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TOPOLOGICAL ASPECTS BORON TRIANGULAR NANOTUBE
AND BORON- α NANOTUBE[#]

P. S. Hemavathi¹, V. Lokesha², M. Manjunath², P. S. K. Reddy³, R. Shruti²

¹ Siddaganga Institute of Technology, Tumkur 572 103, Karnataka, India;

² Vijayanagara Sri Krishnadevaraya University, Ballari 583 105, Karnataka, India;

³ Sri Jayachamarajendra College of Engineering, JSS Science and Technology University,
Mysuru 570 006, Karnataka, India

E-mail: psh@sit.ac.in, v.lokesha@gmail.com, manju3479@gmail.com,
pskreddy@jssstuniv.in, shrutichinnu77@gmail.com

Abstract. Topological graph indices have been used in a lot of areas to study required properties of different objects such as atoms and molecules. Such indices have been described and studied by many mathematicians and chemists since most graphs are generated from molecules by replacing each atom with a vertex and each chemical bond with an edge. These indices are also topological graph invariants measuring several chemical, physical, biological, pharmacological, pharmaceutical, etc. properties of graphs corresponding to real life situations. 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 compute the third Zagreb index, harmonic index, forgotten index, inverse sum index, modified Zagreb index and symmetric division deg index by applying subdivision and semi total point graph for boron triangular and boron- α nanotubes.

Key words: topological indices, Zagreb indices, harmonic index, forgotten index, inverse sum index and symmetric division deg index, boron triangular and boron- α nanotubes.

Mathematical Subject Classification (2010): 05C05, 05C12, 05C75.

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1. Introduction and Preliminaries

A systematic study of topological indices is one of the most striking aspects in many branches of Mathematics with its applications and various other fields of science and technology. Several different topological indices have been investigated so far, most of them useful topological indices are distance based or degree based. This indices may be used to

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derive the quantitative structure property relationship (QSPR) or quantitative structure activity relationship (QSAR). Topological index to correlated the physico-chemical properties of chemical compounds with their molecular structure. Topological indices are the numerical value associated with chemical constitution for correlation of chemical structure with various physical properties, chemical reactivity or biological activity.

The third Zagreb index

$$M_3(G) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)| \quad (1.1)$$

was introduced by Fath-Tabar in [1].

The harmonic index $H(G)$ is introduced in [2] and is defined as:

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}. \quad (1.2)$$

Unfortunately, another degree based graph invariant has not attracted any attention in the literature of Mathematical Chemistry for more than forty years. In view of this fact, Furtula et al. [3] named it as forgotten topological index and is defined as:

$$F(G) = \sum_{uv \in E(G)} [d_G(u)^2 + d_G(v)^2]. \quad (1.3)$$

The inverse sum index [4] is given by

$$I(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}. \quad (1.4)$$

For more details on this important topological indices, we refer to [5, 6]. According to the article in [7], both first and second Zagreb indices give greater weights to the inner vertices and edges, and smaller weights to outer vertices and edges which oppose intuitive reasoning. The second modified Zagreb index is:

$${}^m M_2(G) = \sum_{uv \in E(G)} \frac{1}{d_u \cdot d_v}. \quad (1.5)$$

Among 148 discrete Adriatic indices [8, 9], we considered symmetric division deg discrete adriatic index. The symmetric division deg index is defined as (see [10]):

$$SDD(G) = \sum_{uv \in E(G)} \frac{d_u^2 + d_v^2}{d_u \cdot d_v}. \quad (1.6)$$

The subdivision graph $S(G)$ is the graph obtained by replacing each of its edge by a path of length 2 or equivalently, by inserting an additional vertex into each edge of G .

The semi total point $R(G)$ graph is obtained from G by adding a new vertex corresponding to every edge of G and by joining each new vertex to the end vertices of the edge corresponding to it.

Boron nanotubes: In last 20 years, various type of boron containing nanomaterials. Boron nanomaterials have been considered as excellent material for enhancing the characteristics of optoelectronic nano devices because of their broad elastic modulus,

high melting point, excessive conductivity. These materials can carry excessive emission current, which recommends that they may have great prospective applications in field emission area [11]. Boron nanomaterials some best properties such as excessive resistance to oxidation at high temperatures, great chemical stability and are stable broad band-gap semiconductor [12, 13]. Moreover, the extensive range of boron nanomaterials themselves could be the building blocks for combining with other existing nanomaterial to design and create materials with new properties. The boron triangular nanotube was created in 2004 [11] and obtained from a carbon hexagonal nanotube by adding an extra atom to the centre of each hexagon. Also, a special boron nanotube was fabricated from a carbon hexagonal nanotube in 2008, by adding an extra atom to the centre of certain hexagons [14, 15]. This nanotube is designed by generating a mixture of hexagons and triangles called boron- α nanotube. These nanotubes are important materials for optical, electronic, bio and chemical sensing applications. The comparison study about some computational aspects of boron triangular and boron- α nanotubes has been investigated in [16]. The 3D perceptions of boron triangular and boron- α nanotube are presented in the Fig. 1.

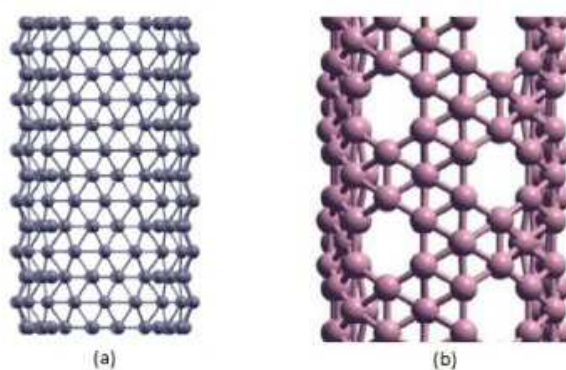


Fig. 1 (a) 3D-perception of boron triangular nanotube, (b) 3D-perception of boron- α nanotube.

