusion of various anionic borate groups. This general concept was demonstrated previously by Helberg *et al.* (2020), where an anionic sulfonamide substituent greatly enhanced reactivity. We are currently investigating a family of triaryl(pyridin-3-yl)borate catalysts derived from the reaction of trifluoro(pyridin-3-yl)borate with various arylmagnesium bromides (Fig. 1). When using [4-(dibutylamino)phenyl]magnesium bromide as the nucleophile, the expected triaryl(pyridin-3-yl)borate was not obtained from the reaction. Instead, **1**, a tetramer of bis[4-(di-*n*-butylamino)phenyl](pyridin-3-yl)borane, was isolated (Scheme 1). At the core of this compound is a 16-membered ring comprised of four (pyridin-3-yl)borane groups. A survey of the Cambridge Structural Database (CSD; Version 5.43, with June 2022 updates; Groom *et al.*, 2016) revealed that this core ring system has been reported twice previously, but with very different conformational geometries than observed in **1**.

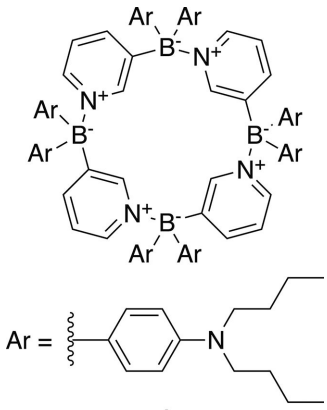


2. Experimental

2.1. Synthesis and crystallization

In a two-necked round-bottomed flask equipped with a septum and an addition funnel, freshly burnished magnesium

turnings (224 mg, 9.21 mmol, 5.11 equiv.) were suspended in tetrahydrofuran (THF, 10 ml) under argon and 4 drops of dibromoethane were added as an initiator. Upon warming to



1
Scheme 1

313 K, 1-bromo-4-(di-*n*-butylamino)benzene (2.56 g, 9.01 mmol, 5.01 equiv.) dissolved in THF (10 ml) was added dropwise over a period of 30 min. After stirring for an additional 4 h, during which time the magnesium was consumed, the reaction mixture was cooled to 273 K and potassium trifluoro(pyridin-3-yl)borate (Petruzziello *et al.*, 2013) (333 mg, 1.80 mmol, 1.00 equiv.) was added in one portion. The resulting solution was allowed to warm to room temperature over the course of 1 h and then refluxed for 14 h. It was subsequently quenched at room temperature with concentrated aqueous K_2CO_3 (10 ml) and extracted twice with dichloromethane (DCM, 2 × 50 ml). The combined DCM layers were concentrated and the residual material dissolved in the minimal amount of DCM. This solution was then triturated into ethyl acetate (100 ml) and became milky looking, but upon filtration the orange–white product changed rapidly to a dark-red waxy solid. This waxy material was dissolved in ethyl acetate and, upon standing for one week, white crystals (yield: 85 mg, 0.043 mmol, 2%) of **1** formed. ^{1}H NMR spectroscopic analysis of the crude material showed no evidence of the formation of the desired triarylborate and the low isolated yield is due to losses during the crystallization process since the product is

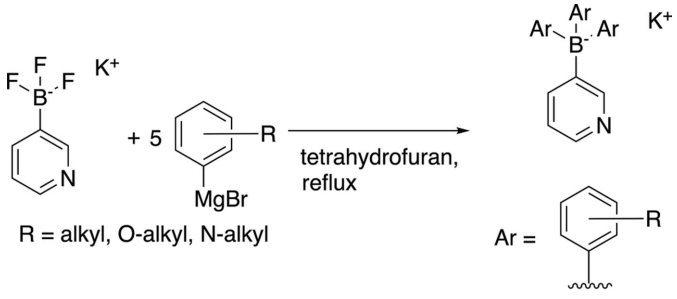


Figure 1
The reaction used to synthesize **1**. On the right is the expected product of the reaction.

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{132}H_{192}B_4N_{12}$
M_r	1990.22
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	130
a, b, c (Å)	15.5952 (11), 15.7968 (11), 25.7779 (15)
α, β, γ (°)	74.729 (2), 85.878 (2), 89.857 (2)
V (Å^3)	6109.5 (7)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.06
Crystal size (mm)	0.15 × 0.05 × 0.05
Data collection	
Diffractometer	Bruker Photon-III CPAD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.709, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	181628, 25030, 19004
R_{int}	0.043
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.140, 1.02
No. of reflections	25030
No. of parameters	1446
No. of restraints	20
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.84, −0.31

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2016), *SHELXT2018* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *ShelXle* (Hübschle *et al.*, 2011), and *Mercury* (Macrae *et al.*, 2020).

relatively soluble in ethyl acetate. The ^{1}H and ^{13}C NMR spectra of **1** are provided in the supporting information.

2.2. Refinement

All H atoms were placed in ideal positions with the following bond lengths: 0.95 Å for aromatic C—H bonds, 0.99 Å for methylene C—H bonds, and 0.98 Å for methyl C—H bonds. H atoms were refined as riding atoms with relative isotropic displacement parameters set at 1.2 times (methylene H atoms) and 1.5 times (methyl H atoms) the U_{eq} value of the atom to which they are attached. The reflections $1\overline{2}3$ and 102 were omitted due to suspected interference from the beamstop. The largest remaining Fourier peak has a value of 0.84 e Å^{-3} and is located at 0.676, 0.972, 0.012. This peak is located between two disordered butyl groups and the closest atom is C130, which is 1.084 Å away. The peak is most likely the result of the disorder of the *n*-butyl groups. For each of the disordered *n*-butyl groups, the C atoms making up the lesser occupied part have their bond lengths and angles restrained to those of the more abundant part (SAME restraint). Due to their proximity in space, the same isotropic or anisotropic displacement parameters are used for all the following pairs of atoms (EADP constraint): C30/C30′, C31/C31′, C33/C32′, C63/C63, C64/C65′, C66/C66′, C99/C99′, C125/C133′, C128/C136, C129/C137, and C132/C140. In total, 20 restraints were added. See Section 3.1 for more details

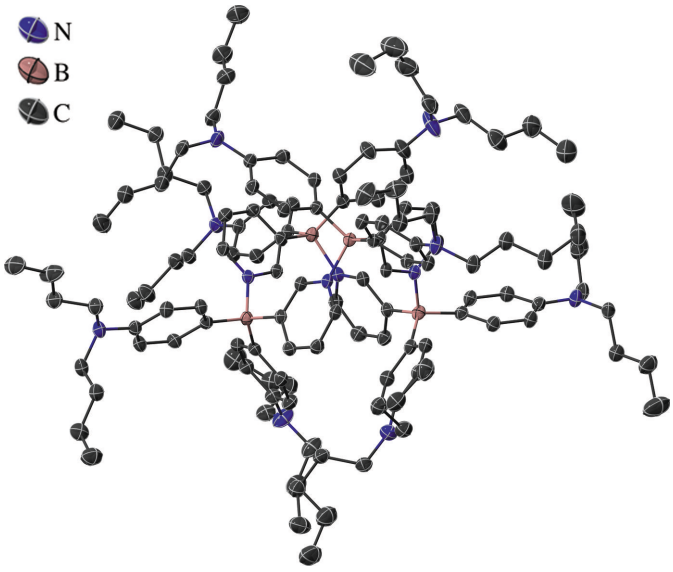


Figure 2
The crystal structure of **1**, with atoms drawn as displacement ellipsoids at the 50% probability level. Only the major parts of the disordered fragments are shown and H atoms have been omitted for clarity.

about the disorder. Additional crystal and refinement information is provided in Table 1.

2.3. Computational details

12 model compounds were generated using the crystallographic coordinates for the core rings of the bis[4-(di-*n*-butylamino)phenyl](pyridin-3-yl)borane (**1**), diethyl(pyridin-3-yl)borane (**2**; Sugihara *et al.*, 1994) and dimethyl(pyridin-3-yl)borane (**3**; Wakabayashi *et al.*, 2008) tetramers as the starting points for the initial structures, and either two methyl, phenyl, 2,6-dimethylphenyl, or *tert*-butyl groups were added to each B atom using the *GaussView* computer program (Dennington *et al.*, 2016). All 12 structures were fully optimized using *GAUSSIAN16* (Frisch *et al.*, 2016) with the M06-2X functional (Zhao & Truhlar, 2008) and the 6-31+G(d) (Hehre *et al.*, 1986) basis set with D3 empirical dispersion corrections (Grimme *et al.*, 2010). Vibrational frequencies were then computed for each species, and all 12 compounds were found to correspond to energy minima (*i.e.* they only have positive vibrational frequencies).

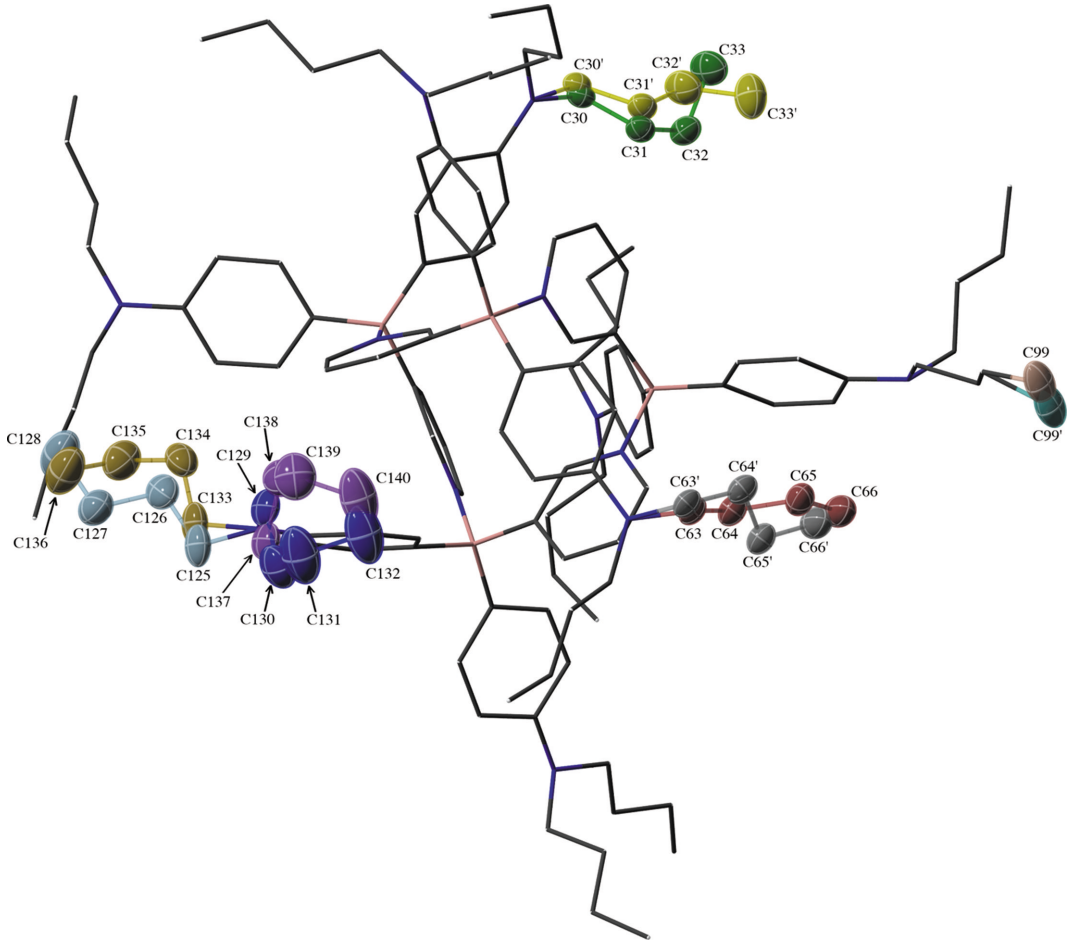


Figure 3
An image highlighting the disorder present in the crystal structure of **1**, where the nondisordered parts of the molecule are drawn as wireframes and H atoms have been omitted for clarity. The atoms are drawn as displacement ellipsoids at the 50% probability level. Each highlighted color (green, yellow, red, grey, teal, pink, blue, purple, light blue, and brown) represents a different disordered part with partial occupancy.

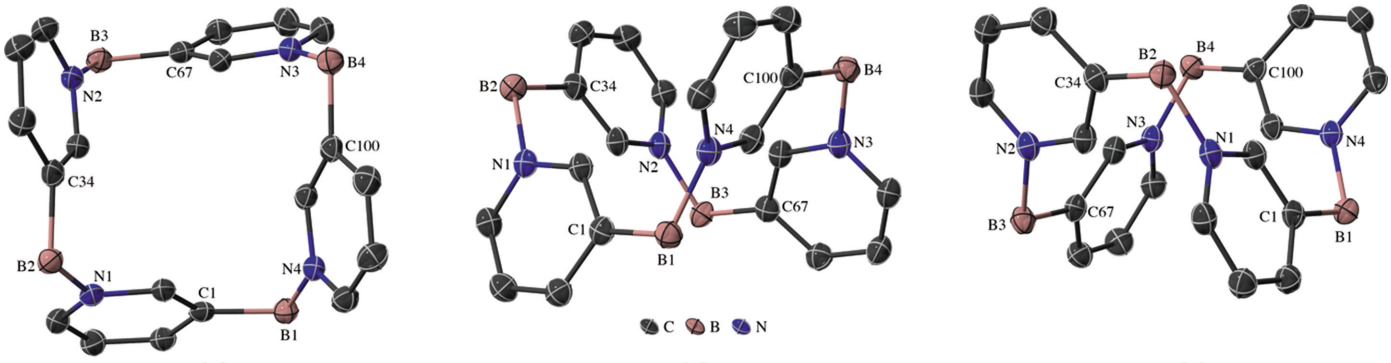


Figure 4
Three different views of the core ring structure of **1**, with atoms drawn as displacement ellipsoids at the 50% probability level and H atoms omitted for clarity.

3. Results and discussion

3.1. Structural features

Tetramer **1** crystallizes in the space group $P\overline{1}$ with $Z = 2$ and $Z' = 1$ (Fig. 2). There is some disorder present in the structure, which is not unexpected considering the molecule has 16 *n*-butyl groups, as well as the relatively high data collection temperature (130 K). Each disordered fragment has been modeled in two partially occupied parts. The first of these is an *n*-butyl group consisting of atoms C30–C33 and C30′–C33′, with occupancies of 71.7 (4) and 28.3 (4)%, respectively (Fig. 3, green and yellow highlights). The second disordered fragment is a different *n*-butyl group containing atoms C63–C66 and C63′–C66′ with respective occupancies of 81.6 (3) and 18.4 (3)% (Fig. 3, red and gray highlights). Another disordered section is a terminal methyl group consisting of atoms C99 and C99′, along with two sets of methylene H atoms on C98. These occupancies are 59.3 (15)% for C99, H98*A*, and H98*B*, and 40.7 (15)% for C99′, H98*C*, and H98*D* (Fig. 3, teal and pink highlights). A fourth disordered part is the *n*-butyl group represented by atoms C125–C128 and C133–C136, with occupancies of 63.5 (5) and 36.5 (5)%, respectively (Fig. 3, light-blue and brown highlights). The final area of disorder is the *n*-butyl group made up of C129–C132 and C137–C140, with respective occupancies of 71.7 (4) and 28.3 (4)% (Fig. 3, dark-blue and purple highlights).

The most interesting part of the structure of **1** is the core 16-membered ring comprised of four (pyridin-3-yl)borate groups (Fig. 4). It adopts a square-shaped conformation that has near S_4 symmetry. This can be seen by first noting that the four N atoms lie in a plane and form an approximate square which has the following side lengths and angles: N1···N2 = 4.205 (2) Å, N2···N3 = 4.159 (2) Å, N3···N4 = 4.211 (2) Å, N4···N1 = 4.250 (2) Å, N1—N2—N3 = 92.45 (4)°, N1—N4—N3 = 91.08 (3)°, N2—N1—N4 = 87.60 (3)°, and N2—N3—N4 = 88.72 (3)° (Fig. 5). The distances between diagonally related N atoms are N1···N3 = 6.039 (2) Å and N2···N4 = 5.852 (2) Å. Two diagonally related B atoms are located above the plane formed by the four N atoms and the other pair of diagonally related B atoms are located below it. The distances between adjacent and diagonally related B atoms are as follows: B1···B2 = 5.194 (3) Å, B2···B3 = 5.227 (2) Å, B3···B4 = 5.204 (2) Å, B4···B1 = 5.224 (3) Å, B1···B3 = 6.160 (3) Å, and B2···B4 = 6.357 (2) Å. If the ring system had true S_4 symmetry, the distances between the adjacent and diagonally related pairs of B and N atoms would be identical, and the angles in the square formed by the N atoms would all be 90°. This is not the case, but the deviations are relatively small and the structure has pseudo-S_4 symmetry.

The pyridine rings in the core of **1** are arranged in a similar manner to the B atoms, with two of them primarily located above the plane of the four N atoms and the other two largely below it. Each pyridine ring is also tilted away from the center of the 16-membered core, giving a 'bowl' shape to the ring structure.

3.2. Intermolecular interactions and Hirshfeld analysis

The two molecules of **1** in the unit cell appear to primarily interact through van der Waals interactions between alkyl

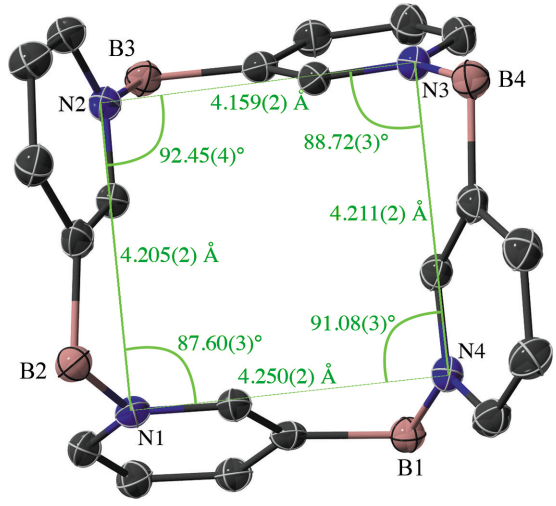


Figure 5
An image of the core 16-membered ring of **1**, showing the angles and side lengths of the approximate square made by the four N atoms. Atoms are drawn as displacement ellipsoids at the 50% probability level. B, N, and C atoms are colored pink, blue, and black, respectively.

