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Chemical Trees with Extreme Values of a Few Types of Multiplicative Zagreb Indices

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Abstract

We obtain sharp upper bounds for the second multiplicative Zagreb index and multiplicative sum Zagreb index and lower bound for the first multiplicative Zagreb index among the class of chemical trees. Also, we characterize those chemical trees achieving extremal values of multiplicative Zagreb indices that we considered.

1 Introduction

In this paper we consider only finite simple graphs. Let $G = (V, E)$ be a graph with $n = |V(G)|$ vertices and $m = |E(G)|$ edges. For each vertex $v \in V$, let $d_G(v)$ denotes the degree of a vertex v in G and $\Delta(G)$ the maximum vertex degree of the graph G. We will omit the subscript G whenever the graph is clear from the context.

The first and the second multiplicative Zagreb indices are defined as:

$$\Pi_1(G) := \prod_{u \in V(G)} d_G^2(u), \qquad \Pi_2(G) := \prod_{uv \in E(G)} d_G(u) \cdot d_G(v).$$

These two multiplicative variants of ordinary Zagreb indices were introduced by Todeschini et al. in [6,7] and called *multiplicative Zagreb indices* by Gutman in [2]. In the same paper, Gutman treated extremal values of those indices over the set of all trees $\mathcal{T}(n)$ of order $n \geqslant 4$ and found that path P_n is maximal with respect to Π_1, but minimal with respect to Π_2, while star S_n is maximal with respect to Π_2 and minimal to Π_1.

Eliasi, Iranmanesh and Gutman introduced a new graphical invariant in [1] :

$$\Pi_1^*(G) := \prod_{uv \in E(G)} (d_G(u) + d_G(v)) .$$

In [8] Xu and Das named it as *multiplicative sum Zagreb index* and characterized the trees, unicyclic and bicyclic graphs extremal with respect to this topological index. They found that the path P_n is minimal, while the star S_n is maximal with respect to Π_1^*, among all trees of order $n \geqslant 4$.

The main goal of this article is to give sharp upper bounds for Π_2 and Π_1^* and lower bound for Π_1 over the class $\mathcal{H}(n)$ of chemical trees with n vertices. Also, we will characterize trees with extremal values of considered multiplicative Zagreb indices over the class $\mathcal{H}(n)$.

Let us denote by $\mathcal{T}_1^r(n)$, $r \geqslant 2$, the class of all trees with only pendent vertices and vertices of degree r and by $\mathcal{T}_k^r(n)$, $2 \leqslant k < r$, the class of all trees with exactly one vertex of degree k, while the other vertices are pendent or of degree r. The reason we introduced such notation is because we will prove that the extremal graphs we are looking for belong to those classes. Also, we find that the subclass when $r = 4$ is of particular importance among the class of chemical trees, and thus we simplify notation by $\mathcal{H}_i(n) = \mathcal{T}_i^4(n)$, $i = 1, 2, 3$.

2 First Multiplicative Zagreb Index

In this section, we characterize the class of chemical trees with minimal Π_1 index. Clearly, finding the minimum of Π_1 index over some class of graphs is equivalent to finding the minimum of Narumi-Katayama index

$$NK(G) := \prod_{u \in V(G)} d_G(u)$$

over the same class of graphs.

Since our primary focus is on the class of chemical graphs $\mathcal{H}(n)$ and the set $\{NK(G) \mid G \in \mathcal{H}(n)\}$ is a subset of the set of natural numbers, there must exist a chemical tree $G_0 \in \mathcal{H}(n)$ such that

$$NK(G_0) = \min\{NK(G) \mid G \in \mathcal{H}(n)\}.$$

The following theorem describes some necessary conditions which G_0 must satisfy.

Theorem 2.1. *Let $G_0 \in \mathcal{H}(n)$ be such that*

$$NK(G_0) = \min\{NK(G) \mid G \in \mathcal{H}(n)\}.$$

Then $G_0 \in \mathcal{H}_1(n) \cup \mathcal{H}_2(n) \cup \mathcal{H}_3(n)$.

