Symmetry properties of single-walled boron nitride nanotubes

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(Received 27 April 2001; published 20 September 2001)

The symmetry operations for armchair, zigzag, and chiral boron nitride nanotubes (BN-NT's) are identified. It is found that each type belongs to a different family of *nonsymmorphic* rod groups. Armchair BN-NT's with even index n are found to be *centrosymmetric*. We determine the numbers of Raman- and infrared-active vibrations in single-walled BN-NT's. We find that, in contrast to achiral carbon nanotubes, zigzag BN-NT's possess almost twice the Raman- and infrared-active vibrations as armchair BN-NT's.

DOI: 10.1103/PhysRevB.64.153408 PACS number(s): 61.48.+c, 78.30.Na, 63.20.Dj, 02.20.−a

Boron nitride nanotubes (BN-NT's) are a recently synthesized[1] type of tubular materials, combining stable insulating properties[2,3] and high strength.[4] *Ab initio* studies of the spatial *structure* of BN-NT's have predicted the buckling of B-N bonds, which is the formation of a concentric inner "B cylinder" and outer "N cylinder."[3,5] The classification of BN-NT spatial *symmetries*, on the other hand, has been rather partial so far, being limited to a determination of their chiralities only.[2,6] Owing to the subset relation between the plane groups of two-dimensional (2D) hexagonal BN and graphite nets, $p3m1 \subseteq p6mm$, single-walled BN-NT's (hereafter, BN-NT's) are characterized by the pair of indices n and m,[2,6] as carbon nanotubes (C-NT's) do:[7] $(n,m=n)$ armchair, $(n,m=0)$ zigzag, and $(n,0<m<n)$ chiral. Thus, the (n,m) BN- and C-NT's possess the same lattice period T_z (Ref. 6) and number N of hexagons within their unit cells.

The profound implication of the symmetry properties of BN-NT's on physical effects can be seen in the recent work of Král *et al.*,[8] who predicted noncentrosymmetry- and polarity-based photogalvanic effects in BN-NT's. More specifically, the direction of the induced photocurrent was shown to depend on the BN-NT chirality. As will be shown below, however, armchair BN-NT's with even index n are *centrosymmetric*. Nevertheless and in contrast to 2D and 3D centrosymmetric and polar crystalline materials, they (should) exhibit the azimuthal photocurrents predicted in Ref. 8. It is the purpose of this work to complete the identification of BN-NT symmetries and determine their rod groups. The implications of symmetry on BN-NT vibrational spectroscopy is studied thereafter. We determine the numbers of Raman- and infrared-active vibrations in BN-NT's and compare them to the recently reexamined numbers in C-NT's.[9]

In order to account for all the symmetries in BN-NT's one can identify those symmetry operations in the plane group $p3m1$ which "survive" the rolling of a 2D hexagonal BN net into the BN-NT cylinder. Of course, one has to account for various newly generated symmetry operations. Alternatively, one can identify the rod groups of BN-NT's as *subgroups* of C-NT rod groups.[10] For instance, C-NT's possess perpendicular C_2 axes;[10] BN-NT's, on the other hand, cannot possess such axes because $p3m1$ do not possess C_2 axes. Choosing to follow the second approach, let us briefly recall the symmetries of C-NT's. The nonsymmorphic rod group[10] describing achiral C-NT's with index n can be decomposed in the following manner (the 13th family of rod groups[11]):

$$\begin{aligned}\mathcal{G}[n] &= \mathcal{L}_{T_z} \times \mathcal{D}_{nh} \times [\mathbf{E} \oplus \mathbf{S}_{2n}] \\ &= \mathcal{L}_{T_z} \times \mathcal{D}_{nd} \times [\mathbf{E} \oplus \mathbf{S}_{2n}] \\ &= \mathcal{L}_{T_z} \times [\mathcal{D}_{nh}|_{z=0} \oplus (\mathcal{D}_{nd}|_{z=T_z/4} \ominus \mathcal{C}_{nv}) \oplus \mathcal{C}_{nv} \times \mathbf{S}_{2n}],\end{aligned} \tag{1}$$