Table 2
Absolute and relative zero-point corrected electronic energies of the fully optimized core ring structures **1**–**3** with two methyl, phenyl, 2,6-dimethylphenyl, or *tert*-butyl substituents attached to each B atom.

Core ring conformation	Optimized energy, methyl substituents (kcal mol^{-1})	Optimized energy, phenyl substituents (kcal mol^{-1})	Optimized energy, 2,6-dimethylphenyl substituents (kcal mol^{-1})	Optimized energy, *tert*-butyl substituents (kcal mol^{-1})
1	−883814.07	−1845754.34	−2239939.24	−1475072.98
2	−883814.34	−1845743.07	−2239927.90	−1475090.07
3	−883814.16	−1845743.15	−2239926.22	−1475096.90
Energy differences				
1–**2**	0.27	−11.27	−11.34	17.09
1–**3**	0.09	−11.19	−13.02	23.92
2–**3**	−0.18	0.08	−1.68	6.83

groups. To confirm this, the Hirshfeld surface (Spackman & Jayatilaka, 2009) of **1** was calculated and colored based on the d_{norm} parameter using the *CrystalExplorer* software package (Fig. 6) (Spackman *et al.*, 2021). It indicates that the closest intermolecular contacts in the crystal are between atoms H99*A* and H13*W*^{i} [symmetry code: (i) $-x$, $-y+1$, $-z+2$], with a distance of 1.546 Å. Analysis of the fingerprint plots of the Hirshfeld surface (Fig. 7) indicate that H···H contacts account for 88.3% of the contacts on the surface, with C···H/H···C contacts accounting for 10.7% and N···H/H···N interactions accounting for the remaining 1.0%. The area in the lower left of the plot corresponding to low d_i and d_e values shows four notable spikes indicative of close contacts between H atoms. These data are consistent with the van der Waals contacts being the primary interactions between molecules in the crystal.

3.3. Database survey

The Cambridge Structural Database (CSD) was surveyed using the WebCSD search tool (Groom *et al.*, 2016). Two structures containing 16-membered (pyridin-3-yl)borane tetramer rings were reported previously by Sugihara and Wakabayashi in the crystal structures of diethyl(pyridin-3-yl)borane (**2**; CSD refcode POGKAX; Sugihara *et al.*, 1994) and dimethyl(pyridin-3-yl)borane tetramers (**3**; CSD refcode YIVFOZ; Wakabayashi *et al.*, 2008), respectively. In these two structures, the core 16-membered ring adopts slightly different conformations, with the ring system for **2** possessing twofold rotational symmetry and a 'cone' shape [Fig. 8(*a*)], whereas **3** has inversion symmetry and a 'paddle' shape [Fig. 8(*b*)]. These compounds differ only slightly in their chemical compositions, with **2** having two ethyl groups attached to each of the B atoms, whereas there are methyl groups in **3**. In the conformations of both **2** and **3**, the B atoms are all located in the same plane, and form an approximate rectangle. The positions of the pyridine rings within the cores of **2** and **3** are relatively similar, with the main difference being the orientation of the pyridine rings with respect to the plane formed by the B atoms. In compound **2**, the majority of all four pyridine rings are located to one side of the plane formed by the B atoms. For **3**, the majority of rings *E* and *F* are located outside and on

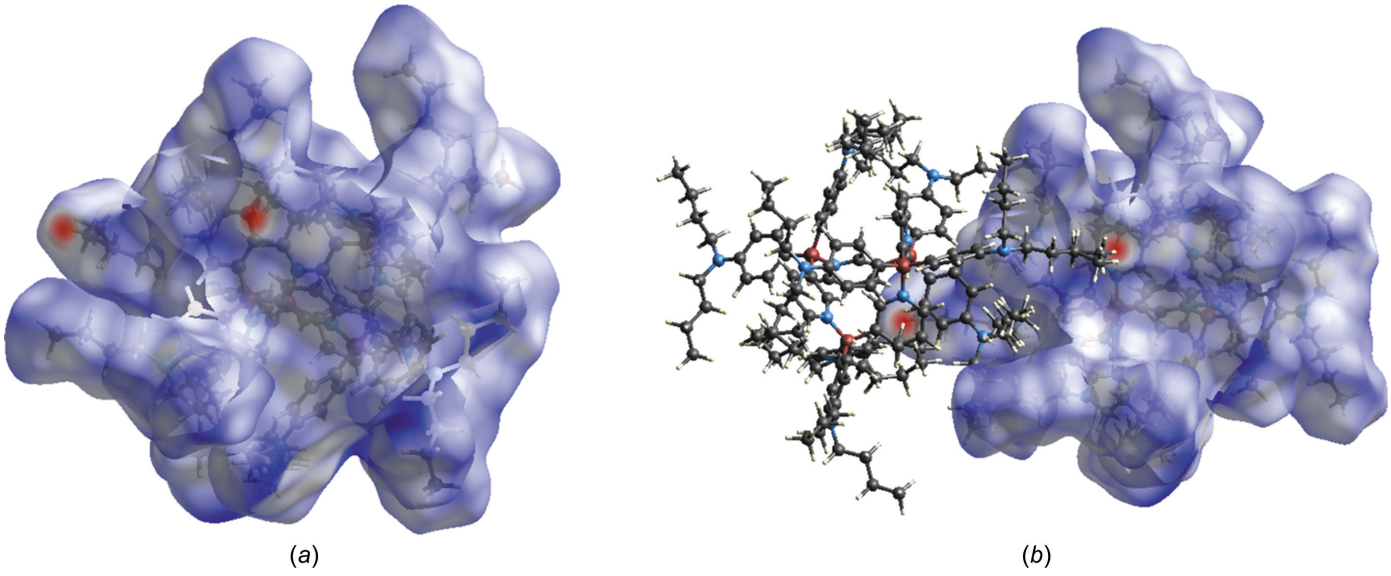


Figure 6
(*a*) Hirshfeld surface (d_{norm}) of **1** and (*b*) an image showing the interactions of the surface with an adjacent molecule. C atoms are illustrated in black, N atoms are given in blue, B atoms are shown in red, and all of the atoms are drawn as fixed-size balls.

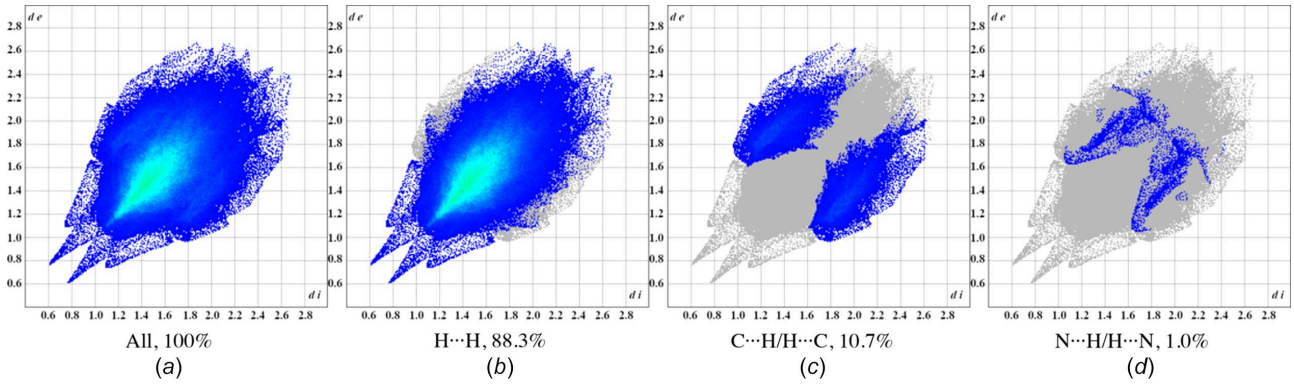


Figure 7
Fingerprint plots of (*a*) the entire Hirshfeld surface of **1**, (*b*) H···H contacts, (*c*) C···H/H···C contacts, and (*d*) N···H/H···N contacts.

opposite sides of the plane formed by the B atoms, while rings *G* and *H* are located within this plane. Overall, the core rings of **2** and **3** are much more similar in shape to one another than **1**.

3.4. Computations

In order to investigate the conformational differences between the core rings of **1**, **2**, and **3**, gas-phase density functional theory (DFT) computations were carried out on all three conformers. At first glance, the differences in conformation appear to be sterically driven. Compounds **2** and **3** have small alkyl substituents and similar conformations, whereas **1** has a much larger 4-(dibutylamino)phenyl substituent, causing the core ring to contort to the observed geometry. 12 model structures were created and optimized using the methods outlined in Section 2.3. Their energies are summarized in Table 2 and show that when methyl groups are attached to the B atoms, the energies of each ring system are nearly the same (*i.e.* within 0.3 kcal mol^{-1} of each other). When larger phenyl rings are used, the ring conformation in **1** is found to be approximately 11 kcal mol^{-1} more stable than those for both **2** and **3**. The same thing is observed when 2,6-dimethylphenyl rings are present, with **1** being more stable than **2** and **3** by approximately 11 and 13 kcal mol^{-1}, respectively. However, when the substituents on boron are *tert*-butyl groups, a significant change in the stability of the ring conformations is observed, with **3** being nearly 7 and 24 kcal mol^{-1} more stable than **2** and **1**, respectively.

To help explain the favorable energies of the conformation seen in **1** when phenyl and 2,6-dimethylphenyl groups are present, the crystal structure of **1** and computed structures containing the phenyl and 2,6-dimethylphenyl substituents for conformations **1**, **2**, and **3** were examined for the presence of intramolecular C—H···π interactions between H atoms located *ortho* to the pyridine N atoms on the core ring and the π-systems of the aryl substituents. These contacts between the electron-poor H atoms and electron-rich aromatic C atoms could be indicative of a stabilizing interaction that could explain the stability of **1** relative to **2** and **3**. Several close contacts in the range 2.299–2.987 Å were observed in all of the structures. The number and distances of these contacts in each of the structures, however, do not correlate with the computed energy differences. Based on this, it seems more likely that

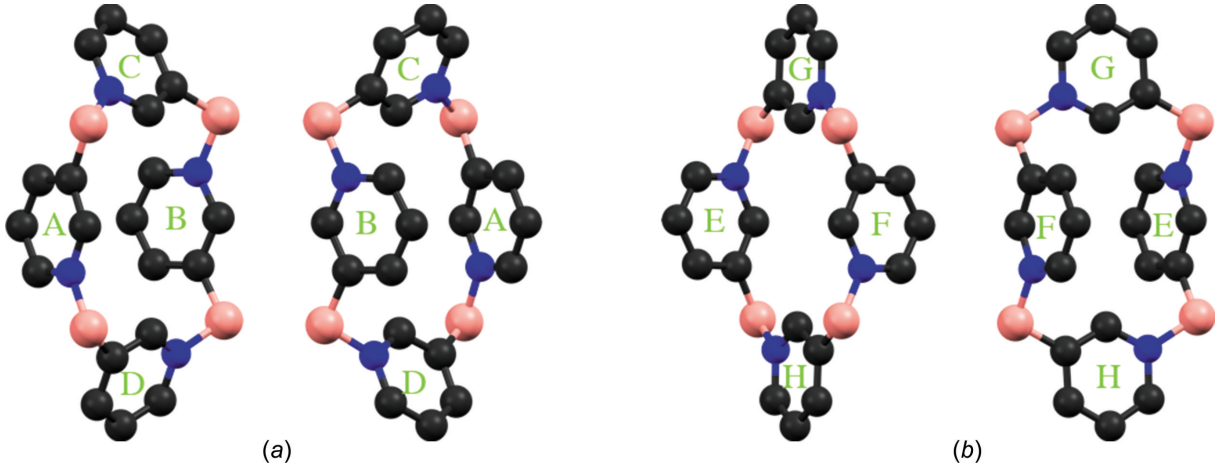


Figure 8
Two views of the core ring systems of (*a*) the diethyl(pyridin-3-yl)borane tetramer (**2**; Sugihara *et al.*, 1994) and (*b*) the dimethyl(pyridin-3-yl)borane tetramer (**3**; Wakabayashi *et al.*, 2008). Atoms are drawn as fixed-size colored balls with B, N, and C atoms in pink, blue, and black, respectively. The alkyl substituents (methyl and ethyl) have been omitted for clarity to highlight the ring conformations.

these close contacts are the result of the steric demands of the system rather than attractive C—H$\cdots\pi$ interactions that determine the conformation. The computations also reveal that the conformation of the 16-membered core ring system is affected by the substituents that are present on the B atoms, and that when they are phenyl and 2,6-dimethylphenyl, the specific steric environment of the system results in the conformation observed in **1** being the most stable.

4. Conclusions

The tetramer of bis[4-(di-*n*-butylamino)phenyl](pyridin-3-yl)-borane exhibits a pseudo-S_4 conformation of the core 16-membered ring that is very different from the two previously reported conformations of this ring. Computations determined that when methyl groups are present on the B atoms of the tetramer, the three reported ring conformations are all roughly equal in energy. When phenyl and 2,6-dimethylphenyl groups are present on the B atoms, the pseudo-S_4 ring conformation observed in **1** is more stable than the other two conformations by approximately 11 and 12 kcal mol^{-1}, respectively. Observations of intramolecular contacts of the crystal and computed structures suggest that this stability is due to the unique steric environment present when phenyl and 2,6-dimethylphenyl substituents are present on the core 16-membered ring rather than attractive intramolecular C—H$\cdots\pi$ interactions

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supporting information

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Structure determination of a bis[4-(di-*n*-butylamino)phenyl](pyridin-3-yl)borane tetramer highlighting a unique geometric conformation of the core 16-membered ring

Alex Lovstedt, Stephen H. Dempsey and Steven R. Kass

Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: SHELXT2018 (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015*b*); molecular graphics: ShelXle (Hübschle *et al.*, 2011) and *Mercury* (Macrae *et al.*, 2020); software used to prepare material for publication: *SHELXL2018* (Sheldrick, 2015*b*).

2,2,8,8,14,14,20,20-Octakis[4-(dibutylamino)phenyl]-1,7,13,19-tetraaza-2,8,14,20-tetraborapentacyclo[19.3.1.1^{3,7}.1^{9,13}.1^{15,19}]octacosa-1(25),3,5,7(28),9(27),10,12,15(26),16,18,21,23-dodecaene-1,7,13,19-tetrakis(ylium)

Crystal data

$C_{132}H_{192}B_4N_{12}$
M_r = 1990.22
Triclinic, $P\overline{1}$
a = 15.5952 (11) Å
b = 15.7968 (11) Å
c = 25.7779 (15) Å
α = 74.729 (2)°
β = 85.878 (2)°
γ = 89.857 (2)°
V = 6109.5 (7) Å^3
Z = 2
$F(000)$ = 2176
D_x = 1.082 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9627 reflections
θ = 2.6–26.4°
μ = 0.06 mm^{-1}
T = 130 K
Rod, white
0.15 × 0.05 × 0.05 mm

Data collection

Bruker Photon-III CMOS diffractometer
Radiation source: micro
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.709, T_{max} = 0.745
181628 measured reflections
25030 independent reflections
19004 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 26.4°, θ_{min} = 1.9°
h = −19→19
k = −19→19
l = −32→32

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.140$
$S = 1.02$
25030 reflections
1446 parameters
20 restraints

Primary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0604P)^2 + 3.2856P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.84$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
N1	0.45468 (8)	0.44718 (8)	0.70760 (5)	0.0236 (3)	
N2	0.23259 (8)	0.28934 (8)	0.72351 (5)	0.0228 (3)	
N3	0.07865 (8)	0.47031 (8)	0.77590 (5)	0.0222 (3)	
N4	0.30026 (8)	0.62560 (8)	0.76940 (5)	0.0221 (3)	
N5	0.35408 (9)	0.00188 (9)	0.60062 (6)	0.0328 (3)	
N6	−0.03377 (9)	0.52372 (10)	0.56259 (6)	0.0336 (3)	
N7	−0.26174 (9)	0.20726 (9)	0.84934 (6)	0.0309 (3)	
N8	0.20919 (10)	0.52450 (10)	0.99154 (6)	0.0365 (3)	
N9	0.46396 (10)	0.72407 (13)	0.52673 (6)	0.0463 (4)	
N10	0.09181 (9)	0.97890 (9)	0.79526 (6)	0.0307 (3)	
N11	0.81683 (8)	0.63631 (9)	0.75295 (6)	0.0284 (3)	
N12	0.41039 (13)	0.08478 (11)	0.88908 (9)	0.0623 (6)	
C1	0.35040 (10)	0.38926 (10)	0.65917 (6)	0.0238 (3)	
C2	0.38154 (10)	0.40186 (10)	0.70570 (6)	0.0238 (3)	
H2	0.349182	0.376819	0.738856	0.029*	
C3	0.50038 (10)	0.48429 (11)	0.66100 (7)	0.0288 (3)	
H3	0.551350	0.516813	0.661460	0.035*	
C4	0.47457 (11)	0.47597 (12)	0.61245 (7)	0.0323 (4)	
H4	0.507509	0.502811	0.579808	0.039*	
C5	0.40069 (10)	0.42849 (11)	0.61145 (7)	0.0290 (3)	
H5	0.383631	0.422271	0.577980	0.035*	
C6	0.29149 (10)	0.24482 (10)	0.63686 (6)	0.0246 (3)	
C7	0.37453 (10)	0.21150 (11)	0.63784 (6)	0.0270 (3)	
H7	0.418936	0.244023	0.647633	0.032*	
C8	0.39576 (10)	0.13352 (11)	0.62529 (6)	0.0279 (3)	
H8	0.453753	0.114964	0.626229	0.034*	
C9	0.33312 (11)	0.08146 (11)	0.61122 (6)	0.0273 (3)	
C10	0.24923 (11)	0.11411 (11)	0.60936 (7)	0.0303 (4)	
H10	0.204644	0.081581	0.599755	0.036*	

