Research Article

Topological Aspects of Boron Nanotubes

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The degree-based topological indices are used to correlate the physical and chemical properties of a molecule with its chemical structure. Boron nanotubular structures are high-interest materials due to the presence of multicenter bonds and have novel electronic properties. These materials have some important issues in nanodevice applications like mechanical and thermal stability. Therefore, they require theoretical studies on the other properties. In this paper, we present certain degree-based topological indices such as ABC , the fourth ABC , GA , and the fifth GA indices for boron triangular and boron- α nanotubes.

1. Introduction

Mathematical chemistry is a branch of theoretical chemistry in which we get information about the molecular structure by using mathematical techniques without assigning that structure to quantum mechanics [1, 2]. Chemical graph theory is a branch of mathematical chemistry which implements graph theory to study mathematical modeling of chemical aspects [3]. This theory shows a prominent effect on the extension of the chemical sciences [4].

The chemical structure of a molecule is strongly related to its chemical properties such as strain energy, boiling point, and heat of formation. Molecular graphs can be used to model the chemical structures of molecules and molecular compounds by considering atoms as vertices and the chemical bonds between the atoms as edges. Consider molecular graph G having vertex set V_G and edge set E_G . Let I_G be the set of edges of G that are incident with a vertex $p \in V_p$, then the degree of p is defined as the cardinality of the set I_G and $\delta_p = \sum_{q \in N_p} d_q$, where set N_p consists of all neighbor vertices of p , that is, $N_p = \{q \in V_G \mid pq \in E_G\}$.

A topological index is the graph invariant which is used to correlate the physical and chemical properties of a chemical compound with its molecular graph. In this sense, topological indices are based on several topological aspects of the corresponding molecular graph. The use of topological indices is particularly important when using

experimental methods leads to waste of time and financial expenditures in large amounts and theoretical methods have not been successful. Topological indices are used to correlate physical properties of chemical structures in QSPR/QSAR studies and provide a measure of structural similarity/stability/diversity of chemical databases. The relative stability of the fullerenes has been correlated with topological indices in [5]. In [6], topological indices are also used to predict the stable isomers of a given fullerene, and for detailed study, we refer [7].

Generally, topological indices can be categorized in three classes: degree-based, distance-based, and spectrum-based indices. In this paper, certain degree-based topological indices are going to be discussed because of their great applications in chemical graph theory. For recent study of distance-based indices, we refer [8, 9], and for spectrum-based indices, we refer [10, 11].

The first degree-based topological index is the Randić connectivity index which was presented by Randić [12] and is defined as

$$\chi(G) = \sum_{pq \in E_G} \frac{1}{\sqrt{d_p d_q}} \quad (1)$$

This index has been shown to reflect molecular branching and is deeply examined by chemists and mathematicians [13, 14]. Many physical and chemical properties depend on

FIGURE 1: (a) A 3D perception of boron triangular nanotube. (b) A 3D perception of boron- α nanotube.

such factors which are different rather than branching. With this motivation, Estrada et al. [15] presented the atom-bond connectivity index, which is defined as

$$ABC(G) = \sum_{pq \in E_G} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}}. \quad (2)$$

It is reported in [15–17] that this index can be applied in modeling thermodynamic features of organic chemical compounds. In addition, Estrada [16] interpreted a new quantum theory which presented that this index implements a model for consideration of 1,2-, 1,3-, and 1,4-interactions in the carbon-atom skeleton of saturated hydrocarbons, and in this sense, it can be applied for rationalizing steric effects in such compounds.

Recently, Ghorbani and Hosseinzadeh [18] presented the fourth atom-bond connectivity index which is defined as

$$ABC_4(G) = \sum_{pq \in E_G} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}}. \quad (3)$$

The sense for presenting a new index is to increase prediction of some property of molecules. One of the successors of the Randić connectivity index called the geometric-arithmetic (GA) connectivity index which is presented by Vukičević and Furtula [19] is defined as

$$GA(G) = \sum_{pq \in E_G} \frac{2\sqrt{d_p d_q}}{(d_p + d_q)}. \quad (4)$$

It is reported in [19, 20] that this index provides better prediction rate than the Randić index in various physico-chemical properties such as entropy, enthalpy of formation, and standard enthalpy of vaporization. Furthermore, the enhancement in the prediction accuracy rate of the GA index comparing to the Randić index is more than 9% for the standard enthalpy of vaporization. In [21], it also presents that there forms excellent correlation between heat of formation of benzenoid hydrocarbons and the GA index (the correlation coefficient is 0.972).

Recently, the fifth GA index is presented by Graovac et al. [22] and is defined as

$$GA_5(G) = \sum_{pq \in E_G} \frac{2\sqrt{\delta_p \delta_q}}{(\delta_p + \delta_q)}. \quad (5)$$

In this paper, we present ABC , ABC_4 , GA , and GA_5 topological indices for new classes of nanotubes fabricated from carbon hexagonal nanotubes called the boron triangular and boron- α nanotubes.