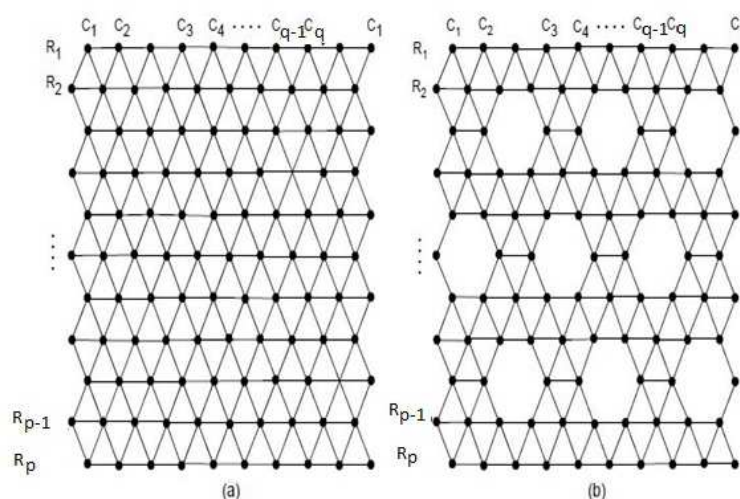


Fig. 2 (a) 2D-sheet of boron triangular nanotube $BT[p, q]$, (b) 2D-sheet of boron- α nanotube $BA[p, q]$.

Recently Jia-Bao, Hani Shaker and et al. [17] worked on topological aspects of boron nanotubes. Motivated from these works, we compute the third Zagreb index, harmonic index,

forgotten index, inverse sum index, modified Zagreb index and symmetric division deg index by applying subdivision and semi total point graph for boron triangular and boron- α nanotubes.

This paper is organized as follows: In Section 2, we get topological indices of boron triangular nanotube, subdivision and semi total point graph of boron triangular nanotube. In Section 3, the topological indices of boron- α nanotube, subdivision and semi total point graph of boron- α nanotube $BA(X)[p, q]$ are obtained. Finally, in Section 4, we presented the topological indices of boron- α nanotube, subdivision and semi total point graph of boron- α nanotube $BA(Y)[p, q]$.

2. Boron triangular nanotube, subdivision and semi total point graph of boron triangular nanotube

We denote the molecular graphs of boron triangular and boron- α nanotubes by $BT[p, q]$ and $BA[p, q]$ respectively, where p is the number of rows and q be the number of columns in 2D sheet of $BT[p, q]$ and $BA[p, q]$ as shown in the Fig. 2. Then boron- α nanotubes can be categorized into two classes with respect to p , denoted these classes as $BA(X)[p, q]$ and $BA(Y)[p, q]$.

Table 1. The order and size of triangular boron nanotubes

Molecular graph	$BT[p, q]$	$S = BT[p, q]$	$R = BT[p, q]$
Order	$\frac{3pq}{2}$	$3q(2p - 1)$	$3q(2p - 1)$
Size	$\frac{3q(3p-2)}{2}$	$3q(3p - 2)$	$\frac{9q(3p-2)}{2}$

Theorem 2.1. Consider the boron triangular nanotube $BT[p, q]$, where $p \geq 3$ and q is even, then

- $M_3(BT[p, q]) = 12q,$
- $H(BT[p, q]) = \frac{3}{4}pq + \frac{3}{4}q + \frac{6}{5}q - 2q,$
- $F(BT[p, q]) = 324pq - 864q + 96q + 312q,$
- $I(BT[p, q]) = \frac{27}{2}pq - 36q + 6q + \frac{72}{5}q,$
- ${}^mM_2(BT[p, q]) = \frac{1}{8}pq - \frac{1}{3}q + \frac{3}{16}q + \frac{1}{4}q,$
- $SDD(BT[p, q]) = 9pq - 24q + 6q + 13q.$

\triangleleft Consider the boron triangular nanotube $G = BT[p, q]$. There are three edge partitions corresponding to the degree of end vertices which are presented as $E_{4,4} = \{uv \in E_G \mid d_u = 4, d_v = 4\}$, $E_{4,6} = \{uv \in E_G \mid d_u = 4, d_v = 6\}$ and $E_{6,6} = \{uv \in E_G \mid d_u = 6, d_v = 6\}$.

Therefore, we have $|E_{4,4}| = 3q$, $|E_{4,6}| = 6q$ and $|E_{6,6}| = \frac{3q(3p-8)}{2}$. The respective edge partitions are shown in Fig. 3 in which edges belong to $E_{4,4}$, $E_{4,6}$ and $E_{6,6}$ respectively. Hence applying the topological indices definitions (Equation (1.1) to (1.6)) we get required results. \triangleright

Theorem 2.2. Consider the subdivision graph of boron triangular nanotube $BT[p, q]$, then

- $M_3(BT[p, q]) = 36pq + 24q - 72q,$
- $H(BT[p, q]) = \frac{9}{4}pq + 4q - \frac{9}{2}q,$
- $F(BT[p, q]) = 360pq + 240q - 720q,$
- $I(BT[p, q]) = \frac{27}{2}pq + 16q - 27q,$

- ${}^m M_2(BT[p, q]) = \frac{3}{4}pq + \frac{3}{2}q - \frac{3}{2}q,$
- $SDD(BT[p, q]) = 30pq + 30q - 60q.$

◁ Consider the subdivision graph of boron triangular nanotube $S = BT[p, q]$. There are two edge partitions corresponding to the degree of end vertices which are presented as $E_{2,4} = \{uv \in E_S \mid d_u = 2, d_v = 4\}$ and $E_{2,6} = \{uv \in E_S \mid d_u = 2, d_v = 6\}$.

