Molecular Properties of Single-Walled Titania Nanotubes

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Abstract

In chemical graph theory, a topological index is a numerical representation of a chemical structure while a topological descriptor correlates certain physico-chemical characteristics of underlying chemical compounds besides its numerical representation. Graph theory plays an important role in modeling and designing any chemical network. A large number of properties like physico-chemical properties, thermodynamic properties, chemical activity and biological activity are determined by the chemical applications of graph theory. These properties can be characterized by certain graph invariants referred to as topological indices. In this paper, we discuss the titania nanotube $TNT_3[m,n]$, titania nanotube $TNT_6[m,n]$, and computed exact results for degree based topological indices.

Keywords: *Titania nanotube $TNT_3[m,n]$; titania nanotube $TNT_6[m,n]$; Zagreb type indices; augmented zagreb index; Balaban index; Forgotten topological index.*

1 Introduction

Graph theory is a champion among the most uncommon and unique branch of arithmetic by which the appearing of any structure is made conceivable. Starting late, it accomplishes much thought among researchers because of its broad assortment of uses in Computer science, electrical frameworks, interconnected frameworks, natural systems, and in science, et cetera. The chemical graph theory is the rapidly creating zone among researchers. It helps in understanding about the essential properties of an atomic diagram. There are an impressive measure of atomic mixes, which have collection of uses in the fields of business, business, mechanical, pharmaceutical science, consistently life and in investigate office.

The numerical encoding of chemical structure with topological indices is at present developing in significance in restorative science, pharmaceutical and bioinformatics. This approach permits the quick gathering, explanation, recovery, examination and mining of concoction structures inside expansive databases. topological records can in this manner be utilized to look for quantitative structure–activity relationships(QSAR), which are models associating synthetic structure with biological activity. At the end of the nineteenth century, there was a blast in the presentation and meaning of new topological Indices [3].

Another subject specifically Chem-informatics which is a mix of chemistry, arithmetic and data science serves to examines ($QSAR$) and ($QSPR$) associations that are utilized to foresee the bioactivity and physiochemical properties of chemical compounds. A topological index is a numerical regard that is handled scientifically from the molecular graph. It is connected with compound constitution exhibiting for relationship of substance structure with various physical, synthetic properties and natural activities [1, 2].

For a given $G = (V, E)$ diagram where V to be the vertex set and E to be the edge set of G. The degree $\xi(r)$ of r is the amount of edges of G episode with r. The length of a most restricted way in a diagram G is a separation $d(r, s)$ among r and s. A graph can be spoken by a polynomial, a numerical esteem or by network shape. There are certain sorts of topological indices principally degree based indices and distances based indices.

In 1972, Gutman and Trinajestić [4, 5] define the Zagreb indices as:

$$M_1(G) = \sum_{rs \in E(G)} (\zeta(r) + \zeta(s)) \tag{1}$$

$$M_2(G) = \sum_{uv \in E(G)} (\zeta(r) \times \zeta(s)) \tag{2}$$

In 2008, Došlić introduces the first and second Zagreb coindex as: [6]:

$$\overline{M_1} = \overline{M_1}(G) = \sum_{rs \notin E(G)} [\zeta(r) + \zeta(s)] \tag{3}$$

$$\overline{M_2} = \overline{M_2}(G) = \sum_{rs \notin E(G)} \zeta(r)\zeta(s) \tag{4}$$

In 2016, I. Gutman *et al.* [7] proves the following Theorems:

Theorem 1. *Let G be a graph with $|V(G)|$ vertices and $|E(G)|$ edges and $M_1(G)$ represent the first Zagreb index, then*

$$\overline{M_1}(G) = 2|E(G)|\Big(|V(G) - 1\Big) - M_1(G) \tag{5}$$

Theorem 2. *Let G be a graph with $|V(G)|$ vertices and $|E(G)|$ edges and $M_1(G)$, $M_2(G)$ represent the first and second Zagreb index respectively, then*

$$\overline{M_2}(G) = 2|E(G)|^2 - \frac{1}{2}M_1(G) - M_2(G) \tag{6}$$

M. Ghorbani and N. Azimi [8] define first and second multiple Zagreb indcies as:

$$PM_1(G) = \prod_{rs \in E(G)} [\zeta(r) + \zeta(s)] \tag{7}$$

$$PM_2(G) = \prod_{rs \in E(G)} [\zeta(r) \times \zeta(s)] \tag{8}$$

The properties of $PM_1(G), PM_2(G)$ indices for some chemical structures have been studied in [9]. B. Furtula and I. Gutman [10] introduced forgotten topological index (also called F-index) as:

$$F(G) = \sum_{rs \in E(G)} \left(\zeta(r)^2 + \zeta(s)^2\right) \tag{9}$$

Some latest results regarding forgotten topological index see [11, 12]

Spurred by the achievement of the ABC index, Furtula [13] *et. al.*, set forth its changed adaptation and they named it "augmented Zagreb index" and is characterized as:

$$AZI(G) = \sum_{rs \in E(G)} \left(\frac{\zeta(r) \times \zeta(s)}{\zeta(r) + \zeta(s) - 2} \right)^3 \tag{10}$$

Another topological index in view of the level of the vertex is the Balaban index [14, 15]. This index for a graph G of order n, size m is characterized as:

$$J(G) = \frac{m}{m - n + 2} \sum_{rs \in E(G)} \frac{1}{\sqrt{\zeta(r) \times \zeta(s)}} \tag{11}$$

Ranjini et al. [16] reclassified the Zagreb indices to be specific the re-imagined in the first place, second and third Zagreb indices for a graph G as;

$$ReZG_1(G) = \sum_{rs \in E(G)} \frac{\zeta(r) + \zeta(s)}{\zeta(r)\zeta(s)} \tag{12}$$

$$ReZG_2(G) = \sum_{rs \in E(G)} \frac{\zeta(r)\zeta(s)}{\zeta(r) + \zeta(s)} \tag{13}$$

$$ReZG_3(G) = \sum_{rs \in E(G)} \zeta(r)\zeta(s)(\zeta(r) + \zeta(s)) \tag{14}$$

Nowadays there is an extensive research activity on these topological indices and their variants see [17, 20, 21, 18, 19].

2 Methods

For the calculation of our outcomes, we used a methodology for combinatorial enlisting, a vertex segment procedure, an edge parcel procedure, diagram theoretical instruments, logical frameworks, a degree-tallying technique, and a degrees of neighbors system. Also, we utilized Matlab for logical estimations and affirmations. We moreover used Maple for plotting numerical outcomes.

3 Three Layered Titania Nanotube $TNT_3[m, n]$

Titania nanotubes exists in nature in two forms namely single-walled titania nanotubes ($SWTiO_2NT_s$) and multiwalled titania nanotubes ($MWTiO_2NT_s$). Our study mainly focuses on the ($SWTiO_2NT_s$) because we consider their chemical graphs to work on molecular descriptors. Anatase is one of the three mineral forms of titanium dioxide, the other two being brookite and rutile. Titania nanotubes are formed by rolling up t toichiometric two-periodic (2D) sheets cut from the energetically stable anatase surface, which contains either six ($O - Ti - O_O - Ti - O$) or three ($O - Ti - O$) layers. The 3-layer model of the anatase slab consists of three atomic layers ($O - Ti - O$), however, its structural optimization results in formation of fluorite-type slab. In Figure 1, 3-layered hexagonal and 6-layered centered rectangular titania sheets are depicted. The graph of 3-layered titania nanotube can be viewed as in Figure 2. We denote the 2-parametric chemical graph of 3-layered titania nanotube as $TNT_3[m, n]$, where m and n are number of titanium atoms in each column and row respectively see detail in [22].

