ADV MATH SCI JOURNAL
Advances in Mathematics: Scientific Journal **10** (2021), no.3, 1273–1284
ISSN: 1857-8365 (printed); 1857-8438 (electronic)
https://doi.org/10.37418/amsj.10.3.15

ZAGREB ALLIANCE INDICES

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ABSTRACT. Topological indices are numerical invariants associated with a graph that describes its molecular structures and provide a mathematical language to predict properties such as boiling points, viscosity, the radius of gyrations etc. In this paper, we compute the Zagreb Alliance indices of molecular graphs of Nanostar Dendrimers, PDI-cored dendrimers, Tri-hexagonal Boron Nanotube, Tri-Hexagonal boron nanotorus and Tri-Hexagonal boron α nanotorus.

1. INTRODUCTION

A defensive alliance [2] in a graph G is a subset of its vertex set satisfying the property that each vertex in it has at least as many neighbors in the alliance (including itself) than neighbors not belonging to the alliance. The minimum cardinality of a minimal defensive alliance of G is called alliance number of the graph G and it is denoted by $a(G)$. Let v be a vertex of G. Then we define the alliance number of G at v, denoted by $a_G(v)$, as the least cardinality of an alliance set of G containing the vertex v.

Topological index is the graph invariant number used for modeling the biological and chemical properties of molecules in the quantitative structure relationship studies and the quantitative structure interaction relationship studies.

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2020 *Mathematics Subject Classification.* 97K30, 05C07, 05C69.
Key words and phrases. defensive alliance set, zagreb index, defensive degree.
Submitted: 17.02.2021; *Accepted:* 04.03.2021; *Published:* 16.03.2021.

For the similar work on Topological indices we refer to [2–6]. Zagreb indices are the oldest given by Gutman and Trinajstic [1] defined as:

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

These indices are based on degree of the vertices. Now, in this expression if we replace degree of the vertex by an alliance number with respect to the vertex of G we get Zagreb alliance indices. It is defined as follows:

i) Zagreb alliance index: $A_1(G) = \sum_{uv \in E}[a_G(v) + a_G(u)]$.
ii) Second Zagreb alliance index: $A_2(G) = \sum_{uv \in E}[a_G(v) \times a_G(u)]$.
iii) First Multiplicative Zagreb alliance index= $MA_1 = \prod_{uv \in E}[a_G(v)+a_G(u)]$.
iv) Second Multiplicative Zagreb alliance index= $MA_2 = \prod_{uv \in E}[a_G(v) \times a_G(u)]$.

Remark 1.1. *If v is a pendant vertex of a graph G, then $a_G(v) = 1$.*

Remark 1.2. *For any vertex v of a graph G, $a_G(v) \geq \lceil \frac{\deg_G(v)}{2} \rceil$, where $\deg_G(v)$ is the degree of v in G.*

Theorem 1.1. *For a complete graph K_n, $A_1(K_n) = n(n-1)\lceil \frac{n}{2} \rceil$ and $A_2(K_n) = \frac{n(n-1)}{2}\lceil \frac{n}{2} \rceil^2$.*

Proof. Let S be a defensive set with respect to every vertex in K_n. For every vertices in a complete graph K_n to be defensive we need atleast $\lceil \frac{n}{2} \rceil$ vertices in S so as to satisfy $|N_G[v] \cap S| \geq |N_G[v] - S|$. Therefore $a_{K_n}(v) = \lceil \frac{n}{2} \rceil$, for all $v \in V(K_n)$. Also number of edges in $K_n = \binom{n}{2}$. Hence $A_1(K_n)$ =2× no of edges×$\lceil \frac{n}{2} \rceil = n(n-1)\lceil \frac{n}{2} \rceil$. And $A_2(K_n)$= no of edges $\times \lceil \frac{n}{2} \rceil^2 = \frac{n(n-1)}{2}\lceil \frac{n}{2} \rceil^2$. □

2. Zagreb alliance indices of Dendrimers

Dendrimers are nano-sized, radially symmetric particles with very much characterized, homogeneous, and mono disperse structure that has a normally symmetric center, an internal shell, and an external shell. An assortment of dendrimers exist, and each has natural properties, for example, polyvalency, self-amassing, electrostatic communications, compound dependability, low cytotoxicity, and solvency. These fluctuated attributes settle on dendrimers a decent decision in the clinical field, and this audit covers their different applications.