where the reference point $z=0$ denotes the crossing of horizontal, σ_h, and vertical, σ_v, reflection planes (see Fig. 1). $\mathcal{L}_{T_z}$ is the one-dimensional translation group with the primitive translation $T_z = |\mathbf{T}_z|$. $\mathbf{E}$ is the identity operation. The screw axis $\mathbf{S}_{2n} = (z \to z + T_z/2, \varphi \to \varphi + \pi/n)$ involves the lattice smallest nonprimitive translation and rotation. The subtraction of the point group $\mathcal{C}_{nv}$ in Eq. (1) reflects the set relation $\mathcal{D}_{nh}|_{z=0} \cap \mathcal{D}_{nd}|_{z=T_z/4} = \mathcal{C}_{nv}$ for all n's. The glide plane $\mathbf{g}$ is also presented in Fig. 1. It fulfills the multiplication relation $\mathbf{g} = \mathbf{S}_{2n}\sigma_v$. The existence of n distinct glide planes in $\mathcal{G}[n]$ stems from the last term in Eq. (1). The point group of the rod group, $\mathcal{G}_0[n]$, is obtained by setting all translations (including the nonprimitive ones) in $\mathcal{G}[n]$ equal to zero. From Eq. (1) we obtain

$$\mathcal{G}_0[n] = \mathcal{D}_{nh} \times [\mathbf{E} \oplus C_{2n}] = \mathcal{D}_{nd} \times [\mathbf{E} \oplus C_{2n}] = \mathcal{D}_{2nh}, \tag{2}$$

where $C_{2n} = (\varphi \to \varphi + \pi/n)$ is the rotation embedded in $\mathbf{S}_{2n}$. The nonsymmorphic rod group[10] describing the (n,m)-chiral C-NT can be decomposed as follows (the fifth family of rod groups[11]):

$$\begin{aligned}\mathcal{G}[N] &= \mathcal{L}_{T_z} \times \mathcal{D}_d \times \left[\sum_{j=0}^{N/d-1} \mathbf{S}_{N/d}^j\right] \\ &= \mathcal{L}_{T_z} \times \mathcal{D}_1 \times \left[\sum_{j=0}^{N-1} \mathbf{S}_N^j\right].\end{aligned} \tag{3}$$

$N = 2(n^2 + m^2 + nm)/d_R$, where d_R is the greatest common divisor of $2n+m$ and $2m+n$.[7] d is the greatest common divisor of n and m. $\mathbf{S}_{N/d}$ and $\mathbf{S}_N$ are screw-axis operations with the orders of N/d and N, respectively. The point group of the rod group is readily obtained from Eq. (3),

