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Research Article

ON THE GENERALIZED ZAGREB INDEX OF DENDRIMER NANOSTARS

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ABSTRACT

In this paper, we focus on the structure of molecular graph "Dendrimer Nanostars $D_3[n]$" $(\forall n\in\mathbb{N}\cup\{0\})$ and present some new results about the Generalized Zagreb index of Dendrimer Nanostars.

Keywords: Molecular graph; Dendrimer Nanostars; Zagreb indices; Generalized Zagreb Index.

1. INTRODUCTION

Let $G=(V,E)$ be a simple connected graph of finite order n and the sets of vertices and edges of G are denoted by $V=V(G)$ and $E=E(G)$, respectively. In such a simple molecular graph, vertices represent atoms and edges represent bonds. We denote degree and distance by d_v and $d(u,v)$, that the degree of a vertex v of G which is defined as the number of edges incident to v and the distance $d(u,v)$ between the vertices u and v of the graph G is equal to the length of (number of edges in) the shortest path that connects u and v A general reference for the notation in graph theory is [1-6].

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In chemistry, graph invariants are known as topological indices. In graph theory, we have many different topological indices of arbitrary graph *G*. A topological index of a graph is a number related to a graph which is invariant under graph automorphisms. Obviously, every topological index defines a counting polynomial and vice versa.

The Wiener index *W(G)* is the oldest based structure descriptor introduced by *Harold Wiener* in 1947[7], is the first topological index in chemistry. The Wiener index of *G* is defined as the sum of distances between all pairs of vertices of *G* and is equal as follow:

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

where *d(u,v)* is distance between the vertices *u* and *v* of the graph *G* [7-11].

More than forty years ago by *I. Gutman* and *N. Trinajstić* introduced the *First Zagreb index* $M_1(G)$ [4,5]. It is defined as the sum of squares of the vertex degrees d_u and d_v of vertices *u* and *v* in *G*. Recently, we know the *Second Zagreb index* $M_2(G)$. The first and second Zagreb indices of *G* are denoted by $M_1(G)$ *and* $M_2(G)$, respectively and defined as follows:

$$M_1(G)=\sum_{v\in V(G)} (d_v^2) \text{ or } \sum_{e=uv\in E(G)} (d_v+d_v)$$

$$M_2(G)=\sum_{e=uv\in E(G)} (d_v\times d_v)$$

where d_u and d_v are the degrees of *u* and *v*, respectively.

Also, we know that their polynomials (the *First Zagreb polynomial* $M_1(G,x)$ and the *Second Zagreb polynomial* $M_2(G,x)$) as follow:

$$M_1(G,x)=\sum_{e=uv\in E(G)} x^{(d_v+d_v)}$$

$$M_2(G,x)=\sum_{e=uv\in E(G)} x^{(d_v\times d_v)}$$

On the other hands, one can see that the First Zagreb index $M_1(G)$ and the Second Zagreb index $M_2(G)$ are equal to first derivative of its polynomial (at x=1) $\forall i=1,2,$ respectively as:

$$M_i(G)=\frac{\partial M_i(G,x)}{\partial x}|_{x=1}$$

The readers interested in more information on the Zagreb indices and topological indices can be referred to [11-29] and to the references therein.

In 2011, *A. Iranmanesh et.al* [30] introduced the generalized Zagreb index of a connected graph *G,* based on degree of vertices of *G*. The *Generalized Zagreb index* is defined as:

Definition 1: [30] Let *G* be a graph with the set of vertices *V*(*G*) and the set of edges *E*(*G*). The Generalized Zagreb index of *G* is defined for arbitrary non-negative integer *r* and *s* as follows $(\forall r,s\in\mathbb{N})$:

$$M_{\{r,s\}}(G)=\sum_{e=uv\in E(G)} (d_u^r d_v^s+d_u^s d_v^r)$$

Corollary 1. [30,31] Let G be a graph with the vertex and edge sets $V(G)$ and $E(G)$. Some of the properties of the generalized Zagreb index of G are as

$$M_{\{0,0\}}(G)=2\sum_{v\in V(G)}=2|E(G)|$$

$$M_{\{1,0\}}(G)=M_1(G)$$

$$M_{\{r-1,0\}}(G)=\sum_{v\in V(G)} d_v^r$$

$$M_{\{1,1\}}(G)=2M_2(G)$$

$$M_{\{r,r\}}(G)=2\sum_{uv\in E(G)}(d_u\times d_v)^r$$

The goal of this paper is computing the *Generalized Zagreb index* of an infinite class of Dendrimer Nanostars $D_3[n]$ $(\forall n\in\mathbb{N}\cup\{0\})$.

2. RESULTS AND DISCUSSION

A Dendrimer Nanostars an artificially manufactured or synthesized molecule built up from branched units called monomers and is one of the main objects of Nano biotechnology that is prepared in a step-wise fashion from simple branched monomer units, the nature and functionality of which can be easily controlled and varied. The first terms of this family of Nanostars are shown Fig.1 and Fig.2. For more study about Dendrimer Nanostars, we encourage the reader to consult papers and books [32-39].

Now, we present some new results about this general version of Zagreb indices an infinite class of Dendrimer Nanostars $D_3[n]$ $(\forall n\in\mathbb{N}\cup\{0\})$.

By these terminologies, we can present the main results of this paper in following theorem.

Theorem 1. Let $D_3[n]$ be the n^{th} growth of Dendrimer Nanostar $(\forall n\in\mathbb{N}\cup\{0\})$. Then, the generalized Zagreb index of $D_3[n]$ is equal to $(\forall r,s\in\mathbb{N})$:

$$M_{\{r,s\}}(D_3[n])=3(2^n)(3^r+3^s-2(3^{r+s}))+4\zeta_n(3^{r+s}+3^r2^s+3^s2^r+2^{r+s})$$

Proof of Theorem 1. Consider the Dendrimer Nanostar $D_3[n]$ $(\forall n\in\mathbb{N}\cup\{0\})$. Now, for

achieve our favorite topological indices of this class of Dendrimer Nanostars, we present the following notations.

For a graph $G=(V;E)$, we have several partitions of the vertex set $V(G)$ and the edge set $E(G)$ of G, as follow [20]:

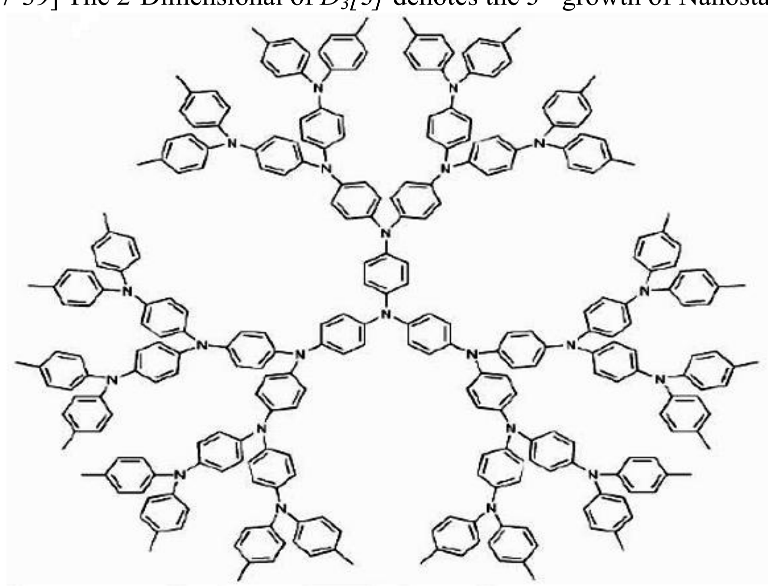
$$\forall k:\ \delta\le k\le\Delta,\ V_k(G)=\{v\in V(G)|\ d_v=k\}$$

