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Structural Study of Boron Nanotubes by Shigehalli, Kanabur, and Sanskruti Indices Along with their Multiplicative Invariants

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Abstract: Nanotechnology revolutionized the 21st century because of its applications in many important fields like defense and security, electronics, optical engineering, nano devices, nano fabrics, computer, medicine drugs, cosmetics, and nano biotechnology. Boron nanoclusters, boron nanowires, and boron nanotubes have all been developed in the previous 20 years. Keeping in view the sensitivity of boron nanostructures, we have calculated the Shigehalli, Kanabur invariants and their multiplicative versions MSK, MSK_1 and MSK_2 indices of boron tri-hexagonal, boron tri-angular, and boron alpha nanotubes (BANT) are useful in estimating these nanostructures' chemical properties.

Keywords: nano-technology; boron nanotubes; multiplicative Shigehalli and Kanabur indices; Shigehalli and Kanabur index; Sanskruti index.

1. Introduction

The combined study of graphs, chemistry, and information science is a relatively new discipline called Cheminformatics. In chemical sciences, chemical graph theory plays a significant role. Chemical graph theory is a subfield of mathematical chemistry that graph theory concerns the mathematical description of chemical occurrences. In the previous decades, a great deal of study has been done in this field. Topological indices are the real numbers that describe the properties of chemical structures that are represented in the form of graphs. These are useful in knowing the variety of physicochemical characteristics, chemical reactivity, or biological activity. Topological indices are a notable contrivance of mathematical chemistry and play a vital role in the (QSAR)/(QSPR) investigation among all topological indices because the accuracy of physicochemical parameters for chemical compounds determines the uniqueness of QSAR/QSPR models [1-3].

Actually, topological indices are based on the translation of a molecular graph into a number that describes the network's topology. Using molecular modeling, we examine the link between chemical substance structure, characteristics, and activity. Topological indices have an important part in key courses regarding chemical structures, such as chemistry and pharmacology. In the graphs of chemical compounds, atoms and bonds are represented by vertices and edges, respectively. In this manuscript, we have addressed the multiplicative version of Shigehalli and Kanabur (MSK Index, MSK_1 Index and MSK_2 Index) indices of boron tri-hexagonal, boron tri-angular, and boron α nanotubes are useful in estimating these nano structures' properties. There is a number of topological indices that have applications in Chemistry. Readers interested in learning about graph theory might look for beginning talks on the subject [4-7].

Shigehalli and Kanabur [8] presented the following new degree-based topological indices; Shigehalli and Kanabur indices are characterized as follows:

$$SK(G) = \sum_{uv\in E(G)} \frac{d_u+d_v}{2} \quad (1)$$
$$SK_1(G) = \sum_{uv\in E(G)} \frac{d_u.d_v}{2} \quad (2)$$
$$SK_2(G) = \sum_{uv\in E(G)} [\frac{d_u+d_v}{2}]^2 \quad (3)$$
$$SK_3(G) = \sum_{uv\in E(G)} \frac{(\delta_u+\delta_v)}{2} \quad (4)$$

where δ_u is the degree sum of neighbors of end vertices.

In 2016, the Sanskruti index of a graph G has been defined [9] as follows:

$$S(G) = \sum_{uv\in E(G)} [\frac{(\delta_u+\delta_v)}{\delta_u+\delta_v-2}]^3 \quad (5)$$

Multiplicative Shigehalli and Kanabur indices are defined as follows:

$$MSK(G) = \prod_{uv\in E(G)} \frac{d_u+d_v}{2} \quad (6)$$
$$MSK(G) = \prod_{uv\in E(G)} \frac{d_u+d_v}{2} \quad (7)$$
$$MSK_2(G) = \prod_{uv\in E(G)} [\frac{d_u+d_v}{2}]^2 \quad (8)$$

Nanotubes have a wide range of properties (structural, thermal, chemical, biological, electrical) that vary by their structure depending upon their length, diameter, chirality, or twist. *SK* indices are useful in the estimation of these properties of nanotubes according to their structures. Nanotubes can have multiple walls (MWNTs)-cylinders within other cylinders, in addition, to having a single cylindrical wall. Readers interested in learning more about Topological Indices (SK) are directed to read recent work on it [10, 11].

2. Materials and Methods

In the field of Nano-Technology, many materials and devices were created, like boron nanoclusters, boron nanowires, and boron nanotubes have all been developed in the previous 20 years. They all have a wide range of applications. After the discovery of carbon nanotubes, it took thirteen years to discover Boron nanotubes. This discovery proves their chemical stability, chemical sensing, and high-level protection oxidation at high temperatures. Electronic and optical properties calibrated structural stability and structure [12] are of great importance in studying boron nanotubes.