C11	0.23037 (10)	0.19312 (11)	0.62132 (6)	0.0283 (3)
H11	0.172976	0.213250	0.618841	0.034*
C12	0.44413 (11)	−0.01704 (12)	0.58963 (7)	0.0339 (4)
H12A	0.473771	0.037806	0.568368	0.041*
H12B	0.447114	−0.059227	0.567186	0.041*
C13	0.49196 (12)	−0.05453 (12)	0.63966 (8)	0.0358 (4)
H13A	0.467442	−0.113153	0.658697	0.043*
H13B	0.483803	−0.016037	0.664283	0.043*
C14	0.58747 (13)	−0.06267 (15)	0.62604 (9)	0.0486 (5)
H14A	0.611340	−0.004335	0.605833	0.058*
H14B	0.595449	−0.102597	0.602291	0.058*
C15	0.63719 (17)	−0.09730 (18)	0.67565 (12)	0.0704 (7)
H15A	0.698207	−0.101110	0.664558	0.106*
H15B	0.614859	−0.155711	0.695386	0.106*
H15C	0.630592	−0.057421	0.699001	0.106*
C16	0.28991 (11)	−0.04927 (11)	0.58304 (7)	0.0323 (4)
H16A	0.235307	−0.049269	0.605145	0.039*
H16B	0.309142	−0.110756	0.589959	0.039*
C17	0.27273 (13)	−0.01627 (12)	0.52402 (7)	0.0384 (4)
H17A	0.325208	−0.022688	0.501466	0.046*
H17B	0.259021	0.046887	0.515836	0.046*
C18	0.19874 (15)	−0.06634 (15)	0.50993 (8)	0.0514 (5)
H18A	0.213367	−0.129223	0.517451	0.062*
H18B	0.146985	−0.061358	0.533458	0.062*
C19	0.1780 (2)	−0.0339 (2)	0.45197 (10)	0.0803 (9)
H19A	0.130220	−0.068894	0.445333	0.120*
H19B	0.228634	−0.039627	0.428375	0.120*
H19C	0.161739	0.027838	0.444458	0.120*
C20	0.18520 (10)	0.38418 (10)	0.63082 (6)	0.0248 (3)
C21	0.10039 (10)	0.35123 (11)	0.64320 (6)	0.0274 (3)
H21	0.091696	0.294718	0.667553	0.033*
C22	0.02876 (11)	0.39562 (11)	0.62227 (7)	0.0290 (3)
H22	−0.026751	0.369671	0.633174	0.035*
C23	0.03706 (10)	0.47867 (11)	0.58505 (6)	0.0284 (3)
C24	0.12094 (11)	0.51334 (11)	0.57193 (7)	0.0303 (4)
H24	0.129818	0.569470	0.547168	0.036*
C25	0.19153 (11)	0.46733 (11)	0.59438 (6)	0.0287 (3)
H25	0.246966	0.493882	0.584389	0.034*
C26	−0.12116 (11)	0.48873 (13)	0.57824 (7)	0.0356 (4)
H26A	−0.120086	0.424146	0.584639	0.043*
H26B	−0.157409	0.512192	0.547851	0.043*
C27	−0.16267 (12)	0.51035 (13)	0.62848 (7)	0.0371 (4)
H27A	−0.166948	0.574873	0.621442	0.045*
H27B	−0.125041	0.489720	0.658475	0.045*
C28	−0.25227 (12)	0.46898 (14)	0.64590 (8)	0.0424 (4)
H28A	−0.284358	0.503065	0.667880	0.051*
H28B	−0.283781	0.472516	0.613413	0.051*
C29	−0.24960 (15)	0.37398 (15)	0.67822 (9)	0.0526 (5)

H29A	−0.308411	0.350741	0.688251	0.079*	
H29B	−0.219711	0.370148	0.710905	0.079*	
H29C	−0.218957	0.339597	0.656411	0.079*	
C30	−0.0200 (7)	0.6103 (5)	0.5246 (5)	0.0317 (12)	0.717 (4)
H30A	−0.069849	0.623449	0.502214	0.038*	0.717 (4)
H30B	0.031530	0.608263	0.500142	0.038*	0.717 (4)
C31	−0.0079 (2)	0.6851 (2)	0.55103 (13)	0.0347 (6)	0.717 (4)
H31A	−0.062291	0.693290	0.571249	0.042*	0.717 (4)
H31B	0.036880	0.668935	0.577089	0.042*	0.717 (4)
C32	0.01826 (18)	0.77113 (18)	0.50971 (11)	0.0406 (7)	0.717 (4)
H32A	0.031636	0.815325	0.529093	0.049*	0.717 (4)
H32B	0.071429	0.761783	0.488679	0.049*	0.717 (4)
C33	−0.0497 (2)	0.8074 (2)	0.47103 (14)	0.0546 (8)	0.717 (4)
H33A	−0.030710	0.865008	0.447964	0.082*	0.717 (4)
H33B	−0.103733	0.813339	0.491503	0.082*	0.717 (4)
H33C	−0.058491	0.767273	0.448579	0.082*	0.717 (4)
C30′	−0.032 (2)	0.6043 (13)	0.5201 (13)	0.0317 (12)	0.283 (4)
H30C	−0.084153	0.604413	0.500062	0.038*	0.283 (4)
H30D	0.018229	0.603251	0.494793	0.038*	0.283 (4)
C31′	−0.0292 (7)	0.6901 (6)	0.5358 (4)	0.0347 (6)	0.283 (4)
H31C	−0.080118	0.693266	0.560398	0.042*	0.283 (4)
H31D	0.022746	0.691762	0.555498	0.042*	0.283 (4)
C32′	−0.0274 (7)	0.7688 (6)	0.4873 (4)	0.0546 (8)	0.283 (4)
H32C	0.029101	0.771086	0.466788	0.066*	0.283 (4)
H32D	−0.071856	0.759592	0.463707	0.066*	0.283 (4)
C33′	−0.0418 (7)	0.8558 (5)	0.4987 (4)	0.066 (3)	0.283 (4)
H33D	−0.043127	0.901419	0.464644	0.099*	0.283 (4)
H33E	0.005046	0.868851	0.518985	0.099*	0.283 (4)
H33F	−0.096644	0.854289	0.520028	0.099*	0.283 (4)
C34	0.14902 (10)	0.31691 (10)	0.80023 (6)	0.0231 (3)	
C35	0.18464 (9)	0.34193 (10)	0.74752 (6)	0.0226 (3)	
H35	0.174735	0.399958	0.726809	0.027*	
C36	0.25196 (10)	0.20938 (10)	0.75307 (6)	0.0264 (3)	
H36	0.287125	0.172586	0.737015	0.032*	
C37	0.22172 (11)	0.17936 (11)	0.80659 (7)	0.0292 (3)	
H37	0.237099	0.123037	0.827374	0.035*	
C38	0.16883 (10)	0.23223 (10)	0.82951 (6)	0.0269 (3)	
H38	0.145627	0.210668	0.865716	0.032*	
C39	−0.01352 (10)	0.33029 (10)	0.83224 (6)	0.0234 (3)	
C40	−0.04077 (10)	0.28619 (10)	0.79550 (6)	0.0259 (3)	
H40	−0.001929	0.283525	0.765862	0.031*	
C41	−0.12094 (10)	0.24633 (11)	0.79989 (6)	0.0269 (3)	
H41	−0.135688	0.218266	0.773302	0.032*	
C42	−0.18054 (10)	0.24696 (10)	0.84316 (6)	0.0259 (3)	
C43	−0.15478 (10)	0.29019 (11)	0.88057 (6)	0.0289 (3)	
H43	−0.193362	0.292458	0.910395	0.035*	
C44	−0.07398 (10)	0.32985 (11)	0.87498 (6)	0.0271 (3)	
H44	−0.059178	0.358015	0.901510	0.033*	

C45	−0.28378 (11)	0.15538 (11)	0.81294 (7)	0.0323 (4)
H45A	−0.263537	0.187592	0.775695	0.039*
H45B	−0.347188	0.150010	0.814289	0.039*
C46	−0.24643 (12)	0.06348 (12)	0.82507 (8)	0.0360 (4)
H46A	−0.183057	0.068489	0.818720	0.043*
H46B	−0.260173	0.033535	0.863635	0.043*
C47	−0.28039 (13)	0.00776 (13)	0.79098 (8)	0.0430 (5)
H47A	−0.343999	0.006163	0.795371	0.052*
H47B	−0.263123	0.035611	0.752546	0.052*
C48	−0.24795 (17)	−0.08550 (14)	0.80565 (10)	0.0591 (6)
H48A	−0.273108	−0.118649	0.783092	0.089*
H48B	−0.264621	−0.113503	0.843692	0.089*
H48C	−0.185150	−0.084628	0.799643	0.089*
C49	−0.30765 (11)	0.18271 (11)	0.90288 (7)	0.0328 (4)
H49A	−0.264708	0.168826	0.930250	0.039*
H49B	−0.341681	0.128449	0.906270	0.039*
C50	−0.36762 (11)	0.25153 (12)	0.91586 (7)	0.0334 (4)
H50A	−0.334562	0.306293	0.912733	0.040*
H50B	−0.412205	0.264798	0.889538	0.040*
C51	−0.41037 (13)	0.21946 (16)	0.97242 (8)	0.0487 (5)
H51A	−0.442977	0.164642	0.974988	0.058*
H51B	−0.365039	0.205023	0.998196	0.058*
C52	−0.47054 (14)	0.28386 (17)	0.98924 (9)	0.0561 (6)
H52A	−0.495802	0.257870	1.025919	0.084*
H52B	−0.516388	0.297955	0.964414	0.084*
H52C	−0.438546	0.337609	0.988332	0.084*
C53	0.11199 (10)	0.40672 (10)	0.87565 (6)	0.0234 (3)
C54	0.18764 (10)	0.37951 (10)	0.90061 (6)	0.0262 (3)
H54	0.219169	0.333966	0.890664	0.031*
C55	0.21912 (11)	0.41570 (11)	0.93925 (7)	0.0298 (4)
H55	0.270497	0.393758	0.955225	0.036*
C56	0.17639 (11)	0.48393 (11)	0.95504 (6)	0.0280 (3)
C57	0.09824 (11)	0.50977 (11)	0.93228 (7)	0.0308 (4)
H57	0.065415	0.553640	0.943235	0.037*
C58	0.06842 (10)	0.47209 (11)	0.89406 (6)	0.0281 (3)
H58	0.015403	0.491694	0.879495	0.034*
C59	0.29786 (12)	0.50943 (13)	1.00615 (7)	0.0385 (4)
H59A	0.321686	0.564129	1.011717	0.046*
H59B	0.332496	0.495925	0.975696	0.046*
C60	0.30702 (12)	0.43568 (13)	1.05636 (7)	0.0399 (4)
H60A	0.281526	0.381334	1.051314	0.048*
H60B	0.274100	0.450077	1.087129	0.048*
C61	0.39953 (13)	0.41870 (15)	1.07006 (9)	0.0478 (5)
H61A	0.433407	0.408016	1.038483	0.057*
H61B	0.423948	0.471657	1.077581	0.057*
C62	0.40806 (14)	0.34103 (16)	1.11826 (9)	0.0542 (5)
H62A	0.469051	0.330611	1.124004	0.081*
H62B	0.381890	0.288847	1.111672	0.081*

H62C	0.378756	0.353306	1.150354	0.081*	
C63	0.1729 (2)	0.6047 (2)	0.99942 (14)	0.0351 (7)	0.816 (3)
H63A	0.190473	0.613085	1.033918	0.042*	0.816 (3)
H63B	0.109442	0.599409	1.002103	0.042*	0.816 (3)
C64	0.20152 (19)	0.68581 (16)	0.95344 (10)	0.0390 (6)	0.816 (3)
H64A	0.264888	0.692039	0.951696	0.047*	0.816 (3)
H64B	0.186052	0.676123	0.918841	0.047*	0.816 (3)
C65	0.16171 (18)	0.77057 (16)	0.95972 (10)	0.0453 (7)	0.816 (3)
H65A	0.167351	0.774801	0.996967	0.054*	0.816 (3)
H65B	0.099622	0.769226	0.954165	0.054*	0.816 (3)
C66	0.2033 (2)	0.8512 (2)	0.92030 (15)	0.0553 (8)	0.816 (3)
H66A	0.173580	0.903819	0.924849	0.083*	0.816 (3)
H66B	0.199154	0.846740	0.883356	0.083*	0.816 (3)
H66C	0.263892	0.855132	0.927250	0.083*	0.816 (3)
C63′	0.1536 (13)	0.5885 (10)	1.0108 (7)	0.0351 (7)	0.184 (3)
H63C	0.173594	0.592877	1.045666	0.042*	0.184 (3)
H63D	0.094425	0.563679	1.018213	0.042*	0.184 (3)
C64′	0.1493 (7)	0.6812 (6)	0.9743 (4)	0.037 (3)	0.184 (3)
H64C	0.123203	0.677891	0.940938	0.045*	0.184 (3)
H64D	0.110318	0.715524	0.992615	0.045*	0.184 (3)
C65′	0.2328 (7)	0.7300 (7)	0.9586 (4)	0.0390 (6)	0.184 (3)
H65C	0.272149	0.695967	0.940291	0.047*	0.184 (3)
H65D	0.258873	0.734286	0.991773	0.047*	0.184 (3)
C66′	0.2257 (12)	0.8217 (9)	0.9219 (8)	0.0553 (8)	0.184 (3)
H66D	0.282577	0.850337	0.914606	0.083*	0.184 (3)
H66E	0.186326	0.855846	0.939438	0.083*	0.184 (3)
H66F	0.203621	0.818050	0.887883	0.083*	0.184 (3)
C67	0.15617 (10)	0.60533 (10)	0.72923 (6)	0.0228 (3)	
C68	0.14629 (10)	0.52697 (10)	0.76921 (6)	0.0229 (3)	
H68	0.190058	0.511892	0.793679	0.028*	
C69	0.01745 (10)	0.48959 (10)	0.74076 (6)	0.0249 (3)	
H69	−0.029660	0.449924	0.744411	0.030*	
C70	0.02156 (10)	0.56578 (11)	0.69948 (7)	0.0279 (3)	
H70	−0.021937	0.578075	0.674688	0.033*	
C71	0.08941 (10)	0.62408 (10)	0.69446 (6)	0.0259 (3)	
H71	0.090904	0.677773	0.667000	0.031*	
C72	0.29224 (10)	0.69710 (10)	0.66771 (6)	0.0238 (3)	
C73	0.26748 (11)	0.67922 (11)	0.62059 (6)	0.0282 (3)	
H73	0.210442	0.658470	0.620304	0.034*	
C74	0.32201 (11)	0.69023 (12)	0.57408 (7)	0.0332 (4)	
H74	0.300519	0.679095	0.542906	0.040*	
C75	0.40789 (11)	0.71735 (11)	0.57218 (7)	0.0313 (4)	
C76	0.43432 (11)	0.73616 (11)	0.61873 (7)	0.0295 (3)	
H76	0.491841	0.755283	0.619406	0.035*	
C77	0.37764 (10)	0.72726 (10)	0.66390 (6)	0.0268 (3)	
H77	0.397895	0.742545	0.694183	0.032*	
C78	0.43613 (13)	0.70153 (15)	0.47962 (8)	0.0476 (5)	
H78A	0.395985	0.650507	0.491460	0.057*	

H78B	0.486716	0.683745	0.459761	0.057*
C79	0.39259 (14)	0.77513 (15)	0.44216 (8)	0.0505 (5)
H79A	0.430130	0.828226	0.432972	0.061*
H79B	0.338344	0.788773	0.460467	0.061*
C80	0.37286 (16)	0.75131 (17)	0.39026 (9)	0.0576 (6)
H80A	0.423347	0.722030	0.377652	0.069*
H80B	0.323883	0.708976	0.398348	0.069*
C81	0.35162 (19)	0.82855 (18)	0.34633 (10)	0.0710 (7)
H81A	0.334477	0.808811	0.315532	0.106*
H81B	0.402162	0.867564	0.335170	0.106*
H81C	0.304194	0.860251	0.359305	0.106*
C82	0.55271 (11)	0.75334 (13)	0.52321 (7)	0.0382 (4)
H82A	0.557695	0.793945	0.546302	0.046*
H82B	0.569687	0.786242	0.485559	0.046*
C83	0.61450 (13)	0.67740 (13)	0.54063 (8)	0.0457 (5)
H83A	0.598843	0.646112	0.578754	0.055*
H83B	0.607407	0.635479	0.518617	0.055*
C84	0.70860 (13)	0.70651 (15)	0.53493 (9)	0.0483 (5)
H84A	0.745321	0.654322	0.538788	0.058*
H84B	0.722017	0.745668	0.498358	0.058*
C85	0.72988 (15)	0.75412 (18)	0.57629 (10)	0.0604 (6)
H85A	0.791844	0.766632	0.573074	0.091*
H85B	0.713037	0.717257	0.612546	0.091*
H85C	0.698564	0.809335	0.570054	0.091*
C86	0.19466 (10)	0.76016 (10)	0.74279 (6)	0.0235 (3)
C87	0.22825 (10)	0.84600 (10)	0.72303 (6)	0.0271 (3)
H87	0.276391	0.855972	0.697292	0.033*
C88	0.19433 (11)	0.91678 (11)	0.73936 (7)	0.0301 (4)
H88	0.219806	0.973394	0.724725	0.036*
C89	0.12318 (10)	0.90648 (10)	0.77707 (6)	0.0268 (3)
C90	0.08814 (10)	0.82192 (11)	0.79708 (7)	0.0285 (3)
H90	0.039513	0.812154	0.822441	0.034*
C91	0.12368 (10)	0.75163 (10)	0.78026 (6)	0.0264 (3)
H91	0.098354	0.694983	0.795035	0.032*
C92	0.07361 (11)	1.05804 (11)	0.75278 (7)	0.0317 (4)
H92A	0.119713	1.066361	0.723326	0.038*
H92B	0.075503	1.109482	0.767844	0.038*
C93	−0.01267 (11)	1.05590 (12)	0.72905 (7)	0.0342 (4)
H93A	−0.016612	1.002630	0.715910	0.041*
H93B	−0.059426	1.052407	0.757664	0.041*
C94	−0.02495 (12)	1.13616 (13)	0.68299 (8)	0.0409 (4)
H94A	0.019818	1.137330	0.653555	0.049*
H94B	−0.016741	1.189370	0.695642	0.049*
C95	−0.11261 (14)	1.13915 (16)	0.66076 (9)	0.0517 (5)
H95A	−0.115385	1.190876	0.630042	0.078*
H95B	−0.157191	1.142523	0.688911	0.078*
H95C	−0.121935	1.085999	0.648955	0.078*
C96	0.02787 (12)	0.95835 (12)	0.84128 (7)	0.0338 (4)