Here we discus the Zagreb alliance indices of Nanostar Dendrimers $D_1(n)$ and PDI-cored dendrimers $D_2(n)$.

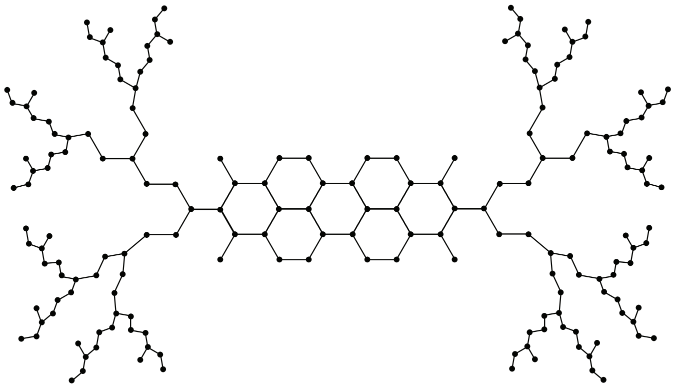


FIGURE 1. Nanostar Dendrimers $D_1(n)$ with $n = 3$

Theorem 2.1. *For the molecular graph* $D_1(n)$ *we have (i)* $A_1(D_1(n)) = 43 \cdot 2^{n+1} + 112$ *(ii)* $A_2(D_1(n)) = 4[5 \cdot 2^{n+2} + 26]$ *(iii)* $MA_1(D_1(n) = 2^{2n+14} \cdot 3^3 \cdot 11^2 \cdot (2^n + 1)(2^{n-1} + 1)$ *(iv)*$MA_2(D_1(n) = 2^{2n+11} \cdot 3 \cdot 11^2(2^n + 1)(2^{n-1} + 1)$.

Proof. In Figure 1, it is clear that $D_1(n)$ has $4(2^n + 1$ pendant vertices. By the remark 1.1, for all the pendant vertices v, $a_G(v) = 1$. Also all the vertices u having degree 2 are adjacent to the vertices of degree 2 and degree 3. Hence $a_G(u) = 2$. Further, the vertices w with degree 3 are adjacent to the vertices of degree atmost 3, so $a_G(w) = 2$. The molecular graph $D_1(n) = (V, E)$ have $|E| = 20 \cdot 2^n + 26$. The edge set E consists of edges of the form $\{e_{1,2}, e_{1,3}, e_{2,2}, e_{2,3}, e_{3,3}\}$, where $e_{i,j}$ denotes an edge joining the vertices having degree i with degree j. We denote $E_{i,j} = \{(e_{i,j})\}$. From Figure 1, $|E_{1,2}| = 4(2^n + 1)$, $|E_{1,3}| = 4(2^{n-1} + 1)$, $|E_{2,2}| = 3 \cdot 2^{n+1}$, $|E_{2,3}| = 22 \cdot 2^{n-1}$ and $|E_{3,3}| = 22$. Now, using these values we can find the following:

(i) Zagreb alliance index:

$$
\begin{aligned}
& A_1(D_1(n)) \\
&= \sum_{uv \in E} [a_G(v) + a_G(u)] \\
&= 3|E_{1,2}| + 3|E_{1,3}| + 4|E_{2,2}| + 4|E_{2,3}| + 4|E_{3,3}| \\
&= 3[4(2^n + 1)] + 3[4(2^{n-1} + 1)] + 4[3 \cdot 2^{n+1}] + 4[22 \cdot 2^{n-1}] + 4[22] \\
&= 43 \cdot 2^{n+1} + 112.
\end{aligned}
$$

(ii) Second Zagreb alliance index:

$$\begin{aligned}
&A_2(D_1(n))\\
&= \sum_{uv\in E}[a_G(v) \times a_G(u)]\\
&= 2|E_{1,2}| + 2|E_{1,3}| + 4|E_{2,2}| + 4|E_{2,3}| + 4|E_{3,3}|\\
&= 2[4(2^n+1)] + 2[4(2^{n-1}+1)] + 4[3\cdot 2^{n+1}] + 4[22\cdot 2^{n-1}] + 4[22]\\
&= 20\cdot 2^{n+2} + 104\\
&= 4[5\cdot 2^{n+2} + 26].
\end{aligned}$$