Topological Indices are gaining favor in the field of research since they simply need computing and do not require any physical experimentation. In the last two decades, boron nanotubes have become very attractive to study in different fields of nanosciences because of their thermal and mechanical stability. Modern topological indices are the best flavor to study nanotechnology's structural behavior because of their increasing applications and uses. Different indices of the same nanotube have also been calculated by Zobair et al. in [13, 14]. Boron triangular nanotubes are formed by adding an atom to the center of each hexagon in carbon nanotubes. Tri-hexagonal boron nanotube is a new class of boron nanotube that is constructed from triangles and hexagons [15]. By removing some atoms from tri-angular nanotubes, tri-hexagonal boron nanotubes are formed. After relaxation, tri-hexagonal boron nanotubes remain flat, metallic, and sparser than the other boron nanotubes. The three-dimensional structure of the tri-hexagonal boron nanotube is shown in Figure 1. Trihexagonal boron nanotube is denoted as $\mathrm{C_3C_6(H)[p,q]}$ where the number of hexagons in one column is p, and the number of hexagons in one row is q in a two-dimensional lattice of $\mathrm{C_3C_6(H)[p,q]}$ nanotube. In this section, we have calculated the Shigehalli and Kanabur indices along with their multiplicative version of the MSK Index, $\mathrm{MSK_1}$ Index and $\mathrm{MSK_2}$ indices of boron tri-hexagonal, boron tri-angular, and boron alpha nano are useful in estimating the actual properties like chemical reactivity, physical features, biological activity, thermal stability, and electrical conductivity of the nanotubes. Boron nanotubes have taken much interest from scientists and researchers in the last few years because of their rare properties and applications in technology. For more studies regarding the topological indices [16-20].

3. Results and Discussion

The $3D$ and $2D$ graphical portrayal of $C_3C_6(H)[p,q]$ nanotube is displayed in Figures 1 and 2. This nanotube has $8pq$ number of vertices and $q(18p-1)$ number of edges [5, 16]. Triangular boron nanotube is denoted as $BT[m,n]$ where m is the number of rows and n is the number of columns in a two-dimensional lattice of $BT[m,n]$. This nanotube has $\frac{3mn}{2}$ number of vertices and $\frac{3n(3m-2)}{2}$ number of edges.

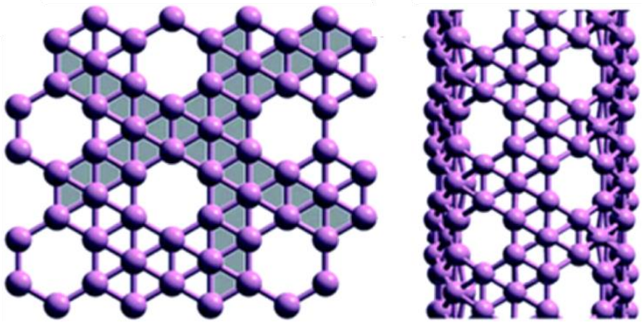

Figure 1. Molecular structure of Tri-Hexagonal boron nanotube.

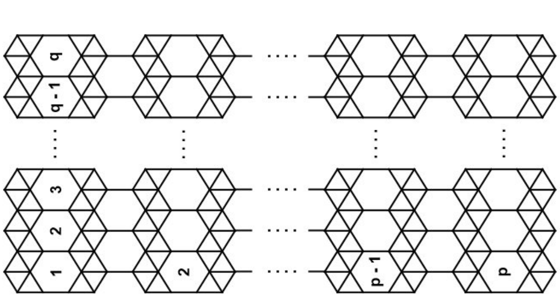

Figure 2. The graph of $C_3C_6(H)[p,q]$ nanotube.

Theorem 3.1. *Consider the Tri-Hexagonal boron nanotube $C_3C_6(H)[p,q]$, then*

$$MSK(H) = 51840(2p-1)^2pq^4 \qquad (9)$$

$$MSK_1(H) = 1080000(2p-1)^2pq^4 \qquad (10)$$

Proof. Four different edge sets as per the degree of end nodes of $C_3C_6(H)[p,q]$ are $E_1 = uv \in E(H)|d_u = 3$ and $d_v = 5$, $E_2 = uv \in E(H)|d_u = d_v = 4$, $E_3 = uv \in E(H)|d_u =$

4 and $d_v = 5$, also, $E_4 = uv \in E(H)|d_u = d_v = 5$. Figure 3 illustrates these partitions E_1, E_2, E_3, and E_4 with four different colors as red, green, black, and blue, respectively.

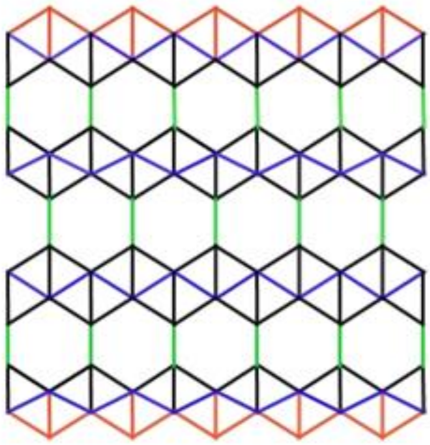

Figure 3. The graph of $C_3C_6(H)[p,q]$ nanotube with $p = 2$ and $q = 5$.

These partitions are shown in Table 1 as per their order and size.

Table 1. Edge partition data of H.

