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# Non-neighbor sum-connectivity index and ABC index

**S.B. Chandrakala**
*Department of Mathematics, Nitte Meenakshi Institute of Technology, Yelahanka, Bengaluru, India. Pin 560 064*
chandrakalasb14@gmail.com

**G.R. Roshini***
*Department of Mathematics, Nitte Meenakshi Institute of Technology, Yelahanka, Bengaluru, India. Pin 560 064*
gr.roshini@gmail.com

**B. Sooryanarayana**
*Department of Mathematics, Dr.Ambedkar Institute of Technology, B.D.A. Outer Ring Road, Mallathahalli, Bengaluru, Karnataka State, India. Pin 560 056*
dr_bsnrao@dr-ait.org

**Michaela Mihoková**
*Department of Mathematics, Faculty of Natural Sciences, Matej Bel University, Tajovského 40, 974 01 Banská Bystrica, Slovakia*
michaela.mihokova@umb.sk

**Abstract**

Topological indices have a significant importance in the study of physicochemical properties of chemical compounds. Among them, degree based topological indices have played a prominent role to study the chemical properties of nanostructure materials. In this paper, we compute non-neighbor sum-connectivity index (SCI), non-neighbor ABC index, multiplicative non-neighbor SCI and multiplicative non-neighbor ABC index for some standard classes of graphs and for corona products of some graphs. We have also obtained the same for some nano-structures.

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## 1 Introduction

We consider a graph $G$ to be a finite, undirected, simple graph having $n$ vertices with $m$ edges. Let $V(G)$ be the vertex set and $E(G)$ be the edge set of $G$, $d_G(u)$ denotes the degree of a vertex $u$, $\delta$ and $\Delta$ be the minimum degree and the maximum degree of a graph $G$ respectively, $d(u, v)$ is the distance between the vertices $u$ and $v$. A vertex $v \in V(G)$ is called a full degree vertex, if $d_G(v) = n - 1$. Also, $uv$ represents an edge between the two vertices $u$ and $v$. For undefined terminologies we refer to [3].

*corresponding author

A topological index is a numeric value mathematically derived from the graph representing a molecule. The mathematical and computational chemistry involving the computation of topological indices is a trending research topic. Topological indices are of two main categories, one depends on vertex distance and the other depends on vertex degree.

Zagreb indices are the oldest among the topological indices, given by Gutman and Trinajstic [2] defined as

$$M_1(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]$$

and

$$M_2(G) = \sum_{uv \in E(G)} [d_G(u) \times d_G(v)].$$

As the years passed many degree based topological indices were introduced, among which sum-connectivity index (SCI) and atom bond connectivity (ABC) index are two such topological indices. Sum-connectivity index, which was introduced in 2009 [14], is defined as

$$SCI(G) = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]^{-1/2}.$$

Atom-bond connectivity (ABC) index, which was introduced in 1998 [1], is defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(u) + d_G(v) - 2}{d_G(u) \times d_G(v)}}.$$

The first multiplicative topological index was introduced in 1984 by Narumi and Katayama [6] and it is defined as

$$NK(G) = \prod_{u \in V(G)} d_G(u).$$

Some of the non-neighbor topological indices are studied in [8]. Also, some work on Randic and multiplicative topological indices can be referred in [9, 10, 11].

Motivated by these works, we define non-neighbor sum-connectivity index, non-neighbor ABC index and multiplicative non-neighbor sum-connectivity index, multiplicative non-neighbor ABC index. We define a set $\overline{N_G(u)}$ of non-neighbors of a vertex $u$ as $\overline{N_G(u)} = \{v \in V(G) : d(u,v) \neq 1\}$ and a non-neighbor degree $\overline{d_G(u)}$ of $u$ as $\overline{d_G(u)} = n - 1 - d_G(u)$, where $n$ is the order of the graph $G$. Let $\overline{\delta}$ and $\overline{\Delta}$ denotes the minimum non-neighbor degree and the maximum non-neighbor degree of a graph $G$, respectively. Throughout this paper we use the notation NN for non-neighbor.

**Definition 1.** Non-neighbor SCI (NN-SCI):

$$\overline{SCI(G)} = \sum_{uv \in E(G)} [\overline{d_G(u)} + \overline{d_G(v)}]^{-1/2}$$

**Definition 2.** Multiplicative non-neighbor SCI:

$$\Pi\overline{SCI(G)} = \prod_{uv \in E(G)} [\overline{d_G(u)} + \overline{d_G(v)}]^{-1/2}$$

**Definition 3.** Non-neighbor ABC index (NN-ABC):

$$\overline{ABC(G)} = \sum_{uv\in E(G)} \sqrt{\frac{\overline{d_G(u)} + \overline{d_G(v)} - 2}{\overline{d_G(u)} \times \overline{d_G(v)}}}$$

**Definition 4.** Multiplicative non-neighbor ABC index:

$$\Pi\overline{ABC(G)} = \prod_{uv\in E(G)} \sqrt{\frac{\overline{d_G(u)} + \overline{d_G(v)} - 2}{\overline{d_G(u)} \times \overline{d_G(v)}}}$$

Boron nanotubes have been considered as excellent nanomaterial because of their remarkable properties such as high chemical stability, high resistance to oxidation at high temperatures and being a stable wide band-gap semiconductor, due to which they can be used for applications at high temperatures or in corrosive environments such as batteries, fuel cells, super capacitors, high speed machines as solid lubricants. The stability, mechanical and electronic properties have been discussed in [7, 13]. In 2009, Y. Liu et al. [12] predicted a new class of boron nanotubes, which are covered by hexagons and triangles. Such a nanotube was called Tri-Hexagonal boron nanotube and its 3D perception is shown in the Figure 1. Some of the degree based topological indices are studied for Tri-Hexagonal boron nanotube in [5].

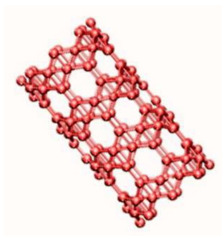

Figure 1. A 3D perception of Tri-Hexagonal boron nanotube.

In this article, NN-SCI, NN-ABC index and multiplicative NN-SCI, multiplicative NN-ABC index are introduced. In Section 2, these new indices are obtained for some classes of graphs. In Section 3, the indices are computed for some corona products of graphs. Finally, in Section 4, the new indices are computed for some nano-structures.