2. Boron Nanotubes

In last 20 years, various types of boron-containing nanomaterials such as boron nanoclusters, boron nanowires, boron nanotubes, boron nanobelts, boron nanoribbons, boron nanosheets, and boron fullerenes have been experimentally synthesized and identified. Boron nanomaterials have been considered as excellent materials for enhancing the characteristics of optoelectronic nanodevices because of their broad elastic modulus, high-melting

FIGURE 2: (a) A 2D sheet of boron triangular nanotube $BT[m, n]$. (b) A 2D sheet of boron- α nanotube $BA[m, n]$.

point, excessive conductivity, great emission uniformity, and low turn-on field. These materials can carry excessive emission current, which recommends that they may have great prospective applications in the field emission area [23]. Furthermore, boron nanomaterials also have some better properties compared to carbon nanomaterials such as excessive resistance to oxidation at high temperatures and great chemical stability and are stable broad band-gap semiconductor [24, 25]. Due to these properties, boron nanomaterials may have great applications at high temperatures or in corrosive environments functioning as supercapacitors, solid lubricants, fuel cells, and batteries [26]. Moreover, the extensive range of boron nanomaterials themselves could be the building blocks for combining with other existing nanomaterials to design and create materials with new properties. For this reason, the boron-nitrogen clusters have been developed in [27, 28], and boron-nitrogen cages have been computed in [29]. The boron fullerenes are the cage molecules [30] which can serve as the building blocks for fabrication of new hybrid nanostructures with novel properties.

The boron triangular nanotube was created in 2004 [23] and obtained from a carbon hexagonal nanotube by adding an extra atom to the center of each hexagon. Also, a special boron nanotube was fabricated from a carbon hexagonal nanotube in 2008, by adding an extra atom to the center of certain hexagons [31, 32]. This nanotube is designed by generating a mixture of hexagons and triangles called the boron- α nanotube. It is reported in [33, 34] that these nanotubes are important materials for optical, electronic, chemical, and biosensing applications. The comparison study about some computational aspects of boron triangular and boron- α nanotubes has been investigated in [35]. The 3D perceptions of boron triangular and boron- α nanotube are presented in Figure 1.

3. Main Results

We denote the molecular graphs of boron triangular and boron- α nanotubes by $BT[m, n]$ and $BA[m, n]$, respectively, where m is the number of rows and n is the number of columns in a 2D sheet of $BT[m, n]$ or $BA[m, n]$ as shown in

TABLE 1: The order and size of boron nanotubes.

Molecular graph	Order	Size
$BT[m, n]$	$3mn/2$	$3n(3m-2)/2$
$BA(X)[m, n]$	$n(4m+1)/3$	$n(7m-2)/2$
$BA(Y)[m, n]$	$4mn/3$	$n(7m-4)/2$

Figure 2. We categorize the boron- α nanotubes into two classes with respect to m . We denote these classes as $BA(X)[m, n]$ and $BA(Y)[m, n]$ for $m \equiv 2 \pmod{3}$ and $m \equiv 0 \pmod{3}$, respectively. The order and size of $BT[m, n]$, $BA(X)[m, n]$, and $BA(Y)[m, n]$ are given in Table 1. In the following theorem, we compute the ABC index, fourth ABC , GA , and fifth GA indices for $BT[m, n]$.

Theorem 1. Consider the boron triangular nanotube $BT[m, n]$, where $m \geq 3$ and n even, then

$$\begin{aligned}
 ABC(BT[m, n]) &= \frac{3\sqrt{10}}{4}mn + \frac{3\sqrt{6}}{4}n - 2\sqrt{10}n + 2\sqrt{3}n, \\
 GA(BT[m, n]) &= \frac{9}{2}mn + \frac{12\sqrt{6}}{5}n - 9n, \\
 ABC_4(BT[m, n]) &= \frac{\sqrt{70}}{8}mn - \frac{7\sqrt{70}}{12}n + \frac{3\sqrt{62}}{32}n \\
 &\quad + \frac{3\sqrt{38}}{20}n + \frac{\sqrt{33}}{4}n + \frac{3\sqrt{5}}{4}n, \\
 GA_5(BT[m, n]) &= \frac{9}{2}mn + \frac{72\sqrt{2}}{17}n + \frac{24\sqrt{10}}{13}n - 15n.
 \end{aligned} \tag{6}$$

Proof. Consider the boron triangular nanotube $G = BT[m, n]$. There are three partite subsets of the edge set E_G corresponding to the degree of end vertices which are presented as

FIGURE 3: The edge partitions of BT [7, 4] nanotube: (a) with respect to degree of end vertices; (b) with respect to degree sum of neighbor vertices.

$$\begin{aligned}
 E_{4,4} &= \{pq \in E_G \mid d_p = d_q = 4\}, \\
 E_{4,6} &= \{pq \in E_G \mid d_p = 4 \text{ and } d_q = 6\}, \\
 E_{6,6} &= \{pq \in E_G \mid d_p = d_q = 6\}.
 \end{aligned} \quad (7)$$

