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Fixed-Order Chemical Trees with Given Segments and Their Maximum Multiplicative Sum Zagreb Index

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Abstract: Topological indices are often used to predict the physicochemical properties of molecules. The multiplicative sum Zagreb index is one of the multiplicative versions of the Zagreb indices, which belong to the class of most-examined topological indices. For a graph G with edge set $E = \{e_1, e_2, \cdots, e_m\}$, its multiplicative sum Zagreb index is defined as the product of the numbers $D(e_1), D(e_2), \cdots, D(e_m)$, where $D(e_i)$ is the sum of the degrees of the end vertices of e_i. A chemical tree is a tree of maximum degree at most 4. In this research work, graphs possessing the maximum multiplicative sum Zagreb index are determined from the class of chemical trees with a given order and fixed number of segments. The values of the multiplicative sum Zagreb index of the obtained extremal trees are also obtained.

Keywords: topological index; multiplicative sum Zagreb indices; chemical trees; segments; extremal problem

MSC: 05C05; 05C07; 05C09; 05C35

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1. Introduction

A characteristic of a graph that is preserved under graph isomorphism is commonly referred to as a graph invariant [1]. In chemical graph theory, graphical invariants that take numerical quantities are usually named topological invariants, or simply, topological indices. Zagreb indices, particularly the first and second Zagreb indices denoted by M_1 and M_2, respectively, belong to well-examined categories of topological indices. Initially, they appeared in connection with the study molecules [2,3]. These indices can be defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v) = \sum_{x \in V(G)} d_x^2 \quad \textit{and} \quad M_2(G) = \sum_{uv \in E(G)} d_u d_v,$$

where uv is an edge between the vertices u and v, while d_x is the degree of the vertex x. Some information about the chemical applications of M_1 and M_2 can be found in [4,5]. These indices have also been the subject of extensive research into their relationship, comparison, and other mathematical properties [6–14]. Many existing facts of the Zagreb indices can be found in survey papers [15–19].

In 2010, Todeschini et al. [20] proposed to consider the multiplicative versions of topological indices. The multiplicative versions of M_1 and M_2 are defined [21] as follows:

$$\Pi_1 = \Pi_1(G) = \Pi_{u \in V(G)} d_u^2 \quad \textit{and} \quad \Pi_2 = \Pi_2(G) = \Pi_{uv \in E(G)} d_u d_v.$$

Bozovic et al. [22] discussed extreme values of multiplicative Zagreb indices for chemical trees. Wang et al. [23] examined the extremum multiplicative Zagreb indices of trees with a specific number of vertices and maximum degree. Further mathematical features of these two multiplicative indices can be found in [21,24–31].

In 2012, Eliasi et al. [25] introduced a modification of the multiplicative first Zagreb index known as the multiplicative sum Zagreb index [32]. The mathematical formulation of the multiplicative sum Zagreb index is as follows:

$$\Pi_1^* = \Pi_1^*(G) = \Pi_{uv\in E(G)}(d_u + d_v).$$

In [25], it was shown that the path has the least Π_1^*-value across all connected graphs with the specified order. The trees achieving the second least Π_1^*-value were also determined in [25]. Xu and Das [31] described the extremal trees, unicyclic graphs and bicyclic graphs of a specified order with respect to Π_1^*. Azari and Iranmanesh [33] established bounds on Π_1^* for graph operations. Further mathematical features of Π_1^* can be found in [27,34].

The focus of this work is strictly on the mathematical structure of chemical graphs. (Such graphs have found applications in chemistry; see, for example, the recent article [35]). More precisely, in this study, graphs possessing the greatest Π_1^*-values are determined from the class of chemical trees with a given order and fixed number of segments. The Π_1^*-values of the obtained extremal trees are also obtained.

2. Preliminaries

In this section, some definitions as well as notations used in this paper are given. Undefined terminology from graph theory can be found in some standard books. The graphs under discussion here are simple, undirected, and finite. The degree of a vertex v is represented by d_v. The distance between two vertices u and v is denoted by $d(u,v)$. A tree of maximum degree at most four is called a chemical tree. The notion $|A|$ represents the cardinality of the set A. Consider a non-trivial path $P_{i,j} = v_1v_2\cdots v_k$ in a tree such that $d_{v_1} = i$ and $d_{v_k} = j$. If $k \geq 3$, then every vertex of $P_{i,j}$ different from vertex v_1 and v_k is called an internal vertex of $P_{i,j}$. The path $P_{i,j}$ is referred to as an internal path if $i, j \geq 3$ provided that all internal vertices have degree 2 (if exist). Furthermore, the path $P_{i,j}$ is an external path if one of the two numbers i, j, is equal to 1 and the other has a value greater than 2 provided that all internal vertices have degree 2 (if exist). A branching vertex in a tree is a vertex with a degree greater than 2. If S is an external path or an internal path in a tree G, then S is called a segment of the graph G. We call the path graph P_n of order n also a segment of P_n. Thus, a path graph has only one segment and there is no graph with exactly two segments. Let $G(n,s)$ denote the class of all chemical trees with exactly n vertices and s segments, where $3 \leq s \leq n-1$. Let $\mathsf{D}(G)$ be the degree sequence of a graph G. Define $x_i = |\{x \in V(G) : d_x = i\}|$. For a chemical tree G, we write (for the sake of simplicity) the degree sequence of G as

$$\mathsf{D}(G) = ((x_4)_4, (x_3)_3, (x_2)_2, (x_1)_1).$$

For example, if a chemical tree has the degree sequence $(4,4,1,1,1,1,1,1)$ then we write it as $((2)_4, (0)_3, (0)_2, (6)_1)$. Let $N_G(u)$ be the set of neighbors of the vertex $u \in G$. In a graph G, let $\mathcal{E}_{i,j}(G)$ (or simply $\mathcal{E}_{i,j}$, when there is no confusion about G) be the set of edges of G with end vertices of degrees i and j. Certainly, $\mathcal{E}_{i,j}(G) = \mathcal{E}_{j,i}(G)$. For $e \in \mathcal{E}_{i,j}$, define $w(e) = i + j$.

3. Main Results

Before proceeding to our main results, we give some crucial lemmas that provide some useful information on obtaining the greatest possible value of the multiplicative sum Zagreb index for trees belonging to the class $G(n,s)$.

Lemma 1. *For a chemical tree $G_m \in G(n,s)$ with maximum multiplicative sum Zagreb index, the following statements are true:*

(a) *If $s \geq 5$ then $\mid \mathcal{E}_{1,2} \mid = 0$,*
(b) *If $3 \leq s \leq 4$ then $\mid \mathcal{E}_{1,2} \mid \leq 1$,*
(c) *If there is an internal path of the form $P_{i,j}$ in G_m of length 1, then there is no internal path of the form $P_{p,q}$ in G_m, with $p+q < i+j$, having length larger than 1.*
(d) *If a path $P_{i,j}$, with $6 \leq i+j \leq 8$, contains an internal vertex of degree four then $\mid \mathcal{E}_{1,3} \mid = 0$.*
(e) *The graph G_m does not possess an internal path having a length of 1 and an internal path having a length larger than 2 simultaneously.*
(f) *If G_m has exactly two vertices of degree 3 then G_m does not possess simultaneously the internal paths $P_{3,3}$ and $P_{4,4}$ both of length 1.*

Proof. Throughout this proof, whenever the degree notion d_α is used, it represents the degree of a vertex α in the graph G_m.

(a) If $\mid \mathcal{E}_{1,2} \mid \neq 0$ then there must be a vertex, say v_2, of degree two laying on an external path $v_1 v_2 \cdots v_i$ of G_m where $d_{v_1} = 1$, $d_{v_i} \in \{3,4\}$, and $i \geq 3$. Since $s \geq 5$, G_m has another branching vertex, say v_j $(i < j)$, which forms an internal path $v_i - v_j$ in the graph G_m. Let v_{i+1} be the neighbor of v_i that lies on the path $v_i - v_j$ (the vertex v_{i+1} may coincide with v_j).
Now, we consider a tree G_{m_1} that can be found in the class $G(n,s)$ and is obtained from G_m by the following operation:

$$G_{m_1} = G_m - \{v_1 v_2, v_i v_{i+1}\} + \{v_1 v_i, v_2 v_{i+1}\}.$$

There exists a positive real number Θ such that these two graphs satisfy the following:

$$\Pi_1^*(G_{m_1}) - \Pi_1^*(G_m) = \Theta\big[(d_{v_i+1} + 2)(d_{v_i} + 1) - 3(d_{v_i+1} + d_{v_i})\big]. \quad (1)$$

Since $d_{v_i+1} \geq 2$ and $3 \leq d_{v_i} \leq 4$, Equation (1) yields $\Pi_1^*(G_{m_1}) - \Pi_1^*(G_m) > 0$, a contradiction.

