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Kinetic Stability of Azaborafullerene $C_{58}BN$ as Predicted by the Bond Resonance Energy Model

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The kinetic stability of a polyatomic molecule is very hard to judge. We utilized the bond resonance energy (BRE) model to estimate the kinetic stability of azaborafullerenes $C_{58}BN$. In marked contrast to $C_{58}B_2$ and $C_{58}N_2$, all truncated icosahedron-shaped isomers of $C_{58}BN$ were found to lack chemically reactive substructures. On this theoretical basis, these isomers are presumed to be kinetically fairly stable even under harsh reactor conditions. This explains well why $C_{58}BN$ can be detected by mass spectrometry. At least some of the isomers will be isolated in macroscopic amounts in the near future.

There is continuous interest in the synthesis and characterization of heterofullerenes, in which one or more C atoms of the fullerene cage are substituted by heteroatoms, such as B or N atoms.[1—3] Borafullerenes are generated abundantly by the laser vaporization of a graphite pellet containing boron or boron nitride. However, they cannot be isolated in macroscopic amounts.[1—5] In contrast, the evidence for the formation of azafullerenes by arc synthesis is far from being clear-cut.[1—3] Azafullerenes are not produced by the laser ablation of a boron nitride-graphite composite rod.[1]

The bond resonance energy (BRE) model has been used successfully for predicitng kinetic stability for fullerenes, planar polycyclic aromatic and antiaromatic hydrocarbons, and their molecular ions.[6—15] By kinetic stability, we mean stability against any possible chemical reaction and decomposition.[16] In general, a molecule that has one or more π bonds with a large negative BRE is kinetically very unstable.[6—15] All borafullerenes are chemically reactive in this sense. The kinetic instability of azafullerenes has been presumed to be due to their tendency to liberate N_2 and/or CN during the synthetic process.[15]

The next synthetic target must naturally be azaborafullerenes.[1—3] In fact, there have been some reports on the formation of $C_{58}BN$ in gas-phase heterofullerene preparation experiments.[19,20] However, nobody has succeeded in isolating $C_{58}BN$ in macroscopic quantities. In this paper, we evaluate the BREs for all truncated icosahedron-shaped isomers of $C_{58}BN$ to complement the experiment and estimate their degrees of kinetic stability or chemical inertness. This kind of investigation will give us an important clue to exploring the possibility of producing azaborafullerenes and their molecular ions in large amounts.

Theory

The BRE model has been described repeatedly.[6—15] In brief, the BRE, defined within the framework of simple Hückel theory, represents the contribution of every π bond to the topological resonance energy of the molecule.[21,22] The minimum or smallest BRE in a molecule (min BRE) is closely associated with the kinetic stability of the molecule.[16] If the min BRE is smaller than $-0.100|\beta|$, the molecule is presumed to have chemically reactive substructures. It is noteworthy that the isolated pentagon rule (IPR) and the kinetic stability of fullerene molecular anions have been verified using the BRE model.[6,10,14]

In order to obtain chemically meaningful BREs for all π bonds in $C_{58}BN$, one must select the best set of Hückel heteroatom parameters for such heterofullerenes. We utilize Van-Catledge's parameters listed in Table 1[23] because they are the only ones determined consistently with each other. He reported all necessary parameters in this study. The same parameter set was previously applied to borafullerenes and azafullerenes.[14,15]

Results and Discussion

$C_{58}BN$ has 31 truncated icosahedron-shaped isomers, all of which are isoelectronic with C_{60}.[24] These isomers are designated as follows. First, the carbon atoms are numbered as indicated in the Schlegel diagram of C_{60} in Fig. 1. An N atom substitutes the carbon atom at the 1-position and a B

Table 1. Hückel Parameters for Boron and Nitrogen Atoms

Parameter	Van-Catledge's value[a)]
h_B	−0.45
h_N	1.37
k_{CB}	0.73
k_{CN}	0.89
k_{BN}	0.53

a) Ref. 23.