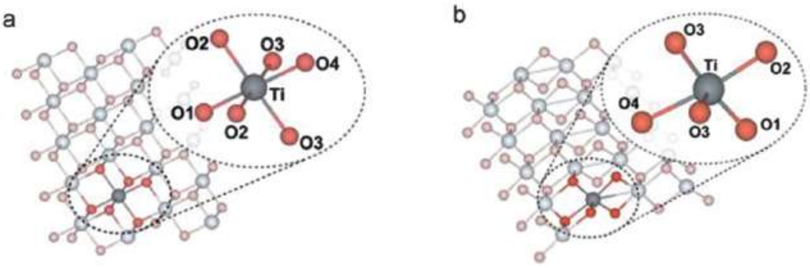


Figure 1: Two different types of coordination for Ti atoms in: (a) 3-layered hexagonal titania sheets (six-fold) and (b) 6-layered centered rectangular titania sheets (five-fold) .

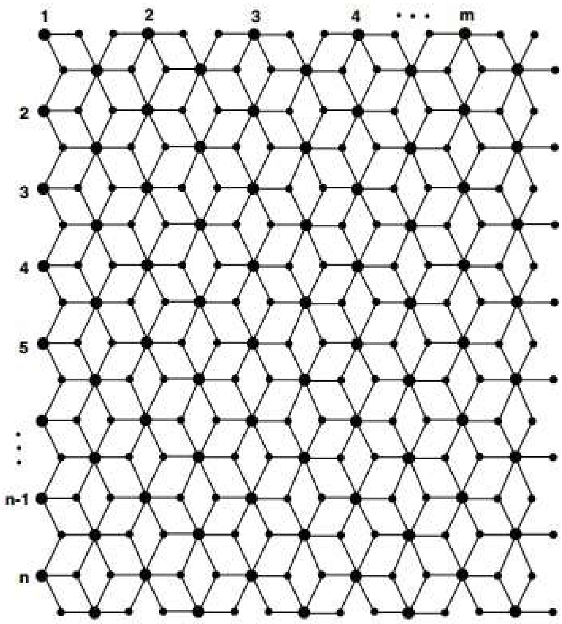


Figure 2: The graph of 3-layered titania nanotube $TNT_3[m, n]$.

3.1 Results for Three Layered Titania Nanotube $TNT_3[m, n]$

The number of vertices and edges in the three layered Titania Nanotube $TNT_3[m, n]$ are $7mn - 2m - 2n + 1$ and $12mn - 4m - 3n + 1$ respctively. To compute our main results, namely degree based topological indices for $TNT_3[m, n]$, we first make the partitions of edges based on the degree of vertices. The first edge partition contains 1 edge rs, where $\zeta(r) = 1$ and $\zeta(s) = 4$. The second edge partition contains n edges rs, where $\zeta(r) = 1$ and $\zeta(s) = 6$. The third edge partition contains 1 edge rs, where $\zeta(r) = 2$ and $\zeta(s) = 2$. The fourth edge partition contains 2 edge rs, where $\zeta(r) = 2$ and $\zeta(s) = 3$. The fifth edge partition contains $4m - 2$ edges rs, where $\zeta(r) = 2$ and $\zeta(s) = 4$. The sixth edge partition contains $4m + 2n - 6$ edges rs, where $\zeta(r) = 2$ and $\zeta(s) = 6$. The seventh edge partition contains $3n - 4$ edge rs, where $\zeta(r) = 3$ and $\zeta(s) = 3$. The eighth edge partition contains $4m - 3$ edges rs, where $\zeta(r) = 3$ and $\zeta(s) = 4$. The ninth edge partition contains $12mn - 16m - 9n + 12$ edges rs, where $\zeta(r) = 3$ and $\zeta(s) = 6$.

- **The first and second Zagreb indices of $TNT_3[m, n]$**

Using equation 1, equation 2 and the edge partition of Titania Nanotube $TNT_3[m, n]$, we computed our required result as follows:

$$
\begin{aligned}
M_1(G) &= \sum_{rs\in E(G)} (\zeta(r)+\zeta(s)) \\
M_1(TNT_3[m,n]) &= (1+4)(1)+(1+6)(n)+(2+2)(1)+(2+3)(2)+(2+4)(4m-2) \\
&+ (2+6)(4m+2n-6)+(3+3)(3n-4)+(3+4)(4m-3) \\
&+ (3+6)(12mn-16m-9n+12) \\
&= 108mn-60m-40n+22
\end{aligned}
$$

$$
\begin{aligned}
M_2(G) &= \sum_{rs\in E(G)} (\zeta(r)\times\zeta(s)) \\
M_2(TNT_3[m,n]) &= (1\times4)(1)+(1\times6)(n)+(2\times2)(1)+(2\times3)(2)+(2\times4)(4m-2) \\
&+ (2\times6)(4m+2n-6)+(3\times3)(3n-4)+(3\times4)(4m-3) \\
&+ (3\times6)(12mn-16m-9n+12) \\
&= 216mn-160m-105n+76
\end{aligned}
$$

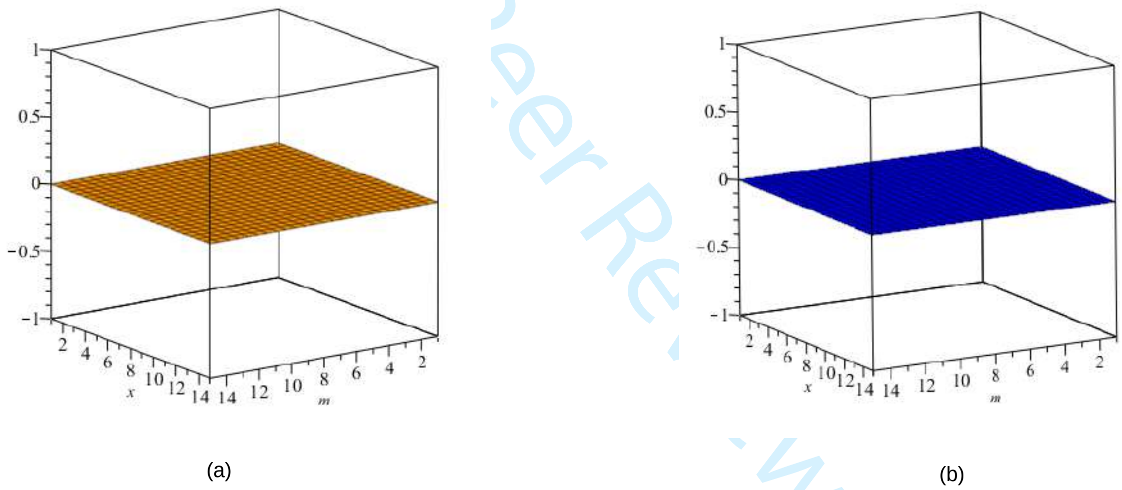


Figure 3: (a)First Zagreb index (b)Second Zagreb index.