**Proposition 5.** *For a graph $G$ of order $n \geq 3$ with the diameter $diam(G) \geq 2$,*

(i) $\overline{SCI(G)}$, $\Pi\overline{SCI(G)}$ *exist and* $\overline{SCI(G)}$, $\Pi\overline{SCI(G)} > 0$,

(ii) *if* $\overline{ABC(G)}$, $\Pi\overline{ABC(G)}$ *exist, then there does not exist a full degree vertex in $G$. Moreover,* $\overline{ABC(G)}$, $\Pi\overline{ABC(G)} \geq 0$.

**Proposition 6.** *Let $G$ be a connected graph of order $n \geq 3$. Then for each $u \in V(G)$, $\overline{d_G(u)} \geq 0$.*

**Proposition 7.** *Let $G$ be a connected graph of order $n$ and size $m$. Then*

$$\sum_{u\in V(G)} \overline{d_G(u)} = n(n-1) - 2m.$$

## 2 NN-SCI, NN-ABC index and multiplicative NN-SCI, multiplicative NN-ABC index for some classes of graphs

Here formulas for NN-SCI, NN-ABC index and multiplicative NN-SCI, multiplicative NN-ABC index of a $k$-regular graph, a cycle, a path, a complete bipartite graph, a star graph and a wheel graph are computed.

**Theorem 8.** *For a $k$-regular graph $G$ of order $n \geq 3$ with $2 \leq k \leq n-2$,*

$$\overline{SCI(G)} = \frac{nk}{2\sqrt{2(n-1-k)}} \qquad \text{and} \qquad \overline{ABC(G)} = \frac{nk}{n-1-k}\sqrt{\frac{n-2-k}{2}}.$$

*Proof.* A $k$-regular graph of order $n \geq 3$ has $nk/2$ number of edges. In these graphs the NN-degree of each vertex is $n-1-k$. Hence for a $k$-regular graph $G$,

$$\overline{SCI(G)} = \frac{nk}{2}\left[\frac{1}{\sqrt{2(n-1-k)}}\right] = \frac{nk}{2\sqrt{2(n-1-k)}}$$

and

$$\overline{ABC(G)} = \frac{nk}{2}\left[\sqrt{\frac{2(n-1-k)-2}{(n-1-k)^2}}\right] = \frac{nk}{n-1-k}\sqrt{\frac{n-2-k}{2}}.$$

□

**Corollary 9.** *For a $k$-regular graph $G$ of order $n \geq 3$ with $2 \leq k \leq n-2$,*

$$\Pi\overline{SCI(G)} = [2(n-1-k)]^{-\frac{nk}{4}} \quad \text{and} \quad \Pi\overline{ABC(G)} = \left[\frac{\sqrt{2(n-2-k)}}{n-1-k}\right]^{\frac{nk}{2}}.$$

**Corollary 10.** *For a cycle $C_n$ $(n \geq 4)$,*

$$\overline{SCI(C_n)} = n[2(n-3)]^{-\frac{1}{2}} \ ; \quad \overline{ABC(C_n)} = \frac{n}{n-3}\sqrt{2(n-4)}$$

*and*

$$\Pi\overline{SCI(C_n)} = [2(n-3)]^{-\frac{n}{2}} \ ; \quad \Pi\overline{ABC(C_n)} = \left[\frac{\sqrt{2(n-4)}}{n-3}\right]^{n}.$$

**Remark 11.** The diameter of a complete graph is 1 and hence NN-topological indices are not defined for it.

**Theorem 12.** *For a path $P_n$ $(n \geq 4)$,*

$$\overline{SCI(P_n)} = \frac{2}{\sqrt{2n-5}} + \sqrt{\frac{n-3}{2}} \quad \text{and} \quad \overline{ABC(P_n)} = 2\sqrt{\frac{2n-7}{(n-2)(n-3)}} + \sqrt{2(n-4)}.$$

*Proof.* Let $u \in V(P_n)$. Then

$$\overline{d_{P_n}(u)} = \begin{cases} n-2 & \text{if } d_{P_n}(u) = 1 \\ n-3 & \text{if } d_{P_n}(u) = 2 \end{cases} \qquad \text{and} \qquad |E(P_n)| = n-1.$$

By Definition 1 and 3,

$$\overline{SCI(P_n)} = \frac{2}{\sqrt{(n-2)+(n-3)}} + \frac{n-3}{\sqrt{2(n-3)}} = \frac{2}{\sqrt{2n-5}} + \sqrt{\frac{n-3}{2}}$$

and

$$\begin{aligned}\overline{ABC(P_n)} &= 2\sqrt{\frac{(n-2)+(n-3)-2}{(n-2)(n-3)}} + (n-3)\sqrt{\frac{2(n-3)-2}{(n-3)^2}} \\ &= 2\sqrt{\frac{2n-7}{(n-2)(n-3)}} + \sqrt{2(n-4)}.\end{aligned}$$

□

**Corollary 13.** *For a path $P_n$ $(n \geq 4)$,*

$$\begin{aligned}\Pi\overline{SCI(P_n)} &= \frac{1}{2n-5}[2(n-3)]^{-\frac{n-3}{2}}, \\ \Pi\overline{ABC(P_n)} &= \left[\frac{2n-7}{(n-2)(n-3)}\right]\left[\frac{1}{n-3}\sqrt{2(n-4)}\right]^{n-3}.\end{aligned}$$

*Proof.*

$$\begin{aligned}\Pi\overline{SCI(P_n)} &= \left[\frac{1}{\sqrt{(n-2)+(n-3)}}\right]^2 \times \left[\frac{1}{\sqrt{2(n-3)}}\right]^{n-3} = \frac{1}{2n-5}[2(n-3)]^{-\frac{n-3}{2}}, \\ \Pi\overline{ABC(P_n)} &= \left[\sqrt{\frac{(n-2)+(n-3)-2}{(n-2)(n-3)}}\right]^2 \times \left[\sqrt{\frac{2(n-3)-2}{(n-3)^2}}\right]^{n-3} \\ &= \frac{2n-7}{(n-2)(n-3)}\left[\frac{1}{n-3}\sqrt{2(n-4)}\right]^{n-3}.\end{aligned}$$

□

**Remark 14.** $\overline{SCI(P_3)} = 2$, $\Pi\overline{SCI(P_3)} = 1$; indices $\overline{ABC(P_3)}$ and $\Pi\overline{ABC(P_3)}$ do not exist.