Proof.

Let G be a chemical tree and let $x \in V(G)$ be a vertex of a degree 2 or 3. Let us suppose that there exists at least one vertex y in G , $y \neq x$, such that

$$d(x) \leqslant d(y) < 4.$$

We are going to construct chemical tree $H \in \mathcal{H}(n)$ such that

$$NK(H) < NK(G),$$

i.e. NK doesn't achieve minimum on the graph G.

Since G is a tree, there is a unique path P from x to y, and it goes through exactly one of the neighbours of the vertex x. We have already supposed that x has at least two neighbours, so there is a neighbour x_1 that P doesn't go through. (Note that y could be the other neighbour of x.) Let us denote by $G_{x \nsim x_1 \sim y}$ the graph created from G by removing the edge xx_1 and adding the edge x_1y. For the sake of simplicity, the graph $G_{x \nsim x_1 \sim y}$ will be further denoted by H.

It holds

$$NK(G) = \prod_{u \in V(G)} d_G(u) = d_G(x) \cdot d_G(y) \cdot \prod_{\substack{v \in V(G) \\ v \notin \{x,y\}}} d_G(v).$$

Similarly,

$$NK(H) = \prod_{u \in V(H)} d_H(u) = d_H(x) \cdot d_H(y) \cdot \prod_{\substack{v \in V(H) \\ v \notin \{x,y\}}} d_G(v).$$

As $d_H(v) = d_G(v)$, for all $v \notin \{x, y\}$ and $d_H(x) = d_G(x) - 1$, $d_H(y) = d_G(y) + 1$, then

$$\begin{aligned} NK(H) - NK(G) &= \prod_{\substack{v \in V(G) \\ v \notin \{x,y\}}} d_G(v) \cdot \Big[(d_G(x) - 1)(d_G(y) + 1) - d_G(x)d_G(y)\Big] \\ &= \prod_{\substack{v \in V(G) \\ v \notin \{x,y\}}} d_G(v) \cdot \Big[d_G(x) - d_G(y) - 1\Big]. \end{aligned} \tag{1}$$

Since $d_G(x) \leqslant d_G(y)$, then $NK(H) - NK(G) < 0$, and therefore $NK(H) < NK(G)$.

■

Remark: Note that the previous theorem could be generalized in some sense. Namely, if we define

$$\mathcal{T}^r(n) = \{G \in \mathcal{T}(n) \mid \Delta(G) \leqslant r\},\ r \in \mathbb{N},$$

it could be proven, by using the same arguments as we did in the previous theorem, that the minimum of Narumi-Katayama index over the considered class,

$$NK(H_0) = \min\{NK(H) \mid H \in \mathcal{T}^r(n)\},$$

is attained at a graph H_0, such that $H_0 \in \mathcal{T}_k^r(n)$, $1 \leqslant k < r$.

Proposition 2.2. *Let G be a tree such that $G \in \mathcal{T}_k^r(n)$, $1 \leqslant k < r$, $r > 2$. Then*

$$n \equiv k+1 \pmod{(r-1)}.$$

Proof.

Let $G \in \mathcal{T}_k^r(n)$ be a tree with ℓ pendent vertices. From the Handshaking lemma, it follows

$$\sum_{v \in V(G)} d(v) = 2(n-1).$$

Respecting the given conditions and notation, we have

$$\ell + r(n-\ell) = 2n-2, \text{when } k = 1,$$

and

$$\ell + k + r(n-\ell-1) = 2n-2, \text{when } k > 1.$$

From both cases, it comes directly

$$n \equiv k+1 \pmod{(r-1)}.$$

■

Note that the proof of the previous proposition provides a useful relation between parameters n, r, ℓ and k in general and particularly for the class of chemical trees when $r = 4$. Also, when speaking of the minimum of Narumi-Katayama index over the class of chemical trees of degree n, we should realize that Theorem 2.1 highlited the importance of the subset $\mathcal{H}_1(n) \cup \mathcal{H}_2(n) \cup \mathcal{H}_3(n)$ of $\mathcal{H}(n)$.

