On multiplicative Zagreb indices of graphs

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ABSTRACT

Todeschini et al. have recently suggested to consider multiplicative variants of additive graph invariants, which applied to the Zagreb indices would lead to the multiplicative Zagreb indices of a graph *G*, denoted by $\Pi_1(G)$ and $\Pi_2(G)$, under the name first and second multiplicative Zagreb index, respectively. These are define as $\Pi_1(G) = \prod_{v\in V(G)} d_G(v)^2$ and $\Pi_2(G) = \prod_{uv\in E(G)} d_G(v)\, d_G(v)$, where $d_G(v)$ is the degree of the vertex *v*. In this paper we compute these indices for link and splice of graphs. In continuation, with use these graph operations, we compute the first and the second multiplicative Zagreb indices for a class of dendrimers.

Keywords: Multiplicative Zagreb indices, splice, link, chain graphs, dendrimer.

1. INTRODUCTION

In this article, we are concerned with simple graphs, that is finite and undirected graphs without loops and multiple edges. Let *G* be such a graph and *V*(*G*) and *E*(*G*) be its vertex set and edge set, respectively. An edge of *G*, connecting the vertices *u* and *v* will be denoted by *uv*. The degree $d_G(v)$ of a vertex $v \in V(G)$ is the number of vertices of *G* adjacent to *v*.

A molecular graph is a simple graph, such that its vertices correspond to the atoms and the edges to the bonds. Note that hydrogen atoms are often omitted. Molecular descriptors play a significant role in chemistry, pharmacology, etc. Among them, topological indices have a prominent place [10]. The vertex-degree-based graph invariants $M_1(G) = \sum_{v\in V(G)} d_G(v)^2$ and $M_2(G) = \sum_{uv\in E(G)} d_G(u)\, d_G(v)$ are known under the name first and second Zagreb index, respectively. These have been conceived in the 1970s and found considerable applications in chemistry [3,8,13]. The Zagreb indices were subject to a large number of mathematical studies, of which we mention only a few newest [4,7].

Todeschini et al. [9, 11] have recently proposed to consider multiplicative variants of additive graph invariants, which applied to the Zagreb indices would lead to

$$\Pi_1 = \Pi_1(G) = \prod_{v \in V(G)} d_G(v)^2$$

and

$$\Pi_2 = \Pi_2(G) = \prod_{uv \in E(G)} d_G(u)\, d_G(v)\,.$$

One can easily see that

$$\Pi_2(G) = \prod_{u \in V(G)} d_G(u)^{d_G(u)}\,. \qquad (1)$$

Our notation is standard and mainly taken from standard books of chemical graph theory [10,12]. For background materials, see reference [2,5,6].

2. MAIN RESULTS AND DISCUSSION

The goal of this section is obtaining formulas for some graph operations of multiplicative Zagreb indices. In the next section we will applied these graph operations to get some applications in chemistry.

SPLICE AND LINK

Suppose that *G* and *H* are graphs with disjoint vertex sets. Following Došlić [1], for given vertices $u \in V(G)$ and $v \in V(H)$ a splice of *G* and *H* by vertices *u* and *v*, denoted by $(G \bullet H)(u,v)$, is obtained by identifying the vertices *u* and *v* in the union of *G* and *H*. Similarly, a link of *G* and *H* by vertices *u* and *v* is defined as the graph $(G \square H)(u,v)$ obtained by joining *u* and *v* by an edge in the union of these graphs.

Let G_1 and G_2 be graphs as specified above. Denote the vertex obtained by identifying v_1 and v_2 by v_{12}. Then directly from the definition of their splice and link we obtain:

Lemma 1.