- **The first and second Zagreb coindices of** $TNT_3[m,n]$

Now by using Equation (3) and Theorem 1 first Zagreb coindex is computed as below:

$$
\begin{aligned}
\overline{M_1}(G) &= \sum_{rs\notin E(G)} (\zeta(r)+\zeta(s)) \\
\overline{M_1}(G) &= 2|E(G)|\big(|V(G)|-1\big)-M_1(G) \\
&= 2(12mn-4m-3n+1)\big(7mn-2m-2n+1-1\big)-(108mn-60m-40n+22) \\
&= 168m^2n^2-104m^2n-90mn^2-66mn+16m^2+12n^2+56m+36n-22
\end{aligned}
$$

Now, by using Equation (4) and Theorem 2, the second Zagreb coindex is computed as:

$$\begin{aligned}\overline{M_2}(G) &= \sum_{rs\notin E(G)} (\zeta(r)\zeta(s))\\ &= 2|E(G)|^2 - \frac{1}{2}M_1(G) - M_2(G)\\ \overline{M_2}(G) &= 2(12mn-4m-3n+1)^2 - \frac{1}{2}(108mn-60m-40n+22) - (216mn-160m-105n+76)\\ &= 146m^2n^2 - 124m^2n - 78mn^2 - 58mn + 14m^2 + 16n^2 + 66m + 26n - 8\end{aligned}$$

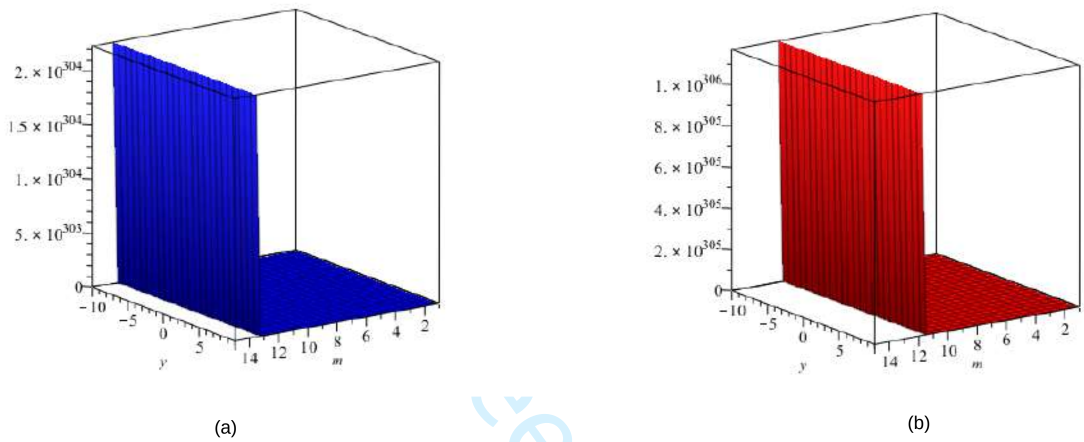


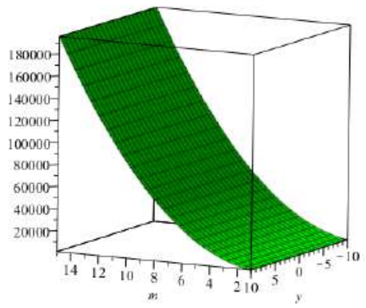
Figure 4: (a)First Zagreb coindex (b)Second Zagreb coindex.

- **Multiple Zagreb indices of $TNT_3[m,n]$**

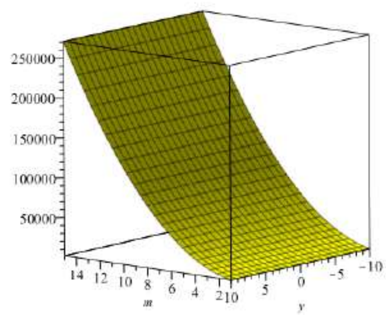
Let G be the graph of $TNT_3[m,n]$. Then, from the edge partition of $TNT_3[m,n]$, its Multiple-Zagreb indices using Equations (7), (8) are computed as:

$$\begin{aligned}PM_1(G) &= \prod_{rs\in E(G)} [\zeta(r)+\zeta(s)]\\ &= (1+4)^{(1)} \times (1+6)^{(n)} \times (2+2)^{(1)} \times (2+3)^{(2)} \times (2+4)^{(4m-2)}\\ &\times (2+6)^{(4m+2n-6)} \times (3+3)^{(3n-4)} \times (3+4)^{(4m-3)}\\ &\times (3+6)^{(12mn-16m-9n+12)}\\ &= 4\times(5)^{(3)} \times (6)^{(4m+3n-6)} \times (7)^{(4m+n-3)} \times (8)^{(4m+2n-6)} \times (9)^{(12mn-16m-9n+12)}\end{aligned}$$

$$
\begin{aligned}
PM_2(G) &= \prod_{rs \in E(G)} [\zeta(r) \times \zeta(s)] \\
&= (1 \times 4)^{(1)} \times (1 \times 6)^{(n)} \times (2 \times 2)^{(1)} \times (2 \times 3)^{(2)} \times (2 \times 4)^{(4m-2)} \\
&\times (2 \times 6)^{(4m+2n-6)} \times (3 \times 3)^{(3n-4)} \times (3 \times 4)^{(4m-3)} \\
&\times (3 \times 6)^{(12mn-16m-9n+12)} \\
&= (4)^{(2)} \times (6)^{(n+2)} \times (8)^{(4m-2)} \times (9)^{(3n-4)} \\
&\times (12)^{(8m+2n-9)} \times (18)^{(12mn-16m-9n+12)}
\end{aligned}
$$



(a)



(b)

Figure 5: (a)First Multiple Zagreb index (b)Second Multiple Zagreb index.

- **Forgotten index, Augmented Zagreb index and Balaban index of** $TNT_3[m, n]$

Let G be the graph of $TNT_3[m, n]$, the forgotten index is computed as:

$$
\begin{aligned}
F(G) &= \sum_{rs \in E(G)} \left(\zeta(r)^2 + \zeta(s)^2\right) \\
&= (1^2 + 4^2)(1) + (1^2 + 6^2)(n) + (2^2 + 2^2)(1) + (2^2 + 3^2)(2) + (2^2 + 4^2)(4m - 2) \\
&+ (2^2 + 6^2)(4m + 2n - 6) + (3^2 + 3^2)(3n - 4) + (3^2 + 4^2)(4m - 3) \\
&+ (3^2 + 6^2)(12mn - 16m - 9n + 12) \\
&= (17)(1) + (37)(n) + (8)(1) + (13)(2) + (20)(4m - 2) + (40)(4m + 2n - 6) \\
&+ (18)(3n - 4) + (25)(4m - 3) + (45)(12mn - 16m - 9n + 12) \\
&= 540mn - 380m - 234n + 164
\end{aligned}
$$

Now by using Equation (10), the augmented Zagreb index is computed as:

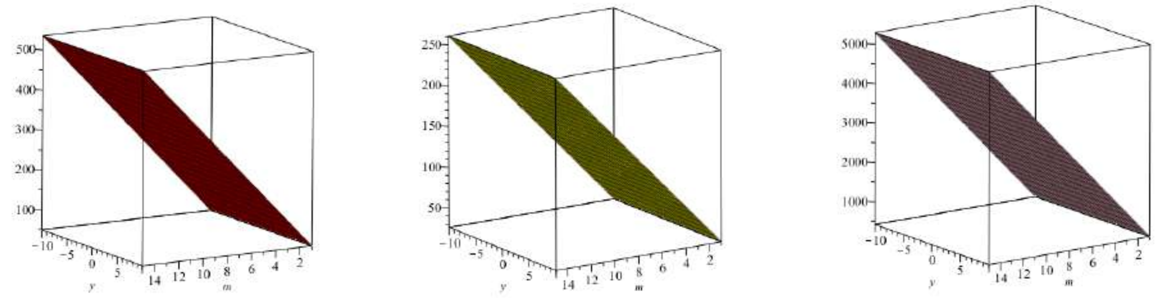
$$\begin{aligned}
AZI(G) &= \sum_{rs\in E(G)} \left(\frac{\zeta(r)\zeta(s)}{\zeta(r)+\zeta(s)-2}\right)^3 \\
&= (1)\left(\frac{1\times 4}{1+4-2}\right)^3 + (n)\left(\frac{1\times 6}{1+6-2}\right)^3 + (1)\left(\frac{2\times 2}{2+2-2}\right)^3 + (2)\left(\frac{2\times 3}{2+3-2}\right)^3 \\
&+ (4m-2)\left(\frac{2\times 4}{2+4-2}\right)^3 + (4m+2n-6)\left(\frac{2\times 6}{2+6-2}\right)^3 + (3n-4)\left(\frac{3\times 3}{3+3-2}\right)^3 \\
&+ (4m-3)\left(\frac{3\times 4}{3+4-2}\right)^3 + (12mn-16m-9n+12)\left(\frac{3\times 6}{3+6-2}\right)^3 \\
&= \left(\frac{64}{27}\right) + (n)\left(\frac{216}{125}\right) + \left(\frac{64}{8}\right) + (2)\left(\frac{216}{27}\right) + (4m-2)\left(\frac{512}{64}\right) \\
&+ (4m+2n-6)\left(\frac{1728}{216}\right) + (3n-4)\left(\frac{729}{64}\right) + (4m-3)\left(\frac{1728}{125}\right) \\
&+ (12mn-16m-9n+12)\left(\frac{5832}{343}\right) \\
&= 64m+16n-104 + \left(\frac{496}{27}\right) + \left(\frac{6912m+216n-5184}{125}\right) + \left(\frac{2187n-2916}{64}\right)
\end{aligned}$$