Corollary 2.3. *Let G be a chemical tree with n vertices such that $G \in \mathcal{H}_1(n) \cup \mathcal{H}_2(n) \cup \mathcal{H}_3(n)$. Then*

a. $n \equiv 2 \pmod 3$ *and* $\ell = \frac{2+2n}{3}$, *if* $G \in \mathcal{H}_1(n)$*;*

b. $n \equiv 0 \pmod 3$ *and* $\ell = \frac{2n}{3}$, *if* $G \in \mathcal{H}_2(n)$*;*

c. $n \equiv 1 \pmod 3$ *and* $\ell = \frac{1+2n}{3}$, *if* $G \in \mathcal{H}_3(n)$*.*

Proposition 2.4. *Let G be a chemical tree with n vertices such that $G \in \mathcal{H}_1(n) \cup \mathcal{H}_2(n) \cup \mathcal{H}_3(n)$. Then*

$$\Pi_1(G) = \begin{cases} 4^{\frac{2}{3}n-\frac{4}{3}}, & G \in \mathcal{H}_1(n) \\ 4^{\frac{2}{3}n-1}, & G \in \mathcal{H}_2(n) \\ 9 \cdot 4^{\frac{2}{3}n-\frac{8}{3}}, & G \in \mathcal{H}_3(n). \end{cases}$$

Proof. From the Corollary 2.3, it follows that if $G \in \mathcal{H}_1(n)$ then $n \equiv 2 \pmod 3$ and $\ell = \frac{2n+2}{3}$. Consequently,

$$\Pi_1(G) = \prod_{d(v)=1} d^2(v) \cdot \prod_{d(v)=4} d^2(v) = 4^{\frac{2}{3}n-\frac{4}{3}}.$$

Similarly, if $G \in \mathcal{H}_2(n)$, then $n \equiv 0 \pmod 3$, $\ell = \frac{2n}{3}$, so

$$\Pi_1(G) = 4 \cdot \prod_{d(v)=4} d^2(v) = 4 \cdot 4^{2(n-\frac{2n}{3}-1)} = 4^{\frac{2}{3}n-1},$$

and if $G \in \mathcal{H}_3(n)$, then $n \equiv 1 \pmod 3$, $\ell = \frac{2n+1}{3}$, so

$$\Pi_1(G) = 9 \cdot \prod_{d(v)=4} d^2(v) = 9 \cdot 4^{2(n-1-\frac{2n+1}{3})} = 9 \cdot 4^{\frac{2}{3}n-\frac{8}{3}}.$$

∎

The final conclusion of this section, following directly from the previous assertions, is that

$$\min_{G \in \mathcal{H}(n)} \Pi_1(G) = \begin{cases} 4^{\frac{2}{3}n-\frac{4}{3}}, & n \equiv 2 \pmod 3 \\ 4^{\frac{2}{3}n-1}, & n \equiv 0 \pmod 3 \\ 9 \cdot 4^{\frac{2}{3}n-\frac{8}{3}}, & n \equiv 1 \pmod 3). \end{cases}$$

3 Second Multiplicative Zagreb Index

In this section we find the subclass of chemical trees at which Π_2 attains its maximal value. As it is done in Lemma 3.1 in [2], we use equivalent form of the second multiplicative Zagreb index as:

$$\Pi_2(G) = \prod_{v \in V(G)} d(v)^{d(v)}.$$

The following theorem, same as Theorem 2.1, will again emphasize the importance of subclass $\mathcal{H}_1(n) \cup \mathcal{H}_2(n) \cup \mathcal{H}_3(n)$ of chemical trees.

Theorem 3.1. *Let $G_0 \in \mathcal{H}(n)$ be such that*

$$\Pi_2(G_0) = \max\{\Pi_2(G) \mid G \in \mathcal{H}(n)\}.$$

Then $G_0 \in \mathcal{H}_1(n) \cup \mathcal{H}_2(n) \cup \mathcal{H}_3(n)$.