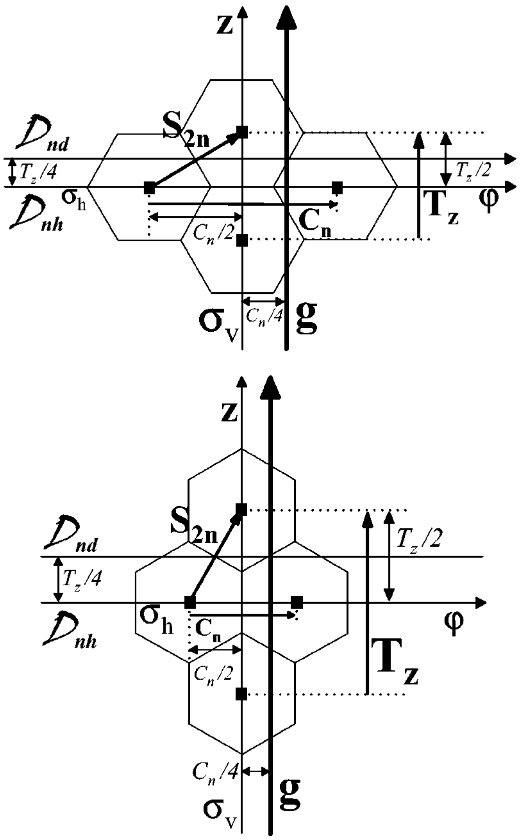

FIG. 1. 2D projection of various symmetries in achiral C-NT's (armchair segment, top; zigzag segment, bottom): $\mathbf{T}_z$ is the primitive translation; $\mathbf{S}_{2n}$ is the screw axis with nonprimitive translation and rotation, denoted by $T_z/2$ and $C_n/2$, respectively; $\mathbf{g}$ is a glide plane; $\mathcal{D}_{nh}|_{z=0}$ and $\mathcal{D}_{nd}|_{z=T_z/4}$ stand for the corresponding point-group operations, among which σ_h, σ_v and $\mathbf{C}_n$ are denoted. Note the $T_z/4$ shift between $\mathcal{D}_{nh}|_{z=0}$ and $\mathcal{D}_{nd}|_{z=T_z/4}$, which coexist in all achiral C-NT's.

$$\mathcal{G}_0[N] = \sum_{j=0}^{N/d-1} C_{N/d}^j \times \mathcal{D}_d = \sum_{j=0}^{N-1} C_N^j \times \mathcal{D}_1 = \mathcal{D}_N, \qquad (4)$$

where $C_{N/d}=(\varphi\rightarrow\varphi+2d\pi/N)$ and $C_N=(\varphi\rightarrow\varphi+2\pi/N)$ are the rotations embedded in $\mathbf{S}_{N/d}$ and $\mathbf{S}_N$, respectively.

Let us consider first the achiral BN-NT's with the rotation axis of order n, that is, the (n,n)-armchair (Fig. 2) or $(n,0)$-zigzag (Fig. 3) BN-NT's. Unlike the situation for C-NT's, they do not possess the same symmetry operations, owing to the lower symmetry $p3m1\subseteq p6mm$. More specifically, the (n,n)-armchair BN-NT possesses *horizontal* planes (see Fig. 2). The lack of C_2 axes (recall that there are no C_2 axes in $p3m1$) leads to the absence of vertical planes in this case. Consequently, the $\mathcal{D}_{nh}$ and $\mathcal{D}_{nd}$ point groups in armchair C-NT's [see Fig. 1 (top) and Eq. (1)] reduce to $\mathcal{C}_{nh}$ and $\mathcal{S}_{2n}$, respectively (see Fig. 2). The reverse is true for the (n,0)-zigzag BN-NT, which has *vertical* planes (see Fig. 3), but no horizontal ones. Consequently, both $\mathcal{D}_{nh}$ and $\mathcal{D}_{nd}$ point groups in zigzag C-NT's [see Fig. 1 (bottom) and Eq. (1)] reduce to $\mathcal{C}_{nv}$ (see Fig. 3). Nevertheless, achiral BN-NT's still possess symmetries of *nonsymmorphic* rod groups

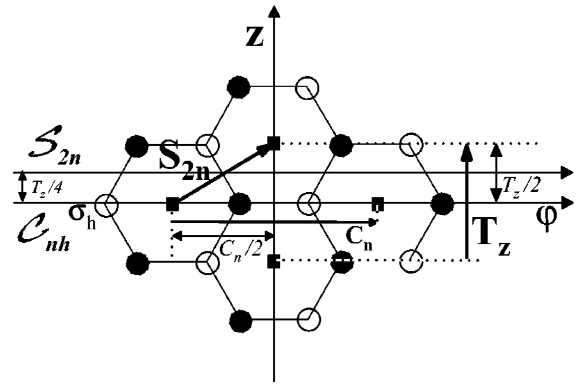

FIG. 2. 2D projection of various symmetries in armchair BN-NT's (●, B; ○, N): $\mathbf{T}_z$ is the primitive translation; $\mathbf{S}_{2n}$ is the screw axis with nonprimitive translation and rotation, denoted by $T_z/2$ and $C_n/2$, respectively; $\mathcal{C}_{nh}|_{z=0}$ and $\mathcal{S}_{2n}|_{z=T_z/4}$ stand for the corresponding point-group operations, among which σ_h and $\mathbf{C}_n$ are denoted. Note the $T_z/4$ shift between $\mathcal{C}_{nh}|_{z=0}$ and $\mathcal{S}_{2n}|_{z=T_z/4}$, which coexist in all armchair BN-NT's.