(i) $$d_{(G_1 \bullet G_2)(v_1,v_2)}\left(u\right) = \begin{cases} d_{G_i}(u) & u \in V(G_i) \quad \text{and} \quad u \neq v_i \\ d_{G_1}(v_1) + d_{G_2}(v_2) & u = v_{12} \end{cases},$$

(ii) $$d_{(G_1 \square G_2)(v_1,v_2)}(u) = \begin{cases} d_{G_i}(u) & u \in V(G_i)\ \left(i = 1,2\right) \quad \text{and} \quad u \neq v_i \\ d_{G_i}(u) + 1 & u = v_i\ ;\ i = 1,2 \end{cases}.$$

Theorem 2. The first multiplicative Zagreb index of the splice and link of *G₁* and *G₂* satisfies the relations

$$\Pi_1\left(G_1 \bullet G_2\right)\left(v_1, v_2\right) = \left(\frac{d_{G_1}(v_1) + d_{G_2}(v_2)}{d_{G_1}(v_1)\, d_{G_2}(v_2)}\right)^2 \Pi_1\left(G_1\right) \Pi_1\left(G_2\right)$$

$$\Pi_1\left(G_1 \square G_2\right)\left(v_1, v_2\right) = \left(\frac{\left(d_{G_1}(v_1) + 1\right)\left(d_{G_2}(v_2) + 1\right)}{d_{G_1}(v_1)\ d_{G_2}(v_2)}\right)^2 \Pi_1\left(G_1\right) \Pi_1\left(G_2\right)$$

Proof.
For the splice of G_1 and G_2we have

$$V(G_1 \bullet G_2) = \left[V(G_1) \setminus \{v_1\}\right] \cup \left[V(G_2) \setminus \{v_2\}\right] \cup \{v_{12}\}$$

which implies

$$\Pi_1\left(G_1 \bullet G_2\right)\left(v_1, v_2\right) = \left[\prod_{x \in V(G_1) \setminus \{v_1\}} d_{G_1}(x)^2\right]\left[\prod_{y \in V(G_2) \setminus \{v_2\}} d_{G_2}(y)^2\right]\left[d_{G_1 \bullet G_2}(v_{12})^2\right]$$

$$= \left[\frac{1}{d_{G_1}(v_1)^2} \prod_{x \in V(G_1)} d_{G_1}(x)^2\right]\left[\frac{1}{d_{G_2}(v_2)^2} \prod_{y \in V(G_2)} d_{G_2}(y)^2\right]\left[d_{G_1}(v_1) + d_{G_2}(v_2)\right]^2$$

$$= \left[\frac{1}{d_{G_1}(v_1)^2} \Pi_1(G_1)\right]\left[\frac{1}{d_{G_2}(v_2)^2} \Pi_1(G_2)\right]\left[d_{G_1}(v_1) + d_{G_2}(v_2)\right]^2$$

from which the first formula follows. Further, by part (ii) of Lemma 1,

$$\Pi_1\left(G_1 \sim G_2\right)\left(v_1,v_2\right)=\left[\prod_{x\in V(G_1)\setminus\{v_1\}} d_{G_1}(x)^2\right]\left[\prod_{y\in V(G_2)\setminus\{v_2\}} d_{G_2}(y)^2\right]\left[d_{G_1\sim G_2}(v_1)^2 d_{G_1\sim G_2}(v_2)^2\right]$$

$$=\left[\frac{1}{d_{G_1}(v_1)^2}\prod_{x\in V(G_1)} d_{G_1}(x)^2\right]\left[\frac{1}{d_{G_2}(v_2)^2}\prod_{y\in V(G_2)} d_{G_2}(y)^2\right]\left[[d_{G_1}(v_1)+1]^2[d_{G_2}(v_2)+1]^2\right]$$

$$=\left[\frac{1}{d_{G_1}(v_1)^2}\Pi_1(G_1)\right]\left[\frac{1}{d_{G_2}(v_2)^2}\Pi_1(G_2)\right]\left[[d_{G_1}(v_1)+1][d_{G_2}(v_2)+1]\right]^2$$

from which the second formula follows. ■

In a fully analogous manner, bearing in mind Eq. (1), we can prove:

Theorem 3. The second multiplicative Zagreb index of the splice and link of G_1 and G_2 satisfies the relations

$$\Pi_2\left(G_1\bullet G_2\right)\left(v_1,v_2\right)=\frac{[d_{G_1}(v_1)+d_{G_2}(v_2)]^{d_{G_1}(v_1)+d_{G_2}(v_2)}}{d_{G_1}(v_1)^{d_{G_1}(v_1)}\, d_{G_2}(v_2)^{d_{G_2}(v_2)}}\Pi_2\left(G_1\right)\Pi_2\left(G_2\right)$$

$$\Pi_2\left(G_1 \sim G_2\right)\left(v_1,v_2\right)=\frac{\left(d_{G_1}(v_1)+1\right)^{d_{G_1}(v_1)+1}\left(d_{G_2}(v_2)+1\right)^{d_{G_2}(v_2)+1}}{d_{G_1}(v_1)^{d_{G_1}(v_1)}\, d_{G_2}(v_2)^{d_{G_2}(v_2)}}\Pi_2\left(G_1\right)\Pi_2\left(G_2\right).$$