**Theorem 15.** *For a complete bipartite graph $K_{p,q}$,*

(i) $\overline{SCI(K_{p,q})} = \frac{pq}{\sqrt{p+q-2}}$, *where $p \geq 1$, $q \geq 2$ (or reverse order),*

(ii) $\overline{ABC(K_{p,q})} = pq\sqrt{\frac{p+q-4}{(p-1)(q-1)}}$, *where $p, q \geq 2$.*

*Proof.* Let $V_1$ and $V_2$ be the bi-partitions of $K_{p,q}$ with $|V_1| = p$ and $|V_2| = q$. Then for each $u \in V(K_{p,q})$, we have

$$\overline{d_{K_{p,q}}(u)} = \begin{cases} p-1 & \text{if } u \in V_1 \\ q-1 & \text{if } u \in V_2 \end{cases} \qquad \text{and} \qquad |E(K_{p,q})| = pq.$$

So, by Definition 1 and 3,

$$\overline{SCI(K_{p,q})} = pq\left[\frac{1}{\sqrt{(p-1)+(q-1)}}\right] = \frac{pq}{\sqrt{p+q-2}}$$

and

$$\overline{ABC(K_{p,q})} = pq\sqrt{\frac{(p-1)+(q-1)-2}{(p-1)(q-1)}} = pq\sqrt{\frac{p+q-4}{(p-1)(q-1)}}.$$

□

**Corollary 16.** *For a complete bipartite graph $K_{p,q}$,*

(i) $\Pi\overline{SCI(K_{p,q})} = [p+q-2]^{-\frac{pq}{2}}$, *where $p \geq 1$, $q \geq 2$ (or reverse order),*

(ii) $\Pi\overline{ABC(K_{p,q})} = \left[\frac{p+q-4}{(p-1)(q-1)}\right]^{\frac{pq}{2}}$, *where $p, q \geq 2$.*

*Proof.*

$$\Pi\overline{SCI(K_{p,q})} = \left[\frac{1}{\sqrt{(p-1)+(q-1)}}\right]^{pq} = [p+q-2]^{-\frac{pq}{2}}$$

and

$$\Pi\overline{ABC(K_{p,q})} = \left[\sqrt{\frac{p+q-4}{(p-1)(q-1)}}\right]^{pq} = \left[\frac{p+q-4}{(p-1)(q-1)}\right]^{\frac{pq}{2}}.$$

□

**Corollary 17.** *For a star graph $K_{1,n}$ $(n \geq 2)$,*

$$\overline{SCI(K_{1,n})} = \frac{n}{\sqrt{n-1}} \;;\quad \overline{ABC(K_{1,n})} \text{ does not exist}$$

*and*

$$\Pi\overline{SCI(K_{1,n})} = (n-1)^{-\frac{n}{2}} \;;\quad \Pi\overline{ABC(K_{1,n})} \text{ does not exist.}$$

**Theorem 18.** *For a wheel graph $W_{1,n}$ $(n \geq 4)$,*

$$\overline{SCI(W_{1,n})} = n\left[\frac{\sqrt{2}+1}{\sqrt{2(n-3)}}\right] \quad \textit{and} \quad \overline{ABC(W_{1,n})} \quad \textit{does not exist.}$$

*Proof.* For each vertex $u \in V(W_{1,n})$, we have

$$\overline{d_{W_{1,n}}(u)} = \begin{cases} 0 & \text{if } u \text{ is a central vertex} \\ n-3 & \text{otherwise} \end{cases} \qquad \text{and} \qquad |E(W_{1,n})| = 2n.$$

So, by Definition 1 and 3,

$$\overline{SCI(W_{1,n})} = \frac{n}{\sqrt{n-3}} + \frac{n}{\sqrt{2(n-3)}} = n\left[\frac{\sqrt{2}+1}{\sqrt{2(n-3)}}\right].$$

As $W_{1,n}$ has a full degree vertex, $\overline{ABC(W_{1,n})}$ does not exist. □

**Corollary 19.** *For a wheel graph $W_{1,n}$ $(n \geq 4)$,*

$$\Pi\overline{SCI(W_{1,n})} = [\sqrt{2}(n-3)]^{-n} \quad \text{and} \quad \Pi\overline{ABC(W_{1,n})} \quad \text{does not exist.}$$

*Proof.*

$$\Pi\overline{SCI(W_{1,n})} = \left(\frac{1}{\sqrt{n-3}}\right)^n \left[\frac{1}{\sqrt{2(n-3)}}\right]^n = [\sqrt{2}(n-3)]^{-n}$$

□

## 3 NN-SCI, NN-ABC index and multiplicative NN-SCI, multiplicative NN-ABC index of corona products of graphs

In this section, we give formulas for NN-SCI, NN-ABC index and multiplicative NN-SCI, multiplicative NN-ABC index of a comb graph, a sunlet graph, a helm graph, a fan graph and a friendship graph.

The corona product $G \odot H$ [4] of two graphs $G$ and $H$, is the graph obtained by taking one copy of $G$ and $|V(G)|$ copies of $H$, and by joining each vertex of the $i$-th copy of $H$ to the $i$-th vertex of $G$; where $1 \leq i \leq |V(G)|$.