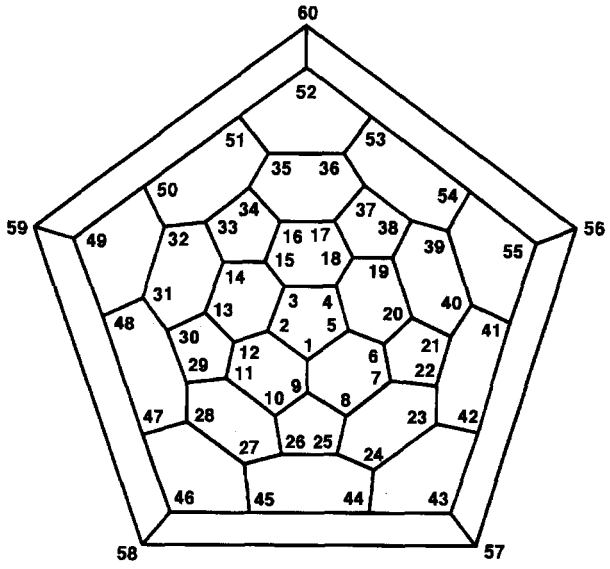

Fig. 1. Schlegel diagram of C_{60}.

atom then substitutes the C atom at the *x*-position to produce isomer **1-*x*** of $C_{58}BN$. $C_{58}BN$ has eight more isomers than $C_{58}B_2$ and $C_{58}N_2$ since the isomers of the former species are lower in molecular symmetry.[26] All isomers have a closed-shell electronic configuration. The highest occupied and lowest unoccupied molecular orbitals are fully bonding and slightly antibonding, respectively.

The min BREs calculated for all isomers of $C_{58}BN$, together with those for $C_{58}B_2$ and $C_{58}N_2$, are presented in Table 2, where the min BREs $< -0.100|\beta|$ are underlined. The min BRE of the prototypical fullerene C_{60} is $0.0822|\beta|$,[6] which implies that all CC bonds contribute to the aromaticity of the molecule. It is noteworthy that all isomers of $C_{58}BN$ have a min BRE $> -0.100|\beta|$. In sharp contrast to $C_{58}B_2$ and $C_{58}N_2$, $C_{58}BN$ has no isomers with a min BRE $< -0.100|\beta|$. Therefore, we can fully expect that all isomers of $C_{58}BN$ are not kinetically very unstable and that at least some of them will be extractable from the products obtained by vaporization of a boron compound-graphite composite rod.

All π bonds with a min BRE are located near the N atom, but are not C–N bonds. As in the case of all-carbon fullerenes,[6,9] relatively weak bonds are 5/6 CC bonds in general. Here, an *m*/*n* bond signifies a π bond shared by *m*- and *n*-membered rings. For seven isomers, 5/6 CB bonds are responsible for the min BRE. For all isomers but **1-7**,

Table 2. Min BREs for Neutral Fullerene Isomers of $C_{58}B_2$, $C_{58}N_2$, and $C_{58}BN$