Therefore, we have $|E_{2,4}| = 12q$, and $|E_{2,6}| = 9q(p - 2)$. Applying the subdivision graph operator to the Fig. 3, then respective edge partitions which edges belong to $E_{2,4}$ and $E_{2,6}$ respectively. Hence applying the topological indices definitions (Equation (1.1) to (1.6)), we get required results. ▷

Theorem 2.3. Consider the semi total point graph of boron triangular nanotube $R = BT[p, q]$, then

- $M_3(BT[p, q]) = 72q + 90pq - 180q + 24q,$
- $H(BT[p, q]) = \frac{12}{5}q + \frac{9}{7}pq - \frac{18}{7}q + \frac{3}{8}q + \frac{3}{5}q + \frac{3}{8}pq - q,$
- $F(BT[p, q]) = 816q + 1332pq - 2664q + 384q + 1248q + 1296pq - 3456q,$
- $I(BT[p, q]) = \frac{96}{5}q + \frac{108}{7}q - \frac{216}{7}q + 12q + \frac{144}{5}q + 27pq - 72q,$
- ${}^m M_2(BT[p, q]) = \frac{3}{4}q + \frac{3}{8}pq - \frac{3}{4}q + \frac{3}{64}q + \frac{1}{16}q + \frac{1}{32}pq - \frac{1}{12}q,$
- $SDD(BT[p, q]) = 51q + \frac{111}{2}pq - 111q + 6q + 13q + 9pq - 24q.$

◁ Consider the semi total point boron triangular nanotube $R = BT[p, q]$. There are five edge partitions corresponding to the degree of end vertices which are presented as $E_{2,8} = \{uv \in E_R \mid d_u = 2, d_v = 8\}$, $E_{2,12} = \{uv \in E_R \mid d_u = 2, d_v = 12\}$, $E_{8,8} = \{uv \in E_R \mid d_u = 8, d_v = 8\}$, $E_{8,12} = \{uv \in E_R \mid d_u = 8, d_v = 12\}$ and $E_{12,12} = \{uv \in E_R \mid d_u = 12, d_v = 12\}$.

Therefore, we have $|E_{2,8}| = 12q$, $|E_{2,12}| = 9q(q - 2)$, $|E_{8,8}| = 3q$, $|E_{8,12}| = 6q$, and $|E_{12,12}| = \frac{3q(3p-8)}{2}$. Applying the semi total point graph operator to the Fig. 3, then respective edge partitions which edges belongs to $E_{2,8}$, $E_{2,12}$, $E_{8,8}$, $E_{8,12}$, and $E_{12,12}$ respectively. Hence applying the topological indices definitions (Equation (1.1) to (1.6)), we get required results. ▷

3. Boron- α nanotube, subdivision and semi total point graph of boron- α nanotube $BA(X)[p, q]$

In this segment, we concentrated basic result on boron- α nanotube, subdivision and semi total point graph of boron- α nanotube $BA(X)[p, q]$.

Table 2. The order and size of boron- α $BA(X)[p, q]$ nanotubes

Molecular graph	$BA(X)[p, q]$	$S_1 = BA(X)[p, q]$	$R_1 = BA(X)[p, q]$
Order	$\frac{q}{3}(4p + 1)$	$\frac{q}{6}(29p - 4)$	$\frac{q}{6}(29p - 4)$
Size	$\frac{q}{2}(7p - 2)$	$q(7p - 2)$	$\frac{3q(7p-2)}{2}$

Theorem 3.1. Consider the boron- α nanotube $BA(X)[p, q]$, then

- $M_3\{BA(X)[p, q]\} = 2pq + 4q - 6q + 4q,$
- $H\{BA(X)[p, q]\} = \frac{3}{4}q + \frac{8}{9}q + \frac{2}{5}q + \frac{3}{10}pq - \frac{4}{5}q + \frac{4}{11}pq - \frac{12}{11}q,$
- $F\{BA(X)[p, q]\} = 96q + 164q + 104q + 75pq - 200q + 122pq - 366q,$

- $I\{BA(X)[p, q]\} = 6q + \frac{80}{9}q + \frac{24}{5}q + \frac{15}{4}pq - 10q + \frac{60}{11}pq - \frac{180}{11}q,$
- ${}^mM_2\{BA(X)[p, q]\} = \frac{3}{16}q + \frac{1}{5}q + \frac{1}{12}q + \frac{3}{50}pq - \frac{4}{25}q + \frac{1}{15}pq - \frac{1}{5}q,$
- $SDD\{BA(X)[p, q]\} = 6q + \frac{41}{5}q + \frac{13}{3}q + 3pq - 8q + \frac{61}{15}pq - \frac{61}{5}q.$

\triangleleft Consider the boron- α nanotube $H = BA(X)[p, q]$. There are five edge partitions corresponding to the degree of end vertices which are presented as $E_{4,4} = \{uv \in E_H \mid d_u = 4, d_v = 4\}$, $E_{4,5} = \{uv \in E_H \mid d_u = 4, d_v = 5\}$, $E_{4,6} = \{uv \in E_H \mid d_u = 4, d_v = 6\}$, $E_{5,5} = \{uv \in E_H \mid d_u = 5, d_v = 5\}$ and $E_{5,6} = \{uv \in E_H \mid d_u = 5, d_v = 6\}$.