(d_u, d_v)	No. of Edges
(3,5)	$6q$
(4,4)	$q(2p-1)$
(4,5)	$6q(2p-1)$
(5,5)	$4pq$

By using edge partitions, we calculated $MSK(H)$, $MSK_1(H)$ and $MSK_2(H)$ for H.

$$MSK(H) = 6q[\frac{3+5}{2}] \times q(2p-1)[\frac{4+4}{2}] \times 6q(2p-1)[(\frac{4+5}{2}] \times 4pq[\frac{5+5}{2}]$$

After simplification, we get

$$MSK(H) = 51840(2p-1)^2pq^4$$

Now, we compute $MSK_1(H)$ for H

$$MSK_1(H) = 6q[\frac{3.5}{2}] \times q(2p-1)[\frac{4.4}{2}] \times 6q(2p-1)[\frac{4.5}{2}] \times 4pq[\frac{5.5}{2}]$$

After simplification, we get

$$MSK_1(H) = 1080000(2p-1)^2pq^4q$$

Now, we shall compute $MSK_2(H)$, $SK(H)$, $SK_1(H)$, $SK_2(H)$ and $SK_3(H)$ indices of $C_3C_6(H)[p,q]$ nanotube in the following theorems.

Theorem 3.2. *Consider the Tri-Hexagonal boron nanotube $C_3C_6(H)[p,q]$,then*

$$MSK_2(H) = 18662400(2p-1)^2pq^4q$$

Proof. The proof is analogous to the previous theorem.

Theorem 3.3. *Consider the Tri-Hexagonal boron nanotube $C_3C_6(H)[p,q]$, then*

$$SK(H) = 82pq - 7q. \quad (11)$$

$$SK_1(H) = 186pq - 23q. \quad (12)$$

Proof. Consider the tri-hexagonal boron nanotube $C_3C_6(H)[p,q]$. Using basic information from theorem 3.1, Table 1, we calculated $SK(H)$, $SK_1(H)$ and $SK_2(H)$ for H by using the edge partition technique.

$$SK(H) = 6q[\frac{3+5}{2}] + q(2p-1)[\frac{4+4}{2}] + 6q(2p-1)[(\frac{4+5}{2}] + 4pq[\frac{5+5}{2}]$$

After simplification, we get

$$SK(H) = 82pq - 7q$$

Now, we compute $SK_1(H)$ for H

$$SK_1(H) = 6q[\frac{3\times5}{2}] + q(2p-1)[\frac{4\times4}{2}] + 6q(2p-1)[\frac{4\times5}{2}] + 4pq[\frac{5\times5}{2}]$$

After simplification, we get

$$SK_1(H) = 186pq - 23q$$

Theorem 3.4. *Consider the Tri-Hexagonal boron nanotube $C_3C_6(H)[p,q]$, then*

$$SK_2(H) = (375)pq - (\frac{83}{2})q$$

Proof. The proof is analogous to the previous theorem.

Theorem 3.5. *Consider the Tri-Hexagonal boron nanotube $C_3C_6(H)[p,q]$, then*

$$SK_3(H) = 372pq - 46q. \quad (13)$$

$$S(H) = (22912.695323318)pq - (5515.6238130605)q. \quad (14)$$

Proof. Consider the tri-hexagonal boron nanotube $C_3C_6(H)[p,q]$. According to the degree sum of neighbors of end vertices, there are eight separate edge sets that are

$E_1 = uv \in E(H)|\delta_u = 15$ and $\delta_v = 20, E_2 = uv \in E(H)|\delta_u = 15$ and $\delta_v = 21, E_3 = uv \in E(H)|\delta_u = \delta_v = 19,\ E_4 = uv \in E(H)|\delta_u = 19$ and $\delta_v = 20,\ E_5 = uv \in E(H)|\delta_u = 19$ and $\delta_v = 21, E_6 = uv \in E(H)|\delta_u = 19$ and $\delta_v = 22, E_7 = uv \in E(H)|\delta_u = 20$ and $\delta_v = 21,\ E_8 = uv \in E(H)|d_u = d_v = 22$. The representation of these partition sets is shown in Figure 4, in which red, sky blue, green, purple, pink, black, yellow, and blue edges belong to $E_1, E_2, E_3, E_4, E_5, E_6, E_7$ and E_8 respectively.

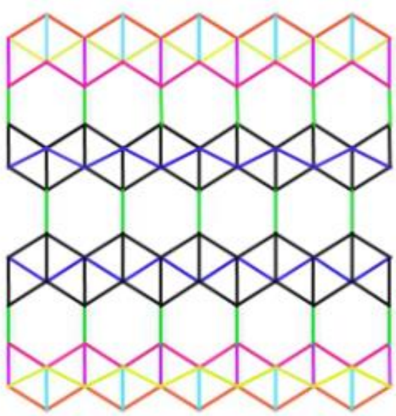

Figure 4. The graph of $C_3C_6(H)[p,q]$ nanotube with $p = 2$ and $q = 5$.

Partitions of edge sets are shown in Table 2 as per their order and size.

Table 2. The edge partition of H corresponds to the degree sum of neighbors of end vertices.