Therefore, we have $|E_{4,4}| = 3n$, $|E_{4,6}| = 6n$, and $|E_{6,6}| = 3n(3m-8)/2$. The representative edges of these partite sets are shown in Figure 3(a) in which blue, red, and black edges belong to $E_{4,4}$, $E_{4,6}$, and $E_{6,6}$, respectively. From (2) and (4), the ABC and GA indices of G are formulated as

$$\begin{aligned}
 ABC(G) &= \sum_{pq \in E_{4,4}} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}} + \sum_{pq \in E_{4,6}} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}} \\
 &\quad + \sum_{pq \in E_{6,6}} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}} \\
 &= \frac{3\sqrt{10}}{4}mn + \frac{3\sqrt{6}}{4}n - 2\sqrt{10}n + 2\sqrt{3}n, \\
 GA(G) &= \sum_{pq \in E_{4,4}} \frac{2\sqrt{d_p d_q}}{d_p + d_q} + \sum_{pq \in E_{4,6}} \frac{2\sqrt{d_p d_q}}{d_p + d_q} + \sum_{pq \in E_{6,6}} \frac{2\sqrt{d_p d_q}}{d_p + d_q} \\
 &= \frac{9}{2}mn + \frac{12\sqrt{6}}{5}n - 9n.
 \end{aligned} \quad (8)$$

Similarly, the edge partite subsets of E_G corresponding to their degree sum of neighbors of end vertices are given as

$$\begin{aligned}
 S_{20,20} &= \{pq \in E_G \mid \delta_p = \delta_q = 20\}, \\
 S_{20,32} &= \{pq \in E_G \mid \delta_p = 20 \text{ and } \delta_q = 32\}, \\
 S_{32,32} &= \{pq \in E_G \mid \delta_p = \delta_q = 32\}, \\
 S_{32,36} &= \{pq \in E_G \mid \delta_p = 32 \text{ and } \delta_q = 36\}, \\
 S_{36,36} &= \{pq \in E_G \mid \delta_p = \delta_q = 36\}.
 \end{aligned} \quad (9)$$

Therefore, we have $|S_{20,20}| = 3q$, $|S_{20,32}| = 6q$, $|S_{32,32}| = 3q$, $|S_{32,36}| = 6q$, and $|S_{36,36}| = 3q(3p-14)/2$. The representatives of these partite sets are shown in Figure 3(b) in which blue, red, yellow, green, and black edges belong to $S_{20,20}$, $S_{20,32}$, $S_{32,32}$, $S_{32,36}$, and $S_{36,36}$, respectively. From (3) and (5), the fourth ABC and fifth GA indices of G are computed as

$$\begin{aligned}
 ABC_4(G) &= \sum_{pq \in S_{20,20}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} + \sum_{pq \in S_{20,32}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\
 &\quad + \sum_{pq \in S_{32,32}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} + \sum_{pq \in S_{32,36}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\
 &\quad + \sum_{pq \in S_{36,36}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\
 &= \frac{\sqrt{70}}{8}mn - \frac{7\sqrt{70}}{12}n + \frac{3\sqrt{62}}{32}n \\
 &\quad + \frac{3\sqrt{38}}{20}n + \frac{\sqrt{33}}{4}n + \frac{3\sqrt{5}}{4}n, \\
 GA_5(G) &= \sum_{pq \in S_{20,20}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{20,32}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{32,32}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\
 &\quad + \sum_{pq \in S_{32,36}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{36,36}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\
 &= \frac{9}{2}mn + \frac{72\sqrt{2}}{17}n + \frac{24\sqrt{10}}{13}n - 15n.
 \end{aligned} \quad (10)$$

In next theorem, we formulate ABC, the fourth ABC, GA, and the fifth GA indices for $BA(X)[m, n]$ nanotubes.

