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BN Alternants: Boron Nitride Cages and Polymers

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BN alternants with borons and nitrogens fully replacing alternant sets of carbons in an alternant hydrocarbon form a special class of species of natural interest. The Hückel model for general BN alternants and certain extended Hückel models for "regular" BN alternants are shown to be simply soluble in terms of the eigensolutions for the corresponding alternant hydrocarbons. The difference in the electronegativities for boron and nitrogen implies the opening of HOMO−LUMO gaps for alternant BN clusters—or equivalently the opening of band gaps (at the Fermi energy) for BN alternant polymers. Infinite classes first of octahedral-symmetry fullerenoid cages and second of "buckytube" polymers are considered.

1. Introduction

Alternant hydrocarbons are those conjugated hydrocarbons whose carbon atoms can be formally divided into two classes ("starred" and "unstarred") such that each atom has only atoms of the other class as nearest neighbors. This class of molecules has been extensively studied both experimentally and theoretically for over 50 years. Since boron and nitrogen bracket carbon in the periodic chart, in their numbers of valence electrons and in their electronegativities, alternant B-N compounds (obtainable for any alternant hydrocarbon by substitution of boron for one class of carbons and nitrogen for all of the other) can often be found to exhibit properties parallelling those of the corresponding organics—the classic example here being borazine $B_3N_3H_6$, the analogue of benzene. See e.g. Niedenzu and Dawson[1] or Geanangel and Shore.[2] Also BN exists in forms analogous both to diamond and to graphite, so that there has been much work[3,4] on these structures—with a view to technological applications such as high-temperature wide-band-gap semiconductors. Thus it seems natural to ask whether boron−nitride analogs exist for newer carbon allotropes such as Buckminsterfullerene, C_{60}.

A trivial answer to this question is "no". Since any fullerene cage contains (essentially by definition) 12 pentagonal rings and hence must be nonalternant, a strict BN alternant cannot exist for such fullerene cages. In correspondence with C_{60}, however, an elegant analogue ($B_{24}N_{24}C_{12}$) with just a portion of the carbons replaced has been proposed,[5] and low-doped cages $C_{60-x}B_x$ and $C_{60-x}N_x$ with $x = 1, 2$ have been observed[6] and computations made.[7] The $B_{36}N_{24}$ species proposed by La Placa *et al.*[8] deviates from our interests in having adjacent B atoms and consequent destabilizing homonuclear bonds.

Another answer to the question of BN alternant fullerene-like cages is "yes"—if we forego the usual (twelve) pentagonal rings and replace them with six square rings. The simplest such possibilities here are the cube and the truncated octahedron, as indeed have already been theoretically studied.[9] In fact, these two species are but the first members of an infinite family of octahedral-symmetry BN alternant cages, as we discuss in section 3.

There is yet another "graphitic" infinite allotropic form for carbon, the buckytube, which is obtained by wrapping a hexagonal net of carbon atoms onto a long tube. Such quasi-one-dimensional tubes have been found experimentally[10] and are the target of much present work.

Since these structures are alternant, BN analogues may exist. In section 4, we discuss these BN-tube analogs utilizing methodologies employed previously to characterize buckytubes.[11] While we employ and solve analytically the Hückel (band-theoretic) model, the method generalizes (due to the symmetry) to any one-electron model with one electron per site. But first in section 2 we consider the general case of BN alternants, extending some earlier results of Bochvar *et al.*[12,13]

⊗ Abstract published in *Advance ACS Abstracts,* March 1, 1995.

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2. The Hückel Model for BN Alternants

In general, for any alternant BN system the simplest Hückel Hamiltonian (for molecular graph G) may be written

$$\mathbf{H} = \beta\mathbf{A} + \mathbf{D} \tag{1}$$

with **A** being the adjacency matrix

$$A_{ij} = \begin{cases} 1;\ i \sim j \text{ in G} \\ 0;\ i \nsim j \text{ in G} \end{cases} \tag{2}$$

and with being **D** a diagonal matrix whose elements are

$$D_{ij} = \begin{cases} \alpha_B;\ i = j & \text{a boron} \\ \alpha_N;\ i = j & \text{a nitrogen} \\ 0;\ i \neq j \end{cases} \tag{3}$$

Here β is a "resonance" integral and α_B, α_N are "Coulomb" integrals.