Isomer	Min BRE/$\lvert\beta\rvert$[a)]		
	$C_{58}B_2$	$C_{58}N_2$	$C_{58}BN$
1-2	−0.3598 (1-2)	−0.2364 (9-10, 11-12)	−0.0091 (9-10)
1-3	−0.1677 (1-5, 3-4)	−0.0838 (8-9, 15-16)	0.0283 (8-9)
1-6	−0.2796 (1-5)	−0.1492 (8-9)	0.0267 (8-9)
1-7	−0.1767 (1-5, 6-7)	−0.1189 (8-9)	0.0212 (7-22)
1-8		The same as **1-6**	0.0186 (8-9)
1-9	−0.2704 (6-7, 11-12)	−0.0897 (6-7, 11-12)	0.0021 (8-9, 9-10)
1-13	−0.1865 (1-5, 13-30)	−0.0190 (6-7, 31-32)	0.0331 (13-30)
1-14	−0.2954 (1-2)	−0.0623 (11-12)	0.0349 (14-15)
1-15	−0.2741 (3-4)	−0.0726 (17-18)	0.0324 (8-9)
1-16	−0.1966 (3-4)	−0.0922 (9-10)	0.0347 (9-10)
1-21		The same as **1-16**	0.0289 (8-9)
1-22		The same as **1-14**	0.0240 (7-22)
1-23	−0.1844 (8-9, 7-22)	−0.0749 (6-7, 8-25)	0.0286 (9-10)
1-24	−0.2245 (6-7, 7-22)	−0.1376 (8-9, 8-25)	0.0301 (7-22)
1-25		The same as **1-15**	0.0239 (25-26)
1-31	−0.1978 (31-48)	−0.1392 (13-30, 29-30)	0.0321 (9-10)
1-32	−0.2328 (1-2)	−0.0738 (11-12)	0.0381 (8-9)
1-33	−0.2028 (11-12, 13-30)	−0.0923 (11-12, 13-30)	0.0343 (9-10)
1-34	−0.2206 (1-2, 16-34)	−0.0627 (6-7, 32-50)	0.0366 (8-9)
1-35	−0.2007 (1-2)	−0.1083 (6-7, 33-34)	0.0351 (9-10)
1-41	−0.1738 (1-5, 40-41)	−0.0482 (6-7, 21-22)	0.0338 (9-10)
1-42		The same as **1-32**	0.0359 (9-10)
1-43		The same as **1-35**	0.0355 (9-10)
1-44		The same as **1-31**	0.0294 (25-26)
1-49	−0.2075 (49-50)	−0.0794 (8-9)	0.0365 (8-9)
1-50	−0.1537 (1-5, 49-50)	−0.0456 (11-12, 33-34)	0.0381 (9-10)
1-51		The same as **1-49**	0.0367 (8-9)
1-52	−0.1912 (6-7, 11-12, 54-55, 49-50)	−0.0527 (6-7, 11-12, 49-50, 54-55)	0.0370 (8-9, 9-10)
1-56	−0.2394 (9-10, 54-55)	−0.1006 (9-10, 54-55)	0.0313 (9-10)
1-57	−0.1731 (1-5, 57-58)	−0.0579 (9-10, 42-43)	0.0336 (9-10)
1-60	−0.1494 (6-7, 11-12, 49-50, 54-55)	−0.0425 (6-7, 11-12, 49-50, 54-55)	0.0359 (8-9, 9-10)

a) Bonds with a min BRE are indicated in parentheses.

even the min BRE has a positive value. As 5/6 CN bonds are parts of aromatic pyrrole substructures, they have a fairly large positive BRE. All 6/6 bonds are kinetically stable with a BRE $> -0.100|\beta|$. According to Chen et al.,[24,25] the thermodynamic stability of $C_{58}BN$ decreases with increasing distance between B and N atoms. However, kinetic stability is indifferent to the distance between the two heteroatoms.

In 1999 Nakamura et al. measured the laser desorption/ionization mass spectra of the products obtained by laser ablation of a BC_2N-graphite composite rod in argon.[21] The mass peak at *m/z* 721 can be attributed to not only $C_{58}{}^{11}B^{14}N$ but also $^{12}C_{59}{}^{13}C$.[3] However, they noticed that the intensity ratio of the *m/z* 721 peak to the 720 peak (83.9 : 100) is higher compared with that of a pure C_{60} sample (70.2 : 100). This is a strong indication that a small amount of $C_{58}BN$ is produced together with C_{60}. The composition of this cluster was further confirmed by producing ^{15}N-labelled clusters.[20] These observations are compatible with the prediction that $C_{58}BN$ is kinetically stable. Nakamura et al. speculated that BN is generated first and then reacts with carbon clusters to form $C_{58}BN$.[20]