(b) Assume that the hypothesis holds but the conclusion does not hold; that is, suppose that the inequality $|\mathcal{E}_{1,2}| > 1$ holds. Let v denotes the only branching vertex in G_m (as $3 \leq s \leq 4$) with two distinct external paths $v_1 v_2 \cdots v_r v$ and $\acute{v}_1 \acute{v}_2 \cdots \acute{v}_s v$, each one having length of at least 2. Now, a new tree G_{m_1} is constructed from G_m using the following operation:

$$G_{m_1} = G_m - \{v_1 v_2, \acute{v}_s v\} + \{v_1 v, v_2 \acute{v}_s\}.$$

This operation emphasizes that $G_{m_1} \in G(n,s)$. There is $\Theta > 0$ such that

$$\Pi_1^*(G_{m_1}) - \Pi_1^*(G_m) = \Theta[4(d_v + 1) - 3(d_v + 2)]. \quad (2)$$

Since $d_v \geq 3$, Equation (2) gives $\Pi_1^*(G_{m_1}) - \Pi_1^*(G_m) > 0$, a contradiction.

(c) Assume contrarily that G_m possesses an internal path of the form $P_{p,q}$ of length larger than 1, such that $p+q < i+j$. Suppose that $P_{p,q} : v_1 v_2 \cdots v_k$ and $P_{i,j} : uv$, where $(d_u, d_v, d_{v_1}, d_{v_k}) = (i,j,p,q)$ and $k \geq 3$. Then, a tree $G_{m_1} \in G(n,s)$ is considered that is obtained using the following operation:

$$G_{m_1} = G_m - \{uv, v_1 v_2, v_2 v_3\} + \{uv_2, v_2 v, v_1 v_3\}.$$

There is a number $\Theta > 0$, such that

$$\Pi_1^*(G_{m_1}) - \Pi_1^*(G_m) = \Theta[(i+2)(j+2)(p + d_{v_3}) - (i+j)(p+2)(d_{v_3} + 2)]. \quad (3)$$

The following possible cases are discussed next:
Case (1): $i = j = 4$.

In this case, $p+q \leq 7$. Thus, $5 \leq p + d_{v_3} \leq 7$ and consequently, Equation (3) gives

$$\Pi_1^*(G_{m_1}) - \Pi_1^*(G_m) = 4\Theta[9(p+d_{v_3}) - 2(p+2)(d_{v_3}+2)] > 0,$$

a contradiction.

Case (2): Either $i = 3$ and $j = 4$ or $i = 4$ and $j = 3$.

In this case, $p+q \leq 6$. Thus, $5 \leq p + d_{v_3} \leq 6$ and consequently, Equation (3) gives

$$\Pi_1^*(G_{m_1}) - \Pi_1^*(G_m) = \Theta[30(p+d_{v_3}) - 7(p+2)(d_{v_3}+2)] > 0,$$

a contradiction again.
In both possible cases, we arrive at

$$\Pi_1^*(G_{m_1}) - \Pi_1^*(G_m) > 0,$$

a contradiction because of our contrary assumption that G_m possess an internal path of the form $P_{p,q}$ of length larger than 1, such that $p+q < i+j$.

(d) Contrarily, assume that $\mid \mathcal{E}_{1,3} \mid \neq 0$. Then, there exists $yz \in \mathcal{E}_{1,3}$, such that $d_y = 1$ and $d_z = 3$. Let $P_{i,j} : u_0 u_1 \cdots u_{k-1} u_k u_{k+1} \cdots u_g$ be a path with an internal vertex u_k of degree 4, such that $6 \leq i+j \leq 8$. Without loss of generality, suppose that u_k is the only internal vertex on $P_{i,j}$; otherwise, we may consider a subpath $P'_{i',j'}$ of $P_{i,j}$ containing exactly one internal vertex of degree 4, such that $6 \leq i' + j' \leq 8$. The following cases are to be discussed here:

Case (1): $d_{u_{k-1}} = d_{u_{k+1}} = 2$

If $u_{k+1} = u_g$, then we assume that u_{k+2} is a neighbor of u_{k+1} not lying on the path $P_{i,j}$; otherwise, we assume that u_{k+2} is a neighbor of u_{k+1} lying on the $u_{k+1} - u_g$ path. Whether z lies on $P_{i,j}$ or not, in either of the two cases, we define a new graph as follows:

$$G_{m_1} = G_m - \{yz, u_{k-1}u_k, u_{k+1}u_{k+2}\} + \{yu_k, u_{k+1}z, u_{k-1}u_{k+2}\}.$$

Note that the tree G_{m_1} belongs to the collection $G(n,s)$. Whether z lies on $P_{i,j}$ or not, in either of the two cases, there exists a positive real number Θ, such that

$$\Pi_1^*(G_{m_1}) - \Pi_1^*(G_m) = \Theta\big(d_{u_{k+2}} + 2\big) > 0,$$

which is a contradiction.

Case (2): $\max\{d_{u_{k-1}}, d_{u_{k+1}}\} = 3$.

In this case, we consider a tree $G_{m_1} \in G(n,s)$ obtained using the operation described as follows:

$$G_{m_1} = G_m - \{yz, u_{k-1}u_k, u_k u_{k+1}\} + \{yu_k, u_k z, u_{k-1}u_{k+1}\}.$$

Whether z lies on $P_{i,j}$ or not, in either of the two cases, there exists a positive real number Θ, such that

$$\Pi_1^*(G_{m_1}) - \Pi_1^*(G_m) = \Theta\big[35(d_{u_k-1} + d_{u_k+1}) - 4(d_{u_k-1}+4)(d_{u_k+1}+4)\big]. \tag{4}$$

Note that there are the following three possibilities concerning the degrees of the vertices u_{k-1} and u_{k+1}:

- $d_{u_{k-1}} = 2$ and $d_{u_{k+1}} = 3$,
- $d_{u_{k-1}} = 3$ and $d_{u_{k+1}} = 2$,
- $d_{u_{k-1}} = 3 = d_{u_{k+1}}$.

In every case, Equation (4) gives

$$\Pi_1^*(G_{m_1}) - \Pi_1^*(G_m) > 0,$$

a contradiction.

(e) Although the proof of this part is slightly different from that of part (c), we provide its proof here for the sake of completeness. Assume contrarily that G_m simultaneously possesses an internal path $P_{p,q} : v_1v_2 \cdots v_k$ of length $k-1 \geq 3$ and an internal path $P_{i,j} : uv$ of length 1, where $(d_u, d_v, d_{v_1}, d_{v_k}) = (i, j, p, q)$. Then, a tree $G_{m_1} \in G(n,s)$ is considered that is obtained using the following operation:

$$G_{m_1} = G_m - \{uv, v_1v_2, v_2v_3\} + \{uv_2, v_2v, v_1v_3\}.$$

There is a number $\Theta > 0$, such that

$$\Pi_1^*(G_{m_1}) - \Pi_1^*(G_m) = \Theta(p+2)[(i+2)(j+2) - 4(i+j)]. \tag{5}$$

Since $3 \leq i \leq 4$ and $3 \leq j \leq 4$, Equation (5) provides

$$\Pi_1^*(G_{m_1}) - \Pi_1^*(G_m) > 0,$$

a contradiction.

(f) Assume contrarily that G_m possesses simultaneously the internal paths $P_{3,3}$ and $P_{4,4}$ both of length 1. Let $xy, uv \in V(G_m)$, such that $d_y = 3 = d_x$, the distance $d(y,u)$ is minimum, and $d_v = 4 = d_u$. Note that y and u lie on the unique $x - v$ path. Let y_1 be the neighbor of y lying on the $y - u$ path. By part (c), the degree of y_1 is 4.
First, we discuss the case when $y_1 = u$. Consider a tree $G_{m_1} \in G(n,s)$ that is obtained using the following operation:

$$G_{m_1} = G_m - \{uv, xy\} + \{ux, yv\}.$$

Then, we obtain $\Pi_1^*(G_{m_1}) > \Pi_1^*(G_m)$, a contradiction.
Next, consider the case when $y_1 \neq u$. Then, y_1 has a neighbor, say y_2, of degree 2 lying on the $y_1 - u$ path. Let y_3 be the neighbor of y_2 lying on the $y_2 - u$ path. The vertices y_3 and u may be the same. By part (e), $d_{y_3} = 4$. Now, consider a tree $G_{m_2} \in G(n,s)$ that is obtained using the following operation:

$$G_{m_2} = G_m - \{uv, y_1y_2, y_2y_3\} + \{uy_2, y_2v, y_1y_3\}.$$

Certainly, $\Pi_1^*(G_{m_2}) = \Pi_1^*(G_m)$. Now, define

$$G_{m_3} = G_{m_2} - \{y_1y_3, xy\} + \{y_1x, y_3y\}.$$

Then, $G_{m_3} \in G(n,s)$ and $\Pi_1^*(G_{m_3}) > \Pi_1^*(G_{m_2}) = \Pi_1^*(G_m)$, which yields a contradiction again.

