# Proposed Boron Nanotubes†

**Asta Gindulytė,[‖,‡] William N. Lipscomb,*[,§] and Lou Massa[‖,‡]**

Department of Chemistry, Hunter College, 695 Park Avenue, New York, New York 10021, The Graduate School, City University of New York, 33 West 42nd Street, New York, New York 10036, and Gibbs Chemical Laboratory, Harvard University, Cambridge, Massachusetts 02138

*Received May 19, 1998*

Carbon nanotubes are cylindrical structures related to carbon fullerene structures. Indeed, carbon nanotube cylinders are often "capped" at their ends with "hemispherical" carbon fullerenes, illustrating the close relation of the two types of structure. Nanotube structures are of great interest because of their mechanical and one-dimensional electrical properties.[1−4]

In earlier papers[5−7] we explored the dual (reciprocal) geometries of boron and carbon fullerenes. These dual relationships were based upon the Descartes−Euler formula

$$P - C + F = 2 \quad (1)$$

where in a polyhedral type of molecule, *P*, *C*, and *F* are counts of points (vertexes), connections (bonds), and faces, respectively. The molecules considered in refs[5−7] were based upon consideration of highly spherical compounds, either singly or compounded as "multicage" molecules. The molecules considered here, nanotubes, are based upon the geometry of a cylinder. In the search for boron nanotubes, the duals of carbon nanotubes, we employ a generalization of the above equation, viz., the Euler−Poincare formula for a cylinder,

$$P - C + F = 0 \quad (2)$$

where *P*, *C*, and *F* retain their previous meanings.

Of course there is any number of different possible nanotubes. In this paper, for purposes of efficiency, we restrict our discussions to a few types. They are sufficiently general that the analysis shown here can be adapted afterward to any other case. In Figures 1−3 we show selected examples of carbon nanotubes and their boron duals derived from the Euler−Poincare formula, eq 2. The boron duals may be imagined as arising from a correspondence between a boron atom and the center of each of the carbon faces in the carbon nanotubes. If the formula for a given carbon nanotube is taken to be $C_P$, then the formula for its boron dual nanotube is $B_FH_F$. In the Figures, the hydrogen atoms, which extend radially outward from each boron atom, are not shown in order to simplify the drawing. Moreover, it may be possible to synthesize boron nanotubes (and boron fullerenes) as pure boron compounds, i.e., without bonds to hydrogen atoms. We would expect the basic boron geometrical structure to be the same with or without the hydrogen atoms attached. But, we recognize the electronic structure associated with the boron geometry will be greatly modified by the formation of BH bonds.

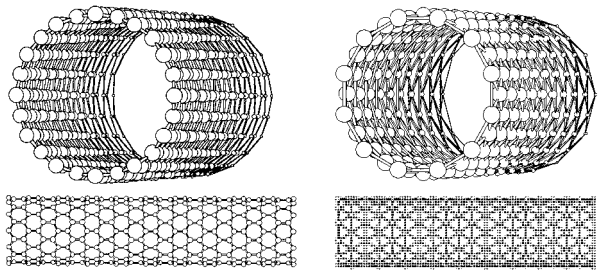

**Figure 1.** Carbon (left) and boron (right) nanotubes, shown as end-on (top) and side (bottom) views. The case shown is the "zigzag" geometry corresponding to $(n, m) = (12,0)$.

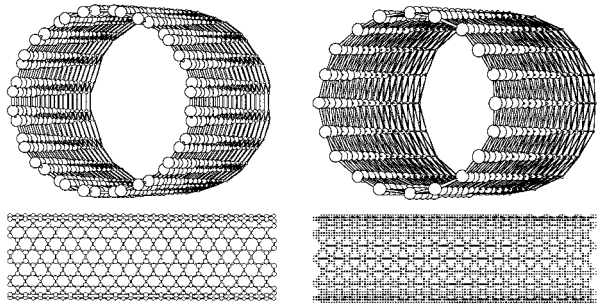

**Figure 2.** Carbon and boron nanotubes viewed as in Figure 1; the "armchair" geometry corresponds to $(n, m) = (10,10)$.

