International Journal of Applied Graph Theory
Vol.4, No.1 (2020), 29 - 49.
$ISSN(Online) : 2456 - 7884$

Non-Neighbor F-index and Randic index

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Abstract

A topological index is a graph invariant number, used for modeling biological and chemical properties of molecules in quantitative structure property relationship studies and quantitative structure activity relationship studies. In this paper, we compute non-neighbor F-index, non-neighbor Randic index, multiplicative non-neighbor F-index and multiplicative non-neighbor Randic index of some standard classes of graphs and for some corona products of graphs. We obtained the same for some nano-structures. We have also given some realization of graphs for the above indices.

Key words: topological index, non-neighbor vertices, nano-structures

2010 Mathematics Subject Classification : 97K30, 05C07

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Ψ Received on July 15, 2019 / Accepted on December 24, 2019

1 Introduction

We consider finite, undirected, simple graph G, 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 vertex u, $d(u,v)$ 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 represent an edge between the two vertices u and v. For $u, v \in V(G)$, $u \sim v$ denotes u is adjacent to v and $u \nsim v$ denotes u is not adjacent to v . For undefined terminologies we refer to [1].

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 depend on vertex degree.

Among the topological indices, Zagreb indices are the oldest given by Gutman and Trinajstic [3] defined as

$$M_1(G) = \sum_{uv\in E(G)} [d_G(u) + d_G(v)] \; and \; M_2(G) = \sum_{uv\in E(G)} [d_G(u) \times d_G(v)]$$

Among the many degree based topological indices, F-index and Randic index are two such degree based topological indices. Forgotten topological index or F-index [2] was introduced by Furtula and Gutman which is defined as

$$F(G) = \sum_{u\in V(G)} d_G(u)^3 = \sum_{uv\in E(G)} [d_G(u)^2 + d_G(v)^2]$$

Randic index [8] was introduced in 1975 which is defined as

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

The first multiplicative topological index was introduced in 1984 by Narumi and Katayama [5] which is defined as

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

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

Motivated by these works, we define non-neighbor F-index, non-neighbor Randic index and multiplicative non-neighbor F-index, multiplicative non-neighbor Randic index. We define a set $\overline{N_G(u)}$ of non-neighbors of a vertex u as $\overline{N_G(u)} = \{v \in V(G) : d(u,v) > 1\}$ 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. Throughout this paper we use the notation NN for non-neighbor.

Definition 1.1. Non-neighbor F-index (NN-F index):

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

Definition 1.2. Multiplicative non-neighbor F- index:

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

Definition 1.3. Non-neighbor Randic index (NN-R index):

$$\overline{R(G)} = \sum_{uv \in E(G)} \frac{1}{\sqrt{\overline{d_G(u)} \times \overline{d_G(v)}}}$$

Definition 1.4. Multiplicative non-neighbor Randic index:

$$\Pi\overline{R(G)} = \prod_{uv \in E(G)} \frac{1}{\sqrt{\overline{d_G(u)} \times \overline{d_G(v)}}}$$

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 are 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 lubricant. The stability, mechanical and electronic properties has been discussed in[7, 13]. In 2009, Y. Liu et al.[12] predicted a new class of boron nanotube which is covered by hexagons and triangles and was called as Tri-Hexagonal boron nanotube. A 3D perception of Tri-Hexagonal boron nanotube is shown in the Figure 1. Some of the degree based topological indices are studied for tri-hexagonal boron nanotube[6].

In this article, NN-F index, NN-R index, multiplicative NN-F index and multiplicative NN-R index are introduced. In Section 2, these new indices are obtained for some classes of graphs. In Section 3, these new indices are computed for some corona products of graphs. In Section 4, these new indices are computed for some nano-structures. Finally, in Section 5, we give the realization of graphs for some of the above indices.

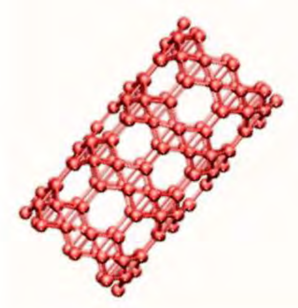

Figure 1: Three-dimensional perception of Tri- Hexagonal boron nanotube.

Proposition 1.5. For a graph G of order $n \geq 3$ and the diameter $diam(G) \geq 2$, there exists a NN-topological index.

Proposition 1.6. Let G be a connected graph of order $n \geq 3$. Then for $u \in V(G)$, $\overline{d_G(u)} \geq 0$.

Proposition 1.7. Let G be a connected graph of order n and size m. Then

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

Proposition 1.8. For a graph G of order $n \geq 3$, if G has a full degree vertex then $\overline{R(G)} = \Pi\overline{R(G)} =$ does not exists.