$$\forall i,j:\ \delta\le i,j\le\Delta,\ E_{\{i,j\}}(G)=\{uv\in E(G)|d_u=I\ \&\ d_v=j\}$$

such that $V(G)=\bigcup_{i=\delta}^{\Delta}V_i(G)$, $E(G)=\bigcup_i E_{\{i,j\}}(G)$, where $\delta=Min\{d_v|v\in V(G)\}$ and $\Delta=Max\{d_v|v\in V(G)\}$ be the minimum degree and the maximum degree of vertices of G, respectively.

From the 2-Dimensional structure of Dendrimer Nanostar $D_3[n]$ (depicted in Figure 1) and a "Core $D_3[0]$" and "*Leaf*" (depicted in Figure 2), we see that $D_3[n]$ create by add $3(2^n)$ leafs to $D_3[n-1]$ in the n^{th} growth of Dendrimer Nanostar. Thus, there are $\zeta_n=3\sum_{i=0}^{n}(2^i)=3\left(\frac{2^{n+1}-1}{2-1}\right)=3(2^{n+1}-1)$ leafs (C_6) in Dendrimer $D_3[n]$.

Figure 1. [37-39] The 2-Dimensional of $D_3[3]$ denotes the 3^{th} growth of Nanostar Dendrimer.



Therefore, by using above notations and reference [37-39], we have

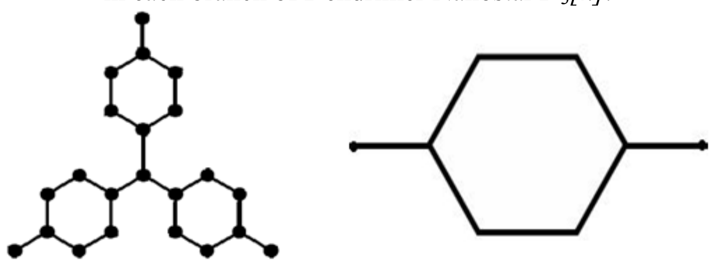
$$V_1=\{v\in V(D_3[n])|\ d_v=1\}\rightarrow|V_1(D_3[n])|=2\times|V_1(D_3[n-1])|=3(2^n)$$

$$V_2=\{v\in V(D_3[n])|\ d_v=2\}\rightarrow|V_2(D_3[n])||=V_2(D_3[n-1])|+4\times3(2^n)=12(2^{n+1}-1)$$

$$V_3=\{v\in V(D_3[n])|\ d_v=3\}\rightarrow|V_3(D_3[n])|=15(2^n)$$

Thus $V(D_3[n])=V_1 \cup V_2 \cup V_3 \rightarrow |V(D_3[n])|=4(3(2^{n+1})-5)$.

Figure 2. [37-39] A "Core $D_3[0]$" is the primal structure (A) and a "Leaf" is the added graph in each branch of Dendrimer Nanostar $D_3[n]$.



(A) (B)

Also, from the structure of Dendrimer Nanostar $D_3[n]$ in Figure 1) [37-39], one can see that

$$E_{\{1+3\}}=\{ uv\in E(D_3[n]) |\ d_u=1 \& d_v=3\} \rightarrow |E_{\{1+3\}}|=3(2^n)$$
$$E_{\{2+2\}}=\{ uv\in E(D_3[n]) |\ d_u=d_v=2\} \rightarrow |E_{\{2+2\}}|=2\zeta_n=6(2^{n+1}-1)$$
$$E_{\{2+3\}}=\{e=uv\in E(D_3[n]) |\ d_u=3 \ \& d_v=2\} \rightarrow |E_{\{2+3\}}|=4\zeta_n=12(2^{n+1}-1)$$
$$E_{\{3+3\}}=\{e=uv\in E(D_3[n]) |\ d_u=d_v=3\} \rightarrow |E_{\{3+3\}}|=2\zeta_n-3(2^n)=9(2^n)-6$$