(iii) First Multiplicative Zagreb alliance index:

$$\begin{aligned}
&MA_1(D_1(n))\\
&= \prod_{uv\in E}[a_G(v) + a_G(u)]\\
&= 3|E_{1,2}| \times 3|E_{1,3}| \times 4|E_{2,2}| \times 4|E_{2,3}| \times 4|E_{3,3}|\\
&= 3[4(2^n+1)] \times 3[4(2^{n-1}+1)] \times 4[3\cdot 2^{n+1}] \times 4[22\cdot 2^{n-1}] \times 4[22]\\
&= 2^{2n+14}\cdot 3^3\cdot 11^2\cdot (2^n+1)(2^{n-1}+1).
\end{aligned}$$

(iv) Second Multiplicative Zagreb alliance index:

$$\begin{aligned}
&MA_2(D_1(n))\\
&= \prod_{uv\in E}[a_G(v) \times a_G(u)]\\
&= 2|E_{1,2}| \times 2|E_{1,3}| \times 4|E_{2,2}| \times 4|E_{2,3}| \times 4|E_{3,3}|\\
&= 2[4(2^n+1)] \times 2[4(2^{n-1}+1)] \times 4[3\cdot 2^{n+1}] \times 4[22\cdot 2^{n-1}]x4[22]\\
&= 2^{2n+11}\cdot 3\cdot 11^2(2^n+1)(2^{n-1}+1).
\end{aligned}$$

□

Let $D_2(n)$ be the second type molecular graph of the PDI-core dendrimer, where $D_2(n)$ is the generation stage of $D_2(n)$. It consists of four similar branches and a single core. The total number of edges of the molecular graph $D_2(n)$ is $136\times 2^n - 30$.

Theorem 2.2. *For a molecular graph $D_2(n)$,*

i) $A_1(D_2(n)) = 12[43\cdot 2^n - 9]$

ii) $A_2(D_2(n)) = 4[121\cdot 2^n - 24]$

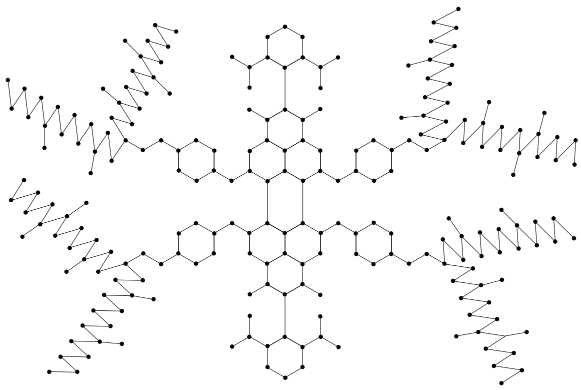


FIGURE 2. PDI-core dendrimer $D_2(n)$ with $n = 1$

iii) $MA_1(D_2(n)2^{n+16} \cdot 3^3(2^{n+1} - 1)(7 \cdot 2^n - 5)(11 \cdot 2^n - 1)(2^{n+2} + 13)$
iv) $MA_2(D_2(n) = 2^{n+18} \cdot 3(2^{n+1} - 1)(7 \cdot 2^n - 5)(11 \cdot 2^n - 1)(2^{n+2} + 13)$.

Proof. For the PDI-core dendrimes the number of edges are given by $136 \cdot 2^n - 30$. Dendrimes consists all vertices of degree atmost 3. In Figure 2, it is clear that $D_2(n)$ has $20 \cdot 2^n$ pendant vertices. By Remark 1.1, for all the pendant vertices v, $a_G(v) = 1$. Also all the vertices u having degree 2 are adjacent to the vertices of degree 2 and degree 3. Hence $a_G(u) = 2$. The molecular graph $D_1(n) = (V, E)$ have $|E| = 20 \cdot 2^n + 26$. The edge set E consists of edges of the form $\{e_{1,2}, e_{1,3}, e_{2,2}, e_{2,3}, e_{3,3}\}$, where $e_{i,j}$ denotes an edge joining the vertices having degree i with degree j. We denote $E_{i,j} = \{(e_{i,j})\}$. From Figure 2, $|E_{1,2}| = 2^{n+2}$, $|E_{1,3}| = 24 \cdot 2^n - 12$, $|E_{2,2}| = 8(7 \cdot 2^n - 5)$, $|E_{2,3}| = 4(11 \cdot 2^n - 1)$ and $|E_{3,3}| = 8 \cdot 2^n + 26$. Now, using these values we can find the following:

(i) Zagreb alliance index:

$$
\begin{aligned}
&A_1(D_2(n)) \\
&= \sum_{uv \in E} [a_G(v) + a_G(u)] \\
&= 3|E_{1,2}| + 3|E_{1,3}| + 4|E_{2,2}| + 4|E_{2,3}| + 4|E_{3,3}| \\
&= 3[2^{n+2}] + 3[24 \cdot 2^n - 12] + 4[8(7 \cdot 2^n - 5)] + 4[4(11 \cdot 2^n - 1)] + 4[8 \cdot 2^n + 26] \\
&= 12[43 \cdot 2^n - 9].
\end{aligned}
$$

(ii) Second Zagreb alliance index:

$$
\begin{aligned}
& A_2(D_2(n)) \\
&= \sum_{uv \in E} [a_G(v) \times a_G(u)] \\
&= 2|E_{1,2}| + 2|E_{1,3}| + 4|E_{2,2}| + 4|E_{2,3}| + 4|E_{3,3}| \\
&= 2[2^{n+2}] + 2[24 \cdot 2^n - 12] + 4[8(7 \cdot 2^n - 5)] + 4[4(11 \cdot 2^n - 1)] + 4[8 \cdot 2^n + 26] \\
&= 4[121 \cdot 2^n - 24].
\end{aligned}
$$

(iii) First Multiplicative Zagreb alliance index:

$$
\begin{aligned}
& MA_1(D_2(n)) \\
&= \prod_{uv \in E} [a_G(v) + a_G(u)] \\
&= 3|E_{1,2}| \times 3|E_{1,3}| \times 4|E_{2,2}| \times 4|E_{2,3}| \times 4|E_{3,3}| \\
&= 3[2^{n+2}] \times 3[24 \cdot 2^n - 12] \times 4[8(7 \cdot 2^n - 5)] \times 4[4(11 \cdot 2^n - 1)] \times 4[8 \cdot 2^n + 26] \\
&= 2^{n+16} \cdot 3^3(2^{n+1} - 1)(7 \cdot 2^n - 5)(11 \cdot 2^n - 1)(2^{n+2} + 13).
\end{aligned}
$$

(iv) Second Multiplicative Zagreb alliance index:

$$
\begin{aligned}
& MA_2(D_2(n)) \\
&= \prod_{uv \in E} [a_G(v) \times a_G(u)] \\
&= 2|E_{1,2}| \times 2|E_{1,3}| \times 4|E_{2,2}| \times 4|E_{2,3}| \times 4|E_{3,3}| \\
&= 2[2^{n+2}] \times 2[24 \cdot 2^n - 12] \times 4[8(7 \cdot 2^n - 5)] \times 4[4(11 \cdot 2^n - 1)] \times 4[8 \cdot 2^n + 26] \\
&= 2^{n+18} \cdot 3(2^{n+1} - 1)(7 \cdot 2^n - 5)(11 \cdot 2^n - 1)(2^{n+2} + 13).
\end{aligned}
$$

□

3. Zagreb indices of Boron Nanotubes

Boron nanotubes have been considered as incredible nano material due to their amazing properties like, at high temperatures it has high protection from oxidation, high synthetic strength and are a stable wide band hole semiconductor. In light of their unique properties it very well may be utilized for applications at high temperatures and furthermore in destructive conditions, for example, batteries, fast machines as strong grease, super capacitors and energy components. In this section, we find Zagreb indices of three kinds of nanotubes: (a)Tri-hexagonal Boron Nanotube $C_3C_6(H)[c;r]$ (b)Tri-Hexagonal boron nanotorus $THBC_3C_6[c;r]$ and (c)Tri-Hexagonal boron α nanotorus $THBAC_3C_6[c;r]$, where c is the number of hexagons in one column and r is the number of hexagons in one row in two-dimensional lattice of nanotube.

