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On the Zagreb indices of nanostar dendrimers

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Let G be a graph. The first and second Zagreb index of G is defined as $M_1(G)=\sum_{v\in V(G)}\deg_G(v)^2$ and $M_2(G)=\sum_{uv\in E(G)}\deg_G(u)\deg_G(v)$ respectively. In this paper we compute Zagreb indices of chain graphs.

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1. Introduction

Dendrimers are macromolecular nanoscale objects that are widely recognized as precise, mathematically defined, covalent core-shell assemblies. Since dendrimers are well defined organic molecules in the size range of (1 to 15) nm and are known to act as hosts for guest molecules, they are promising candidates as templates for the formation of inorganic nanoclusters [1,2].

Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena [3]. This theory had an important effect on the development of the chemical sciences. Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by V(G) and E(G), respectively. A topological index of a graph G is a numeric quantity related to G. The oldest topological index is the Wiener index which introduced by Harold Wiener [4]. The name of topological index was introduced by Haro Hosoya [5]. We encourage the reader to consult [6] for historical background material as well as basic computational techniques. Two topological indices, symbolized by M_1 and M_2 are defined in terms of vertex-degrees as follows [7, 8]:

$M_1(G)=\sum_{v\in V(G)}\deg_G(v)^2$ and $M_2(G)=\sum_{uv\in E(G)}\deg_G(u)\deg_G(v)$.

In this paper by using definition of chain graphs we compute two Zagreb indices of nanostar dendrimers. Herein, our notation is standard and taken from the standard book of graph theory [9-17].

2. Main results and discussion

Suppose G_is $(1 \le i \le n)$ be some graphs and $v_i \in V(G_i)$. A chain graph denoted by $G=G(G_1,\dots,G_n,v_1,\dots,v_n)$ is the union of G_is together with edges v_iv_{i+1} $(1 \le i \le n-1)$, see Fig. 1. Then $|V(G)|=\sum_{i=1}^{n}|V(G_i)|$ and $|E(G)|=(n-1)+\sum_{i=1}^{n}|E(G_i)|$.

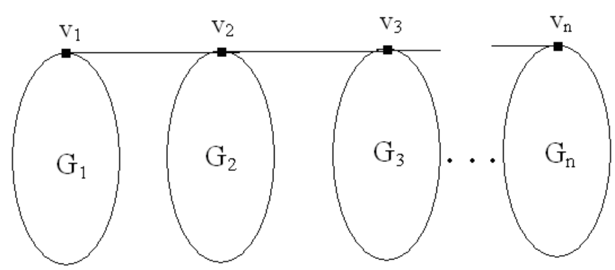

Fig. 1. The chain graph $G=G(G_1,\dots,G_n,v_1,\dots,v_n)$.

Before calculating the Zagreb indices for nanostar dendrimers, we must compute these indices, for some well-known class of graphs.

Example 1. Consider the ladder graph L_n, with $2n$ vertices (Fig. 2). It is easy to see that $|E(L_n)|=3n-2$, $M_1(L_n)=18n-20$ and $M_2(L_n)=27n-40$ $(n\ge 3)$.

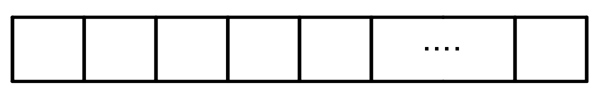

Fig. 2. Graph of ladder with 2n vertices.

Example 2. Consider the wheel graph W_n, with $n+1$ vertices (Fig. 3). One can see that $|E(W_n)|=2n$, $M_1(W_n)=n^2+4n$ and $M_2(W_n)=3n^2-9n$.

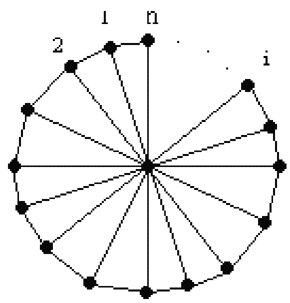

Fig. 3. Graph of wheel on n + 1 vertices.

Example 3. Let $GP(n,k)$ be generalized Petersen graph with parameters n and k, the vertex set $V=\{x_1,...,x_n,y_1,...,y_n\}$ and the edge set $E=\{x_1x_2,x_2x_3,...,x_nx_1,x_1y_1,x_2y_2,...,x_ny_n,y_1y_{k+1},y_2y_{k+2},...,y_ny_{k+n}\}$ (mod n) respectively. It is easy to see that $|E(GP(n,k))|=\begin{cases}3n & \text{if } n\neq 2k\\ \frac{5n}{2} & \text{if } n=2k\end{cases}$ and so, we have $M_1(GP(n,k))=\begin{cases}18n & \text{if } n\neq 2k\\ 13n & \text{if } n=2k\end{cases}$ and $M_2(GP(n,k))=\begin{cases}27n & \text{if } n\neq 2k\\ 17n & \text{if } n=2k\end{cases}$.