2 NN-F index, NN-R index and multiplicative NN-F index, multiplicative NN-R index for classes of graphs

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

Theorem 2.1. For a k-regular graph G $(k \geq 2)$ of order $n \geq 3$,

$$\overline{F(G)} = nk(n-1-k)^2 \; and \; \overline{R(G)} = \frac{nk}{2(n-1-k)}.$$

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,

$$\overline{F(G)} = \frac{nk}{2}[2(n-1-k)^2] = nk(n-1-k)^2$$

and

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

Hence the result. ∎

Corollary 2.2. For a k-regular graph G $(k \geq 2)$ of order $n \geq 3$,

$$\Pi\overline{F(G)} = [\sqrt{2}(n-1-k)]^{nk} \;\; ; \;\; \Pi\overline{R(G)} = [n-1-k]^{-\frac{nk}{2}}.$$

Proof: By definitions, we have $\Pi\overline{F(G)} = [2(n-1-k)^2]^{\frac{nk}{2}} = [\sqrt{2}(n-1-k)]^{nk}$ and $\Pi\overline{R(G)} = \left(\frac{1}{\sqrt{(n-1-k)^2}}\right)^{\frac{nk}{2}} = [n-1-k]^{-\frac{nk}{2}}$. ∎

Corollary 2.3. For a cycle C_n $(n \geq 4)$,

$$\overline{F(C_n)} = 2n(n-3)^2 \;\; ; \;\; \overline{R(C_n)} = \frac{n}{(n-3)}; \;\; \Pi\overline{F(C_n)} = 2^n(n-3)^{2n} \; ; \;\; \Pi\overline{R(C_n)} = (n-3)^{-n}.$$

Proof: Taking $k = 2$, in Theorem 2.1 we get the results. ∎

Remark 2.4. In the complete graph K_n, diameter is 1. Hence NN topological indices cannot be defined for it.

Theorem 2.5. For a path P_n $(n \geq 3)$, $\overline{F(P_n)} = 2(n-2)(n^2-5n+7)$; $\overline{R(P_n)} = \frac{2}{\sqrt{(n-2)(n-3)}}+1$

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

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

By Definition 1.1 and 1.3,

$$\overline{F(P_n)} = 2[(n-2)^2 + (n-3)^2] + (n-3)[2(n-3)^2] = 2(n-2)(n^2-5n+7)$$

and

$$\overline{R(P_n)} = \frac{2}{\sqrt{(n-2)(n-3)}} + \frac{(n-3)}{\sqrt{(n-3)^2}} = \frac{2}{\sqrt{(n-2)(n-3)}} + 1$$

∎

Corollary 2.6. For a path P_n $(n > 3)$,

$$\Pi\overline{F(P_n)} = [2(n-3)^2]^{(n-3)}[(n-2)^2 + (n-3)^2]^2 \ ;$$
$$\Pi\overline{R(P_n)} = [(n-2)(n-3)^{(n-2)}]^{-1}.$$

Proof: $\Pi\overline{F(P_n)} = [(n-2)^2+(n-3)^2]^2[2(n-3)^2]^{(n-3)} = [2(n-3)^2]^{(n-3)}[(n-2)^2+(n-3)^2]^2$ and $\Pi\overline{R(P_n)} = \left(\frac{1}{\sqrt{(n-2)(n-3)}}\right)^2\left(\frac{1}{\sqrt{(n-3)^2}}\right)^{(n-3)} = [(n-2)(n-3)^{(n-2)}]^{-1}$. ∎

Theorem 2.7. For a complete bipartite graph $K_{p,q}$ $(p, q \geq 1)$,

$$\overline{F(K_{p,q})} = pq[p^2 + q^2 + 2(1-p-q)] \ ; \ \overline{R(K_{p,q})} = \frac{pq}{\sqrt{pq - p - q + 1}}.$$

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

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

So, by Definition 1.1 and 1.3,

$$\overline{F(K_{p,q})} = pq[(p-1)^2 + (q-1)^2] = pq[p^2 + q^2 + 2(1-p-q)] \qquad \text{and}$$
$$\overline{R(K_{p,q})} = pq\left[\frac{1}{\sqrt{(p-1)(q-1)}}\right] = \frac{pq}{\sqrt{pq - p - q + 1}}.$$

∎

Corollary 2.8. For a complete bipartite graph $K_{p,q}$,

$$\Pi\overline{F(K_{p,q})} = [p^2 + q^2 + 2(1-p-q)]^{pq} \quad ; \quad \Pi\overline{R(K_{p,q})} = [pq - p - q + 1]^{-\frac{pq}{2}}.$$

Proof:

$$\Pi\overline{F(K_{p,q})} = [(p-1)^2 + (q-1)^2]^{pq} = [p^2 + q^2 + 2(1-p-q)]^{pq} \qquad \text{and}$$
$$\Pi\overline{R(K_{p,q})} = \left[\frac{1}{\sqrt{(p-1)(q-1)}}\right]^{pq} = [pq - p - q + 1]^{-\frac{pq}{2}}.$$

