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The second eccentric Zagreb index of the N^{TH} growth nanostar dendrimer $D_3[N]$

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Abstract. Let $G = (V,E)$ be an ordered pair, where $V(G)$ is a non-empty set of vertices and $E(G)$ is a set of edges called a graph. We denote a vertex by v, where $v \in V(G)$ and edge by e, where $e = uv \in E(G)$. We denote degree of vertex v by d_v which is defined as the number of edges adjacent with vertex v. The distance between two vertices of G is the length of a shortest path connecting these two vertices which is denoted by $d(u,v)$ where $u,v \in V(G)$. The eccentricity $ecc(v)$ of a vertex v in G is the distance between vertex v and vertex farthest from v in G. In this paper, we consider an infinite family of nanostar dendrimers and then we compute its second eccentric Zagreb index. Ghorbani and Hosseinzadeh introduced the second eccentric Zagreb index as $EM_2(G) = \sum_{uv\in E(G)} \big(ecc(u) \times ecc(v)\big)$, that $ecc(u)$ denotes the eccentricity of vertex u and $ecc(v)$ denotes the eccentricity of vertex v of G.

Keywords. molecular graph, eccentricity, Zagreb topological index, nanostar dendrimer, $D_3[n]$.

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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 [23], just to name a few. Carbon allotropes such as carbon nanocones and carbon nanotubes have been proposed as possible molecular gas storage devices [1,32].

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 [24,29–31].

Let $G = (V, E)$ be a simple connected molecular graph, the vertex and edge sets of graph G are denoted by $V(G)$ and $E(G)$, respectively. Throughout this paper, graph means simple connected graph [17,18,28]. 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 $ecc(u)$ 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 [27] as,

$$\xi(G) = \sum_{u \in V(G)} d_v ecc(v),$$

where d_v is the degree of the vertex v and $ecc(v)$ is the eccentricity of the vertex v.

The Zagreb topological indices was introduced by I. Gutman and N. Trinajstić in 1972 [17,18]. The first and second zagreb indices are defined as

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

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

where d_v denotes the degree of v. Mathematical properties of the first Zagreb index for general graphs can be found in [17,18,26,28].

Recently in 2012, the *second eccentric Zagreb index* was introduced by Ghorbani and Hosseinzadeh that is the eccentric version of second Zagreb index of the molecular graph G and it is equal to [15]

$$EM_2(G) = \sum_{uv \in E(G)} [ecc(u) \times ecc(v)],$$

where $ecc(u)$ is the eccentricity of the vertex u and $ecc(v)$ is the eccentricity of the vertex v.

In this study, we consider an infinite family of nanostar dendrimers and compute its second eccentric Zagreb index.

2 Results And Discussion

Here, we compute the second eccentric Zagreb index of an infinite family of nanostar dendrimers, we denote the n^{th} growth of nanostar dendrimer for all$n \geq 1$ 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 [11–13]. Also, the nanostar dendrimer $D_3[n]$ has a core depicted in Figure 2 and the repeated element cycle C_6 that we named by *leaf*, and obviously the n^{th} growth of nanostar dendrimer has

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

of leafs, see Figure 2.

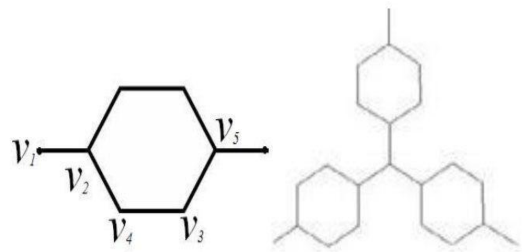

Figure 1. An example of the nanostar dendrimer $D_3[n]$, for $n = 3$ [11–14].

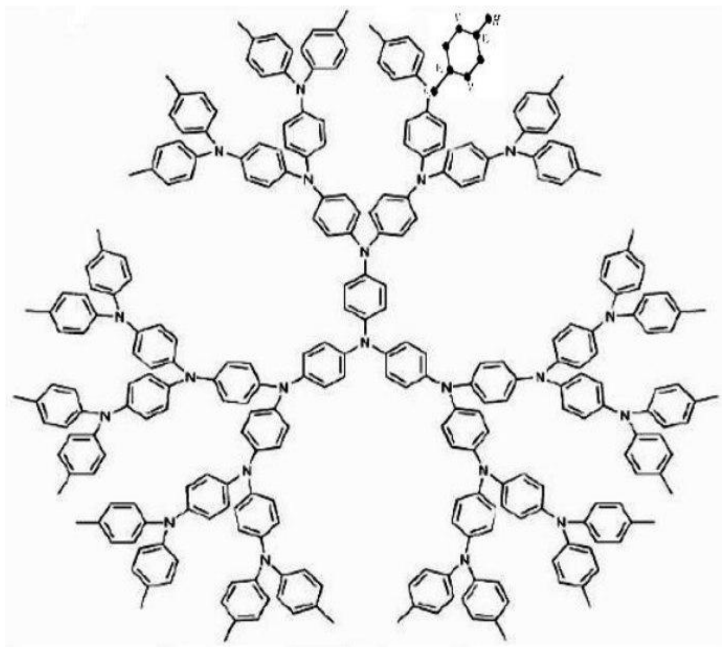

Figure 2. The added graph in each branch and $D_3[0]$ is the primal structure of nanostar dendrimer $D_3[n]$ [11–14].