CHAIN GRAPHS

Let G_i $(1 \le i \le n)$ be some graphs and $v_i \in V(G_i)$. A chain graph, denoted by $G=G(G_1,\ldots,G_n,v_1,\ldots,v_n)$, is obtained from the union of the graphs G_i, $i=1,2,\ldots,n$, by adding the edges $v_i v_{i+1}$ $(1 \le i \le n-1)$, see Figure 1. Then $|V(G)|=\sum_{i=1}^{n}|V(G_i)|$ and $|E(G)|=(n-1)+\sum_{i=1}^{n}|E(G_i)|$.

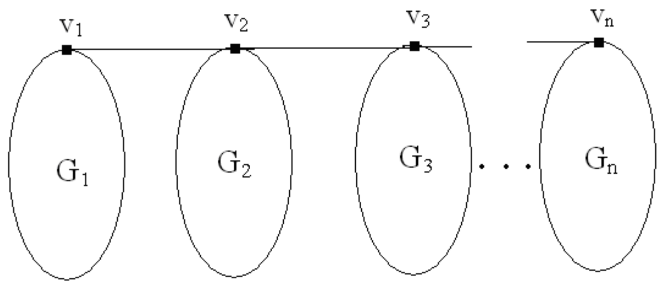

Figure 1. The Chain Graph $G = G(G_1,...,G_n,v_1,...,v_n)$.

One can see that $G\left(G_1,G_2,v_1,v_2\right) \cong \left(G_1 \square G_2\right)\left(v_1,v_2\right)$.

It is worth noting that the above-specified class of chain graphs embraces, as special cases, all trees and all unicyclic graphs. In addition, the molecular graphs of many polymers and dendrimers are chain graphs.

Lemma 4. Suppose that $G = G(G_1,G_2,...,G_n,v_1,v_2,...,v_n)$ is a chain graph. Then:

$$d_G(u) = \begin{cases} d_{G_i}(u) & u \in V(G_i) \text{ and } u \neq v_i \\ d_{G_i}(u) + 1 & u = v_i,\ \ i = 1,n \\ d_{G_i}(u) + 2 & u = v_i,\ \ 2 \le i \le n-1 \end{cases} .$$

Theorem 5. If $n \ge 3$ and $v_1,...,v_n \neq u_1,...,u_k$, then for $G = G(G_1,G_2,...,G_n,v_1,v_2,...,v_n)$ the following holds:

$$\Pi_1^{(u_1,...,u_k)}(G) = \prod_{i=1}^{n} \Pi_1^{(v_i,u_1,...,u_k)}(G_i) \prod_{j=2}^{n-1} \left(d_{G_j}(v_j) + 2\right)^2 \prod_{k=1,n} \left(d_{G_k}(v_k) + 1\right)^2 ,$$

$$\Pi_2^{(u_1,...,u_k)}(G) = \prod_{i=1}^{n} \Pi_2^{(v_i,u_1,...,u_k)}(G_i) \prod_{j=2}^{n-1} \left(d_{G_j}(v_j) + 2\right)^{d_{G_j}(v_j)+2} \prod_{k=1,n} \left(d_{G_k}(v_k) + 1\right)^{d_{G_k}(v_k)+1}$$

where we use the truncated versions of the two multiplicative Zagreb indices, namely,

$\Pi_1^{(u_1,u_2,...,u_k)}(G) = \prod_{\substack{v \in V(G) \\ v \neq u_1,u_2,...,u_k}} d_G(v)^2$ and $\Pi_2^{(u_1,u_2,...,u_k)}(G) = \prod_{\substack{v \in V(G) \\ v \neq u_1,u_2,...,u_k}} d_G(v)^{d_G(v)}$.

