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Computation of Eccentricity based Topological Properties of a Carbon Nanotube

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Abstract Chemical graph theory is prominent research area in mathematical chemistry, due to its extensive applications especially in quantitative structure-activity relationships (QSARs) where eccentricity based topological invariants are used for the mathematical modeling of biological activities of molecules, identifying structurally similar molecules and used to study the structure and properties of materials, such as polymers and ceramics. Carbon nanotubes (CNTs) are cylindrical structures made up of carbon atoms that are arranged in a unique hexagonal pattern. In this research, we examine the NA_m^n nanotube after considering it in the form of chemical graph and compute eccentricity based topological invariants like eccentric-connectivity index with total-eccentricity index with some versions of the zagreb indices.

Index Terms eccentric-connectivity index, total-eccentricity index, eccentricity based Zagreb indices, nanotube

I. Introduction

Mathematical chemistry is a field of study that involves the application of mathematical models, methods, and algorithms to describe and understand chemical phenomena. It combines mathematical principles with chemistry to develop theories, models, and computational tools to analyze chemical systems and predict their behavior. Chemical graph theory is a subfield of mathematical chemistry that studies the mathematical properties of molecular structures represented as graphs. In chemical graph theory, a molecule is represented as a graph, where atoms are represented as nodes, and bonds between atoms are represented as edges. Chemical graph theory gives numerous essential methods for the evaluation of chemical structures. For chemical compounds the prediction of the biological activities and properties the QSAR and QSPR relationships are applicable significantly. In chemical graph theory some mathematical and computational methods are utilized at atomic level for evaluation of the chemical structures [1], [2]. Chemical graph theory has applications in various fields, such as drug discovery, materials science, and catalysis. It is an essential tool for understanding and designing new molecules and materials, as well as for predicting their properties and behavior.

A graph $G = (V, E)$ contains V as a set of vertices and E as a set of edges, where G is undirected graph without multiple edges and loops. The vertices adjacent with u is its degree denoted by $d(u)$. A walk in G is a sequence of adjacent vertices where a walk without vertex repetition is called a path. Distance is a shortest path between the pair of vertices denoted by $d(u, v)$ [3]. Eccentricity is the distance between u and a vertex that is farthest from u denoted by $\varepsilon(u)$ [3]–[5].

The representation of a graph by a matrix, polynomial, sequence or a numerical quantity has essential features in graph theory. The numerical value of a graph which identify its topology called topological index or graph invariant. A number is called a topological index of a graph G denoted by $Top(G)$ with the property for two isomorphic graphs H and G, we have $Top(H) = Top(G)$. Topological indices in organic chemistry are very helpful for the structure activity relationships, structure property relationships, isomer discrimination, chemical documentation and pharmaceutical drug design. There are several degree-based, distance and eccentricity based graph invariants. Especially eccentricity based topological invariants are useful for the mathematical modeling of several biological activities of molecules of diverse nature. Eccentricity based topological invariants have been shown to be effective in identifying structurally similar molecules, which can be useful in drug design and discovery. Also Eccentricity-based topological indices have been used to study the structure and properties of materials, such as polymers and ceramics. These indices can provide insight into the bonding and electronic properties of these materials, which can be useful in designing new materials with specific properties. [6], [7].

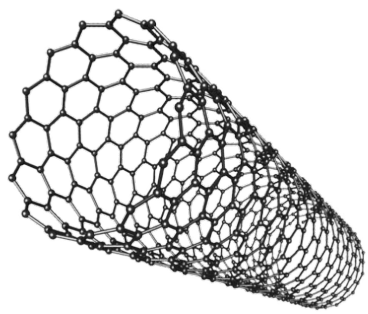

Figure 1: A carbon nanotube.

Concept of topological indices started from Wiener index, which is half sum of the distances divided by 2 between all pairs of vertices [8], given by,

$$W(G) = \frac{1}{2}\sum_{(u,v)} d(u,v). \tag{1}$$

Eccentric connectivity index is a distance-based topological index was presented by Sharma, Goswami, and Madan [9], [10]. As compared to Wiener index, eccentric connectivity index shows greater order predictability and high discriminating power from structure property and structure activity [11]. The mathematical expression is,

$$\xi(G) = \sum_{u\in V(G)} [d(u)\epsilon(u)]. \tag{2}$$

Total-eccentricity index is obtained when the vertex degree is not considered [12]–[14]. The mathematical expression is,

$$\varsigma(G) = \sum_{u\in V(G)} [\epsilon(u)]. \tag{3}$$

Zagreb indices with their variants are very useful in the studies of QSPR and QSAR. Vukičeivc and Graovac presented Zagreb eccentricity indices [15]. Also Modjtaba Ghorbani, Mohammad A. Hosseinzadeh stated the new version of Zagreb indices [16], [17]. The first, second and third zagreb eccentricity indices are described as [18]–[20],

$$M_1^*(G) = \sum_{uv\in E(G)} [\epsilon(u)+\epsilon(v)], \tag{4}$$

$$M_1^{**}(G) = \sum_{v\in V(G)} [\epsilon(v)]^2, \tag{5}$$

$$M_2^*(G) = \sum_{uv\in E(G)} [\epsilon(u)\epsilon(v)]. \tag{6}$$

For more detailed study on eccentricity based topological indices see [21].

Carbon nanotubes (CNTs) are cylindrical structures made up of carbon atoms that are arranged in a unique hexagonal pattern shown in Fig.1. They are a type of nanomaterial with remarkable mechanical, electrical, and thermal properties, which make them attractive for a wide range of applications, including electronics, energy storage, and materials science. In this research we consider a carbon nanotube in the form of a sheet.

Let the quadrilateral section P_m^n with dimensions $m \times n$. We have $n \geq 2$ hexagons on lateral side with $m \geq 2$ hexagons on upper and lower sides. In Figure.2 the hexagonal lattice L is shown. Consider the vertices u_0^j and u_m^j by identifying two lateral sides of P_m^n by taking $j = \{0,1,2,...,n\}$, we acquire NA_m^n.

In our research, let NA_m^n in replacement of P_m^n with $n = m$, we compute eccentric connectivity index with total-eccentricity index and some Zagreb eccentricity indices for various cases.

II. Main Results

In this section we discuss our main results.

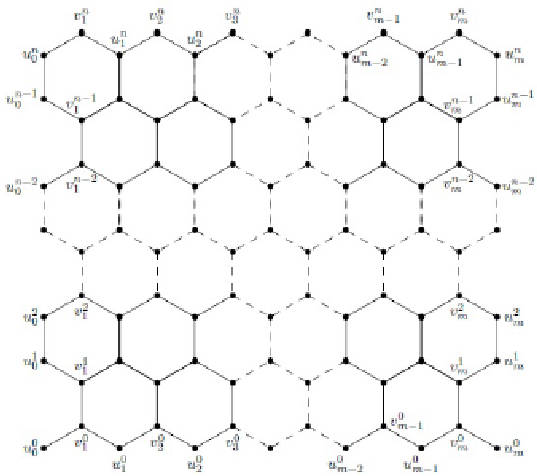

Figure 2: NA_m^n nanotube with vertices labelling

A. Eccentric connectivity index of NA_m^n nanotube

Theorem 1. *Let $G \cong NA_m^n$ with $n \equiv 0(mod2)$. The eccentric-connectivity index is,*

$$\xi(G) = 10n + \sum_{m=1}^{\frac{n}{2},n>2}(6nt-2mt) + \sum_{m=\frac{n}{2}}^{n,n>2}(4nt+2mt) + \sum_{m=0}\left[\sum_{k=2}^{n-2,n>2}(6nt-2mt-2kt-12n+4m+4k)\right] + \sum_{m=1}^{\frac{n}{2}}\left[\sum_{k\equiv 0(mod2)}^{n}(\tfrac{9}{2}nt^2-\tfrac{3}{2}mt^2-\tfrac{3}{2}kt^2-\tfrac{9}{2}nt+\tfrac{3}{2}mt+\tfrac{3}{2}kt)\right] + \sum_{m=\frac{n}{2}}^{n}\left[\sum_{k\equiv 0(mod2)}^{n}(3nt^2+\tfrac{3}{2}mt^2-\tfrac{3}{2}kt^2-2nt-\tfrac{3}{2}mt+\tfrac{3}{2}kt)\right] + \sum_{m=0}^{\frac{n}{2}}\left[\sum_{k\equiv 1(mod2)}^{n-1}(\tfrac{9}{2}nt^2-\tfrac{3}{2}mt^2-\tfrac{3}{2}kt^2+9nt-3mt-3kt)\right] + \sum_{m=\frac{n}{2}}^{n-1}\left[\sum_{k\equiv 1(mod2)}^{n-1}(3nt^2+\tfrac{3}{2}mt^2-\tfrac{3}{2}kt^2-6nt-3mt-3kt)\right] + \sum_{m\equiv 0(mod2)}\left[\sum_{k\equiv 1(mod2)}^{n-1}(4nt+2mt-2kt)\right] + 46.$$