Therefore, we have $|E_{4,4}| = 3q$, $|E_{4,5}| = 4q$, $|E_{4,6}| = 2q$, $|E_{5,5}| = \frac{q(3p-8)}{2}$, and $|E_{5,6}| = 2q(p-3)$. The respective edge partitions are shown in Fig. 4 in which edges belong to $E_{4,4}$, $E_{4,5}$, $E_{4,6}$, $E_{5,5}$ and $E_{5,6}$ respectively. Hence applying the topological indices definitions (Equation (1.1) to (1.6)), we get required results. \triangleright

Theorem 3.2. Consider the subdivision graph of boron- α nanotube $S_1 = BA(X)[p, q]$,

- $M_3\{BA(X)[p, q]\} = 24q + 15pq - 30q + 8pq - 16q,$
- $H\{BA(X)[p, q]\} = 4q + \frac{10}{7}pq - \frac{20}{7}q + \frac{1}{2}pq - q,$
- $F\{BA(X)[p, q]\} = 240q + 145pq - 290q + 80pq - 160q,$
- $I\{BA(X)[p, q]\} = 16q + \frac{50}{7}pq - \frac{100}{7}q + 3pq - 6q,$
- ${}^mM_2\{BA(X)[p, q]\} = \frac{3}{2}pq + \frac{1}{2}q - q + \frac{1}{6}pq - \frac{1}{3}q,$
- $SDD\{BA(X)[p, q]\} = 30q + \frac{29}{2}pq - 29q + \frac{20}{3}pq - \frac{40}{3}q.$

\triangleleft Consider the subdivision graph of boron- α nanotube $S_1 = BA(X)[p, q]$. There are three edge partitions corresponding to the degree of end vertices which are presented as $E_{2,4} = \{uv \in E_{S_1} \mid d_u = 2, d_v = 4\}$, $E_{2,5} = \{uv \in E_{S_1} \mid d_u = 2, d_v = 5\}$ and $E_{2,6} = \{uv \in E_{S_1} \mid d_u = 2, d_v = 6\}$.

Therefore, we have $|E_{2,4}| = 12q$, $|E_{2,5}| = 5q(p-2)$ and $|E_{2,6}| = 2q(p-2)$. Applying the subdivision graph operator to the Fig. 4, then respective edge partitions which edges belongs to $E_{2,4}$, $E_{2,5}$ and $E_{2,6}$ respectively. Hence applying the topological indices definitions (Equation (1.1) to (1.6)), we get required results. \triangleright

Theorem 3.3. Consider the semi total point graph of boron- α nanotube $R_1 = BA(X)[p, q]$,

- $M_3\{BA(X)[p, q]\} = 72q + 40pq - 80q + 20pq - 40q + 8q + 8q + 4pq - 12q,$
- $H\{BA(X)[p, q]\} = \frac{3}{2}q + \frac{1}{2}pq - q + \frac{1}{6}pq - \frac{1}{3}q + \frac{3}{32}q + \frac{1}{10}q + \frac{1}{24}q + \frac{3}{100}pq$
 $-\frac{2}{25}q + \frac{1}{30}pq + \frac{1}{10}q,$
- $F\{BA(X)[p, q]\} = 816q + 520pq - 1040q + 296pq - 592q + 384q + 656q$
 $+416q + 300pq - 800q + 488pq - 1464q,$
- $I\{BA(X)[p, q]\} = \frac{96}{5}q + \frac{25}{3}pq - \frac{50}{3}q + \frac{24}{7}pq - \frac{48}{7}q + 12q + \frac{160}{9}q + \frac{48}{5}q$
 $+\frac{15}{2}pq - 20q + \frac{120}{11}pq - \frac{360}{11}q,$

- ${}^m M_2\{BA(X)[p, q]\} = \frac{3}{4}q + \frac{1}{4}pq - \frac{1}{2}q + \frac{1}{12}pq - \frac{1}{6}q + \frac{3}{64}q + \frac{1}{20}q + \frac{1}{48}q$
 $+ \frac{3}{200}pq - \frac{1}{25}q + \frac{120}{11}pq - \frac{360}{11}q,$
- $SDD\{BA(X)[p, q]\} = 51q + 26pq - 52q + \frac{37}{3}pq - \frac{74}{3}q + 6q + \frac{41}{5}q + \frac{13}{2}q + 3pq$
 $- 8q + \frac{61}{15}pq - \frac{61}{5}q.$

◁ Consider the semi total point graph of boron- α nanotube $R_1 = BA(X)[p, q]$. There are eight edge partitions corresponding to the degree of end vertices which are presented as $E_{2,8} = \{uv \in E_{R_1} \mid d_u = 2, d_v = 8\}$, $E_{2,10} = \{uv \in E_{R_1} \mid d_u = 2, d_v = 10\}$, $E_{2,12} = \{uv \in E_{R_1} \mid d_u = 2, d_v = 12\}$, $E_{8,8} = \{uv \in E_{R_1} \mid d_u = 8, d_v = 8\}$, $E_{8,10} = \{uv \in E_{R_1} \mid d_u = 8, d_v = 10\}$, $E_{8,12} = \{uv \in E_{R_1} \mid d_u = 8, d_v = 12\}$, $E_{10,10} = \{uv \in E_{R_1} \mid d_u = 10, d_v = 10\}$ and $E_{10,12} = \{uv \in E_{R_1} \mid d_u = 10, d_v = 12\}$.

Therefore, we have $|E_{2,8}| = 12q$, $|E_{2,10}| = 5q(p - 2)$, $|E_{2,12}| = 2q(p - 2)$, $|E_{8,8}| = 3q$, $|E_{8,10}| = 4q$, $|E_{8,12}| = 2q$, $|E_{10,10}| = \frac{q(3p-8)}{2}$, and $|E_{10,12}| = 2q(p - 3)$. Applying the semi total point graph operator to the Fig. 4 and then applying the topological indices definitions (Equation (1.1) to (1.6)), we get required results. ▷

4. Boron- α , subdivision and semi total point graph of boron- α nanotube $BA(Y)[p, q]$

In this section we demonstrated the results on boron- α , subdivision and semi total point graph of boron- α nanotube $BA(Y)[p, q]$.