∎

Corollary 2.9. For a star graph $K_{1,n}$ $(n \geq 2)$,

$$\overline{F(K_{1,n})} = n(n-1)^2 \; ; \; \Pi\overline{F(K_{1,n})} = (n-1)^{2n} \; ;$$
$$\overline{R(K_{1,n})} = \Pi\overline{R(K_{1,n})} = does \; not \; exist.$$

Theorem 2.10. For a wheel graph $W_{1,n}$ $(n \geq 4)$,

$$\overline{F(W_{1,n})} = 3n(n-3)^2 \; ; \; \overline{R(W_{1,n})} = does \; not \; exist.$$

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

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

So, by Definition 1.1 and 1.3,
$\overline{F(W_{1,n})} = n(n-3)^2 + 2n(n-3)^2 = 3n(n-3)^2$ and $\overline{R(W_{1,n})} = does \; not \; exist.$ ∎

Corollary 2.11. For a wheel graph $W_{1,n}$ $(n \geq 4)$,
$\Pi\overline{F(W_{1,n})} = [2(n-3)^4]^n \;\; ; \;\; \Pi\overline{R(W_{1,n})} = does \; not \; exist.$

Proof: $\Pi\overline{F(W_{1,n})} = (n-3)^{2n}[2(n-3)^2]^n = [2(n-3)^4]^n$ and $\Pi\overline{R(W_{1,n})} = does \; not \; exist.$ ∎

3 NN-F index, NN-R index and multiplicative NN-F index, multiplicative NN-R index of some corona products of graphs

In this section, we give formulas for NN-F index, NN-R index and multiplicative NN-F index, multiplicative NN-R 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 3.1. For a comb graph $G = P_n \odot K_1$ $(n \geq 3)$,

$$\overline{F(G)} = 4[4n^3 - 16n^2 + 25n - 15] \; ;$$
$$\overline{R(G)} = 2^{\frac{1}{2}}(2n-3)^{-\frac{1}{2}}[(n-1)^{-\frac{1}{2}} + (n-2)^{-\frac{1}{2}}] + 2^{-1}(n-2)^{\frac{1}{2}}[(n-1)^{-\frac{1}{2}} + (n-3)(n-2)^{-\frac{3}{2}}].$$

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

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

So, by Definition 1.1 and 1.3,

$$\begin{aligned} \overline{F(G)} &= 2[(2(n-1))^2 + (2n-3)^2] + 2[(2n-3)^2 + (2(n-2))^2] \\ &+ (n-2)[(2(n-1))^2 + (2(n-2))^2] + (n-3)[2(2(n-2))^2 \\ &= 4[4n^3 - 16n^2 + 25n - 15] \end{aligned}$$

and

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

■

Corollary 3.2. For a comb graph $G = P_n \odot K_1$ $(n \geq 3)$,

$$\begin{aligned} \Pi\overline{F(G)} &= 2^{(n-3)}(2n-4)^{2(n-3)}[(2n-2)^2 + (2n-3)^2]^2[(2n-3)^2 \\ &\quad + (2n-4)^2]^2[(2n-2)^2 + (2n-4)^2]^{(n-2)} ; \\ \Pi\overline{R(G)} &= 2^{-(2n-3)}(n-1)^{-\frac{n}{2}}(2n-3)^{-2}(n-2)^{-\frac{3(n-2)}{2}}. \end{aligned}$$

Proof: For $G = P_n \odot K_1$,

$$\begin{aligned} \Pi\overline{F(G)} &= [(2(n-1))^2 + (2n-3)^2]^2[(2n-3)^2 + (2(n-2))^2]^2 \\ &\quad [(2(n-1))^2 + (2(n-2))^2]^{(n-2)}[2(2(n-2))^2]^{(n-3)} \\ &= 2^{(n-3)}(2n-4)^{2(n-3)}[(2n-2)^2 + (2n-3)^2]^2[(2n-3)^2 + (2n-4)^2]^2 \\ &\quad [(2n-2)^2 + (2n-4)^2]^{(n-2)} \end{aligned}$$

and

$$\Pi\overline{R(G)} = [2(n-1)(2n-3)]^{-1}[2(2n-3)(n-2)]^{-1}[2^2(n-1)(n-2)]^{-\frac{(n-2)}{2}}$$
$$[2^2(n-2)^2]^{-\frac{(n-3)}{2}}$$
$$= 2^{-(2n-3)}(n-1)^{-\frac{n}{2}}(2n-3)^{-2}(n-2)^{-\frac{3(n-2)}{2}}$$

∎

Theorem 3.3. For a sunlet graph $G = C_n \odot K_1$ $(n \geq 3)$,

$$\overline{F(G)} = 4n[4n^2 - 14n + 13] \ ; \ \overline{R(G)} = n[2(n-2)]^{-1}[(n-1)^{-\frac{1}{2}}(n-2)^{-\frac{1}{2}} + 1].$$