Proof. Let $G \cong NA_m^n$. From Eq. (2), we have,

$$\xi(G) = \sum_{u\in V(G)}[d(u)\epsilon(u)].$$

By utilizing Table 1 in Eq. (2), we get,

$$\xi(G) = 1\times 2\times 3n+2\times 2\times 5+2\times t\times \sum_{m=1,t\neq 2}^{\frac{n}{2},n>2}(3n-m)+2\times 2\times 6+2\times t\times \sum_{m=\frac{n}{2},t\neq 2}^{n,n>2}(2n+m)+2\times(t-2)\times \sum_{m=0}\sum_{k\equiv 0(mod2)}^{n-2,n>2}(3n-m-k)+3\times \tfrac{t^2-t}{2}\times \sum_{m=1}^{\frac{n}{2}}\sum_{k\equiv 0(mod2)}^{n}(3n-m-k)+3\times\tfrac{t^2-t}{2}\times\sum_{m=\frac{n}{2}}^{n}\sum_{k\equiv 0(mod2)}^{n}(2n+m-k)+2\times 1\times(2n+1)+(3)\times(\tfrac{t^2+2t}{2}\times \sum_{m=0}^{\frac{n}{2}}\sum_{k\equiv 1(mod2)}^{n-1}(3n-m-k))+3\times\tfrac{t^2-2t}{2}\times\sum_{m=\frac{n}{2}}^{n-1}\sum_{k\equiv 1(mod2)}^{n-1}(2n+m-k)+2\times t\times\sum_{m\equiv 0(mod2)}\sum_{k\equiv 1(mod2)}^{n-1}(2n+m-k).$$

After simplification, we get

$$\xi(G) = 10n + \sum_{m=1}^{\frac{n}{2},n>2}(6nt-2mt) + \sum_{m=\frac{n}{2}}^{n,n>2}(4nt+2mt) + \sum_{m=0}[\sum_{k=2}^{n-2,n>2}(6nt-2mt-2kt-12n+4m+4k)] +$$

$\sum_{m=1}^{\frac{n}{2}}[\sum_{k\equiv 0(mod2)}^{n}(\frac{9}{2}nt^2-\frac{3}{2}mt^2-\frac{3}{2}kt^2-\frac{9}{2}nt+\frac{3}{2}mt+\frac{3}{2}kt)]+\sum_{m=\frac{n}{2}}^{n}[\sum_{k\equiv 0(mod2)}^{n}(3nt^2+\frac{3}{2}mt^2-\frac{3}{2}kt^2-2nt-\frac{3}{2}mt+\frac{3}{2}kt)]+$
$\sum_{m=0}^{\frac{n}{2}}[\sum_{k\equiv 1(mod2)}^{n-1}(\frac{9}{2}nt^2-\frac{3}{2}mt^2-\frac{3}{2}kt^2+9nt-3mt-3kt)]+\sum_{m=\frac{n}{2}}^{n-1}[\sum_{k\equiv 1(mod2)}^{n-1}3nt^2+\frac{3}{2}mt^2-\frac{3}{2}kt^2-6nt-3mt-3kt)]+$
$\sum_{m\equiv 0(mod2)}[\sum_{k\equiv 1(mod2)}^{n-1}(4nt+2mt-2kt)]+46.$ □

Theorem 2. *Let $G\cong NA_m^n$ with $n\equiv 1(mod2)$. The eccentric-connectivity index is,*

$$\xi(G)=12n+\sum_{m=1}^{\frac{n-1}{2}}(6nt-2mt-6n+2m)+\sum_{m=\frac{n+1}{2}}^{n-1}(4nt+2mt-4n-2m)+\sum_{m=0}[\sum_{k\equiv 0(mod2)}^{n-1}(6nt-2mt-2kt-6n+2m+2k)]+\sum_{m=n}[\sum_{k\equiv 0(mod2)}^{n-1}(4nt+2mt-2kt-4n-2m+2k)]+\sum_{m=1}^{\frac{n-1}{2}}[\sum_{k\equiv 0(mod2)}^{n-1}(\frac{9}{2}nt^2-\frac{3}{2}mt^2-\frac{3}{2}kt^2-9nt+3mt+3kt+\frac{9}{2}n-\frac{3}{2}m-\frac{3}{2}k)]+\sum_{m=\frac{n+1}{2}}^{n-1}[\sum_{k\equiv 0(mod2)}^{n-1}(3nt^2+\frac{3}{2}mt^2-\frac{3}{2}kt^2-6nt-3mt+3kt+3n+\frac{3}{2}m-\frac{3}{2}k)]+\sum_{m=0}^{\frac{n-1}{2}}[\sum_{k\equiv 1(mod2)}^{n}(\frac{9}{2}nt^2-\frac{3}{2}mt^2-\frac{3}{2}kt^2+\frac{9}{2}nt-\frac{3}{2}mt-\frac{3}{2}kt)]+\sum_{m=\frac{n+1}{n}}^{n}[\sum_{k\equiv 1(mod2)}^{n}(3nt^2+\frac{3}{2}mt^2-\frac{3}{2}kt^2+3nt+\frac{3}{2}mt-\frac{3}{2}kt)].$$

Proof. Let $G\cong NA_m^n$. From Eq. (2), we have,

$$\xi(G)=\sum_{u\in V(G)}[d(u)\epsilon(u)].$$

By utilizing Table 2 in Eq. (2), we get,

$$\xi(G)=1\times 4\times 3n+2\times\frac{2t-2}{2}\times\sum_{m=1}^{\frac{n-1}{2}}(3n-m)+\frac{2t-2}{2}\times 2\times\sum_{m=\frac{n+1}{2}}^{n-1}(2n+m)+(t-1)\times 2\times\sum_{m=0}[\sum_{k\equiv 0(mod2)}^{n-1}(3n-m-k)]+(t-1)\times 2\times\sum_{m=n}[\sum_{k\equiv 0(mod2)}^{n-1}(2n+m-k)]+3\times\frac{t^2-2t+1}{2}\times\sum_{m=1}^{\frac{n-1}{2}}[\sum_{k\equiv 0(mod2)}^{n-1}(3n-m-k)]+3\times\frac{t^2-2t+1}{2}\times\sum_{m=\frac{n+1}{2}}^{n-1}[\sum_{k\equiv 0(mod2)}^{n-1}(2n+m-k)]+3\times\frac{t^2+t}{2}\times\sum_{m=0}^{\frac{n-1}{2}}[\sum_{k\equiv 1(mod2)}^{n}(3n-m-k)]+3\times\frac{t^2+t}{2}\times\sum_{m=\frac{n+1}{2}}^{n}[\sum_{k\equiv 1(mod2)}^{n}(2n+m-k)].$$

After simplification, we get,

$$\xi(G)=12n+\sum_{m=1}^{\frac{n-1}{2}}(6nt-2mt-6n+2m)+\sum_{m=\frac{n+1}{2}}^{n-1}(4nt+2mt-4n-2m)+\sum_{m=0}[\sum_{k\equiv 0(mod2)}^{n-1}(6nt-2mt-2kt-6n+2m+2k)]+\sum_{m=n}[\sum_{k\equiv 0(mod2)}^{n-1}(4nt+2mt-2kt-4n-2m+2k)]+\sum_{m=1}^{\frac{n-1}{2}}[\sum_{k\equiv 0(mod2)}^{n-1}(\frac{9}{2}nt^2-\frac{3}{2}mt^2-\frac{3}{2}kt^2-9nt+3mt+3kt+\frac{9}{2}n-\frac{3}{2}m-\frac{3}{2}k)]+\sum_{m=\frac{n+1}{2}}^{n-1}[\sum_{k\equiv 0(mod2)}^{n-1}(3nt^2+\frac{3}{2}mt^2-\frac{3}{2}kt^2-6nt-3mt+3kt+3n+\frac{3}{2}m-\frac{3}{2}k)]+\sum_{m=0}^{\frac{n-1}{2}}[\sum_{k\equiv 1(mod2)}^{n}(\frac{9}{2}nt^2-\frac{3}{2}mt^2-\frac{3}{2}kt^2+\frac{9}{2}nt-\frac{3}{2}mt-\frac{3}{2}kt)]+\sum_{m=\frac{n+1}{n}}^{n}[\sum_{k\equiv 1(mod2)}^{n}(3nt^2+\frac{3}{2}mt^2-\frac{3}{2}kt^2+3nt+\frac{3}{2}mt-\frac{3}{2}kt)].$$ □

B. Total-eccentricity index of NA_m^n nanotube

Theorem 3. *Let $G\cong NA_m^n$ with $n\equiv 0(mod2)$, then total-eccentricity index is,*

Representatives	Degree	Eccentricity	Range	Frequency
$\{u_i^m, u_{n-i}^m\}$	3	$(3n-m-k)$	$(1 \leq m \leq \frac{n}{2})$, $(1 \leq i \leq \frac{n}{2})\ \forall\, m$, $(2 \leq k \leq n)$ k is even. $\forall\, m$.	$\frac{t^2-t}{2}$, t is even.
$\{u_i^m, u_{n-i}^m\}$	2	$(2n+m)$	$\{m=2, n=2\}$, $(\frac{n}{2} \leq m \leq n), n>2$, $\{i=0\}$.	t, t is even. $t \neq 2$.
$\{u_i^m, u_{n-i}^m\}$	3	$(2n+m-k)$	$(\frac{n}{2} \leq m \leq n)$ $(1 \leq i \leq \frac{n}{2})\ \forall\, m$, $(2 \leq k \leq n)$, k is even. $\forall$ m.	$\frac{t^2-t}{2}$, t is even.
$\{u_{\frac{n}{2}}^0\}$	2	$(2n+1)$	$\{m=0, n \equiv 0(mod2)\}$	1
$\{v_i^m, v_{n-i+1}^m\}$	3	$(3n-m-k)$	$(0 \leq m \leq \frac{n}{2})$, $(1 \leq i \leq \frac{n}{2})\ \forall\, m$, $(1 \leq k \leq n-1)$, k is even. $\forall$ m.	$\frac{t^2+2t}{2}$, t is even.
$\{u_i^m, u_{n-i}^m\}$	1	$(3n)$	$\{i=0$, $m=0\}$.	2
$\{u_i^0, u_{n-i}^0\}$	2	$(3n-m-k)$	$\{m=0\}$, $(2 \leq k \leq n-2, n \neq 2)$ k is even. $(1 \leq i \leq \frac{n}{2}-1, n \neq 2)$.	$t-2$, t is even.
$\{v_i^m, v_{n-i+1}^m\}$	3	$(2n+m-k)$	$(\frac{n}{2} \leq m \leq n-1)$, $(1 \leq i \leq \frac{n}{2})\ \forall\, m$, $(1 \leq k \leq n-1)$, k is odd. $\forall\, m$.	$\frac{t^2-2t}{2}$, t is even.
$\{u_i^m, u_{n-i}^m\}$	2	$(3n-m)$	$\{m=1\}, \{n=2\}$, $(1 \leq m \leq \frac{n}{2})\ \{n>2\}$, $\{i=0\}$.	t, t is even. $t \neq 2$.
$\{v_i^m, v_{n-i+1}^m\}$	2	$(2n+m-k)$	$\{m=n \equiv 0(mod2)\}$ $(1 \leq i \leq \frac{n}{2})\ \forall\, m$, $(1 \leq k \leq n-1)$, k is odd. $\forall\, m$.	t, t is even.