$(\boldsymbol{\delta_u}, \boldsymbol{\delta_v})$	**No. of Edges**
(15,20)	$4q$
(15,21)	$2q$
(19,19)	$q(2p-1)$
(19,20)	$2q$
(19,21)	$4q$
(19,22)	$12q(p-1)$
(20,21)	$4q$
(22,22)	$4q(p-1)$

By using the edge partitions technique, we have

$$SK_3(H) = \sum_{uv\in E_1(H)} \frac{(\delta_u+\delta_v)}{2} + \sum_{uv\in E_2(H)} \frac{(\delta_u+\delta_v)}{2} + \sum_{uv\in E_3(H)} \frac{(\delta_u+\delta_v)}{2} + \sum_{uv\in E_4(H)} \frac{(\delta_u+\delta_v)}{2} + \sum_{uv\in E_5(H)} \frac{(\delta_u+\delta_v)}{2} + \sum_{uv\in E_6(H)} \frac{(\delta_u+\delta_v)}{2} + \sum_{uv\in E_7(H)} \frac{(\delta_u+\delta_v)}{2} + \sum_{uv\in E_8(H)} \frac{(\delta_u+\delta_v)}{2}$$

$$= 4q\frac{(15+20)}{2} + 2q\frac{(15+21)}{2} + q(2p-1)\frac{(19+19)}{2} + 2q\frac{(19+20)}{2} + 4q\frac{(19+21)}{2} + 4q(p-1)\frac{(19+22)}{2} + 4q\frac{(20+21)}{2} + 4q(p-1)\frac{(22+22)}{2}$$

After simplification, we get

$$SK_3(H) = 372pq - 46q$$

Now, we compute $S(H)$ for H

$$S(H) = \sum_{uv\in E_1(H)} [\frac{(\delta_u\delta_v)}{\delta_u+\delta_v-2}]^3 + \sum_{uv\in E_2(H)} [\frac{(\delta_u\delta_v)}{\delta_u+\delta_v-2}]^3 + \sum_{uv\in E_3(H)} [\frac{(\delta_u\delta_v)}{\delta_u+\delta_v-2}]^3 + \sum_{uv\in E_4(H)} [\frac{(\delta_u\delta_v)}{\delta_u+\delta_v-2}]^3 + \sum_{uv\in E_5(H)} [\frac{(\delta_u\delta_v)}{\delta_u+\delta_v-2}]^3 + \sum_{uv\in E_6(H)} [\frac{(\delta_u\delta_v)}{\delta_u+\delta_v-2}]^3 + \sum_{uv\in E_7(H)} [\frac{(\delta_u\delta_v)}{\delta_u+\delta_v-2}]^3 + \sum_{uv\in E_8(H)} [\frac{(\delta_u\delta_v)}{\delta_u+\delta_v-2}]^3$$

$$= 4q[\frac{(15\times 20)}{15+20-2}]^3 + 2q[\frac{(15\times 21)}{15+21-2}]^3 + q(2p-1)[\frac{(19\times 19)}{19+19-2}]^3 + 2q[\frac{(19\times 20)}{19+20-2}]^3 + 4q[\frac{(19\times 21)}{19+21-2}]^3 + 12q(p-1)[\frac{(19\times 22)}{19+22-2}]^3 + 4q[\frac{(20\times 21)}{20+21-2}]^3 + 4q(-1)[\frac{(22\times 22)}{22+22-2}]^3$$

After simplification, we get

$$S(H) = (22912.695323318)pq - (5515.6238130605)q$$

3.1. Tri-Angular Boron Nanotubes

The graphical portrayal of $BT[m,n]$ nanotube is displayed in Figure 5. This nanotube is meant as $BT[m,n]$ where the number of columns is m and the number of rows is n in a two-dimensional grid of $BT[m,n]$ nanotube. This nanotube has $\frac{3mn}{2}$ number of vertices (order) and $\frac{3n(3m-2)}{2}$ number of edges (size) [21].

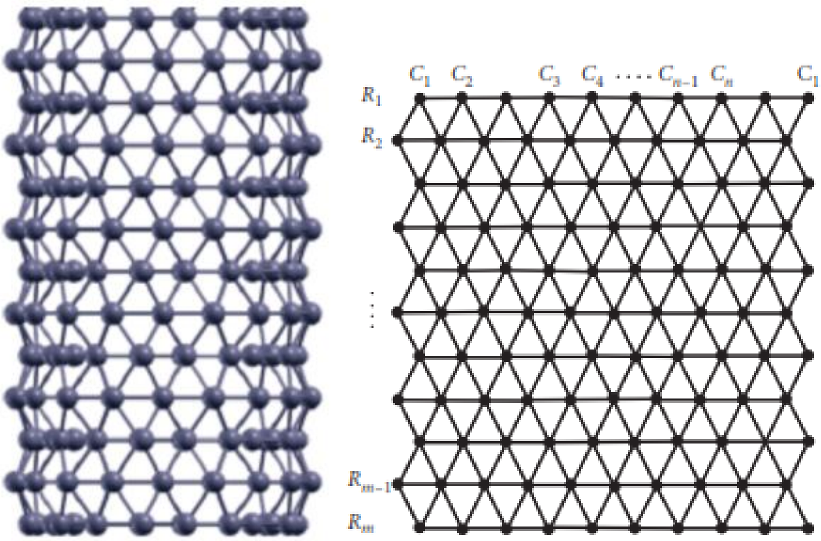

Figure 5. Graphical structure of Tri-Angular boron nanotube.