Among low-energy isomers of $C_{58}BN$ are **1-9** (957.56), **1-2** (974.23), **1-7** (995.40), **1-6** (1001.01), and **1-8** (1003.07), in which values in parentheses are the heats of formation in kcal mol^{-1} calculated using AM1.[24,25] In these isomers, B and N atoms are situated more or less close to each other. Two of the lowest-energy isomers have a B–N bond, which is isoelectronic with a C=C bond. In addition, the HOMO-LUMO energy gap, a conventional index of kinetic stability, is very large for these isomers. Even if their heats of atomization are somewhat smaller than that of C_{60},[24] at least some low-energy isomers must be contained in the laser ablation products.

In this context, $C_{58}N_2$ has been neither isolated nor detected although there are many isomers with a min BRE $> -0.100|\beta|$.[1–3] Smalley et al. reported that the attempted synthesis of N-containing species from N-doped graphite produces N_2 gas rather than substituted fullerenes.[1] Thus, N_2 is very different in reactivity from BN. It has been suggested that $B_{30}N_{30}$ would not be very stable since it would require that the N–N and B–B bonds exist in the molecule.[4] MNDO study confirmed that N–N bonds have a marked destabilizing effect on the azafullerene cage.[27] This may be the primary reason why $C_{58}N_2$ is difficult to produce. To

Table 3. Min BREs for Neutral or Charged Fullerene Isomers of $C_{58}B_2$, $C_{58}N_2$, and $C_{58}BN$ with 60 π Electrons

Isomer	Min BRE/$\|\beta\|$[a]		
	$C_{58}B_2{}^{2-}$	$C_{58}N_2{}^{2-}$	$C_{58}BN$
1-2	0.0338 (1-5, 2-3)	0.0333 (9-10, 11-12)	−0.0091 (9-10)
1-3	0.0435 (1-5, 3-4)	0.0362 (9-10, 14-15)	0.0283 (8-9)
1-6	0.0233 (6-7)	0.0034 (8-9)	0.0267 (8-9)
1-7	0.0228 (1-5, 6-7)	−0.0198 (8-9)	0.0212 (7-22)
1-8		The same as **1-6**	0.0186 (8-9)
1-9	0.0404 (6-7, 11-12)	0.0236 (14-15, 18-19, 23-24, 27-28)	0.0021 (8-9, 9-10)
1-13	0.0415 (2-3, 11-12)	0.0241 (9-10, 14-15)	0.0331 (13-30)
1-14	0.0443 (2-3)	0.0140 (9-10)	0.0349 (14-15)
1-15	0.0420 (15-16)	0.0176 (9-10)	0.0324 (8-9)
1-16	0.0387 (3-4)	0.0271 (8-9)	0.0347 (9-10)
1-21		The same as **1-16**	0.0289 (8-9)
1-22		The same as **1-14**	0.0240 (7-22)
1-23	0.0530 (1-5, 23-24)	0.0180 (7-22, 8-9)	0.0286 (9-10)
1-24	0.0467 (1-2, 24-44)	0.0094 (9-10, 25-26)	0.0301 (7-22)
1-25		The same as **1-15**	0.0239 (25-26)
1-31	0.0467 (1-2)	0.0260 (13-30)	0.0321 (9-10)
1-32	0.0482 (1-5)	0.0286 (9-10)	0.0381 (8-9)
1-33	0.0491 (1-5, 33-34)	0.0365 (8-9, 32-50)	0.0343 (9-10)
1-34	0.0492 (1-5, 33-34)	0.0330 (9-10, 35-36)	0.0366 (8-9)
1-35	0.0478 (1-5)	0.0321 (16-34)	0.0351 (9-10)
1-41	0.0516 (1-2, 41-55)	0.0314 (8-9, 23-42)	0.0338 (9-10)
1-42		The same as **1-32**	0.0359 (9-10)
1-43		The same as **1-35**	0.0355 (9-10)
1-44		The same as **1-31**	0.0294 (25-26)
1-49	0.0482 (49-50)	0.0338 (8-9)	0.0365 (8-9)
1-50	0.0487 (1-5, 49-50)	0.0336 (8-9, 51-52)	0.0381 (9-10)
1-51		The same as **1-49**	0.0367 (8-9)
1-52	0.0503 (1-2, 1-5, 51-52, 52-53)	0.0373 (8-9, 9-10, 56-60, 59-60)	0.0370 (8-9, 9-10)
1-56	0.0496 (1-5, 56-57)	0.0394 (8-9, 41-55)	0.0313 (9-10)
1-57	0.0487 (1-5, 57-58)	0.0347 (8-9, 43-44)	0.0336 (9-10)
1-60	0.0505 (1-2, 1-5, 56-60, 59-60)	0.0366 (8-9, 9-10, 51-52, 52-53)	0.0359 (8-9, 9-10)

