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THE FIRST ECCENTRIC ZAGREB INDEX OF THE N^{TH} GROWTH OF NANOSTAR DENDRIMER $D_3[N]$

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Abstract: Let $G = (V, E)$ be a graph, where $V(G)$ is a non-empty set of vertices and $E(G)$ is a set of edges, $e = uv \in E(G)$, d_u be degree of vertex u. The distance between two vertices of G is the length of a shortest path connecting these two vertices. The eccentricity ϵ_u of a vertex u in G is the largest distance between u and any other vertex of G. In this paper, we consider an infinite family of Nanostar Dendrimers and compute its First Eccentric Zagreb index. The First Eccentric Zagreb index was introduced by Ghorbani and Hosseinzadeh as $Zg_1^*(G) = \sum_{uv\in E(G)} \left(\epsilon_u + \epsilon_v\right)$, that ϵ_u is the eccentricity of a vertex u and ϵ_v is the eccentricity of a vertex v of G.

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1. Introduction

Chemical graph theory is a branch of mathematical chemistry which has an important effect on the development of the chemical sciences. A topological index is a numerical value associated with the chemical constitution of a certain chemical compound aiming to correlate various physical and chemical properties, or some biological activity in it. Carbon nanostructures have found many potential industrial applications such as energy storage, gas sensors, biosensors, nanoelectronic devices and chemical probes [29], just to name a few. Carbon allotropes such as carbon nanocones and carbon nanotubes have been proposed as possible molecular gas storage devices [1, 35].

The Nanostar Dendrimer is a part of a new group of macromolecules that seem photon funnels just like artificial antennas and also is a great resistant of photo bleaching. Recently some people investigated the mathematical properties of these nanostructures in [21-36].

Let $G = (V, E)$ be a simple connected molecular graph, the vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively. Throughout this paper, graph means simple connected graph [23, 24, 34]. If $x, y \in V(G)$ then the distance $d(u, v)$ between u and v is defined as the length of a minimum path connecting u and v. The eccentricity ϵ_u of a vertex u in G is the largest distance between u and any other vertex of G.

The *Eccentric connectivity index* of the molecular graph G, was proposed by Sharma, Goswami and Madan [33] as,

$$\xi(G) = \sum_{u \in V(G)} d_u \epsilon_u$$

where d_u is the degree of the vertex u and ϵ_u is the eccentricity of the vertex u.

The Zagreb topological index Zg_1 was introduced by I. Gutman and N. Trinajstic in 1972 [23, 24] as the sum of the squares of the degrees of all vertices of G

$$Zg_1(G) = \sum_{u \in V(G)} (d(u))^2,$$

where d_u denotes the degree of u. Mathematical properties of the First Zagreb index for general graphs can be found in [23, 24, 31, 34].

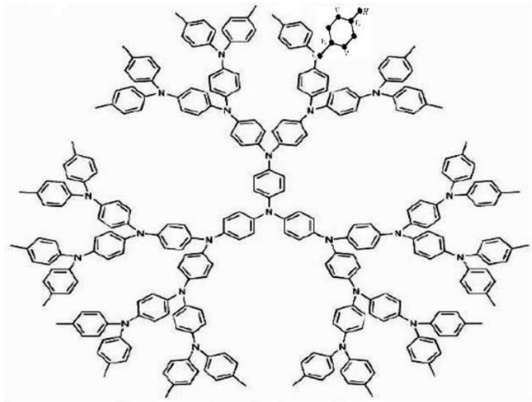

Figure 1: An example of the Nanostar Dendrimer $D_3[n]$, for $n = 3$

Recently in 2012, the *First Eccentric Zagreb index* was introduced by Ghorbani and Hosseinzadeh that is the Eccentric version of first Zagreb index of the molecular graph G and is equal to [21]

$$Zg_1^*(G) = \sum_{uv \in E(G)} [\epsilon_u + \epsilon_v],$$

where ϵ_u is the eccentricity of the vertex u and ϵ_v is the eccentricity of the vertex v.

In this study, we consider an infinite family of Nanostar Dendrimers and compute its First Eccentric Zagreb index and we call this First Eccentric Zagreb index $Zg_1^*(G)$ by the *Third Zagreb index* and denote by $Zg_3(G)$.

2. Results And Discussion

In this sections, we compute the third Zagreb index $Zg_3(G)$ of an infinite family of Nanostar Dendrimers, we denote the n^{th} growth of Nanostar Dendrimer $(\forall n \geq 1)$ by $D_3[n]$.

From Figure 1, one can see that the general representation of this family of Nanostar has $21(2^{n+1}) - 20$ vertices/atoms and $24(2^{n+1} - 1)$ bonds/edges [10]–[19]. Also, the Nanostar Dendrimer $D_3[n]$ has a core depicted in Figure 2 and a repeat element cycle C_6 that we named by *Leaf*, and obviously the n^{th} growth of Nanostar Dendrimer has of leafs, see Figure 2.

$$\xi_n 3 \sum_{i=0}^{n} (2^i) = 3 \left(\frac{2^{n+1} - 1}{2 - 1} \right).$$

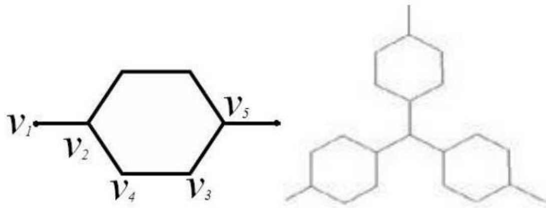

Figure 2: The added graph in each branch and $D_3[0]$ is the primal structure of Nanostar Dendrimer $D_3[n]$.