Theorem 3.6. *Consider the Tri-Angular $BT[m,n]$ boron nanotube, then*

$$MSK(H) = 3240n^3(3m-8) \quad (15)$$

$$MSK_1(H) = 46656n^3(3m-8) \quad (16)$$

Proof. Consider the Tri-Angular boron nanotube $BT[m,n]$. According to degrees of end vertices, there are three separate edge sets which are $E_1 = uv \in E(H)|d_u = d_v = 4$, $E_2 = uv \in E(H)|d_u = 4$ and $d_v = 6$, $E_3 = uv \in E(H)|d_u = d_v = 6$. The representation of these partition sets is shown in Figure 6, in which blue, red and black edges belong to E_1, E_2, and E_3, respectively.

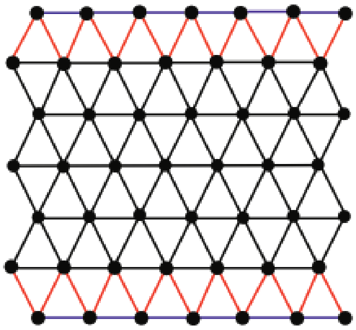

Figure 6: The graph of $BT[m,n]$ nanotube with $m = 7$ and $n = 4$.

Partitions of edge sets are shown in Table 3 as per their order and size.

Table 3. Edge partition data of H.

(d_u, d_v)	No. of Edges
(4,4)	$3n$
(4,6)	$6n$
(6,6)	$\frac{3n(3m-8)}{2}$

Now using the edge partitions technique, we calculate $MSK(H)$, $MSK_1(H)$ and $MSK_2(H)$ for H.

$$MSK(H) = \prod_{uv\in E_1(H)} \frac{d_u+d_v}{2} \times \prod_{uv\in E_2(H)} \frac{d_u+d_v}{2} \times \prod_{uv\in E_3(H)} \frac{d_u+d_v}{2}$$

$$= 3n[\frac{4+4}{2}] \times 6n[\frac{4+6}{2}] \times \frac{3n(3m-8)}{2} [(\frac{6+6}{2}]$$

After simplification, we get

$$MSK(H) = 3240n^3(3m-8)$$

Now, we compute $MSK_1(H)$ for H

$$MSK_1(H) = \prod_{uv\in E_1(H)} \frac{d_u.d_v}{2} \times \prod_{uv\in E_2(H)} \frac{d_u.d_v}{2} \times \prod_{uv\in E_3(H)} \frac{d_u.d_v}{2}$$

$$= 3n[\frac{4.4}{2}] \times 6n[\frac{4.6}{2}] \times \frac{3n(3m-8)}{2} [\frac{6.6}{2}]$$

After simplification, we get

$$MSK_1(H) = 46656n^3(3m-8)$$

Theorem 3.7. *Consider the Tri-Angular boron nanotube $BT[m,n]$, then*

$$MSK_2(H) = 388800n^3(3m-8)$$

Proof. The proof is analogous to the previous theorem.

Theorem 3.8. *Consider the Tri-Angular $BT[m,n]$ boron nanotube, then*

$$SK(H) = (27)mn - (30)n. \quad (17)$$

$$SK_1(H) = (81)mn - (120)n. \quad (18)$$

Proof. Consider the Tri-Angular boron nanotube $BT[m,n]$. Using basic information from Theorem 4.1 and Table 3, we calculated $SK(H)$, $SK_1(H)$ and $SK_2(H)$ for H by using the edge partition technique.

$$SK(H) = \sum_{uv\in E_1(H)} \frac{d_u+d_v}{2} + \sum_{uv\in E_2(H)} \frac{d_u+d_v}{2} + \sum_{uv\in E_3(H)} \frac{d_u+d_v}{2}$$
$$= 3n[\frac{4+4}{2}] + 6n[\frac{4+6}{2}] + \frac{3n(3m-8)}{2}[\frac{6+6}{2}]$$

After simplification, we get

$$SK(H) = (27)mn - (30)n$$

Now, we compute $SK_1(H)$ for H

$$SK_1(H) = \sum_{uv\in E_1(H)} \frac{d_u\times d_v}{2} + \sum_{uv\in E_2(H)} \frac{d_u\times d_v}{2} + \sum_{uv\in E_3(H)} \frac{d_u\times d_v}{2}$$
$$= 3n[\frac{4\times 4}{2}] + 6n[\frac{4\times 6}{2}] + \frac{3n(3m-8)}{2}[\frac{6\times 6}{2}]$$

After simplification, we get

$$SK_1(H) = (81)mn - (120)n$$

Now, we shall compute $SK_2(H)$ the descriptor in the following theorem.