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

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

By Definition 1.1 and 1.3,

$$\overline{F(G)} = n[(2n-2)^2 + 3(2n-4)^2] = 4n[4n^2 - 14n + 13]$$

and

$$\overline{R(G)} = n[2^2(n-1)(n-2)]^{-\frac{1}{2}} + n[2^2(n-2)^2]^{-\frac{1}{2}}$$
$$= n[2(n-2)]^{-1}[(n-1)^{-\frac{1}{2}}(n-2)^{-\frac{1}{2}} + 1]$$

∎

Corollary 3.4. For a sunlet graph $G = C_n \odot K_1$ $(n \geq 3)$,

$$\Pi\overline{F(G)} = 2^{5n}[(n-2)^2(2n^2 - 6n + 5)]^n \quad ; \ \Pi\overline{R(G)} \quad = [2^{2n}[(n-1)(n-2)^3]^{\frac{n}{2}}]^{-1}.$$

Proof:

$$\Pi\overline{F(G)} = [(2n-2)^2 + (2n-4)^2]^n[2(2n-4)^2]^n = 2^{5n}[(n-2)^2(2n^2 - 6n + 5)]^n \text{ and}$$
$$\Pi\overline{R(G)} = [2^2(n-1)(n-2)]^{-\frac{n}{2}}[2^2(n-2)^2]^{-\frac{n}{2}} = [2^{2n}[(n-1)(n-2)^3]^{\frac{n}{2}}]^{-1}.$$

∎

Theorem 3.5. For a helm graph $G = W_{1,n} \odot K_1 \setminus v_o v_o^{'}$ where v_o is the central vertex of $W_{1,n}$ and $v_o^{'}$ is the one and only vertex of K_1,

$$\overline{F(G)} = n[21n^2 - 68n + 65]\ ;\ \overline{R(G)} = n(2n-4)^{-\frac{1}{2}}[(2n-1)^{-\frac{1}{2}} + (2n-4)^{-\frac{1}{2}} + n^{-\frac{1}{2}}].$$

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

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

By Definition 1.1 and 1.3,

$$\begin{aligned} \overline{F(G)} &= n[(2n-1)^2 + 4(2n-4)^2 + n^2] = n[21n^2 - 68n + 65] \qquad \text{and} \\ \overline{R(G)} &= n\Big[[(2n-1)(2n-4)]^{-\frac{1}{2}} + (2n-4)^{-1} + [n(2n-4)]^{-\frac{1}{2}}\Big] \\ &= n(2n-4)^{-\frac{1}{2}}[(2n-1)^{-\frac{1}{2}} + (2n-4)^{-\frac{1}{2}} + n^{-\frac{1}{2}}]. \end{aligned}$$

■

Corollary 3.6. For a helm graph $(n \geq 3)$,

$$\begin{aligned} \Pi\overline{F(G)} &= \Big[2(2n-4)^2[(2n-1)^2 + (2n-4)^2][n^2 + (2n-4)^2]\Big]^n \qquad \text{and} \\ \Pi\overline{R(G)} &= \Big[(2n-4)^2[n(2n-1)]^{\frac{1}{2}}\Big]^{-n}. \end{aligned}$$

Proof: For a helm graph

$$\begin{aligned} \Pi\overline{F(G)} &= [(2n-1)^2 + (2n-4)^2]^n[2(2n-4)^2]^n[(2n-4)^2 + n^2]^n \\ &= \Big[2(2n-4)^2[(2n-1)^2 + (2n-4)^2][n^2 + (2n-4)^2]\Big]^n \qquad \text{and} \\ \Pi\overline{R(G)} &= [(2n-1)(2n-4)]^{-\frac{n}{2}}(2n-4)^{-n}[(2n-4)n]^{-\frac{n}{2}} \\ &= \Big[(2n-4)^2[n(2n-1)]^{\frac{1}{2}}\Big]^{-n}. \end{aligned}$$

■

Theorem 3.7. For a fan graph $f_n = K_1 \odot P_n$ $(n \geq 4)$,

$$\overline{F(G)} = (n-2)[3n^2 - 14n + 25] \quad ; \quad \overline{R(G)} = does\ not\ exist.$$

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

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

By Definition 1.1 and 1.3,

$$\begin{aligned} \overline{F(G)} &= 2(n-2)^2 + (n-2)(n-3)^2 + 2[(n-2)^2 + (n-3)^2] + 2(n-3)^3 \\ &= (n-2)[3n^2 - 14n + 25] \end{aligned}$$

and $\overline{R(G)} = does\ not\ exist.$ ∎

Corollary 3.8. For a fan graph f_n $(n \geq 4)$,

$$\Pi\overline{F(G)} = 2^{(n-3)}(n-2)^4(n-3)^{2(2n-5)}[2n^2 - 10n + 13]^2 \ ; \ \Pi\overline{R(G)} = does\ not\ exist.$$