H96A	0.045474	0.904883	0.867897	0.041*	
H96B	−0.027977	0.945261	0.828840	0.041*	
C97	0.01592 (15)	1.03201 (13)	0.86895 (8)	0.0456 (5)	
H97A	0.072258	1.048054	0.879404	0.055*	
H97B	−0.006085	1.084316	0.843343	0.055*	
C98	−0.04601 (17)	1.00554 (17)	0.91852 (8)	0.0613 (7)	
H98A	−0.099615	0.984484	0.907292	0.074*	0.593 (15)
H98B	−0.021204	0.954467	0.943679	0.074*	0.593 (15)
H98C	−0.029305	0.949762	0.943368	0.074*	0.407 (15)
H98D	−0.105663	0.999854	0.908912	0.074*	0.407 (15)
C99	−0.0704 (7)	1.0681 (7)	0.9492 (3)	0.061 (2)	0.593 (15)
H99A	−0.110775	1.039824	0.979730	0.092*	0.593 (15)
H99B	−0.097908	1.118440	0.925907	0.092*	0.593 (15)
H99C	−0.019049	1.088141	0.962580	0.092*	0.593 (15)
C99′	−0.0346 (10)	1.0913 (10)	0.9453 (5)	0.061 (2)	0.407 (15)
H99D	−0.072139	1.082100	0.978568	0.092*	0.407 (15)
H99E	−0.050518	1.145456	0.919466	0.092*	0.407 (15)
H99F	0.025295	1.095952	0.953471	0.092*	0.407 (15)
C100	0.41331 (10)	0.51826 (10)	0.78742 (6)	0.0235 (3)	
C101	0.42050 (10)	0.53968 (11)	0.83648 (6)	0.0279 (3)	
H101	0.463137	0.512340	0.859554	0.033*	
C102	0.36677 (11)	0.59969 (11)	0.85176 (6)	0.0296 (3)	
H102	0.370413	0.611312	0.885873	0.036*	
C103	0.30755 (10)	0.64285 (10)	0.81706 (6)	0.0260 (3)	
H103	0.271544	0.685312	0.827168	0.031*	
C104	0.35061 (9)	0.56313 (10)	0.75634 (6)	0.0229 (3)	
H104	0.342183	0.549143	0.723395	0.028*	
C105	0.57587 (10)	0.49849 (10)	0.76312 (6)	0.0250 (3)	
C106	0.64956 (10)	0.45722 (11)	0.78520 (6)	0.0270 (3)	
H106	0.646250	0.396112	0.802406	0.032*	
C107	0.72755 (10)	0.50151 (11)	0.78315 (7)	0.0279 (3)	
H107	0.775291	0.469938	0.798879	0.034*	
C108	0.73694 (10)	0.59185 (10)	0.75829 (6)	0.0261 (3)	
C109	0.66367 (10)	0.63451 (11)	0.73662 (7)	0.0279 (3)	
H109	0.666630	0.695778	0.719870	0.033*	
C110	0.58699 (10)	0.58909 (11)	0.73914 (7)	0.0281 (3)	
H110	0.539128	0.620930	0.723797	0.034*	
C111	0.86940 (10)	0.61789 (11)	0.79968 (7)	0.0286 (3)	
H11A	0.930748	0.620833	0.786348	0.034*	
H11B	0.856587	0.557053	0.821513	0.034*	
C112	0.85637 (11)	0.67951 (11)	0.83645 (7)	0.0322 (4)	
H11C	0.872702	0.740136	0.815686	0.039*	
H11D	0.794798	0.678988	0.848941	0.039*	
C113	0.90983 (12)	0.65261 (12)	0.88519 (7)	0.0346 (4)	
H11E	0.891817	0.592715	0.906424	0.042*	
H11F	0.971008	0.650523	0.872416	0.042*	
C114	0.90168 (14)	0.71417 (14)	0.92184 (8)	0.0456 (5)	
H11G	0.937321	0.693091	0.952298	0.068*	

H11H	0.841483	0.715677	0.935352	0.068*	
H11I	0.920983	0.773334	0.901448	0.068*	
C115	0.82158 (10)	0.72737 (11)	0.71977 (7)	0.0291 (3)	
H11J	0.795180	0.765586	0.741179	0.035*	
H11K	0.787223	0.732195	0.688314	0.035*	
C116	0.91244 (11)	0.76090 (11)	0.69958 (7)	0.0311 (4)	
H11L	0.947309	0.755585	0.730862	0.037*	
H11M	0.938701	0.723764	0.677413	0.037*	
C117	0.91473 (12)	0.85568 (12)	0.66628 (8)	0.0391 (4)	
H11N	0.892034	0.893287	0.689173	0.047*	
H11O	0.876721	0.861748	0.636398	0.047*	
C118	1.00494 (13)	0.88759 (13)	0.64295 (8)	0.0431 (5)	
H11P	1.003134	0.949170	0.622256	0.065*	
H11Q	1.026976	0.851916	0.619214	0.065*	
H11R	1.042777	0.882211	0.672360	0.065*	
C119	0.46931 (10)	0.35200 (10)	0.80472 (6)	0.0251 (3)	
C120	0.50428 (10)	0.28085 (11)	0.78787 (7)	0.0303 (4)	
H120	0.543065	0.292813	0.756572	0.036*	
C121	0.48503 (11)	0.19394 (11)	0.81461 (8)	0.0345 (4)	
H121	0.509187	0.148622	0.800516	0.041*	
C122	0.43079 (12)	0.17178 (11)	0.86190 (8)	0.0389 (4)	
C123	0.39645 (12)	0.24146 (11)	0.88008 (8)	0.0366 (4)	
H123	0.359787	0.229418	0.912318	0.044*	
C124	0.41488 (11)	0.32794 (11)	0.85195 (7)	0.0295 (3)	
H124	0.389184	0.373182	0.865465	0.035*	
C125	0.4583 (5)	0.0124 (4)	0.8816 (2)	0.0515 (13)	0.635 (5)
H12C	0.457554	−0.033359	0.916270	0.062*	0.635 (5)
H12D	0.518793	0.031342	0.870366	0.062*	0.635 (5)
C126	0.4226 (3)	−0.0267 (2)	0.83910 (18)	0.0535 (10)	0.635 (5)
H12E	0.360446	−0.039578	0.848226	0.064*	0.635 (5)
H12F	0.429295	0.016960	0.803565	0.064*	0.635 (5)
C127	0.4676 (3)	−0.1102 (2)	0.83521 (16)	0.0592 (11)	0.635 (5)
H12G	0.529551	−0.096984	0.825121	0.071*	0.635 (5)
H12H	0.462339	−0.153279	0.871003	0.071*	0.635 (5)
C128	0.4310 (5)	−0.1503 (4)	0.7943 (2)	0.0837 (14)	0.635 (5)
H12I	0.461181	−0.204634	0.793870	0.126*	0.635 (5)
H12J	0.438329	−0.108929	0.758529	0.126*	0.635 (5)
H12K	0.369646	−0.163504	0.804107	0.126*	0.635 (5)
C129	0.3402 (3)	0.0643 (2)	0.93108 (13)	0.0471 (8)	0.717 (4)
H12L	0.315413	0.005383	0.934193	0.057*	0.717 (4)
H12M	0.294246	0.108101	0.922839	0.057*	0.717 (4)
C130	0.3803 (3)	0.0669 (2)	0.98447 (16)	0.0695 (11)	0.717 (4)
H13C	0.417299	0.015202	0.995442	0.083*	0.717 (4)
H13D	0.417594	0.119982	0.977168	0.083*	0.717 (4)
C131	0.3182 (4)	0.0676 (3)	1.02931 (16)	0.0953 (17)	0.717 (4)
H13E	0.348633	0.053184	1.062872	0.114*	0.717 (4)
H13F	0.275083	0.020257	1.032504	0.114*	0.717 (4)
C132	0.2722 (4)	0.1504 (4)	1.0258 (2)	0.092 (2)	0.717 (4)

H13G	0.230042	0.142737	1.056869	0.137*	0.717 (4)
H13H	0.242549	0.166359	0.992465	0.137*	0.717 (4)
H13I	0.313470	0.197031	1.025908	0.137*	0.717 (4)
C133	0.4424 (9)	0.0131 (8)	0.8623 (4)	0.0515 (13)	0.365 (5)
H13J	0.440661	−0.043914	0.890007	0.062*	0.365 (5)
H13K	0.503147	0.026234	0.848497	0.062*	0.365 (5)
C134	0.3897 (4)	0.0039 (5)	0.8152 (3)	0.0526 (17)	0.365 (5)
H13L	0.330513	−0.016342	0.829348	0.063*	0.365 (5)
H13M	0.386211	0.061919	0.788914	0.063*	0.365 (5)
C135	0.4305 (5)	−0.0607 (5)	0.7869 (3)	0.065 (2)	0.365 (5)
H13N	0.398980	−0.059275	0.754643	0.077*	0.365 (5)
H13O	0.490413	−0.041155	0.774224	0.077*	0.365 (5)
C136	0.4314 (10)	−0.1542 (7)	0.8211 (4)	0.0837 (14)	0.365 (5)
H13P	0.455939	−0.191895	0.799314	0.126*	0.365 (5)
H13Q	0.372542	−0.173972	0.834561	0.126*	0.365 (5)
H13R	0.466431	−0.157353	0.851605	0.126*	0.365 (5)
C137	0.3762 (6)	0.0647 (6)	0.9479 (4)	0.0471 (8)	0.283 (4)
H13S	0.393027	0.005540	0.968360	0.057*	0.283 (4)
H13T	0.396710	0.108873	0.965371	0.057*	0.283 (4)
C138	0.2807 (6)	0.0697 (6)	0.9430 (4)	0.061 (2)	0.283 (4)
H13U	0.267416	0.127734	0.919191	0.073*	0.283 (4)
H13V	0.262939	0.024378	0.925590	0.073*	0.283 (4)
C139	0.2290 (7)	0.0571 (7)	0.9957 (4)	0.075 (3)	0.283 (4)
H13W	0.169044	0.040481	0.992039	0.090*	0.283 (4)
H13X	0.253544	0.009305	1.023442	0.090*	0.283 (4)
C140	0.2302 (12)	0.1402 (10)	1.0126 (7)	0.092 (2)	0.283 (4)
H14C	0.192314	0.133777	1.045418	0.137*	0.283 (4)
H14D	0.210195	0.188186	0.983753	0.137*	0.283 (4)
H14E	0.289004	0.153239	1.019616	0.137*	0.283 (4)
B1	0.26552 (11)	0.32896 (12)	0.65910 (7)	0.0247 (4)	
B2	0.08061 (11)	0.37749 (11)	0.82430 (7)	0.0230 (3)	
B3	0.23393 (11)	0.67598 (11)	0.72498 (7)	0.0232 (3)	
B4	0.48146 (11)	0.45247 (12)	0.76794 (7)	0.0247 (4)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0217 (6)	0.0215 (6)	0.0280 (7)	−0.0004 (5)	0.0000 (5)	−0.0078 (5)
N2	0.0206 (6)	0.0239 (7)	0.0258 (6)	−0.0018 (5)	−0.0008 (5)	−0.0101 (5)
N3	0.0220 (6)	0.0228 (6)	0.0239 (6)	−0.0004 (5)	0.0000 (5)	−0.0102 (5)
N4	0.0211 (6)	0.0208 (6)	0.0246 (6)	−0.0028 (5)	0.0000 (5)	−0.0067 (5)
N5	0.0300 (7)	0.0319 (8)	0.0427 (8)	0.0035 (6)	−0.0059 (6)	−0.0199 (7)
N6	0.0268 (7)	0.0352 (8)	0.0374 (8)	0.0032 (6)	−0.0037 (6)	−0.0068 (6)
N7	0.0240 (7)	0.0345 (8)	0.0377 (8)	−0.0073 (6)	0.0041 (6)	−0.0175 (6)
N8	0.0424 (9)	0.0365 (8)	0.0379 (8)	0.0026 (7)	−0.0139 (7)	−0.0197 (7)
N9	0.0339 (9)	0.0741 (12)	0.0343 (8)	−0.0091 (8)	0.0075 (7)	−0.0230 (8)
N10	0.0333 (8)	0.0243 (7)	0.0361 (8)	0.0036 (6)	−0.0011 (6)	−0.0111 (6)
N11	0.0242 (7)	0.0256 (7)	0.0344 (7)	−0.0039 (5)	−0.0061 (6)	−0.0048 (6)

N12	0.0719 (13)	0.0229 (8)	0.0815 (14)	−0.0039 (8)	0.0281 (11)	−0.0038 (9)
C1	0.0229 (8)	0.0220 (8)	0.0278 (8)	0.0027 (6)	0.0002 (6)	−0.0092 (6)
C2	0.0211 (7)	0.0220 (8)	0.0286 (8)	−0.0006 (6)	0.0010 (6)	−0.0080 (6)
C3	0.0242 (8)	0.0280 (8)	0.0334 (9)	−0.0054 (6)	0.0028 (6)	−0.0079 (7)
C4	0.0299 (9)	0.0361 (9)	0.0288 (8)	−0.0063 (7)	0.0057 (7)	−0.0070 (7)
C5	0.0290 (8)	0.0316 (9)	0.0274 (8)	−0.0018 (7)	0.0004 (6)	−0.0104 (7)
C6	0.0252 (8)	0.0266 (8)	0.0224 (7)	−0.0008 (6)	0.0011 (6)	−0.0083 (6)
C7	0.0246 (8)	0.0290 (8)	0.0294 (8)	−0.0030 (6)	0.0004 (6)	−0.0120 (7)
C8	0.0237 (8)	0.0303 (9)	0.0306 (8)	0.0013 (6)	0.0010 (6)	−0.0104 (7)
C9	0.0313 (9)	0.0272 (8)	0.0249 (8)	0.0005 (7)	−0.0003 (6)	−0.0099 (6)
C10	0.0282 (8)	0.0328 (9)	0.0342 (9)	−0.0019 (7)	−0.0048 (7)	−0.0160 (7)
C11	0.0255 (8)	0.0313 (9)	0.0309 (8)	0.0025 (7)	−0.0032 (6)	−0.0126 (7)
C12	0.0342 (9)	0.0317 (9)	0.0404 (10)	0.0041 (7)	−0.0018 (7)	−0.0179 (8)
C13	0.0373 (10)	0.0260 (9)	0.0470 (10)	0.0036 (7)	−0.0062 (8)	−0.0138 (8)
C14	0.0379 (11)	0.0483 (12)	0.0661 (14)	0.0091 (9)	−0.0116 (10)	−0.0249 (10)
C15	0.0555 (15)	0.0627 (16)	0.096 (2)	0.0211 (12)	−0.0314 (14)	−0.0199 (14)
C16	0.0364 (9)	0.0270 (9)	0.0366 (9)	0.0001 (7)	−0.0055 (7)	−0.0130 (7)
C17	0.0458 (11)	0.0349 (10)	0.0370 (10)	−0.0021 (8)	−0.0073 (8)	−0.0125 (8)
C18	0.0555 (13)	0.0572 (13)	0.0456 (12)	−0.0088 (10)	−0.0132 (10)	−0.0180 (10)
C19	0.0818 (19)	0.107 (2)	0.0508 (14)	−0.0273 (17)	−0.0212 (13)	−0.0146 (15)
C20	0.0258 (8)	0.0265 (8)	0.0249 (7)	−0.0003 (6)	0.0007 (6)	−0.0123 (6)
C21	0.0281 (8)	0.0280 (8)	0.0280 (8)	−0.0015 (7)	−0.0009 (6)	−0.0107 (7)
C22	0.0246 (8)	0.0326 (9)	0.0320 (8)	−0.0023 (7)	−0.0019 (6)	−0.0124 (7)
C23	0.0276 (8)	0.0325 (9)	0.0276 (8)	0.0034 (7)	−0.0024 (6)	−0.0124 (7)
C24	0.0314 (9)	0.0300 (9)	0.0279 (8)	0.0005 (7)	−0.0009 (7)	−0.0053 (7)
C25	0.0259 (8)	0.0311 (9)	0.0301 (8)	−0.0024 (7)	0.0016 (6)	−0.0105 (7)
C26	0.0294 (9)	0.0407 (10)	0.0381 (9)	0.0037 (8)	−0.0066 (7)	−0.0119 (8)
C27	0.0334 (9)	0.0405 (10)	0.0408 (10)	0.0009 (8)	−0.0062 (8)	−0.0158 (8)
C28	0.0324 (10)	0.0551 (12)	0.0425 (10)	−0.0008 (9)	−0.0025 (8)	−0.0178 (9)
C29	0.0518 (13)	0.0526 (13)	0.0560 (13)	−0.0110 (10)	0.0032 (10)	−0.0206 (10)
C30	0.028 (4)	0.0361 (14)	0.031 (2)	0.0030 (16)	−0.0070 (19)	−0.0082 (10)
C31	0.0365 (19)	0.0399 (12)	0.0296 (19)	0.0047 (12)	−0.0072 (11)	−0.0112 (13)
C32	0.0439 (16)	0.0403 (15)	0.0387 (15)	−0.0053 (12)	−0.0061 (12)	−0.0117 (12)
C33	0.058 (2)	0.050 (2)	0.0476 (19)	−0.0021 (16)	−0.0110 (14)	0.0029 (16)
C30′	0.028 (4)	0.0361 (14)	0.031 (2)	0.0030 (16)	−0.0070 (19)	−0.0082 (10)
C31′	0.0365 (19)	0.0399 (12)	0.0296 (19)	0.0047 (12)	−0.0072 (11)	−0.0112 (13)
C32′	0.058 (2)	0.050 (2)	0.0476 (19)	−0.0021 (16)	−0.0110 (14)	0.0029 (16)
C33′	0.077 (6)	0.042 (5)	0.074 (6)	0.003 (4)	0.006 (5)	−0.008 (4)
C34	0.0208 (7)	0.0247 (8)	0.0262 (8)	−0.0051 (6)	−0.0016 (6)	−0.0107 (6)
C35	0.0202 (7)	0.0225 (8)	0.0273 (8)	−0.0013 (6)	−0.0007 (6)	−0.0105 (6)
C36	0.0254 (8)	0.0261 (8)	0.0306 (8)	0.0014 (6)	−0.0023 (6)	−0.0124 (7)
C37	0.0326 (9)	0.0247 (8)	0.0304 (8)	0.0017 (7)	−0.0031 (7)	−0.0073 (7)
C38	0.0294 (8)	0.0265 (8)	0.0256 (8)	−0.0028 (6)	0.0002 (6)	−0.0088 (6)
C39	0.0241 (8)	0.0224 (8)	0.0242 (7)	−0.0007 (6)	0.0000 (6)	−0.0077 (6)
C40	0.0260 (8)	0.0269 (8)	0.0256 (8)	−0.0023 (6)	0.0029 (6)	−0.0096 (6)
C41	0.0277 (8)	0.0278 (8)	0.0284 (8)	−0.0027 (6)	−0.0010 (6)	−0.0134 (7)
C42	0.0230 (8)	0.0247 (8)	0.0306 (8)	−0.0014 (6)	−0.0007 (6)	−0.0085 (6)
C43	0.0262 (8)	0.0341 (9)	0.0285 (8)	−0.0026 (7)	0.0040 (6)	−0.0133 (7)