Proof.

$$\Pi_1^{(u_1,u_2,...,u_k)}(G) = \prod_{\substack{v \in V(G) \\ v \neq u_1,u_2,...,u_k}} d_G(v)^2$$

$$= \prod_{i=1}^{n}\left(\prod_{\substack{v\in V(G_i)\\ v\neq v_i,u_1,u_2,\ldots,u_k}} d_{G_i}(v)^2\right)\left(d_{G_1}(v_1)+1\right)^2\left(d_{G_2}(v_2)+2\right)^2\cdots\left(d_{G_{n-1}}(v_{n-1})+2\right)^2\left(d_{G_n}(v_n)+1\right)^2$$

$$= \prod_{i=1}^{n}\Pi_1^{(v_i,u_1,\ldots,u_k)}(G_i)\prod_{j=2}^{n-1}\left(d_{G_j}(v_j)+2\right)^2\prod_{k=1,n}\left(d_{G_k}(v_k)+1\right)^2,$$

and similarly

$$\Pi_2^{(u_1,u_2,\ldots,u_k)}(G) = \prod_{\substack{v\in V(G)\\ v\neq u_1,u_2,\ldots,u_k}} d_G(v)^{d_G(v)}$$

$$= \prod_{i=1}^{n}\left(\prod_{\substack{v\in V(G_i)\\ v\neq v_i,u_1,u_2,\ldots,u_k}} d_{G_i}(v)^{d_{G_i}(v)}\right)\prod_{j=2}^{n-1}\left(d_{G_j}(v_j)+2\right)^{d_{G_j}(v_j)+2}\prod_{k=1,n}\left(d_{G_k}(v_k)+1\right)^{d_{G_k}(v_k)+1}$$

$$= \prod_{i=1}^{n}\Pi_2^{(v_i,u_1,\ldots,u_k)}(G_i)\prod_{j=2}^{n-1}\left(d_{G_j}(v_j)+2\right)^{d_{G_j}(v_j)+2}\prod_{k=1,n}\left(d_{G_k}(v_k)+1\right)^{d_{G_k}(v_k)+1}.$$

3. APPLICATION

The goal of this section is computing the truncated Zagreb indices of an infinite class of dendrimers. To do this, we use Theorems 2 and 3. The truncated Zagreb indices for other classes of dendrimers, can be computed similarly. Consider the graph G_1 shown in Fig. 2. It is easy to see that

$$\Pi_1(G_1) = 2^{30}3^8 \text{ and } \Pi_2(G_1) = 2^{30}3^{12},$$

$$\Pi_1^{(v_1)}(G_1) = \Pi_1^{(v_2)}(G_1) = \Pi_1^{(v_3)}(G_1) = \Pi_1^{(v)}(G_1) = 2^{28}3^8$$

and

$$\Pi_2^{(v_1)}(G_1) = \Pi_2^{(v_2)}(G_1) = \Pi_2^{(v_3)}(G_1) = \Pi_2^{(v)}(G_1) = 2^{28}3^{12},$$

and so, for $1 \le i, j \le 3, i \neq j$,

$$\Pi_1^{(v,v)}(G_1) = \Pi_1^{(v_i,v_j)}(G_1) = 2^{26}3^8 \text{ and } \Pi_2^{(v,v)}(G_1) = \Pi_2^{(v_i,v_j)}(G_1) = 2^{26}3^{12}.$$

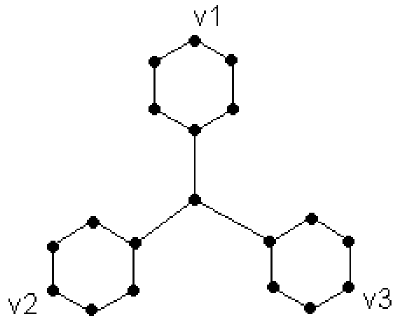

Figure 2. The Graph of Dendrimer G_n for n=1.