**Theorem 20.** *For a comb graph $G = P_n \odot K_1$ $(n \geq 3)$,*

$$\begin{aligned}\overline{SCI(G)} &= 2\left[(4n-5)^{-\frac{1}{2}} + (4n-7)^{-\frac{1}{2}}\right] \\ &\quad + (n-2)\left[(4n-6)^{-\frac{1}{2}} + 2^{-1}(n-3)(n-2)^{-\frac{3}{2}}\right],\end{aligned}$$

$$\overline{ABC(G)} = \sqrt{\frac{2}{2n-3}}\left(\sqrt{\frac{4n-7}{n-1}} + \sqrt{\frac{4n-9}{n-2}}\right) + (n-2)\left[\frac{1}{\sqrt{n-1}} + \frac{n-3}{(n-2)^2}\sqrt{\frac{2n-5}{2}}\right].$$

*Proof.* Let $u \in V(G)$. Then

$$\overline{d_G(u)} = \begin{cases} 2n-2 & \text{if } d_G(u) = 1 \\ 2n-3 & \text{if } d_G(u) = 2 \\ 2(n-2) & \text{if } d_G(u) = 3 \end{cases} \qquad \text{and} \qquad |E(G)| = 2n-1.$$

So, by Definition 1 and 3,

$$\begin{aligned}\overline{SCI(G)} &= 2[(2n-2)+(2n-3)]^{-\frac{1}{2}} + 2[(2n-3)+(2n-4)]^{-\frac{1}{2}} \\ &\quad + (n-2)[(2n-2)+(2n-4)]^{-\frac{1}{2}} + (n-3)\left[2^2(n-2)\right]^{-\frac{1}{2}} \\ &= 2\left[(4n-5)^{-\frac{1}{2}} + (4n-7)^{-\frac{1}{2}}\right] + (n-2)\left[(4n-6)^{-\frac{1}{2}} + 2^{-1}(n-3)(n-2)^{-\frac{3}{2}}\right]\end{aligned}$$

and

$$\begin{aligned}\overline{ABC(G)} &= 2\sqrt{\frac{(2n-2)+(2n-3)-2}{(2n-2)(2n-3)}} + 2\sqrt{\frac{(2n-4)+(2n-3)-2}{(2n-4)(2n-3)}} \\ &\quad + (n-2)\sqrt{\frac{(2n-2)+(2n-4)-2}{(2n-2)(2n-4)}} + (n-3)\sqrt{\frac{2(2n-4)-2}{(2n-4)^2}} \\ &= \sqrt{\frac{2}{2n-3}}\left(\sqrt{\frac{4n-7}{n-1}} + \sqrt{\frac{4n-9}{n-2}}\right) + (n-2)\left[\frac{1}{\sqrt{n-1}} + \frac{n-3}{(n-2)^2}\sqrt{\frac{2n-5}{2}}\right].\end{aligned}$$

□

**Corollary 21.** *For a comb graph $G = P_n \odot K_1$ $(n \geq 3)$,*

$$\Pi\overline{SCI(G)} = \left[2^{\frac{3n-8}{2}}(4n-5)(4n-7)(2n-3)^{\frac{n-2}{2}}(n-2)^{\frac{n-3}{2}}\right]^{-1},$$
$$\Pi\overline{ABC(G)} = 2^{-\frac{n+1}{2}}(n-1)^{-\frac{n}{2}}(4n-7)(4n-9)(2n-5)^{\frac{n-3}{2}}(2n-3)^{-2}(n-2)^{-(n-2)}.$$

*Proof.* For $G = P_n \odot K_1$,

$$\begin{aligned}\Pi\overline{SCI(G)} &= [(2n-2)+(2n-3)]^{-1}[(2n-3)+(2n-4)]^{-1}[(2n-2)\\ &\quad + (2n-4)]^{-\frac{n-2}{2}}\left[2^2(n-2)\right]^{-\frac{n-3}{2}}\\ &= \left[2^{\frac{3n-8}{2}}(4n-5)(4n-7)(2n-3)^{\frac{n-2}{2}}(n-2)^{\frac{n-3}{2}}\right]^{-1}\end{aligned}$$

and

$$\begin{aligned}\Pi\overline{ABC(G)} &= \left[\sqrt{\frac{(2n-2)+(2n-3)-2}{(2n-2)(2n-3)}}\right]^2\left[\sqrt{\frac{(2n-4)+(2n-3)-2}{(2n-4)(2n-3)}}\right]^2\\ &\quad \left[\sqrt{\frac{(2n-2)+(2n-4)-2}{(2n-2)(2n-4)}}\right]^{n-2}\left[\sqrt{\frac{2(2n-4)-2}{(2n-4)^2}}\right]^{n-3}\\ &= 2^{-\frac{n+1}{2}}(n-1)^{-\frac{n}{2}}(4n-7)(4n-9)(2n-5)^{\frac{n-3}{2}}(2n-3)^{-2}(n-2)^{-(n-2)}.\end{aligned}$$

□

**Theorem 22.** *For a sunlet graph $G = C_n \odot K_1$ $(n \geq 3)$*

$$\overline{SCI(G)} = \frac{n}{2}\left[2^{\frac{1}{2}}(2n-3)^{-\frac{1}{2}} + (n-2)^{-\frac{1}{2}}\right],$$
$$\overline{ABC(G)} = n\left[(n-1)^{-\frac{1}{2}} + 2^{-\frac{1}{2}}(n-2)^{-1}(2n-5)^{\frac{1}{2}}\right].$$

*Proof.* Let $u \in V(G)$. Then

$$\overline{d_G(u)} = \begin{cases} 2(n-1) & \text{if } d_G(u) = 1 \\ 2(n-2) & \text{if } d_G(u) = 3 \end{cases} \qquad \text{and} \qquad |E(G)| = 2n.$$

By Definition 1 and 3,

$$\begin{aligned}\overline{SCI(G)} &= n[(2n-2)+(2n-4)]^{-\frac{1}{2}} + n[2(2n-4)]^{-\frac{1}{2}}\\ &= \frac{n}{2}\left[2^{\frac{1}{2}}(2n-3)^{-\frac{1}{2}} + (n-2)^{-\frac{1}{2}}\right]\end{aligned}$$

and

$$\begin{aligned}\overline{ABC(G)} &= n\sqrt{\frac{(2n-2)+(2n-4)-2}{(2n-2)(2n-4)}} + n\sqrt{\frac{2(2n-4)-2}{(2n-4)^2}}\\ &= n\left[(n-1)^{-\frac{1}{2}} + 2^{-\frac{1}{2}}(n-2)^{-1}(2n-5)^{\frac{1}{2}}\right].\end{aligned}$$