Table 1: Vertices eccentricity according to degree of vertices when $n \equiv 0(mod2)$

$$\varsigma(G) = 8n + \sum_{m=1}^{\frac{n}{2}, n>2}(3nt-mt) + \sum_{m=\frac{n}{2}}^{n, n>2}(2nt+mt) + \sum_{m=0}[\sum_{k\equiv 0(mod2)}^{n-2}(3nt-mt-kt-6n+2m+2k)] + \sum_{m=1}^{\frac{n}{2}}[\sum_{k\equiv 0(mod2)}^{n}(\tfrac{3}{2}nt^2 - \tfrac{1}{2}mt^2 - \tfrac{1}{2}kt^2 - \tfrac{3}{2}nt + \tfrac{1}{2}mt + \tfrac{1}{2}mk)] + \sum_{m=\frac{n}{2}}^{n}[\sum_{k\equiv 0(mod2)}^{n}(nt^2 + \tfrac{1}{2}mt^2 - \tfrac{1}{2}kt^2 - nt - \tfrac{1}{2}mt + \tfrac{1}{2}kt)] + \sum_{m=0}^{\frac{n}{2}}[\sum_{k\equiv 1(mod2)}^{n-1}(\tfrac{3}{2}nt^2 - \tfrac{1}{2}mt^2 - \tfrac{1}{2}kt^2 + 3nt - mt - kt)] + \sum_{m=\frac{n}{2}}^{n-1}[\sum_{k\equiv 1(mod2)}^{n-1}(nt^2 + \tfrac{1}{2}mt^2 - \tfrac{1}{2}kt^2 - 2nt - mt + kt)] + \sum_{m\equiv 0(mod2)}[\sum_{k\equiv 1(mod2)}^{n-1}(2nt + mt - kt)] + 23.$$

Proof. Let $G \cong NA_m^n$. Then from Eq. (3), we have,

$$\varsigma(G) = \sum_{u \in V(G)} \epsilon(u).$$

By utilizing Table 1 into Eq. (2), we get,

$$\varsigma(G) = 2 \times 3n + 2 \times 5 + t \times \sum_{m=1}^{\frac{n}{2}, n>2}(3n-m) + 6 \times 2 + t \times \sum_{m=\frac{n}{2}}^{n, n>2}(2n+m) + (t-2) \times \sum_{m=0}[\sum_{k\equiv 0(mod2)}^{n-2}(3n-m-k)] + \frac{t^2-t}{2} \times (\sum_{m=1}^{\frac{n}{2}}[\sum_{k\equiv 0(mod2)}^{n}(3n-m-k)]) + \frac{t^2-t}{2} \times \sum_{m=\frac{n}{2}}^{n}[\sum_{k\equiv 0(mod2)}^{n}(2n+m-k)] + 2n \times 1 + 1 + \frac{t^2+2t}{2} \times \sum_{m=0}^{\frac{n}{2}}[\sum_{k\equiv 1(mod2)}^{n-1}(3n - m - k)] + \frac{t^2-2t}{2} \times \sum_{m=\frac{n}{2}}^{n-1}[\sum_{k\equiv 1(mod2)}^{n-1}(2n+m-k)] + t \times \sum_{m\equiv 0(mod2)}[\sum_{k\equiv 1(mod2)}^{n-1}(2n+m-k)].$$

After simplification, we get

Representatives	Degree	Eccentricity	Range	Frequency
$\{u_i^m, u_{n-i}^m\}$	1	$(3n)$	$\{m=0, m=n\}$, $\{i=0\}$	4
$\{u_i^m, u_{n-i}^m\}$	2	$(3n-m)$	$(1 \leq m \leq \frac{n-1}{2})$, $\{i=0\}, \forall m$	$\frac{2t-2}{2}$, t is odd.
$\{u_i^m, u_{n-i}^m\}$	3	$(3n-m-k)$	$(1 \leq m \leq \frac{n-1}{2})$, $(1 \leq i \leq \frac{n-1}{2})\ \forall\, m$, $(2 \leq k \leq n-1)\ \forall\, m$, k is even.	$\frac{t^2-2t+1}{2}$, t is odd.
$\{u_i^0, u_{n-i}^0\}$	2	$(3n-m-k)$	$\{m=0\}$, $(1 \leq i \leq \frac{n-1}{2})\ \forall\, m$, $(2 \leq k \leq n-1)\ \forall\, m$, k is even.	$t-1$, t is odd.
$\{u_i^m, u_{n-i}^m\}$	2	$(2n+m)$	$(\frac{n+1}{2} \leq m \leq n-1)$, $\{i=0\}, \forall$ m .	$\frac{2t-2}{2}$, t is odd.
$\{v_i^m, v_{n-i+1}^m\}$	3	$(3n-m-k)$	$(0 \leq m \leq \frac{n-1}{2})$, $(1 \leq i \leq \frac{n+1}{2})\ \forall\, m$, $(1 \leq k \leq n)\ \forall\, m$, k is odd.	$\frac{t^2+t}{2}$, t is odd.
$\{u_i^m, u_{n-i}^m\}$	3	$(2n+m-k)$	$(\frac{n+1}{2} \leq m \leq n-1)$, $(1 \leq i \leq \frac{n-1}{2})\ \forall\, m$, $(2 \leq k \leq n-1)\ \forall\, m$, k is even.	$\frac{t^2-2t+1}{2}$, t is odd.
$\{v_i^m, v_{n-i+1}^m\}$	3	$(2n+m-k)$	$(\frac{n+1}{2} \leq m \leq n)$, $(1 \leq i \leq \frac{n+1}{2})\ \forall\, m$, $(1 \leq k \leq n)\ \forall\, m$, k is odd.	$\frac{t^2+t}{2}$, t is odd.
$\{u_i^m, u_{n-i}^m\}$	2	$(2n+m-k)$	$\{m=n\}$, $(1 \leq i \leq \frac{n-1}{2})\ \forall\, m$, $(2 \leq k \leq n-1)\ \forall\, m$, k is even.	$t-1$, t is odd.

Table 2: Vertices eccentricity according to degree of vertices when $n \equiv 1(mod2)$

$$\varsigma(G) = 8n + \sum_{m=1}^{\frac{n}{2}, n>2}(3nt-mt) + \sum_{m=\frac{n}{2}}^{n, n>2}(2nt+mt) + \sum_{m=0}[\sum_{k\equiv 0(mod2)}^{n-2}(3nt-mt-kt-6n+2m+2k)] + \sum_{m=1}^{\frac{n}{2}}[\sum_{k\equiv 0(mod2)}^{n}(\tfrac{3}{2}nt^2 - \tfrac{1}{2}mt^2 - \tfrac{1}{2}kt^2 - \tfrac{3}{2}nt + \tfrac{1}{2}mt + \tfrac{1}{2}mk)] + \sum_{m=\frac{n}{2}}^{n}[\sum_{k\equiv 0(mod2)}^{n}(nt^2 + \tfrac{1}{2}mt^2 - \tfrac{1}{2}kt^2 - nt - \tfrac{1}{2}mt + \tfrac{1}{2}kt)] + \sum_{m=0}^{\frac{n}{2}}[\sum_{k\equiv 1(mod2)}^{n-1}(\tfrac{3}{2}nt^2 - \tfrac{1}{2}mt^2 - \tfrac{1}{2}kt^2 + 3nt - mt - kt)] + \sum_{m=\frac{n}{2}}^{n-1}[\sum_{k\equiv 1(mod2)}^{n-1}(nt^2 + \tfrac{1}{2}mt^2 - \tfrac{1}{2}kt^2 - 2nt - mt + kt)] + \sum_{m\equiv 0(mod2)}[\sum_{k\equiv 1(mod2)}^{n-1}(2nt+mt-kt)] + 23. \qquad \square$$