□

If we consider the class $G(n,s)$ for $s \in \{3,4\}$, then we note that $G(n,s)$ consists of exactly one element for every $(n,s) \in \{(4,3),(5,3),(5,4),(6,4)\}$. For $n \geq s+3$ with $s \in \{3,4\}$, we have the next result, which follows from Lemma 1(b).

Corollary 1. *The graph constructed by attaching $s-1$ pendent vertices to a single pendent vertex of the path $P_{n-(s-1)}$ possesses uniquely the greatest multiplicative sum Zagreb index in $G(n,s)$ for every $n \geq s+3$ with $s \in \{3,4\}$. The mentioned greatest value is $3(s+2)(s+1)^{s-1}4^{n-s-2}$.*

Because of Corollary 1, in the rest of the current section, we focus on the case when $5 \le s \le n-1$ for the class $G(n,s)$. To prove our next lemma, we need the following existing result:

Lemma 2 ([36]). *For every graph $G \in G(n,s)$, the following statements holds:*

(a) *The equation $x_3 = 0$ holds if and only if $x_2 = n-s-1$, $x_1 = \frac{2s+4}{3}$, $x_4 = \frac{s-1}{3}$, $s = 3t+1$ for some positive integer t.*

(b) *The equation $x_3 = 1$ holds if and only if $x_2 = n-s-1$, $x_1 = \frac{2s+3}{3}$, $x_4 = \frac{s-3}{3}$, $s = 3t$ for some positive integer t.*

(c) *The equation $x_3 = 2$ holds if and only if $x_2 = n-s-1$, $x_1 = \frac{2s+2}{3}$ $x_4 = \frac{s-5}{3}$, $s = 3t+2$ for some positive integer t.*

Lemma 3. *Let $G_m \in G(n,s)$ be a chemical tree with maximum multiplicative sum Zagreb index and t be a positive integer. Then,*

$$D(G_m) = \begin{cases} \left(\left(\frac{s-1}{3}\right)_4, (0)_3, (n-s-1)_2, \left(\frac{2s+4}{3}\right)_1\right) & \text{if } s = 3t+1 \\ \left(\left(\frac{s-3}{3}\right)_4, (1)_3, (n-s-1)_2, \left(\frac{2s+3}{3}\right)_1\right) & \text{if } s = 3t \\ \left(\left(\frac{s-5}{3}\right)_4, (2)_3, (n-s-1)_2, \left(\frac{2s+2}{3}\right)_1\right) & \text{if } s = 3t+2. \end{cases}$$

Proof. Throughout this proof, whenever the degree notion d_α is used, it represents the degree of a vertex α in the graph G_m. First, we show that $x_3 \le 2$. We suppose on the contrary that the inequality $x_3 \ge 3$ holds. Take $p, q, r \in V(G_m)$, such that $d_p = d_q = d_r = 3$. If all these three vertices are on one path, then (without loss of generality) suppose that q lies on the unique $p-r$ path in G_m. In either of the two cases, suppose that $N_{G_m}(r) = \{r_1, r_2, r_3\}$ is the set of neighbors of r with the condition that r_1 is located on $p-r$ path (r_1 may coincide with q). Now, a chemical tree G_{m_1} is obtained in the collection $G(n,s)$ using the following operation:

$$G_{m_1} = G_m - \{rr_2, rr_3\} + \{pr_2, qr_3\}.$$

For the case when all the three vertices p, q, r, are on one path, see Figure 1.

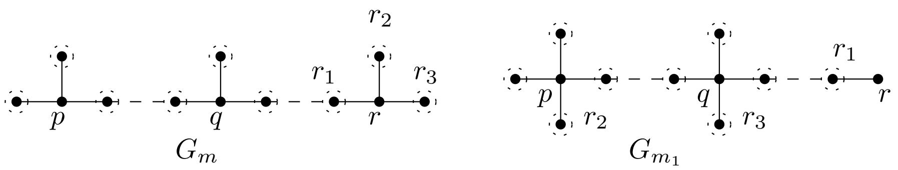

Figure 1. The transformation applied on the graph G_m to obtain a new graph G_{m_1} in Lemma 3.

Note that there is a real number $\Theta > 0$, such that

$$\begin{aligned} \Pi_1^*(G_{m_1}) - \Pi_1^*(G_m) = \Theta\Bigg(& (d_{r_1}+1) \prod_{q' \in N_{G_m}(q)} (d_{q'}+4) \prod_{p' \in N_{G_m}(p)} (d_{p'}+4) \prod_{i=2}^{3} (d_{r_i}+4) \\ & - \prod_{i=1}^{3} (d_{r_i}+3) \prod_{q' \in N_{G_m}(q)} (d_{q'}+3) \prod_{p' \in N_{G_m}(p)} (d_{p'}+3) \Bigg) \\ > \Theta\Bigg(& (d_{r_1}+1) \prod_{p' \in N_{G_m}(p)} (d_{p'}+4) \prod_{i=2}^{3} (d_{r_i}+4) \\ & - \prod_{i=1}^{3} (d_{r_i}+3) \prod_{p' \in N_{G_m}(p)} (d_{p'}+3) \Bigg). \end{aligned} \tag{6}$$

Since $2 \leq d_{r_1} \leq 4$, inequality (6) yields

$$\Pi_1^*(G_{m_1}) - \Pi_1^*(G_m) > 0,$$

a contradiction. Hence, the inequality $x_3 \leq 2$ holds, which together with Lemma 2 gives the required result. $\square$

We now define three subclasses of $G(n,s)$ as follows when $n \geq 8$ and $s = 3t+1$ for some integer $t \geq 2$:

- $\mathbb{G}_1 = \{T \in G(n,s) : x_2 = 0 = x_3\}$.
- $\mathbb{G}_2$ consists of those members of $G(n,s)$ that obey $1 \leq x_2 \leq x_4 - 1$ and $|\ \mathcal{E}_{2,4}\ | = 2x_2$ and $|\ \mathcal{E}_{1,2}\ | = |\ \mathcal{E}_{2,2}\ | = 0 = x_3$.
- $\mathbb{G}_3$ consists of those members of $G(n,s)$ that obey $|\ \mathcal{E}_{1,2}\ | = |\ \mathcal{E}_{4,4}\ | = 0 = x_3$ and $x_2 > x_4 - 1$.

Three examples G_1, G_2, and G_3, one from each of the classes $\mathbb{G}_1$, $\mathbb{G}_2$, and $\mathbb{G}_3$, respectively, are depicted in Figure 2.

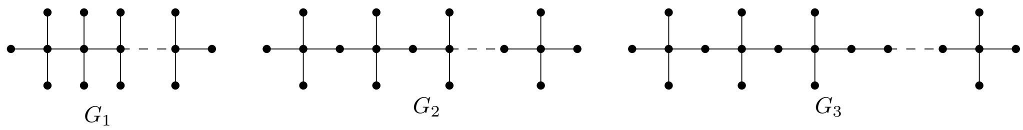

Figure 2. Three examples G_1, G_2, and G_3, one from each of the classes $\mathbb{G}_1$, $\mathbb{G}_2$, and $\mathbb{G}_3$, respectively.