Theorem 3.9. *Consider the Tri-Angular $BT[m,n]$ boron nanotube, then*

$$SK_2(H) = (162)mn - (234)n$$

Proof. Consider the Tri-Angular boron nanotube. Now, we calculate $SK_2(G)$ for G.

$$SK_2(H) = \sum_{uv\in E_1(H)} [\frac{d_u+d_v}{2}]^2 + \sum_{uv\in E_2(H)} [\frac{d_u+d_v}{2}]^2 + \sum_{uv\in E_3(H)} [\frac{d_u+d_v}{2}]^2$$
$$= 3n[\frac{4+4}{2}]^2 + 6n[\frac{4+5}{2}]^2 + \frac{3n(3m-8)}{2}[\frac{6+6}{2}]^2$$

After simplification, we get

$$SK_2(H) = (162)mn - (234)n$$

3.2. Boron- α Nanotubes

The graphical portrayal of $BANT[m,n]$ nanotube is displayed in Figure 7. This nanotube is meant as $BANT[m,n]$ where the number of columns is m, and the number of rows is n in a two-dimensional grid of $BANT[m,n]$ nanotube. With regard to m, we divide this Boron- α NT into two classes. We define these classes as $BANT(X)[m,n]$ with a number of vertices $\frac{n(4m+1)}{3}$ (order) and edges $\frac{n(7m-2)}{2}$ (size) and $BANT(Y)[m,n]$ with the number of vertices $\frac{4mn}{3}$ (order) and edges $\frac{n(7m-4)}{2}$ (size) for $m = 2\,mod3$ and $m = 0\,mod3$, respectively[21].

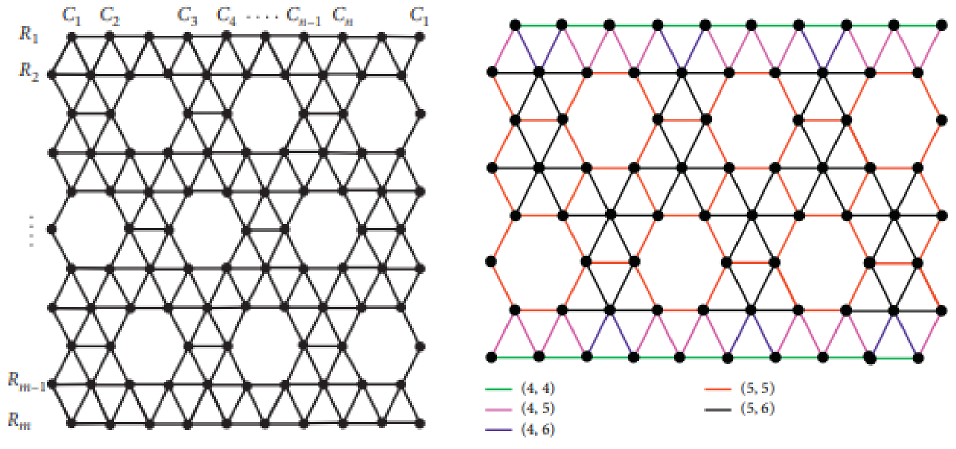

Figure 7. The graph of $BANT(X)[m,n]$ nanotube.

Theorem 3.10. *Consider the Boron- α NT $L = BANT(H)[m,n]$, then*

$$MSK(H) = 59400n^5(3m-8)(m-3) \quad (19)$$

$$MSK_1(H) = 4320000n^5(3m-8)(m-3) \quad (20)$$

Proof. Consider the Boron- α NT $BANT(H)[m,n]$. According to degrees of end vertices, there are five separate edge sets which are $E_1 = uv \in E(H)|d_u = d_v = 4$, $E_2 = uv \in E(H)|d_u = 4$ and $d_v = 5$, $E_3 = uv \in E(H)|d_u = 4$ and $d_v = 6$, $E_4 = uv \in E(H)|d_u = d_v = 5$, $E_5 = uv \in E(H)|d_u = 5$ and $d_v = 6$. The representation of these partition sets is shown in Figure 7. Table 4 shows the partition of edge sets of H corresponding to their degree of end vertices.

Table 4. The edge partition of H corresponds to the degree of end vertices.

(d_u, d_v)	No. of Edges
(4,4)	$3n$
(4,5)	$4n$
(4,6)	$2n$
(5,5)	$\frac{n(3m-8)}{2}$
(5,6)	$2n(m-3)$

By using edge partitions, we calculated $MSK(H)$, $MSK_1(H)$ and $MSK_2(H)$ for $BANT(H)[m,n]$.

$$MSK(H) = \prod_{uv\in E_1(H)} \frac{d_u+d_v}{2} \times \prod_{uv\in E_2(H)} \frac{d_u+d_v}{2} \times \prod_{uv\in E_3(H)} \frac{d_u+d_v}{2}$$

$$\times \prod_{uv\in E_4(H)} \frac{d_u+d_v}{2} \times \prod_{uv\in E_5(H)} \frac{d_u+d_v}{2}$$

$$= 3n[\frac{4+4}{2}] \times 4n[\frac{4+5}{2}] \times 2n[(\frac{4+6}{2}] \times \frac{n(3m-8)}{2}[\frac{5+5}{2}] \times 2n(m-3)[\frac{5+6}{2}]$$

After simplification, we get

$$MSK(H) = 59400n^5(3m-8)(m-3)$$

Now, we compute $SK_1(H)$ for H

$$MSK_1(H) = 3n[\frac{4.4}{2}] \times 4n[\frac{4.5}{2}] \times 2n[\frac{4.6}{2}] \times \frac{n(3m-8)}{2}[\frac{5.5}{2}] \times 2n(m-3)[\frac{5.6}{2}]$$

After simplification, we get

$$MSK_1(H) = 4320000n^5(3m-8)(m-3)$$

Now, we shall compute $MSK_2(H)$ the descriptor in the following theorem.