Theorem 4. *Let $G \cong NA_m^n$ with $n \equiv 1(mod2)$, then total-eccentricity index is,*

$$\varsigma(G) = 12n + \sum_{m=1}^{\frac{n-1}{2}}(3nt - mt - 3n + m) + \sum_{m=\frac{n+1}{2}}^{n-1}(2nt + mt - 2n - m) + \sum_{m=0}[\sum_{k\equiv 0(mod2)}^{n-1}(3nt - mt - kt - 3n + m + k)] + \sum_{m=n}[\sum_{k\equiv 0(mod2)}^{n-1}(2nt + mt - kt - 2n - m + k)] + \sum_{m=1}^{\frac{n-1}{2}}[\sum_{k\equiv 0(mod2)}^{n-1}(\tfrac{3}{2}nt^2 - \tfrac{1}{2}mt^2 - \tfrac{1}{2}kt^2 - 3nt + mt + kt + \tfrac{3}{2}n - \tfrac{1}{2}m - \tfrac{1}{2}k)] + \sum_{m=\frac{n+1}{2}}^{n-1}[\sum_{k\equiv 0(mod2)}^{n-1}(nt^2 + \tfrac{1}{2}mt^2 - \tfrac{1}{2}kt^2 - 2nt - mt + kt + n + \tfrac{1}{2}m - \tfrac{1}{2}k)] + \sum_{m=0}^{\frac{n-1}{2}}[\sum_{k\equiv 1(mod2)}^{n}(\tfrac{3}{2}nt^2 - \tfrac{1}{2}mt^2 - \tfrac{1}{2}kt^2 + \tfrac{3}{2}nt - \tfrac{1}{2}mt - \tfrac{1}{2}kt)] + \sum_{m=\frac{n+1}{2}}^{n}[\sum_{k\equiv 1(mod2)}^{n}(nt^2 + \tfrac{1}{2}mt^2 - \tfrac{1}{2}kt^2 + nt + \tfrac{1}{2}mt - \tfrac{1}{2}kt)].$$

Proof. Let $G \cong NA_m^n$. Then from Eq. (3), we have,

$$\varsigma(G) = \sum_{u\in V(G)} \epsilon(u)$$

By utilizing Table 2 into Eq. (2), we get,

$$\varsigma(G) = 4\times 3n + \frac{2t-2}{2}\times \sum_{m=1}^{\frac{n-1}{2}}(3n-m) + \frac{2t-2}{2}\times \sum_{m=\frac{n+1}{2}}^{n-1}(2n+m) + (t-1)\times \sum_{m=0}[\sum_{k\equiv 0(mod2)}^{n-1}(3n-m-k)] + (t-1)\times \sum_{m=n}[\sum_{k\equiv 0(mod2)}^{n-1}(2n+m-k)] + (\frac{t^2-2t+1}{2})\times \sum_{m=1}^{\frac{n-1}{2}}[\sum_{k\equiv 0(mod2)}^{n-1}(3n-m-k)] + \frac{t^2-2t+1}{2}\times \sum_{m=\frac{n+1}{2}}^{n-1}[\sum_{k\equiv 0(mod2)}^{n-1}(2n+m-k)] + \frac{t^2+t}{2}\times \sum_{m=0}^{\frac{n-1}{2}}[\sum_{k\equiv 1(mod2)}^{n}(3n-m-k)] + (\frac{t^2+t}{2})\times \sum_{m=\frac{n+1}{2}}^{n}[\sum_{k\equiv 1(mod2)}^{n}(2n+m-k)].$$

After simplification, we get,

$$\varsigma(G) = 12n + \sum_{m=1}^{\frac{n-1}{2}}(3nt-mt-3n+m) + \sum_{m=\frac{n+1}{2}}^{n-1}(2nt+mt-2n-m) + \sum_{m=0}[\sum_{k\equiv 0(mod2)}^{n-1}(3nt-mt-kt-3n+m+k)] + \sum_{m=n}[\sum_{k\equiv 0(mod2)}^{n-1}(2nt+mt-kt-2n-m+k)] + \sum_{m=1}^{\frac{n-1}{2}}[\sum_{k\equiv 0(mod2)}^{n-1}(\frac{3}{2}nt^2-\frac{1}{2}mt^2-\frac{1}{2}kt^2-3nt+mt+kt+\frac{3}{2}n-\frac{1}{2}m-\frac{1}{2}k)] + \sum_{m=\frac{n+1}{2}}^{n-1}[\sum_{k\equiv 0(mod2)}^{n-1}(nt^2+\frac{1}{2}mt^2-\frac{1}{2}kt^2-2nt-mt+kt+n+\frac{1}{2}m-\frac{1}{2}k)] + \sum_{m=0}^{\frac{n-1}{2}}[\sum_{k\equiv 1(mod2)}^{n}(\frac{3}{2}nt^2-\frac{1}{2}mt^2-\frac{1}{2}kt^2+\frac{3}{2}nt-\frac{1}{2}mt-\frac{1}{2}kt)] + \sum_{m=\frac{n+1}{2}}^{n}[\sum_{k\equiv 1(mod2)}^{n}(nt^2+\frac{1}{2}mt^2-\frac{1}{2}kt^2+nt+\frac{1}{2}mt-\frac{1}{2}kt)].$$ □

C. First Zagreb-eccentricity index of NA_m^n nanotube

Theorem 5. *Let $G \cong NA_m^n$ with $n \equiv 0(mod2)$. The first Zagreb-eccentricity index is,*

$$M_1^*(G) = \sum_{i=1}^{\frac{n}{2}}\sum_{p=2n-\frac{n}{2}}^{2n-1}(12ip+6i-6p-3) + \sum_{p=n\equiv 0(mod2)}(12np+3n) + \sum_{p=n\equiv 0(mod2)}(8p+4) + \sum_{i=\frac{n}{2}+3}(\frac{n}{2}-1)\underbrace{times}(6i-16)\times \sum_{p=2n+1}^{3n-\frac{n}{2}-1}(2p+1) + \sum_{i=3n+6j,0\le j\le \frac{n}{2}-1}\sum_{p=3n-\frac{n}{2}}^{3n-1}(12np+6n-2ip-i).$$

Proof. Let $G \cong NA_m^n$. From Eq. (4), we have,

$$M_1^*(G) = \sum_{uv\in E(G)}[\epsilon(u)+\epsilon(v)].$$

By utilizing Table 3, we get,

$$M_1^*(G) = \sum_{i=1}^{\frac{n}{2}}(6i-3)\times \sum_{p=2n-\frac{n}{2}}^{2n-1}(p+p+1) + 3n\times \sum_{p=n\equiv 0(mod2)}(2p+2p+1) + 2\times \sum_{p=n\equiv 0(mod2)}(2p+1+2p+1) + \sum_{i=\frac{n}{2}+3}(\frac{n}{2}-1)\underbrace{times}(6i-16)\times \sum_{p=2n+1}^{3n-\frac{n}{2}-1}(p+p+1) + \sum_{i=3n+6j,0\le j\le \frac{n}{2}-1}\times \sum_{p=3n-\frac{n}{2}}^{3n-1}(p+p+1).$$

After simplification, we get

$$M_1^*(G)=\sum_{i=1}^{\frac{n}{2}}\sum_{p=2n-\frac{n}{2}}^{2n-1}(12ip+6i-6p-3)+\sum_{p=n\equiv 0(mod2)}(12np+3n)+\sum_{p=n\equiv 0(mod2)}(8p+4)+\sum_{i=\frac{n}{2}+3}(\tfrac{n}{2}-1)\underbrace{times}(6i-16)\times\sum_{p=2n+1}^{3n-\frac{n}{2}-1}(2p+1)+\sum_{i=3n+6j,0\leq j\leq\frac{n}{2}-1}\sum_{p=3n-\frac{n}{2}}^{3n-1}(12np+6n-2ip-i).$$ □

Theorem 6. *Let $G\cong NA_m^n$ with $n\equiv 1(mod4)$. The first Zagreb-eccentricity index is,*

$$M_1^*(G)=\sum_{p=\frac{3n+1}{2}}(2p)+\sum_{i=(\frac{n-1}{2})\underbrace{times}2}\sum_{p=\frac{3n+1}{2}}^{\frac{5n-1}{2},p\equiv 0(mod2)}(2ip)+\sum_{i=1}^{\frac{n-3}{2},i\equiv 1(mod2)}\sum_{p=\frac{3n+1}{2}}^{2n-2,p\equiv 0(mod2)}(8ip+4i)+\sum_{i=2}^{\frac{n-1}{2},i\equiv 0(mod2)}\sum_{p=\frac{3n+3}{2}}^{2n-1,p\equiv 1(mod2)}(16ip+8i-4p-2)+\sum_{i=2n+2}(\tfrac{n+3}{4})\underbrace{times}i\times\sum_{p=2n}^{\frac{5n-1}{2},p\equiv 0(mod2)}(2p+1)+\sum_{i=4n}(\tfrac{n-1}{4})\underbrace{times}i\times\sum_{p=2n+1}^{\frac{5n-3}{2},p\equiv 1(mod2)}(2p+1)+\sum_{i=\frac{n-1}{4}}^{1}\sum_{p=\frac{5n+1}{2}}^{3n-2,p\equiv 1(mod2)}(32ip+16i)+\sum_{i=\frac{n-3}{2}}^{1,i\equiv 1(mod2)}\sum_{p=\frac{5n+3}{2}}^{3n-1,p\equiv 0(mod2)}(8ip+4i).$$

Proof. Let $G\cong NA_m^n$. From Eq. (4), we have,

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

By utilizing Table 4, we get,

$$M_1^*(G)=1\times\sum_{p=\frac{3n+1}{2}}(p+p)+\sum_{i=(\frac{n-1}{2})\underbrace{times}2}i\times\sum_{p=\frac{3n+1}{2}}^{\frac{5n-1}{2},p\equiv 0(mod2)}(p+p)+\sum_{i=1}^{\frac{n-3}{2},i\equiv 1(mod2)}4i\times sum_{p=\frac{3n+1}{2}}^{2n-2,p\equiv 0(mod2)}(p+p+1)+\sum_{i=2}^{\frac{n-1}{2},i\equiv 0(mod2)}(8i-2)\times\sum_{p=\frac{3n+3}{2}}^{2n-1,p\equiv 1(mod2)}(p+p+1)+\sum_{i=2n+2}(\tfrac{n+3}{4})\underbrace{times}i\times\sum_{p=2n}^{\frac{5n-1}{2},p\equiv 0(mod2)}(p+p+1)+\sum_{i=4n}(\tfrac{n-1}{4})\underbrace{times}i\times\sum_{p=2n+1}^{\frac{5n-3}{2},p\equiv 1(mod2)}(p+p+1)+\sum_{i=\frac{n-1}{4}}^{1}16i\times\sum_{p=\frac{5n+1}{2}}^{3n-2,p\equiv 1(mod2)}(p+p+1)+\sum_{i=\frac{n-3}{2}}^{1,i\equiv 1(mod2)}4i\times\sum_{p=\frac{5n+3}{2}}^{3n-1,p\equiv 0(mod2)}(p+p+1).$$