Theorem 1. *Let $G_m \in G(n,s)$ be a chemical tree with maximum multiplicative sum Zagreb index such that $n \geq 8$ and $s = 3t+1$ for some integer $t \geq 2$. Then $G_m \in \mathbb{G}_1 \cup \mathbb{G}_2 \cup \mathbb{G}_3$.*

Proof. By Lemma 3, it holds that $x_3 = 0$. If $x_2 = 0$ then $G_m \in \mathbb{G}_1$ and we are done. If $x_2 \neq 0$ then Lemma 1(a) confirms that $|\ \mathcal{E}_{1,2}\ | = 0$. Now, the conclusion is obtained from Lemma 1(e). $\square$

Next, we define five subclasses of $G(n,s)$ as follows when $n \geq 8$ and $s = 3t$ for some integer $t \geq 2$:

- $\mathbb{H}_1 = \{H_5 \in G(n,6) : x_2 \geq 1\}$, where H_5 is given Figure 3.
- $\mathbb{H}_2 = \{H_6 \in G(n,9) : x_2 \geq 0;$ if $x_2 \geq 2$ then $|\ \mathcal{E}_{3,4}\ | = 0\}$, where H_6 is shown Figure 3.
- $\mathbb{H}_3 = \{T \in G(n,s) : x_3 = 1,\ 0 \leq x_2 \leq x_4 - 3, |\ \mathcal{E}_{3,4}\ | = 3,\ |\ \mathcal{E}_{2,2}\ | = |\ \mathcal{E}_{1,2}\ | = 0,\ |\ \mathcal{E}_{2,4}\ | = 2x_2, |\ \mathcal{E}_{1,4}\ | = x_1,\ s \geq 12\}$. For example, the graphs H_2 and H_4 given in Figure 3 belong to $\mathbb{H}_3$.
- $\mathbb{H}_4 = \{T \in G(n,s) : x_3 = 1,\ 0 \leq x_4 - 3 < x_2 \leq x_4, |\ \mathcal{E}_{2,3}\ | = x_2 - (x_4 - 3), |\ \mathcal{E}_{3,4}\ | = x_4 - x_2, |\ \mathcal{E}_{1,4}\ | = x_1, |\ \mathcal{E}_{2,2}\ | = |\ \mathcal{E}_{1,2}\ | = |\ \mathcal{E}_{1,3}\ | = |\ \mathcal{E}_{4,4}\ | = 0,\ s \geq 12\}$. For example, the graph H_7 given in Figure 3 belongs to $\mathbb{H}_4$.
- $\mathbb{H}_5 = \{T \in G(n,s) : x_3 = 1,\ x_2 > x_4 \geq 3, |\ \mathcal{E}_{2,3}\ | = 3, |\ \mathcal{E}_{2,4}\ | = 2x_4 - 3, |\ \mathcal{E}_{1,4}\ | = x_1, |\ \mathcal{E}_{3,4}\ | = |\ \mathcal{E}_{1,2}\ | = |\ \mathcal{E}_{1,3}\ | = |\ \mathcal{E}_{4,4}\ | = 0,\ s \geq 12\}$. For example, the graph H_8 given in Figure 3 belongs to $\mathbb{H}_5$.

Theorem 2. *Let $G_m \in G(n,s)$ be a chemical tree with maximum multiplicative sum Zagreb index such that $n \geq 8$ and $s = 3t$ for some integer $t \geq 2$. Then $G_m \in \cup_{i=1}^{5}\mathbb{H}_i$.*

Proof. By Lemma 3, it holds that $x_3 = 1$. If $s = 6$ then Lemma 1(a) implies that $G_m \in \mathbb{H}_1$. If $s = 9$, then by the parts (a), (d), and (e) of Lemma 1, we have $G_m \in \mathbb{H}_2$. If (i) $s \geq 12$ and $0 \leq x_2 \leq x_4 - 3$, or (ii) $s \geq 12$ and $0 \leq x_4 - 3 < x_2 \leq x_4$, or (iii) $s \geq 12$ and $x_2 > x_4 \geq 3$, then by the parts (a), (c), (d), and (e) of Lemma 1, we conclude that $G_m \in \mathbb{H}_3$, or $G_m \in \mathbb{H}_4$, or $G_m \in \mathbb{H}_5$, respectively. $\square$

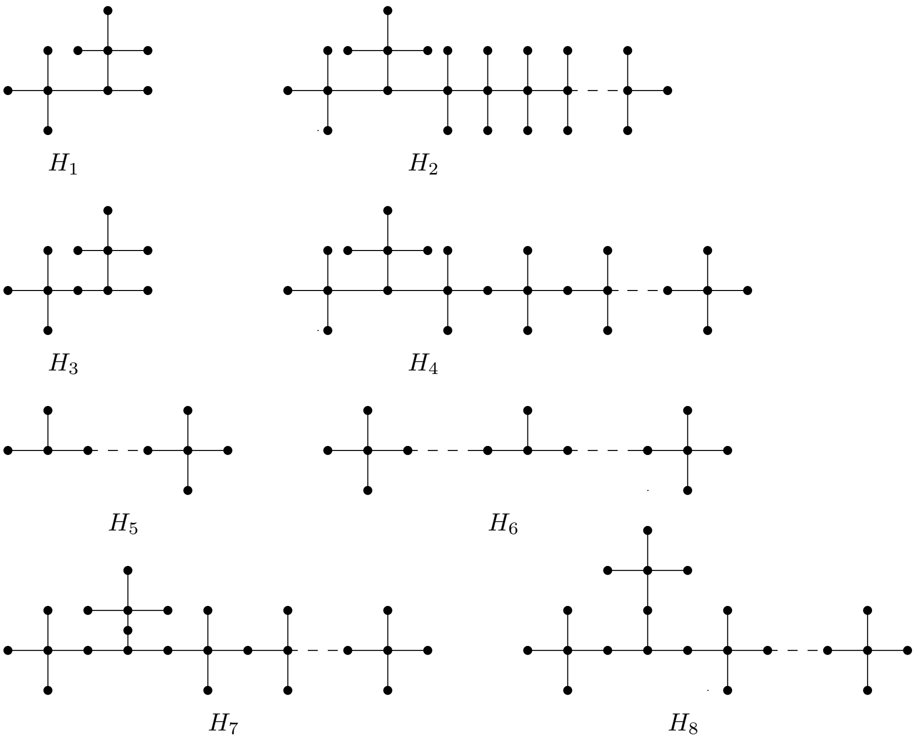

Figure 3. Some chemical trees with $x_3 = 1$.

We next define six subclasses of $G(n, s)$ as follows when $n \geq 7$ and $s = 3t + 2$ for some integer $t \geq 1$:

- $\mathbb{I}_1 = \{T \in G(n, 5) : x_3 = 2, x_2 \geq 1, x_4 = 0, x_1 = |\ \mathcal{E}_{1,3}\ | = 4, |\ \mathcal{E}_{2,3}\ | = 2, |\ \mathcal{E}_{2,2}\ | = n - 7\}$.
- $\mathbb{I}_2 = \{T \in G(n, s) : 8 \leq s \leq 17,\ n \leq \frac{4s-2}{3},\ x_3 = 2, |\ \mathcal{E}_{1,2}\ | = |\ \mathcal{E}_{2,2}\ | = |\ \mathcal{E}_{4,4}\ | = 0, |\ \mathcal{E}_{1,3}\ | = \frac{17-s}{3}, |\ \mathcal{E}_{1,4}\ | = s - 5, |\ \mathcal{E}_{2,3}\ | = |\ \mathcal{E}_{2,4}\ | = x_2, |\ \mathcal{E}_{3,3}\ | = 1\}$. For example, the graphs I_0, I_1, I_2, I_3, I_4, and I_7 given in Figure 4 belong to $\mathbb{I}_2$.
- $\mathbb{I}_3 = \{T \in G(n, s) : 8 \leq s \leq 17,\ n > \frac{4s-2}{3},\ x_3 = 2, |\ \mathcal{E}_{1,2}\ | = |\ \mathcal{E}_{3,3}\ | = |\ \mathcal{E}_{3,4}\ | = |\ \mathcal{E}_{4,4}\ | = 0, |\ \mathcal{E}_{1,3}\ | = \frac{17-s}{3}, |\ \mathcal{E}_{1,4}\ | = s - 5, |\ \mathcal{E}_{2,3}\ | = \frac{s+1}{3}, |\ \mathcal{E}_{2,4}\ | = x_4\}$. For example, the graph I_5 depicted in Figure 4 belongs to $\mathbb{I}_3$.
- $\mathbb{I}_4 = \{T \in G(n, s) : s > 17,\ n \leq \frac{4s-17}{3},\ x_3 = 2, |\ \mathcal{E}_{1,4}\ | = x_1, |\ \mathcal{E}_{2,4}\ | = 2x_2, |\ \mathcal{E}_{3,4}\ | = 6, |\ \mathcal{E}_{1,2}\ | = |\ \mathcal{E}_{3,3}\ | = |\ \mathcal{E}_{1,3}\ | = |\ \mathcal{E}_{2,2}\ | = |\ \mathcal{E}_{2,3}\ | = 0\}$. For example, the graph I_6 given in Figure 4 belongs to $\mathbb{I}_4$.
- $\mathbb{I}_5 = \{T \in G(n, s) : s > 17,\ \frac{4s-17}{3} < n \leq \frac{4s+1}{3},\ x_3 = 2, |\ \mathcal{E}_{1,4}\ | = x_1, |\ \mathcal{E}_{2,3}\ | = \frac{3n-4s+17}{3}, |\ \mathcal{E}_{2,4}\ | = \frac{3n-2s-23}{3}, |\ \mathcal{E}_{1,2}\ | = |\ \mathcal{E}_{3,3}\ | = |\ \mathcal{E}_{1,3}\ | = |\ \mathcal{E}_{2,2}\ | = |\ \mathcal{E}_{4,4}\ | = 0\}$. For example, the graph I_8 shown in Figure 4 belongs to $\mathbb{I}_5$.
- $\mathbb{I}_6 = \{T \in G(n, s) : s > 17,\ n > \frac{4s+1}{3},\ x_3 = 2, |\ \mathcal{E}_{1,4}\ | = x_1, |\ \mathcal{E}_{2,3}\ | = 6, |\ \mathcal{E}_{2,4}\ | = \frac{2s-22}{3}, |\ \mathcal{E}_{1,2}\ | = |\ \mathcal{E}_{3,3}\ | = |\ \mathcal{E}_{1,3}\ | = |\ \mathcal{E}_{3,4}\ | = |\ \mathcal{E}_{4,4}\ | = 0\}$.