Theorem 3.11. *Consider the Boron- α NT $H = BANT[m,n]$, then*

$$MSK_2(H) = 1176120000n^5(3m-8)(m-3)$$

Proof. The proof is analogous to Theorem 5.1.

By using edge partitions, we calculated $MSK(H)$, $MSK_1(H)$ and $MSK_2(H)$ for the Boron- α NT $BANT(H)[m,n]$.

Theorem 3.12. *Consider the Boron- α NT $H = BANT(H)[m,n]$, then*

$$MSK(H) = \frac{200475}{2}n^8(3m-8)(2m-5) \quad (21)$$

$$MSK_1(H) = 41006250n^8(3m-8)(2m-5) \quad (22)$$

Proof. Consider the Boron- α NT $BANT(H)[m,n]$. According to degrees of end vertices, there are eight separate edge sets which are $E_1 = uv \in E(H)|d_u = d_v = 3$, $E_2 = uv \in E(H)|d_u = 3$ and $d_v = 5$, $E_3 = uv \in E(H)|d_u = 3$ and $d_v = 6$, $E_4 = uv \in E(H)|d_u = d_v = 4$, $E_5 = uv \in E(H)|d_u = 4$ and $d_v = 5$, $E_6 = uv \in E(H)|d_u = 4$ and $d_v = 6$, $E_7 = uv \in E(H)|d_u = d_v = 5$, $E_8 = uv \in E(H)|d_u = 5$ and $d_v = 6$.

The representation of these partition sets is shown in Figure 8.

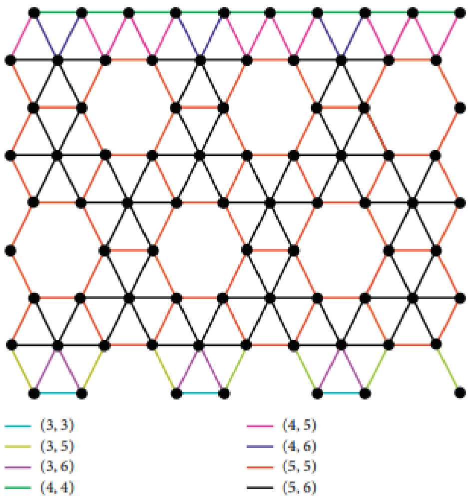

Figure 8. The graph of $BANT(H)[m,n]$ nanotube with $m = 9$ and $n = 6$.

Table 5 shows the partition of edge sets of H corresponding to their degree of end vertices.

Table 5. Edge partition data of H.

(d_u, d_v)	No. of Edges
(3,3)	$n/2$
(3,5)	n
(3,6)	n
(4,4)	$3n/2$
(4,5)	$2n$
(4,6)	n
(5,5)	$\frac{n(3m-8)}{2}$
(5,6)	$n(2m-5)$

By using edge partitions, we calculated $MSK(H)$, $MSK_1(H)$ and $MSK_2(H)$ for H.

$$MSK(H) = \prod_{uv\in E_1(H)} \frac{d_u+d_v}{2} \times \prod_{uv\in E_2(H)} \frac{d_u+d_v}{2} \times \prod_{uv\in E_3(H)} \frac{d_u+d_v}{2}$$
$$\times \prod_{uv\in E_4(H)} \frac{d_u+d_v}{2} \times \prod_{uv\in E_5(H)} \frac{d_u+d_v}{2} \times \prod_{uv\in E_6(H)} \frac{d_u+d_v}{2}$$
$$\times \prod_{uv\in E_7(H)} \frac{d_u+d_v}{2} \times \prod_{uv\in E_8(H)} \frac{d_u+d_v}{2}$$
$$= \frac{n}{2}[\frac{3+3}{2}] \times n[\frac{3+5}{2}] \times n[(\frac{3+6}{2}] \times \frac{3n}{2}[\frac{4+4}{2}] \times 2n[\frac{4+5}{2}] \times n[(\frac{4+6}{2}]$$
$$\times \frac{n(3m-8)}{2}[\frac{5+5}{2}] \times n(2m-5)[\frac{5+6}{2}]$$

After simplification, we get

$$MSK(H) = \frac{200475}{2} n^8 (3m-8)(2m-5)$$

Now, we compute $SK_1(H)$ for H

$$MSK_1(H) = \frac{n}{2}[\frac{3.3}{2}] \times n[\frac{3.5}{2}] \times n[\frac{3.6}{2}] \times \frac{3n}{2}[\frac{4.4}{2}] \times 2n[\frac{4.5}{2}] \times n[\frac{4.6}{2}]$$
$$\times \frac{n(3m-8)}{2}[\frac{5.5}{2}] \times n(2m-5)[\frac{5.6}{2}]$$

After simplification, we get

$$MSK_1(H) = 41006250 n^8 (3m-8)(2m-5)$$

Now, we shall compute $MSK_2(H)$ the descriptor in the following theorem.