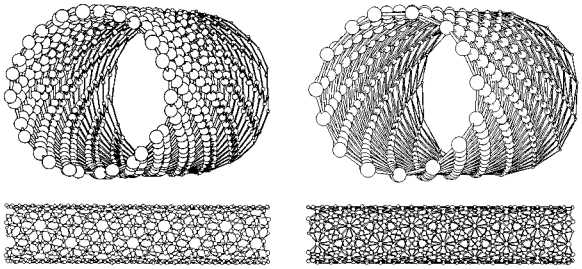

**Figure 3.** Carbon and boron nanotubes viewed as in Figure 1; an example chiral geometry corresponding to $(n, m) = (10,5)$.

**Table 1.** Carbon and Boron Dual Nanotubes; Listed Are the Factors of the Euler−Poincare Formula for a Cylinder, viz. $P - C + F = 0$

| formula | *P* | *F* | *C* | (*n*, *m*) | tube type | *P* | *F* | formula |
|---|---|---|---|---|---|---|---|---|
| $C_{480}$ | 480 | 240 | 720 | (12, 0) | zigzag | 240 | 480 | $B_{240}H_{240}$ |
| $C_{720}$ | 720 | 360 | 1080 | (10, 10) | armchair | 360 | 720 | $B_{360}H_{360}$ |
| $C_{600}$ | 600 | 300 | 900 | (10, 5) | chiral | 300 | 600 | $B_{300}H_{300}$ |

In Table 1 we display a count of *P*, *C*, and *F* for each of the molecules displayed in Figures 1−3. It may be seen how the Euler−Poincare formula is satisfied in each case. Notice in particular how the roles of *P* and *F* are interchanged in going

† This paper is dedicated to M. Frederick Hawthorne on the occasion of his 70th birthday.

* Corresponding author.
‖ Hunter College.
‡ City University of New York.
§ Harvard University.

(1) Dresselhaus, M. S.; Dresselhaus, G.; Eklund, P. C. *Science of Fullerenes and Carbon Nanotubes*; Academic: San Diego, 1996.
(2) Mintmire, J. W.; Dunlap, B. I.; White, C. T. *Phys. Rev. Lett.* **1992**, *68*, 631.
(3) Bethune, D. S.; Kiang, C.-H.; de Vries, M. S.; Gorman, G.; Savoy, R.; Vazquez, J.; Beyers, R. *Nature* **1993**, *363*, 605.
(4) Iijima, S.; Ichihashi, T. *Nature* **1993**, *363*, 603.
(5) Lipscomb, W. N.; Massa, L. *Inorg. Chem.* **1992**, *31*, 2297−2299.
(6) Dereckei-Kovacs, A.; Dunlap, B. I.; Lipscomb, W. N.; Lowrey, A.; Marynick, D. S.; Massa, L. *Inorg. Chem.* **1994**, *33*, 5617−5619.
(7) Lipscomb, W. N.; Massa, L. *Inorg. Chem.* **1994**, *33*, 5155−5156.