□

**Corollary 23.** *For a sunlet graph* $G = C_n \odot K_1$ $(n \geq 3)$,

$$\Pi\overline{SCI(G)} = \left[2^3(n-2)(2n-3)\right]^{-\frac{n}{2}} \quad \text{and} \quad \Pi\overline{ABC(G)} = \left[\frac{1}{n-2}\sqrt{\frac{2n-5}{2(n-1)}}\right]^n.$$

*Proof.*

$$\Pi\overline{SCI(G)} = [(2n-2)+(2n-4)]^{-\frac{n}{2}}[2(2n-4)]^{-\frac{n}{2}} = \left[2^3(n-2)(2n-3)\right]^{-\frac{n}{2}}$$

and

$$\begin{aligned}\Pi\overline{ABC(G)} &= \left[\sqrt{\frac{(2n-2)+(2n-4)-2}{(2n-2)(2n-4)}}\right]^n \left[\sqrt{\frac{2(2n-4)-2}{(2n-4)^2}}\right]^n \\ &= \left[\frac{1}{n-2}\sqrt{\frac{2n-5}{2(n-1)}}\right]^n.\end{aligned}$$

□

**Theorem 24.** *For a helm graph* $G = W_{1,n} \odot K_1 \setminus v_o v_o^{'}$ $(n \geq 3)$, *where* $v_o$ *is the central vertex of* $W_{1,n}$ *and* $v_o^{'}$ *is the one and only vertex of* $K_1$,

$$\overline{SCI(G)} = n[(4n-5)^{-\frac{1}{2}} + 2^{-1}(n-2)^{-\frac{1}{2}} + (3n-4)^{-\frac{1}{2}}],$$

$$\overline{ABC(G)} = \frac{n}{\sqrt{2}}\left[\sqrt{\frac{4n-7}{(2n-1)(n-2)}} + \frac{\sqrt{2n-5}}{n-2} + \sqrt{\frac{3}{n}}\right].$$

*Proof.* For any $u \in V(G)$, we have

$$\overline{d_G(u)} = \begin{cases} 2n-1 & \text{if } d_G(u) = 1 \\ 2(n-2) & \text{if } d_G(u) = 4 \\ n & \text{if } d_G(u) = n \end{cases} \qquad \text{and} \qquad |E(G)| = 3n.$$

By Definition 1 and 3,

$$\begin{aligned}\overline{SCI(G)} &= n\left\{[(2n-1)+(2n-4)]^{-\frac{1}{2}} + [2(2n-4)]^{-\frac{1}{2}} + [n+(2n-4)]^{-\frac{1}{2}}\right\} \\ &= n\left[(4n-5)^{-\frac{1}{2}} + 2^{-1}(n-2)^{-\frac{1}{2}} + (3n-4)^{-\frac{1}{2}}\right]\end{aligned}$$

and

$$\begin{aligned}\overline{ABC(G)} &= n\left[\sqrt{\frac{(2n-1)+(2n-4)-2}{(2n-1)(2n-4)}} + \sqrt{\frac{2(2n-4)-2}{(2n-4)^2}} + \sqrt{\frac{n+(2n-4)-2}{n(2n-4)}}\right] \\ &= \frac{n}{\sqrt{2}}\left[\sqrt{\frac{4n-7}{(2n-1)(n-2)}} + \frac{\sqrt{2n-5}}{n-2} + \sqrt{\frac{3}{n}}\right].\end{aligned}$$

□

**Corollary 25.** *For a helm graph* $G = W_{1,n} \odot K_1 \setminus v_o v_o^{'}$ $(n \geq 3)$, *where* $v_o$ *is the central vertex of* $W_{1,n}$ *and* $v_o^{'}$ *is the one and only vertex of* $K_1$,

$$\Pi\overline{SCI(G)} = 2^{-n}\left[(4n-5)(n-2)(3n-4)\right]^{-\frac{n}{2}},$$

$$\Pi\overline{ABC(G)} = \left[\frac{3(4n-7)(2n-5)}{n(2n-1)(2n-4)^3}\right]^{\frac{n}{2}}.$$

*Proof.*

$$\Pi\overline{SCI(G)} = \left\{[(2n-1)+(2n-4)]^{-\frac{1}{2}} \times [2(2n-4)]^{-\frac{1}{2}} \times [n+(2n-4)]^{-\frac{1}{2}}\right\}^n$$
$$= 2^{-n}\big[(4n-5)(n-2)(3n-4)\big]^{-\frac{n}{2}}$$

and

$$\Pi\overline{ABC(G)} = \left[\sqrt{\frac{(2n-1)+(2n-4)-2}{(2n-1)(2n-4)}} \times \sqrt{\frac{2(2n-4)-2}{(2n-4)^2}} \times \sqrt{\frac{n+(2n-4)-2}{n(2n-4)}}\right]^n$$
$$= \left[\frac{3(4n-7)(2n-5)}{n(2n-1)(2n-4)^3}\right]^{\frac{n}{2}}.$$

□

**Theorem 26.** *For a fan graph $f_n = K_1 \odot P_n$ $(n \geq 4)$,*

$$\overline{SCI(f_n)} = 2\left[(n-2)^{-\frac{1}{2}} + (2n-5)^{-\frac{1}{2}} + 2^{-\frac{3}{2}}(n-3)^{\frac{1}{2}}\right] + (n-2)(n-3)^{-\frac{1}{2}},$$

*$\overline{ABC(f_n)}$ does not exist.*

*Proof.* For any $u \in V(f_n)$, we have

$$\overline{d_{f_n}(u)} = \begin{cases} n-2 & \text{if } d_{f_n}(u) = 2 \\ n-3 & \text{if } d_{f_n}(u) = 3 \\ 0 & \text{if } d_{f_n}(u) = n \end{cases} \qquad \text{and} \qquad |E(f_n)| = 2n-1.$$

By Definition 1 and 3,

$$\overline{SCI(f_n)} = 2(n-2)^{-\frac{1}{2}} + (n-2)(n-3)^{-\frac{1}{2}} + 2\left[(n-2)+(n-3)\right]^{-\frac{1}{2}}$$
$$+ (n-3)[2(n-3)]^{-\frac{1}{2}}$$
$$= 2\left[(n-2)^{-\frac{1}{2}} + (2n-5)^{-\frac{1}{2}} + 2^{-\frac{3}{2}}(n-3)^{\frac{1}{2}}\right] + (n-2)(n-3)^{-\frac{1}{2}}.$$