Proof.
Let G be a chemical tree and let $x \in V(G)$ such that $d(x) \in \{2, 3\}$. Suppose that there is $y \in V(G)$, $y \neq x$, such that $d(y) \geqslant d(x)$ and $d(y) < 4$. Let $H = G_{x \nsim x_1 \sim y}$ be the tree constructed as in the proof of Theorem 2.1. Then we have

$$\Pi_2(G) = d(x)^{d(x)} \cdot d(y)^{d(y)} \cdot \prod_{v \in V(G) \setminus \{x,y\}} d(v)^{d(v)}$$

and

$$\Pi_2(H) = (d(x)-1)^{d(x)-1} \cdot (d(y)+1)^{d(y)+1} \cdot \prod_{v \in V(G) \setminus \{x,y\}} d(v)^{d(v)},$$

where $d(v) = d_G(v)$, for each vertex v.

$d(x)$	$d(y)$	$d(x)^{d(x)} \cdot d(y)^{d(y)}$	$(d(x)-1)^{d(x)-1} \cdot (d(y)+1)^{d(y)+1}$
2	2	16	27
2	3	108	256
3	3	729	1024

It follows

$$\Pi_2(G) < \Pi_2(H).$$

■

Proposition 3.2. *Let G be a chemical tree such that $G \in \mathcal{H}_1(n) \cup \mathcal{H}_2(n) \cup \mathcal{H}_3(n)$. Then*

$$\Pi_2(G) = \begin{cases} 4^{\frac{4(n-2)}{3}}, & G \in \mathcal{H}_1(n) \\ 4^{\frac{4n}{3}-3}, & G \in \mathcal{H}_2(n) \\ 3^3 \cdot 4^{\frac{4(n-1)}{3}-4}, & G \in \mathcal{H}_3(n). \end{cases}$$

Proof.

If $G \in \mathcal{H}_1(n)$ then $n \equiv 2 \pmod 3$, G has $\frac{n-2}{3}$ vertices of degree 4, while all other vertices are pendent. It follows that

$$\Pi_2(G) = 4^{4\frac{n-2}{3}}.$$

If $G \in \mathcal{H}_2(n)$ then $n \equiv 0 \pmod 3$, G has $\frac{n}{3} - 1$ vertices of degree 4, one vertex of degree 2, and all other vertices are pendent. Thus

$$\Pi_2(G) = 2^2 \cdot 4^{4\frac{n}{3}-4} = 4^{4\frac{n}{3}-3}.$$

If $G \in \mathcal{H}_3(n)$ then $n \equiv 1 \pmod 3$, G has $\frac{n-1}{3} - 1$ vertices of degree 4, one vertex of degree 3, and all other vertices are pendent. Therefore

$$\Pi_2(G) = 3^3 \cdot 4^{4\frac{n-1}{3}-4}.$$

■

As a conclusion, from the assertions of this section, we have

$$\max_{G \in \mathcal{H}(n)} \Pi_2(G) = \begin{cases} 4^{\frac{4(n-2)}{3}}, & n \equiv 2 \pmod 3 \\ 4^{\frac{4n}{3}-3}, & n \equiv 0 \pmod 3 \\ 3^3 \cdot 4^{\frac{4(n-1)}{3}-4}, & n \equiv 1 \pmod 3). \end{cases}$$

4 Multiplicative sum Zagreb Index

In this section we give sharp upper bound of the multiplicative sum Zagreb index of chemical trees and characterize the case when that bound is attained.

Suppose that G is a chemical tree with a vertex x such that $d(x) \in \{2, 3\}$ and there is a vertex $y \neq x$ of G such that $d(x) \leqslant d(y) < 4$. We describe how a graph G can be transformed to the graph $G' \in \mathcal{H}_1(n) \cup \mathcal{H}_2(n) \cup \mathcal{H}_3(n)$ that has greater multiplicative sum Zagreb index, i.e $\Pi_1^*(G') > \Pi_1^*(G)$.