After simplification, we get

$$M_1^*(G)=\sum_{p=\frac{3n+1}{2}}(2p)+\sum_{i=(\frac{n-1}{2})\underbrace{times}2}\sum_{p=\frac{3n+1}{2}}^{\frac{5n-1}{2},p\equiv 0(mod2)}(2ip)+\sum_{i=1}^{\frac{n-3}{2},i\equiv 1(mod2)}\sum_{p=\frac{3n+1}{2}}^{2n-2,p\equiv 0(mod2)}(8ip+4i)+\sum_{i=2}^{\frac{n-1}{2},i\equiv 0(mod2)}\sum_{p=\frac{3n+3}{2}}^{2n-1,p\equiv 1(mod2)}(16ip+8i-4p-2)+\sum_{i=2n+2}(\tfrac{n+3}{4})\underbrace{times}i\times\sum_{p=2n}^{\frac{5n-1}{2},p\equiv 0(mod2)}(2p+1)+\sum_{i=4n}(\tfrac{n-1}{4})\underbrace{times}i\times\sum_{p=2n+1}^{\frac{5n-3}{2},p\equiv 1(mod2)}(2p+1)+\sum_{i=\frac{n-1}{4}}^{1}\sum_{p=\frac{5n+1}{2}}^{3n-2,p\equiv 1(mod2)}(32ip+16i)+\sum_{i=\frac{n-3}{2}}^{1,i\equiv 1(mod2)}\sum_{p=\frac{5n+3}{2}}^{3n-1,p\equiv 0(mod2)}(8ip+4i).$$ □

Theorem 7. *Let $G\cong NA_m^n$ with $n\equiv 3(mod4)$. The first Zagreb-eccentricity index is,*

$$M_1^*(G)=\sum_{i=\underbrace{(\frac{n+1}{2})\,times}2}\sum_{p=\frac{3n+3}{2}}^{\frac{5n+1}{2},p\equiv 0(mod2)}(2ip)+\sum_{i=1}^{\frac{n+1}{4}}\sum_{p=\frac{3n+1}{2}}^{2n-1,p\equiv 1(mod2)}(32ip+16i-20p-10)+\sum_{i=1}^{\frac{n+1}{4}}\sum_{p=\frac{3n+3}{2}}^{2n,p\equiv 0(mod2)}(16ip+8i)+\sum_{i=4n}\underbrace{(\frac{n+1}{4})\,times}\,i\times\sum_{p=2n+1}^{\frac{5n-1}{2},p\equiv 1(mod2)}(2p+1)+\sum_{i=2n+2,n\neq 3}\underbrace{(\frac{n-3}{4})\,times}\,i\times\sum_{p=2n+2,n\neq 3}^{\frac{5n-3}{2},p\equiv 0(mod2)}(2p+1)+\sum_{i=1,n\neq 3}^{\frac{n-3}{4}}\sum_{p=\frac{5n+3}{2},n\neq 3}^{3n-2,p\equiv 1(mod2)}(32ip+16i)+\sum_{i=\frac{n+1}{4}}^{1}\sum_{p=\frac{5n+1}{2}}^{3n-1,p\equiv 0(mod2)}(16ip+8i-8p-4).$$

Proof. Let $G\cong NA_m^n$. From Eq. (4), we have

$$M_1^*(G)=\sum_{uv\in E(G)}[\epsilon(u)+\epsilon(v)].$$

By utilizing Table 5, we get,

$$M_1^*(G)=\sum_{i=\underbrace{(\frac{n+1}{2})\,times}2}i\times\sum_{p=\frac{3n+3}{2}}^{\frac{5n+1}{2},p\equiv 0(mod2)}(p+p)+\sum_{i=1}^{\frac{n+1}{4}}(16i-10)\times\sum_{p=\frac{3n+1}{2}}^{2n-1,p\equiv 1(mod2)}(p+p+1)+\sum_{i=1}^{\frac{n+1}{4}}8i\times\sum_{p=\frac{3n+3}{2}}^{2n,p\equiv 0(mod2)}(p+p+1)+\sum_{i=4n}\underbrace{(\frac{n+1}{4})\,times}\,i\times\sum_{p=2n+1}^{\frac{5n-1}{2},p\equiv 1(mod2)}(p+p+1)+\sum_{i=2n+2,n\neq 3}\underbrace{(\frac{n-3}{4})\,times}\,i\times\sum_{p=2n+2,n\neq 3}^{\frac{5n-3}{2},p\equiv 0(mod2)}(p+p+1)+\sum_{i=1,n\neq 3}^{\frac{n-3}{4}}16i\times\sum_{p=\frac{5n+3}{2},n\neq 3}^{3n-2,p\equiv 1(mod2)}(p+p+1)+\sum_{i=\frac{n+1}{4}}^{1}(8i-4)\times\sum_{p=\frac{5n+1}{2}}^{3n-1,p\equiv 0(mod2)}(p+p+1).$$

After simplification, we get

$$M_1^*(G)=\sum_{i=\underbrace{(\frac{n+1}{2})\,times}2}\sum_{p=\frac{3n+3}{2}}^{\frac{5n+1}{2},p\equiv 0(mod2)}(2ip)+\sum_{i=1}^{\frac{n+1}{4}}\sum_{p=\frac{3n+1}{2}}^{2n-1,p\equiv 1(mod2)}(32ip+16i-20p-10)+\sum_{i=1}^{\frac{n+1}{4}}\sum_{p=\frac{3n+3}{2}}^{2n,p\equiv 0(mod2)}(16ip+8i)+\sum_{i=4n}\underbrace{(\frac{n+1}{4})\,times}\,i\times\sum_{p=2n+1}^{\frac{5n-1}{2},p\equiv 1(mod2)}(2p+1)+\sum_{i=2n+2,n\neq 3}\underbrace{(\frac{n-3}{4})\,times}\,i\times\sum_{p=2n+2,n\neq 3}^{\frac{5n-3}{2},p\equiv 0(mod2)}(2p+1)+\sum_{i=1,n\neq 3}^{\frac{n-3}{4}}\sum_{p=\frac{5n+3}{2},n\neq 3}^{3n-2,p\equiv 1(mod2)}(32ip+16i)+\sum_{i=\frac{n+1}{4}}^{1}\sum_{p=\frac{5n+1}{2}}^{3n-1,p\equiv 0(mod2)}(16ip+8i-8p-4).\quad\square$$

D. Second Zagreb-eccentricity index of NA_m^n nanotube

Theorem 8. *Let $G\cong NA_m^n$ with $n\equiv 0(mod2)$. The second Zagreb-eccentricity index is,*

$$M_1^{**}(G)=22n^2+4n+\sum_{m=1}^{\frac{n}{2},n>2}(9n^2t+m^2t-6nmt)+\sum_{m=\frac{n}{2}}^{n,n>2}(4n^2t+m^2t+4nmt)+\sum_{m=0}[\sum_{k\equiv 0(mod2)}^{n-2,n>2}(9n^2t+m^2t+k^2t-6nmt+2mkt-6nkt-18n^2-2m^2-2k^2+12nm-4mk+12nk)]+\sum_{m=1}^{\frac{n}{2}}[\sum_{k\equiv 0(mod2)}^{n}(\frac{9}{2}n^2t^2+\frac{1}{2}m^2t^2+\frac{1}{2}k^2t^2-3nmt^2+mkt^2-3nkt^2-\frac{9}{2}n^2t-\frac{1}{2}m^2t-\frac{1}{2}k^2t+3nmt-mkt+3nkt)+\sum_{m=\frac{n}{2}}^{n}[\sum_{k\equiv 0(mod2)}^{n}(2n^2t^2+\frac{1}{2}m^2t^2+\frac{1}{2}k^2t^2+2nmt^2-mkt^2-2nkt^2-2n^2t-\frac{1}{2}m^2t-\frac{1}{2}k^2t-2nmt+mkt+2nkt)]+\sum_{m=0}^{\frac{n}{2}}[\sum_{k\equiv 1(mod2)}^{n-1}(\frac{9}{2}n^2t^2+\frac{1}{2}m^2t^2+\frac{1}{2}k^2t^2-3nmt^2+mkt^2-3nkt^2+9n^2t+m^2t+k^2t-6nmt+2mkt-6nkt)]+\sum_{m=\frac{n}{2}}^{n-1}[\sum_{k\equiv 1(mod2)}^{n-1}(2n^2t^2+\frac{1}{2}m^2t^2+\frac{1}{2}k^2t^2+2nmt^2-mkt^2-2nkt^2-4n^2t-m^2t-k^2t-4nmt+2mkt+4nkt)]+\sum_{m\equiv 0(mod2)}[\sum_{k\equiv 1(mod2)}^{n-1}(4n^2t+m^2t+k^2t+4nmt-2mkt-4nkt)]+123.$$