because the screw axis $\mathbf{S}_{2n}$ "survives" the symmetry lowering described above (see Figs. 2 and 3). Consequently, the *smallest* building block in constructing achiral BN-NT's is composed of one B and one N atom, rather than of a rectangular cell comprising two B and two N atoms, as employed recently by Kim *et al.*[12] The nonsymmorphic rod group describing the (n,n)-armchair BN-NT with (either odd or even) index n can be decomposed in the following manner:

$$\begin{aligned}\mathcal{G}^{arm}[n] &= \mathcal{L}_{T_z}\times\mathcal{C}_{nh}\times[\mathbf{E}\oplus\mathbf{S}_{2n}]\\ &= \mathcal{L}_{T_z}\times\mathcal{S}_{2n}\times[\mathbf{E}\oplus\mathbf{S}_{2n}]\\ &= \mathcal{L}_{T_z}\times[\mathcal{C}_{nh}|_{z=0}\oplus(\mathcal{S}_{2n}|_{z=T_z/4}\ominus\mathcal{C}_n)\oplus\mathcal{C}_n\times\mathbf{S}_{2n}];\end{aligned} \qquad (5)$$

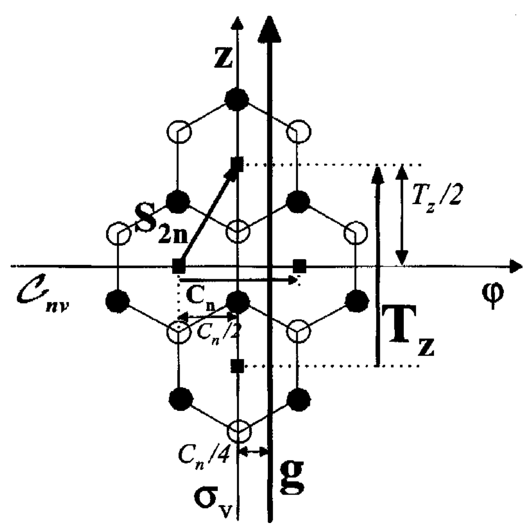

FIG. 3. 2D projection of various symmetries in zigzag BN-NT's (●, B; ○, N): $\mathbf{T}_z$ is the primitive translation; $\mathbf{S}_{2n}$ is the screw axis with nonprimitive translation and rotation, denoted by $T_z/2$ and $C_n/2$, respectively; $\mathbf{g}$ is a glide plane; $\mathcal{C}_{nv}$ stands for the corresponding point-group operations, among which σ_v and $\mathbf{C}_n$ are denoted.

i.e., $\mathcal{G}^{arm}[n]$ belongs to the fourth family of rod groups.[11] The reference point $z=0$ denotes the crossing of the horizontal reflection plane $\boldsymbol{\sigma}_h$ and the n-fold rotation axis $\mathbf{C}_n$ (see Fig. 2). The subtraction of the point group $\mathcal{C}_n$ in Eq. (5) reflects the set relation $\mathcal{C}_{nh}|_{z=0}\cap\mathcal{S}_{2n}|_{z=T_z/4}=\mathcal{C}_n$ for all n's. Note that while an hexagonal BN-net ($p3m1$) does not possess the inversion symmetry, armchair BN-NT's with even index n do possess it. In addition, let us point out that the buckling of B-N bonds[3,5] has no effect on the spatial symmetries of BN-NT's because the B and N atoms form two concentric cylinders[5] in the BN-NT's. The point group of the rod group is readily obtained from Eq. (5),

$$\mathcal{G}_0^{arm}[n]=\mathcal{C}_{nh}\times[\mathbf{E}\oplus C_{2n}]=\mathcal{S}_{2n}\times[\mathbf{E}\oplus C_{2n}]=\mathcal{C}_{2nh}. \quad (6)$$