Now by using Equations (11), Balaban index is computed as below:

$$\begin{aligned}
J(G) &= \frac{m}{m-n+2}\sum_{rs\in E(G)} \frac{1}{\sqrt{\zeta(r)\times\zeta(s)}} \\
&= \frac{12mn-4m-3n+1}{12mn-4m-3n+1-7mn+2m+2n-1+2}\left[\frac{1}{\sqrt{1\times 4}} + \frac{n}{\sqrt{1\times 6}} + \frac{1}{\sqrt{2\times 2}} + \frac{2}{\sqrt{2\times 3}}\right] \\
&+ \frac{12mn-4m-3n+1}{12mn-4m-3n+1-7mn+2m+2n-1+2}\left[\frac{(4m-2)}{\sqrt{2\times 4}} + \frac{(4m+2n-6)}{\sqrt{2\times 6}} + \frac{3n-4}{\sqrt{3\times 3}}\right] \\
&+ \frac{12mn-4m-3n+1}{12mn-4m-3n+1-7mn+2m+2n-1+2}\left[\frac{(4m-3)}{\sqrt{3\times 4}} + \frac{(12mn-16m-9n+12)}{\sqrt{3\times 6}}\right] \\
&= \frac{12mn-4m-3n+1}{5mn-2m-n+2}\left[\frac{1}{\sqrt{4}} + \frac{n}{\sqrt{6}} + \frac{1}{\sqrt{4}} + \frac{2}{\sqrt{6}} + \frac{(4m-2)}{\sqrt{8}} + \frac{(4m+2n-6)}{\sqrt{12}}\right] \\
&+ \frac{12mn-4m-3n+1}{5mn-2m-n+2}\left[\frac{3n-4}{\sqrt{9}} + \frac{(4m-3)}{\sqrt{12}} + \frac{(12mn-16m-9n+12)}{\sqrt{18}}\right] \\
&= \frac{12mn-4m-3n+1}{5mn-2m-n+2}\left[1 + \frac{n+2}{\sqrt{6}} + \frac{(4m-2)}{\sqrt{8}} + \frac{(8m+2n-9)}{\sqrt{12}}\right] \\
&+ \frac{12mn-4m-3n+1}{5mn-2m-n+2}\left[\frac{3n-4}{\sqrt{9}} + \frac{(12mn-16m-9n+12)}{\sqrt{18}}\right]
\end{aligned}$$

- **The redefine first, second, and third Zegreb index of $TNT_3[m,n]$**

Let G be the graph of $TNT_3[m,n]$. Then by using Equation (12), the redefine first Zagreb index is



(a) (b) (c)

Figure 6: (a)Forgotten index (b)Augmented Zagreb index (c)Balaban index.

computed as:

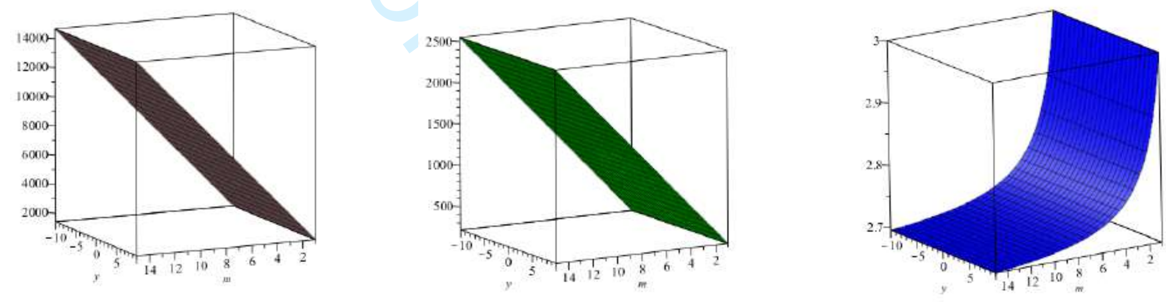
$$
\begin{aligned}
ReZG_1(G) &= \sum_{rs \in E(G)} \frac{\zeta(r)+\zeta(s)}{\zeta(r)\zeta(s)} \\
&= (1)\Big(\frac{1+4}{1\times 4}\Big) + (n)\Big(\frac{1+6}{1\times 6}\Big) + (1)\Big(\frac{2+2}{2\times 2}\Big) \\
&+ (2)\Big(\frac{2+3}{2\times 3}\Big) + (4m-2)\Big(\frac{2+4}{2\times 4}\Big) + (4m+2n-6)\Big(\frac{2+6}{2\times 6}\Big) \\
&+ (3n-4)\Big(\frac{3+3}{3\times 3}\Big) + (4m-3)\Big(\frac{3+4}{3\times 4}\Big) + (12mn-16m-9n+12)\Big(\frac{3+6}{3\times 6}\Big) \\
&= 1 + \Big(\frac{5}{4}\Big) + \Big(\frac{7n}{6}\Big) + \Big(\frac{5}{3}\Big) + (4m-2)\Big(\frac{3}{4}\Big) + (4m+2n-6)\Big(\frac{2}{3}\Big) \\
&+ (3n-4)\Big(\frac{2}{3}\Big) + (4m-3)\Big(\frac{7}{12}\Big) + (12mn-16m-9n+12)\Big(\frac{1}{2}\Big)
\end{aligned}
$$

By using Equations (13), the second redefine Zagreb index is computed as below:

$$
\begin{aligned}
ReZG_2(G) &= \sum_{rs \in E(G)} \frac{\zeta(r)\zeta(s)}{\zeta(r)+\zeta(s)} \\
&= (1)\Big(\frac{1\times 4}{1+4}\Big) + (n)\Big(\frac{1\times 6}{1+6}\Big) + (1)\Big(\frac{2\times 2}{2+2}\Big) \\
&+ (2)\Big(\frac{2\times 3}{2+3}\Big) + (4m-2)\Big(\frac{2\times 4}{2+4}\Big) + (4m+2n-6)\Big(\frac{2\times 6}{2+6}\Big) \\
&+ (3n-4)\Big(\frac{3\times 3}{3+3}\Big) + (4m-3)\Big(\frac{3\times 4}{3+4}\Big) + (12mn-16m-9n+12)\Big(\frac{3\times 6}{3+6}\Big) \\
&= 1 + \Big(\frac{4}{5}\Big) + \Big(\frac{6n}{7}\Big) + \Big(\frac{3}{5}\Big) + (4m-2)\Big(\frac{4}{5}\Big) + (4m+2n-6)\Big(\frac{3}{2}\Big) \\
&+ (3n-4)\Big(\frac{3}{2}\Big) + (4m-3)\Big(\frac{12}{7}\Big) + (12mn-16m-9n+12)(2)
\end{aligned}
$$