Proof. Let $G \cong NA_m^n$. From Eq. (5), we have,

$$M_1^{**}(G) = \sum_{v \in V(G)} [\epsilon(v)]^2.$$

By utilizing Table 1, we get,

$$M_1^{**}(G) = 2\times(3n)^2 + 2\times(5)^2 + t\times\sum_{m=1}^{\frac{n}{2},n>2}(3n-m)^2 + 2\times(6)^2 + t\times\sum_{m=\frac{n}{2}}^{n,n>2}(2n+m)^2 + (t-2)\times\sum_{m=0}[\sum_{k\equiv 0(mod2)}^{n-2,n>2}(3n-m-k)^2] + (\frac{t^2-t}{2})\times\sum_{m=1}^{\frac{n}{2}}[\sum_{k\equiv 0(mod2)}^{n}(3n-m-k)^2 + \frac{t^2-t}{2}\times\sum_{m=\frac{n}{2}}^{n}[\sum_{k\equiv 0(mod2)}^{n}(2n+m-k)^2] + (1)\times\sum_{n\equiv 0(mod2)}(2n+1)^2 + \frac{t^2+2t}{2}\times\sum_{m=0}^{\frac{n}{2}}[\sum_{k\equiv 1(mod2)}^{n-1}(3n-m-k)^2] + \frac{t^2-2t}{2}\times\sum_{m=\frac{n}{2}}^{n-1}[\sum_{k\equiv 1(mod2)}^{n-1}(2n+m-k)^2] + t\times\sum_{m\equiv 0(mod2)}[\sum_{k\equiv 1(mod2)}^{n-1}(2n+m-k)^2].$$

After simplification, we get,

$$M_1^{**}(G) = 22n^2 + 4n + \sum_{m=1}^{\frac{n}{2},n>2}(9n^2t + m^2t - 6nmt) + \sum_{m=\frac{n}{2}}^{n,n>2}(4n^2t + m^2t + 4nmt) + \sum_{m=0}[\sum_{k\equiv 0(mod2)}^{n-2,n>2}(9n^2t + m^2t + k^2t - 6nmt + 2mkt - 6nkt - 18n^2 - 2m^2 - 2k^2 + 12nm - 4mk + 12nk)] + \sum_{m=1}^{\frac{n}{2}}[\sum_{k\equiv 0(mod2)}^{n}(\frac{9}{2}n^2t^2 + \frac{1}{2}m^2t^2 + \frac{1}{2}k^2t^2 - 3nmt^2 + mkt^2 - 3nkt^2 - \frac{9}{2}n^2t - \frac{1}{2}m^2t - \frac{1}{2}k^2t + 3nmt - mkt + 3nkt) + \sum_{m=\frac{n}{2}}^{n}[\sum_{k\equiv 0(mod2)}^{n}(2n^2t^2 + \frac{1}{2}m^2t^2 + \frac{1}{2}k^2t^2 + 2nmt^2 - mkt^2 - 2nkt^2 - 2n^2t - \frac{1}{2}m^2t - \frac{1}{2}k^2t - 2nmt + mkt + 2nkt)] + \sum_{m=0}^{\frac{n}{2}}[\sum_{k\equiv 1(mod2)}^{n-1}(\frac{9}{2}n^2t^2 + \frac{1}{2}m^2t^2 + \frac{1}{2}k^2t^2 - 3nmt^2 + mkt^2 - 3nkt^2 + 9n^2t + m^2t + k^2t - 6nmt + 2mkt - 6nkt)] + \sum_{m=\frac{n}{2}}^{n-1}[\sum_{k\equiv 1(mod2)}^{n-1}(2n^2t^2 + \frac{1}{2}m^2t^2 + \frac{1}{2}k^2t^2 + 2nmt^2 - mkt^2 - 2nkt^2 - 4n^2t - m^2t - k^2t - 4nmt + 2mkt + 4nkt)] + \sum_{m\equiv 0(mod2)}[\sum_{k\equiv 1(mod2)}^{n-1}(4n^2t + m^2t + k^2t + 4nmt - 2mkt - 4nkt)] + 123. \qquad \square$$

Theorem 9. *Let $G \cong NA_m^n$ with $n \equiv 1(mod2)$. The second Zagreb-eccentricity index is,*

$$M_1^{**}(G) = 36n^2 + \sum_{m=1}^{\frac{n-1}{2}}(9n^2t + m^2t - 6nmt - 9n^2 - m^2 + 6nm) + \sum_{m=\frac{n+1}{2}}^{n-1}(4n^2t + m^2t + 4nmt - 4n^2 - m^2 - 4nm) + \sum_{m=0}[\sum_{k\equiv 0(mod2)}^{n-1}(9n^2t + m^2t + k^2t - 6nmt + 2mkt - 6nkt - 9n^2 - m^2 - k^2 + 6nm - 2mk + 6nk)] + \sum_{m=n}[\sum_{k\equiv 0(mod2)}^{n-1}(4n^2t + m^2t + k^2t + 4nmt - 2mkt - 4nkt - 4n^2 - m^2 - k^2 - 4nm + 2mk + 4nk)] + \sum_{m=1}^{\frac{n-1}{2}}[\sum_{k\equiv 0(mod2)}^{n-1}(\frac{9}{2}n^2t^2 + \frac{1}{2}m^2t^2 + \frac{1}{2}k^2t^2 - 3nmt^2 + mkt^2 - 3nkt^2 - 9n^2t - m^2t - k^2t + 6nmt - 2mkt + 6nkt + \frac{9}{2}n^2 + \frac{1}{2}m^2 + \frac{1}{2}k^2 - 3nm + mk - 3nk)] + \sum_{m=\frac{n+1}{2}}^{n-1}[\sum_{k\equiv 0(mod2)}^{n-1}(2n^2t^2 + \frac{1}{2}m^2t^2 + \frac{1}{2}k^2t^2 + 2nmt^2 - mkt^2 - 2nkt^2 - 4n^2t - m^2t - k^2t - 4nmt + 2mkt + 4nkt + 2n^2 + \frac{1}{2}m^2 + \frac{1}{2}k^2 + 2nm - mk - 2nk)] + \sum_{m=0}^{\frac{n-1}{2}}[\sum_{k\equiv 1(mod2)}^{n}(\frac{9}{2}n^2t^2 + \frac{1}{2}m^2t^2 + \frac{1}{2}k^2t^2 - 3nmt^2 + mkt^2 - 3nkt^2 + \frac{9}{2}n^2t + \frac{1}{2}m^2t + \frac{1}{2}k^2t - 3nmt + mkt - 3nkt)] + \sum_{m=\frac{n+1}{2}}^{n}[\sum_{k\equiv 1(mod2)}^{n}(2n^2t^2 + \frac{1}{2}m^2t^2 + \frac{1}{2}k^2t^2 + 2nmt^2 - mkt^2 - 2nkt^2 + 2n^2t + \frac{1}{2}m^2t + \frac{1}{2}k^2t + 2nmt - mkt - 2nkt)].$$

Proof. Let $G \cong NA_m^n$. From Eq. (5), we have,

$$M_1^{**}(G) = \sum_{v \in V(G)} [\epsilon(v)]^2.$$

By utilizing Table 2, we get,

$$M_1^{**}(G) = 4\times(3n)^2 + \frac{2t-2}{2}\times\sum_{m=1}^{\frac{n-1}{2}}(3n-m)^2 + \frac{2t-2}{2}\times\sum_{m=\frac{n+1}{2}}^{n-1}(2n+m)^2 + (t-1)\times\sum_{m=0}[\sum_{k\equiv 0(mod2)}^{n-1}(3n-m-k)^2] + (t-1)\times\sum_{m=n}[\sum_{k\equiv 0(mod2)}^{n-1}(2n+m-k)^2] + \frac{t^2-2t+1}{2}\times\sum_{m=1}^{\frac{n-1}{2}}[\sum_{k\equiv 0(mod2)}^{n-1}(3n-m-k)^2] + \frac{t^2-2t+1}{2}\times\sum_{m=\frac{n+1}{2}}^{n-1}[\sum_{k\equiv 0(mod2)}^{n-1}(2n+m-k)^2] + \frac{t^2+t}{2}\times\sum_{m=0}^{\frac{n-1}{2}}[\sum_{k\equiv 1(mod2)}^{n}(3n-m-k)^2] + \frac{t^2+t}{2}\times\sum_{m=\frac{n+1}{2}}^{n}[\sum_{k\equiv 1(mod2)}^{n}(2n+m-k)^2].$$