Similarly, the nonsymmorphic rod group describing the $(n,0)$-zigzag BN-NT with (either odd or even) index n can be decomposed in the following manner:

$$\mathcal{G}^{zig}[n]=\mathcal{L}_{T_z}\times\mathcal{C}_{nv}\times[\mathbf{E}\oplus\mathbf{S}_{2n}]; \quad (7)$$

namely, $\mathcal{G}^{zig}[n]$ belongs to the eighth family of rod groups.[11] Note that the glide planes in zigzag CN-NT's [see Fig. 1 (bottom) and Eq. (1)] are preserved in zigzag BN-NT's [see Fig. 3 and Eq. (7)]. The point group of the rod group is readily obtained from Eq. (7),

$$\mathcal{G}_0^{arm}[n]=\mathcal{C}_{nv}\times[\mathbf{E}\oplus C_{2n}]=\mathcal{C}_{2nv}. \quad (8)$$

Finally, let us discuss the (n,m)-chiral BN-NT. Since there are no C_2 axes in $p3m1$, the $\mathcal{D}_d$ point group in the (n,m)-chiral C-NT [see Eq. (3)] reduces to $\mathcal{C}_d$ in the (n,m)-chiral BN-NT. Nevertheless, chiral BN-NT's still possess the nonsymmorphic rod-group symmetries, since the screw axis $\mathbf{S}_N$ "survives" this symmetry lowering. Consequently, the nonsymmorphic rod group describing the (n,m)-chiral BN-NT can be decomposed as follows:

$$\mathcal{G}^{ch}[N]=\mathcal{L}_{T_z}\times\mathcal{C}_d\times\left[\sum_{j=0}^{N/d-1}\mathbf{S}_{N/d}^{j}\right]=\mathcal{L}_{T_z}\times\left[\sum_{j=0}^{N-1}\mathbf{S}_{N}^{j}\right]. \quad (9)$$

Thus, $\mathcal{G}^{ch}[N]$ belongs to the first family of rod groups.[11] From Eq. (9) we easily find the point group of the rod group,

$$\mathcal{G}_0^{ch}[N]=\mathcal{C}_d\times\left[\sum_{j=0}^{N/d-1}C_{N/d}^{j}\right]=\sum_{j=0}^{N-1}C_N^{j}=\mathcal{C}_N. \quad (10)$$

Having identified their rod-group symmetries, we would like to find the number of optically active vibrations in BN-NT's. Aiming at characterizing the symmetry of phonons at the $\Gamma(k=0)$-point, we have to consider the irreducible representations (irrep's) of the above *nonsymmorphic* rod groups at Γ. As known from the theory of space groups,[13] these irrep's are in a one-to-one correspondence with the irrep's of the corresponding factor groups of the wave vector $k=0$, which are isomorphic to the point groups of the rod groups, $\mathcal{G}_0^{arm}[n]=\mathcal{C}_{2nh}$, $\mathcal{G}_0^{zig}[n]=\mathcal{C}_{2nv}$, and $\mathcal{G}_0^{ch}[N]=\mathcal{C}_N$. We have to analyze separately armchair, zigzag, and chiral BN-NT's, owing to the different point groups mentioned above.

In order to determine the symmetries (at the Γ point) of the $6N$ phonon modes in armchair BN-NT's and how many modes are Raman or IR active we have to associate them with the irrep's of $\mathcal{G}_0^{arm}[n]=\mathcal{C}_{2nh}$. Recall that the character table of $\mathcal{C}_{2nh}$ possesses $4n$ irrep's,[14] $\Gamma_{\mathcal{C}_{2nh}}=A_g\oplus B_g\oplus A_u\oplus B_u\oplus\boldsymbol{\Sigma}_{j=1}^{n-1}\{E_{jg}^{\pm}\oplus E_{ju}^{\pm}\}$. The $6N$ phonon modes transform according to the following irrep's:

$$\begin{aligned}\Gamma_{6N}^{arm}&=\Gamma_{\mathrm{a}}^{arm}\otimes\Gamma_{\mathrm{v}}\\&=4A_g\oplus2B_g\oplus2A_u\oplus4B_u\\&\quad\oplus2E_{1g}^{\pm}\oplus4E_{2g}^{\pm}\oplus2E_{3g}^{\pm}\oplus\cdots\oplus[3+(-1)^{n-1}]E_{(n-1)g}^{\pm}\\&\quad\oplus4E_{1u}^{\pm}\oplus2E_{2u}^{\pm}\oplus4E_{3u}^{\pm}\oplus\cdots\oplus[3-(-1)^{n-1}]E_{(n-1)u}^{\pm},\end{aligned} \quad (11)$$