Now by using Equations (14), the third redefine Zagreb index is computed as:

$$\begin{aligned}
ReZG_3(G) &= \sum_{rs\in E(G)} \Big(\zeta(r)\times\zeta(s)\Big)\Big(\zeta(r)+\zeta(s)\Big)\\
&= (1)\Big[(1\times 4)(1+4)\Big]+(n)\Big[(1\times 6)(1+6)\Big]+(1)\Big[(2\times 2)(2+2)\Big]\\
&+ (2)\Big[(2\times 3)(2+3)\Big]+(4m-2)\Big[(2\times 4)(2+4)\Big]+(4m+2n-6)\Big[(2\times 6)(2+6)\Big]\\
&+ (3n-4)\Big[(3\times 3)(3+3)\Big]+(4m-3)\Big[(3\times 4)(3+4)\Big]\\
&+ (12mn-16m-9n+12)\Big[(3\times 6)(3+6)\Big]\\
&= 96+42n+48(4m-2)+96(4m+2n-6)+54(3n-4)+87(4m-3)\\
&+ 172(12mn-16m-9n+12)\\
&= 2064mn-1828m-1152n+1011
\end{aligned}$$



(a) (b) (c)

Figure 7: (a)First redefine Zagreb index (b)Second redefine Zagreb index (c)Third redefine Zagreb index.

4 Six Layered Titania Nanotube $TNT_6[m,n]$

As we have already mentioned that, titania nanotubes are formed by rolling up the stoichiometric two-periodic (2D) sheets cut from the energetically stable anatase surface, which contains either six $(O-Ti-O_O-Ti-O)$ or three $(O-Ti-O)$ layers. The 6-layer model of the anatase slab consists of three atomic layers $(O-Ti-O_O-Ti-O)$, however, its structural optimization results in formation of fluorite-type slab. The graph of 6-layered titania nanotube can be viewed as in Figure 8. We denote the 2-parametric chemical graph of 6-layered titania nanotube as $TNT_6[m,n]$, where m is defined periodically as shown in Figure 3 and n are number of titanium atoms in each row.

4.1 Results for Six Layered Titania Nanotube $TNT_6[m,n]$

The number of vertices and edges in $TNT_6[m,n]$ are $8mn-2m-2n+8$ and $20mn-4m-2n$ respectively. Now first we compute degree based topological indices for $TNT_6[m,n]$ nanotube. There are nine types of edge partitions based on the end degrees for each vertex.

The first edge partition contains 2 edges rs, where $\zeta(r) = 1$ and $\zeta(s) = 4$. The second edge partition contains $2n - 2$ edges rs, where $\zeta(r) = 1$ and $\zeta(s) = 5$. The third edge partition contains 1 edges rs, where $\zeta(r) = 2$ and $\zeta(s) = 2$. The fourth edge partition contains 2 edges rs, where $\zeta(r) = 2$ and $\zeta(s) = 3$. The fifth edge partition contains $12m - 5$ edge rs, where $\zeta(r) = 2$ and $\zeta(s) = 4$. The sixth edge partition contains $8mn - 4m - 4n + 3$ edges rs, where $\zeta(r) = 2$ and $\zeta(s) = 5$. The seventh edge partition contains $3n - 4$ edges rs, where $\zeta(r) = 3$ and $\zeta(s) = 3$. The eighth edge partition contains $4m - 1$ edge rs, where $\zeta(r) = 3$ and $\zeta(s) = 4$. The ninth edge partition contains $12mn - 16m - 3n + 4$ edges rs, where $\zeta(r) = 3$ and $\zeta(s) = 5$.

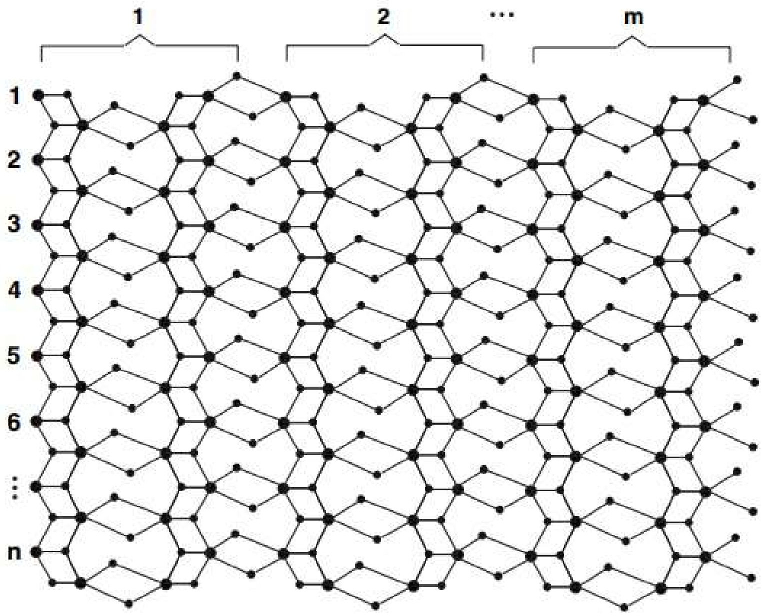


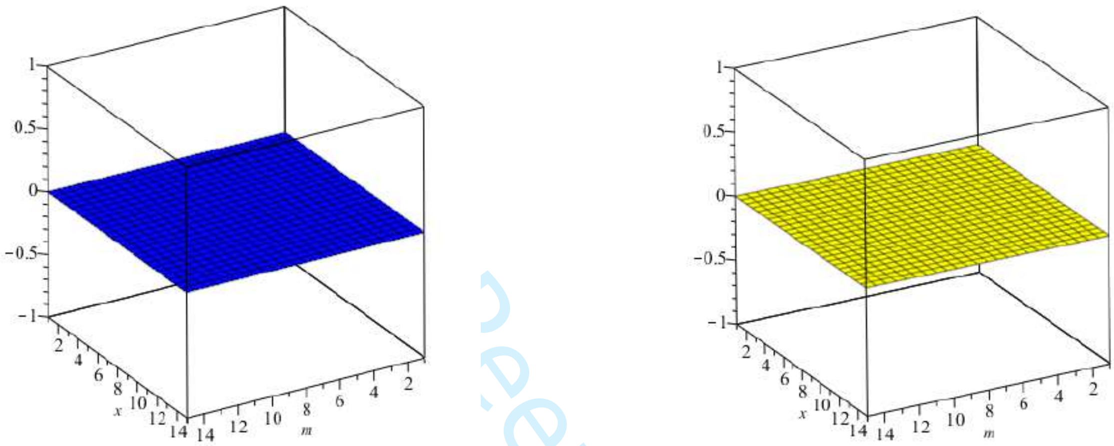
Figure 8: The graph of 6-layered titania nanotube $TNT_6[m, n]$.