Theorem 2. Consider the boron- α nanotube $BA(X)[m, n]$, then

$$\begin{aligned}
 ABC(BA(X)[m, n]) &= \frac{3\sqrt{2}}{5}mn + \frac{6}{\sqrt{30}}mn + \frac{3\sqrt{6}}{4}n \\
 &\quad + \frac{4\sqrt{7}}{\sqrt{20}}n + \frac{2}{\sqrt{3}}n - \frac{8\sqrt{2}}{5}n - \frac{18}{\sqrt{30}}n, \\
 GA(BA(X)[m, n]) &= \frac{4\sqrt{30}}{11}mn + \frac{3}{2}mn + \frac{16\sqrt{5}}{9}n \\
 &\quad + \frac{8\sqrt{6}}{10}n - \frac{12\sqrt{30}}{11}n - n, \\
 ABC_4(BA(X)[m, n]) &= \frac{\sqrt{13}}{9}mn + \frac{\sqrt{22}}{9}mn + \frac{2\sqrt{35}}{3\sqrt{38}}n \\
 &\quad + \frac{\sqrt{10}}{3\sqrt{3}}n + \frac{\sqrt{41}}{6}n + \frac{3\sqrt{5}}{\sqrt{133}}n \\
 &\quad + \frac{7}{9\sqrt{2}}n + \frac{5}{\sqrt{84}}n + \frac{6}{19}n + \frac{\sqrt{46}}{24}n \\
 &\quad + \frac{\sqrt{53}}{3\sqrt{21}}n - \frac{14\sqrt{13}}{27}n - \frac{5\sqrt{22}}{9}n, \\
 GA_5(BA(X)[m, n]) &= \frac{36\sqrt{10}}{57}mn + \frac{3}{2}mn + \frac{12\sqrt{38}}{37}n \\
 &\quad + \frac{8\sqrt{3}}{7}n + \frac{8\sqrt{114}}{43}n + \frac{8\sqrt{133}}{47}n \\
 &\quad + \frac{24\sqrt{2}}{17}n + \frac{4\sqrt{42}}{13}n \\
 &\quad + \frac{24\sqrt{21}}{55}n - \frac{180\sqrt{10}}{57}n - 5n.
 \end{aligned} \tag{11}$$

Proof. Consider the boron- α nanotube $H = BA(X)[m, n]$. There are five partite subsets of the edge set E_H corresponding to the degree of end vertices which are given as

$$\begin{aligned}
 E_{4,4} &= \{pq \in E_H \mid d_p = d_q = 4\}, \\
 E_{4,5} &= \{pq \in E_H \mid d_p = 4 \text{ and } d_q = 5\}, \\
 E_{4,6} &= \{pq \in E_H \mid d_p = 4 \text{ and } d_q = 6\}, \\
 E_{5,5} &= \{pq \in E_H \mid d_p = d_q = 5\}, \\
 E_{5,6} &= \{pq \in E_H \mid d_p = 5 \text{ and } d_q = 6\}.
 \end{aligned} \tag{12}$$

Therefore, we have $|E_{4,4}| = 3n$, $|E_{4,5}| = 4n$, $|E_{4,6}| = 2n$, $|E_{5,5}| = n(3m - 8)/2$, and $|E_{5,6}| = 2n(m - 3)$. The

FIGURE 4: The edge partitions of $BA(X)[8, 6]$ with respect to degree of end vertices.

representative edges of these partite sets are presented in Figure 4. From (2) and (4), the ABC and GA indices of H are formulated as

$$\begin{aligned}
 ABC(H) &= \sum_{pq \in E_{4,4}} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}} + \sum_{pq \in E_{4,5}} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}} \\
 &\quad + \sum_{pq \in E_{4,6}} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}} + \sum_{pq \in E_{5,5}} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}} \\
 &\quad + \sum_{pq \in E_{5,6}} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}} \\
 &= \frac{3\sqrt{2}}{5}mn + \frac{6}{\sqrt{30}}mn + \frac{3\sqrt{6}}{4}n + \frac{4\sqrt{7}}{\sqrt{20}}n \\
 &\quad + \frac{2}{\sqrt{3}}n - \frac{8\sqrt{2}}{5}n - \frac{18}{\sqrt{30}}n, \\
 GA(H) &= \sum_{pq \in E_{4,4}} \frac{2\sqrt{d_p d_q}}{d_p + d_q} + \sum_{pq \in E_{4,5}} \frac{2\sqrt{d_p d_q}}{d_p + d_q} \\
 &\quad + \sum_{pq \in E_{4,6}} \frac{2\sqrt{d_p d_q}}{d_p + d_q} + \sum_{pq \in E_{5,5}} \frac{2\sqrt{d_p d_q}}{d_p + d_q} \\
 &\quad + \sum_{pq \in E_{5,6}} \frac{2\sqrt{d_p d_q}}{d_p + d_q}
 \end{aligned}$$

$$\begin{aligned}
&= \frac{4\sqrt{30}}{11}mn + \frac{3}{2}mn + \frac{16\sqrt{5}}{9}n \\
&\quad + \frac{8\sqrt{6}}{10}n - \frac{12\sqrt{30}}{11}n - n.
\end{aligned} \tag{13}$$