where

$$\Gamma_{\mathrm{a}}^{arm}=2\left(A_g\oplus B_u\oplus\sum_{j=2,4,6,\ldots}^{N-1}E_{jg}^{\pm}\oplus\sum_{j=1,3,5,\ldots}^{N-1}E_{ju}^{\pm}\right)$$

stands for the reducible representation of the B and N atom positions inside the unit cell. The prefactor of 2 in $\Gamma_{\mathrm{a}}^{arm}$ reflects the two equivalent and disjoint sublattices made by the B and N atoms in the BN-NT's. $\Gamma_{\mathrm{v}}=A_u\oplus E_{1u}^{\pm}$ is the vector representation. Of these modes, the ones that transform according to $\Gamma_{\mathrm{t}}=A_g\oplus E_{1g}^{\pm}\oplus E_{2g}^{\pm}$ (the tensor representation) or Γ_{v} are Raman or IR active, respectively. Out of the $6N$ phonon modes, four (which transform as Γ_{v} and $\Gamma_{R_z}=A_g$) have vanishing frequencies.[15] Consequently, the symmetries and numbers of optically active phonon modes in armchair BN-NT's are given by

$$\Gamma_{\mathrm{Raman}}^{arm}=3A_g\oplus2E_{1g}^{\pm}\oplus4E_{2g}^{\pm}\Rightarrow n_{\mathrm{Raman}}^{arm}=9, \quad (12)$$

$$\Gamma_{\mathrm{IR}}^{arm}=A_u\oplus3E_{1u}^{\pm}\Rightarrow n_{\mathrm{IR}}^{arm}=4. \quad (13)$$

Note that the numbers of Raman- and IR-active phonon modes found for armchair BN-NT's are almost the same as for armchair C-NT's (8 Raman- and 3 IR-active modes).[9]

Analogously to the treatment given above for armchair BN-NT's, we would like to discuss the irrep's of $\mathcal{G}_0^{zig}[n]=\mathcal{C}_{2nv}$. Recall that the character table of $\mathcal{C}_{2nv}$ possesses $n+3$ irrep's,[14] $\Gamma_{\mathcal{C}_{2nv}}=A_1\oplus A_2\oplus B_1\oplus B_2\oplus\boldsymbol{\Sigma}_{j=1}^{n-1}E_j$. The $6N$ phonon modes transform according to the following reducible representation:

$$\Gamma_{6N}^{zig}=\Gamma_{\mathrm{a}}^{zig}\otimes\Gamma_{\mathrm{v}}=4A_1\oplus2A_2\oplus4B_1\oplus2B_2\oplus\sum_{j=1}^{N-1}6E_j, \quad (14)$$

where $\Gamma_{\mathrm{a}}^{zig}=2(A_1\oplus B_1\oplus\boldsymbol{\Sigma}_{j=1}^{n-1}E_j)$ and $\Gamma_{\mathrm{v}}=A_1\oplus E_1$. Of these modes, the ones that transform according to $\Gamma_{\mathrm{t}}=A_1\oplus E_1\oplus E_2$ and/or Γ_{v} are Raman and/or IR active, respectively. Four of the $6N$ phonon modes, those which transform as Γ_{v} and $\Gamma_{R_z}=A_2$, have vanishing frequencies.[15] Consequently, the symmetries and numbers of optically active phonon modes are given by

$$\Gamma^{zig}_{\mathrm{Raman}} = 3A_1 \oplus 5E_1 \oplus 6E_2 \Rightarrow n^{zig}_{\mathrm{Raman}} = 14, \tag{15}$$

$$\Gamma^{zig}_{\mathrm{IR}} = 3A_1 \oplus 5E_1 \Rightarrow n^{zig}_{\mathrm{IR}} = 8. \tag{16}$$

Note that the numbers of Raman- and IR-active phonon modes found for zigzag BN-NT's are almost twice as for zigzag C-NT's (8 Raman- and 3 IR-active modes)[9] or armchair BN-NT's [see Eqs. (12) and (13). In addition, as a result of the lowered symmetry with respect to and in contrast to the situation for zigzag C-NT's, *all* eight IR-active modes are Raman active as well.