Proof:

$$\begin{aligned} \Pi\overline{F(G)} &= (n-2)^4(n-3)^{2(n-2)}[(n-2)^2 + (n-3)^2]^2[2(n-3)^2]^{(n-3)} \\ &= 2^{(n-3)}(n-2)^4(n-3)^{2(2n-5)}[2n^2 - 10n + 13]^2 \end{aligned}$$

and $\Pi\overline{R(G)} = does\ not\ exist.$ ∎

Theorem 3.9. For a friendship graph $F_n = K_1 \odot nK_2$ $(n \geq 2)$,

$$\overline{F(G)} = 2^4 n(n-1)^2 \ ; \ \overline{R(G)} = does\ not\ exists.$$

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

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

By Definition 1.1 and 1.3,

$$\overline{F(G)} = 2n[2^2(n-1)^2] + n[2^3(n-1)^2] = 2^4 n(n-1)^2$$

and $\overline{R(G)} = does\ not\ exist.$ ∎

Corollary 3.10. For a friendship graph $F_n = K_1 \odot nK_2$ $(n \geq 2)$,

$$\Pi\overline{F(G)} = 2^{7n}(n-1)^{6n} \quad ; \quad \Pi\overline{R(G)} = does\ not\ exists.$$

Proof: $\Pi\overline{F(G)} = [2(n-1)]^{4n}[2(2n-2)^2]^n = 2^{7n}(n-1)^{6n}$ and $\Pi\overline{R(G)} = does\ not\ exists.$ ∎

4 NN-F index, NN-R index and multiplicative NN-F index, multiplicative NN-R 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-α nanotube $THBAC_3C_6[p,q]$. We will compute NN-F index, NN-R index and multiplicative NN-F index, multiplicative NN-R index of $C_3C_6(H)[p,q]$, $THBC_3C_6[p,q]$ and $THBAC_3C_6[p,q]$. 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.

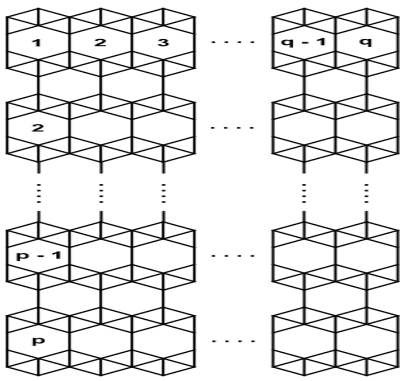

Figure 2: A 2-D molecular graph of tri-hexagonal boron nanotube - $C_3C_6(H)[p,q]$.

Theorem 4.1. For the tri-hexagonal boron nanotube $G = C_3C_6(H)[p,q]$ for some $p,q \geq 1$,

$$\overline{F(G)} = 6q(8pq-4)^2 + 20pq(8pq-6)^2 + 8q(2p-1)(8pq-5)^2 \quad ;$$

$$\overline{R(G)} = (8pq-6)^{-\frac{1}{2}}[6q(8pq-4)^{-\frac{1}{2}} + [6q(2p-1)](8pq-5)^{-\frac{1}{2}} + 4pq(8pq-6)^{-\frac{1}{2}}] + q(2p-1)(8pq-5)^{-1}.$$

Proof: Let G be the graph representing tri-hexagonal boron nanotube $G = C_3C_6(H)[p,q]$. There are four partitions of the edge set corresponding to their non-neighbor 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, $\overline{F(G)}$ and $\overline{R(G)}$ of G can be computed. By Definition 1.1 and 1.3,

$$\begin{aligned}\overline{F(G)} &= 6q[(8pq-4)^2 + (8pq-6)^2] + [q(2p-1)][2(8pq-5)^2] \\ &\quad + [6q(2p-1)][(8pq-5)^2 + (8pq-6)^2] + 4pq[2(8pq-6)^2] \\ &= 6q(8pq-4)^2 + 20pq(8pq-6)^2 + 8q(2p-1)(8pq-5)^2 \\ \overline{R(G)} &= 6q[(8pq-4)(8pq-6)]^{-\frac{1}{2}} + [q(2p-1)](8pq-5)^{-1} \\ &\quad + [6q(2p-1)][(8pq-5)(8pq-6)]^{-\frac{1}{2}} + 4pq(8pq-6)^{-1} \\ &= (8pq-6)^{-\frac{1}{2}}[6q(8pq-4)^{-\frac{1}{2}} + [6q(2p-1)](8pq-5)^{-\frac{1}{2}} + 4pq(8pq-6)^{-\frac{1}{2}}] \\ &\quad + q(2p-1)(8pq-5)^{-1}\end{aligned}$$

Which is the required result. ∎

Corollary 4.2. For the tri-hexagonal boron nanotube $G = C_3C_6(H)[p,q]$,

$$\begin{aligned}\Pi\overline{F(G)} &= 2^{q(6p-1)}(8pq-5)^{2q(2p-1)}(8pq-6)^{8pq}[(8pq-4)^2 + (8pq-6)^2]^{6q} \\ &\quad [(8pq-5)^2 + (8pq-6)^2]^{6q(2p-1)} ; \\ \Pi\overline{R(G)} &= (8pq-4)^{-3q}(8pq-5)^{-4q(2p-1)}(8pq-6)^{-10pq}.\end{aligned}$$

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.