After simplification, we get,

$$M_1^{**}(G) = 36n^2 + \sum_{m=1}^{\frac{n-1}{2}}(9n^2t+m^2t-6nmt-9n^2-m^2+6nm) + \sum_{m=\frac{n+1}{2}}^{n-1}(4n^2t+m^2t+4nmt-4n^2-m^2-4nm) + \sum_{m=0}[\sum_{k\equiv 0(mod2)}^{n-1}(9n^2t+m^2t+k^2t-6nmt+2mkt-6nkt-9n^2-m^2-k^2+6nm-2mk+6nk)] + \sum_{m=n}[\sum_{k\equiv 0(mod2)}^{n-1}(4n^2t+m^2t+k^2t+4nmt-2mkt-4nkt-4n^2-m^2-k^2-4nm+2mk+4nk)] + \sum_{m=1}^{\frac{n-1}{2}}[\sum_{k\equiv 0(mod2)}^{n-1}(\frac{9}{2}n^2t^2+\frac{1}{2}m^2t^2+\frac{1}{2}k^2t^2-3nmt^2+mkt^2-3nkt^2-9n^2t-m^2t-k^2t+6nmt-2mkt+6nkt+\frac{9}{2}n^2+\frac{1}{2}m^2+\frac{1}{2}k^2-3nm+mk-3nk)] + \sum_{m=\frac{n+1}{2}}^{n-1}[\sum_{k\equiv 0(mod2)}^{n-1}(2n^2t^2+\frac{1}{2}m^2t^2+\frac{1}{2}k^2t^2+2nmt^2-mkt^2-2nkt^2-4n^2t-m^2t-k^2t-4nmt+2mkt+4nkt+2n^2+\frac{1}{2}m^2+\frac{1}{2}k^2+2nm-mk-2nk)] + \sum_{m=0}^{\frac{n-1}{2}}[\sum_{k\equiv 1(mod2)}^{n}(\frac{9}{2}n^2t^2+\frac{1}{2}m^2t^2+\frac{1}{2}k^2t^2-3nmt^2+mkt^2-3nkt^2+\frac{9}{2}n^2t+\frac{1}{2}m^2t+\frac{1}{2}k^2t-3nmt+mkt-3nkt)] + \sum_{m=\frac{n+1}{2}}^{n}[\sum_{k\equiv 1(mod2)}^{n}(2n^2t^2+\frac{1}{2}m^2t^2+\frac{1}{2}k^2t^2+2nmt^2-mkt^2-2nkt^2+2n^2t+\frac{1}{2}m^2t+\frac{1}{2}k^2t+2nmt-mkt-2nkt)]. \quad \square$$

E. Third Zagreb-eccentricity index of NA_m^n nanotube

Theorem 10. *Let $G \cong NA_m^n$ with $n \equiv 0(mod2)$. The third Zagreb-eccentricity index is equal to,*

$$M_2^*(G) = \sum_{i=1}^{\frac{n}{2}}\sum_{p=2n-\frac{n}{2}}^{2n-1}(6ip^2-3p^2+6ip-3p) + \sum_{p=n\equiv 0(mod2)}(12np^2+6np) + \sum_{p=n\equiv 0(mod2)}(8p^2+8p+2) + \sum_{i=\frac{n}{2}+3}(\frac{n}{2}-1)\underbrace{times}(6i-16)\times\sum_{p=2n+1}^{3n-\frac{n}{2}-1}(p^2+p) + \sum_{i=3n+6j,0\le j\le\frac{n}{2}-1}\sum_{p=3n-\frac{n}{2}}^{3n-1}(6np^2-ip^2+6np-ip).$$

Proof. Let $G \cong NA_m^n$. From Eq. (6), we have,

$$M_2^*(G) = \sum_{uv\in E(G)}\epsilon(u).\epsilon(v).$$

By utilizing Table 3, we get,

$$M_2^*(G) = \sum_{i=1}^{\frac{n}{2}}(6i-3)\times\sum_{p=2n-\frac{n}{2}}^{2n-1}(p).(p+1) + \sum_{p=n\equiv 0(mod2)}3n\times(p).(2p+1) + \sum_{p=n\equiv 0(mod2)}2\times(2p+1).(2p+1) + \sum_{i=\frac{n}{2}+3}(\frac{n}{2}-1)\underbrace{times}(6i-16)\times\sum_{p=2n+1}^{3n-\frac{n}{2}-1}(p).(p+1) + \sum_{i=3n+6j,0\le j\le\frac{n}{2}-1}(6n-i)\times\sum_{p=3n-\frac{n}{2}}^{3n-1}(p).(p+1).$$

After simplification, we get

$[\epsilon_u, \epsilon_v]$	Range	Frequency	Range
$[p, p+1]$	$(2n - \frac{n}{2} \leq p \leq 2n-1)$	$(3+6(i-1))$	$(1 \leq i \leq \frac{n}{2})$
$[2p, 2p+1]$	$(p = n \equiv 0(mod2))$	$(3n)$	$(n \equiv 0(mod2))$
$[2p+1, 2p+1]$	$(p = n \equiv 0(mod2))$	(2)	$(i = \frac{n}{2}+2)$
$[p, p+1]$	$(2n+1 \leq p \leq 3n - \frac{n}{2} - 1)$	$((\frac{n}{2}-1)\underbrace{times}[6i-16)])$	$(i = \frac{n}{2}+3)$
$[p, p+1]$	$(3n-1 \geq p \geq 3n - \frac{n}{2})$	$(6n-i)$	$(i = 3n+6j)$, where $(0 \leq j \leq \frac{n}{2}-1)$.

Table 3: The edge partition according to eccentricity of vertices when $n \equiv 0(mod2)$

$$M_2^*(G) = \sum_{i=1}^{\frac{n}{2}} \sum_{p=2n-\frac{n}{2}}^{2n-1} (6ip^2 - 3p^2 + 6ip - 3p) + \sum_{p=n\equiv 0(mod2)} (12np^2 + 6np) + \sum_{p=n\equiv 0(mod2)} (8p^2 + 8p + 2) + \sum_{i=\frac{n}{2}+3} (\frac{n}{2} - 1)\underbrace{times}(6i-16) \times \sum_{p=2n+1}^{3n-\frac{n}{2}-1} (p^2+p) + \sum_{i=3n+6j, 0\leq j \leq \frac{n}{2}-1} \sum_{p=3n-\frac{n}{2}}^{3n-1} (6np^2 - ip^2 + 6np - ip).$$ □

Theorem 11. *Let $G \cong NA_m^n$ with $n \equiv 1(mod2)$. The third Zagreb-eccentricity index is,*

$$M_2^*(G) = \sum_{p=\frac{3n+1}{2}} (p^2) + \sum_{i=(\frac{n-1}{2})\underbrace{times}2} \sum_{p=\frac{3n+1}{2}}^{\frac{5n-1}{2}, p\equiv 0(mod2)} (ip^2) + \sum_{i\equiv 1(mod2)}^{\frac{n-3}{2}} \sum_{p=\frac{3n+1}{2}}^{2n-2, p\equiv 0(mod2)} (4ip^2 + 4ip) + \sum_{i\equiv 0(mod2)}^{\frac{n-1}{2}} \sum_{p=\frac{3n+3}{2}}^{2n-1, p\equiv 1(mod2)} (8ip^2 - 2p^2 + 8ip - 2p) + \sum_{i=2n+2} (\frac{n+3}{4})\underbrace{times}i \times \sum_{p=2n}^{\frac{5n-1}{2}, p\equiv 0(mod2)} (p^2+p) + \sum_{i=4n} (\frac{n-1}{4})\underbrace{times}i \times \sum_{p=2n+1}^{\frac{5n-3}{2}, p\equiv 1(mod2)} (p^2+p) + \sum_{i=\frac{n-1}{4}}^{1} 16i \times \sum_{p=\frac{5n+1}{2}}^{3n-2, p\equiv 1(mod2)} (p^2+p) + \sum_{i=\frac{n-3}{2}}^{1, i\equiv 1(mod2)} 4i \times \sum_{p=\frac{5n+3}{2}}^{3n-1, p\equiv 0(mod2)} (p^2+p).$$

Proof. Let $G \cong NA_m^n$. From Eq. (6), we have

$$M_2^*(G) = \sum_{uv \in E(G)} \epsilon(u).\epsilon(v).$$

By utilizing Table 4, we get,

$$M_2^*(G) = 1 \times \sum_{p=\frac{3n+1}{2}} (p).(p) + \sum_{i=(\frac{n-1}{2})\underbrace{times}2} i \times \sum_{p=\frac{3n+1}{2}}^{\frac{5n-1}{2}, p\equiv 0(mod2)} (p).(p) + \sum_{i\equiv 1(mod2)}^{\frac{n-3}{2}} 4i \times \sum_{p=\frac{3n+1}{2}}^{2n-2, p\equiv 0(mod2)} (p).(p+1) + \sum_{i\equiv 0(mod2)}^{\frac{n-1}{2}} (8i-2) \times \sum_{p=\frac{3n+3}{2}}^{2n-1, p\equiv 1(mod2)} p).(p+1) + \sum_{i=2n+2} (\frac{n+3}{4})\underbrace{times}i \times \sum_{p=2n}^{\frac{5n-1}{2}, p\equiv 0(mod2)} (p).(p+1) + \sum_{i=4n} (\frac{n-1}{4})\underbrace{times} \times \sum_{p=2n+1}^{\frac{5n-3}{2}, p\equiv 1(mod2)} (p).(p+1) + \sum_{i=\frac{n-1}{4}}^{1} 16i \times \sum_{p=\frac{5n+1}{2}}^{3n-2, p\equiv 1(mod2)} (p).(p+1) + \sum_{i=\frac{n-3}{2}}^{1, i\equiv 1(mod2)} 4i \times \sum_{p=\frac{5n+3}{2}}^{3n-1, p\equiv 0(mod2)} (p).(p+1).$$

After simplification, we get,

$$M_2^*(G) = \sum_{p=\frac{3n+1}{2}} (p^2) + \sum_{i=(\frac{n-1}{2})\underbrace{times}2} \sum_{p=\frac{3n+1}{2}}^{\frac{5n-1}{2}, p\equiv 0(mod2)} (ip^2) + \sum_{i\equiv 1(mod2)}^{\frac{n-3}{2}} \sum_{p=\frac{3n+1}{2}}^{2n-2, p\equiv 0(mod2)} (4ip^2 + 4ip) + \sum_{i\equiv 0(mod2)}^{\frac{n-1}{2}} \sum_{p=\frac{3n+3}{2}}^{2n-1, p\equiv 1(mod2)} (8ip^2 - 2p^2 + 8ip - 2p) + \sum_{i=2n+2} (\frac{n+3}{4})\underbrace{times}i \times \sum_{p=2n}^{\frac{5n-1}{2}, p\equiv 0(mod2)} (p^2+p) + \sum_{i=4n} (\frac{n-1}{4})\underbrace{times}i \times \sum_{p=2n+1}^{\frac{5n-3}{2}, p\equiv 1(mod2)} (p^2+p) + \sum_{i=\frac{n-1}{4}}^{1} 16i \times \sum_{p=\frac{5n+1}{2}}^{3n-2, p\equiv 1(mod2)} (p^2+p) + \sum_{i=\frac{n-3}{2}}^{1, i\equiv 1(mod2)} 4i \times \sum_{p=\frac{5n+3}{2}}^{3n-1, p\equiv 0(mod2)} (p^2+p).$$ □