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. Also, for the vertices of $V_5[i]$, 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 $D_3[n]$.

Theorem 2.1. *We consider the graph of nanostar dendrimer $D_3[n]$. Then second eccentric Zagreb index is equal to*

$$\begin{aligned} EM_2(D_3[n]) &= EM_2(D_3[0]) + 3\sum_{\forall i=1,\dots,n} 2^i(100i^2+110i+30) \\ &+ 6\sum_{\forall i=1,\dots,n} 2^i(100i^2+130i+42) + 6\sum_{\forall i=1,\dots,n} 2^i(100i^2+150i+56) \\ &+ 6\sum_{\forall i=1,\dots,n} 2^i(100i^2+170i+72) + 3(2^n)(100n^2+190n+90). \end{aligned}$$

Proof. Let G be the graph of nanostar dendrimer $D_3[n]$. Hence, we have

$$\begin{aligned} EM_2(D_3[n]) &= EM_2(D_3[0]) + \sum_{\forall i=1,\dots,n; uv\in E(D_3[n]) u\in V_1[i], v\in V_2[i]} \big(ecc(u)\times ecc(v)\big) \\ &+ \sum_{\forall i=1,\dots,n; uv\in E(D_3[n]) u\in V_2[i], v\in V_3[i]} \big(ecc(u)\times ecc(v)\big) \\ &+ \sum_{\forall i=1,\dots,n; uv\in E(D_3[n]) u\in V_3[i], v\in V_4[i]} \big(ecc(u)\times ecc(v)\big) \\ &+ \sum_{\forall i=1,\dots,n; uv\in E(D_3[n]) u\in V_4[i], v\in V_5[i]} \big(ecc(u)\times ecc(v)\big) \\ &+ \sum_{vH\in(D_3[n]), H\in V_1[n+1], v\in V_5[n]} \big(ecc(H)\times ecc(v)\big), \end{aligned}$$

$$\begin{aligned} EM_2(D_3[n]) &= EM_2(D_3[0]) + \sum_{\forall i=1,\dots,n} 3(2^i)\big(ecc(V_1[i])\times ecc(V_2[i])\big) \\ &+ \sum_{\forall i=1,\dots,n} 3(2^i)\big(ecc(V_2[i])\times ecc(V_3[i])\big) \\ &+ \sum_{\forall i=1,\dots,n} 3(2^i)\big(ecc(V_3[i])\times ecc(V_4[i])\big) \\ &+ \sum_{\forall i=1,\dots,n} 3(2^i)\big(ecc(V_4[i])\times ecc(V_5[i])\big) \\ &+ 3(2^n)\big(ecc(H)\times ecc(V_5[n])\big). \end{aligned}$$

By using above values we get

$$\begin{aligned}EM_2(D_3[n]) = EM_2(D_3[0]) &+ \sum_{\forall i=1,\dots,n} 3(2^i)\big((10i+5)\times(10i+6)\big)\\ &+ \sum_{\forall i=1,\dots,n} 3(2^{i+1})\big((10i+6)\times(10i+7)\big)\\ &+ \sum_{\forall i=1,\dots,n} 3(2^{i+1})\big((10i+7)\times(10i+8)\big)\\ &+ \sum_{\forall i=1,\dots,n} 3(2^{i+1})\big((10i+8)\times(10i+9)\big)\\ &+ 3(2^n)\big((10n+10)\times(10n+9)\big).\end{aligned}$$

After doing some calculations, we have

$$\begin{aligned}EM_2(D_3[n]) = EM_2(D_3[0]) &+ 3\sum_{\forall i=1,\dots,n} 2^i(100i^2+110i+30)\\ &+ 6\sum_{\forall i=1,\dots,n} 2^i(100i^2+130i+42) + 6\sum_{\forall i=1,\dots,n} 2^i(100i^2+150i+56)\\ &+ 6\sum_{\forall i=1,\dots,n} 2^i(100i^2+170i+72) + 3(2^n)(100n^2+190n+90).\end{aligned}$$

□

3 Conclusion

In this paper, we discussed the eccentric connectivity index, first Zagreb index and second Zagreb index. We have considered an infinite family of nanostar dendrimers and we computed its second eccentric Zagreb index.

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