As $f_n$ has a full degree vertex, $\overline{ABC(f_n)}$ does not exist. □

**Corollary 27.** *For a fan graph $f_n = K_1 \odot P_n$ $(n \geq 4)$,*

$$\Pi\overline{SCI(f_n)} = \left[2^{\frac{n-3}{2}}(n-2)(2n-5)(n-3)^{\frac{2n-5}{2}}\right]^{-1} \quad \textit{and} \quad \Pi\overline{ABC(f_n)} \textit{ does not exist.}$$

*Proof.*

$$\Pi\overline{SCI(f_n)} = (n-2)^{-1}(n-3)^{-\frac{n-2}{2}}[(n-2)+(n-3)]^{-1}[2(n-3)]^{-\frac{n-3}{2}}$$
$$= \left[2^{\frac{n-3}{2}}(n-2)(2n-5)(n-3)^{\frac{2n-5}{2}}\right]^{-1}$$

□

**Theorem 28.** *For a friendship graph $F_n = K_1 \odot nK_2$ $(n \geq 2)$,*

$$\overline{SCI(F_n)} = 2^{\frac{1}{2}}n(n-1)^{-\frac{1}{2}}\left(1+2^{-\frac{3}{2}}\right) \qquad \textit{and} \qquad \overline{ABC(F_n)} \textit{ does not exist.}$$

*Proof.* For any $u \in V(F_n)$, we have

$$\overline{d_{F_n}(u)} = \begin{cases} 2n-2 & \text{if } d_{F_n}(u) = 2 \\ 0 & \text{if } d_{F_n}(u) = 2n \end{cases} \qquad \text{and} \qquad |E(F_n)| = 3n.$$

By Definition 1 and 3,

$$\overline{SCI(F_n)} = 2n[2(n-1)]^{-\frac{1}{2}} + n[4(n-1)]^{-\frac{1}{2}} = 2^{\frac{1}{2}} n(n-1)^{-\frac{1}{2}} \left(1 + 2^{-\frac{3}{2}}\right).$$

As $F_n$ has a full degree vertex, $\overline{ABC(F_n)}$ does not exist. □

**Corollary 29.** *For a friendship graph $F_n = K_1 \odot nK_2$ $(n \geq 2)$,*

$$\Pi\overline{SCI(F_n)} = \left[2^2(n-1)^{\frac{3}{2}}\right]^{-n} \qquad \textit{and} \qquad \Pi\overline{ABC(F_n)} \textit{ does not exist.}$$

*Proof.* $\Pi\overline{SCI(F_n)} = [2(n-1)]^{-n}[2(2n-2)]^{-\frac{n}{2}} = \left[2^2(n-1)^{\frac{3}{2}}\right]^{-n}$ □

## 4 NN-SCI, NN-ABC index and multiplicative NN-SCI, multiplicative NN-ABC index of some nano-structures

In this section, we consider Tri-Hexagonal boron nanotube $C_3C_6(H)[p,q]$, Tri-Hexagonal boron nanotorus $THBC_3C_6[p,q]$ and Tri-Hexagonal boron-$\alpha$ nanotube $THBAC_3C_6[p,q]$. We will compute NN-SCI, NN-ABC index and multiplicative NN-SCI, multiplicative NN-ABC index of these nano-structures. To compute certain topological indices of these, we will partition the edge set based on NN degrees of end vertices of each edge of the graph.

### 4.1 Tri-Hexagonal boron nanotube

In this section, we calculate some topological indices of $C_3C_6(H)[p,q]$, where $p$ denotes the number of hexagons in a column and $q$ denotes the number of hexagons in a row of the 2D graph of $G = C_3C_6(H)[p,q]$ nanotube. It is easy to see that $|V(G)| = 8pq$ and $|E(G)| = q(18p-1)$. The molecular graph of $G = C_3C_6(H)[p,q]$ nanotube is shown in the Figure 2.

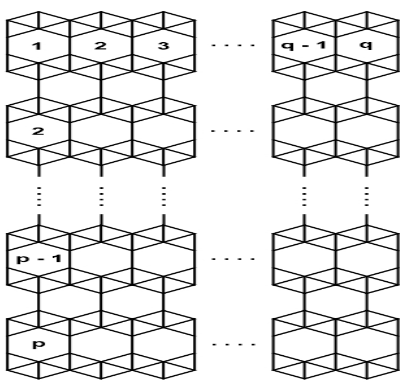


Figure 2. A 2D molecular graph of Tri-Hexagonal boron nanotube - $C_3C_6(H)[p,q]$.

**Theorem 30.** *For Tri-Hexagonal boron nanotube $G = C_3C_6(H)[p,q]$, where $p, q \geq 1$,*

$$\overline{SCI(G)} = q\left[\frac{6}{\sqrt{16pq-10}} + \frac{(2p-1)}{\sqrt{2(8pq-5)}} + \frac{6(2p-1)}{\sqrt{16pq-11}} + \frac{2p}{\sqrt{4pq-3}}\right],$$

$$\overline{ABC(G)} = \frac{q}{\sqrt{8pq-6}}\left[6\sqrt{\frac{4pq-3}{2pq-1}} + \frac{\sqrt{2}(2p-1)(8pq-6)}{8pq-5} + 6(2p-1)\sqrt{\frac{16pq-13}{8pq-5}} + 4p\sqrt{\frac{8pq-7}{4pq-3}}\right].$$

*Proof.* There are four partitions of the edge set corresponding to their NN degrees of end vertices of $G$, which are

$$E_1 = E_{(8pq-4,8pq-6)} = \{uv \in E(G) | \overline{d_G(u)} = 8pq-4 \ and \ \overline{d_G(v)} = 8pq-6\};$$
$$|E_1| = 6q$$
$$E_2 = E_{(8pq-5,8pq-5)} = \{uv \in E(G) | \overline{d_G(u)} = \overline{d_G(v)} = 8pq-5\};$$
$$|E_2| = q(2p-1)$$
$$E_3 = E_{(8pq-5,8pq-6)} = \{uv \in E(G) | \overline{d_G(u)} = 8pq-5 \ and \ \overline{d_G(v)} = 8pq-6\};$$
$$|E_3| = 6q(2p-1)$$
$$E_4 = E_{(8pq-6,8pq-6)} = \{uv \in E(G) | \overline{d_G(u)} = \overline{d_G(v)} = 8pq-6\};$$
$$|E_4| = 4pq$$