- **The first and second Zagreb indices of $TNT_6[m, n]$**

Using equation 1, equation 2 and the edge portions of Titania Nanotube $TNT_6[m, n]$, we computed our required result as follows:

$$\begin{aligned}
M_1(G) &= \sum_{rs \in E(G)} (\zeta(r) + \zeta(s)) \\
M_1(TNT_6[m, n]) &= (1+4)(2) + (1+5)(2n-2) + (2+2)(1) + (2+3)(2) + (2+4)(12m-5) \\
&+ (2+5)(8mn - 4m - 4n + 3) + (3+3)(3n-4) + (3+4)(4m-1) \\
&+ (3+5)(12mn - 16m - 3n + 4) \\
&= 152mn - 56m - 22n + 4
\end{aligned}$$

$$
\begin{aligned}
M_2(G) &= \sum_{rs\in E(G)} (\zeta(r)\times\zeta(s)) \\
M_2(TNT_6[m,n]) &= (1\times4)(2)+(1\times5)(2n-2)+(2\times2)(1)+(2\times3)(2)+(2\times4)(12m-5) \\
&+ (2\times5)(8mn-4m-4n+3)+(3\times3)(3n-4)+(3\times4)(4m-1) \\
&+ (3\times5)(12mn-16m-3n+4) \\
&= 236mn-140m-125n+68
\end{aligned}
$$



(a) (b)

Figure 9: (a)First Zagreb index (b)Second Zagreb index.

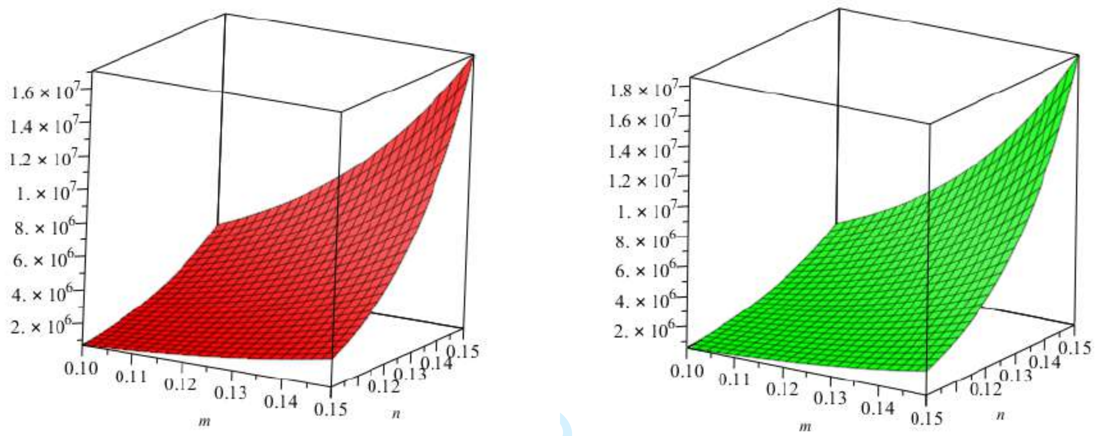
- **The first and second Zagreb coindices of $TNT_6[m,n]$**

Now by using Equations (3) and Theorem 1 first Zagreb coindex is computed as below:

$$
\begin{aligned}
\overline{M_1}(G) &= \sum_{rs\notin E(G)} (\zeta(r)+\zeta(s)) \\
\overline{M_1}(G) &= 2|E(G)|\big(|V(G)|-1\big)-M_1(G) \\
&= 2(20mn-4m-2n)\big(8mn-2m-2n+8-1\big)-(152mn-56m-22n+4) \\
&= 494m^2n^2+644m^2n+120m^2+264mn^2+164mn-66m+64n^2-20n+2
\end{aligned}
$$

Now, by using Equations (4) and Theorem 2, the second Zagreb coindex is computed as:

$$\begin{aligned}
\overline{M_2}(G) &= \sum_{rs \notin E(G)} (\zeta(r)\zeta(s)) \\
&= 2|E(G)|^2 - \frac{1}{2}M_1(G) - M_2(G) \\
\overline{M_2}(G) &= 2(20mn - 4m - 2n)^2 - \frac{1}{2}(152mn - 56m - 22n + 4) - (236mn - 140m - 125n + 68) \\
&= 448m^2n^2 + 664m^2n + 186m^2 + 242mn^2 - 42mn - 142m + 62n^2 - 32n + 8
\end{aligned}$$



(a) (b)

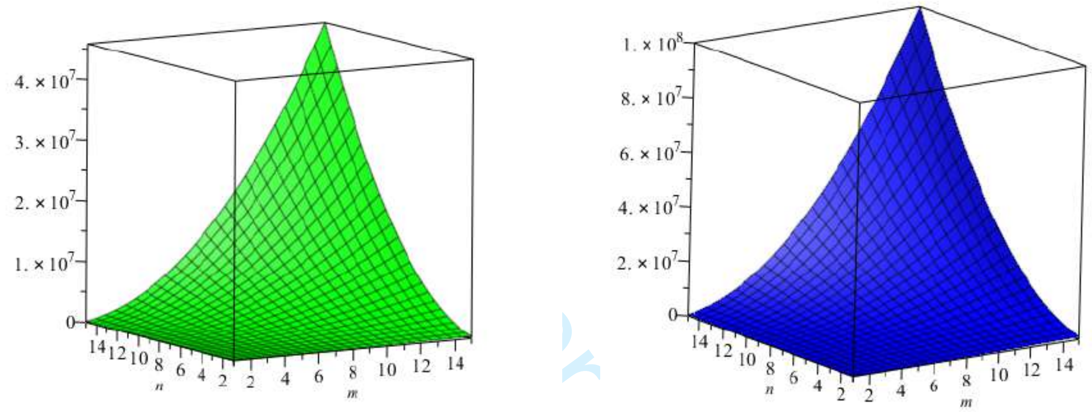
Figure 10: (a)First Zagreb coindex (b)Second Zagreb coindex.

- **Multiple Zagreb indices of $TNT_6[m, n]$**

Let G be the graph of $TNT_6[m, n]$. Then, from the edge partition of $TNT_6[m, n]$, its Multiple-Zagreb indices using Equations (7), (8) are computed as:

$$\begin{aligned}
PM_1(G) &= \prod_{rs \in E(G)} [\zeta(r) + \zeta(s)] \\
&= (1+4)^{(2)} \times (1+6)^{(2n-2)} \times (2+2)^{(1)} \times (2+3)^{(2)} \times (2+4)^{(12m-5)} \\
&\times \ (2+5)^{(8mn-4m-4n+3)} \times (3+3)^{(3n-4)} \times (3+4)^{(4m-1)} \\
&\times \ (3+5)^{(12mn-16m-3n+4)} \\
&= 4 \times (5)^{(4)} \times (6)^{(12m+3n-9)} \times (7)^{(8mn-2n)} \times (8)^{(12mn-16m-3n+4)}
\end{aligned}$$

$$
\begin{aligned}
PM_2(G) &= \prod_{rs\in E(G)} [\zeta(r)\times\zeta(s)] \\
&= (1\times 4)^{(1)} \times (1\times 5)^{(2n-2)} \times (2\times 2)^{(1)} \times (2\times 3)^{(2)} \times (2\times 4)^{(12m-5)} \\
&\times\ (2\times 5)^{(8mn-4m-4n+3)} \times (3\times 3)^{(3n-4)} \times (3\times 4)^{(4m-1)} \\
&\times\ (3\times 5)^{(12mn-16m-3n+4)} \\
&= (4)^{(2)} \times (5)^{(2n-2)} \times (6)^{(2)} \times (8)^{(12m-5)} \times (9)^{(3n-4)} \\
&\times\ (10)^{(8mn-4m-4n+3)} (12)^{(4m-1)} \times (15)^{(12mn-16m-3n+4)}
\end{aligned}
$$



(a) (b)

Figure 11: (a)First Multiple Zagreb index (b)Second Multiple Zagreb index.