Consider the $n-1$th growth of Nanostar Dendrimer in $D_3[n-1]$ and we would like to construct $D_3[n]$. In every branch of $D_3[n]$, the leaf graph added. From Figure.2, one can see that the maximum eccentricity of a leaf of $D_3[n]$ is 6, and also, the eccentricity of previous vertices of core $D_3[0]$ are equal to 10.

Thus, for eccentric of vertices in added leaf of Nanostar Dendrimer $D_3[n-1]$ to $D_3[n]$, we can following results:

For all $i = 1, 2, ..., n$ We have $3(2^{i-1})$ vertices of kind labeled $V_1[i]$ with eccentricity $5i + 5(i + 1)$ and have $3(2^i)$ vertices of kind labeled $V_2[i]$ with eccentricity $5i + 5(i + 1)$. Also there are $3(2^{i+1})$ vertices of $V_3[i]$ and $V_4[i]$, with eccentricity $10i + 7$ and $10i + 8$, respectively. And $3(2^i)$ vertices $V_5[i]$, its eccentricity is $10i + 9$.

Therefore, by using above mention results, we have the following computations for third Zagreb index of the n^{th} growth of Nanostar Dendrimer $D_3[n]$ as:

Theorem 1. *We consider the graph of Nanostar Dendrimer $D_3[n]$. Then third Zagreb index is equal to*

$$Zg_3(D_3[n]) = zg_3(D_3[0]) + \sum_{\forall i=1,\ldots,n} 2^i(20i+1) + 6 \sum_{\forall i=1,\ldots,n} 2^i(20i+13) + 6 \sum_{\forall i=1,\ldots,n} 2^i(20i+15) + 6 \sum_{\forall i=1,\ldots,n} 2^i(20i+17) + 3(2^n)(20n+19).$$

Proof. Let G be the graph of Nanostar Dendrimer $D_3[n]$. Since we have

$$Zg_3(D_3[n]) = zg_3(D_3[0]) + \sum_{\forall i=1,\ldots,n;uv\in E(D_3[n])u\in V_1[i],v\in V_2[i]} \left(\epsilon_u + \epsilon_v\right) + \sum_{\forall i=1,\ldots,n;uv\in E(D_3[n])u\in V_2[i],v\in V_3[i]} \left(\epsilon_u + \epsilon_v\right)$$

$$
\begin{aligned}
&+ \sum_{\forall i=1,\ldots,n; uv\in E(D_3[n]) u\in V_3[i], v\in V_4[i]} \big(\epsilon_u + \epsilon_v\big)\\
&+ \sum_{\forall i=1,\ldots,n; uv\in E(D_3[n]) u\in V_4[i], v\in V_5[i]} \big(\epsilon_u + \epsilon_v\big)\\
&+ \sum_{vH\in (D_3[n]), H\in V_1[n+1], v\in V_5[n]} \big(ecc\epsilon_H + \epsilon_v\big),
\end{aligned}
$$

$$
\begin{aligned}
Zg_3(D_3[n]) =& zg_3(D_3[0]) + \sum_{\forall i=1,\ldots,n} 3(2^i)\big(\epsilon_{V_1[i]}\\
&+ \epsilon_{V_2[i]}\big) + \sum_{\forall i=1,\ldots,n} 3(2^i)\big(\epsilon_{V_2[i]}\\
&+ \epsilon_{V_3[i]}\big) + \sum_{\forall i=1,\ldots,n} 3(2^i)\big(\epsilon_{V_3[i]} + \epsilon_{V_4[i]}\big)\\
&+ \sum_{\forall i=1,\ldots,n} 3(2^i)\big(\epsilon_{V_4[i]} + \epsilon_{V_5[i]}\big) + 3(2^n)\big(\epsilon_H + \epsilon_{V_5[n]}\big).
\end{aligned}
$$

By using above values we obtain

$$
\begin{aligned}
Zg_3(D_3[n]) =& zg_3(D_3[0]) + \sum_{\forall i=1,\ldots,n} 3(2^i)(10i+5+10i+6)\\
&+ \sum_{\forall i=1,\ldots,n} 3(2^{i+1})(10i+6+10i+7)\\
&+ \sum_{\forall i=1,\ldots,n} 3(2^{i+1})(10i+7+10i+8)\\
&+ \sum_{\forall i=1,\ldots,n} 3(2^{i+1})(10i+8+10i+9) + 3(2^n)(10n+10+10n+9).
\end{aligned}
$$

After doing some calculations:

$$
\begin{aligned}
Zg_3(D_3[n]) =& zg_3(D_3[0]) + \sum_{\forall i=1,\ldots,n} 2^i(20i+1) + 6\sum_{\forall i=1,\ldots,n} 2^i(20i+13)\\
&+ 6\sum_{\forall i=1,\ldots,n} 2^i(20i+15) + 6\sum_{\forall i=1,\ldots,n} 2^i(20i+17) + 3(2^n)(20n+19). \qquad \square
\end{aligned}
$$

3. Conclusion

In this paper, we have discussed the Eccentric connectivity index, First Zagreb index and Third Zagreb index. We have considered an infinite family of

Nanostar Dendrimers and we have computed its Third Zagreb index.

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