C44	0.0270 (8)	0.0307 (9)	0.0268 (8)	−0.0033 (7)	−0.0001 (6)	−0.0138 (7)
C45	0.0245 (8)	0.0346 (9)	0.0419 (10)	−0.0030 (7)	−0.0034 (7)	−0.0169 (8)
C46	0.0329 (9)	0.0367 (10)	0.0420 (10)	−0.0018 (8)	−0.0032 (8)	−0.0164 (8)
C47	0.0448 (11)	0.0382 (10)	0.0520 (12)	−0.0026 (9)	−0.0053 (9)	−0.0220 (9)
C48	0.0746 (16)	0.0409 (12)	0.0706 (15)	0.0032 (11)	−0.0125 (12)	−0.0281 (11)
C49	0.0276 (9)	0.0319 (9)	0.0390 (9)	−0.0060 (7)	0.0026 (7)	−0.0107 (7)
C50	0.0278 (9)	0.0365 (10)	0.0376 (9)	−0.0033 (7)	0.0019 (7)	−0.0138 (8)
C51	0.0411 (11)	0.0680 (14)	0.0365 (10)	0.0067 (10)	0.0037 (8)	−0.0146 (10)
C52	0.0454 (12)	0.0773 (16)	0.0545 (13)	−0.0039 (11)	0.0089 (10)	−0.0359 (12)
C53	0.0237 (8)	0.0241 (8)	0.0228 (7)	−0.0038 (6)	0.0010 (6)	−0.0075 (6)
C54	0.0274 (8)	0.0252 (8)	0.0273 (8)	0.0005 (6)	−0.0010 (6)	−0.0095 (6)
C55	0.0288 (9)	0.0320 (9)	0.0297 (8)	0.0011 (7)	−0.0063 (7)	−0.0092 (7)
C56	0.0329 (9)	0.0269 (8)	0.0255 (8)	−0.0029 (7)	−0.0040 (6)	−0.0088 (6)
C57	0.0334 (9)	0.0308 (9)	0.0324 (9)	0.0038 (7)	−0.0040 (7)	−0.0154 (7)
C58	0.0265 (8)	0.0302 (9)	0.0309 (8)	0.0017 (7)	−0.0058 (6)	−0.0129 (7)
C59	0.0410 (10)	0.0419 (10)	0.0370 (10)	−0.0047 (8)	−0.0110 (8)	−0.0159 (8)
C60	0.0369 (10)	0.0493 (11)	0.0343 (9)	−0.0027 (8)	−0.0040 (8)	−0.0122 (8)
C61	0.0378 (11)	0.0559 (13)	0.0511 (12)	0.0010 (9)	−0.0090 (9)	−0.0151 (10)
C62	0.0451 (12)	0.0651 (15)	0.0525 (13)	0.0065 (10)	−0.0134 (10)	−0.0134 (11)
C63	0.043 (2)	0.0375 (17)	0.0313 (18)	−0.0016 (12)	−0.0050 (12)	−0.0192 (13)
C64	0.0455 (15)	0.0377 (14)	0.0369 (12)	−0.0048 (11)	−0.0014 (11)	−0.0161 (10)
C65	0.0583 (16)	0.0378 (14)	0.0433 (13)	0.0016 (11)	−0.0114 (11)	−0.0150 (11)
C66	0.062 (2)	0.0389 (19)	0.0643 (16)	−0.0033 (14)	−0.0231 (15)	−0.0075 (16)
C63′	0.043 (2)	0.0375 (17)	0.0313 (18)	−0.0016 (12)	−0.0050 (12)	−0.0192 (13)
C64′	0.044 (7)	0.042 (6)	0.030 (5)	−0.003 (5)	−0.002 (5)	−0.018 (4)
C65′	0.0455 (15)	0.0377 (14)	0.0369 (12)	−0.0048 (11)	−0.0014 (11)	−0.0161 (10)
C66′	0.062 (2)	0.0389 (19)	0.0643 (16)	−0.0033 (14)	−0.0231 (15)	−0.0075 (16)
C67	0.0230 (8)	0.0226 (8)	0.0244 (7)	0.0018 (6)	0.0009 (6)	−0.0098 (6)
C68	0.0209 (7)	0.0244 (8)	0.0258 (7)	−0.0007 (6)	−0.0009 (6)	−0.0106 (6)
C69	0.0229 (8)	0.0265 (8)	0.0286 (8)	−0.0016 (6)	−0.0026 (6)	−0.0127 (6)
C70	0.0255 (8)	0.0295 (8)	0.0310 (8)	0.0020 (7)	−0.0065 (6)	−0.0111 (7)
C71	0.0268 (8)	0.0243 (8)	0.0268 (8)	0.0026 (6)	−0.0020 (6)	−0.0073 (6)
C72	0.0250 (8)	0.0196 (7)	0.0262 (8)	0.0017 (6)	−0.0011 (6)	−0.0050 (6)
C73	0.0266 (8)	0.0293 (8)	0.0290 (8)	−0.0016 (7)	−0.0010 (6)	−0.0083 (7)
C74	0.0359 (9)	0.0390 (10)	0.0266 (8)	−0.0024 (8)	−0.0007 (7)	−0.0125 (7)
C75	0.0301 (9)	0.0333 (9)	0.0292 (8)	−0.0007 (7)	0.0037 (7)	−0.0074 (7)
C76	0.0258 (8)	0.0299 (9)	0.0314 (8)	−0.0029 (7)	0.0011 (6)	−0.0067 (7)
C77	0.0299 (8)	0.0245 (8)	0.0263 (8)	−0.0004 (6)	−0.0018 (6)	−0.0075 (6)
C78	0.0411 (11)	0.0704 (15)	0.0354 (10)	−0.0097 (10)	0.0088 (8)	−0.0239 (10)
C79	0.0442 (12)	0.0633 (14)	0.0440 (11)	−0.0154 (10)	0.0011 (9)	−0.0151 (10)
C80	0.0577 (14)	0.0654 (15)	0.0513 (13)	−0.0083 (11)	−0.0098 (10)	−0.0169 (11)
C81	0.0827 (19)	0.0719 (17)	0.0581 (15)	−0.0151 (14)	−0.0261 (13)	−0.0112 (13)
C82	0.0322 (9)	0.0486 (11)	0.0311 (9)	−0.0037 (8)	0.0066 (7)	−0.0079 (8)
C83	0.0513 (12)	0.0410 (11)	0.0432 (11)	−0.0013 (9)	0.0011 (9)	−0.0095 (9)
C84	0.0411 (11)	0.0542 (13)	0.0472 (11)	0.0093 (9)	0.0013 (9)	−0.0104 (10)
C85	0.0444 (13)	0.0734 (16)	0.0673 (15)	0.0027 (11)	−0.0035 (11)	−0.0257 (13)
C86	0.0227 (8)	0.0243 (8)	0.0246 (7)	0.0012 (6)	−0.0032 (6)	−0.0077 (6)
C87	0.0256 (8)	0.0266 (8)	0.0281 (8)	−0.0002 (6)	0.0014 (6)	−0.0062 (6)

C88	0.0322 (9)	0.0226 (8)	0.0346 (9)	−0.0029 (7)	−0.0003 (7)	−0.0067 (7)
C89	0.0271 (8)	0.0247 (8)	0.0310 (8)	0.0030 (6)	−0.0053 (6)	−0.0105 (7)
C90	0.0255 (8)	0.0295 (9)	0.0318 (8)	−0.0011 (7)	0.0024 (6)	−0.0118 (7)
C91	0.0262 (8)	0.0221 (8)	0.0313 (8)	−0.0024 (6)	0.0004 (6)	−0.0084 (6)
C92	0.0314 (9)	0.0240 (8)	0.0410 (9)	0.0006 (7)	−0.0020 (7)	−0.0108 (7)
C93	0.0347 (9)	0.0308 (9)	0.0382 (9)	−0.0023 (7)	−0.0029 (7)	−0.0110 (7)
C94	0.0363 (10)	0.0427 (11)	0.0411 (10)	−0.0007 (8)	−0.0017 (8)	−0.0066 (8)
C95	0.0495 (12)	0.0577 (13)	0.0469 (12)	0.0020 (10)	−0.0137 (9)	−0.0092 (10)
C96	0.0375 (10)	0.0324 (9)	0.0338 (9)	0.0061 (7)	−0.0021 (7)	−0.0128 (7)
C97	0.0656 (14)	0.0386 (11)	0.0374 (10)	0.0201 (10)	−0.0091 (9)	−0.0172 (8)
C98	0.0745 (16)	0.0788 (17)	0.0358 (11)	0.0402 (13)	−0.0087 (10)	−0.0232 (11)
C99	0.087 (6)	0.061 (5)	0.0400 (18)	0.033 (4)	−0.007 (4)	−0.021 (3)
C99′	0.087 (6)	0.061 (5)	0.0400 (18)	0.033 (4)	−0.007 (4)	−0.021 (3)
C100	0.0216 (7)	0.0207 (7)	0.0271 (8)	−0.0053 (6)	−0.0004 (6)	−0.0045 (6)
C101	0.0278 (8)	0.0273 (8)	0.0285 (8)	−0.0008 (7)	−0.0064 (6)	−0.0060 (7)
C102	0.0344 (9)	0.0307 (9)	0.0254 (8)	−0.0004 (7)	−0.0038 (7)	−0.0100 (7)
C103	0.0276 (8)	0.0250 (8)	0.0261 (8)	−0.0013 (6)	0.0012 (6)	−0.0091 (6)
C104	0.0217 (7)	0.0222 (8)	0.0256 (7)	−0.0036 (6)	0.0001 (6)	−0.0081 (6)
C105	0.0235 (8)	0.0245 (8)	0.0279 (8)	−0.0016 (6)	−0.0013 (6)	−0.0086 (6)
C106	0.0269 (8)	0.0232 (8)	0.0301 (8)	−0.0015 (6)	−0.0015 (6)	−0.0058 (6)
C107	0.0236 (8)	0.0275 (8)	0.0328 (8)	0.0013 (6)	−0.0049 (6)	−0.0074 (7)
C108	0.0232 (8)	0.0272 (8)	0.0291 (8)	−0.0023 (6)	−0.0017 (6)	−0.0099 (6)
C109	0.0266 (8)	0.0214 (8)	0.0347 (9)	−0.0015 (6)	−0.0031 (7)	−0.0055 (6)
C110	0.0234 (8)	0.0258 (8)	0.0344 (9)	0.0004 (6)	−0.0040 (6)	−0.0061 (7)
C111	0.0235 (8)	0.0277 (8)	0.0344 (9)	−0.0005 (6)	−0.0049 (6)	−0.0071 (7)
C112	0.0296 (9)	0.0309 (9)	0.0356 (9)	0.0002 (7)	−0.0005 (7)	−0.0084 (7)
C113	0.0331 (9)	0.0362 (10)	0.0351 (9)	0.0000 (7)	−0.0025 (7)	−0.0106 (8)
C114	0.0477 (12)	0.0506 (12)	0.0419 (11)	−0.0073 (9)	0.0007 (9)	−0.0195 (9)
C115	0.0257 (8)	0.0256 (8)	0.0345 (9)	−0.0026 (6)	−0.0051 (7)	−0.0044 (7)
C116	0.0263 (8)	0.0298 (9)	0.0357 (9)	−0.0031 (7)	−0.0029 (7)	−0.0056 (7)
C117	0.0332 (10)	0.0311 (9)	0.0492 (11)	−0.0052 (8)	−0.0039 (8)	−0.0039 (8)
C118	0.0409 (11)	0.0398 (11)	0.0442 (11)	−0.0121 (8)	0.0026 (8)	−0.0050 (8)
C119	0.0206 (7)	0.0236 (8)	0.0315 (8)	−0.0011 (6)	−0.0047 (6)	−0.0071 (6)
C120	0.0240 (8)	0.0285 (9)	0.0385 (9)	−0.0008 (7)	−0.0006 (7)	−0.0096 (7)
C121	0.0278 (9)	0.0257 (9)	0.0514 (11)	0.0008 (7)	−0.0011 (8)	−0.0129 (8)
C122	0.0353 (10)	0.0240 (9)	0.0532 (11)	−0.0024 (7)	0.0008 (8)	−0.0040 (8)
C123	0.0353 (10)	0.0275 (9)	0.0422 (10)	−0.0028 (7)	0.0062 (8)	−0.0034 (7)
C124	0.0290 (9)	0.0246 (8)	0.0344 (9)	0.0001 (7)	−0.0014 (7)	−0.0070 (7)
C125	0.067 (3)	0.0260 (11)	0.055 (4)	0.0001 (16)	0.011 (3)	−0.004 (3)
C126	0.048 (2)	0.038 (2)	0.069 (3)	−0.0097 (17)	−0.0031 (19)	−0.0037 (19)
C127	0.063 (2)	0.050 (2)	0.066 (2)	−0.0070 (18)	−0.0102 (19)	−0.0161 (18)
C128	0.124 (3)	0.060 (2)	0.070 (4)	−0.012 (2)	−0.016 (4)	−0.020 (3)
C129	0.056 (3)	0.0278 (12)	0.053 (2)	−0.0098 (16)	0.0029 (16)	−0.0035 (13)
C130	0.084 (3)	0.056 (2)	0.061 (2)	0.0197 (19)	−0.0116 (19)	−0.0004 (17)
C131	0.144 (5)	0.076 (3)	0.057 (2)	0.036 (3)	0.000 (3)	−0.005 (2)
C132	0.130 (6)	0.075 (3)	0.061 (3)	0.034 (4)	0.022 (3)	−0.010 (2)
C133	0.067 (3)	0.0260 (11)	0.055 (4)	0.0001 (16)	0.011 (3)	−0.004 (3)
C134	0.037 (3)	0.044 (4)	0.072 (5)	0.002 (3)	−0.002 (3)	−0.009 (3)

C135	0.058 (4)	0.071 (5)	0.071 (5)	−0.005 (3)	0.008 (3)	−0.033 (4)
C136	0.124 (3)	0.060 (2)	0.070 (4)	−0.012 (2)	−0.016 (4)	−0.020 (3)
C137	0.056 (3)	0.0278 (12)	0.053 (2)	−0.0098 (16)	0.0029 (16)	−0.0035 (13)
C138	0.051 (5)	0.056 (5)	0.076 (6)	−0.004 (4)	−0.001 (5)	−0.017 (4)
C139	0.075 (7)	0.073 (7)	0.068 (6)	−0.005 (5)	0.019 (5)	−0.011 (5)
C140	0.130 (6)	0.075 (3)	0.061 (3)	0.034 (4)	0.022 (3)	−0.010 (2)
B1	0.0239 (9)	0.0268 (9)	0.0243 (8)	−0.0022 (7)	0.0023 (7)	−0.0095 (7)
B2	0.0234 (9)	0.0229 (9)	0.0237 (8)	−0.0019 (7)	−0.0004 (6)	−0.0084 (7)
B3	0.0225 (8)	0.0230 (9)	0.0247 (8)	0.0004 (7)	−0.0026 (7)	−0.0070 (7)
B4	0.0223 (9)	0.0256 (9)	0.0267 (9)	−0.0012 (7)	−0.0020 (7)	−0.0077 (7)

Geometric parameters (Å, º)

N1—C3	1.342 (2)	C65—H65A	0.9900
N1—C2	1.359 (2)	C65—H65B	0.9900
N1—B4	1.662 (2)	C66—H66A	0.9800
N2—C36	1.339 (2)	C66—H66B	0.9800
N2—C35	1.3541 (19)	C66—H66C	0.9800
N2—B1	1.656 (2)	C63′—C64′	1.523 (14)
N3—C69	1.342 (2)	C63′—H63C	0.9900
N3—C68	1.3568 (19)	C63′—H63D	0.9900
N3—B2	1.658 (2)	C64′—C65′	1.490 (12)
N4—C103	1.339 (2)	C64′—H64C	0.9900
N4—C104	1.3553 (19)	C64′—H64D	0.9900
N4—B3	1.643 (2)	C65′—C66′	1.515 (14)
N5—C9	1.388 (2)	C65′—H65C	0.9900
N5—C16	1.457 (2)	C65′—H65D	0.9900
N5—C12	1.458 (2)	C66′—H66D	0.9800
N6—C23	1.390 (2)	C66′—H66E	0.9800
N6—C30′	1.44 (3)	C66′—H66F	0.9800
N6—C26	1.461 (2)	C67—C68	1.387 (2)
N6—C30	1.464 (10)	C67—C71	1.403 (2)
N7—C42	1.395 (2)	C67—B3	1.628 (2)
N7—C45	1.457 (2)	C68—H68	0.9500
N7—C49	1.465 (2)	C69—C70	1.379 (2)
N8—C56	1.395 (2)	C69—H69	0.9500
N8—C63	1.443 (4)	C70—C71	1.381 (2)
N8—C59	1.462 (2)	C70—H70	0.9500
N8—C63′	1.49 (2)	C71—H71	0.9500
N9—C75	1.391 (2)	C72—C73	1.397 (2)
N9—C78	1.447 (2)	C72—C77	1.404 (2)
N9—C82	1.449 (2)	C72—B3	1.633 (2)
N10—C89	1.420 (2)	C73—C74	1.391 (2)
N10—C96	1.461 (2)	C73—H73	0.9500
N10—C92	1.471 (2)	C74—C75	1.401 (2)
N11—C108	1.412 (2)	C74—H74	0.9500
N11—C115	1.466 (2)	C75—C76	1.399 (2)
N11—C111	1.471 (2)	C76—C77	1.387 (2)