Also, there are eleven edge partite subsets of E_G corresponding to their degree sum of neighbors of end vertices, which are given as

$$\begin{aligned}
S_{18,19} &= \{pq \in E_H \mid \delta_p = 18 \text{ and } \delta_q = 19\}, \\
S_{18,24} &= \{pq \in E_H \mid \delta_p = 18 \text{ and } \delta_q = 24\}, \\
S_{19,19} &= \{pq \in E_H \mid \delta_p = \delta_q = 19\}, \\
S_{19,24} &= \{pq \in E_H \mid \delta_p = 19 \text{ and } \delta_q = 24\}, \\
S_{19,28} &= \{pq \in E_H \mid \delta_p = 19 \text{ and } \delta_q = 28\}, \\
S_{24,24} &= \{pq \in E_H \mid \delta_p = \delta_q = 24\}, \\
S_{24,27} &= \{pq \in E_H \mid \delta_p = 24 \text{ and } \delta_q = 27\}, \\
S_{24,28} &= \{pq \in E_H \mid \delta_p = 24 \text{ and } \delta_q = 28\}, \\
S_{27,27} &= \{pq \in E_H \mid \delta_p = \delta_q = 27\}, \\
S_{27,28} &= \{pq \in E_H \mid \delta_p = 27 \text{ and } \delta_q = 28\}, \\
S_{27,30} &= \{pq \in E_H \mid \delta_p = 27 \text{ and } \delta_q = 30\}.
\end{aligned} \tag{14}$$

Therefore, we have $|S_{18,19}| = 2n$, $|S_{18,24}| = 2n$, $|S_{19,19}| = n$, $|S_{19,24}| = 2n$, $|S_{19,28}| = 2n$, $|S_{24,24}| = n$, $|S_{24,27}| = 2n$, $|S_{24,28}| = 2n$, $|S_{27,27}| = n(3m-14)/2$, $|S_{27,28}| = 2n$, and $|S_{27,30}| = 2n(m-5)$. The representative edges of these partite sets are presented in Figure 5. From (3) and (5), the fourth ABC index and fifth GA index are computed as

$$\begin{aligned}
ABC_4(G) &= \sum_{pq \in S_{18,19}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} + \sum_{pq \in S_{18,24}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\
&\quad + \sum_{pq \in S_{19,19}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} + \sum_{pq \in S_{19,24}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\
&\quad + \sum_{pq \in S_{19,28}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} + \sum_{pq \in S_{24,24}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\
&\quad + \sum_{pq \in S_{24,27}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} + \sum_{pq \in S_{24,28}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}}
\end{aligned}$$

FIGURE 5: The edge partitions of $BA(X)[8,6]$ with respect to degree sum of neighbor vertices.

$$\begin{aligned}
&+ \sum_{pq \in S_{27,27}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} + \sum_{pq \in S_{27,28}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\
&+ \sum_{pq \in S_{27,30}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\
&= \frac{\sqrt{13}}{9}mn + \frac{\sqrt{22}}{9}mn + \frac{2\sqrt{35}}{3\sqrt{38}}n + \frac{\sqrt{10}}{3\sqrt{3}}n \\
&\quad + \frac{\sqrt{41}}{6}n + \frac{3\sqrt{5}}{\sqrt{133}}n + \frac{7}{9\sqrt{2}}n + \frac{5}{\sqrt{84}}n \\
&\quad + \frac{6}{19}n + \frac{\sqrt{46}}{24}n + \frac{\sqrt{53}}{3\sqrt{21}}n - \frac{14\sqrt{13}}{27}n - \frac{5\sqrt{22}}{9}n,
\end{aligned}$$

$$\begin{aligned}
GA_5(G) &= \sum_{pq \in S_{18,19}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{18,24}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\
&\quad + \sum_{pq \in S_{19,19}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{19,24}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\
&\quad + \sum_{pq \in S_{19,28}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{24,24}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\
&\quad + \sum_{pq \in S_{24,27}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{24,28}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q}
\end{aligned}$$

$$\begin{aligned}
& + \sum_{pq \in S_{27,27}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{27,28}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\
& + \sum_{pq \in S_{27,30}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\
& = \frac{36\sqrt{10}}{57}mn + \frac{3}{2}mn + \frac{12\sqrt{38}}{37}n + \frac{8\sqrt{3}}{7}n + \frac{8\sqrt{114}}{43}n \\
& + \frac{8\sqrt{133}}{47}n + \frac{24\sqrt{2}}{17}n + \frac{4\sqrt{42}}{13}n \\
& + \frac{24\sqrt{21}}{55}n - \frac{180\sqrt{10}}{57}n - 5n.
\end{aligned} \tag{15}$$

For $BA(Y)[m, n]$ nanotube, ABC , the fourth ABC , GA and the fifth GA indices are formulated in Theorem 3.