Now, $\overline{SCI(G)}$ and $\overline{ABC(G)}$ can be computed. By Definition 1 and 3,

$$\begin{aligned}
\overline{SCI(G)} &= \frac{6q}{\sqrt{(8pq-4)+(8pq-6)}} + \frac{q(2p-1)}{\sqrt{2(8pq-5)}} \\
&+ \frac{6q(2p-1)}{\sqrt{(8pq-5)+(8pq-6)}} + \frac{4pq}{\sqrt{2(8pq-6)}} \\
&= q\left[\frac{6}{\sqrt{16pq-10}} + \frac{2p-1}{\sqrt{2(8pq-5)}} + \frac{6(2p-1)}{\sqrt{16pq-11}} + \frac{2p}{\sqrt{4pq-3}}\right], \\
\overline{ABC(G)} &= 6q\sqrt{\frac{(8pq-4)+(8pq-6)-2}{(8pq-4)(8pq-6)}} + q(2p-1)\sqrt{\frac{2(8pq-5)-2}{(8pq-5)^2}} \\
&+ 6q(2p-1)\sqrt{\frac{(8pq-5)+(8pq-6)-2}{(8pq-5)(8pq-6)}} + 4pq\sqrt{\frac{2(8pq-6)-2}{(8pq-6)^2}} \\
&= \frac{q}{\sqrt{8pq-6}}\left[6\sqrt{\frac{4pq-3}{2pq-1}} + \frac{\sqrt{2}(2p-1)(8pq-6)}{8pq-5}\right. \\
&\left. + 6(2p-1)\sqrt{\frac{16pq-13}{8pq-5}} + 4p\sqrt{\frac{8pq-7}{4pq-3}}\right],
\end{aligned}$$

which is the required result. □

**Corollary 31.** *For Tri-Hexagonal boron nanotube $C_3C_6(H)[p,q]$, where $p,q \geq 1$,*

$$\begin{aligned}\Pi\overline{SCI(G)} &= 2^{-\frac{q}{2}(6p-1)}(8pq-5)^{-\frac{q}{2}(2p-1)}(8pq-6)^{-2pq}\\ &\quad\times(16pq-10)^{-3q}(16pq-11)^{-3q(2p-1)},\\ \Pi\overline{ABC(G)} &= 2^{\frac{q}{2}(6p+11)}(4pq-3)^{3q}(8pq-4)^{-3q}(8pq-5)^{-4q(2p-1)}(8pq-6)^{-q(9p+\frac{1}{2})}\\ &\quad\times(8pq-7)^{2pq}(16pq-13)^{3q(2p-1)}.\end{aligned}$$

### 4.2 Tri-Hexagonal boron nanotorus

In this section, we calculate some topological indices of $THBC_3C_6[p,q]$, where $p$ denotes the number of hexagons in a column and $q$ denotes the number of hexagons in a row of the 2D graph of $G = THBC_3C_6[p,q]$ nanotorus. It is easy to see that $|V(G)| = 8pq$ and $|E(G)| = 18pq$. The molecular graph of $G = THBC_3C_6[p,q]$ nanotorus is shown in the Figure 3.

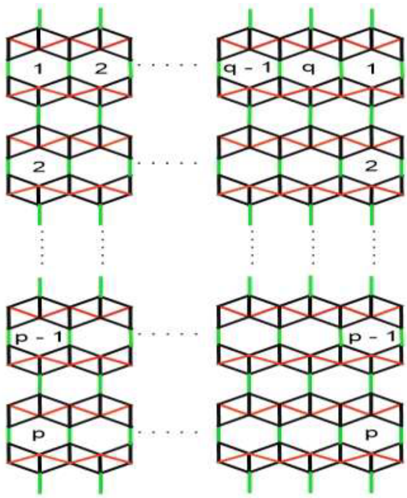


Figure 3. A 2D molecular graph of Tri-Hexagonal boron nanotorus - $THBC_3C_6[p,q]$.

**Theorem 32.** *For Tri-Hexagonal boron nanotorus $G = THBC_3C_6[p,q]$, where $p,q \geq 1$,*

$$\overline{SCI(G)} = 2pq\left[\frac{1}{\sqrt{2(8pq-5)}} + \frac{6}{\sqrt{16pq-11}} + \frac{1}{\sqrt{4pq-3}}\right],$$

$$\overline{ABC(G)} = 4pq\left[\frac{\sqrt{4pq-3}}{8pq-5} + 3\sqrt{\frac{16pq-13}{(8pq-5)(8pq-6)}} + \frac{\sqrt{2(8pq-7)}}{8pq-6}\right].$$

*Proof.* There are three partitions of the edge set corresponding to their NN degrees of end vertices of $G$, which are

$$E_1 = E_{(8pq-5,8pq-5)} = \{uv \in E(G) | \ \overline{d_G(u)} = \overline{d_G(v)} = 8pq - 5\};$$
$$|E_1| = 2pq$$
$$E_2 = E_{(8pq-5,8pq-6)} = \{uv \in E(G) | \ \overline{d_G(u)} = 8pq - 5 \ and \ \overline{d_G(v)} = 8pq - 6\};$$
$$|E_2| = 12pq$$
$$E_3 = E_{(8pq-6,8pq-6)} = \{uv \in E(G) | \ \overline{d_G(u)} = \overline{d_G(v)} = 8pq - 6\};$$
$$|E_3| = 4pq$$