The eigenproblem for the adjacency matrix is

$$\mathbf{A}|\lambda\rangle = \lambda|\lambda\rangle \tag{4}$$

By the Coulson–Rushbrooke pairing theorem[14] Hückel eigensolutions for alternant hydrocarbons occur in pairs (at least for $\lambda \neq 0$)

$$|\pm\lambda\rangle = |\lambda,\mathrm{N}\rangle \pm |\lambda,\mathrm{B}\rangle \tag{5}$$

where $|\lambda,\mathrm{N}\rangle$ and $|\lambda,\mathrm{B}\rangle$, respectively, have nonzero coefficients only at "starred" and "unstarred" sites (to be identified as N and B). As it turns out, the two-dimensional space spanned by a pair $\{|\lambda,\mathrm{N}\rangle, |\lambda,\mathrm{B}\rangle\}$ is invariant under the action of the BN-alternant Hamiltonian

$$\begin{aligned} \mathbf{H}|\lambda,\mathrm{N}\rangle &= \beta\mathbf{A}|\lambda,\mathrm{N}\rangle + \alpha_N|\lambda,\mathrm{N}\rangle \\ &= \beta\lambda|\lambda,\mathrm{B}\rangle + \alpha_N|\lambda,\mathrm{N}\rangle \end{aligned} \tag{6}$$

and

$$\begin{aligned} \mathbf{H}|\lambda,\mathrm{B}\rangle &= \beta\mathbf{A}|\lambda,\mathrm{B}\rangle + \alpha_B|\lambda,\mathrm{B}\rangle \\ &= \beta\lambda|\lambda,\mathrm{N}\rangle + \alpha_B|\lambda,\mathrm{B}\rangle \end{aligned} \tag{7}$$

which can be easily seen by substitution for $|\lambda,\mathrm{N}\rangle$ and $|\lambda,\mathrm{B}\rangle$ in terms of $|\pm\lambda\rangle$. Thus the eigenproblem reduces generally to the treatment of a set of 2 × 2 matrices

$$\begin{pmatrix} \alpha_N & \beta\lambda \\ \beta\lambda & \alpha_B \end{pmatrix} \tag{8}$$

where λ are eigenvalues to the adjacency matrix **A** alone. The Hamiltonian eigenvalues are

$$\begin{aligned} \epsilon_\pm &= \bar{\alpha} \pm \sqrt{\Delta^2 + \beta^2\lambda^2} \\ \bar{\alpha} &= (\alpha_B + \alpha_N)/2 \\ \Delta &= (\alpha_B - \alpha_N)/2 \end{aligned} \tag{9}$$

with $\bar{\alpha}$ similar to that for carbon and Δ nearly[15] the size of $|\beta|$. Via a related argument, Bochvar and Stankevich[12] reached this same result some time ago.

A special point concerns the states corresponding to nonbonding MOs for the hydrocarbons—i.e., the case with $\lambda = 0$. The Coulson–Rushbrooke result of (5) is based upon properties of the so-called *alternancy* operator $\hat{\mathbf{a}}$ which changes orbital signs on starred (N) sites (so that $\hat{\mathbf{a}}$ is like the **D** operator but with α_N and α_B replaced by -1 and $+1$). The readily seen anticommutation of $\hat{\mathbf{a}}$ with **A** leads directly to the result of (5) with $\lambda \neq 0$, and the same argument still tells us that application of $\hat{\mathbf{a}}$ to a $\lambda = 0$-eigenvalue eigenvector $|0\rangle$ yields back an eigenvector with eigenvalue $-\lambda = 0$—it is just that the resultant eigenvector might be the same one (up to a sign). In any event, a linearly independent set of 0-eigenvalue eigenvectors may be chosen each entirely localized on one set (B or N) of sites. Thus those on the B subset are acted on by the full model Hamiltonian to give an eigenvalue of $\epsilon = \alpha_B$, while for those on the N subset yield $\epsilon = \alpha_N$. Overall, we then still have a gap of at least 2Δ with the numbers of levels below and above this gap being respectively the numbers of nitrogen and boron atoms. Thus for neutral BN alternants, the HOMO–LUMO (or band) gap is at least 2Δ. That is, there are no radicaloid BN alternants.