Lemma 1. Suppose $G=G(G_1,G_2,...,G_n,v_1,v_2,...,v_n)$ be a chain graph. So, we have:

(i) $|V(G(G_1,G_2,...,G_n,v_1,v_2,...,v_n))|=\sum_{i=1}^{n}|V(G_i)|$,

(ii) $|E(G(G_1,G_2,...,G_n,v_1,v_2,...,v_n))|=\sum_{i=1}^{n}|E(G_i)|+n-1$,

(iii) $G(G_1,G_2,...,G_n,v_1,v_2,...,v_n)$ is connected if and only if G_i ($1\le i\le n$) be connected,

(iv) $deg_G(a)=\begin{cases}deg_{G_i}(a) & a\in V(G_i) \text{ and } a\neq v_i\\ deg_{G_i}(a)+1 & a=v_i,\ i=1,n\\ deg_{G_i}(a)+2 & a=v_i,\ 2\le i\le n-1\end{cases}$.

Proof. The proof is straightforward.

Theorem 2. For the chain graph $G=G(G_1,G_2,v_1,v_2)$ we have:

$$M_1(G)=M_1(G_1)+M_1(G_2)+2(deg_{G_1}(v_1)+deg_{G_2}(v_2)+1)$$

and

$$M_2(G)=M_2(G_1)+M_2(G_2)+\sum_{i=1}^{2}\sum_{j=1}^{deg_{G_i}(v_i)}deg_{G_i}(u_{ij})+(deg_{G_1}(v_1)+1)(deg_{G_2}(v_2)+1)$$

in which vertices u_{ij} and v_i are adjacent.

Proof. By using definition of Zagreb index, one can see that

$$M_1(G)=\sum_{v\in V(G)}deg_G(v)^2=\sum_{\substack{v\in V(G_1)\\ v\neq v_1}}deg_{G_1}(v)^2+\sum_{\substack{v\in V(G_2)\\ v\neq v_2}}deg_{G_2}(v)^2$$

$$+\ (deg_{G_1}(v_1)+1)^2+(deg_{G_2}(v_2)+1)^2$$

$$=\ M_1(G_1)+M_1(G_2)+2(deg_{G_1}(v_1)+deg_{G_2}(v_2)+1)$$

and so,

$$M_2(G)=\sum_{uv\in E(G)}deg_G(u)deg_G(v)=\sum_{\substack{uv\in E(G_1)\\ u,v\neq v_1}}deg_{G_1}(u)deg_{G_1}(v)+\sum_{\substack{uv\in E(G_2)\\ u,v\neq v_2}}deg_{G_2}(u)deg_{G_2}(v)$$

$$+\sum_{i=1}^{2}\sum_{uv_i\in E(G_i)}(deg_{G_i}(v_i)+1)deg_{G_i}(u)+(deg_{G_1}(v_1)+1)(deg_{G_2}(v_2)+1)$$

$$=\ M_2(G_1)+M_2(G_2)+\sum_{i=1}^{2}\sum_{j=1}^{deg_{G_i}(v_i)}deg_{G_i}(u_{ij})+(deg_{G_1}(v_1)+1)(deg_{G_2}(v_2)+1)$$

Theorem 3. Consider the chain graph $G=G(G_1,G_2,...,G_n,v_1,v_2,...,v_n)$ ($n\ge 3$). We have:

$$M_1(G)=\sum_{i=1}^{n}M_1(G_i)+2\sum_{i=1,n}deg_{G_i}(v_i)+4\sum_{i=2}^{n-1}deg_{G_i}(v_i)+2(2n-3)$$

$$M_2(G)=\sum_{i=1}^{n}M_2(G_i)+\sum_{i=1,n}\sum_{j=1}^{deg_{G_i}(v_i)}deg_{G_i}(u_{ij})+2\sum_{i=2}^{n-1}\sum_{j=1}^{deg_{G_i}(v_i)}deg_{G_i}(u_{ij})$$

$$+\ (deg_{G_1}(v_1)+1)(deg_{G_2}(v_2)+2)+(deg_{G_{n-1}}(v_{n-1})+2)(deg_{G_n}(v_n)+1)$$

$$+\sum_{i=2}^{n-2}(deg_{G_i}(v_i)+2)(deg_{G_{i+1}}(v_{i+1})+2),$$

in which vertices u_{ij} are adjacent to the vertices v_i.