Theorem 3. Consider the boron- α nanotube $BA(Y)[m, n]$, then

$$\begin{aligned}
ABC(BA(Y)[m, n]) &= \frac{6}{\sqrt{50}}mn + \frac{\sqrt{30}}{5}mn + \frac{3\sqrt{6}}{8}n \\
&+ \sqrt{\frac{2}{5}}n + \frac{\sqrt{7}}{3\sqrt{2}}n + \frac{\sqrt{7}}{\sqrt{5}}n + \frac{1}{\sqrt{3}}n \\
&+ \frac{1}{3}n - \frac{8\sqrt{2}}{5}n - \frac{\sqrt{30}}{2}n, \\
GA(BA(Y)[m, n]) &= \frac{4\sqrt{30}}{11}mn + \frac{3}{2}mn + \frac{\sqrt{15}}{4}n \\
&+ \frac{2\sqrt{2}}{3}n + \frac{8\sqrt{5}}{9}n \\
&+ \frac{2\sqrt{6}}{5}n - \frac{10\sqrt{30}}{11}n - 2n, \\
ABC_4(BA(Y)[m, n]) &= \frac{\sqrt{13}}{9}mn + \frac{2\sqrt{5}}{9}mn + \frac{\sqrt{26}}{28}n \\
&+ \frac{\sqrt{37}}{5\sqrt{14}}n + \frac{\sqrt{38}}{2\sqrt{91}}n + \frac{\sqrt{35}}{3\sqrt{38}}n \\
&+ \frac{\sqrt{10}}{6\sqrt{3}}n + \frac{3}{19}n + \frac{\sqrt{41}}{2\sqrt{114}}n \\
&+ \frac{3\sqrt{5}}{2\sqrt{133}}n + \frac{\sqrt{46}}{48}n + \frac{7}{18\sqrt{2}}n \\
&+ \frac{5}{4\sqrt{21}}n + \frac{2\sqrt{3}}{25}n + \frac{7}{5\sqrt{26}}n
\end{aligned}$$

$$\begin{aligned}
& + \frac{\sqrt{2}}{3\sqrt{3}}n + \frac{\sqrt{53}}{5\sqrt{30}}n + \frac{\sqrt{17}}{3\sqrt{26}}n \\
& + \frac{\sqrt{53}}{6\sqrt{21}}n - \frac{14\sqrt{13}}{27}n - \frac{10\sqrt{5}}{9}n, \\
GA_5(BA(Y)[m, n]) &= \frac{12\sqrt{10}}{19}mn + \frac{3}{2}mn \\
& + \frac{10\sqrt{14}}{39}n + \frac{\sqrt{91}}{10}n + \frac{6\sqrt{38}}{37}n \\
& + \frac{4\sqrt{3}}{7}n + \frac{4\sqrt{114}}{43}n + \frac{4\sqrt{133}}{47}n \\
& + \frac{12\sqrt{2}}{17}n + \frac{2\sqrt{42}}{13}n + \frac{10\sqrt{26}}{51}n \\
& + \frac{15\sqrt{3}}{26}n + \frac{2\sqrt{30}}{11}n + \frac{6\sqrt{78}}{53}n \\
& + \frac{12\sqrt{21}}{55}n - \frac{60\sqrt{10}}{19}n - 5n.
\end{aligned} \tag{16}$$

Proof. Consider the boron- α nanotube $K = BA(Y)[m, n]$. From Figure 6, we can see that there are eight partite subsets of edge set E_K corresponding to their degree of end vertices which are given as

$$\begin{aligned}
E_{3,3} &= \{pq \in E_K \mid d_p = d_q = 3\}, \\
E_{3,5} &= \{pq \in E_K \mid d_p = 3 \text{ and } d_q = 5\}, \\
E_{3,6} &= \{pq \in E_K \mid d_p = 3 \text{ and } d_v = 6\}, \\
E_{4,4} &= \{pq \in E_K \mid d_p = d_q = 4\}, \\
E_{4,5} &= \{pq \in E_K \mid d_u = 4 \text{ and } d_v = 5\}, \\
E_{4,6} &= \{pq \in E_K \mid d_p = 4 \text{ and } d_q = 6\}, \\
E_{5,5} &= \{pq \in E_K \mid d_p = d_q = 5\}, \\
E_{5,6} &= \{pq \in E_K \mid d_p = 5 \text{ and } d_v = 6\}.
\end{aligned} \tag{17}$$

Therefore, we have $|E_{3,3}| = n/2$, $|E_{3,5}| = n$, $|E_{3,6}| = n$, $|E_{4,4}| = 3n/2$, $|E_{4,5}| = 2n$, $|E_{4,6}| = n$, $|E_{5,5}| = n(3m-8)/2$, and $|E_{5,6}| = n(2m-5)$. From (2) and (4), the ABC and GA indices of K are computed as

FIGURE 6: The edge partitions of BA(Y) [9, 6] with respect to degree of end vertices.