The question arises as to whether any of the general results of the preceding two paragraphs extend beyond the simple Hückel model. First, if nearest-neighbor resonance integrals are allowed to vary with individual BN bond lengths, our results and in particular (9) still apply—all one need to do is let the unit elements of **A** vary away from 1 and still denote its eigenvalues by λ. The same proofs apply and the HOMO–LUMO (or band) gap remains at least 2Δ.

If we specialize to the case of *regular* BN alternants wherein all B and N atoms have the same degree d in the alternant graph, then related results may be proved for an extended Hückel model. Many BN alternants are not so regular,[1,2] but the cyclic ones (which have historically played a key role) are, as also are the cages and tubes of sections 3 and 4. The simple standard extension of the Hückel model[16] takes β-integrals to next-nearest neighbors and utilizes an overlap matrix

$$\mathbf{S} = 1 + s\mathbf{A} \tag{10}$$

with the nearest-neighbor overlap integral $s \approx 0.25$. Now $(\mathbf{A}^2 - d\mathbf{1})$ (with **1** the identity matrix and d the degree of connection) may be seen to connect next-nearest neighbor sites, and if there are no four-membered rings, all the nonzero elements of $\mathbf{A}^2 - d\mathbf{1}$ take the same value 1. In this case, we may write our extended Hückel model Hamiltonian matrix as

$$\mathbf{H}_{ex} = \mathbf{D} + \beta\mathbf{A} + \beta'(\mathbf{A}^2 - d\mathbf{1}) \tag{11}$$

with β' a next-nearest neighbor resonance integral. Following the procedure in (6) and (7), one similarly arrives at the representation of $\mathbf{H}_{ex}$ on the same basis $\{|\lambda,\mathrm{N}\rangle, |\lambda,\mathrm{B}\rangle\}$

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(15) See, e.g.: Streitweiser, A., Jr. *Molecular Orbital Theory*; John Wiley & Sons: New York, 1961; Chapter 5.

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$$\begin{pmatrix} \alpha_N + \beta'\lambda^2 - \beta'd & \beta\lambda \\ \beta\lambda & \alpha_B + \beta'\lambda^2 - \beta'd \end{pmatrix} \qquad (12)$$

and of course **S** has a like-blocked representation

$$\begin{pmatrix} 1 & s\lambda \\ s\lambda & 1 \end{pmatrix} \qquad (13)$$

Thus our extended Hückel eigenvalues are

$$\epsilon_{\pm} = \frac{\bar{a} - s\beta\lambda^2 \pm \sqrt{\Delta^2 + (\beta - sa_B)(\beta - sa_N)\lambda^2}}{1 - s^2\lambda^2} \qquad (14)$$

where $\bar{a}$, a_N, and a_B are modified "Coulomb" parameters

$$a_N = \alpha_N + \beta'\lambda^2 - \beta'd$$

$$a_B = \alpha_B + \beta'\lambda^2 - \beta'd \qquad (15)$$

$$\bar{a} = (a_N + a_B)/2$$

Of course not all of the next-nearest neighbors have resonance integrals exactly as assumed in (11), but it is only a correction itself which will be best for either regular-polygon cycles or for benzenoid structures, including those of section 4. Again presuming that the minimum possible HOMO–LUMO gap corresponds to $\lambda = 0$, we see from (14) that it must still be at least of size 2Δ. Refinement of the Hückel model evidently introduces no tendency toward radicaloid behavior of regular BN alternants.

3. "Octahedral-Symmetry" Fullerenoid Cages

All of these cages are to have models constructable by cutting equal equilateral triangular fragments from the honeycomb lattice and then pasting eight such fragments onto the faces of an octahedron such that the cut bonds match together on the boundaries of the faces. Indeed this is much the same scheme as already used to construct icosahedral-symmetry fullerene cages.[17–19] The equilateral triangles cut from the (graphitic) honeycomb lattice have the apices of each triangle in the centers of hexagonal faces, as indicated in Figure 1. The possible triangles are identified by an indication of the location of one of such a triangle's apices relative to another of its apices. This is conveniently specified by the length of a walk along "principal" directions oriented from center-to-center of adjacent hexagons on the underlying honeycomb lattice. Needing only two such principal directions (for a two-dimensional lattice), we choose the first to be oriented noninternally (to the triangle) as directly as possible from the first to the second apex, while the second direction is oriented at 120° to the first—and all are further chosen so that the number of $h > 0$ steps taken in the first direction is at least as great as the number k of steps taken in the second direction (as one proceeds from the first to the second apex). For instance, the triangles of Figure 1 are of type $(h, k) = (2, 0)$ and the one of Figure 2 is of type (3, 2).

