RAIRO-Oper. Res. 59 (2025) 2615–2632
https://doi.org/10.1051/ro/2025084

RAIRO Operations Research
www.rairo-ro.org

EXTREMAL VALUES OF TWO MULTIPLICATIVE TYPE TOPOLOGICAL INDICES

Chunlei Xu[1], Kinkar Chandra Das[2,*], Guanru Li[1] and Yiming Lei[3]

Abstract. The multiplicative-type topological index of a graph is defined as the product of a symmetric function of the degrees of all adjacent vertices. It can be regarded as the multiplicative version of the vertex-degree-based topological index of the graph. Based on some graph operations, the extremal values of the multiplicative sum Zagreb index for trees with at most three branch vertices are determined. Some upper bounds of the multiplicative sum Zagreb index in relation to graph parameters are also provided. Furthermore, the extremal values of the multiplicative Sombor index for chemical graphs and chemical trees are completely characterized, respectively.

Mathematics Subject Classification. 05C35, 05C09, 92E10, 05C07.

Received November 18, 2024. Accepted June 20, 2025.

1. Introduction

In mathematical chemistry and chemical graph theory, topological indices can be seen as descriptors of a molecule graph. Since the Wiener index was introduced in 1972, a series of topological indices have been defined over the past fifty years. Among the most well-known are the first Zagreb index and the second Zagreb index, defined as follows:

$$M_1(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v)) = \sum_{u \in V(G)} d_G(u)^2$$

and

$$M_2(G) = \sum_{uv \in E(G)} d_G(u) d_G(v),$$

where G is a graph with vertex set $V(G)$ and edge set $E(G)$, $d_G(u) = d_u$ denotes the degree of the vertex $u \in V(G)$ (sometimes d_i is used to denote the degree of the vertex v_i). For discussions on the mathematical properties and chemical applications of M_1 and M_2, see [2, 3, 5–8, 13, 16, 17, 19, 26, 28, 30]. The main results concerning the properties of these indices are summarized in [10, 15, 23, 24].

Keywords. Extremal value, topological index, chromatic number, tree.

[1] College of Mathematics Science, Inner Mongolia Minzu University, Tongliao 028000, P.R. China.
[2] Department of Mathematics, Sungkyunkwan University, Suwon 16419, Republic of Korea
[3] School of Mathematical Sciences, Bohai University, Jinzhou 121013, P.R. China.
*Corresponding author: kinkardas2003@gmail.com

The general formula for a multiplicative version of a topological index is given as

$$\mathrm{MTI} = \mathrm{MTI}(G) = \prod_{1\le i\le j\le n-1} F(d_i, d_j)^{x_{ij}} = \prod_{1\le i\le j\le n-1} F_{ij}^{x_{ij}},$$

where $F(d_i, d_j) = F_{ij}$ is a symmetric function, and x_{ij} represents the number of edges between vertices of degrees i and j. Different choices of F_{ij} yield various multiplicative topological indices. For example, $F_{ij} = d_i d_j$, $F_{ij} = d_i + d_j$, and $F_{ij} = \sqrt{d_i^2 + d_j^2}$ correspond to the *second multiplicative Zagreb index* $\Pi_2(G) = \prod_{v_iv_j\in E(G)} d_i\, d_j$, the *multiplicative sum Zagreb index* $\Pi_1^*(G) = \prod_{v_iv_j\in E(G)} (d_i + d_j)$, and the *multiplicative Sombor index* $\Pi_{\mathrm{SO}}(G) = \prod_{v_iv_j\in E(G)} \sqrt{d_i^2 + d_j^2}$, respectively. The multiplicative second Zagreb index was proposed by Todeschini and Consonni [27] and further studied by Gutman [14], while the *multiplicative sum Zagreb index* was introduced by Eliasi *et al.* [12] in 2012. The *Multiplicative Sombor index* was introduced by Kulli [21] and further explored in [22, 32]. For recent results associated with the multiplicative sum Zagreb index, see [9, 11, 12, 18, 20, 29, 31]. Very recently, several researchers have explored various aspects of the topological indices of graphs as discussed in [1, 4, 25].

We now recall some useful definitions and notations used in this article. Let $\Omega(n, p)$ denote the class of all trees with p branch vertices and n vertices. Let $\mathcal{T}_n$ denote the class of all trees of order n, and let P_n and $S_n \cong K_{1,n-1}$ represent the path and star of order n, respectively. The double star of order n, denoted by $\mathrm{DS}(p, q)$ with $p+q+2 = n$, is constructed by joining the central vertices of two stars $K_{1,p}$ and $K_{1,q}$ by an edge. Other definitions and notations will be introduced as needed.

This paper is organized as follows. In Sections 2 and 3, we determine the extremal values for the multiplicative versions of topological indices. In particular, the extremal Π_1^*-values for trees with at most three branch vertices are entirely characterized. In Section 4, some upper bounds for Π_1^* in terms of graph parameters are obtained. Sections 5 and 6 are devoted to determining the extremal Π_{SO}-values for chemical graphs and chemical trees, respectively.