Theorem 3.13. *Consider the Boron- α NT $H = BANT(H)[m,n]$ then,*

$$MSK_2(H) = 13396741875 n^8 (3m-8)(2m-5)$$

Proof. The proof is analogous to Theorem 5.3.

Theorem 3.14. *Consider the boron triangular nanotube* $BT[m,n]$, *then*

$$SK_3(H) = 162mn - 240n. \quad (23)$$

$$SK(H) = (28558.36884)mn - (71768.15745)n \quad (24)$$

Proof. Consider the boron triangular nanotube $BT[m,n]$. According to the degree sum of neighbors of end vertices, there are five separate edge sets which are $E_1 = uv \in E(H)|\delta_u = \delta_v = 20$, $E_2 = uv \in E(H)|\delta_u = 20$ and $\delta_v = 32$, $E_3 = uv \in E(H)|\delta_u = \delta_v = 32$, $E_4 = uv \in E(H)|\delta_u = 32$ and $\delta_v = 36$, $E_5 = uv \in E(H)|d_u = d_v = 36$.
The representation of these partition sets is shown in Figure 9, in which blue, red, purple, yellow, green, and black edges belong to E_1, E_2, E_3, E_4, E_5 respectively.

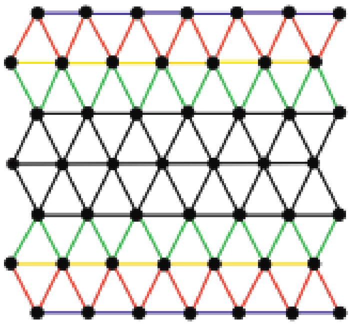

Figure 9. The graph of $BT[m,n]$ nanotube with $m = 7$ and $n = 4$.

Table 6 shows the partition of edge sets of H corresponding to their degree sum of neighbors of end vertices.

Table 6. The edge partition of H corresponds to the degree sum of neighbors of end vertices.

(δ_u, δ_v)	No. of Edges
(20,20)	$3n$
(20,32)	$6n$
(32,32)	$3n$
(32,36)	$6n$
(36,36)	$\frac{3n(3m-14)}{2}$

By using edge partitions,

$$SK_3(H) = \sum_{uv\in E_1(H)} \frac{(\delta_u+\delta_v)}{2} + \sum_{uv\in E_2(H)} \frac{(\delta_u+\delta_v)}{2} + \sum_{uv\in E_3(H)} \frac{(\delta_u+\delta_v)}{2} + \sum_{uv\in E_4(H)} \frac{(\delta_u+\delta_v)}{2} + \sum_{uv\in E_5(H)} \frac{(\delta_u+\delta_v)}{2}$$

$$= 3n\frac{(20+20)}{2} + 6n\frac{(20+32)}{2} + 3n\frac{(32+32)}{2} + 6n\frac{(32+36)}{2} + 3n(3m - 14)/2\frac{(36+36)}{2}$$

After simplification, we get

$$SK_3(H) = 162mn - 240n$$

Now, we compute $SK(H)$ for H

$$SK(H) = \sum_{uv\in E_1(H)} [\frac{(\delta_u\delta_v)}{\delta_u+\delta_v-2}]^3 + \sum_{uv\in E_2(H)} [\frac{(\delta_u\delta_v)}{\delta_u+\delta_v-2}]^3 + \sum_{uv\in E_3(H)} [\frac{(\delta_u\delta_v)}{\delta_u+\delta_v-2}]^3$$

$$+ \sum_{uv\in E_4(H)} [\frac{(\delta_u\delta_v)}{\delta_u+\delta_v-2}]^3 + \sum_{uv\in E_5(H)} [\frac{(\delta_u\delta_v)}{\delta_u+\delta_v-2}]^3$$

$$= 3n[\frac{(20\times 20)}{20+20-2}]^3 + 6n[\frac{(20\times 32)}{20+32-2}]^3 + 3n(2p-1)[\frac{(32\times 32)}{32+32-2}]^3 + 6n[\frac{(32\times 36)}{32+36-2}]^3 + \frac{3n(3m-14)}{2}[\frac{(36\times 36)}{36+36-2}]^3$$

After simplification, we get

$$SK(H) = (28558.36884)mn - (71768.15745)n$$

4. Conclusion

Topological indices play a significant role in the investigation of physic-chemical properties of molecular compounds. Boron nanotubes are remarkably important due to their different synthetic properties like stability, electronic, and enthalpy with high prescient power. Boron nanotubes have been studied in several directions by researchers who have computed their energetics and vibrational spectra, keeping their importance in chemical graph theory. In this regard, we have calculated the multiplicative versions of Shigehalli and Kanabur indices, i.e., MSK Index, MSK_1 Index and MSK_2 Index of boron tri-hexagonal, boron tri-angular, and boron alpha nanotubes are useful in estimating the chemical properties of these nanostructures.

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Conflict of interest

The authors declare that there is no conflict of interest.

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