Thus we have identified an infinite class of "octahedral-symmetry" cages from which BN alternants may be constructed.

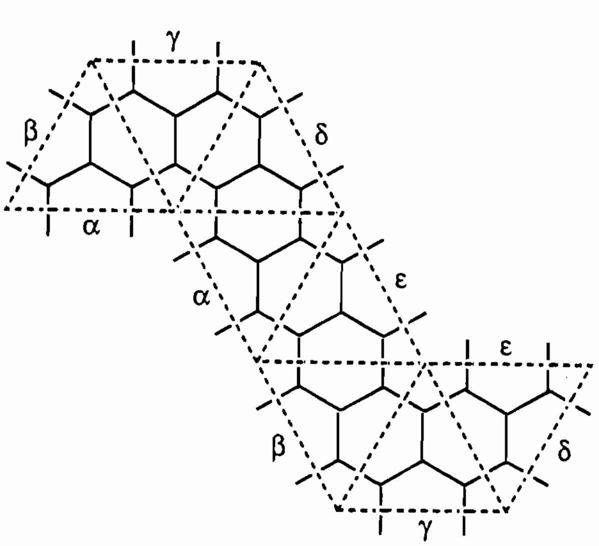

Figure 1. Portion of the honeycomb lattice showing eight triangles to be joined together on the eight faces of an octahedron. When this is done the triangle's edges with the same label (α, β, γ, δ, or ϵ) will join.

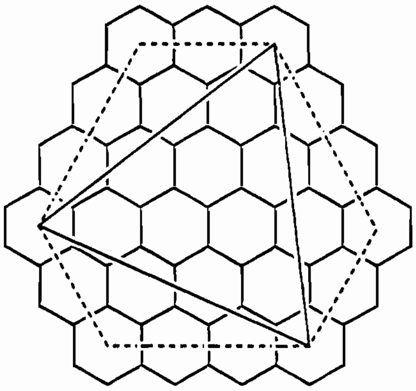

Figure 2. Triangle of type $(h, k) = (3, 2)$ drawn with solid lines. The dotted lines indicate the $h = 3$ steps and $k = 2$ steps in consecutive "principal" directions to move from one triangle apex to the next.

The usual point-group symmetry is just D_{3h}, but if the remaining elements of O_h are augmented with a "color" change between B and N, one obtains an octahedral symmetry, which has consequences[20] reflected in Hamiltonian eigenspectra. These cages each correspond to an ordered pair of integers (h, k) such that

$$0 < h \geq k \geq 0 \qquad (16)$$

Each cage has

$$v = 8(h^2 + kh + k^2) \qquad (17)$$

vertices of which half are B-sites and half are N-sites. Each cage has six square faces at the apices of the underlying octahedron while all (or any) other faces are hexagonal. Those with $k = 0$ or $k = h$ are (or, if not distorted, can be) achiral while all others are necessarily chiral. For these latter we could utilize the pair (k, h) if we wished to distinguish mirror images. A very reasonable coordinate representation of the cages may be readily obtained using the scheme of Manolopolous and Fowler[21] —this for our present case simply means using the

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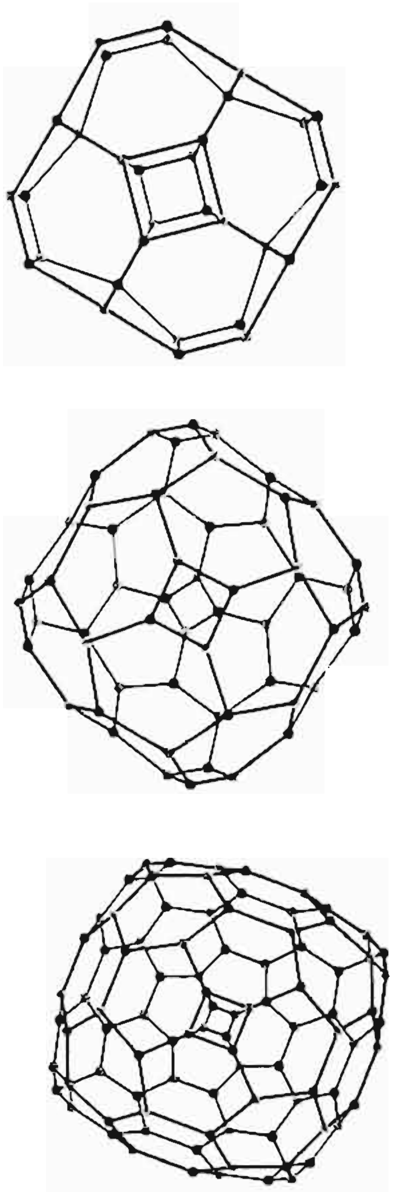