- **Forgotten index, Augmented Zagreb index and Balaban index of** $TNT_6[m,n]$

Let G be the graph of $TNT_6[m,n]$. Then by using Equation (9), the forgotten index is computed as:

$$
\begin{aligned}
F(G) &= \sum_{rs\in E(G)} \left(\zeta(r)^2+\zeta(s)^2\right) \\
&= (1^2+4^2)(2)+(1^2+5^2)(2n-2)+(2^2+2^2)(1)+(2^2+3^2)(2)+(2^2+4^2)(12m-5) \\
&+\ (2^2+5^2)(8mn-4m-4n+3)+(3^2+3^2)(3n-4)+(3^2+4^2)(4m-1) \\
&+\ (3^2+5^2)(12mn-16m-3n+4) \\
&= 650mn-46m-12n+26
\end{aligned}
$$

Now by using Equation (10), the augmented Zagreb index is computed as:

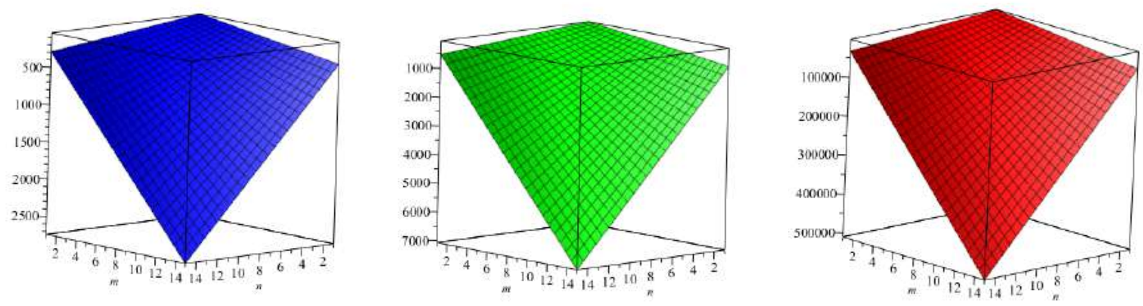
$$
\begin{aligned}
AZI(G) &= \sum_{rs\in E(G)} \left(\frac{\zeta(r)\zeta(s)}{\zeta(r)+\zeta(s)-2}\right)^3 \\
&= (1)\left(\frac{1\times 4}{1+4-2}\right)^3 + (n)\left(\frac{1\times 5}{1+5-2}\right)^3 + (1)\left(\frac{2\times 2}{2+2-2}\right)^3 + (2)\left(\frac{2\times 3}{2+3-2}\right)^3 \\
&+ (12m-5)\left(\frac{2\times 4}{2+4-2}\right)^3 + (18mn-4m-4n+3)\left(\frac{2\times 5}{2+5-2}\right)^3 + (3n-4)\left(\frac{3\times 3}{3+3-2}\right)^3 \\
&+ (4m-1)\left(\frac{3\times 4}{3+4-2}\right)^3 + (12mn-16m-3n+4)\left(\frac{3\times 5}{3+5-2}\right)^3 \\
&= \left(\frac{64}{27}\right) + (n)\left(\frac{125}{64}\right) + \left(\frac{64}{8}\right) + (2)\left(\frac{216}{27}\right) + (12m-5)\left(\frac{216}{64}\right) \\
&+ (18mn-4m-4n+3)\left(\frac{1000}{125}\right) + (3n-4)\left(\frac{729}{64}\right) + (4m-1)\left(\frac{343}{125}\right) \\
&+ (12mn-16m-3n+4)\left(\frac{3375}{216}\right) \\
&= \left(\frac{496}{27}\right) + \left(\frac{2312n+2592m+2348}{64}\right) + \\
&+ \left(\frac{1000(18mn-4m-4n+3)+343(4m-1)}{125}\right) + \left(\frac{3375(12mn-16m-3n+4)}{216}\right)
\end{aligned}
$$

Now by using Equations (11), Balaban index is computed as below:

$$
\begin{aligned}
J(G) &= \frac{m}{m-n+2} \sum_{rs\in E(G)} \frac{1}{\sqrt{\zeta(r)\times\zeta(s)}} \\
&= \frac{20mn-4m-2n}{20mn-4m-2n-8mn-2m-2n+8+2}\left[\frac{2}{\sqrt{1\times 4}} + \frac{2n-2}{\sqrt{1\times 5}} + \frac{1}{\sqrt{2\times 2}} + \frac{2}{\sqrt{2\times 3}}\right] \\
&+ \frac{20mn-4m-2n}{20mn-4m-2n-8mn-2m-2n+8+2}\left[\frac{(12m-5)}{\sqrt{2\times 4}} + \frac{(8mn-4m-4n+3)}{\sqrt{2\times 5}} + \frac{3n-4}{\sqrt{3\times 3}}\right] \\
&+ \frac{20mn-4m-2n}{20mn-4m-2n-8mn-2m-2n+8+2}\left[\frac{(4m-1)}{\sqrt{3\times 4}} + \frac{(12mn-16m-3n+4)}{\sqrt{3\times 5}}\right] \\
&= \frac{20mn-4m-2n}{12mn-6m-4n+10}\left[\frac{3}{\sqrt{2}} + \frac{2n-2}{\sqrt{5}} + \frac{2}{\sqrt{6}} + \frac{(12m-5)}{\sqrt{8}} + \frac{(8mn-4m-4n+3)}{\sqrt{10}}\right] \\
&+ \frac{20mn-4m-2n}{12mn-6m-4n+10}\left[\frac{3n-4}{\sqrt{9}} + \frac{(4m-1)}{\sqrt{12}} + \frac{(12mn-16m-3n+4)}{\sqrt{15}}\right]
\end{aligned}
$$

- **The redefine first, second, and third Zegreb index of $TNT_6[m,n]$**

Let G be the graph of $TNT_6[m,n]$. Then by using Equation (12), the redefine first Zagreb index is



(a) (b) (c)

Figure 12: (a)Forgotten index (b)Augmented Zagreb index (c)Balaban index.

computed as:

$$\begin{aligned}
ReZG_1(G) &= \sum_{rs\in E(G)} \frac{\zeta(r)+\zeta(s)}{\zeta(r)\zeta(s)} \\
&= (2)\Big(\frac{1+4}{1\times 4}\Big) + (2n-2)\Big(\frac{1+5}{1\times 5}\Big) + (1)\Big(\frac{2+2}{2\times 2}\Big) \\
&+ (2)\Big(\frac{2+3}{2\times 3}\Big) + (12m-5)\Big(\frac{2+4}{2\times 4}\Big) + (8mn-4m-4n+3)\Big(\frac{2+5}{2\times 5}\Big) \\
&+ (3n-4)\Big(\frac{3+3}{3\times 3}\Big) + (4m-1)\Big(\frac{3+4}{3\times 4}\Big) + (12mn-16m-3n+4)\Big(\frac{3+5}{3\times 5}\Big) \\
&= 1+\Big(\frac{5}{4}\Big) + \Big(\frac{6(2n-2)}{5}\Big) + \Big(\frac{5}{3}\Big) + (12m-5)\Big(\frac{3}{4}\Big) + (8mn-4m-4n+3)\Big(\frac{7}{10}\Big) \\
&+ (3n-4)\Big(\frac{2}{3}\Big) + (4m-1)\Big(\frac{7}{12}\Big) + (12mn-16m-3n+4)\Big(\frac{8}{15}\Big)
\end{aligned}$$