There are two cases to consider, depending on degree of the vertex x.

Case 1. Let $d(x) = 2$ and let $N(x) = \{x_1, x_2\}$. Since G is a tree, there is unique path P from x to y and it goes through exactly one of the neighbours of the vertex x. Let it be the vertex x_2.

We will prove that

$$\Pi_1^*(G) < \Pi_1^*(H),$$

where $H = G_{x \nsim x_1 \sim y}$.

Now, we have two possibilities: $d(y) = 2$ and $d(y) = 3$.

Case 1.1. Let us consider the first case, the one where $d(y) = 2$. If y is not a neighbour of x, then let y_1 and y_2 be neighbours of the vertex y.
Let $S_G = \{xx_1, xx_2, yy_1, yy_2\} \subset E(G)$ and $S_H = \{yx_1, xx_2, yy_1, yy_2\} \subset E(H)$.

From the definition of multiplicative sum Zagreb index we have

$$\begin{aligned}\Pi_1^*(G) &= \prod_{uv \in E(G)} (d_G(u) + d_G(v)) \\ &= \prod_{i=1}^{2}(d_G(x) + d_G(x_i)) \cdot \prod_{i=1}^{2}(d_G(y) + d_G(y_i)) \cdot \prod_{\substack{uv \in E(G) \\ uv \notin S_G}} (d_G(u) + d_G(v))\end{aligned}$$

and

$$\begin{aligned}\Pi_1^*(H) =& (d_H(x) + d_H(x_2))(d_H(y) + d_H(x_1)) \cdot \prod_{i=1}^{2}(d_H(y) + d_H(y_i)) \cdot \\ & \cdot \prod_{\substack{uv \in E(H) \\ uv \notin S_H}} (d_H(u) + d_H(v)) .\end{aligned}$$

Hence,

$$\Pi_1^*(G) < \Pi_1^*(H)$$

if and only if

$$(2 + d(x_1))(2 + d(x_2))(2 + d(y_1))(2 + d(y_2)) < (1 + d(x_2))(3 + d(x_1))(3 + d(y_1))(3 + d(y_2))$$

i.e. if and only if

$$1 + \frac{1}{1 + d(x_2)} < \left(1 + \frac{1}{2 + d(x_1)}\right)\left(1 + \frac{1}{2 + d(y_1)}\right)\left(1 + \frac{1}{2 + d(y_2)}\right). \qquad (2)$$

Since $1 \leqslant d(x_2)$, the left-hand side of (2) is not greater than $\frac{3}{2}$. Similarly, the minimum value of the right-hand side of (2) is $\left(1+\frac{1}{6}\right)^3 = \frac{7^3}{6^3}$. Therefore, inequality (2) holds due to $\frac{3}{2} < \frac{7^3}{6^3}$, so $\Pi_1^*(G) < \Pi_1^*(H)$.

Note that, if y is a neighbour of x, then $S_G = \{xx_1, xy, yy_1\}$, $S_H = \{yx_1, yy_1, xy\}$ and using the same arguments as above we have

$$\Pi_1^*(G) < \Pi_1^*(H) \Longleftrightarrow 4 \cdot (2 + d(x_1))(2 + d(y_1)) < 4 \cdot (3 + d(x_1))(3 + d(y_1))$$
$$\Longleftrightarrow 1 < \left(1 + \frac{1}{2 + d(x_1)}\right)\left(1 + \frac{1}{2 + d(y_1)}\right),$$

which is always true.