Figure 3. The three octahedral symmetry cages, from top to bottom, with $(h, k) = (2, 0), (2, 1), (2, 2)$.

triple of eigenvector components of the highest t_1-symmetry eigenvectors to **A** as the coordinates of the various atomic vertices. In Figure 3 we show the three cages with $h = 2$. Further, following earlier arguments,[17] it may be seen that the described octahedral-symmetry polyhedron cages are *all* those that are possible with four- and six-sided faces only. Finally, the arguments of the preceding section establish that all these cages are stable with a large HOMO−LUMO gap (exceeding 2Δ, at least within the Hückel and slightly extended Hückel models, though the corresponding octahedral-symmetry carbon cages often have a zero band gap due to symmetry). This is in agreement with the more sophisticated computations earlier reported on the $h = k = 1$ cage.[7]

4. Band Structure of BN Buckytubes

In section 2 we showed that the eigenvectors and eigenvalues for BN analogs can immediately be obtained from those for the related buckytube for which results have already been analytically determined.[11] We therefore here only briefly review the symmetry treatment for hexagonal wrappings of tubes.

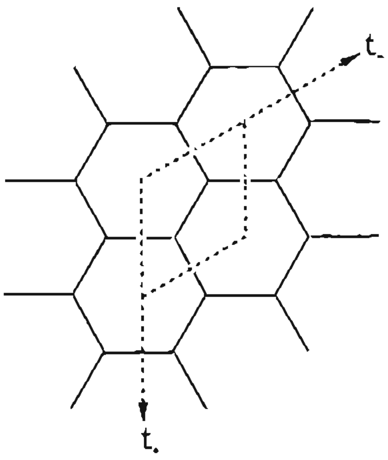

Figure 4. The 2-site reduced unit cell enclosed within dotted lines. Also shown are the directions taken to make the t_+ and t_- counts of the text.

Figure 4 shows the two-site (diamond-shaped) reduced unit cell where on each site there is a π-like orbital oriented normal to the tube surface. In general, the Hückel resonance integrals along different directions will be different but here we take them all to be equal (though the general treatment here and in section 2 is not dependent on this assumption). Now any tube is characterized by the values t_+ and t_- ($t_+ \geq t_-$) which are the lengths of paths oriented along "principal" directions through the centers of adjacent hexagons, much as the paths in section 3. For two such paths radiating (at 120° to one another) from one hexagon, the two paths will eventually intersect (if they are chosen not to wind in opposite directions along the tube and if we have not gone to the "planar" limit). Letting t_+ and t_- be the larger and lesser (or equal) numbers of steps along the two paths uniquely specifies the tubes. Here then we have

$$0 < t_+ \geq t_- \geq 0 \tag{18}$$

(in an interesting analogy to (16)). Here (t_+, t_-) determine a tubes' "helicity"—again $t_- = 0$ and $t_+ = t_-$ both correspond to purely achiral rotationally symmetric tubes (Figure 5a,e) whereas $t_0 = t_+ - t_- > 0$ implies helical structures (Figure 5b−d). For a standard lattice (i.e., the bonds on a hexagon have the same length), the tube radius r is given (from elementary trigonometric arguments) as

$$r = \frac{l}{2\pi}\sqrt{3(t_+^2 + t_-^2 + t_+t_-)} \tag{19}$$

where l is the nearest-neighbor distance (i.e., the in-plane bond length).