Finally, let us discuss the irrep's of $\mathcal{G}^{ch}_0[N] = \mathcal{C}_N$. Recall that the character table of $\mathcal{C}_N$ possesses N irrep's,[14] $\Gamma_{\mathcal{C}_N} = A \oplus B \oplus \Sigma_{j=1}^{N/2-1} E^{\pm}_j$ (N is always even for BN-NT's). The $6N$ phonon modes transform according to the following reducible representation:

$$\Gamma^{ch}_{6N} = \Gamma^{zig}_{\mathrm{a}} \otimes \Gamma_{\mathrm{v}} = 6A \oplus 6B \oplus \sum_{j=1}^{N/2-1} 6E^{\pm}_j, \tag{17}$$

where $\Gamma^{ch}_{\mathrm{a}} = 2(A \oplus B \oplus \Sigma_{j=1}^{N/2-1} E^{\pm}_j) = 2\Gamma_{\mathcal{C}_N}$ and $\Gamma_{\mathrm{v}} = A \oplus E^{\pm}_1$. Of these modes, the ones that transform according to $\Gamma_{\mathrm{t}} = A \oplus E^{\pm}_1 \oplus E^{\pm}_2$ and/or Γ_{v} are Raman and/or IR active, respectively. Four of the $6N$ phonon modes, those which transform as Γ_{v} and $\Gamma_{R_z} = A$ have vanishing frequencies.[15] Consequently, the symmetries and numbers of optically active phonon modes are given by

$$\Gamma^{ch}_{\mathrm{Raman}} = 4A \oplus 5E^{\pm}_1 \oplus 6E^{\pm}_2 \Rightarrow n^{zig}_{\mathrm{Raman}} = 15, \tag{18}$$

$$\Gamma^{ch}_{\mathrm{IR}} = 4A \oplus 5E^{\pm}_1 \Rightarrow n^{zig}_{\mathrm{IR}} = 9. \tag{19}$$

Note that the numbers of Raman- and IR-active phonon modes found for chiral BN-NT's are almost the same as for chiral C-NT's (14 Raman- and 6 IR-active modes).[9]

In conclusion, we identified three families of rod groups which are relevant for the description of BN-NT's: the fourth for the armchair, the eighth for the zigzag, and the first for the chiral BN-NT's. Like their carbon ''ancestors'' (achiral, the 13th family; chiral, the fifth family[10]) all BN-NT's possess the symmetries of *nonsymmorphic* rod groups. Contrary to achiral C-NT's, however, armchair and zigzag BN-NT's belong to different rod-group families. In addition, we showed that armchair BN-NT's with even index n are *centrosymmetric* materials. Nevertheless, and in contrast to 2D and 3D centrosymmetric *and* polar crystalline materials, they are expected to exhibit the photogalvanic effects discussed in Ref. 8. Having preserved the Nth-order screw-axis symmetry existing in C-NT's, BN-NT's could also serve as candidates for the selective generation of high-order harmonics, as recently proposed by Alon *et al.* for C-NT's.[16]

By utilizing the symmetries of the factor groups $\mathcal{C}_{2nh}$, $\mathcal{C}_{2nv}$ and $\mathcal{C}_N$ we have found that all armchair BN-NT's have 9 Raman- and 4 IR-active phonon modes; all armchair BN-NT's have 14 Raman- and 8 IR-active phonon modes; all chiral BN-NT's have 15 Raman- and 9 IR-active phonon modes. Especially and unlike the situation for achiral CN-NT's,[9] the numbers of Raman- and infrared-active vibrations in zigzag BN-NT's are almost twice as in armchair BN-NT's.

Note added in proof. BN-NT spatial symmetry has recently and independently been determined by Damnjanović *et al.*[17]

This work was supported in part by the Basic Research Foundation administered by the Israeli Academy of Sciences and Humanities and by the Fund for the Promotion of Research at Technion. The author wishes to thank Professor N. Moiseyev, Dr. V. Averbukh, Professor U. Peskin, and Dr. P. Král for many helpful discussions and comments.

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