Table 3. The order and size of boron- α nanotubes of $BA(Y)[p, q]$

Molecular graph	$BA(Y)[p, q]$	$S_2 = BA(Y)[p, q]$	$R_2 = BA(Y)[p, q]$
Order	$\frac{4}{3}pq$	$\frac{q}{6}(29p - 12)$	$\frac{q}{6}(29p - 12)$
Size	$\frac{q}{2}(7p - 4)$	$q(7p - 4)$	$\frac{3q(7p-4)}{2}$

Theorem 4.1. Consider the boron- α nanotube $BA(Y)[p, q]$, then

- $M_3\{BA(Y)[p, q]\} = 2q + 3q + 2q + 2q + 2pq - 5q,$
- $H\{BA(Y)[p, q]\} = \frac{1}{6}q + \frac{1}{4}q + \frac{2}{9}q + \frac{3}{8}q + \frac{4}{9}q + \frac{1}{5}q + \frac{3}{10}pq - \frac{4}{5}q + \frac{4}{11}pq - \frac{10}{11}q,$
- $F\{BA(Y)[p, q]\} = 9q + 34q + 45q + 48q + 82q + 52q + 75pq - 200q + 122pq - 305q,$
- $I\{BA(Y)[p, q]\} = \frac{3}{4}q + \frac{15}{8}q + 2q + 3q + \frac{40}{9}q + \frac{12}{5}q + \frac{15}{4}pq - 10q + \frac{60}{11}pq - \frac{150}{11}q,$
- ${}^m M_2\{BA(Y)[p, q]\} = \frac{1}{18}q + \frac{1}{15}q + \frac{1}{18}q + \frac{3}{32}q + \frac{1}{10}q + \frac{1}{24}q + \frac{3}{50}pq - \frac{4}{25}q + \frac{1}{15}pq - \frac{1}{6}q,$
- $SDD\{BA(Y)[p, q]\} = q + \frac{34}{15}q + \frac{5}{2}q + 3q + \frac{41}{10}q + \frac{13}{6}q + 3pq - 8q + \frac{61}{15}pq - \frac{61}{6}q.$

◁ Consider the boron- α nanotube $K = BA(Y)[p, q]$. There are eight edge partitions corresponding to the degree of end vertices which are presented as $E_{3,3} = \{uv \in E_K \mid d_u = 3, d_v = 3\}$, $E_{3,5} = \{uv \in E_K \mid d_u = 3, d_v = 5\}$, $E_{3,6} = \{uv \in E_K \mid d_u = 3, d_v = 6\}$, $E_{4,4} = \{uv \in E_K \mid d_u = 4, d_v = 4\}$, $E_{4,5} = \{uv \in E_K \mid d_u = 4, d_v = 5\}$, $E_{4,6} = \{uv \in E_K \mid d_u = 4, d_v = 6\}$, $E_{5,5} = \{uv \in E_K \mid d_u = 5, d_v = 5\}$ and $E_{5,6} = \{uv \in E_K \mid d_u = 5, d_v = 6\}$.

Therefore, we have $|E_{3,3}| = \frac{q}{2}$, $|E_{3,5}| = q$, $|E_{3,6}| = q$, $|E_{4,4}| = \frac{3q}{2}$, $|E_{4,5}| = 2q$, $|E_{4,6}| = q$, $|E_{5,5}| = \frac{q(3p-8)}{2}$, and $|E_{5,6}| = q(2p-5)$. Hence applying the topological indices definitions (Equation (1.1) to (1.6)), we get required results. \triangleright

Theorem 4.2. Consider the subdivision graph of boron- α nanotube $S_2 = BA(Y)[p, q]$,

- $M_3\{BA(Y)[p, q]\} = 3q + 12q + 15pq - 30q + 8pq - 12q,$
- $H\{BA(Y)[p, q]\} = \frac{6}{5}q + 2q + \frac{10}{7}pq - \frac{20}{7}q + \frac{1}{2}pq - \frac{3}{4}q,$
- $F\{BA(Y)[p, q]\} = 39q + 120q + 145pq - 290q + 80pq - 120q,$
- $I\{BA(Y)[p, q]\} = \frac{18}{5}q + 8q + \frac{50}{7}pq - \frac{100}{7}q + 3pq - \frac{9}{2}q,$
- ${}^mM_2\{BA(Y)[p, q]\} = \frac{1}{2}q + \frac{3}{4}q + \frac{1}{2}pq - q + \frac{1}{6}pq - \frac{1}{4}q,$
- $SDD\{BA(Y)[p, q]\} = \frac{13}{2}q + 15q + \frac{29}{2}pq - 29q + \frac{20}{3}pq - 10q.$

\triangleleft Consider the subdivision graph of boron- α nanotube $S_2 = \{BA(Y)[p, q]\}$. There are four edge partitions corresponding to the degree of end vertices which are presented as $E_{2,3} = \{uv \in E_{S_2} \mid d_u = 2, d_v = 3\}$, $E_{2,4} = \{uv \in E_{S_2} \mid d_u = 2, d_v = 4\}$, $E_{2,5} = \{uv \in E_{S_2} \mid d_u = 2, d_v = 5\}$ and $E_{2,6} = \{uv \in E_{S_2} \mid d_u = 2, d_v = 6\}$.