By using Equations (13), the second redefine Zagreb index is computed as below:

$$\begin{aligned}
ReZG_2(G) &= \sum_{rs\in E(G)} \frac{\zeta(r)\zeta(s)}{\zeta(r)+\zeta(s)} \\
&= (1)\Big(\frac{1\times 4}{1+4}\Big) + (2n-2)\Big(\frac{1\times 5}{1+5}\Big) + (1)\Big(\frac{2\times 2}{2+2}\Big) \\
&+ (2)\Big(\frac{2\times 3}{2+3}\Big) + (12m-5)\Big(\frac{2\times 4}{2+4}\Big) + (8mn-4m-4n+3)\Big(\frac{2\times 5}{2+5}\Big) \\
&+ (3n-4)\Big(\frac{3\times 3}{3+3}\Big) + (4m-1)\Big(\frac{3\times 4}{3+4}\Big) + (12mn-16m-3n+4)\Big(\frac{3\times 5}{3+5}\Big) \\
&= 1+\Big(\frac{4}{5}\Big) + \Big(\frac{5(2n-2)}{6}\Big) + \Big(\frac{12}{5}\Big) + (12m-5)\Big(\frac{4}{3}\Big) + (8mn-4m-4n+3)\Big(\frac{10}{7}\Big) \\
&+ (3n-4)\Big(\frac{3}{2}\Big) + (4m-1)\Big(\frac{12}{7}\Big) + (12mn-16m-3n+4)\Big(\frac{15}{18}\Big)
\end{aligned}$$

Now by using Equations (14), the third redefine Zagreb index is computed as:

$$\begin{aligned}
ReZG_3(G) &= \sum_{rs\in E(G)} \Big(\zeta(r)\times\zeta(s)\Big)\Big(\zeta(r)+\zeta(s)\Big) \\
&= (1)\Big[(1\times 4)(1+4)\Big] + (2n-2)\Big[(1\times 5)(1+5)\Big] + (1)\Big[(2\times 2)(2+2)\Big] \\
&+ (2)\Big[(2\times 3)(2+3)\Big] + (12m-5)\Big[(2\times 4)(2+4)\Big] \\
&+ (3n-4)\Big[(3\times 3)(3+3)\Big] + (4m-1)\Big[(3\times 4)(3+4)\Big] \\
&+ (12mn-16m-3n+4)\Big[(3\times 5)(3+5)\Big] \\
&+ (8mn-4m-4n+3)\Big[(2\times 5)(2+5)\Big] \\
&= 1868mn-1626m-1052n+1242
\end{aligned}$$

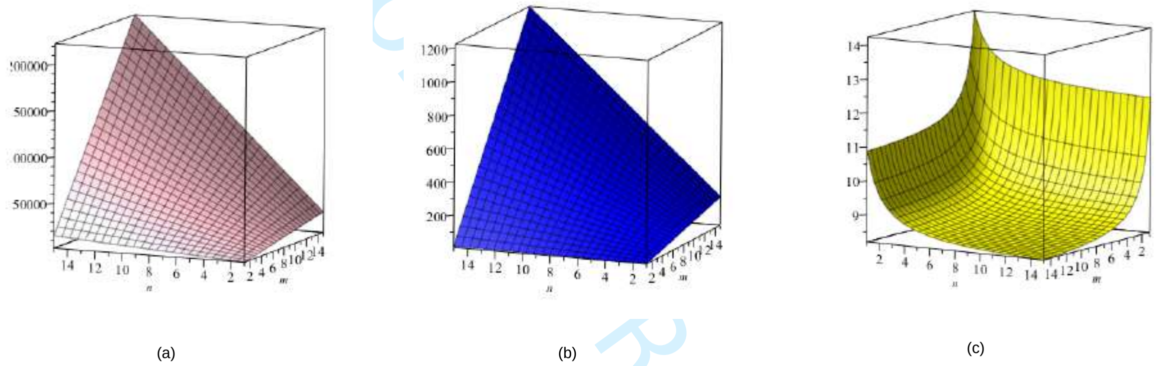


Figure 13: (a)First redefine Zagreb index (b)Second redefine Zagreb index (c)Third redefine Zagreb index.

5 Comparisons and Discussion

- For the comparison of these indices numerically for $TNT_3[m,n]$, we computed all indices for different values of m,n. Now, from Table 1, Table 2, we can easily see that all indices are in increasing order as the values of m,n are increasing. The graphical representations of the topological indices for $TNT_3[m,n]$ are depicted in Figure 3, Figure 4, Figure 5, Figure 6 and Figure 7 for certain values of m,n.

Table 1: Numerical computation of all indices for $TNT_3[m,n]$.

$[m,n]$	$M_1(G)$	$M_2(G)$	$\overline{M_1}(G)$	$\overline{M_2}(G)$	$PM_1(G)$	$PM_2(G)$
$[1,1]$	30	27	1612	2194	4.2×10^3	5.5×10^5
$[2,2]$	210	198	5276	7244	6.3×10^4	10.7×10^7
$[3,3]$	740	698	12268	12698	8.4×10^5	14.3×10^9
$[4,4]$	1420	1380	18788	22756	12.3×10^{10}	18.4×10^{15}

Table 2: Numerical computation of all indices for $TNT_3[m,n]$.

$[m,n]$	$F(G)$	$AZI(G)$	$J(G)$	$ReZ_1(G)$	$ReZ_2(G)$	$ReZ_3(G)$
[1,1]	1214	232.4	32.2	50	26.3	720
[2,2]	2454	479.8	54.2	84.5	43.6	1068
[3,3]	4306	646.6	82.5	119.3	59.5	1416
[4,4]	5246	813.5	104.7	154	76.5	1764

- For the comparison of these indices numerically for $TNT_6[m,n]$, we computed all indices for different values of m, n. Now, from Table 3, Table 4, we can easily see that all indices are in increasing order as the values of m, n are increasing. The graphical representations of the topological indices for $TNT_6[m,n]$ are depicted in Figure 9, Figure 10, Figure 11, Figure 12 and Figure 13, for certain values of m, n.

Table 3: Numerical computation of all indices for $TNT_6[m,n]$.

$[m,n]$	$M_1(G)$	$M_2(G)$	$\overline{M_1(G)}$	$\overline{M_2(G)}$	$PM_1(G)$	$PM_2(G)$
[1,1]	78	39	1612	2194	6.3×10^6	6.5×10^7
[2,2]	186	166	6412	6354	7.3×10^9	12.7×10^{11}
[3,3]	426	542	16258	12878	11.5×10^{12}	17.4×10^{15}
[4,4]	864	924	22758	41766	18.2×10^{16}	22.5×10^{19}

Table 4: Numerical computation of all indices for $TNT_6[m,n]$.

$[m,n]$	$F(G)$	$AZI(G)$	$J(G)$	$ReZ_1(G)$	$ReZ_2(G)$	$ReZ_3(G)$
[1,1]	1084	324.6	15.3	30	34.3	2808
[2,2]	4480	468.5	17.5	80	53.3	10080
[3,3]	9176	666.8	19.6	152	79.2	21600
[4,4]	14372	987.5	25.8	246	96.7	37368

- The Zagreb types indices and polynomials were found to occur for the computation of the total π-electron energy of molecules [24]; thus, the total π-electron energy in increasing order in the case of $TNT_3[m,n]$, and $TNT_6[m,n]$, for higher values of m, n.
  The forgotten topological index is helpful for testing the substance and pharmacological properties of drug nuclear structures. So in the case of bismuth tri-iodides $TNT_3[m,n]$, and $TNT_6[m,n]$, its increasing value is useful for quick action during chemical reaction for drugs.
  The augmented Zagreb index displays a good correlation with the formation heat of heptanes and octane. So our computation for AZI index is play an important rule for formation heat of heptanes and octane as its values are in increasing order.

6 Conclusion

In this paper, we have studied and computed some degree based topological indices for the $TNT_3[m,n]$, and $TNT_6[m,n]$. The exact results have been computed of first and second zegreb coindices, Multiple Zagreb indices, forgotten index, the augmented Zagreb index, Balaban index, redefine first, second and third zegrab indices, of $TNT_3[m,n]$, and $TNT_6[m,n]$ are computed. As these result are help in chemical point of you as well as pharmaceutical science. We are looking forward in future to compute other topological indices for $TNT_3[m,n]$, and $TNT_6[m,n]$.

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