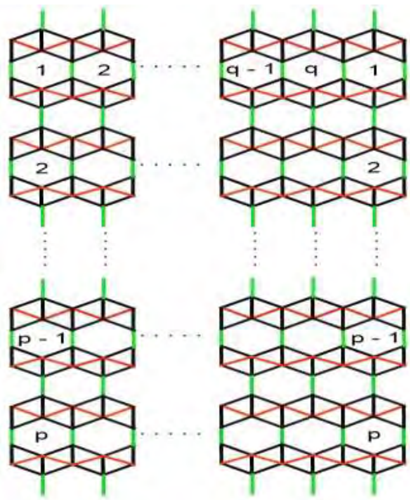

Figure 3: A 2-D molecular graph of Tri-Hexagonal boron nanotorus - $THBC_3C_6[p,q]$.

Theorem 4.3. For the Tri-Hexagonal boron nanotorus $G = THBC_3C_6[p,q]$ for some $p, q \geq 1$,

$$\overline{F(G)} = 16pq(8pq-5)^2 + 20pq(8pq-6)^2 \quad ;$$
$$\overline{R(G)} = 2pq\Big\{(8pq-5)^{-1} + 2pq(8pq-6)^{-\frac{1}{2}}[3(8pq-5)^{-\frac{1}{2}} + (8pq-6)^{-\frac{1}{2}}]\Big\}.$$

Proof: Let G be the graph representing Tri-Hexagonal boron nanotorus $G = THBC_3C_6[p,q]$. There are three partitions of the edge set corresponding to their non-neighbor 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, by Definition 1.1 and 1.3,

$$\begin{aligned}\overline{F(G)} &= 2pq[2(8pq-5)^2] + 12pq[(8pq-5)^2 + (8pq-6)^2] + 4pq[2(8pq-6)^2] \\ &= 16pq(8pq-5)^2 + 20pq(8pq-6)^2 \\ \overline{R(G)} &= 2pq(8pq-5)^{-1} + 12pq(8pq-5)^{-\frac{1}{2}}(8pq-6)^{-\frac{1}{2}} + 4pq(8pq-6)^{-1} \\ &= 2pq\Big\{(8pq-5)^{-1} + 2pq(8pq-6)^{-\frac{1}{2}}[3(8pq-5)^{-\frac{1}{2}} + (8pq-6)^{-\frac{1}{2}}]\Big\}\end{aligned}$$

which is the required result. ■

Corollary 4.4. For the Tri-Hexagonal boron nanotorus $G = THBC_3C_6[p,q]$,

$$\Pi\overline{F(G)} = 2^{6pq}(8pq-5)^{4pq}(8pq-6)^{8pq}[(8pq-5)^2 + (8pq-6)^2]^{12pq} \quad ;$$
$$\Pi\overline{R(G)} = \Big[(8pq-5)^4(8pq-6)^5\Big]^{-2pq}.$$

4.3 Tri-Hexagonal boron-α 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.

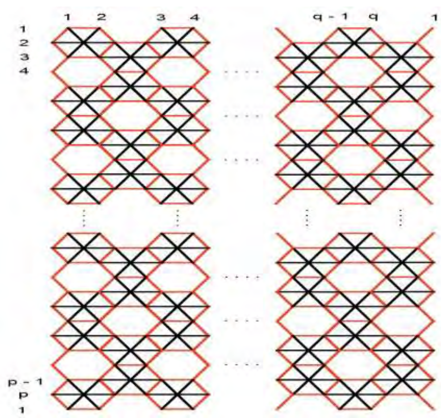

Figure 4: A 2-D molecular graph of Tri-Hexagonal boron-α nanotorus- $THBAC_3C_6[p,q]$.

Theorem 4.5. For the Tri-Hexagonal boron-α nanotorus $G = THBAC_3C_6[p,q]$ for some

$p, q \geq 1$,

$$\overline{F(G)} = 5pq\Big(\frac{4}{3}pq - 6\Big)^2 + 2pq\Big(\frac{4}{3}pq - 7\Big)^2 \ ;$$
$$\overline{R(G)} = pq\Big(\frac{4}{3}pq - 6\Big)^{-\frac{1}{2}}\Big[\frac{3}{2}\Big(\frac{4}{3}pq - 6\Big)^{-\frac{1}{2}} + 2\Big(\frac{4}{3}pq - 7\Big)^{-\frac{1}{2}}\Big].$$

Proof: Let G be the graph representing Tri-Hexagonal boron-α nanotorus $G = THBAC_3C_6[p, q]$. There are two partitions of the edge set corresponding to their non-neighbor degrees of end vertices of G which are