N12—C122	1.394 (2)	C76—H76	0.9500
N12—C125	1.412 (7)	C77—H77	0.9500
N12—C129	1.456 (4)	C78—C79	1.498 (3)
N12—C137	1.520 (11)	C78—H78A	0.9900
N12—C133	1.540 (13)	C78—H78B	0.9900
C1—C2	1.387 (2)	C79—C80	1.533 (3)
C1—C5	1.405 (2)	C79—H79A	0.9900
C1—B1	1.633 (2)	C79—H79B	0.9900
C2—H2	0.9500	C80—C81	1.485 (3)
C3—C4	1.380 (2)	C80—H80A	0.9900
C3—H3	0.9500	C80—H80B	0.9900
C4—C5	1.382 (2)	C81—H81A	0.9800
C4—H4	0.9500	C81—H81B	0.9800
C5—H5	0.9500	C81—H81C	0.9800
C6—C7	1.396 (2)	C82—C83	1.530 (3)
C6—C11	1.403 (2)	C82—H82A	0.9900
C6—B1	1.620 (2)	C82—H82B	0.9900
C7—C8	1.387 (2)	C83—C84	1.524 (3)
C7—H7	0.9500	C83—H83A	0.9900
C8—C9	1.405 (2)	C83—H83B	0.9900
C8—H8	0.9500	C84—C85	1.512 (3)
C9—C10	1.404 (2)	C84—H84A	0.9900
C10—C11	1.388 (2)	C84—H84B	0.9900
C10—H10	0.9500	C85—H85A	0.9800
C11—H11	0.9500	C85—H85B	0.9800
C12—C13	1.518 (3)	C85—H85C	0.9800
C12—H12A	0.9900	C86—C91	1.398 (2)
C12—H12B	0.9900	C86—C87	1.405 (2)
C13—C14	1.519 (3)	C86—B3	1.622 (2)
C13—H13A	0.9900	C87—C88	1.386 (2)
C13—H13B	0.9900	C87—H87	0.9500
C14—C15	1.519 (3)	C88—C89	1.402 (2)
C14—H14A	0.9900	C88—H88	0.9500
C14—H14B	0.9900	C89—C90	1.396 (2)
C15—H15A	0.9800	C90—C91	1.394 (2)
C15—H15B	0.9800	C90—H90	0.9500
C15—H15C	0.9800	C91—H91	0.9500
C16—C17	1.516 (2)	C92—C93	1.522 (2)
C16—H16A	0.9900	C92—H92A	0.9900
C16—H16B	0.9900	C92—H92B	0.9900
C17—C18	1.518 (3)	C93—C94	1.514 (3)
C17—H17A	0.9900	C93—H93A	0.9900
C17—H17B	0.9900	C93—H93B	0.9900
C18—C19	1.505 (3)	C94—C95	1.516 (3)
C18—H18A	0.9900	C94—H94A	0.9900
C18—H18B	0.9900	C94—H94B	0.9900
C19—H19A	0.9800	C95—H95A	0.9800
C19—H19B	0.9800	C95—H95B	0.9800

C19—H19C	0.9800	C95—H95C	0.9800
C20—C25	1.398 (2)	C96—C97	1.521 (2)
C20—C21	1.406 (2)	C96—H96A	0.9900
C20—B1	1.629 (2)	C96—H96B	0.9900
C21—C22	1.384 (2)	C97—C98	1.511 (3)
C21—H21	0.9500	C97—H97A	0.9900
C22—C23	1.407 (2)	C97—H97B	0.9900
C22—H22	0.9500	C98—C99	1.453 (8)
C23—C24	1.403 (2)	C98—C99′	1.689 (14)
C24—C25	1.393 (2)	C98—H98A	0.9900
C24—H24	0.9500	C98—H98B	0.9900
C25—H25	0.9500	C98—H98C	0.9900
C26—C27	1.525 (2)	C98—H98D	0.9900
C26—H26A	0.9900	C99—H99A	0.9800
C26—H26B	0.9900	C99—H99B	0.9800
C27—C28	1.530 (3)	C99—H99C	0.9800
C27—H27A	0.9900	C99′—H99D	0.9800
C27—H27B	0.9900	C99′—H99E	0.9800
C28—C29	1.515 (3)	C99′—H99F	0.9800
C28—H28A	0.9900	C100—C104	1.382 (2)
C28—H28B	0.9900	C100—C101	1.405 (2)
C29—H29A	0.9800	C100—B4	1.629 (2)
C29—H29B	0.9800	C101—C102	1.379 (2)
C29—H29C	0.9800	C101—H101	0.9500
C30—C31	1.530 (5)	C102—C103	1.383 (2)
C30—H30A	0.9900	C102—H102	0.9500
C30—H30B	0.9900	C103—H103	0.9500
C31—C32	1.525 (4)	C104—H104	0.9500
C31—H31A	0.9900	C105—C106	1.402 (2)
C31—H31B	0.9900	C105—C110	1.407 (2)
C32—C33	1.514 (4)	C105—B4	1.626 (2)
C32—H32A	0.9900	C106—C107	1.395 (2)
C32—H32B	0.9900	C106—H106	0.9500
C33—H33A	0.9800	C107—C108	1.405 (2)
C33—H33B	0.9800	C107—H107	0.9500
C33—H33C	0.9800	C108—C109	1.401 (2)
C30′—C31′	1.515 (14)	C109—C110	1.385 (2)
C30′—H30C	0.9900	C109—H109	0.9500
C30′—H30D	0.9900	C110—H110	0.9500
C31′—C32′	1.512 (11)	C111—C112	1.531 (2)
C31′—H31C	0.9900	C111—H11A	0.9900
C31′—H31D	0.9900	C111—H11B	0.9900
C32′—C33′	1.493 (11)	C112—C113	1.524 (2)
C32′—H32C	0.9900	C112—H11C	0.9900
C32′—H32D	0.9900	C112—H11D	0.9900
C33′—H33D	0.9800	C113—C114	1.523 (3)
C33′—H33E	0.9800	C113—H11E	0.9900
C33′—H33F	0.9800	C113—H11F	0.9900

C34—C35	1.386 (2)	C114—H11G	0.9800
C34—C38	1.398 (2)	C114—H11H	0.9800
C34—B2	1.628 (2)	C114—H11I	0.9800
C35—H35	0.9500	C115—C116	1.521 (2)
C36—C37	1.383 (2)	C115—H11J	0.9900
C36—H36	0.9500	C115—H11K	0.9900
C37—C38	1.383 (2)	C116—C117	1.516 (2)
C37—H37	0.9500	C116—H11L	0.9900
C38—H38	0.9500	C116—H11M	0.9900
C39—C44	1.396 (2)	C117—C118	1.522 (3)
C39—C40	1.404 (2)	C117—H11N	0.9900
C39—B2	1.623 (2)	C117—H11O	0.9900
C40—C41	1.385 (2)	C118—H11P	0.9800
C40—H40	0.9500	C118—H11Q	0.9800
C41—C42	1.402 (2)	C118—H11R	0.9800
C41—H41	0.9500	C119—C124	1.399 (2)
C42—C43	1.400 (2)	C119—C120	1.403 (2)
C43—C44	1.390 (2)	C119—B4	1.624 (2)
C43—H43	0.9500	C120—C121	1.387 (2)
C44—H44	0.9500	C120—H120	0.9500
C45—C46	1.526 (2)	C121—C122	1.397 (3)
C45—H45A	0.9900	C121—H121	0.9500
C45—H45B	0.9900	C122—C123	1.397 (3)
C46—C47	1.518 (2)	C123—C124	1.387 (2)
C46—H46A	0.9900	C123—H123	0.9500
C46—H46B	0.9900	C124—H124	0.9500
C47—C48	1.516 (3)	C125—C126	1.528 (6)
C47—H47A	0.9900	C125—H12C	0.9900
C47—H47B	0.9900	C125—H12D	0.9900
C48—H48A	0.9800	C126—C127	1.515 (5)
C48—H48B	0.9800	C126—H12E	0.9900
C48—H48C	0.9800	C126—H12F	0.9900
C49—C50	1.520 (2)	C127—C128	1.509 (6)
C49—H49A	0.9900	C127—H12G	0.9900
C49—H49B	0.9900	C127—H12H	0.9900
C50—C51	1.516 (3)	C128—H12I	0.9800
C50—H50A	0.9900	C128—H12J	0.9800
C50—H50B	0.9900	C128—H12K	0.9800
C51—C52	1.508 (3)	C129—C130	1.562 (5)
C51—H51A	0.9900	C129—H12L	0.9900
C51—H51B	0.9900	C129—H12M	0.9900
C52—H52A	0.9800	C130—C131	1.456 (6)
C52—H52B	0.9800	C130—H13C	0.9900
C52—H52C	0.9800	C130—H13D	0.9900
C53—C54	1.397 (2)	C131—C132	1.475 (6)
C53—C58	1.401 (2)	C131—H13E	0.9900
C53—B2	1.619 (2)	C131—H13F	0.9900
C54—C55	1.390 (2)	C132—H13G	0.9800

C54—H54	0.9500	C132—H13H	0.9800
C55—C56	1.400 (2)	C132—H13I	0.9800
C55—H55	0.9500	C133—C134	1.552 (10)
C56—C57	1.404 (2)	C133—H13J	0.9900
C57—C58	1.385 (2)	C133—H13K	0.9900
C57—H57	0.9500	C134—C135	1.516 (8)
C58—H58	0.9500	C134—H13L	0.9900
C59—C60	1.511 (3)	C134—H13M	0.9900
C59—H59A	0.9900	C135—C136	1.508 (11)
C59—H59B	0.9900	C135—H13N	0.9900
C60—C61	1.516 (3)	C135—H13O	0.9900
C60—H60A	0.9900	C136—H13P	0.9800
C60—H60B	0.9900	C136—H13Q	0.9800
C61—C62	1.512 (3)	C136—H13R	0.9800
C61—H61A	0.9900	C137—C138	1.504 (11)
C61—H61B	0.9900	C137—H13S	0.9900
C62—H62A	0.9800	C137—H13T	0.9900
C62—H62B	0.9800	C138—C139	1.496 (11)
C62—H62C	0.9800	C138—H13U	0.9900
C63—C64	1.540 (4)	C138—H13V	0.9900
C63—H63A	0.9900	C139—C140	1.487 (14)
C63—H63B	0.9900	C139—H13W	0.9900
C64—C65	1.517 (3)	C139—H13X	0.9900
C64—H64A	0.9900	C140—H14C	0.9800
C64—H64B	0.9900	C140—H14D	0.9800
C65—C66	1.517 (4)	C140—H14E	0.9800

C3—N1—C2	118.20 (13)	H66D—C66′—H66F	109.5
C3—N1—B4	124.49 (13)	H66E—C66′—H66F	109.5
C2—N1—B4	117.31 (12)	C68—C67—C71	114.97 (14)
C36—N2—C35	118.58 (13)	C68—C67—B3	123.77 (13)
C36—N2—B1	123.75 (13)	C71—C67—B3	121.04 (13)
C35—N2—B1	117.65 (12)	N3—C68—C67	124.74 (14)
C69—N3—C68	118.31 (13)	N3—C68—H68	117.6
C69—N3—B2	123.86 (12)	C67—C68—H68	117.6
C68—N3—B2	117.66 (12)	N3—C69—C70	121.35 (14)
C103—N4—C104	118.64 (13)	N3—C69—H69	119.3
C103—N4—B3	124.09 (13)	C70—C69—H69	119.3
C104—N4—B3	117.27 (12)	C69—C70—C71	119.46 (15)
C9—N5—C16	120.69 (14)	C69—C70—H70	120.3
C9—N5—C12	119.22 (14)	C71—C70—H70	120.3
C16—N5—C12	117.07 (13)	C70—C71—C67	121.10 (15)
C23—N6—C30′	126.7 (13)	C70—C71—H71	119.5
C23—N6—C26	121.55 (14)	C67—C71—H71	119.5
C30′—N6—C26	111.7 (13)	C73—C72—C77	113.74 (14)
C23—N6—C30	118.7 (4)	C73—C72—B3	125.08 (14)
C26—N6—C30	119.7 (4)	C77—C72—B3	120.85 (13)
C42—N7—C45	119.65 (13)	C74—C73—C72	123.42 (15)

C42—N7—C49	119.12 (14)	C74—C73—H73	118.3
C45—N7—C49	115.45 (13)	C72—C73—H73	118.3
C56—N8—C63	120.9 (2)	C73—C74—C75	121.48 (15)
C56—N8—C59	120.10 (15)	C73—C74—H74	119.3
C63—N8—C59	114.8 (2)	C75—C74—H74	119.3
C56—N8—C63′	117.7 (9)	N9—C75—C76	121.96 (16)
C59—N8—C63′	122.0 (9)	N9—C75—C74	121.76 (16)
C75—N9—C78	121.12 (16)	C76—C75—C74	116.28 (15)
C75—N9—C82	123.05 (15)	C77—C76—C75	120.85 (15)
C78—N9—C82	115.84 (15)	C77—C76—H76	119.6
C89—N10—C96	116.09 (13)	C75—C76—H76	119.6
C89—N10—C92	115.73 (13)	C76—C77—C72	124.14 (15)
C96—N10—C92	114.35 (13)	C76—C77—H77	117.9
C108—N11—C115	116.92 (13)	C72—C77—H77	117.9
C108—N11—C111	118.30 (13)	N9—C78—C79	113.40 (19)
C115—N11—C111	114.89 (13)	N9—C78—H78A	108.9
C122—N12—C125	123.9 (3)	C79—C78—H78A	108.9
C122—N12—C129	120.3 (2)	N9—C78—H78B	108.9
C122—N12—C137	118.2 (4)	C79—C78—H78B	108.9
C122—N12—C133	117.6 (5)	H78A—C78—H78B	107.7
C2—C1—C5	114.70 (14)	C78—C79—C80	111.33 (19)
C2—C1—B1	123.54 (14)	C78—C79—H79A	109.4
C5—C1—B1	121.66 (14)	C80—C79—H79A	109.4
N1—C2—C1	125.15 (14)	C78—C79—H79B	109.4
N1—C2—H2	117.4	C80—C79—H79B	109.4
C1—C2—H2	117.4	H79A—C79—H79B	108.0
N1—C3—C4	121.11 (15)	C81—C80—C79	113.2 (2)
N1—C3—H3	119.4	C81—C80—H80A	108.9
C4—C3—H3	119.4	C79—C80—H80A	108.9
C3—C4—C5	119.81 (15)	C81—C80—H80B	108.9
C3—C4—H4	120.1	C79—C80—H80B	108.9
C5—C4—H4	120.1	H80A—C80—H80B	107.8
C4—C5—C1	121.02 (15)	C80—C81—H81A	109.5
C4—C5—H5	119.5	C80—C81—H81B	109.5
C1—C5—H5	119.5	H81A—C81—H81B	109.5
C7—C6—C11	114.27 (14)	C80—C81—H81C	109.5
C7—C6—B1	122.72 (14)	H81A—C81—H81C	109.5
C11—C6—B1	122.56 (14)	H81B—C81—H81C	109.5
C8—C7—C6	123.60 (15)	N9—C82—C83	112.73 (17)
C8—C7—H7	118.2	N9—C82—H82A	109.0
C6—C7—H7	118.2	C83—C82—H82A	109.0
C7—C8—C9	121.25 (15)	N9—C82—H82B	109.0
C7—C8—H8	119.4	C83—C82—H82B	109.0
C9—C8—H8	119.4	H82A—C82—H82B	107.8
N5—C9—C10	122.75 (15)	C84—C83—C82	113.53 (17)
N5—C9—C8	121.04 (15)	C84—C83—H83A	108.9
C10—C9—C8	116.20 (15)	C82—C83—H83A	108.9
C11—C10—C9	121.11 (15)	C84—C83—H83B	108.9

C11—C10—H10	119.4	C82—C83—H83B	108.9
C9—C10—H10	119.4	H83A—C83—H83B	107.7
C10—C11—C6	123.53 (15)	C85—C84—C83	112.66 (18)
C10—C11—H11	118.2	C85—C84—H84A	109.1
C6—C11—H11	118.2	C83—C84—H84A	109.1
N5—C12—C13	114.39 (15)	C85—C84—H84B	109.1
N5—C12—H12A	108.7	C83—C84—H84B	109.1
C13—C12—H12A	108.7	H84A—C84—H84B	107.8
N5—C12—H12B	108.7	C84—C85—H85A	109.5
C13—C12—H12B	108.7	C84—C85—H85B	109.5
H12A—C12—H12B	107.6	H85A—C85—H85B	109.5
C12—C13—C14	111.97 (16)	C84—C85—H85C	109.5
C12—C13—H13A	109.2	H85A—C85—H85C	109.5
C14—C13—H13A	109.2	H85B—C85—H85C	109.5
C12—C13—H13B	109.2	C91—C86—C87	114.62 (14)
C14—C13—H13B	109.2	C91—C86—B3	121.40 (14)
H13A—C13—H13B	107.9	C87—C86—B3	123.97 (14)
C13—C14—C15	112.9 (2)	C88—C87—C86	122.98 (15)
C13—C14—H14A	109.0	C88—C87—H87	118.5
C15—C14—H14A	109.0	C86—C87—H87	118.5
C13—C14—H14B	109.0	C87—C88—C89	121.29 (15)
C15—C14—H14B	109.0	C87—C88—H88	119.4
H14A—C14—H14B	107.8	C89—C88—H88	119.4
C14—C15—H15A	109.5	C90—C89—C88	116.90 (14)
C14—C15—H15B	109.5	C90—C89—N10	122.51 (15)
H15A—C15—H15B	109.5	C88—C89—N10	120.53 (14)
C14—C15—H15C	109.5	C91—C90—C89	120.76 (15)
H15A—C15—H15C	109.5	C91—C90—H90	119.6
H15B—C15—H15C	109.5	C89—C90—H90	119.6
N5—C16—C17	114.49 (15)	C90—C91—C86	123.44 (15)
N5—C16—H16A	108.6	C90—C91—H91	118.3
C17—C16—H16A	108.6	C86—C91—H91	118.3
N5—C16—H16B	108.6	N10—C92—C93	114.61 (14)
C17—C16—H16B	108.6	N10—C92—H92A	108.6
H16A—C16—H16B	107.6	C93—C92—H92A	108.6
C16—C17—C18	111.63 (16)	N10—C92—H92B	108.6
C16—C17—H17A	109.3	C93—C92—H92B	108.6
C18—C17—H17A	109.3	H92A—C92—H92B	107.6
C16—C17—H17B	109.3	C94—C93—C92	112.09 (15)
C18—C17—H17B	109.3	C94—C93—H93A	109.2
H17A—C17—H17B	108.0	C92—C93—H93A	109.2
C19—C18—C17	113.31 (19)	C94—C93—H93B	109.2
C19—C18—H18A	108.9	C92—C93—H93B	109.2
C17—C18—H18A	108.9	H93A—C93—H93B	107.9
C19—C18—H18B	108.9	C93—C94—C95	113.53 (17)
C17—C18—H18B	108.9	C93—C94—H94A	108.9
H18A—C18—H18B	107.7	C95—C94—H94A	108.9
C18—C19—H19A	109.5	C93—C94—H94B	108.9