Consider now the graph $G_n = (G_{n-1} \square H_1)(v_1, u_1)$, shown in Figure 2 (for $n=1$) and Figure 3, respectively. It is easy to see that $H_i \cong G_1$ ($1 \le i \le n-1$) and

$$
\begin{aligned}
&G_n = (G_{n-1} \square H_1)(v_1, u_1)\\
&G_{n-1} = (G_{n-2} \square H_2)(v_2, u_2)\\
&\vdots\\
&G_{n-i} = (G_{n-i-1} \square H_{i+1})(v_{i+1}, u_{i+1})\\
&\vdots\\
&G_2 = (G_1 \square H_{n-1})(v_{n-1}, u_{n-1}).
\end{aligned}
$$

Then by using Theorem2, we have the following relations:

$$
\begin{aligned}
&\Pi_1(G_n) = \Pi_1^{(v_1)}(G_{n-1})\Pi_1^{(u_1)}(H_1)\times 3^4\\
&\Pi_1^{(v_1)}(G_{n-1}) = \Pi_1^{(v_2)}(G_{n-2})\Pi_1^{(v_1,u_2)}(H_2)\times 3^4\\
&\vdots\\
&\Pi_1^{(v_i)}(G_{n-i}) = \Pi_1^{(v_{i+1})}(G_{n-i-1})\Pi_1^{(v_i,u_{i+1})}(H_{i+1})\times 3^4\\
&\vdots\\
&\Pi_1^{(v_{n-2})}(G_2) = \Pi_1^{(v_{n-1})}(G_1)\Pi_1^{(v_{n-2},u_{n-1})}(H_{n-1})\times 3^4.
\end{aligned}
$$

Multiplication of these relations yields

$$\Pi_1(G_n) = \Pi_1^{(v_{n-1})}(G_1)\Pi_1^{(u_1)}(H_1)\prod_{i=2}^{n-1}\Pi_1^{(v_{i-1},u_i)}(H_i)\times 3^{4(n-1)},$$

and it is easy to obtain

$$\Pi_1(G_n) = \left(\Pi_1^{(v_1)}(G_1)\right)^2\left(\Pi_1^{(v_1,v_2)}(G_1)\right)^{n-2}\times 3^{4(n-1)}$$

$$= 2^{26n+4}3^{12n-4}.$$

In other words we arrived at the following:

Theorem 6. Consider the graph $G_n = (G_{n-1} \square H_1)(v_1, u_1)$ $(n \geq 2)$, shown in Figure 3. Then,

$$\Pi_1(G_n) = 2^{26n+4}3^{12n-4}.$$

Corollary7. Consider the dendrimer D, shown in Figure 4. Then,

$$\Pi_1(D) = 2^{26n+4}3^{12n-4},$$

Where n is the number of repetition of the fragment G_1.

Now for the second truncated Zagreb index, by using Theorem 3, the following relations are hold:

$$\Pi_2(G_n) = \Pi_2^{(v_1)}(G_{n-1})\Pi_2^{(u_1)}(H_1) \times 3^6$$
$$\Pi_2^{(v_1)}(G_{n-1}) = \Pi_2^{(v_2)}(G_{n-2})\Pi_2^{(v_1,u_2)}(H_2) \times 3^6$$
$$\vdots$$
$$\Pi_2^{(v_i)}(G_{n-i}) = \Pi_2^{(v_{i+1})}(G_{n-i-1})\Pi_2^{(v_i,u_{i+1})}(H_{i+1}) \times 3^6$$
$$\vdots$$
$$\Pi_2^{(v_{n-2})}(G_2) = \Pi_2^{(v_{n-1})}(G_1)\Pi_2^{(v_{n-2},u_{n-1})}(H_{n-1}) \times 3^6.$$

So by production of two sides of these relations, we have

$$\Pi_2(G_n) = \Pi_2^{(v_{n-1})}(G_1)\Pi_2^{(u_1)}(H_1)\prod_{i=2}^{n-1}\Pi_2^{(v_{i-1},u_i)}(H_i) \times 3^{6(n-1)},$$

and it is easy to see that

$$\Pi_2(G_n) = \left(\Pi_2^{(v_1)}(G_1)\right)^2 \left(\Pi_2^{(v_1,v_2)}(G_1)\right)^{n-2} \times 3^{6(n-1)}$$
$$= 2^{26n+4}3^{18n-6}.$$

Theorem 8. Consider the graph $G_n = (G_{n-1} \square H_1)(v_1, u_1)$ $(n \geq 2)$, shown in Figure 3. Then,

$$\Pi_2(G_n) = 2^{26n+4}3^{18n-6}.$$

Corollary 9. Consider the dendrimer D, shown in Figure 4. Then,

$$\Pi_2(D) = 2^{26n+4}3^{18n-6},$$

Where n is the number of repetition of the fragment G_1.