Theorem 3. *Let $G_m \in G(n, s)$ be a chemical tree with the greatest multiplicative sum Zagreb index such that $n \geq 7$ and $s = 3t + 2$ for some integer $t \geq 1$. Then $G_m \in \cup_{i=1}^{6} \mathbb{I}_i$.*

Proof. By Lemma 3, it holds that $x_3 = 2$. If $s = 5$ then Lemma 1(a) implies that $G_m \in \mathbb{I}_1$. If (i) $8 \leq s \leq 17$ and $n \leq \frac{4s-2}{3}$, or (ii) $8 \leq s \leq 17$ and $n > \frac{4s-2}{3}$, or (iii) $s > 17$ and $n \leq \frac{4s-17}{3}$, or (iv) $s > 17$ and $\frac{4s-17}{3} < n \leq \frac{4s+1}{3}$, or (v) $s > 17$ and $n > \frac{4s+1}{3}$, then by Lemma 3, we conclude that $G_m \in \mathbb{I}_2$, or $G_m \in \mathbb{I}_3$, or $G_m \in \mathbb{I}_4$, or $G_m \in \mathbb{I}_5$, or $G_m \in \mathbb{I}_6$, respectively. $\square$

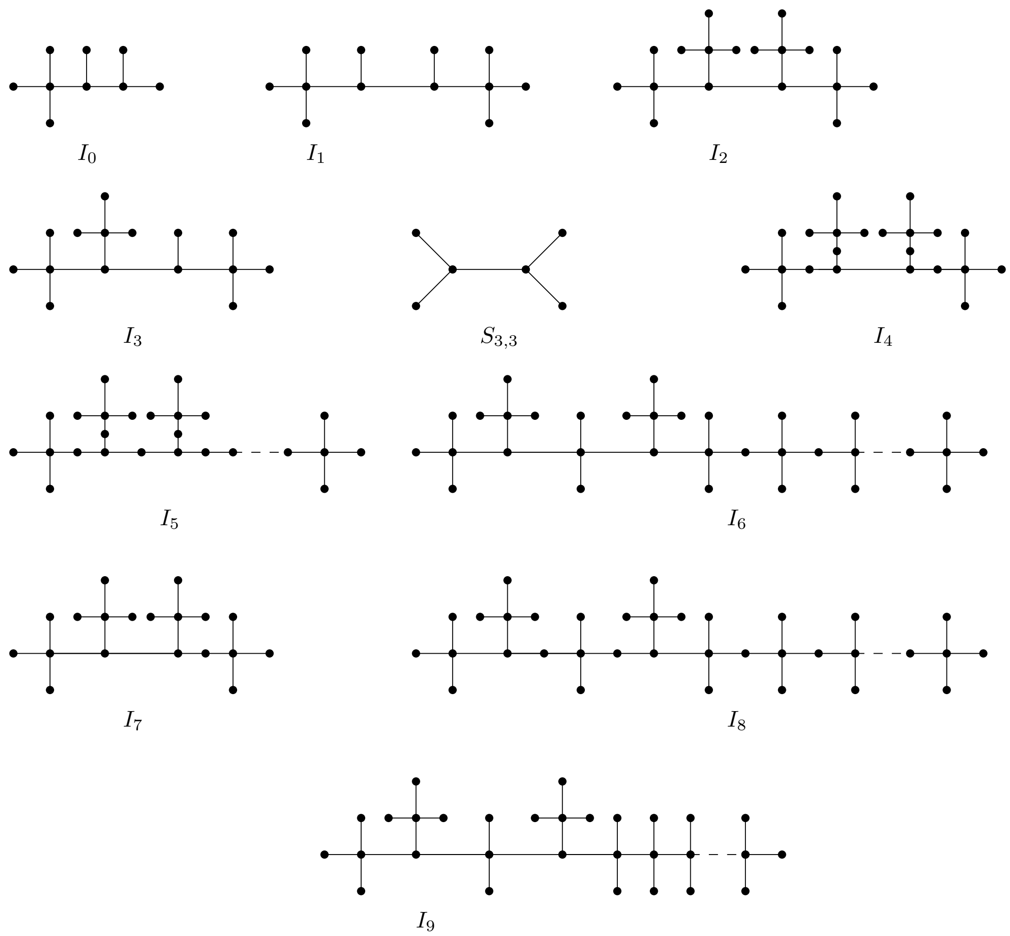

Figure 4. Some chemical trees with $x_3 = 2$.

Theorem 4. *Let $G_m \in G(n,s)$ be a chemical tree with maximum multiplicative sum Zagreb index such that $s = 3t+1$ for some integer $t \geq 2$. Then,*

$$\Pi_1^*(G_m) = \begin{cases} 2^{s-4} \times 5^{\frac{2s+4}{3}} & \text{if } n = s+1, \\ 2^{4s-3n-1} \times 5^{\frac{2s+4}{3}} \times 6^{2(n-s-1)} & \text{if } s+1 < n \leq \frac{4s-1}{3}, \\ 2^{\frac{2(3n-4s+1)}{3}} \times 5^{\frac{2s+4}{3}} \times 6^{\frac{2(s-4)}{3}} & \text{if } n > \frac{4s-1}{3}. \end{cases}$$

Proof. By Lemma 3, we have

$$\mathsf{D}(G_m) = \left(\left(\frac{s-1}{3}\right)_4, (0)_3, (n-s-1)_2, \left(\frac{2s+4}{3}\right)_1 \right).$$

The following cases arise:

Case (1): $n = s+1$.

By using the above degree sequence of G_m, we have $x_2 = 0$. Thus, in this case, G_m consists of vertices of degree 4 and 1 only. Consequently, we have $| \mathcal{E}_{1,4} | = x_1$ and $| \mathcal{E}_{4,4} | = x_4 - 1$. Hence,

$$| \mathcal{E}_{i,j} | = \begin{cases} x_1 = \dfrac{2s+4}{3} & \text{if } i = 1 \text{ and } j = 4, \\ x_4 - 1 = \dfrac{s-4}{3} & \text{if } i = j = 4. \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 2^{s-4} \times 5^{\frac{2s+4}{3}}.$$

Case (2): $s+1 < n \leq \frac{4s-1}{3}$.

Note, in this case, that $1 \leq x_2 \leq x_4 - 1$. By keeping in mind Lemma 1, we obtain

$$|\ \mathcal{E}_{i,j}\ | = \begin{cases} 0 & \text{if either } (i,j) = (1,2) \text{ or } i = j = 2, \\ x_1 = \frac{2s+4}{3} & \text{if } i = 1 \text{ and } j = 4, \\ 2x_2 = 2(n-s-1) & \text{if } i = 2 \text{ and } j = 4, \\ (x_4 - 1) - x_2 = \frac{4s-3n-1}{3} & \text{if } \ i = j = 4. \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 2^{4s-3n-1} \times 5^{\frac{2s+4}{3}} \times 6^{2(n-s-1)}.$$

Case (3): $n > \frac{4s-1}{3}$.