Case 1.2. Let us now observe the case when $d(y) = 3$.
If y is not a neighbour of x then suppose $N(y) = \{y_1, y_2, y_3\}$. Let

$$S_G = \{xx_1, xx_2, yy_1, yy_2, yy_3\} \subset E(G) \text{ and } S_H = \{yx_1, xx_2, yy_1, yy_2, yy_3\} \subset E(H).$$

By employing the definition of multiplicative sum Zagreb index we have

$$\Pi_1^*(G) = \prod_{i=1}^{2}(d_G(x) + d_G(x_i)) \cdot \prod_{i=1}^{3}(d_G(y) + d_G(y_i)) \cdot \prod_{\substack{uv \in E(G) \\ uv \notin S_G}} (d_G(u) + d_G(v))$$

and

$$\Pi_1^*(H) = (d_H(x) + d_H(x_2)) \cdot (d_H(y) + d_H(x_1)) \cdot \prod_{i=1}^{3}(d_H(y) + d_H(y_i))$$
$$\cdot \prod_{\substack{uv \in E(H) \\ uv \notin S_H}} (d_H(u) + d_H(v)).$$

It follows that

$$\Pi_1^*(G) < \Pi_1^*(H)$$
$$\Updownarrow$$
$$\prod_{i=1}^{2}(2 + d(x_i)) \cdot \prod_{i=1}^{3}(3 + d(y_i)) < (4 + d(x_1))(1 + d(x_2)) \prod_{i=1}^{3}(4 + d(y_i))$$
$$\Updownarrow$$
$$1 + \frac{1}{1 + d(x_2)} < \left(1 + \frac{2}{2 + d(x_1)}\right) \prod_{i=1}^{3}\left(1 + \frac{1}{3 + d(y_i)}\right). \tag{3}$$

The inequality (3) holds, since the left side is not greater than $\frac{3}{2}$ and the minimum value of the right side is $\left(1+\frac{2}{6}\right)\left(1+\frac{1}{7}\right)^3 = \frac{4}{3}\cdot\frac{8^3}{7^3}$. Hence, $\Pi_1^*(G) < \Pi_1^*(H)$.

Note that, if y is a neighbour of x, then as in the previous case we will have the same result.

Case 2. Let us suppose that G is a chemical tree with vertices x, y so that $d(x) = d(y) = 3$. By using the same technique as in the previous cases we construct chemical tree H so that

$$\Pi^*(G) < \Pi^*(H).$$

If y is not a neighbour of x, then suppose $N(x) = \{x_1, x_2, x_3\}$, $N(y) = \{y_1, y_2, y_3\}$ and let unique $(x-y)$ path goes through the vertex x_2. Let us denote $H = G_{x \nsim x_1 \sim y}$, $S_G = \{xx_1, xx_2, xx_3, yy_1, yy_2, yy_3\} \subset E(G)$ and $S_H = \{yx_1, xx_2, xx_3, yy_1, yy_2, yy_3\} \subset E(H)$. Consequently,

$$\Pi_1^*(G) = \prod_{i=1}^{3}(d_G(x)+d_G(x_i)) \cdot \prod_{i=1}^{3}(d_G(y)+d_G(y_i)) \cdot \prod_{\substack{uv\in E(G)\\ uv\notin S_G}} (d_G(u)+d_G(v))$$

and

$$\begin{aligned}\Pi_1^*(H) =& (d_H(y)+d_H(x_1))\prod_{i=1}^{2}(d_H(x)+d_H(x_{i+1})) \cdot \prod_{i=1}^{3}(d_H(y)+d_H(y_i)) \\ &\cdot \prod_{\substack{uv\in E(H)\\ uv\notin S_H}} (d_H(u)+d_H(v)) .\end{aligned}$$

Therefore, it follows that

$$\Pi_1^*(G) < \Pi_1^*(H)$$

$$\Updownarrow$$

$$\prod_{i=1}^{3}(3+d(x_i)) \cdot \prod_{i=1}^{3}(3+d(y_i)) < (4+d(x_1)) \cdot \prod_{i=1}^{2}(2+d(x_{i+1})) \cdot \prod_{i=1}^{3}(4+d(y_i))$$

$$\Updownarrow$$

$$\left(1+\frac{1}{1+d(x_2)}\right)\left(1+\frac{1}{1+d(x_3)}\right) < \left(1+\frac{1}{3+d(x_1)}\right)\prod_{i=1}^{3}\left(1+\frac{1}{3+d(y_i)}\right). \qquad (4)$$