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

Now, $\overline{F(G)}$ and $\overline{R(G)}$ of G can be computed. By Definition 1.1 and 1.3,

$$\overline{F(G)} = \frac{3}{2}pq\left[2\left(\frac{4}{3}pq - 6\right)^2\right] + 2pq\left[\left(\frac{4}{3}pq - 6\right) + \left(\frac{4}{3}pq - 7\right)^2\right]$$
$$= 5pq\left(\frac{4}{3}pq - 6\right)^2 + 2pq\left(\frac{4}{3}pq - 7\right)^2$$
$$\overline{R(G)} = \frac{3}{2}pq\left(\frac{4}{3}pq - 6\right)^{-1} + 2pq\left(\frac{4}{3}pq - 6\right)^{-\frac{1}{2}}\left(\frac{4}{3}pq - 7\right)^{-\frac{1}{2}}$$
$$= pq\left(\frac{4}{3}pq - 6\right)^{-\frac{1}{2}}\left[\frac{3}{2}\left(\frac{4}{3}pq - 6\right)^{-\frac{1}{2}} + 2\left(\frac{4}{3}pq - 7\right)^{-\frac{1}{2}}\right]$$

which is the required result. ∎

Corollary 4.6. For the Tri-Hexagonal boron-α nanotorus $G = THBAC_3C_6[p, q]$,

$$\Pi\overline{F(G)} = \Big[2^{\frac{3}{2}}\Big(\frac{4}{3}pq - 6\Big)^3\Big[\Big(\frac{4}{3}pq - 6\Big)^2 + \Big(\frac{4}{3}pq - 7\Big)^2\Big]^2\Big]^{pq} \ ;$$
$$\Pi\overline{R(G)} = \Big[\Big(\frac{4}{3}pq - 6\Big)^{\frac{5}{2}}\Big(\frac{4}{3}pq - 7\Big)\Big]^{-pq}.$$

5 Realization of some topological indices

Proposition 5.1. Let G be a connected graph then $\overline{F(G)} \geq 2$.

Theorem 5.2. There is a connected graph G if and only if $\overline{F(G)} = even.$

Proof: Let G be a connected graph. By Definition 1.1 we have,

$$\begin{aligned}\overline{F(G)} &= \sum_{uv\in E(G)} [(\overline{d_G(u)})^2 + (\overline{d_G(v)})^2] \\ &= \sum_{uv\in E(G)} [(n-1-d_G(u))^2 + (n-1-d_G(v))^2] \\ &= \sum_{uv\in E(G)} 2(n-1)^2 + \sum_{uv\in E(G)} [d_G(u)^2 + d_G(v)^2] \\ &- 2(n-1) \sum_{uv\in E(G)} [d_G(u) + d_G(v)]\end{aligned}$$

We see that the first and third terms of the above equations are even integers. Suppose the second term is odd, as $\sum_{uv\in E(G)}[d_G(u)^2 + d_G(v)^2]$ can be written as $\sum_{v\in V(G)} d_G(u)^3$ is odd then it implies that there are odd number of terms in the summation $\Rightarrow \sum_{v\in V(G)} d_G(u) = odd$, a contradiction. Therefore, second term is also an even integer. Hence $\overline{F(G)} = even.$

Conversely, let $\overline{F(G)} = even.$ Then by Section 2 and Section 3, we see that for $\overline{F(G)} = even$, there exist a connected graph G. ∎

Proposition 5.3. For a connected graph G, $\Pi\overline{F(G)} = K_1 \times K_2 \times \cdots \times K_n$ where each $K_i(1 \le i \le n) = (a_i^2 + b_i^2)$.

Theorem 5.4. For a connected graph G of order n, $\Pi\overline{F(G)} = 0$ if and only if G has at least two full degree vertices.

Proof: Let G be a graph of order n. Let u and v be any two full degree vertices in graph G i.e $d_G(u) = d_G(v) = n-1$. Hence $\overline{d_G(u)} = \overline{d_G(v)} = 0$. Also, there is an edge between u and v in G. Hence by definition, due to this edge uv, $0^2 + 0^2$ is one of the factor of $\Pi\overline{F(G)}$. Therefore, $\Pi\overline{F(G)} = 0$.

Conversely, let $\Pi\overline{F(G)} = 0$, this implies there is an edge xy due to which $0^2 + 0^2$ is one of the factor of $\Pi\overline{F(G)}$. This implies that $\overline{d_G(x)} = \overline{d_G(y)} = 0$ i.e $d_G(x) = d_G(y) = n-1$. Hence we see that x and y are full degree vertices in G. ∎

Theorem 5.5. For a connected graph G of order n, $\Pi\overline{F(G)} = 1$ if and only if $G \cong P_3$.

Proof: By Proposition 1.5, P_3 is the graph of minimum order with $diam(G) = 2$. By Definition 1.2, $\Pi\overline{F(G)} = 1$.
Conversely, $\Pi\overline{F(G)} = 1$. By Proposition 5.3, 1 can be written as $(1^2 + 0^2)^k$ for some $k \in \mathbb{Z}$.

Here k represents number of edges in graph G with NN-degree of its end vertices 1 and 0. The only possible graph of minimal order is P_3. Hence the proof. ∎

Corollary 5.6. Let G be a connected graph. Then $\Pi\overline{F(G)} \geq 1$.