Note, in the present case, that $x_2 > x_4 - 1$. Bearing in mind Lemma 1, we obtain

$$|\ \mathcal{E}_{i,j}\ | = \begin{cases} 0 & \text{if either } i = j = 4 \text{ or } (i,j) = (1,2), \\ x_1 = \frac{2s+4}{3} & \text{if } i = 1 \text{ and } j = 4, \\ (n-1) - x_1 - 2(x_4 - 1) = \frac{3n-4s+1}{3} & \text{if } i = j = 2, \\ 2(x_4 - 1) = \frac{2(s-4)}{3} & \text{if } i = 2 \text{ and } j = 4. \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 2^{\frac{2(3n-4s+1)}{3}} \times 5^{\frac{2s+4}{3}} \times 6^{\frac{2(s-4)}{3}}.$$

□

Theorem 5. *Let $G_m \in G(n,s)$ be the chemical tree with maximum multiplicative sum Zagreb index such that $s = 3\,t$ for some integer $t \geq 2$. Then,*

$$\Pi_1^*(G_m) = \begin{cases} 2^{\frac{2(12-s)}{3}} \times 5^{s-3} \times 7^{\frac{s-3}{3}} & \textit{if } \ n = s+1 \textit{ and } s \leq 9, \\ 7^3 \times 2^{s-12} \times 5^{\frac{2s+3}{3}} & \textit{if } \ n = s+1 \textit{ and } s > 9, \\ 2^{\frac{2(12-s)}{3}} \times 5^{n-4} \times 6^{n-s-1} \times 7^{\frac{4s-3n}{3}} & \textit{if } \ s+1 < n \leq \frac{4s}{3} \textit{ and } s \leq 9, \\ 7^3 \times 2^{4s-3n-9} \times 5^{\frac{2s+3}{3}} \times 6^{2(n-s-1)} & \textit{if } \ s+1 < n \leq \frac{4s-9}{3} \textit{ and } \ s > 9, \\ 5^{\frac{3n-2s+12}{3}} \times 6^{\frac{3n-2s-15}{3}} \times 7^{\frac{4s-3n}{3}} & \textit{if } \ \frac{4s-9}{3} < n \leq \frac{4s}{3} \textit{ and } \ s > 9, \\ 4^{\frac{3n-5s+12}{3}} \times 5^{\frac{4s-12}{3}} \times 6^{\frac{s-3}{3}} & \textit{if } \ n > \frac{4s}{3} \textit{ and } s \leq 9, \\ 4^{\frac{3n-4s}{3}} \times 5^{\frac{2s+12}{3}} \times 6^{\frac{2s-15}{3}} & \textit{if } \ n > \frac{4s}{3} \textit{ and } \ s > 9. \end{cases}$$

Proof. By Lemma 3, we have

$$\mathsf{D}(G_m) = \left(\left(\frac{s-3}{3} \right)_4, (1)_3, (n-s-1)_2, \left(\frac{2s+3}{3} \right)_1 \right). \tag{7}$$

Case (1): $n = s+1$.

In the present case, it holds that $x_2 = 0$. We discuss two possible subcases of the present case as follows:

Subcase (1.1): $s \le 9$.

Note, in the present subcase, that $s \in \{6, 9\}$. Since $x_2 = 0$ in the consider case, if $s = 6$ then Equation (7) yields

$$\mathsf{D}(G_m) = ((1)_4, (1)_3, (0)_2, (5)_1),$$

and hence $n = 7$. Thus, G_m is the graph constructed by attaching two new pendent vertices to a pendent vertex of the star S_5. Similarly, if $s = 9$, then Equation (7) gives

$$\mathsf{D}(G_m) = ((2)_4, (1)_3, (0)_2, (7)_1),$$

and hence $n = 10$. Thus, by Lemma 1(e), G_m is the graph H_1 depicted in Figure 3. Hence, if $s \in \{6, 9\}$, then

$$|\mathcal{E}_{i,j}| = \begin{cases} 0 & \text{if } i = j = 4, \\ \frac{12-s}{3} & \text{if } i = 1 \text{ and } j = 3, \\ s - 3 & \text{if } i = 1 \text{ and } j = 4, \\ \frac{s-3}{3} & \text{if } i = 3 \text{ and } j = 4. \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 2^{\frac{2(12-s)}{3}} \times 5^{s-3} \times 7^{\frac{s-3}{3}}.$$

Subcase (1.2): $s > 9$.

Note, in the present subcase, that $s \ge 12$. Recall also that $x_2 = 0$ in the present case. By Lemma 1(d), every neighbor of the unique vertex of degree 3 in G_m is of degree 4; for example, see H_2 in Figure 3. Hence,

$$|\mathcal{E}_{i,j}| = \begin{cases} 0 & \text{if } i = 1 \text{ and } j = 3, \\ s - x_4 = \frac{2s+3}{3} & \text{if } i = 1 \text{ and } j = 4, \\ 3 & \text{if } i = 3 \text{ and } j = 4, \\ x_4 - 3 = \frac{s-12}{3} & \text{if } i = j = 4. \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 7^3 \times 2^{s-12} \times 5^{\frac{2s+3}{3}}.$$

Case (2): $s + 1 < n \le \frac{4s}{3}$.

Observe, in the current case, that $x_2 \ge 1$. In the following, we discuss two subcases according to whether $s \le 9$ or $s > 9$.

Subcase (2.1): $s \le 9$.

Observe that $s \in \{6, 9\}$. If $s = 6$, then $n = 8$ and hence by Equation (7), we have

$$\mathsf{D}(G_m) = ((1)_4, (1)_3, (1)_2, (5)_1).$$

Thus, by Lemma 1, G_m is a particular case of H_5 shown in Figure 3. If $s = 9$ then $10 < n \le 12$, and by Equation (7), we have

$$\mathsf{D}(G_m) = ((2)_4, (1)_3, (n-10)_2, (7)_1).$$

If $n = 11$ then, by Lemma 1, G_m is the graph H_3 depicted in Figure 3. If $n = 12$ then, again by Lemma 1, G_m is the graph constructed from H_3 by inserting a vertex of degree 2 on its unique internal path of length 1. Thus, all possible non-zero values of $\mid \mathcal{E}_{i,j} \mid$ are given as follows:

$$\mid \mathcal{E}_{i,j} \mid = \begin{cases} \frac{12-s}{3} & \text{if } i = 1 \text{ and } j = 3, \\ s-3 & \text{if } i = 1 \text{ and } j = 4, \\ n-s-1 & \text{if either } (i,j) = (2,3) \text{ or } (i,j) = (2,4), \\ \frac{4s-3n}{3} & \text{if } i = 3 \text{ and } j = 4. \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 2^{\frac{2(12-s)}{3}} \times 5^{n-4} \times 6^{n-s-1} \times 7^{\frac{4s-3n}{3}}.$$

Subcase (2.2): $s > 9$.

Observe, in the current subcase, that $s \geq 12$ and $x_2 \geq 1$.

Subcase (2.2.1): $s \geq 12$ and $\frac{4s-9}{3} < n \leq \frac{4s}{3}$

Note that

$$x_4 - 3 = \frac{4s-9}{3} - s - 1 < n - s - 1 = x_2 \leq \frac{s-3}{3} = x_4,$$

that is, $x_4 - 3 < x_2 \leq x_4$. Hence, by Lemma 1, every internal path of the form $P_{4,4}$ (in G_m) has length 2, and its unique vertex of degree 3 is adjacent to $3 - [x_2 - (x_4 - 3)]$ vertex/vertices of degree 4; for example, consider a graph constructed from the graph H_4 (shown in Figure 3) by inserting a vertex of degree 2 on each of the $x_2 - (x_4 - 3)$ internal path(s) of the form $P_{3,4}$. Hence, the possible non-zero values of $\mid \mathcal{E}_{i,j} \mid$ of G_m are given as follows:

$$\mid \mathcal{E}_{i,j} \mid = \begin{cases} x_1 = \frac{2s+3}{3} & \text{if } i = 1 \text{ and } j = 4, \\ x_2 - (x_4 - 3) = \frac{3n-4s+9}{3} & \text{if } i = 2 \text{ and } j = 3, \\ 3 - [x_2 - (x_4 - 3)] = \frac{4s-3n}{3} & \text{if } i = 3 \text{ and } j = 4, \\ (n-1) - \mid \mathcal{E}_{1,4} \mid - \mid \mathcal{E}_{2,3} \mid - \mid \mathcal{E}_{3,4} \mid = \frac{3n-2s-15}{3} & \text{if } i = 2 \text{ and } j = 4. \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 5^{\frac{3n-2s+12}{3}} \times 6^{\frac{3n-2s-15}{3}} \times 7^{\frac{4s-3n}{3}}.$$

Subcase (2.2.2): $s \geq 12$ and $s + 1 < n \leq \frac{4s-9}{3}$.