From section 2 and ref 11 we therefore obtain the band structure for BN buckytubes

$$\epsilon_{\pm}(m,k) = \bar{\alpha} \pm \sqrt{\Delta^2 + \lambda_{\pm}(m,k)} \tag{20}$$

where $\bar{\alpha}$ and Δ are given in (9) and

$$\lambda_{\pm}(m,k) = \pm\beta|1 + e^{iK} + e^{ik}| \tag{21}$$

Here also K is a (essentially continuous) *wavevector*, ranging from $-\pi$ to $+\pi$ and k is a quasi-discrete quantity with values

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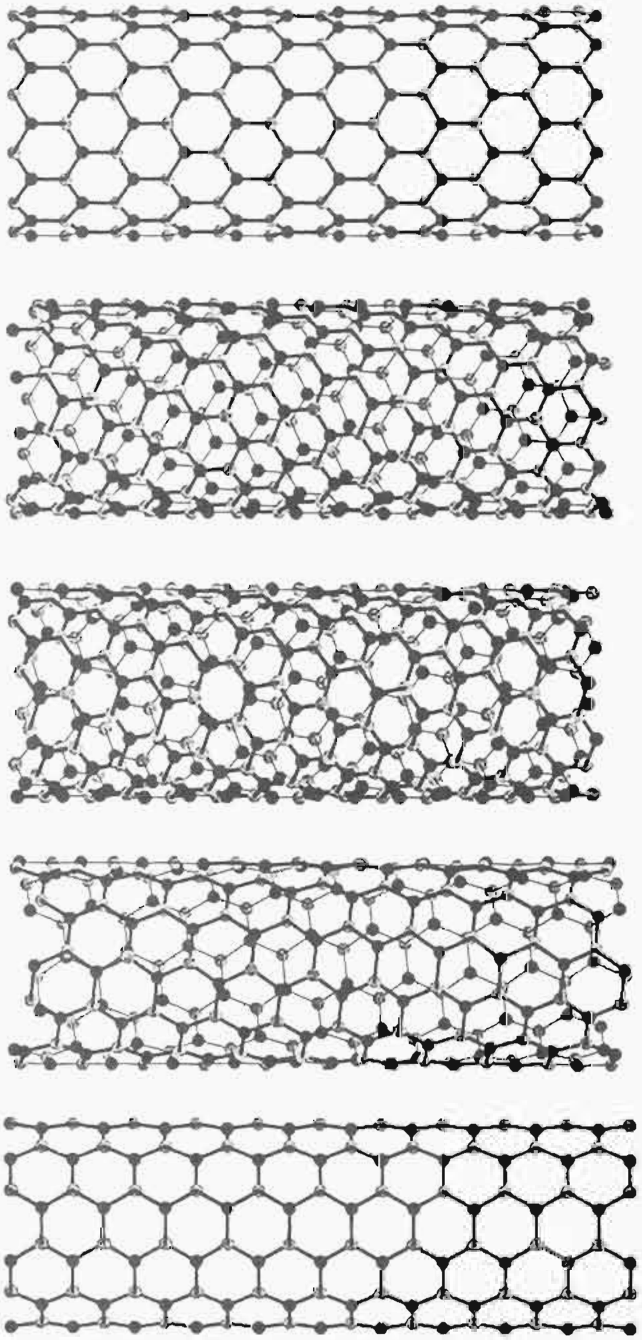

Figure 5. Portions of BN-alternant buckytubes, with different values of (t_+, t_-), from top to bottom: (a) (12, 0); (b) (12, 1); (c) (12, 2); (d) (6, 5); (e) (6, 6).

$$k = \begin{cases} \frac{2\pi m}{t_+}; \text{ if } t_- = 0 \text{ and } m = 0, 1, ..., t_+ \\ \frac{2\pi m}{t_-} + \frac{t_- K}{t_-}; \text{ if } t_- \neq 0 \text{ and } m = 0, 1, ..., t_- \end{cases} \qquad (22)$$

The band structures for the tubes of Figure 5 are given in Figure 6 when $\alpha_B = \alpha_N = 0$ and in Figure 7 when $\alpha_B = -\alpha_N = |\beta|$. It is seen in all cases that the band gap grows as the electronegativity difference grows. The case with $t_+ = 12$ and $t_- = 0$ shows the minimum band gap (β) due to the presence of Δ in eq 20. In the carbon tube, these would have zero band gap. (The presence of fewer bands when $t_- = 1, 2$ corresponds to the fact that for $t_- = 1$ the tube can be viewed as being generated by a single helical hexagonal strip winding around the tube so that the surface is completely covered while $t_- = 2$ would generate the tube via two interfacing helicies.) Much the same results apply with the extended Hückel model, as indicated in Figure 8. As a consequence, all these BN-alternant buckytubes are insulators, at least when undoped.