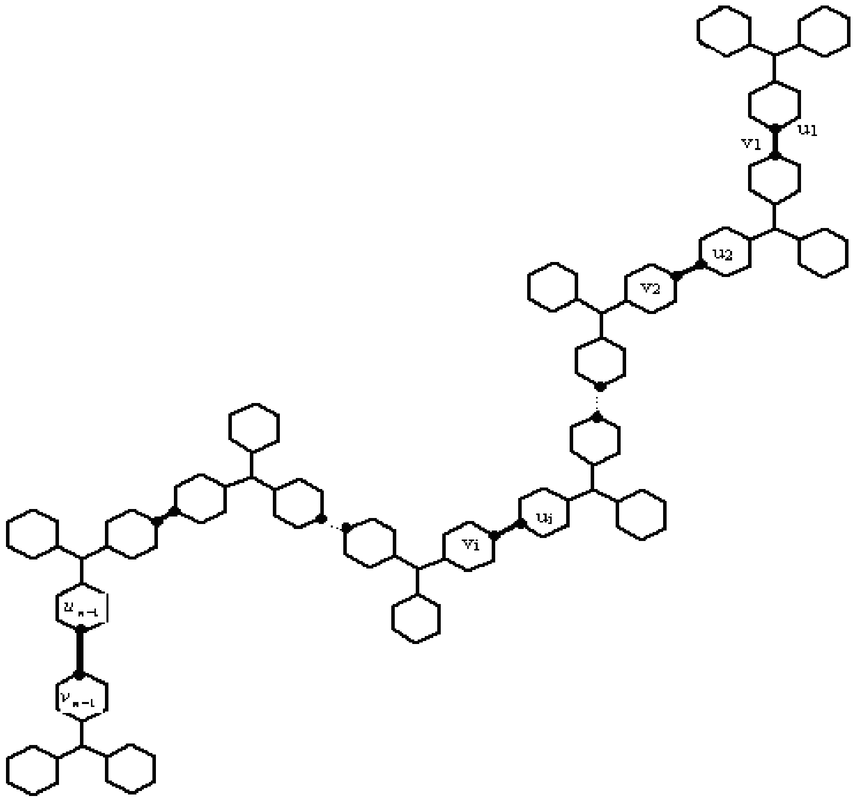

Figure 3. The graph G_n and the labeling of its vertices.

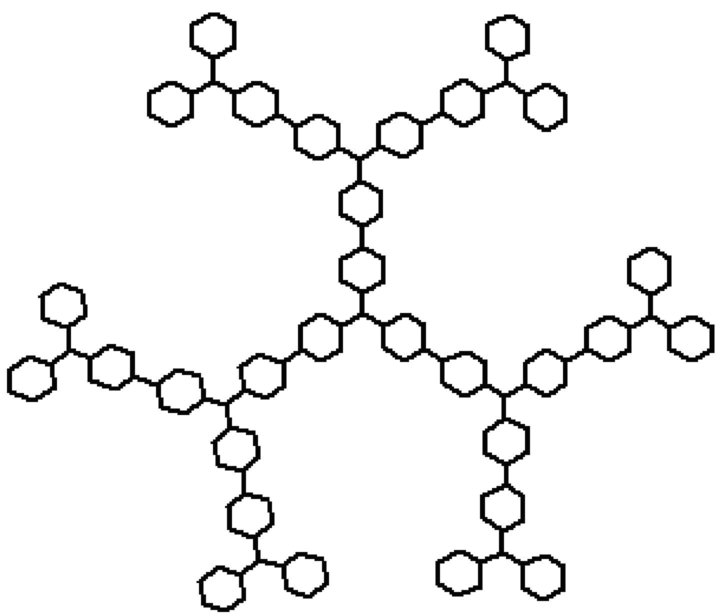

Figure 4. The Graph of the Dendrimer *D*.

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