Observe, in the current subcase, that $s \geq 15$. Note that

$$x_4 - 3 = \frac{4s-9}{3} - s - 1 \geq n - s - 1 = x_2,$$

that is, $x_2 \leq x_4 - 3$. Hence, by Lemma 1, x_2 internal path(s) of the form $P_{4,4}$ in G_m has/have length 2; for example, consider a graph constructed from the graph H_2 (shown in Figure 3) by inserting a vertex of degree 2 on each of the x_2 internal path(s) of the form $P_{4,4}$. Hence, the possible non-zero values of $\mid \mathcal{E}_{i,j} \mid$ are given as follows:

$$\mid \mathcal{E}_{i,j} \mid = \begin{cases} x_1 = \frac{2s+3}{3} & \text{if } i = 1 \text{ and } j = 4, \\ 2x_2 = 2(n-s-1) & \text{if } i = 2 \text{ and } j = 4, \\ 3 & \text{if } i = 3 \text{ and } j = 4, \\ n - x_1 - 2x_2 - 4 = \frac{4s-3n-9}{3} & \text{if } i = j = 4. \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 7^3 \times 2^{4s-3n-9} \times 5^{\frac{2s+3}{3}} \times 6^{2(n-s-1)}.$$

Case (3): $n > \frac{4s}{3}$.

In the following, we discuss subcases for the current case.

Subcase (3.1): $s \leq 9$.

Observe, in the present subcase, that $s \in \{6, 9\}$. If $s = 6$ then $n \geq 9$, and Equation (7) yields

$$\mathsf{D}(G_m) = ((1)_4, (1)_3, (n-7)_2, (5)_1).$$

Thus, by Lemma 1, G_m is of the form H_5 given in Figure 3.

If $s = 9$ then $n \geq 13$, and Equation (7) gives

$$\mathsf{D}(G_m) = ((2)_4, (1)_3, (n-10)_2, (7)_1).$$

Thus, by Lemma 1, G_m is a graph constructed from H_1 (given in Figure 3) by inserting at least one vertex of degree 2 on each of two internal paths of length 1.

Hence, for $s \in \{6, 9\}$, the possible non-zero values of $\mid \mathcal{E}_{i,j} \mid$ are given as

$$\mid \mathcal{E}_{i,j} \mid = \begin{cases} \frac{12-s}{3} & \text{if } i = 1 \text{ and } j = 3, \\ s - 3 & \text{if } i = 1 \text{ and } j = 4, \\ \frac{3n-4s}{3} & \text{if } i = j = 2, \\ \frac{s-3}{3} & \text{if either } (i,j) = (2,3) \text{ or } (i,j) = (2,4). \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 4^{\frac{3n-5s+12}{3}} \times 5^{\frac{4s-12}{3}} \times 6^{\frac{s-3}{3}}.$$

Subcase (3.2): $s > 9$.

Since $n > \frac{4s}{3}$, we have

$$x_2 = n - s - 1 > \frac{s-3}{3} = x_4.$$

Thus, by Lemma 1, every internal path of G_m has a length of at least 2; for example, consider a graph constructed from H_7 (given in Figure 3) by inserting at least one vertex of degree 2 on some internal path(s). Hence, all possible non-zero values of $\mid \mathcal{E}_{i,j} \mid$ are as follows:

$$\mid \mathcal{E}_{i,j} \mid = \begin{cases} x_1 = \frac{2s+3}{3} & \text{if } i = 1 \text{ and } j = 4, \\ 3 & \text{if } i = 2 \text{ and } j = 3, \\ 2x_4 - 3 = \frac{2s-15}{3} & \text{if } i = 2 \text{ and } j = 4, \\ n - 1 - \mid \mathcal{E}_{1,4} \mid - \mid \mathcal{E}_{2,3} \mid - \mid \mathcal{E}_{2,4} \mid = \frac{3n-4s}{3} & \text{if } \; i = j = 2. \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 4^{\frac{3n-4s}{3}} \times 5^{\frac{2s+12}{3}} \times 6^{\frac{2s-15}{3}}.$$

Consequently, the proof is now completed. □

Theorem 6. *Let $G_m \in G(n,s)$ be a chemical tree with maximum multiplicative sum Zagreb index such that $s = 3t + 2$ for some integer $t \geq 1$. Then*

$$\Pi_1^*(G_m) = \begin{cases} 6 \times 4^{\frac{17-s}{3}} \times 5^{s-5} \times 7^{\frac{s-5}{3}} & \text{if } \; n = s+1 \text{ and } s \leq 17, \\ 7^6 \times 2^{s-20} \times 5^{\frac{2s+2}{3}} & \text{if } \; n = s+1 \text{ and } s > 17, \\ 25 \times 2^{2(n-3)} & \text{if } \; n \neq s+1 \text{ and } s = 5, \\ 4^{\frac{17-s}{3}} \times 5^{n-6} \times 6^{n-s} \times 7^{\frac{4s-3n-2}{3}} & \text{if } \; s+1 < n \leq \frac{4s-2}{3} \text{ and } 5 < s \leq 17, \\ 4^{\frac{3n-5s+16}{3}} \times 5^{\frac{4s-14}{3}} \times 6^{\frac{s-5}{3}} & \text{if } \; n > \frac{4s-2}{3} \text{ and } 5 < s \leq 17, \\ 7^6 \times 5^{\frac{2s+2}{3}} \times 6^{2(n-s-1)} \times 2^{4s-3n-17} & \text{if } \; s+1 < n \leq \frac{4s-17}{3} \text{ and } s > 17, \\ 5^{\frac{3n-2s+19}{3}} \times 6^{\frac{3n-2s-23}{3}} \times 7^{\frac{4s-3n+1}{3}} & \text{if } \; \frac{4s-17}{3} < n \leq \frac{4s+1}{3} \text{ and } s > 17, \\ 4^{\frac{3n-4s-1}{3}} \times 5^{\frac{2s+20}{3}} \times 6^{\frac{2s-22}{3}} & \text{if } \; n > \frac{4s+1}{3} \text{ and } s > 17. \end{cases}$$

Proof. By Lemma 3, it holds that

$$\mathsf{D}(G_m) = \left(\left(\frac{s-5}{3} \right)_4, (2)_3, (n-s-1)_2, \left(\frac{2s+2}{3} \right)_1 \right). \tag{8}$$

Case (1): $n = s + 1$.

Certainly, in the current case, $x_2 = 0$. The following subcases are further discussed:

Subcase (1.1): $s \leq 17$.

Here, $s \in \{5, 8, 11, 14, 17\}$ and hence $(n,s) \in \{(6,5), (9,8), (12,11), (15,14), (18,17)\}$. Now, Equation (8) gives

$$\mathsf{D}(G_m) = \begin{cases} ((0)_4, (2)_3, (0)_2, (4)_1) & \text{if } (n,s) = (6,5), \\ ((1)_4, (2)_3, (0)_2, (6)_1) & \text{if } (n,s) = (9,8), \\ ((2)_4, (2)_3, (0)_2, (8)_1) & \text{if } (n,s) = (12,11), \\ ((3)_4, (2)_3, (0)_2, (10)_1) & \text{if } (n,s) = (15,14), \\ ((4)_4, (2)_3, (0)_2, (12)_1) & \text{if } (n,s) = (18,17). \end{cases}$$

Because of Lemma 1, G_m is isomorphic to $S_{3,3}$, I_0, I_1, I_3, or I_2 when (n,s) is equal to $(6,5)$, $(9,8)$, $(12,11)$, $(15,14)$, or $(18,17)$, respectively. Hence, all possible non-zero values of $\mid \mathcal{E}_{i,j} \mid$ are as follows:

$$\mid \mathcal{E}_{i,j} \mid = \begin{cases} \frac{17-s}{3} & \text{if } i = 1 \text{ and } j = 3, \\ s-5 & \text{if } i = 1 \text{ and } j = 4, \\ 1 & \text{if } i = j = 3, \\ \frac{s-5}{3} & \text{if } i = 3 \text{ and } j = 4. \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 6 \times 4^{\frac{17-s}{3}} \times 5^{s-5} \times 7^{\frac{s-5}{3}}.$$

Subcase (1.2): $s > 17$.

Clearly, $s \geq 20$. By Lemma 1, all possible non-zero values of $\mid \mathcal{E}_{i,j} \mid$ in G_m (for example, see I_9 shown in Figure 4) are as follows:

$$\mid \mathcal{E}_{i,j} \mid = \begin{cases} x_1 = \frac{2s+2}{3} & \text{if } i = 1 \text{ and } j = 4, \\ 6 & \text{if } i = 3 \text{ and } j = 4, \\ \frac{s-20}{3} & \text{if } i = j = 4. \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 7^6 \times 2^{s-20} \times 5^{\frac{2s+2}{3}}.$$

Case (2): $n > s+1$.

In this case, we have $x_2 \neq 0$. The following subcases are further considered:

Subcase (2.1): $s = 5$.