C18—C19—H19B	109.5	C95—C94—H94B	108.9
H19A—C19—H19B	109.5	H94A—C94—H94B	107.7
C18—C19—H19C	109.5	C94—C95—H95A	109.5
H19A—C19—H19C	109.5	C94—C95—H95B	109.5
H19B—C19—H19C	109.5	H95A—C95—H95B	109.5
C25—C20—C21	113.62 (14)	C94—C95—H95C	109.5
C25—C20—B1	125.25 (14)	H95A—C95—H95C	109.5
C21—C20—B1	121.09 (14)	H95B—C95—H95C	109.5
C22—C21—C20	124.36 (16)	N10—C96—C97	113.51 (16)
C22—C21—H21	117.8	N10—C96—H96A	108.9
C20—C21—H21	117.8	C97—C96—H96A	108.9
C21—C22—C23	120.85 (15)	N10—C96—H96B	108.9
C21—C22—H22	119.6	C97—C96—H96B	108.9
C23—C22—H22	119.6	H96A—C96—H96B	107.7
N6—C23—C24	121.98 (15)	C98—C97—C96	111.66 (18)
N6—C23—C22	121.91 (15)	C98—C97—H97A	109.3
C24—C23—C22	116.11 (15)	C96—C97—H97A	109.3
C25—C24—C23	121.50 (16)	C98—C97—H97B	109.3
C25—C24—H24	119.3	C96—C97—H97B	109.3
C23—C24—H24	119.3	H97A—C97—H97B	107.9
C24—C25—C20	123.54 (15)	C99—C98—C97	120.6 (5)
C24—C25—H25	118.2	C97—C98—C99′	101.1 (5)
C20—C25—H25	118.2	C99—C98—H98A	107.2
N6—C26—C27	114.34 (15)	C97—C98—H98A	107.2
N6—C26—H26A	108.7	C99—C98—H98B	107.2
C27—C26—H26A	108.7	C97—C98—H98B	107.2
N6—C26—H26B	108.7	H98A—C98—H98B	106.8
C27—C26—H26B	108.7	C97—C98—H98C	111.6
H26A—C26—H26B	107.6	C99′—C98—H98C	111.6
C26—C27—C28	113.47 (15)	C97—C98—H98D	111.6
C26—C27—H27A	108.9	C99′—C98—H98D	111.6
C28—C27—H27A	108.9	H98C—C98—H98D	109.4
C26—C27—H27B	108.9	C98—C99—H99A	109.5
C28—C27—H27B	108.9	C98—C99—H99B	109.5
H27A—C27—H27B	107.7	H99A—C99—H99B	109.5
C29—C28—C27	112.82 (17)	C98—C99—H99C	109.5
C29—C28—H28A	109.0	H99A—C99—H99C	109.5
C27—C28—H28A	109.0	H99B—C99—H99C	109.5
C29—C28—H28B	109.0	C98—C99′—H99D	109.5
C27—C28—H28B	109.0	C98—C99′—H99E	109.5
H28A—C28—H28B	107.8	H99D—C99′—H99E	109.5
C28—C29—H29A	109.5	C98—C99′—H99F	109.5
C28—C29—H29B	109.5	H99D—C99′—H99F	109.5
H29A—C29—H29B	109.5	H99E—C99′—H99F	109.5
C28—C29—H29C	109.5	C104—C100—C101	114.80 (14)
H29A—C29—H29C	109.5	C104—C100—B4	124.32 (14)
H29B—C29—H29C	109.5	C101—C100—B4	120.61 (14)
N6—C30—C31	114.4 (7)	C102—C101—C100	121.17 (15)

N6—C30—H30A	108.7	C102—C101—H101	119.4
C31—C30—H30A	108.7	C100—C101—H101	119.4
N6—C30—H30B	108.7	C101—C102—C103	119.51 (15)
C31—C30—H30B	108.7	C101—C102—H102	120.2
H30A—C30—H30B	107.6	C103—C102—H102	120.2
C32—C31—C30	112.1 (5)	N4—C103—C102	120.91 (15)
C32—C31—H31A	109.2	N4—C103—H103	119.5
C30—C31—H31A	109.2	C102—C103—H103	119.5
C32—C31—H31B	109.2	N4—C104—C100	124.83 (14)
C30—C31—H31B	109.2	N4—C104—H104	117.6
H31A—C31—H31B	107.9	C100—C104—H104	117.6
C33—C32—C31	114.0 (3)	C106—C105—C110	114.09 (14)
C33—C32—H32A	108.7	C106—C105—B4	125.62 (14)
C31—C32—H32A	108.7	C110—C105—B4	120.06 (14)
C33—C32—H32B	108.7	C107—C106—C105	123.19 (15)
C31—C32—H32B	108.7	C107—C106—H106	118.4
H32A—C32—H32B	107.6	C105—C106—H106	118.4
C32—C33—H33A	109.5	C106—C107—C108	121.37 (15)
C32—C33—H33B	109.5	C106—C107—H107	119.3
H33A—C33—H33B	109.5	C108—C107—H107	119.3
C32—C33—H33C	109.5	C109—C108—C107	116.29 (14)
H33A—C33—H33C	109.5	C109—C108—N11	121.73 (14)
H33B—C33—H33C	109.5	C107—C108—N11	121.91 (14)
N6—C30′—C31′	118.0 (19)	C110—C109—C108	121.26 (15)
N6—C30′—H30C	107.8	C110—C109—H109	119.4
C31′—C30′—H30C	107.8	C108—C109—H109	119.4
N6—C30′—H30D	107.8	C109—C110—C105	123.79 (15)
C31′—C30′—H30D	107.8	C109—C110—H110	118.1
H30C—C30′—H30D	107.1	C105—C110—H110	118.1
C32′—C31′—C30′	112.2 (13)	N11—C111—C112	115.47 (14)
C32′—C31′—H31C	109.2	N11—C111—H11A	108.4
C30′—C31′—H31C	109.2	C112—C111—H11A	108.4
C32′—C31′—H31D	109.2	N11—C111—H11B	108.4
C30′—C31′—H31D	109.2	C112—C111—H11B	108.4
H31C—C31′—H31D	107.9	H11A—C111—H11B	107.5
C33′—C32′—C31′	116.3 (8)	C113—C112—C111	111.75 (14)
C33′—C32′—H32C	108.2	C113—C112—H11C	109.3
C31′—C32′—H32C	108.2	C111—C112—H11C	109.3
C33′—C32′—H32D	108.2	C113—C112—H11D	109.3
C31′—C32′—H32D	108.2	C111—C112—H11D	109.3
H32C—C32′—H32D	107.4	H11C—C112—H11D	107.9
C32′—C33′—H33D	109.5	C114—C113—C112	113.65 (16)
C32′—C33′—H33E	109.5	C114—C113—H11E	108.8
H33D—C33′—H33E	109.5	C112—C113—H11E	108.8
C32′—C33′—H33F	109.5	C114—C113—H11F	108.8
H33D—C33′—H33F	109.5	C112—C113—H11F	108.8
H33E—C33′—H33F	109.5	H11E—C113—H11F	107.7
C35—C34—C38	115.28 (14)	C113—C114—H11G	109.5

C35—C34—B2	122.31 (14)	C113—C114—H11H	109.5
C38—C34—B2	122.09 (13)	H11G—C114—H11H	109.5
N2—C35—C34	124.49 (14)	C113—C114—H11I	109.5
N2—C35—H35	117.8	H11G—C114—H11I	109.5
C34—C35—H35	117.8	H11H—C114—H11I	109.5
N2—C36—C37	121.20 (14)	N11—C115—C116	114.11 (13)
N2—C36—H36	119.4	N11—C115—H11J	108.7
C37—C36—H36	119.4	C116—C115—H11J	108.7
C36—C37—C38	119.28 (15)	N11—C115—H11K	108.7
C36—C37—H37	120.4	C116—C115—H11K	108.7
C38—C37—H37	120.4	H11J—C115—H11K	107.6
C37—C38—C34	121.01 (15)	C117—C116—C115	112.49 (14)
C37—C38—H38	119.5	C117—C116—H11L	109.1
C34—C38—H38	119.5	C115—C116—H11L	109.1
C44—C39—C40	114.29 (14)	C117—C116—H11M	109.1
C44—C39—B2	124.08 (13)	C115—C116—H11M	109.1
C40—C39—B2	121.63 (13)	H11L—C116—H11M	107.8
C41—C40—C39	123.87 (14)	C116—C117—C118	112.59 (16)
C41—C40—H40	118.1	C116—C117—H11N	109.1
C39—C40—H40	118.1	C118—C117—H11N	109.1
C40—C41—C42	120.69 (14)	C116—C117—H11O	109.1
C40—C41—H41	119.7	C118—C117—H11O	109.1
C42—C41—H41	119.7	H11N—C117—H11O	107.8
N7—C42—C43	120.81 (14)	C117—C118—H11P	109.5
N7—C42—C41	122.62 (14)	C117—C118—H11Q	109.5
C43—C42—C41	116.58 (14)	H11P—C118—H11Q	109.5
C44—C43—C42	121.41 (14)	C117—C118—H11R	109.5
C44—C43—H43	119.3	H11P—C118—H11R	109.5
C42—C43—H43	119.3	H11Q—C118—H11R	109.5
C43—C44—C39	123.15 (14)	C124—C119—C120	114.23 (14)
C43—C44—H44	118.4	C124—C119—B4	123.19 (14)
C39—C44—H44	118.4	C120—C119—B4	122.10 (14)
N7—C45—C46	115.03 (15)	C121—C120—C119	123.28 (16)
N7—C45—H45A	108.5	C121—C120—H120	118.4
C46—C45—H45A	108.5	C119—C120—H120	118.4
N7—C45—H45B	108.5	C120—C121—C122	121.25 (16)
C46—C45—H45B	108.5	C120—C121—H121	119.4
H45A—C45—H45B	107.5	C122—C121—H121	119.4
C47—C46—C45	113.14 (15)	N12—C122—C123	121.49 (17)
C47—C46—H46A	109.0	N12—C122—C121	121.96 (17)
C45—C46—H46A	109.0	C123—C122—C121	116.54 (16)
C47—C46—H46B	109.0	C124—C123—C122	121.23 (17)
C45—C46—H46B	109.0	C124—C123—H123	119.4
H46A—C46—H46B	107.8	C122—C123—H123	119.4
C48—C47—C46	113.13 (17)	C123—C124—C119	123.44 (16)
C48—C47—H47A	109.0	C123—C124—H124	118.3
C46—C47—H47A	109.0	C119—C124—H124	118.3
C48—C47—H47B	109.0	N12—C125—C126	112.1 (4)

C46—C47—H47B	109.0	N12—C125—H12C	109.2
H47A—C47—H47B	107.8	C126—C125—H12C	109.2
C47—C48—H48A	109.5	N12—C125—H12D	109.2
C47—C48—H48B	109.5	C126—C125—H12D	109.2
H48A—C48—H48B	109.5	H12C—C125—H12D	107.9
C47—C48—H48C	109.5	C127—C126—C125	112.4 (4)
H48A—C48—H48C	109.5	C127—C126—H12E	109.1
H48B—C48—H48C	109.5	C125—C126—H12E	109.1
N7—C49—C50	115.54 (15)	C127—C126—H12F	109.1
N7—C49—H49A	108.4	C125—C126—H12F	109.1
C50—C49—H49A	108.4	H12E—C126—H12F	107.9
N7—C49—H49B	108.4	C128—C127—C126	112.5 (4)
C50—C49—H49B	108.4	C128—C127—H12G	109.1
H49A—C49—H49B	107.5	C126—C127—H12G	109.1
C51—C50—C49	110.81 (16)	C128—C127—H12H	109.1
C51—C50—H50A	109.5	C126—C127—H12H	109.1
C49—C50—H50A	109.5	H12G—C127—H12H	107.8
C51—C50—H50B	109.5	C127—C128—H12I	109.5
C49—C50—H50B	109.5	C127—C128—H12J	109.5
H50A—C50—H50B	108.1	H12I—C128—H12J	109.5
C52—C51—C50	114.71 (19)	C127—C128—H12K	109.5
C52—C51—H51A	108.6	H12I—C128—H12K	109.5
C50—C51—H51A	108.6	H12J—C128—H12K	109.5
C52—C51—H51B	108.6	N12—C129—C130	106.0 (3)
C50—C51—H51B	108.6	N12—C129—H12L	110.5
H51A—C51—H51B	107.6	C130—C129—H12L	110.5
C51—C52—H52A	109.5	N12—C129—H12M	110.5
C51—C52—H52B	109.5	C130—C129—H12M	110.5
H52A—C52—H52B	109.5	H12L—C129—H12M	108.7
C51—C52—H52C	109.5	C131—C130—C129	114.9 (4)
H52A—C52—H52C	109.5	C131—C130—H13C	108.5
H52B—C52—H52C	109.5	C129—C130—H13C	108.5
C54—C53—C58	114.34 (14)	C131—C130—H13D	108.5
C54—C53—B2	124.92 (14)	C129—C130—H13D	108.5
C58—C53—B2	120.26 (14)	H13C—C130—H13D	107.5
C55—C54—C53	123.33 (15)	C130—C131—C132	116.1 (4)
C55—C54—H54	118.3	C130—C131—H13E	108.3
C53—C54—H54	118.3	C132—C131—H13E	108.3
C54—C55—C56	121.11 (15)	C130—C131—H13F	108.2
C54—C55—H55	119.4	C132—C131—H13F	108.2
C56—C55—H55	119.4	H13E—C131—H13F	107.4
N8—C56—C55	122.14 (15)	C131—C132—H13G	109.5
N8—C56—C57	121.29 (15)	C131—C132—H13H	109.5
C55—C56—C57	116.57 (14)	H13G—C132—H13H	109.5
C58—C57—C56	120.79 (15)	C131—C132—H13I	109.5
C58—C57—H57	119.6	H13G—C132—H13I	109.5
C56—C57—H57	119.6	H13H—C132—H13I	109.5
C57—C58—C53	123.71 (15)	N12—C133—C134	114.3 (8)

C57—C58—H58	118.1	N12—C133—H13J	108.7
C53—C58—H58	118.1	C134—C133—H13J	108.7
N8—C59—C60	113.87 (16)	N12—C133—H13K	108.7
N8—C59—H59A	108.8	C134—C133—H13K	108.7
C60—C59—H59A	108.8	H13J—C133—H13K	107.6
N8—C59—H59B	108.8	C135—C134—C133	111.3 (7)
C60—C59—H59B	108.8	C135—C134—H13L	109.4
H59A—C59—H59B	107.7	C133—C134—H13L	109.4
C59—C60—C61	113.38 (16)	C135—C134—H13M	109.4
C59—C60—H60A	108.9	C133—C134—H13M	109.4
C61—C60—H60A	108.9	H13L—C134—H13M	108.0
C59—C60—H60B	108.9	C136—C135—C134	114.7 (7)
C61—C60—H60B	108.9	C136—C135—H13N	108.6
H60A—C60—H60B	107.7	C134—C135—H13N	108.6
C62—C61—C60	112.71 (18)	C136—C135—H13O	108.6
C62—C61—H61A	109.0	C134—C135—H13O	108.6
C60—C61—H61A	109.0	H13N—C135—H13O	107.6
C62—C61—H61B	109.0	C135—C136—H13P	109.5
C60—C61—H61B	109.0	C135—C136—H13Q	109.5
H61A—C61—H61B	107.8	H13P—C136—H13Q	109.5
C61—C62—H62A	109.5	C135—C136—H13R	109.5
C61—C62—H62B	109.5	H13P—C136—H13R	109.5
H62A—C62—H62B	109.5	H13Q—C136—H13R	109.5
C61—C62—H62C	109.5	C138—C137—N12	101.7 (7)
H62A—C62—H62C	109.5	C138—C137—H13S	111.4
H62B—C62—H62C	109.5	N12—C137—H13S	111.4
N8—C63—C64	112.7 (2)	C138—C137—H13T	111.4
N8—C63—H63A	109.1	N12—C137—H13T	111.4
C64—C63—H63A	109.1	H13S—C137—H13T	109.3
N8—C63—H63B	109.1	C139—C138—C137	113.9 (8)
C64—C63—H63B	109.1	C139—C138—H13U	108.8
H63A—C63—H63B	107.8	C137—C138—H13U	108.8
C65—C64—C63	113.8 (2)	C139—C138—H13V	108.8
C65—C64—H64A	108.8	C137—C138—H13V	108.8
C63—C64—H64A	108.8	H13U—C138—H13V	107.7
C65—C64—H64B	108.8	C140—C139—C138	109.3 (10)
C63—C64—H64B	108.8	C140—C139—H13W	109.8
H64A—C64—H64B	107.7	C138—C139—H13W	109.8
C64—C65—C66	112.7 (2)	C140—C139—H13X	109.8
C64—C65—H65A	109.1	C138—C139—H13X	109.8
C66—C65—H65A	109.1	H13W—C139—H13X	108.3
C64—C65—H65B	109.1	C139—C140—H14C	109.5
C66—C65—H65B	109.1	C139—C140—H14D	109.5
H65A—C65—H65B	107.8	H14C—C140—H14D	109.5
C65—C66—H66A	109.5	C139—C140—H14E	109.5
C65—C66—H66B	109.5	H14C—C140—H14E	109.5
H66A—C66—H66B	109.5	H14D—C140—H14E	109.5
C65—C66—H66C	109.5	C6—B1—C20	114.39 (13)