And these imply that

$$E(D_3[n])=E_{\{1+3\}} \cup E_{\{2+2\}} \cup E_{\{2+3\}} \cup E_{\{3+3\}} \rightarrow |E(D_3[n])|=8\zeta_n=24(2^{n+1}-1)$$

Now, we have following computations for the generalized Zagreb index of the n^{th} growth of Dendrimer Nanostar $D_3[n]$ $(\forall n\in \mathbb{N}\cup\{0\})$ as:

$$\begin{aligned}
M_{\{r,s\}}\left(D_3[n]\right) &= \sum_{e=uv\in E(D_3[n])}\left(d_u^{\ r} d_v^{\ s}+d_u^{\ s} d_v^{\ r}\right)\\
&=\sum_{uv\in E_{\{1,3\}}}\left(3^r1^s+3^s1^r\right)+\sum_{e=uv\in E_{\{2,2\}}}\left(2^r2^s+2^s2^r\right)+\sum_{e=uv\in E_{\{2,3\}}}\left(3^r2^s+3^s2^r\right)+\sum_{e=uv\in E_{\{3,3\}}}\left(3^r3^s+3^s3^r\right)\\
&=\sum_{uv\in E_{\{1,3\}}}\left(3^r+3^s\right)+\sum_{uv\in E_{\{2,2\}}}2\left(2^{r+s}\right)+\sum_{uv\in E_{\{2,3\}}}\left(3^r2^s+3^s2^r\right)+\sum_{uv\in E_{\{3,3\}}}2\left(3^{r+s}\right)\\
&=\left(3^r+3^s\right)\times(3\left(2^n\right))+2\left(2^{r+s}\right)\times(6\left(2^{n+1}-1\right))+\left(3^r2^s+3^s2^r\right)\times\left(12\left(2^{n+1}-1\right)\right)+2\left(3^{r+s}\right)\times\left(9\left(2^n\right)-6\right)\\
&=\left(3^r+3^s\right)\times(3\left(2^n\right))+2\left(2^{r+s}\right)\times(2\zeta_n)+\left(3^r2^s+3^s2^r\right)\times\left(4\zeta_n\right)+2\left(3^{r+s}\right)\times\left(2\zeta_n-3\left(2^n\right)\right)\\
&=3\left(2^n\right)\left(3^r+3^s-2\left(3^{r+s}\right)\right)+4\zeta_n\left(3^{r+s}+3^r2^s+3^s2^r+2^{r+s}\right).
\end{aligned}$$

Finally, the generalized Zagreb index of Dendrimer Nanostar $D_3[n]$ is equal to

$$M_{\{r,s\}}(D_3[n])=3(2^n)(x+y-2xy)+4\zeta_n(xy+xt+yz+tz)$$

In which $x=3^r$, $y=3^s$, $z=2^r$, $t=2^s$ and $\zeta_n=3(2^{n+1}-1)$ and this completed the proof of the Theorem1.■

Corollary 2. Consider the Dendrimer Nanostars $D_3[n]$ for all non-negative integer number n, thus the first and second Zagreb indices of $D_3[n]$ are equal to

$$M_1(D_3[n])=M_{\{1,0\}}(D_3[n])=6(39(2^n)-20)$$

and

$$M_2(D_3[n])=½M_{\{1,1\}}(D_3[n])=6(47(2^n)-25)$$

also

$$|E(D_3[n])|=½\,M_{\{0,0\}}(D_3[n])=8\zeta_n=24(2^{n+1}-1).$$

Proof of Corollary 2. $\forall n\in\mathbb{N}\cup\{0\}$, Consider the Dendrimer Nanostars $D_3[n]$, by using Theorem 1 and Corollary 1 the proof is obvious.

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