a) Bonds with a min BRE are indicated in parentheses.

make matters worse, the lowest-energy isomer has a min BRE $< -0.100|\beta|$.[15] Fortunately, such delicate situations are irrelevant to $C_{58}BN$.

$C_{58}N_2^{2+}$, $C_{58}B_2^{2-}$, and $C_{58}BN$ are formally isoelectronic with a moderately aromatic C_{60} molecule with 60 π electrons. The min BREs for the isomers of these species are compared in Table 3. It is noteworthy that all species have a min BRE $> -0.100|\beta|$ and are predicted to be kinetically stable without exceptions. Relatively weak bonds in diazafullerene isomers are strengthened by the loss of two or more π electrons. It is very likely that 60 is a magic number of π electrons for truncated icosahedron-shaped heterofullerene molecules made up of 60 conjugated atoms.

The molecular anions with 66 π electrons of $C_{58}B_2$, $C_{58}N_2$, and $C_{58}BN$ are isoelectronic with a moderately aromatic C_{60} hexaanion.[7,10] The min BREs for these species are listed in Table 4. The octaanion of $C_{58}BN$ may be unrealistic since the charge is too large. For reference, the min BRE of C_{60}^{6-} is $0.084|\beta|$, which indicates that all CC bonds contribute to the aromaticity of this hexaanion.[10] It was found that all species listed in Table 4 have a min BRE $> -0.100|\beta|$. In other words, all π bonds in these molecular anions are the source of aromaticity. Therefore, all isomers of $C_{58}B_2^{8-}$, $C_{58}N_2^{4-}$, and $C_{58}BN^{6-}$ are predicted to be kinetically stable. Some of them may be isolable as components of salts[28] or as charged carbon cages in endohedral metallofullerenes.[29]

It wad found that the min BRE is slightly negative in sign for some isomers of $C_{58}BN^{2-}$ and $C_{58}BN^{4-}$. Likewise, C_{60}^{2-} and C_{60}^{4-} have a negative min BRE although the absolute value is small.[10] In contrast, all isomers of $C_{58}N_2^{4-}$, $C_{58}B_2^{8-}$, and $C_{58}BN^{6-}$ have a positive min BRE. Thus, it is very likely that 66, as well as 60, is also a magic number of π electrons for truncated icosahedron-shaped heterofullerene molecules.

Concluding Remarks

In fullerene chemistry, synthetic accessibility is determined primarily by kinetic stability but not by aromaticity.[6,7] However, the kinetic stability is very difficult to estimate. The min BRE has been a very useful index of kinetic stability for molecules in which kinetic stability is determined primarily by π electrons. As has been seen, all isomers of $C_{58}BN$ were predicted to be kinetically very or fairly stable in this sense. We can rather safely say that the π-electronic

Table 4. Min BREs for Charged Fullerene Isomers of $C_{58}B_2$, $C_{58}N_2$, and $C_{58}BN$ with 66 π Electrons