Theorem 5.7. There is no connected graph G with $\Pi\overline{F(G)} = 2$.

Proof: If $\Pi\overline{F(G)} = 2$, then by its definition, the only posiible factorization is

$$\Pi\overline{F(G)} = (1^2 + 1^2)(1^2 + 0^2)^r for\ some\ r \in \mathbb{Z}^+ \tag{1}$$

Let u and v be any two adjacent vertices with $\overline{d_G(u)} = \overline{d_G(v)} = 1$ in a graph G. Then we discuss the result in the following two cases:

Case(1) a vertex x not adjacent to u and v in G.

(a) Since G is connected, there is a common vertex y adjacent to both u, v and to x, as in Figure 5. Now $\overline{d_G(x)} = 2$ and Equation 1 is not satisfied. Hence $\Pi\overline{F(G)} \neq 2$.

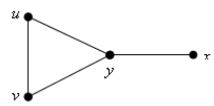

Figure 5: case(1)a

(b) Since G is connected, if there are more than one vertex connecting u, v and x, then now to get the second term of factorization i.e $(1^2 + 0^2)$ all the in between vertices must be full degree vertices. Hence by Theorem 5.4, $\Pi\overline{F(G)} \neq 2$.

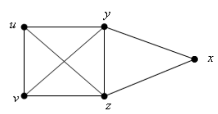

Figure 6: case(1)b

Case(2) two vertices x and y not adjacent to v and u respectively.

(a) if $x \nsim y \Rightarrow \overline{d_G(u)} = \overline{d_G(v)} = 2$. Equation 1 cannot be obtained. Hence $\Pi\overline{F(G)} \neq 2$.

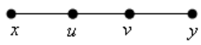

Figure 7: case(2)a

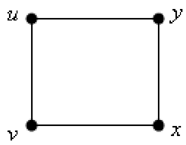

Figure 8: case(2)b

(b) if $x \sim y \Rightarrow \overline{d_G(u)} = \overline{d_G(v)} = 1$. Equation 1 cannot be obtained. Hence $\Pi\overline{F(G)} \neq 2$.

(c) if there is a vertex z and $x \nsim y$. Here $\overline{d_G(u)} = \overline{d_G(v)} = 2$ and z is a full degree vertex. Equation 1 cannot be obtained. Hence $\Pi\overline{F(G)} \neq 2$.

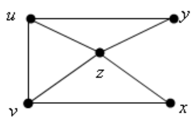

Figure 9: case(2)c

(d) if there is a vertex z and $x \sim y$. Here $\overline{d_G(u)} = \overline{d_G(v)} = \overline{d_G(x)} = \overline{d_G(y)} = 1$ and z is a full degree vertex. Equation 1 cannot be obtained. Hence $\Pi\overline{F(G)} \neq 2$.

(e) if there are more than one vertices connecting u, v, x and y and if $x \sim y$ or $x \nsim y$, as discussed in case (i) part (b) full degree vertices are created. Hence $\Pi\overline{F(G)} \neq 2$.

Hence from all the above cases we can conclude that there is no connected graph G with $\Pi\overline{F(G)} = k = 2$. ■

Theorem 5.8. For any prime number k, there is no connected graph G with $\Pi\overline{F(G)} = k$.

Proof: The only possible way to express $\Pi\overline{F(G)} = k$ is $(1^2 + 0^2)(a_i^2 + b_i^2)$ where $a, b \in \mathbb{Z}$ and $r \in \mathbb{Z}^+$. By constructing a graph having NN-degrees $0, 1, a$, and b, we get additional factors (i.e edges of different degree factors). Hence there is no connected graph G with $\Pi\overline{F(G)} = k$. ■

Theorem 5.9. For a positive integer k, there is no connected graph G with $\Pi\overline{F(G)} = k = 6, 9, 12$.

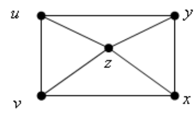

Figure 10: case(2)d

Proof: (i) $\Pi\overline{F(G)} = 6$. The only factor for $6 = 2 \times 3$, since 3 cannot be expressed in the form $(a^2 + b^2)$ where $a, b \in \mathbb{Z}$. Hence there does not exist any connected graph G.

(ii) $\Pi\overline{F(G)} = 9 = (3)^2 = (1^2 + 0^2)^r(3^2 + 0)$ where $r \in \mathbb{Z}^+$. By constructing a graph having factors of degree $(3^2 + 0)$, we get additional edges having different factors. Hence there is no connected graph G.

(iii) $\Pi\overline{F(G)} = 12 = 4 \times 3 = 2^2 \times 3 = 2 \times 6$. From case (i) and case (ii), there is no connected graph G.

∎

Corollary 5.10. For any positive odd integer k, there does not exist a connected graph G with $\Pi\overline{F(G)} = k$.

Proof: Result is evident from Theorem 5.8 and Theorem 5.9. ∎

Acknowlegment : The author's would like to thank the referee for their suggestion which helped in the improvement of the paper.

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