(a) Tri-hexagonal Boron Nanotube by $C_3C_6(H)[r;c]$

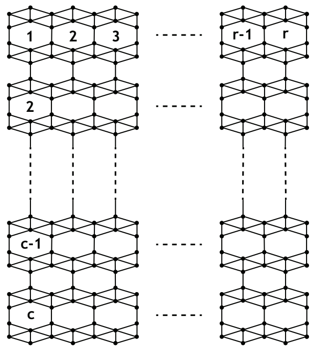


FIGURE 3. Tri-Hexagonal Boron Nanotube

Theorem 3.1. *For a Tri-hexagonal Boron Nanotube* $C_3C_6(H)[r;c]$*:*

(i) $A_1(C_3C_6(H)[r;c]) = 6r[18c-1]$
(ii) $A_2(C_3C_6(H)[r;c]) = 9r[18c-1]$
(iii) $MA_1(C_3C_6(H)[r;c])=6^6 \cdot r^4 \cdot c(2c-1)^2$
(iv) $MA_2(C_3C_6(H)[r;c]) = 3^8 \cdot 6^2 \cdot r^4 \cdot c(2c-1)^2$.

Proof. In a Tri-hexagonal Boron Nanotube $G = C_3C_6(H)[r;c]$, there are $18rc$ vertices and $r(18c-1)$ edges, refer Figure 3. We partition the vertex set in accordance to the degree of the vertices. Let u_i, v_i and w_i be the vertices having degree 3, 4 and 5 respectively. There are $2r$ vertices of the form u_i. All u_i vertices are adjacent to the vertices having degree 5. Hence for every alliance set S with respect to each u_i to be defendable must have atleast 3 cardinality. Therefore $a_G(u_i) = 3$. There are $4rc - 2r$ vertices with degree 4. All the v_i have neighbourhood consisting 3 vertices with degree 5 and one vertex of degree 4. Hence for every alliance set S with respect to each v_i to be defendable must have atleast 3 cardinality. Therefore $a_G(v_i) = 3$. Now, for the $4rc$ vertices w_i with degree 5, obviously every alliance set S with respect to each w_i to be defendable must have atleast 3 cardinality. Therefore $a_G(w_i) = 3$. We have found that for every vertex $v \in G$, $a_G(v) = 3$.

(i) Zagreb alliance index:

$$\begin{aligned} A_1(C_3C_6(H)[r;c]) &= \sum_{uv \in E(G)} [a_G(v) + a_G(u)] \\ &= (\text{number of edges}) \times [a_G(v) + a_G(u)] \\ &= r(18c-1) \times 6 \\ &= 6r(18c-1). \end{aligned}$$

(ii) Second Zagreb alliance index:

$$\begin{aligned} A_2(C_3C_6(H)[r;c]) &= \sum_{uv \in E(G)} [a_G(v) \times a_G(u)] \\ &= (\text{number of edges}) \times [a_G(v) \times a_G(u)] \\ &= r(18c-1) \times 9 \\ &= 9r(18c-1). \end{aligned}$$

(iii) First Multiplicative Zagreb alliance index:

$$\begin{aligned} MA_1(C_3C_6(H)[r;c]) &= \prod_{uv \in E} [a_G(v) + a_G(u)] \\ &= 6 \cdot 6r \times 6 \cdot r(2c-1) \times 6 \cdot 6r(2c-1) \times 6 \cdot 4rc \\ &= 6^6 \cdot r^4 \cdot c(2c-1)^2. \end{aligned}$$

(iv) Second Multiplicative Zagreb alliance index:

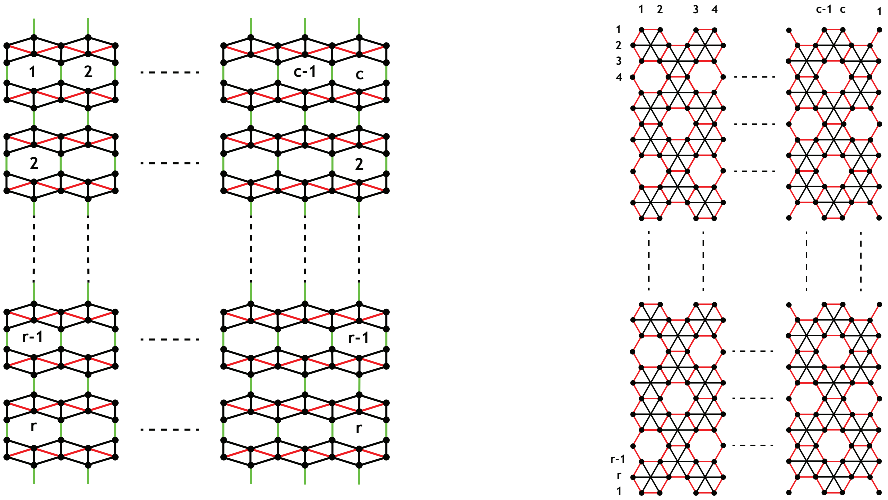
$$\begin{aligned} MA_2(C_3C_6(H)[r;c]) &= \prod_{uv \in E} [a_G(v) \times a_G(u)] \\ &= 9 \cdot 6r \times 9 \cdot r(2c-1) \times 9 \cdot 6r(2c-1) \times 9 \cdot 4rc \\ &= 3^8 \cdot 6^2 \cdot r^4 \cdot c(2c-1)^2. \end{aligned}$$

□

(b) Tri-Hexagonal boron nanotorus, $THBAC_3C_6[r;c]$

Theorem 3.2. *For a molecular graph Tri-Hexagonal boron nanotorus:*

(i) $A_1(THBC_3C_6[r;c]) = 144rc$
(ii) $A_2(THBC_3C_6[r;c]) = 288rc$
(iii) $MA_1(THBC_3C_6[r;c]) = 8^4 \cdot 12rc$



(A) Tri-Hexagonal boron nanotorus

(B) Tri-Hexagonal boron α nanotorus

FIGURE 4. Tri-Hexagonal boron nanotorus

(iv) $MA_2(THBC_3C_6[r;c]) = 16^3 \cdot 96rc$.

Proof. The total number of vertices and edges in the molecular graph Tri-Hexagonal boron nanotorus are $8rc$ and $18rc$ respectively. There are only two types of vertices one with degree 4 and other with degree 5. From Figure 4a it is observed that the vertex u with degree 4 has N(u)=4, among them 3 vertices are with degree 5 and one vertex with degree 4. Hence by Remark 1.2, $a_G(u) \geq 3$. Then S must contain the vertex with degree 5. Therefore for S to be defensive, $|S| = 4$. Hence $a_G(u) = 4$. Also, vertex v with $deg_G(v) = 5$ is adjacent to the three vertices with degree 5 and 2 vertices with degree 4. By Remark 1.2, $a_G(v) \geq 3$, so S must include a vertex with 5. Hence $a_G(v) = 4$. Since $V(THBC_3C_6[r,c])$ has only vertices of degree 4 and 5, the edge set $E(THBC_3C_6[r,c]) = E_{4,4} \cup E_{4,5} \cup E_{5,5}$, where $E_{i,j}$ is a edge joining the vertex with degree i with degree j. From Figure 4a $|E_{4,4}| = 2rc$, $|E_{4,5}| = 12rc$ and $|E_{5,5}| = 4rc$. But for all $v_i \in V(THBC_3C_6[r;c])$ is 4, we have the following:

(i) Zagreb alliance index:

$$A_1(THBC_3C_6[r;c]) = \sum_{uv \in E(G)} [a_G(v) + a_G(u)]$$
$$= \text{(number of edges)} \times [a_G(v) + a_G(u)]$$
$$= 18rc \times 8 = 144rc.$$

(ii)Second Zagreb alliance index:

$$A_2(THBC_3C_6[r;c]) = \sum_{uv\in E(G)} [a_G(v) \times a_G(u)]$$
$$= \text{(number of edges)} \times [a_G(v) \times a_G(u)]$$
$$= 18rc \times 16$$
$$= 288rc.$$