10.1021/ic980559o CCC: $15.00 
Published on Web 11/19/1998

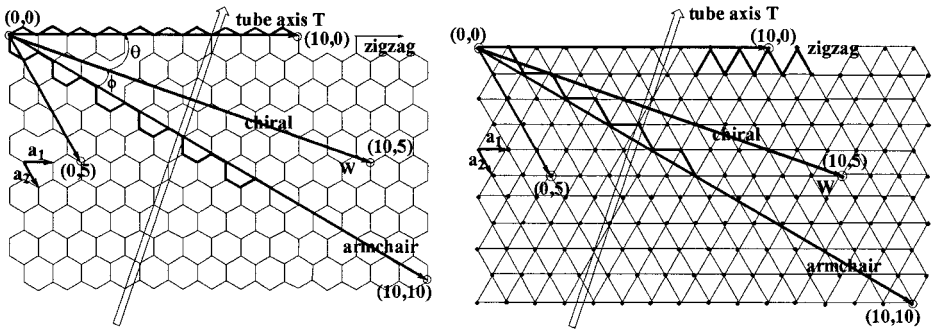


**Figure 4.** Relation between nanotube and lattice for carbon (left) and boron (right), illustrating lattice vectors $\mathbf{a_1}$ and $\mathbf{a_2}$, and the "wrapping" vector $\mathbf{W} = n\mathbf{a_1} + m\mathbf{a_2}$. The extreme cases of "zigzag" ($n$, 0) and "armchair" ($n$, $n$) are indicated. The chiral angle, $\phi$, is that subtended by the general wrapping vector, **W**, and the armchair vector. The sum of the angles $\phi$ and $\theta$ is 30°. The tube axis vector, **T**, is orthogonal to the wrapping vector **W**. The tube diameter, $d = |\mathbf{W}|/\pi$. Notice the boron lattice is mathematically obtained from the carbon lattice by the device of placing a boron point at the center of a carbon face.

from a carbon nanotube to its dual boron nanotube partner. Notice also that the number of bonds is common to the carbon and boron nanotube duals. Obtaining the count of the bonds requires consideration of all dangling bonds in both the carbon and boron cases. Dangling bonds are associated with dangling faces, and these too must be counted to obtain the values listed in the table. We mention in passing that the nanotube cylinders (including their dangling bonds) are topologically related to a torus, for which the Euler−Poincare formula, eq 2, also applies. The nanotubes also map into a flat sheet lattice structure, illustrated in Figure 4.

Following the explanation in ref 1, one may specify a single wall carbon nanotube "by bisecting a $C_{60}$ molecule at the equator and joining the two resulting hemispheres with a cylindrical tube one monolayer thick and with the same diameter as $C_{60}$". Bisecting the $C_{60}$ molecule along different directions will yield carbon nanotubes of differing symmetry. Thus, the "zigzag" and "armchair" carbon nanotubes of Figures 1 and 2 are related to bisections of $C_{60}$ normal to a 3-fold axis and a 5-fold axis, respectively. Analogously, if "spherical" $B_{32}H_{32}$, the geometrical dual[5] of $C_{60}$, is bisected normal to a 5-fold and 3-fold axis one specifies thereby the dual "zigzag" and "armchair" boron nanotubes respectively, as shown in Figures 1 and 2. Additional chiral nanotubes, examples of which are illustrated in Figure 3, can be defined in relation to more general "hemispherical" caps.

Again following the explanation of ref 1, Figure 4 illustrates that a variety of nanotubes may be defined in terms of tube diameter, $d$, angle $\phi$, and wrapping vector $\mathbf{W} = n\mathbf{a_1} + m\mathbf{a_2}$. The "zigzag" and "armchair" nanotubes correspond to angles $\phi$ equal to 0° and 30° respectively. A general chiral nanotube, such as displayed in Figure 3, corresponds to a chiral angle $\phi$, falling between the extremes, 0° and 30°.

A mathematical representation of a general nanotube is formed by "rolling up" the plane of Figure 4, joining the two ends of the chiral vector **W**. Variation of the tube diameter, $d$, and chiral angle, $\phi$, are considered to control the properties of the various nanotubes formed.[1] That carbon nanotubes are semiconducting or metallic depending on variation of $\phi$ and $d$ has been confirmed experimentally.[8,9] It is our expectation that if boron nanotubes could be synthesized, their electrical properties, also controlled by variation of $\phi$ and $d$ parameters, would, like their carbon nanotube duals, be of very great interest.

**Acknowledgment.** We thank Professor Joe Roitberg of Hunter College for valuable topological discussions. This research was supported by an IBM Shared University Research (SUR) grant, a CUNY Research Award, a CUNY Collaborative Award, and a NASA JOVE grant.

IC980559O

(8) Wildöer, J. W. G.; Venema, L. C.; Rinzler, A. G.; Smalley, R. E.; Dekker, C. *Nature* **1998**, *391*, 59−62.
(9) Odom, T. W.; Huang, J.-L.; Kim, P.; Lieber, C. M. *Nature* **1998**, *391*, 62−64.