Therefore, we have $|E_{2,3}| = 3q$, $|E_{2,4}| = 6q$, $|E_{2,5}| = 5q(p-2)$ and $|E_{2,6}| = q(2p-3)$. Applying the subdivision graph operator to the Fig. 5, then respective edge partitions which edges belongs to $E_{2,3}$, $E_{2,4}$, $E_{2,5}$ and $E_{2,6}$ respectively. Hence applying the topological indices definitions (Equation (1.1) to (1.6)), we get required results. \triangleright

Theorem 4.3. Consider the semi total point graph of boron- α nanotube $R_2 = BA(Y)[p, q]$,

- $M_3\{BA(Y)[p, q]\} = 12q + 36q + 40pq - 80q + 20pq - 30q + 4q + 6q + 4q + 4q + 4pq - 10q,$
- $H\{BA(Y)[p, q]\} = \frac{3}{4}q + \frac{6}{5}q + \frac{5}{6}pq - \frac{5}{3}q + \frac{2}{7}pq - \frac{3}{7}q + \frac{1}{12}q + \frac{1}{8}q + \frac{1}{9}q + \frac{3}{16}q + \frac{2}{9}q + \frac{1}{10}q + \frac{3}{20}pq - \frac{2}{5}q + \frac{2}{11}pq - \frac{5}{11}q,$
- $F\{BA(Y)[p, q]\} = 120q + 408q + 520pq - 1040q + 296q - 444q + 36q + 136q + 180q + 192q + 328q + 208q + 300pq - 800q + 488pq - 1220q,$
- $I\{BA(Y)[p, q]\} = \frac{9}{2}q + \frac{48}{5}q + \frac{25}{3}pq - \frac{50}{3}q + \frac{24}{7}pq - \frac{36}{7}q + \frac{3}{2}q + \frac{15}{4}q + 4q + 6q + \frac{80}{9}q + \frac{24}{5}q + \frac{15}{2}pq - 20q + \frac{120}{11}pq - \frac{300}{11}q,$
- ${}^mM_2\{BA(Y)[p, q]\} = \frac{1}{4}q + \frac{3}{8}q + \frac{1}{4}pq - \frac{1}{2}q + \frac{1}{12}pq - \frac{1}{8}q + \frac{1}{72}q + \frac{1}{60}q + \frac{1}{72}q + \frac{3}{128}q + \frac{1}{40}q + \frac{1}{16}q + \frac{3}{200}pq - \frac{1}{25}q + \frac{1}{60}pq - \frac{1}{24}q,$
- $SDD\{BA(Y)[p, q]\} = 10q + \frac{51}{2}q + 26pq - 52q + \frac{37}{3}pq - \frac{37}{2}q + q + \frac{34}{15}q + \frac{5}{2}q + 3q + \frac{41}{10}q + \frac{13}{6}q + 3pq - 8q + \frac{61}{15}pq - \frac{61}{6}q.$

\triangleleft Consider the semi total point graph of boron- α nanotube $R_2 = BA(Y)[p, q]$. There are twelve edge partitions corresponding to the degree of end vertices which are presented

as $E_{2,6} = \{uv \in E_{R_2} \mid d_u = 2, d_v = 6\}$, $E_{2,8} = \{uv \in E_{R_2} \mid d_u = 2, d_v = 8\}$, $E_{2,10} = \{uv \in E_{R_2} \mid d_u = 2, d_v = 10\}$, $E_{2,12} = \{uv \in E_{R_2} \mid d_u = 2, d_v = 12\}$, $E_{6,6} = \{uv \in E_{R_2} \mid d_u = 6, d_v = 6\}$, $E_{6,10} = \{uv \in E_{R_2} \mid d_u = 6, d_v = 10\}$, $E_{6,12} = \{uv \in E_{R_2} \mid d_u = 6, d_v = 12\}$, $E_{8,8} = \{uv \in E_{R_2} \mid d_u = 8, d_v = 8\}$, $E_{8,10} = \{uv \in E_{R_2} \mid d_u = 8, d_v = 10\}$, $E_{8,12} = \{uv \in E_{R_2} \mid d_u = 8, d_v = 12\}$, $E_{10,10} = \{uv \in E_{R_2} \mid d_u = 10, d_v = 10\}$ and $E_{10,12} = \{uv \in E_{R_2} \mid d_u = 10, d_v = 12\}$.

Therefore, we have $|E_{2,6}| = 3q$, $|E_{2,8}| = 6q$, $|E_{2,10}| = 5q(p-2)$, $|E_{2,12}| = q(2p-3)$, $|E_{6,6}| = \frac{q}{2}$, $|E_{6,10}| = q$, $|E_{6,12}| = q$, $|E_{8,8}| = \frac{3q}{2}$, $|E_{8,10}| = 2q$, $|E_{8,12}| = q$, $|E_{10,10}| = \frac{q(3p-8)}{2}$, and $|E_{10,12}| = q(2p-5)$. Applying the semi total point graph operator to the Fig. 5 and then applying the topological indices definitions (Equation (1.1) to (1.6)), we get required results. \triangleright

Table 4. The order and size of boron- α nanotubes of $BA(Y)[p, q]$

Index	$G = BT[p, q]$	$H = BA(X)[p, q]$	$K = BA(Y)[p, q]$
M_3	$12q$	$[2p+2]q$	$[2p+4]q$
H	$[0.75p-0.05]q$	$[0.66364p+0.14798]q$	$[0.66364p-0.05076]q$
F	$[324p-456]q$	$[197p-202]q$	$[197p-235]q$

Table 5. Degree based topological indices of boron nanotubes

I	$[13.5p-15.6]q$	$[9.20455p-6.67475]q$	$[9.20455p-9.16692]q$
mM_2	$[0.125p+0.10417]q$	$[0.12667p+0.11083]q$	$[0.12667p+0.08653]q$
SDD	$[9p-5]q$	$[7.06667p-1.66667]q$	$[7.06667p-3.13333]q$

Table 6. Subdivision graph of degree based topological indices of boron nanotubes

Index	$S = BT[p, q]$	$S_1 = BA(X)[p, q]$	$S_2 = BA(Y)[p, q]$
M_3	$[36p-48]q$	$[23p-22]q$	$[23p-27]q$
H	$[2.25p-0.5]q$	$[1.92857p+0.14286]q$	$[1.92857p-0.40741]q$
F	$[360p-480]q$	$[225p-210]q$	$[225p-251]q$
I	$[13.5p-11]q$	$[10.14286p-4.28571]q$	$[10.14286p-7.18571]q$
mM_2	$0.75pq$	$[0.66667p+0.16667]q$	$0.66667pq$
SDD	$[30p-30]q$	$[21.16667p-12.33333]q$	$[21.16667p-17.5]q$