Isomer	Min BRE/$\|\beta\|$[a)]		
	$C_{58}B_2^{8-}$	$C_{58}N_2^{4-}$	$C_{58}BN^{6-}$
1-2	0.0205 (1-5, 2-3)	0.0166 (9-10, 11-12)	0.0211 (56-60)
1-3	0.0311 (1-5, 3-4)	0.0375 (57-58, 59-60)	0.0362 (56-60)
1-6	0.0468 (6-20)	0.0348 (8-9)	0.0230 (6-7)
1-7	0.0468 (4-5, 6-20)	0.0179 (8-9)	0.0204 (6-7)
1-8		The same as **1-6**	0.0070 (9-10)
1-9	0.0610 (35-51, 36-53, 56-57, 58-59)	0.0048 (1-9)	0.0011 (8-9, 9-10)
1-13	0.0466 (1-2, 12-13)	0.0361 (42-43, 52-53)	0.0130 (11-12)
1-14	0.0490 (3-4)	0.0293 (8-9)	0.0372 (15-16)
1-15	0.0531 (14-15)	0.0141 (57-58)	0.0356 (15-16)
1-16	0.0482 (2-3)	0.0197 (35-36)	0.0279 (57-58)
1-21		The same as **1-16**	0.0191 (6-7)
1-22		The same as **1-14**	0.0153 (6-7)
1-23	0.0455 (1-2, 23-42)	0.0314 (32-50, 51-52)	0.0198 (42-43)
1-24	0.0471 (4-5, 23-42)	0.0128 (35-36, 52-53)	0.0230 (42-43)
1-25		The same as **1-15**	0.0027 (8-9)
1-31	0.0443 (31-32)	0.0064 (6-7)	0.0335 (32-50)
1-32	0.0440 (49-50)	0.0025 (8-9)	0.0338 (32-50)
1-33	0.0514 (1-2, 14-33)	0.0120 (8-9, 32-50)	0.0334 (56-60)
1-34	0.0534 (3-4, 14-15)	0.0111 (42-43, 57-58)	0.0370 (33-34)
1-35	0.0437 (35-51)	−0.0006 (9-10)	0.0205 (35-36)
1-41	0.0444 (2-3, 54-55)	−0.0137 (9-10, 42-43)	0.0363 (41-55)
1-42		The same as **1-32**	0.0235 (42-43)
1-43		The same as **1-35**	0.0222 (42-43)
1-44		The same as **1-31**	0.0208 (42-43)
1-49	0.0429 (1-2)	−0.0028 (59-60)	0.0360 (32-50)
1-50	0.0434 (1-5, 49-50)	−0.0031 (8-9, 51-52)	0.0338 (32-50)
1-51		The same as **1-49**	0.0200 (52-53)
1-52	0.0410 (2-3, 4-5, 35-51, 36-53)	−0.0425 (8-9, 9-10, 56-60, 59-60)	0.0219 (51-52, 52-53)
1-56	0.0412 (1-5, 56-57)	0.0109 (6-7, 42-43)	0.0135 (57-58)
1-57	0.0411 (4-5, 58-59)	−0.0004 (9-10, 42-43)	0.0149 (57-58)
1-60	0.0378 (2-3, 4-5, 56-57, 58-59)	−0.0627 (8-9, 9-10, 51-52, 52-53)	0.0226 (56-60, 59-60)

a) Bonds with a min BRE are indicated in parentheses.

systems in fullerene isomers of $C_{58}BN$ are kinetically stable enough to survive harsh reactor conditions.

However, we pointed out previously that the absence of π bonds with a BRE $< -0.100|\beta|$ is only one of the necessary or very desirable conditions but not a sufficient one for extractability. As in the case of $C_{58}N_2$, many other factors may affect the kinetic stability or instability of the molecule.[15] For example, the uneven charge distribution of $C_{58}BN$ must increase the reactivity toward both electrophiles and nucleophiles.[27] The present approach, based on the BRE, is never universal, but proved to be still very useful for discussing the kinetic stability of heterofullerenes.

Computations were carried out at the Information Processing Center, Shizuoka University.

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