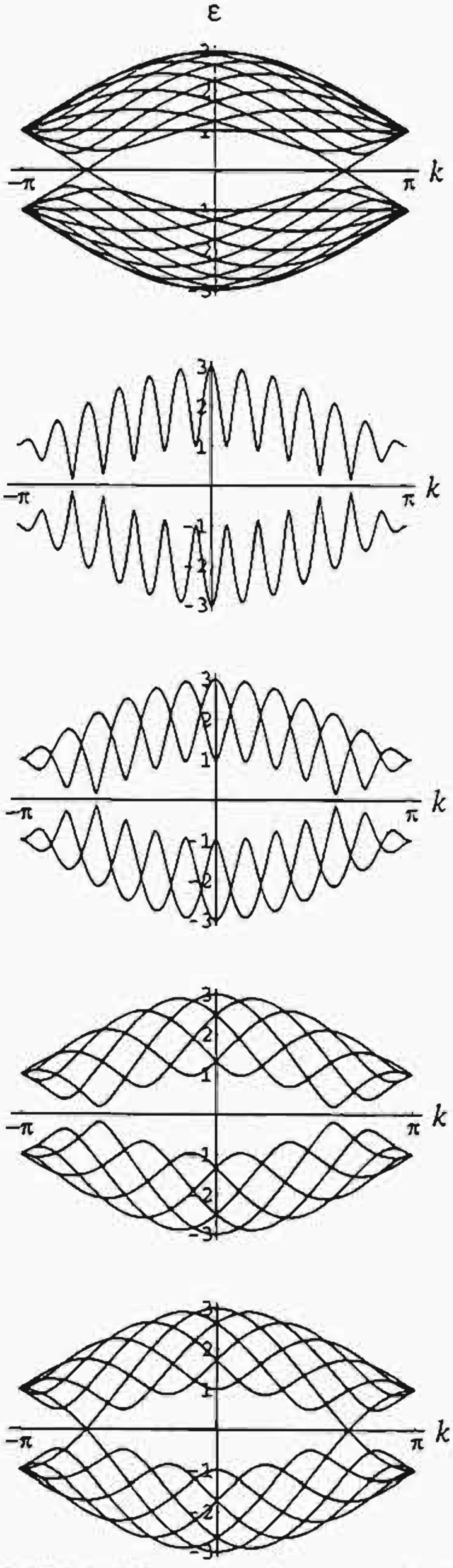

Figure 6. Bands for the homopolar (carbonaceous species with $\alpha_B = \alpha_N = 0$) for the buckytube structures of Figure 5.