Table 7. Semi total point graph of degree based topological indices of boron nanotubes

Index	$R = BT[p, q]$	$R_1 = BA(X)[p, q]$	$R_2 = BA(Y)[p, q]$
M_3	$[90p-84]q$	$[64p-44]q$	$[64p-54]q$
H	$[1.66071p-0.19643]q$	$[0.73p+0.422083]q$	$[1.45087p-0.17062]q$
F	$[2628p-3672]q$	$[1604p-1624]q$	$[1604p-1896]q$
I	$[42.42857p-42.85714]q$	$[30.17099p-17.67330]q$	$[30.17099p-26.04336]q$
mM_2	$[0.40625p+0.02604]q$	$[11.25742p-32.65998]q$	$[0.365p+0.02163]q$
SDD	$[64.5p-65]q$	$[45.4p-25.16667]q$	$[45.4p-38.13333]q$

Conclusion: In this paper, we study important classes of boron nanotubes and formulated M_3 , H , I , mM_2 , SDD indices of their molecular graphs by using edge partition technique. The simplified of these indices for boron triangular nanotube, subdivision and semi total point graph of boron triangular nanotube, boron- α , subdivision and semi total point graph of boron- α nanotube $BA(X)[p, q]$ and boron- α , subdivision and semi total point graph of boron- α nanotube $BA(Y)[p, q]$ are given in Table 1, Table 2 and Table 3. These results can be used in detecting some physical and chemical properties of these boron nanotubes.

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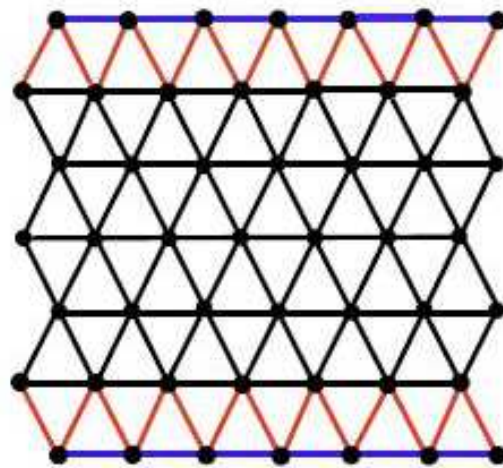


Fig. 3 The edge partitions of $BT[7,4]$ nanotube with respect to degree of end vertices.

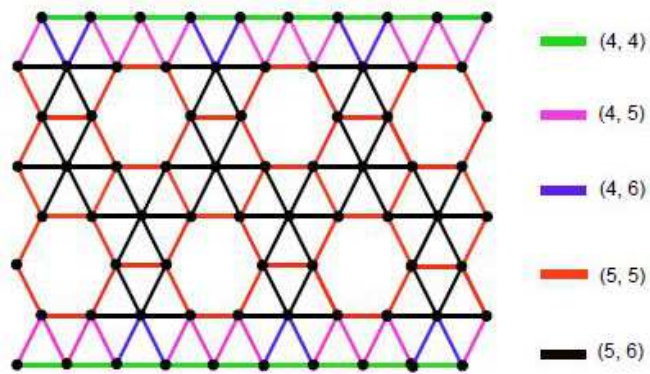


Fig. 4 The edge partitions of $BA(X)[8,6]$ nanotube with respect to degree of end vertices.

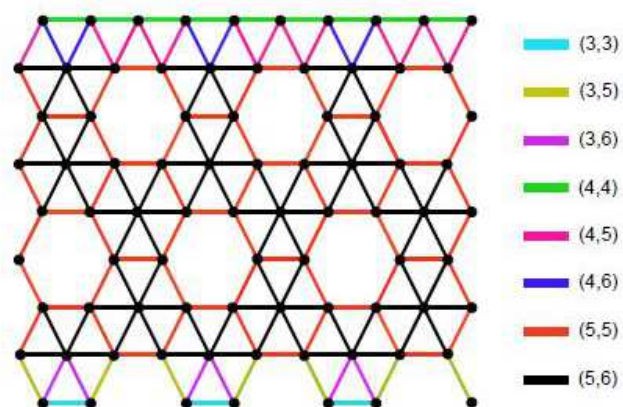


Fig. 5 The edge partitions of $BT(Y)[9,6]$ nanotube with respect to degree of end vertices.