Now, $\overline{SCI(G)}$ and $\overline{ABC(G)}$ can be computed. By Definition 1 and 3,

$$\begin{aligned}\overline{SCI(G)} &= \frac{2pq}{\sqrt{2(8pq-5)}} + \frac{12pq}{\sqrt{(8pq-5)+(8pq-6)}} + \frac{4pq}{\sqrt{2(8pq-6)}} \\ &= 2pq\left[\frac{1}{\sqrt{2(8pq-5)}} + \frac{6}{\sqrt{16pq-11}} + \frac{1}{\sqrt{4pq-3}}\right], \\ \overline{ABC(G)} &= 2pq\sqrt{\frac{2(8pq-5)-2}{(8pq-5)^2}} + 12pq\sqrt{\frac{(8pq-5)+(8pq-6)-2}{(8pq-5)(8pq-6)}} \\ &+ 4pq\sqrt{\frac{2(8pq-6)-2}{(8pq-6)^2}} \\ &= 4pq\left[\frac{\sqrt{4pq-3}}{8pq-5} + 3\sqrt{\frac{16pq-13}{(8pq-5)(8pq-6)}} + \frac{\sqrt{2(8pq-7)}}{8pq-6}\right],\end{aligned}$$

which is the required result. □

**Corollary 33.** *For Tri-Hexagonal boron nanotorus $THBC_3C_6[p,q]$, where $p, q \geq 1$,*

$$\Pi\overline{SCI(G)} = \left[2^5(8pq-5)(16pq-11)^6(4pq-3)^2\right]^{-pq},$$
$$\Pi\overline{ABC(G)} = \left[2^{-6}(4pq-3)^{-9}(8pq-5)^{-8}(8pq-7)^2(16pq-13)^6\right]^{pq}.$$

### 4.3 Tri-Hexagonal boron-$\alpha$ nanotorus

In this section, we calculate some topological indices of $THBAC_3C_6[p,q]$, where $p$ denotes the number of rows and $q$ denotes the number of columns of the 2D graph of $G = THBAC_3C_6[p,q]$ nanotorus. It is easy to see that $|V(G)| = 4pq/3$ and $|E(G)| = 7pq/2$. The molecular graph of $G = THBAC_3C_6[p,q]$ nanotorus is shown in the Figure 4.

**Theorem 34.** *For Tri-Hexagonal boron-$\alpha$ nanotorus $G = THBAC_3C_6[p,q]$, where $p, q \geq 1$,*

$$\overline{SCI(G)} = \frac{pq}{2}\left[\frac{3}{2\sqrt{\frac{2}{3}pq-3}} + \frac{4}{\sqrt{\frac{8}{3}pq-13}}\right],$$
$$\overline{ABC(G)} = \frac{pq}{2\sqrt{\frac{4}{3}pq-6}}\left[3\sqrt{\frac{\frac{4}{3}pq-7}{\frac{2}{3}pq-3}} + 4\sqrt{\frac{\frac{8}{3}pq-15}{\frac{4}{3}pq-7}}\right].$$

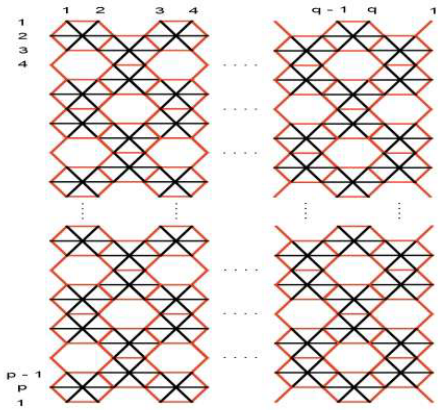


Figure 4. A 2D molecular graph of Tri-Hexagonal boron-$\alpha$ nanotorus - $THBAC_3C_6[p,q]$ .

*Proof.* There are two partitions of the edge set corresponding to their NN degrees of end vertices of $G$, which are

$$\begin{aligned}
E_1 &= E_{\left(\frac{4}{3}pq-6,\frac{4}{3}pq-6\right)} = \left\{uv \in E(G) | \ \overline{d_G(u)} = \overline{d_G(v)} = \frac{4}{3}pq-6\right\};\\
|E_1| &= \frac{3}{2}pq\\
E_2 &= E_{\left(\frac{4}{3}pq-6,\frac{4}{3}pq-7\right)} = \left\{uv \in E(G) | \ \overline{d_G(u)} = \frac{4}{3}pq-6 \ and \ \overline{d_G(v)} = \frac{4}{3}pq-7\right\};\\
|E_2| &= 2pq
\end{aligned}$$

Now, $\overline{SCI(G)}$ and $\overline{ABC(G)}$ can be computed. By Definition 1 and 3,

$$\begin{aligned}
\overline{SCI(G)} &= \frac{3pq}{2\sqrt{2\left(\frac{4}{3}pq-6\right)}} + \frac{2pq}{\sqrt{\left(\frac{4}{3}pq-6\right)+\left(\frac{4}{3}pq-7\right)}}\\
&= \frac{pq}{2}\left[\frac{3}{2\sqrt{\frac{2}{3}pq-3}} + \frac{4}{\sqrt{\frac{8}{3}pq-13}}\right],\\
\overline{ABC(G)} &= \frac{3}{2}pq\sqrt{\frac{2\left(\frac{4}{3}pq-6\right)-2}{\left(\frac{4}{3}pq-6\right)^2}} + 2pq\sqrt{\frac{\left(\frac{4}{3}pq-6\right)+\left(\frac{4}{3}pq-7\right)-2}{\left(\frac{4}{3}pq-6\right)\left(\frac{4}{3}pq-7\right)}}\\
&= \frac{pq}{2\sqrt{\frac{4}{3}pq-6}}\left[3\sqrt{\frac{\frac{4}{3}pq-7}{\frac{2}{3}pq-3}} + 4\sqrt{\frac{\frac{8}{3}pq-15}{\frac{4}{3}pq-7}}\right],
\end{aligned}$$

which is the required result. □

**Corollary 35.** *For Tri-Hexagonal boron-$\alpha$ nanotorus $THBAC_3C_6[p,q]$, where $p,q \geq 1$,*

$$\Pi\overline{SCI(G)} = \left[2^{\frac{3}{2}}\left(\frac{2}{3}pq-3\right)^{\frac{3}{4}}\left(\frac{8}{3}pq-13\right)\right]^{-pq},$$

$$\Pi\overline{ABC(G)} = \left[2^{-\frac{7}{4}}\left(\frac{4}{3}pq-7\right)^{-\frac{1}{4}}\left(\frac{2}{3}pq-3\right)^{-\frac{5}{2}}\left(\frac{8}{3}pq-15\right)\right]^{pq}.$$

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