Since $d(x_2) \geqslant 2$, the left-hand side of (4) is maximal when $d(x_2) = 2$ and $d(x_3) = 1$, so the maximum value is $\frac{5}{3}$. Similarly, the right-hand side of (4) is minimal if $d(x_1) = d(y_1) = d(y_2) = d(y_3) = 4$ and its minimal value is $\frac{8^4}{7^4}$. Since $\frac{5}{3} < \frac{8^4}{7^4}$, assertion follows.

Note that, if $y \in N(x)$, then we get the same result. Repeating the previous transformation, multiplicative Zagreb index increases and the chemical tree G transforms to the chemical tree that belongs to $\mathcal{H}_1(n) \cup \mathcal{H}_2(n) \cup \mathcal{H}_3(n)$. Hence, the next theorem follows immediately.

Theorem 4.1. *Let G be a $n-$vertex chemical tree such that*

$$\Pi_1^*(G) = \max\{\Pi_1^*(H) \mid H \in \mathcal{H}(n)\}.$$

Then $G \in \mathcal{H}_1(n) \cup \mathcal{H}_2(n) \cup \mathcal{H}_3(n)$.

As a simple consequence of the previous theorem, we get exact bounds for Π_1^* over the class of chemical trees in the next propositions.

Proposition 4.2. *Let G be a chemical tree in $\mathcal{H}_1(n)$. Then*

$$\Pi_1^*(G) = 5^{\frac{2n+2}{3}} \cdot 8^{\frac{n-5}{3}}$$

Proof.
According to Corollary 2.3 we have $n \equiv 2 \pmod 3$ and $\ell = \frac{2n+2}{3}$ pendent vertices in G. Therefore,

$$\Pi_1^*(G) = (1+4)^{\ell} \cdot (4+4)^{n-1-\ell} = 5^{\frac{2n+2}{3}} \cdot 8^{\frac{n-5}{3}}.$$

■

Proposition 4.3. *Let G be a chemical tree in $\mathcal{H}_2(n)$ and $x \in V(G)$ be a vertex of degree 2. Then*

$$\Pi_1^*(G) = \begin{cases} 144 \cdot 5^{\frac{2n}{3}-1} \cdot 8^{\frac{n}{3}-3}, & x \text{ is adjacent to a pendent vertex} \\ 180 \cdot 5^{\frac{2n}{3}-1} \cdot 8^{\frac{n}{3}-3}, & x \text{ is not adjacent to a pendent vertex.} \end{cases}$$

Proof.
As stated in Corollary 2.3, $n \equiv 0 \pmod 3$ and there are $\ell = \frac{2n}{3}$ pendent vertices in G. Let e_1 and e_2 be the edges incident to a vertex x.
Assume that unique vertex x of degree 2 is adjacent to some pendent vertex.

We have

$$\Pi_1^*(G) = (1+2) \cdot (4+2) \cdot \prod_{uv \in E(G) \setminus \{e_1, e_2\}} (d(u) + d(v))$$

$$
\begin{aligned}
&= 18 \cdot 5^{\ell-1} \cdot 8^{n-1-(\ell-1)-2} \\
&= 18 \cdot 5^{\frac{2n}{3}-1} \cdot 8^{\frac{n}{3}-2} \\
&= 144 \cdot 5^{\frac{2n}{3}-1} \cdot 8^{\frac{n}{3}-3}.
\end{aligned}
$$

When the vertex x is not adjacent to a pendent vertex, we have

$$
\begin{aligned}
\Pi_1^*(G) &= (4+2) \cdot (4+2) \cdot \prod_{uv \in E(G) \setminus \{e_1, e_2\}} (d(u)+d(v)) \\
&= 36 \cdot 5^{\ell} \cdot 8^{n-1-\ell-2} \\
&= 36 \cdot 5^{\frac{2n}{3}} \cdot 8^{\frac{n}{3}-3} \\
&= 180 \cdot 5^{\frac{2n}{3}-1} \cdot 8^{\frac{n}{3}-3}.
\end{aligned}
$$