References

1. Fath-Tabar, M. Old and New Zagreb Indices of Graphs, *MATCH Commun. Math. Comput. Chem.*, 2011, vol. 65, no. 1, pp. 79–84.
2. Fajtlowicz, S. On Conjectures of Graffiti-II, *Congr. Numer.*, 1987, vol. 60, pp. 187–197.
3. Furtula, B. and Gutman, I. A Forgotten Topological Index, *J. Math. Chem.*, 2015, vol. 53, no. 4, pp. 1184–1190. DOI: 10.1007/s10910-015-0480-z.
4. Balaban, A. T. Highly Discriminating Distance Based Numerical Descriptor, *Chem. Phys. Lett.*, 1982, vol. 89, pp. 399–404. DOI: 10.1016/0009-2614(82)80009-2.
5. Das, K. C. and Gutman, I. Some Properties of the Second Zagreb Index, *MATCH Commun. Math. Comput. Chem.*, 2004, vol. 52, pp. 103–112.
6. Devillers, J. and Balaban, A. T. *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon and Breach Science Publishers, 1999.
7. Milicevic, A., Nikolic, S. and Trinajstić, N. On Reformulated Zagreb Indices, *Molecular Diversity*, 2004, vol. 8, no. 4, pp. 393–399. DOI: 10.1023/b:modi.0000047504.14261.2a.
8. Alexander, V. Upper and Lower Bounds of Symmetric Division deg Index, *Iran. J. Math. Chem.*, 2014, vol. 5, no. 2, pp. 91–98.
9. Vukicevic, D. and Gasperov, M. Bond Additive Modeling 1. Adriatic Indices, *Croat. Chem. Acta*, 2010, vol. 83, no. 3, pp. 243–260.
10. Gupta, C. K., Lokesha, V., Shwetha, S. B. and Ranjini, P. S. On the Symmetric Division deg Index of Graph, *Southeast Asian Bull. Math.*, 2016, vol. 40, no. 1, pp. 59–80.
11. Kunstmann, J. and Quandt, A. Broad Boron Sheets and Boron Nanotubes: Anab Initiostudy of Structural, Electronic, and Mechanical Properties, *Phys. Rev. B*, 2006, vol. 74, no. 3, pp. 1–14. DOI: 10.1103/physrevb.74.035413.
12. Battersby, S. Boron Nanotubes Could Outperform Carbon. *New Scientist*.—URL: www.newscientist.com (accessed on 4 January 2008).
13. Miller, P. Boron Nanotubes Beat Carbon at its Own Game. *Engadget*. URL: www.engadget.com (accessed on 6 January 2008).
14. Lee, R. K. F., Cox, B. J. and Hill, J. M. Ideal Polyhedral Model for Boron Nanotubes with Distinct Bond Lengths, *J. Phys. Chem. C.*, 2009, vol. 113, no. 46, pp. 19794–19805. DOI: 10.1021/jp904985r.
15. Tang, H. and Ismail-Beigi, S. Novel Precursors for Boron Nanotubes, the Competition of Two-center and Three-center Bonding in Boron Sheets, *Phys. Rev. Lett.*, 2007, vol. 99, no. 11, pp. 115501–115504. DOI: 10.1103/physrevlett.99.115501.
16. Manuel, P. Computational Aspects of Carbon and Boron Nanotubes, *Molecules*, 2010, vol. 15, no. 12, pp. 8709–8722. DOI: 10.3390/molecules15128709.
17. Liu, J.-B., Shaker, H., Nadeem, I. and Hussain, M. Topological Aspects of Boron Nanotubes, *Advances in Materials Science and Engineering*, vol. 2018, pp. 1–11. DOI: 10.1155/2018/5729291.

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PANCHANAHALLY SHIVALINGAPPA HEMAVATHI
Siddaganga Institute of Technology,
Tumkur 572 103, Karnataka, India,
Assistant Professor
E-mail: psh@sit.ac.in;

VEERABADHRAIAH LOKESHA
Vijayanagara Sri Krishnadevaraya University,
Ballari 583 105, Karnataka, India,
Professor and Chairman
E-mail: v.lokesha@gmail.com;

MUDDULAPURAM MANJUNATH
Vijayanagara Sri Krishnadevaraya University,
Ballari 583 105, Karnataka, India,
Research Scholar
E-mail: manju3479@gmail.com

POLAEPALLI SIVA KOTA REDDY
Sri Jayachamarajendra College of Engineering,
JSS Science and Technology University,
Mysuru 570 006, Karnataka, India,
Professor
E-mail: pskreddy@jssstuniv.in
RANI SHRUTI
Vijayanagara Sri Krishnadevaraya University,
Ballari 583 105, Karnataka, India,
Research Scholar
E-mail: shrutichinnu77@gmail.com

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ТОПОЛОГИЧЕСКИЕ АСПЕКТЫ
ТРИАНГУЛЯРНЫХ БОРНЫХ НАНОТРУБОК
И АЛЬФА-БОРНЫХ НАНОТРУБОК

Хемавати П. С.¹, Локеша В.², Манджунатх М.², Редди П. С. К.³, Шрути Р.²

¹ Технологический институт Сиддаганга, Тумкур 572 103, Карнатака, Индия;

² Виджаянагара Шри Кришнадеварайский университет, Беллари 583 105, Карнатака, Индия;

³ Научно-технический университет Джагадгуру Шри Шиваратрешвара,
Майсур 570 006, Карнатака, Индия

E-mail: psh@sit.ac.in, v.lokesha@gmail.com, manju3479@gmail.com,
pskreddy@jssstuniv.in, shrutichinnu77@gmail.com

Аннотация. Индексы топологических графов использовались во многих областях для изучения требуемых свойств различных объектов, таких как атомы и молекулы. Такие индексы были описаны и изучены многими математиками и химиками, поскольку большинство графиков генерируются из молекул путем замены каждого атома вершиной, а каждой химической связи — ребром. Эти индексы также являются топологическими инвариантами графа, измеряющими некоторые химические, физические, биологические, фармакологические, фармацевтические и т. д. свойства графов, соответствующие реальным жизненным ситуациям. Основанные на степени топологические индексы используются для корреляции физических и химических свойств молекулы с ее химической структурой. Нанотрубные структуры из бора являются интересными материалами благодаря наличию многоцентровых связей и обладают новыми электронными свойствами. Применение этих материалов в области наноструктур ставит ряд важных вопросов, таких как механическая и термическая стабильность. Поэтому они требуют теоретических исследований по разным свойствам. Статья посвящена подсчету третьего Загребского индекса, гармонического индекса, индекса обратной суммы, модифицированного индекса Загреба и индекса степени симметричного деления с применением к борным нанотрубкам треугольного типа и альфа-борным нанотрубкам.

Ключевые слова: топологический индекс, индекс Загреба, гармонический индекс, индекс обратной суммы, индекс степени симметричного деления, треугольные борные нанотрубки, альфа-борные нанотрубки.

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