With the introduction of impurities, such as O, which in fact

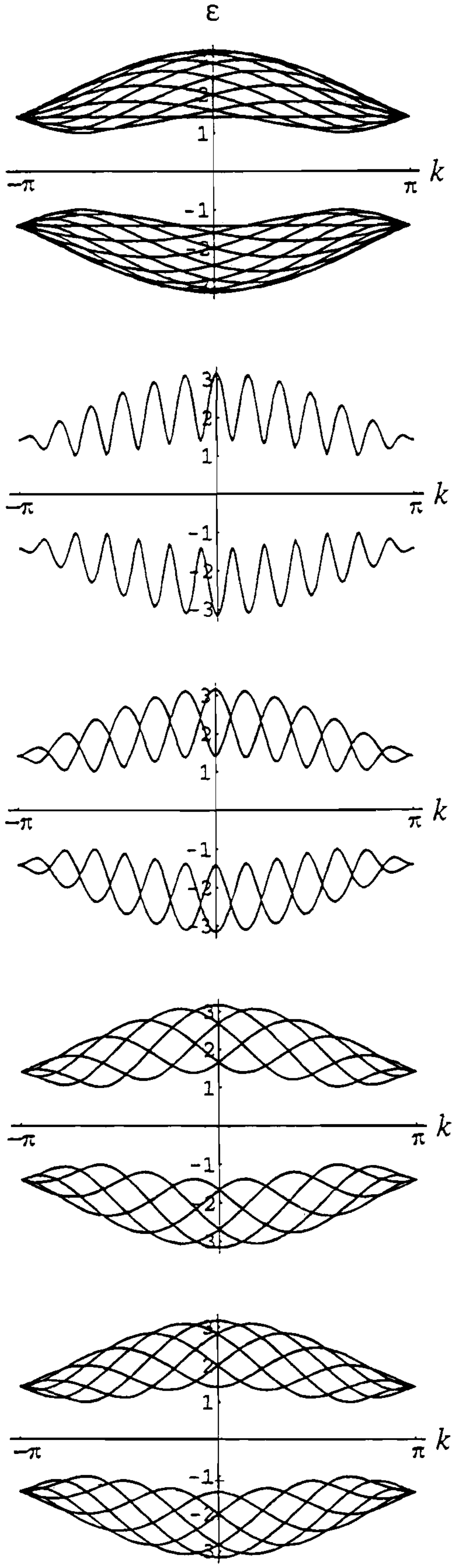

Figure 7. Simple Hückel bands for the BN-alternant structures of Figure 5.

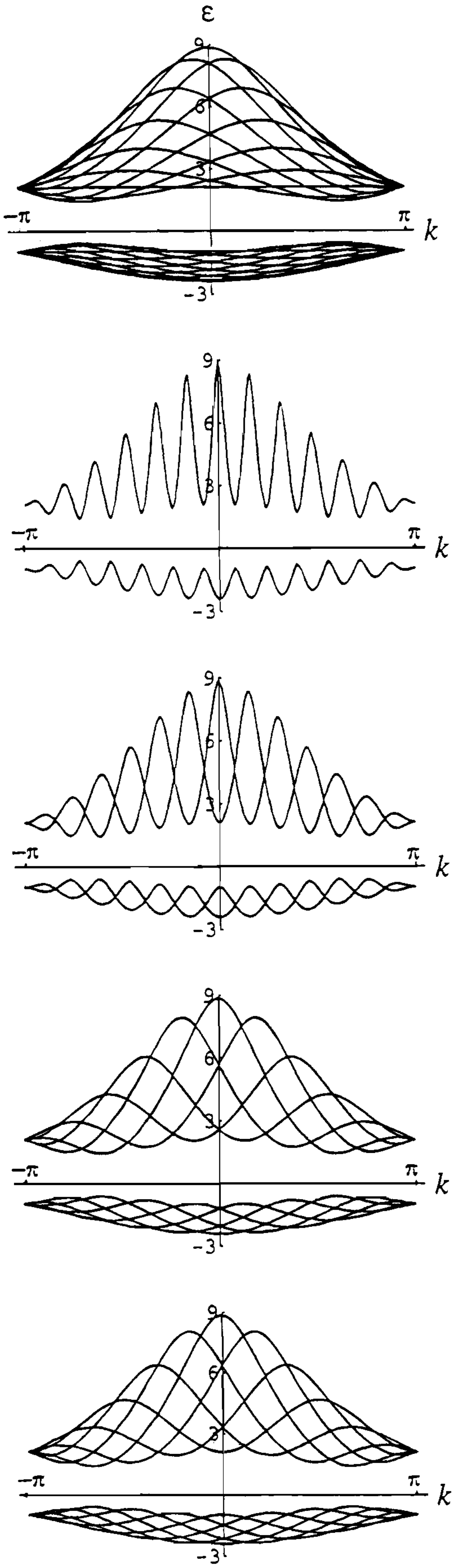

Figure 8. Extended Hückel π-bands for the BN alternants of Figure 5.

often occurs with the chemical-vapor deposited BN films,[4] the possibility of semiconduction arises. The introduction of "softer" impurities such as S or C we believe would offer more likelihood for delocalization. Indeed as the level of carbon-doping increases the band gap can ultimately be closed, at composition CBN where one-third of the B atoms and one-third of the N atoms are (suitably) replaced by C atoms. Evidently C introduces either electrons or holes in a valence bond as it substitutes for B or N. Moreover, such ideas should be relevant in understanding recently synthesized $C_yB_xN_x$ nanotubes.[22]

5. Summary

A general approach for BN analogs of alternant hydrocarbons yields via (9) eigenvalues (and orbitals) depending only on corresponding Hückel eigenvalues and the electronegativity parameters of B and N. When applied to the case of buckytube BN analogs, the results remove the zero band gaps found for some buckytubes and as is found also in more elaborate band-theoretic computation for special-case buckytube structures.[23] The results, however, imply many similarities between carbon and alternant BN tubes and suggest that these are stable species and worthy of synthesis. Success in generating BN tubes might provide clues to the mechanisms for carbon tube formation via the richer chemical structures present in BN tubes.

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