■

Proposition 4.4. *Let G be a chemical tree in $\mathcal{H}_3(n)$ and $x \in V(G)$ is unique vertex of degree 3. Then*

$$
\Pi_1^*(G) = \begin{cases} 7840 \cdot 5^{\frac{2n+1}{3}-2} \cdot 8^{\frac{n-1}{3}-4}, & x \text{ is adjacent to one pendent vertex} \\ 7168 \cdot 5^{\frac{2n+1}{3}-2} \cdot 8^{\frac{n-1}{3}-4}, & x \text{ is adjacent to two pendent vertices} \\ 8575 \cdot 5^{\frac{2n+1}{3}-2} \cdot 8^{\frac{n-1}{3}-4}, & \text{otherwise.} \end{cases}
$$

Proof.
Due to Corollary 2.3, $n \equiv 1 \pmod 3$ and there are $\ell = \frac{2n+1}{3}$ pendent vertices in G.
Let e_1, e_2 and e_3 be the edges incident to a vertex x.
Assume that vertex x is adjacent to only one pendent vertex. Then, we have

$$
\begin{aligned}
\Pi_1^*(G) &= (1+3) \cdot (4+3)^2 \cdot \prod_{uv \in E(G) \setminus \{e_1, e_2, e_3\}} (d(u)+d(v)) \\
&= 196 \cdot 5^{\ell-1} \cdot 8^{n-1-(\ell-1)-3} \\
&= 196 \cdot 5^{\frac{2n+1}{3}-1} \cdot 8^{\frac{n-1}{3}-3} \\
&= 7840 \cdot 5^{\frac{2n+1}{3}-2} \cdot 8^{\frac{n-1}{3}-4}.
\end{aligned}
$$

If the vertex x is adjacent to two pendent vertices, then

$$\begin{aligned}\Pi_1^*(G) &= (1+3)^2 \cdot (4+3) \cdot \prod_{uv \in E(G)\setminus\{e_1,e_2,e_3\}} (d(u)+d(v)) \\ &= 112 \cdot 5^{\ell-2} \cdot 8^{n-1-(\ell-2)-3} \\ &= 112 \cdot 5^{\frac{2n+1}{3}-2} \cdot 8^{\frac{n-1}{3}-2} \\ &= 7168 \cdot 5^{\frac{2n+1}{3}-2} \cdot 8^{\frac{n-1}{3}-4}.\end{aligned}$$

If the vertex x is not adjacent to any pendent vertex, we have

$$\begin{aligned}\Pi_1^*(G) &= (4+3)^3 \cdot \prod_{uv \in E(G)\setminus\{e_1,e_2,e_3\}} (d(u)+d(v)) \\ &= 343 \cdot 5^{\ell} \cdot 8^{n-1-\ell-3} \\ &= 343 \cdot 5^{\frac{2n+1}{3}} \cdot 8^{\frac{n-1}{3}-4} \\ &= 8575 \cdot 5^{\frac{2n+1}{3}-2} \cdot 8^{\frac{n-1}{3}-4}.\end{aligned}$$

■

Finally, from the assertions of this section it follows

$$\max_{G \in \mathcal{H}(n)} \Pi_1^*(G) = \begin{cases} 5^{\frac{2n+2}{3}} \cdot 8^{\frac{n-5}{3}}, & n \equiv 2 \pmod 3 \\ 180 \cdot 5^{\frac{2n}{3}-1} \cdot 8^{\frac{n}{3}-3}, & n \equiv 0 \pmod 3 \\ 8575 \cdot 5^{\frac{2n+1}{3}-2} \cdot 8^{\frac{n-1}{3}-4}, & n \equiv 1 \pmod 3). \end{cases}$$

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