Note, in the current subcase, that $n \geq 7$. By Lemma 1, the graph G_m is constructed by inserting $n-6$ vertices of degree 2 on the internal path of the graph $S_{3,3}$ shown in Figure 4. Hence, all possible non-zero values of $\mid \mathcal{E}_{i,j} \mid$ are mentioned below:

$$\mid \mathcal{E}_{i,j} \mid = \begin{cases} 4 & \text{if } i = 1 \text{ and } j = 3, \\ n-7 & \text{if } i = j = 2, \\ 2 & \text{if } i = 2 \text{ and } j = 3. \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 25 \times 2^{2(n-3)}.$$

Subcase (2.2): $5 < s \leq 17$ and $s+1 < n \leq \frac{4s-2}{3}$.

Note here that $s \in \{8, 11, 14, 17\}$ and hence (n,s) belongs to the set

$$\{(10,8), (13,11), (14,11), (16,14), (17,14), (18,14), (19,17), (20,17), (21,17), (22,17)\}.$$

Now, Equation (8) gives

$$\mathsf{D}(G_m) = \begin{cases} ((1)_4\,,(2)_3\,,(1)_2\,,(6)_1\,) & \text{if } (n,s) = (10,8), \\ ((2)_4\,,(2)_3\,,(1)_2\,,(8)_1\,) & \text{if } (n,s) = (13,11), \\ ((2)_4\,,(2)_3\,,(2)_2\,,(8)_1\,) & \text{if } (n,s) = (14,11), \\ ((3)_4\,,(2)_3\,,(1)_2\,,(10)_1\,) & \text{if } (n,s) = (16,14), \\ ((3)_4\,,(2)_3\,,(2)_2\,,(10)_1\,) & \text{if } (n,s) = (17,14), \\ ((3)_4\,,(2)_3\,,(3)_2\,,(10)_1\,) & \text{if } (n,s) = (18,14), \\ ((4)_4\,,(2)_3\,,(1)_2\,,(12)_1\,) & \text{if } (n,s) = (19,17), \\ ((4)_4\,,(2)_3\,,(2)_2\,,(12)_1\,) & \text{if } (n,s) = (20,17), \\ ((4)_4\,,(2)_3\,,(3)_2\,,(12)_1\,) & \text{if } (n,s) = (21,17), \\ ((4)_4\,,(2)_3\,,(4)_2\,,(12)_1\,) & \text{if } (n,s) = (22,17). \end{cases}$$

Because of Lemma 1, G_m is isomorphic to a graph constructed from I_0, I_1, I_2, or I_3 by inserting one vertex of degree 2 on each of the x_2 internal path(s) of the form $P_{3,4}$. Hence, all possible non-zero values of $|\ \mathcal{E}_{i,j}\ |$ are as follows:

$$|\ \mathcal{E}_{i,j}\ | = \begin{cases} \frac{17-s}{3} & \text{if } i = 1 \text{ and } j = 3, \\ s-5 & \text{if } i = 1 \text{ and } j = 4, \\ n-s-1 & \text{if either } (i,j) = (2,3) \text{ or } (i,j) = (2,4), \\ 1 & \text{if } i = j = 3, \\ \frac{4s-3n-2}{3} & \text{if } i = 3 \text{ and } j = 4. \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 4^{\frac{17-s}{3}} \times 5^{n-6} \times 6^{n-s} \times 7^{\frac{4s-3n-2}{3}}.$$

Subcase (2.3): $5 < s \leq 17$ and $n > \frac{4s-2}{3}$.

By Lemma 1, G_m is isomorphic to a graph constructed from I_0, I_1, I_2, or I_3 by inserting at least one vertex of degree 2 on each its internal path(s). Hence, all possible non-zero values of $|\ \mathcal{E}_{i,j}\ |$ are as follows:

$$|\ \mathcal{E}_{i,j}\ | = \begin{cases} \frac{17-s}{3} & \text{if } i = 1 \text{ and } j = 3, \\ s-5 & \text{if } i = 1 \text{ and } j = 4, \\ \frac{3n-4s-1}{3} & \text{if } i = j = 2, \\ \frac{s+1}{3} & \text{if } i = 2 \text{ and } j = 3, \\ \frac{s-5}{3} & \text{if } i = 2 \text{ and } j = 4. \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 4^{\frac{3n-5s+16}{3}} \times 5^{\frac{4s-14}{3}} \times 6^{\frac{s-5}{3}}.$$

Subcase (2.4): $s + 1 < n \leq \frac{4s-17}{3}$ and $s > 17$.

Note, in the current subcase, that $s \geq 23$ and $x_2 \geq 1$. (If $s = 20$ then we obtain $21 < n \leq 21$, a contradiction.) Also, note that

$$x_2 = n - s - 1 \leq \frac{4s - 17}{3} - s - 1 = x_4 - 5.$$

Thus, by Lemma 1, all possible non-zero values of $|\ \mathcal{E}_{i,j}\ |$ are as follows (for example, G_m may be a graph constructed from I_9 (shown in Figure 4) by inserting a vertex of degree 2 on each of its x_2 internal path(s) of the form $P_{4,4}$):

$$|\ \mathcal{E}_{i,j}\ | = \begin{cases} \frac{2s+2}{3} & \text{if } i = 1 \text{ and } j = 4, \\ 2(n-s-1) & \text{if } i = 2 \text{ and } j = 4, \\ 6 & \text{if } i = 3 \text{ and } j = 4, \\ \frac{4s-3n-17}{3} & \text{if } i = j = 4. \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 7^6 \times 5^{\frac{2s+2}{3}} \times 6^{2(n-s-1)} \times 2^{4s-3n-17}.$$

Subcase (2.5): $s > 17$ and $\frac{4s-17}{3} < n \leq \frac{4s+1}{3}$.

In the current case, observe that $s \geq 20$. Also, note that

$$x_4 - 5 = \frac{4s - 17}{3} - s - 1 < n - s - 1 = x_2 \leq \frac{4s + 1}{3} - s - 1 = x_4 + 1,$$

that is, $x_4 - 5 < x_2 \leq x_4 + 1$. Thus, by Lemma 1, all possible non-zero values of $|\ \mathcal{E}_{i,j}\ |$ are as follows (for example, G_m may be a graph constructed from I_6 (shown in Figure 4) by inserting one vertex of degree 2 on each of its $x_2 - (x_4 - 5)$ internal path(s) of the form $P_{3,4}$):

$$|\ \mathcal{E}_{i,j}\ | = \begin{cases} \frac{2s+2}{3} & \text{if } i = 1 \text{ and } j = 4, \\ \frac{3n-4s+17}{3} & \text{if } i = 2 \text{ and } j = 3, \\ \frac{3n-2s-23}{3} & \text{if } i = 2 \text{ and } j = 4, \\ \frac{4s-3n+1}{3} & \text{if } i = 3 \text{ and } j = 4. \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 5^{\frac{3n-2s+19}{3}} \times 6^{\frac{3n-2s-23}{3}} \times 7^{\frac{4s-3n+1}{3}}.$$

Subcase (2.6): $n > \frac{4s+1}{3}$ and $s > 17$.

Observe, in the current subcase, that

$$x_2 = n - s - 1 > \frac{4s + 1}{3} - s - 1 = x_4 + 1,$$

Thus, by Lemma 1, all possible non-zero values of $\mid \mathcal{E}_{i,j} \mid$ are as follows (for example, G_m may be a graph constructed from I_9 (shown in Figure 4) by inserting at least one vertex of degree 2 on each of its internal paths:

$$\mid \mathcal{E}_{i,j} \mid = \begin{cases} \frac{2s+2}{3} & \text{if } i = 1 \text{ and } j = 4, \\ \frac{3n-4s-1}{3} & \text{if } i = j = 2, \\ 6 & \text{if } i = 2 \text{ and } j = 3, \\ \frac{2s-22}{3} & \text{if } i = 2 \text{ and } j = 4. \end{cases}$$

Therefore,

$$\Pi_1^*(G_m) = 4^{\frac{3n-4s-1}{3}} \times 5^{\frac{2s+20}{3}} \times 6^{\frac{2s-22}{3}}.$$

□

4. Concluding Remarks

In this paper, we have determined graphs possessing the greatest possible values of the multiplicative sum Zagreb (MSZ) index over the class of chemical trees with a given number of segments and fixed order. We have also calculated the values of the MSZ index of the obtained extremal trees. Possible future work toward the study of the maximum MSZ index for chemical trees includes characterizing graphs with the greatest MSZ index from the set of chemical trees with a given order and some additional graph invariants (for example, the number of pendent vertices, matching number, etc.).

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