$$\begin{aligned}
 ABC(K) &= \sum_{pq \in E_{3,3}} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}} + \sum_{pq \in E_{3,5}} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}} \\
 &+ \sum_{pq \in E_{3,6}} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}} + \sum_{pq \in E_{4,4}} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}} \\
 &+ \sum_{pq \in E_{4,5}} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}} + \sum_{pq \in E_{4,6}} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}} \\
 &+ \sum_{pq \in E_{5,5}} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}} + \sum_{pq \in E_{5,6}} \sqrt{\frac{d_p + d_q - 2}{d_p d_q}} \\
 &= \frac{6}{\sqrt{50}}mn + \frac{\sqrt{30}}{5}mn + \frac{3\sqrt{6}}{8}n + \sqrt{\frac{2}{5}}n \\
 &+ \frac{\sqrt{7}}{3\sqrt{2}}n + \frac{\sqrt{7}}{\sqrt{5}}n + \frac{1}{\sqrt{3}}n + \frac{1}{3}n - \frac{8\sqrt{2}}{5}n - \frac{\sqrt{30}}{2}n, \\
 GA(K) &= \sum_{pq \in E_{3,3}} \frac{2\sqrt{d_p d_q}}{d_p + d_q} + \sum_{pq \in E_{3,5}} \frac{2\sqrt{d_p d_q}}{d_p + d_q} \\
 &+ \sum_{pq \in E_{3,6}} \frac{2\sqrt{d_p d_q}}{d_p + d_q} + \sum_{pq \in E_{4,4}} \frac{2\sqrt{d_p d_q}}{d_p + d_q} \\
 &+ \sum_{pq \in E_{4,5}} \frac{2\sqrt{d_p d_q}}{d_p + d_q} + \sum_{pq \in E_{4,6}} \frac{2\sqrt{d_p d_q}}{d_p + d_q}
 \end{aligned}$$

$$\begin{aligned}
 &+ \sum_{pq \in E_{5,5}} \frac{2\sqrt{d_p d_q}}{d_p + d_q} + \sum_{pq \in E_{5,6}} \frac{2\sqrt{d_p d_q}}{d_p + d_q} \\
 &= \frac{4\sqrt{30}}{11}mn + \frac{3}{2}mn + \frac{\sqrt{15}}{4}n + \frac{2\sqrt{2}}{3}n \\
 &+ \frac{8\sqrt{5}}{9}n + \frac{2\sqrt{6}}{5}n - \frac{10\sqrt{30}}{11}n - 2n.
 \end{aligned}$$

(18)

Similarly, there are nineteen edge partite subsets of E_K corresponding to their degree sum of neighbors of end vertices, which are presented as

$$\begin{aligned}
 S_{14,14} &= \{pq \in E_K \mid \delta_p = \delta_q = 14\}, \\
 S_{14,25} &= \{pq \in E_H \mid \delta_p = 14 \text{ and } \delta_q = 25\}, \\
 S_{14,26} &= \{pq \in E_K \mid \delta_p = 14 \text{ and } \delta_q = 26\}, \\
 S_{18,19} &= \{pq \in E_K \mid \delta_p = 18 \text{ and } \delta_q = 19\}, \\
 S_{18,24} &= \{pq \in E_K \mid \delta_p = 18 \text{ and } \delta_q = 24\}, \\
 S_{19,19} &= \{pq \in E_K \mid \delta_p = \delta_q = 19\}, \\
 S_{19,24} &= \{pq \in E_K \mid \delta_p = 19 \text{ and } \delta_q = 24\}, \\
 S_{19,28} &= \{pq \in E_K \mid \delta_p = 19 \text{ and } \delta_q = 28\}, \\
 S_{24,24} &= \{pq \in E_K \mid \delta_p = \delta_q = 24\}, \\
 S_{24,27} &= \{pq \in E_K \mid \delta_p = 24 \text{ and } \delta_q = 27\}, \\
 S_{24,28} &= \{pq \in E_K \mid \delta_p = 24 \text{ and } \delta_q = 28\}, \\
 S_{25,25} &= \{pq \in E_K \mid \delta_p = \delta_q = 25\}, \\
 S_{25,26} &= \{pq \in E_K \mid \delta_p = 25 \text{ and } \delta_q = 26\}, \\
 S_{25,27} &= \{pq \in E_K \mid \delta_p = 25 \text{ and } \delta_q = 27\}, \\
 S_{25,30} &= \{pq \in E_K \mid \delta_p = 25 \text{ and } \delta_q = 30\}, \\
 S_{26,27} &= \{pq \in E_K \mid \delta_p = 26 \text{ and } \delta_q = 27\}, \\
 S_{27,27} &= \{pq \in E_K \mid \delta_p = \delta_q = 27\},
 \end{aligned}$$

$$S_{27,28} = \{pq \in E_K \mid \delta_p = 27 \text{ and } \delta_q = 28\},$$

$$S_{27,30} = \{pq \in E_K \mid \delta_p = 27 \text{ and } \delta_q = 30\}.$$

(19)