H66A—C66—H66C	109.5	C6—B1—C1	110.66 (13)
H66B—C66—H66C	109.5	C20—B1—C1	113.97 (13)
N8—C63′—C64′	117.9 (12)	C6—B1—N2	106.11 (12)
N8—C63′—H63C	107.8	C20—B1—N2	105.77 (12)
C64′—C63′—H63C	107.8	C1—B1—N2	105.05 (12)
N8—C63′—H63D	107.8	C53—B2—C39	116.24 (13)
C64′—C63′—H63D	107.8	C53—B2—C34	113.96 (13)
H63C—C63′—H63D	107.2	C39—B2—C34	108.22 (12)
C65′—C64′—C63′	116.0 (11)	C53—B2—N3	104.57 (12)
C65′—C64′—H64C	108.3	C39—B2—N3	108.50 (12)
C63′—C64′—H64C	108.3	C34—B2—N3	104.52 (12)
C65′—C64′—H64D	108.3	C86—B3—C67	108.43 (12)
C63′—C64′—H64D	108.3	C86—B3—C72	116.22 (13)
H64C—C64′—H64D	107.4	C67—B3—C72	113.51 (13)
C64′—C65′—C66′	114.2 (11)	C86—B3—N4	109.12 (12)
C64′—C65′—H65C	108.7	C67—B3—N4	105.00 (12)
C66′—C65′—H65C	108.7	C72—B3—N4	103.82 (12)
C64′—C65′—H65D	108.7	C119—B4—C105	117.55 (13)
C66′—C65′—H65D	108.7	C119—B4—C100	112.16 (13)
H65C—C65′—H65D	107.6	C105—B4—C100	106.33 (13)
C65′—C66′—H66D	109.5	C119—B4—N1	103.71 (12)
C65′—C66′—H66E	109.5	C105—B4—N1	110.34 (12)
H66D—C66′—H66E	109.5	C100—B4—N1	106.25 (12)
C65′—C66′—H66F	109.5		

C3—N1—C2—C1	1.1 (2)	C89—N10—C92—C93	81.10 (18)
B4—N1—C2—C1	−178.68 (14)	C96—N10—C92—C93	−57.82 (19)
C5—C1—C2—N1	−0.5 (2)	N10—C92—C93—C94	−176.00 (15)
B1—C1—C2—N1	175.87 (14)	C92—C93—C94—C95	−176.22 (17)
C2—N1—C3—C4	−0.7 (2)	C89—N10—C96—C97	163.29 (15)
B4—N1—C3—C4	179.08 (15)	C92—N10—C96—C97	−57.9 (2)
N1—C3—C4—C5	−0.2 (3)	N10—C96—C97—C98	−175.99 (16)
C3—C4—C5—C1	0.9 (3)	C96—C97—C98—C99	−176.4 (5)
C2—C1—C5—C4	−0.5 (2)	C96—C97—C98—C99′	171.6 (5)
B1—C1—C5—C4	−176.96 (15)	C104—C100—C101—C102	1.4 (2)
C11—C6—C7—C8	−0.8 (2)	B4—C100—C101—C102	175.70 (15)
B1—C6—C7—C8	171.73 (15)	C100—C101—C102—C103	−3.2 (2)
C6—C7—C8—C9	−0.9 (3)	C104—N4—C103—C102	1.7 (2)
C16—N5—C9—C10	4.5 (2)	B3—N4—C103—C102	−177.95 (14)
C12—N5—C9—C10	164.24 (16)	C101—C102—C103—N4	1.6 (2)
C16—N5—C9—C8	−176.43 (15)	C103—N4—C104—C100	−3.8 (2)
C12—N5—C9—C8	−16.6 (2)	B3—N4—C104—C100	175.93 (14)
C7—C8—C9—N5	−177.62 (15)	C101—C100—C104—N4	2.2 (2)
C7—C8—C9—C10	1.6 (2)	B4—C100—C104—N4	−171.90 (14)
N5—C9—C10—C11	178.63 (16)	C110—C105—C106—C107	−0.7 (2)
C8—C9—C10—C11	−0.5 (2)	B4—C105—C106—C107	−175.25 (15)
C9—C10—C11—C6	−1.2 (3)	C105—C106—C107—C108	0.0 (3)
C7—C6—C11—C10	1.8 (2)	C106—C107—C108—C109	0.9 (2)

B1—C6—C11—C10	−170.67 (15)	C106—C107—C108—N11	−175.95 (15)
C9—N5—C12—C13	84.50 (19)	C115—N11—C108—C109	−5.0 (2)
C16—N5—C12—C13	−115.00 (17)	C111—N11—C108—C109	139.04 (16)
N5—C12—C13—C14	−173.19 (15)	C115—N11—C108—C107	171.65 (15)
C12—C13—C14—C15	178.14 (18)	C111—N11—C108—C107	−44.3 (2)
C9—N5—C16—C17	78.3 (2)	C107—C108—C109—C110	−0.9 (2)
C12—N5—C16—C17	−81.95 (19)	N11—C108—C109—C110	175.92 (15)
N5—C16—C17—C18	−173.87 (16)	C108—C109—C110—C105	0.1 (3)
C16—C17—C18—C19	178.4 (2)	C106—C105—C110—C109	0.7 (2)
C25—C20—C21—C22	−0.5 (2)	B4—C105—C110—C109	175.55 (15)
B1—C20—C21—C22	177.66 (15)	C108—N11—C111—C112	−92.97 (18)
C20—C21—C22—C23	1.5 (2)	C115—N11—C111—C112	51.78 (19)
C30′—N6—C23—C24	7.0 (11)	N11—C111—C112—C113	177.03 (14)
C26—N6—C23—C24	−177.36 (15)	C111—C112—C113—C114	177.73 (15)
C30—N6—C23—C24	−0.6 (4)	C108—N11—C115—C116	−159.85 (14)
C30′—N6—C23—C22	−173.0 (11)	C111—N11—C115—C116	54.89 (19)
C26—N6—C23—C22	2.7 (2)	N11—C115—C116—C117	−179.01 (15)
C30—N6—C23—C22	179.4 (4)	C115—C116—C117—C118	−176.24 (16)
C21—C22—C23—N6	178.60 (15)	C124—C119—C120—C121	1.7 (2)
C21—C22—C23—C24	−1.4 (2)	B4—C119—C120—C121	−170.60 (16)
N6—C23—C24—C25	−179.51 (15)	C119—C120—C121—C122	−2.2 (3)
C22—C23—C24—C25	0.5 (2)	C125—N12—C122—C123	−163.1 (3)
C23—C24—C25—C20	0.5 (3)	C129—N12—C122—C123	11.9 (4)
C21—C20—C25—C24	−0.5 (2)	C137—N12—C122—C123	−20.8 (5)
B1—C20—C25—C24	−178.53 (15)	C133—N12—C122—C123	172.7 (5)
C23—N6—C26—C27	85.3 (2)	C125—N12—C122—C121	18.2 (4)
C30′—N6—C26—C27	−98.5 (10)	C129—N12—C122—C121	−166.8 (2)
C30—N6—C26—C27	−91.4 (4)	C137—N12—C122—C121	160.6 (5)
N6—C26—C27—C28	−176.90 (15)	C133—N12—C122—C121	−6.0 (6)
C26—C27—C28—C29	81.6 (2)	C120—C121—C122—N12	179.60 (19)
C23—N6—C30—C31	−79.8 (8)	C120—C121—C122—C123	0.9 (3)
C26—N6—C30—C31	97.0 (6)	N12—C122—C123—C124	−177.98 (19)
N6—C30—C31—C32	172.2 (5)	C121—C122—C123—C124	0.8 (3)
C30—C31—C32—C33	64.8 (5)	C122—C123—C124—C119	−1.2 (3)
C23—N6—C30′—C31′	−87 (2)	C120—C119—C124—C123	0.0 (2)
C26—N6—C30′—C31′	97 (2)	B4—C119—C124—C123	172.18 (16)
N6—C30′—C31′—C32′	179.6 (17)	C122—N12—C125—C126	−93.3 (5)
C30′—C31′—C32′—C33′	168.3 (15)	N12—C125—C126—C127	−173.8 (4)
C36—N2—C35—C34	−4.3 (2)	C125—C126—C127—C128	178.5 (5)
B1—N2—C35—C34	176.82 (14)	C122—N12—C129—C130	−87.2 (3)
C38—C34—C35—N2	2.7 (2)	N12—C129—C130—C131	166.9 (3)
B2—C34—C35—N2	−170.84 (14)	C129—C130—C131—C132	−73.1 (6)
C35—N2—C36—C37	2.0 (2)	C122—N12—C133—C134	−76.8 (10)
B1—N2—C36—C37	−179.20 (14)	N12—C133—C134—C135	173.8 (7)
N2—C36—C37—C38	1.5 (2)	C133—C134—C135—C136	65.0 (10)
C36—C37—C38—C34	−3.1 (2)	C122—N12—C137—C138	92.2 (6)
C35—C34—C38—C37	1.1 (2)	N12—C137—C138—C139	−176.9 (7)
B2—C34—C38—C37	174.66 (14)	C137—C138—C139—C140	79.2 (12)

C44—C39—C40—C41	1.0 (2)	C7—C6—B1—C20	152.91 (15)
B2—C39—C40—C41	−178.74 (15)	C11—C6—B1—C20	−35.2 (2)
C39—C40—C41—C42	−0.9 (3)	C7—C6—B1—C1	22.5 (2)
C45—N7—C42—C43	−173.95 (15)	C11—C6—B1—C1	−165.59 (14)
C49—N7—C42—C43	−21.9 (2)	C7—C6—B1—N2	−90.89 (17)
C45—N7—C42—C41	6.3 (2)	C11—C6—B1—N2	80.98 (17)
C49—N7—C42—C41	158.28 (15)	C25—C20—B1—C6	−108.23 (17)
C40—C41—C42—N7	−179.64 (15)	C21—C20—B1—C6	73.87 (18)
C40—C41—C42—C43	0.6 (2)	C25—C20—B1—C1	20.5 (2)
N7—C42—C43—C44	179.85 (15)	C21—C20—B1—C1	−157.41 (14)
C41—C42—C43—C44	−0.4 (2)	C25—C20—B1—N2	135.38 (15)
C42—C43—C44—C39	0.5 (3)	C21—C20—B1—N2	−42.53 (18)
C40—C39—C44—C43	−0.8 (2)	C2—C1—B1—C6	−115.48 (16)
B2—C39—C44—C43	178.96 (15)	C5—C1—B1—C6	60.66 (19)
C42—N7—C45—C46	77.8 (2)	C2—C1—B1—C20	113.93 (16)
C49—N7—C45—C46	−75.17 (19)	C5—C1—B1—C20	−69.93 (19)
N7—C45—C46—C47	172.42 (15)	C2—C1—B1—N2	−1.4 (2)
C45—C46—C47—C48	−176.10 (18)	C5—C1—B1—N2	174.77 (14)
C42—N7—C49—C50	92.00 (19)	C36—N2—B1—C6	19.83 (19)
C45—N7—C49—C50	−114.86 (17)	C35—N2—B1—C6	−161.40 (13)
N7—C49—C50—C51	−179.14 (15)	C36—N2—B1—C20	141.71 (14)
C49—C50—C51—C52	179.38 (17)	C35—N2—B1—C20	−39.52 (17)
C58—C53—C54—C55	−2.0 (2)	C36—N2—B1—C1	−97.43 (16)
B2—C53—C54—C55	170.08 (15)	C35—N2—B1—C1	81.35 (15)
C53—C54—C55—C56	−1.0 (3)	C54—C53—B2—C39	122.93 (16)
C63—N8—C56—C55	168.25 (18)	C58—C53—B2—C39	−65.48 (19)
C59—N8—C56—C55	12.6 (2)	C54—C53—B2—C34	−4.0 (2)
C63′—N8—C56—C55	−172.5 (6)	C58—C53—B2—C34	167.61 (14)
C63—N8—C56—C57	−11.8 (3)	C54—C53—B2—N3	−117.49 (16)
C59—N8—C56—C57	−167.48 (16)	C58—C53—B2—N3	54.10 (17)
C63′—N8—C56—C57	7.4 (6)	C44—C39—B2—C53	13.5 (2)
C54—C55—C56—N8	−176.42 (16)	C40—C39—B2—C53	−166.82 (14)
C54—C55—C56—C57	3.7 (2)	C44—C39—B2—C34	143.20 (15)
N8—C56—C57—C58	176.73 (16)	C40—C39—B2—C34	−37.11 (19)
C55—C56—C57—C58	−3.4 (2)	C44—C39—B2—N3	−103.93 (17)
C56—C57—C58—C53	0.4 (3)	C40—C39—B2—N3	75.75 (17)
C54—C53—C58—C57	2.3 (2)	C35—C34—B2—C53	−120.46 (15)
B2—C53—C58—C57	−170.17 (15)	C38—C34—B2—C53	66.40 (19)
C56—N8—C59—C60	−93.5 (2)	C35—C34—B2—C39	108.57 (16)
C63—N8—C59—C60	109.4 (2)	C38—C34—B2—C39	−64.57 (18)
C63′—N8—C59—C60	91.8 (7)	C35—C34—B2—N3	−6.92 (18)
N8—C59—C60—C61	178.10 (16)	C38—C34—B2—N3	179.94 (13)
C59—C60—C61—C62	−176.29 (18)	C69—N3—B2—C53	−140.54 (14)
C56—N8—C63—C64	−76.9 (3)	C68—N3—B2—C53	44.40 (16)
C59—N8—C63—C64	79.9 (3)	C69—N3—B2—C39	−15.88 (19)
N8—C63—C64—C65	177.9 (2)	C68—N3—B2—C39	169.06 (12)
C63—C64—C65—C66	169.0 (3)	C69—N3—B2—C34	99.42 (15)
C56—N8—C63′—C64′	−80.3 (15)	C68—N3—B2—C34	−75.64 (15)

C59—N8—C63′—C64′	94.5 (15)	C91—C86—B3—C67	30.03 (19)
N8—C63′—C64′—C65′	−57.9 (19)	C87—C86—B3—C67	−150.62 (14)
C63′—C64′—C65′—C66′	179.6 (14)	C91—C86—B3—C72	159.29 (14)
C69—N3—C68—C67	1.8 (2)	C87—C86—B3—C72	−21.4 (2)
B2—N3—C68—C67	177.09 (13)	C91—C86—B3—N4	−83.81 (17)
C71—C67—C68—N3	0.2 (2)	C87—C86—B3—N4	95.54 (17)
B3—C67—C68—N3	174.83 (14)	C68—C67—B3—C86	−107.07 (16)
C68—N3—C69—C70	−1.4 (2)	C71—C67—B3—C86	67.29 (17)
B2—N3—C69—C70	−176.45 (14)	C68—C67—B3—C72	122.18 (15)
N3—C69—C70—C71	−0.8 (2)	C71—C67—B3—C72	−63.46 (18)
C69—C70—C71—C67	2.8 (2)	C68—C67—B3—N4	9.46 (19)
C68—C67—C71—C70	−2.4 (2)	C71—C67—B3—N4	−176.18 (13)
B3—C67—C71—C70	−177.25 (14)	C73—C72—B3—C86	−108.96 (17)
C77—C72—C73—C74	−0.1 (2)	C77—C72—B3—C86	78.03 (18)
B3—C72—C73—C74	−173.52 (15)	C73—C72—B3—C67	17.8 (2)
C72—C73—C74—C75	2.5 (3)	C77—C72—B3—C67	−155.22 (14)
C78—N9—C75—C76	177.93 (18)	C73—C72—B3—N4	131.23 (15)
C82—N9—C75—C76	−1.9 (3)	C77—C72—B3—N4	−41.78 (18)
C78—N9—C75—C74	−1.2 (3)	C103—N4—B3—C86	11.04 (19)
C82—N9—C75—C74	178.93 (18)	C104—N4—B3—C86	−168.65 (12)
C73—C74—C75—N9	176.58 (17)	C103—N4—B3—C67	−105.01 (15)
C73—C74—C75—C76	−2.6 (3)	C104—N4—B3—C67	75.29 (15)
N9—C75—C76—C77	−178.69 (17)	C103—N4—B3—C72	135.57 (14)
C74—C75—C76—C77	0.5 (2)	C104—N4—B3—C72	−44.12 (16)
C75—C76—C77—C72	2.0 (3)	C124—C119—B4—C105	115.35 (17)
C73—C72—C77—C76	−2.1 (2)	C120—C119—B4—C105	−73.0 (2)
B3—C72—C77—C76	171.63 (15)	C124—C119—B4—C100	−8.4 (2)
C75—N9—C78—C79	84.6 (2)	C120—C119—B4—C100	163.26 (14)
C82—N9—C78—C79	−95.5 (2)	C124—C119—B4—N1	−122.59 (15)
N9—C78—C79—C80	174.06 (17)	C120—C119—B4—N1	49.03 (18)
C78—C79—C80—C81	−164.6 (2)	C106—C105—B4—C119	4.3 (2)
C75—N9—C82—C83	92.4 (2)	C110—C105—B4—C119	−169.90 (14)
C78—N9—C82—C83	−87.5 (2)	C106—C105—B4—C100	130.92 (16)
N9—C82—C83—C84	177.53 (16)	C110—C105—B4—C100	−43.30 (19)
C82—C83—C84—C85	71.5 (2)	C106—C105—B4—N1	−114.26 (16)
C91—C86—C87—C88	0.3 (2)	C110—C105—B4—N1	71.51 (18)
B3—C86—C87—C88	−179.10 (15)	C104—C100—B4—C119	−116.36 (16)
C86—C87—C88—C89	−0.2 (3)	C101—C100—B4—C119	69.90 (18)
C87—C88—C89—C90	−0.3 (2)	C104—C100—B4—C105	113.86 (16)
C87—C88—C89—N10	177.00 (15)	C101—C100—B4—C105	−59.87 (18)
C96—N10—C89—C90	7.7 (2)	C104—C100—B4—N1	−3.70 (19)
C92—N10—C89—C90	−130.50 (17)	C101—C100—B4—N1	−177.44 (13)
C96—N10—C89—C88	−169.40 (15)	C3—N1—B4—C119	−133.48 (15)
C92—N10—C89—C88	52.4 (2)	C2—N1—B4—C119	46.32 (16)
C88—C89—C90—C91	0.6 (2)	C3—N1—B4—C105	−6.7 (2)
N10—C89—C90—C91	−176.58 (15)	C2—N1—B4—C105	173.06 (13)
C89—C90—C91—C86	−0.6 (3)	C3—N1—B4—C100	108.12 (16)
C87—C86—C91—C90	0.1 (2)	C2—N1—B4—C100	−72.07 (16)

B3—C86—C91—C90	179.50 (15)