Proof.

$$M_1(G)=\sum_{v\in V(G)}deg_G(v)^2=\sum_{i=1}^{n}\sum_{\substack{v\in V(G_i)\\ v\neq v_i}}deg_{G_i}(v)^2\ +$$

$$\sum_{i=1,n}(deg_{G_i}(v_i)+1)^2+\sum_{i=2}^{n-1}(deg_{G_i}(v_i)+2)^2$$

$$=\sum_{i=1}^{n}M_1(G_i)+2\sum_{i=1,n}deg_{G_i}(v_i)+4\sum_{i=2}^{n-1}deg_{G_i}(v_i)+2(2n-3)$$

and

$$M_2(G)=\sum_{uv\in E(G)}deg_G(u)deg_G(v)=\sum_{i=1}^{n}\sum_{\substack{uv\in E(G_i)\\ u,v\neq v_i}}deg_{G_i}(u)deg_{G_i}(v)$$

$$+\ \sum_{i=1,n}\sum_{uv_i\in E(G_i)}(deg_{G_i}(v_i)+1)deg_{G_i}(u)+\sum_{i=2}^{n-1}\sum_{uv_i\in E(G_i)}(deg_{G_i}(v_i)+2)deg_{G_i}(u)$$

$$+\ (deg_{G_1}(v_1)+1)(deg_{G_2}(v_2)+2)+(deg_{G_{n-1}}(v_{n-1})+2)(deg_{G_n}(v_n)+1)$$

$$+\sum_{i=2}^{n-2}(deg_{G_i}(v_i)+2)(deg_{G_{i+1}}(v_{i+1})+2)$$

$$=\ \sum_{i=1}^{n}M_2(G_i)+\sum_{i=1,n}\sum_{j=1}^{deg_{G_i}(v_i)}deg_{G_i}(u_{ij})+2\sum_{i=2}^{n-1}\sum_{j=1}^{deg_{G_i}(v_i)}deg_{G_i}(u_{ij})$$

$$+\ (deg_{G_1}(v_1)+1)(deg_{G_2}(v_2)+2)+(deg_{G_{n-1}}(v_{n-1})+2)(deg_{G_n}(v_n)+1)$$

$$+\sum_{i=2}^{n-2}(\deg_{G_i}(v_i)+2)(\deg_{G_{i+1}}(v_{i+1})+2).$$

Example 4. Consider the graph G_1 shown in Fig. 4. It is easy to see that $M_1(G_1)=96$ and $M_2(G_1)=111$.

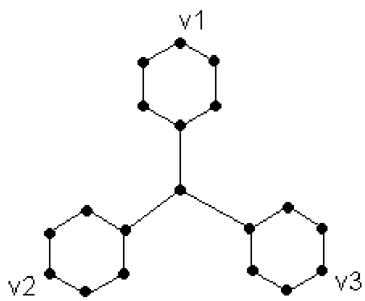

Fig. 4. Graph of nanostar dendrimer for n = 1.

Example 5. Consider the nanostar dendrimer shown in Fig. 5. For the first Zagreb index we have:

$$M_1(G_n)=M_1(G_{n-1})+M_1(G_1)+10,$$

$$M_1(G_{n-1})=M_1(G_{n-2})+M_1(G_1)+10,\cdots$$

and

$$M_1(G_2)=M_1(G_1)+M_1(G_1)+10.$$

Now by summation of these relations we have:

$$M_1(G_n)=M_1(G_1)+(n-1)M_1(G_1)+10(n-1)=nM_1(G_1)+10(n-1)$$

and then by using example 4 we consult $M_1(G_n)=106n-10$.

For the second Zagreb index one can see that $M_2(G_n)=M_2(G_{n-1})+M_2(G_1)+17$, $M_2(G_{n-1})=M_2(G_{n-2})+M_2(G_1)+17$, … and $M_2(G_2)=M_2(G_1)+M_2(G_1)+17$ and by summation of these relations we have $M_2(G_n)=M_2(G_1)+(n-1)M_2(G_1)+17(n-1)=nM_2(G_1)+17(n-1)$ and so, $M_2(G_n)=128n-17$.

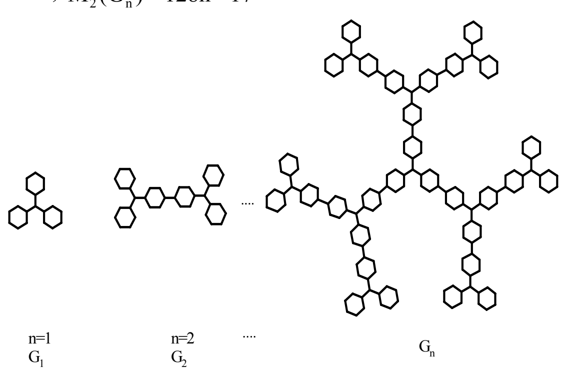

Fig. 5. Graph of nanostar dendrimer.

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