Therefore, we have $|S_{14,14}| = n/2$, $|S_{14,25}| = n$, $|S_{14,26}| = n$, $|S_{18,19}| = n$, $|S_{18,24}| = n$, $|S_{19,19}| = n/2$, $|S_{19,24}| = n$, $|S_{19,28}| = n$, $|S_{24,24}| = n/2$, $|S_{24,27}| = n$, $|S_{24,28}| = n$, $|S_{25,25}| = n/2$, $|S_{25,26}| = n$, $|S_{25,27}| = n$, $|S_{25,30}| = n$, $|S_{26,27}| = n$, $|S_{27,27}| = n(3m-14)/2$, $|S_{27,28}| = n$, and $|S_{27,30}| = 2n(m-5)$. The representative edges of these partite sets corresponding to certain colors are presented in Figure 7. From (3) and (5), the fourth ABC and fifth GA indices of K are computed as

$$\begin{aligned} ABC_4(K) = & \sum_{pq \in S_{14,14}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} + \sum_{pq \in S_{14,25}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\ & + \sum_{pq \in S_{14,26}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} + \sum_{pq \in S_{18,19}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\ & + \sum_{pq \in S_{18,24}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} + \sum_{pq \in S_{19,19}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\ & + \sum_{pq \in S_{19,24}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} + \sum_{pq \in S_{19,28}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\ & + \sum_{pq \in S_{24,24}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} + \sum_{pq \in S_{24,27}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\ & + \sum_{pq \in S_{24,28}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} + \sum_{pq \in S_{25,25}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\ & + \sum_{pq \in S_{25,26}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} + \sum_{pq \in S_{25,27}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\ & + \sum_{pq \in S_{25,30}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} + \sum_{pq \in S_{26,27}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\ & + \sum_{pq \in S_{27,27}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} + \sum_{pq \in S_{27,28}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\ & + \sum_{pq \in S_{27,30}} \sqrt{\frac{\delta_p + \delta_q - 2}{\delta_p \delta_q}} \\ = & \frac{\sqrt{13}}{9}mn + \frac{2\sqrt{5}}{9}mn + \frac{\sqrt{26}}{28}n + \frac{\sqrt{37}}{5\sqrt{14}}n + \frac{\sqrt{38}}{2\sqrt{91}}n \end{aligned}$$

FIGURE 7: The edge partitions of $BA(X)[9, 6]$ with respect to degree sum of neighbor vertices.

$$\begin{aligned} GA_5(K) = & \sum_{pq \in S_{14,14}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{14,25}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\ & + \sum_{pq \in S_{14,26}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{18,19}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\ & + \sum_{pq \in S_{18,24}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{19,19}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\ & + \sum_{pq \in S_{19,24}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{19,28}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\ & + \sum_{pq \in S_{24,24}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{24,27}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\ & + \sum_{pq \in S_{24,28}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{25,25}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\ & + \sum_{pq \in S_{25,26}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{25,27}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\ & + \sum_{pq \in S_{25,30}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{26,27}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\ & + \sum_{pq \in S_{27,27}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{27,28}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\ & + \sum_{pq \in S_{27,30}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \end{aligned}$$

TABLE 2: Degree-based topological indices of boron nanotubes.

Index	BT $[m, n]$	BA (X) $[m, n]$	BA (Y) $[m, n]$
ABC	$(2.37171m - 1.02333)n$	$(1.943973m - 0.190827)n$	$(1.943973m - 0.732831)n$
ABC ₄	$(1.0458m - 0.10448)n$	$(0.921774m + 0.645374)n$	$(0.897521m + 0.023558)n$
GA	$(4.5m - 3.12122)n$	$(3.491718m - 1.040331)n$	$(3.491718m - 2.100829)n$
GA ₅	$(4.5m - 3.17234)n$	$(3.497228m - 1.067682)n$	$(2.498614m + 2.874247)n$

$$\begin{aligned}
& + \sum_{pq \in S_{24,24}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{24,27}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\
& + \sum_{pq \in S_{24,28}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{25,25}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\
& + \sum_{pq \in S_{25,26}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{25,27}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\
& + \sum_{pq \in S_{25,30}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{26,27}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\
& + \sum_{pq \in S_{27,27}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} + \sum_{pq \in S_{27,28}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\
& + \sum_{pq \in S_{27,30}} \frac{2\sqrt{\delta_p \delta_q}}{\delta_p + \delta_q} \\
& = \frac{12\sqrt{10}}{19}mn + \frac{3}{2}mn + \frac{10\sqrt{14}}{39}n + \frac{\sqrt{91}}{10}n + \frac{6\sqrt{38}}{37}n \\
& + \frac{4\sqrt{3}}{7}n + \frac{4\sqrt{114}}{43}n + \frac{4\sqrt{133}}{47}n + \frac{12\sqrt{2}}{17}n \\
& + \frac{2\sqrt{42}}{13}n + \frac{10\sqrt{26}}{51}n + \frac{15\sqrt{3}}{26}n + \frac{2\sqrt{30}}{11}n \\
& + \frac{6\sqrt{78}}{53}n + \frac{12\sqrt{21}}{55}n - \frac{60\sqrt{10}}{19}n - 5n.
\end{aligned} \tag{20}$$

4. Conclusion

In this paper, we study important classes of boron nanotubes and formulated ABC, the fourth ABC, GA and the fifth GA indices of their molecular graphs by using the edge partition technique. The simplified expressions of these indices for boron triangular and boron- α nanotubes are given in Table 2. These results can be used in detecting some physical and chemical properties of these boron nanotubes, and in this sense, these results will be helpful in structural chemistry.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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