(iii) First Multiplicative Zagreb alliance index:

$$MA_1(THBC_3C_6[r;c]) = \prod_{uv\in E} [a_G(v) + a_G(u)]$$
$$= 8|E_{4,4}| \times 8|E_{4,5}| \times 8|E_{5,5}|$$
$$= 8(2rc) \times 8(12rc) \times 8(4rc) = 8^4 \cdot 12rc.$$

(iv) Second Multiplicative Zagreb alliance index:

$$MA_2(THBC_3C_6[r;c]) = \prod_{uv\in E} [a_G(v) \times a_G(u)]$$
$$= 16|E_{4,4}| \times 16|E_{4,5}| \times 16|E_{5,5}|$$
$$= 16(2rc) \times 16(12rc) \times 16(4rc) = 16^3 \cdot 96rc.$$

□

(c)Tri-Hexagonal boron α nanotorus $THBAC_3C_6[r;c]$.

Theorem 3.3. *For a molecular graph Tri-Hexagonal boron α nanotorus:*

(i) $A_1(THBAC_3C_6[r;c])$= $28rc$.
(ii) $A_2(THBAC_3C_6[r;c])$ = $72rc$.
(iii) $MA_1(THBAC_3C_6[r;c]$ = $96r^2c^2$.
(iv) $MA_2(THBAC_3C_6[r;c])$ = $384r^2c^2$.

Proof. The total number of vertices and edges in the molecular graph Tri-Hexagonal boron α nanotorus are $\frac{4rc}{3}$ and $\frac{7rc}{2}$ respectively. There are only two types of vertices one with degree 4 and other with degree 6. From Figure 4b it is observed that the vertex u with degree 5 has one neighbour with vertex degree 6 and remaining vertices with degree 5. Hence by Remark 1.2, $a_G(u) \geq 3$. But then the set S with 3 vertices will not be defensive. Since if $|S| = 3$, then S must either contain all vertices with vertex 5 among which two vertices are not adjacent and hence fails to defend themselves or S must contain the vertex of

degree 6, which will have 4 attackers. Hence $a_G(u) = 4$. Similarly, the vertex v with degree 6 is surrounded by all vertices of degree 5 and by Remark 1.2, $a_G(v) \geq 4$. The set S will be defensive as for any $x \in S$ $|N_G[x] \cap S| \geq |N_G[x] - S|$. Hence $a_G(v) = 4$. The Zagreb indices are calculated as follows:
(i) Zagreb alliance index:

$$\begin{aligned} A_1(THBAC_3C_6[r;c]) &= \sum_{uv \in E(G)} [a_G(v) + a_G(u)] \\ &= \text{(number of edges)} \times [a_G(v) + a_G(u)] \\ &= \frac{7rc}{2} \times 8 \\ &= 28rc. \end{aligned}$$

(ii)Second Zagreb alliance index:

$$\begin{aligned} A_2(THBAC_3C_6[r;c]) &= \sum_{uv \in E(G)} [a_G(v) \times a_G(u)] \\ &= \text{(number of edges)} \times [a_G(v) \times a_G(u)] \\ &= \frac{7rc}{2} \times 16 \\ &= 56rc \end{aligned}$$

(iii) First Multiplicative Zagreb alliance index:

$$\begin{aligned} MA_1(THBAC_3C_6[r;c]) &= \prod_{uv \in E} [a_G(v) + a_G(u)] \\ &= 8|E_{5,5}| \times 8|E_{5,6}| \\ &= 8(\frac{3rc}{2}) \times 8(2rc) = 96r^2c^2. \end{aligned}$$

(iv) Second Multiplicative Zagreb alliance index:

$$\begin{aligned} MA_2(THBAC_3C_6[r;c]) &= \prod_{uv \in E} [a_G(v) \times a_G(u)] \\ &= 16|E_{5,5}| \times 16|E_{5,6}| \\ &= 16(\frac{3rc}{2}) \times 16(2rc) = 384r^2c^2. \end{aligned}$$

□

ACKNOWLEDGMENT

The authors are very much thankful to Visvesvaraya Technological University and Principals of P.A. College of Engineering, Sahyadri College of Engineering and Dr. Ambedkar Institute of Technology for their constant support during the preparation of this paper. Also special thanks to the anonymous referees for their suggestions for the improvement of this paper.

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