Theorem 12. *Let $G \cong NA_m^n$ with $n \equiv 3(mod4)$. The third Zagreb-eccentricity index is,*

$[\epsilon_u, \epsilon_v]$	Range	Frequency	Range
$[p,p]$	$\{p = \frac{3n+1}{2}\}$	$\{1\}$	
$[p,p]$	$(\frac{5n-1}{2} \geq p \geq \frac{3n+1}{2})$, p is even	$\{i\}$	$\{i = (\frac{n-1}{2}) \underbrace{times} 2\}$
$[p,p+1]$	$(3n-1 \geq p \geq \frac{5n+3}{2})$, p is even	$\{4i\}$	$(1 \geq i \geq \frac{n-3}{2}), \{i \equiv 1(mod2)\}$
$[p,p+1]$	$(2n-1 \geq p \geq \frac{3n+3}{2})$, p is even	$\{8i-2\}$	$(\frac{n-1}{2} \geq i \geq 2), \{i \equiv 0(mod2)\}$
$[p,p+1]$	$(\frac{5n-1}{2} \geq p \geq 2n)$, p is even	$\{i = 2n+2\}$	$\{(\frac{n+3}{4}) \underbrace{times}\, i\}$
$[p,p+1]$	$(\frac{5n-3}{2} \geq p \geq 2n+1)$, p is odd	$\{i = 4n\}$	$\{(\frac{n-1}{4}) \underbrace{times}\, i\}$
$[p,p+1]$	$(3n-2 \geq p \geq \frac{5n+1}{2})$, p is odd	$\{16i\}$	$(1 \geq i \geq \frac{n-1}{4})$
$[p,p+1]$	$(2n-2 \geq p \geq \frac{3n+1}{2})$, p is even	$\{4i\}$	$(\frac{n-3}{2} \geq i \geq 1)$, i is even

Table 4: The edge pairs partition according to eccentricity of vertices when $n \equiv 1(mod4)$

$[\epsilon_u, \epsilon_v]$	Range	Frequency	Range
$[p,p]$	$(\frac{3n+3}{2} \leq p \leq \frac{5n+1}{2})$	$\{i\}$	$\{i = (\frac{n+1}{2}) \underbrace{times} 2\}$
$[p,p+1]$	$(\frac{3n+1}{2} \leq p \leq 2n-1)$, p is odd	$\{16i-10\}$	$(1 \leq i \leq \frac{n+1}{4})$
$[p,p+1]$	$(\frac{3n+3}{2} \leq p \leq 2n)$, p is even	$\{8i\}$	$(1 \leq i \leq \frac{n+1}{4})$
$[p,p+1]$	$(2n+1 \leq p \leq \frac{5n-1}{2})$, p is odd	$\{i = 4n\}$	$\{(\frac{n+1}{4}) \underbrace{times}\, i\}$
$[p,p+1]$	$(\frac{5n-3}{2} \geq p \geq 2n+2)$, p is even, $n \neq 3$	$\{i = 2n+2\}, n \neq 3$	$\{(\frac{n-3}{4}) \underbrace{times}\, i\}, n \neq 3$
$[p,p+1]$	$(3n-2 \geq p \geq \frac{5n+3}{2})$, p is odd , $n \neq 3$	$\{16i\}$	$(\frac{n-3}{4} \leq i \leq 1), n \neq 3$
$[p,p+1]$	$(3n-1 \geq p \geq \frac{5n+1}{2})$, p is even	$\{8i-4\}$	$(\frac{n+1}{4} \leq i \leq 1)$

Table 5: The edge pairs partition according to eccentricity of vertices when $n \equiv 3(mod4)$

$$M_2^*(G) = \sum_{i=(\frac{n+1}{2})\underbrace{times}2} \sum_{p=\frac{3n+3}{2}}^{\frac{5n+1}{2}, p\equiv 0(mod2)} (ip^2) + \sum_{i=1}^{\frac{n+1}{4}} \sum_{\frac{3n+1}{2}}^{2n-1, p\equiv 1(mod2)} 16ip^2 - 10p^2 + 16ip - 10p) + \sum_{i=1}^{\frac{n+1}{4}} \sum_{p=\frac{3n+3}{2}}^{2n, p\equiv 0(mod2)} (8ip^2 + 8ip) + \sum_{i=4n} (\frac{n+1}{4})\underbrace{times}\, i \times \sum_{p=2n+1}^{\frac{5n-1}{2}, p\equiv 1(mod2)} (p^2 + p) + \sum_{i=2n+2, n\neq 3} (\frac{n-3}{4})\underbrace{times}\, i \times \sum_{p=2n+2, n\neq 3}^{\frac{5n-3}{2}, p\equiv 0(mod2)} (p^2 + p) + \sum_{i=\frac{n-3}{4}}^{1, n\neq 3} \sum_{p=\frac{5n+3}{2}, n\neq 3}^{3n-2, p\equiv 1(mod2)} (16ip^2 + 16ip) + \sum_{i=\frac{n+1}{4}}^{1} \sum_{p=\frac{5n+1}{2}}^{3n-1, p\equiv 0(mod2)} (8ip^2 - 4p^2 + 8ip - 4p).$$

Proof. Let $G \cong NA_m^n$. From Eq. (6), we have,

$$M_2^*(G) = \sum_{uv\in E(G)} \epsilon(u).\epsilon(v).$$

By utilizing Table 5, we get,

$$M_2^*(G) = \sum_{i=(\frac{n+1}{2})\underbrace{times}2} i \times \sum_{p=\frac{3n+3}{2}}^{\frac{5n+1}{2}, p\equiv 0(mod2)} (p).(p) + \sum_{i=1}^{\frac{n+1}{4}} (16i - 10) \times \sum_{\frac{3n+1}{2}}^{2n-1, p\equiv 1(mod2)} (p).(p+1) + \sum_{i=1}^{\frac{n+1}{4}} 8i \times \sum_{p=\frac{3n+3}{2}}^{2n, p\equiv 0(mod2)} (p).(p+1) + \sum_{i=4n} (\frac{n+1}{4}) times i \times \sum_{p=2n+1}^{\frac{5n-1}{2}, p\equiv 1(mod2)} (p).(p+1) + \sum_{i=2n+2, n\neq 3} (\frac{n-3}{4})\underbrace{times}\, i \times \sum_{p=2n+2, n\neq 3}^{\frac{5n-3}{2}, p\equiv 0(mod2)} p).(p+1) + \sum_{i=\frac{n-3}{4}}^{1, n\neq 3} 16i \times \sum_{p=\frac{5n+3}{2}, n\neq 3}^{3n-2, p\equiv 1(mod2)} (p^2 + p) + \sum_{i=\frac{n+1}{4}}^{1} (8i - 4) \times \sum_{p=\frac{5n+1}{2}}^{3n-1, p\equiv 0(mod2)} p).(p+1).$$

After simplification, we get,

$$M_2^*(G) = \sum_{i=(\frac{n+1}{2})\underbrace{times}2} \sum_{p=\frac{3n+3}{2}}^{\frac{5n+1}{2}, p\equiv 0(mod2)} (ip^2) + \sum_{i=1}^{\frac{n+1}{4}} \sum_{\frac{3n+1}{2}}^{2n-1, p\equiv 1(mod2)} (16ip^2 - 10p^2 + 16ip - 10p) + \sum_{i=1}^{\frac{n+1}{4}} \sum_{p=\frac{3n+3}{2}}^{2n, p\equiv 0(mod2)} (8ip^2 + 8ip) + \sum_{i=4n} (\frac{n+1}{4})\underbrace{times}\, i \times \sum_{p=2n+1}^{\frac{5n-1}{2}, p\equiv 1(mod2)} (p^2 + p) + \sum_{i=2n+2, n\neq 3} (\frac{n-3}{4})\underbrace{times}\, i \times \sum_{p=2n+2, n\neq 3}^{\frac{5n-3}{2}, p\equiv 0(mod2)} (p^2 + p) +$$

$$\sum_{i=\frac{n-3}{4}}^{1,n\neq 3}\sum_{p=\frac{5n+3}{2},n\neq 3}^{3n-2,p\equiv 1(mod2)}(16ip^2+16ip)+\sum_{i=\frac{n+1}{4}}^{1}\sum_{p=\frac{5n+1}{2}}^{3n-1,p\equiv 0(mod2)}(8ip^2-4p^2+8ip-4p). \qquad \square$$

III. Conclusion

In this paper we considered the chemical graph of $G \cong NA_m^n$ and computed eccentric connectivity index with total eccentricity index and some versions of the zagreb indices which are the most prominent eccentricity based graph invariants in chemical graph theory. The results are valid and useful for the modeling of biological activities.

Declarations

Ethical Approval

This declaration is not applicable.

Competing interests

There is no scientific or financial conflict of interests between the authors and we feel convenient to submit.

Authors contributions

The author Wasim Sajjad conducted this research under the supervision of Prof. Xiang-Feng Pan and concluded the results. M. Shoaib Sardar verified the main results of the research article and reviewed it.

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All relevant data is given in the manuscript, there is no hidden or unpublished data.

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