2. Extremal trees on multiplicative sum Zagreb index with at most two branch vertices

In this section, we investigate the extremal Π_1^*-values for trees with at most two branch vertices. Denote by $S(n_1, n_2, \dots, n_k)$ the star-like tree such that $S(n_1, n_2, \dots, n_k) - u = P_{n_1} \cup P_{n_2} \cup \cdots \cup P_{n_k}$, where $u \in V(S(n_1, n_2, \dots, n_k))$, $1 \le n_1 \le n_2 \le \cdots \le n_k$, and $k \ge 3$. Let $\Omega_{n,k}$ denote the class of all star-like trees of order n with a unique vertex of degree $k \ge 3$. For any $T \in \Omega_{n,k}$, denote by k_i the number of branches of length i in T, and by t the length of the longest branch in T. Then

$$\sum_{i=1}^{t} k_i = k \text{ and } \sum_{i=1}^{t} i k_i = n - 1. \tag{1}$$

Theorem 2.1. *If $T \in \Omega_{n,k}$, then*

$$\mathrm{MTI}(T) = (X_k)^{k_1} (Y_k)^{k} F_{22}^{n-1},$$

where $X_k = \frac{F_{1k}F_{22}}{F_{12}F_{2k}}$, and $Y_k = \frac{F_{12}F_{2k}}{F_{22}^2}$.

Proof. If $T \in \Omega_{n,k}$, then the three degrees of vertices in T are only $1, 2, k$. One can easily see that

$$x_{1k} = k_1,\ x_{12} = x_{2k} = k_2 + \cdots + k_t,\ x_{22} = k_3 + 2k_4 + \cdots + (t-2)k_t.$$

Using (1), from the above, we obtain

$$x_{1k} = k_1,\ x_{12} = x_{2k} = k - k_1,\ x_{22} = n - 1 + k_1 - 2k.$$

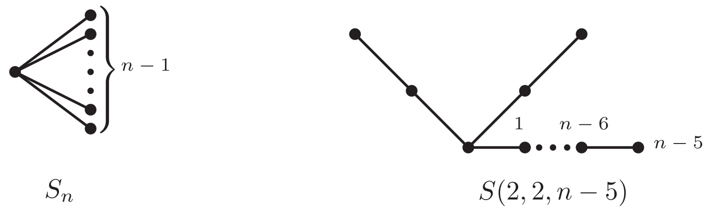


FIGURE 1. Trees S_n and $S(2, 2, n-5)$ in Corollary 2.3.

Therefore, by the definition of MTI,

$$\begin{aligned}\mathrm{MTI}(T) &= F_{12}^{x_{12}} F_{1k}^{x_{1k}} F_{22}^{x_{22}} F_{2k}^{x_{2k}} \\ &= F_{12}^{k-k_1} F_{1k}^{k_1} F_{22}^{n-1+k_1-2k} F_{2k}^{k-k_1} = \left(\frac{F_{1k}F_{22}}{F_{12}F_{2k}}\right)^{k_1} \left(\frac{F_{12}F_{2k}}{F_{22}^2}\right)^{k} F_{22}^{n-1}.\end{aligned}$$

We complete the proof of this theorem. □

Corollary 2.2. *Let MTI be the multiplicative version of a topological index. Also let $T \in \Omega_{n,k}$ and $X_k \geq 1$.*

(a) *Then MTI attains maximal value if and only if $T \cong S(\underbrace{1,1,\dots,1}_{k-1}, n-k)$.*

(b) *If $n \geq 2k+1$, then MTI attains minimal value if and only if $T \cong S(\underbrace{2,2,\dots,2}_{k-1}, n+1-2k)$. Otherwise, MTI attains minimal value if and only if $T \cong S(\underbrace{1,1,\dots,1}_{2k+1-n}, \underbrace{2,2,\dots,2}_{n-1-k})$.*

Proof. For a pair $A, B \in \Omega_{n,k}$,

$$\frac{\mathrm{MTI}(B)}{\mathrm{MTI}(A)} = X_k^{k_1(B)-k_1(A)}$$

by Theorem 2.1. Thus, we distinguish the two cases in the following.

(a) If $X_k \geq 1$, then the MTI-value attains it maximum when T is isomorphic to the tree with the greatest number of branch vertices of length 1, that is, $T \cong S(\underbrace{1,1,\dots,1}_{k-1}, n-k)$.

(b) If $X_k \geq 1$, then the MTI-value attains it minimum when T is isomorphic to the tree with the fewest branches of length 1.

(i) If $n \geq 2k+1$, then $S(\underbrace{2,2,\dots,2}_{k-1}, n+1-2k)$ admit $k_1(S) = 0$.

(ii) If $k+1 \leq n < 2k+1$, then $S(\underbrace{1,1,\dots,1}_{2k+1-n}, \underbrace{2,2,\dots,2}_{n-1-k})$ has the minimum number of branches of length 1 (Fig. 1).

□

According to the discussion in Theorem 2.1, we can determine the extremal Π_1^*-values in the following corollary.

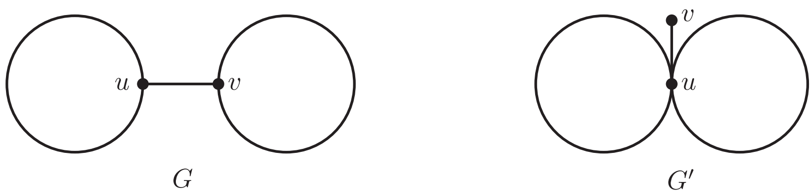


FIGURE 2. Graphs G and G' in Lemma 2.4.

Corollary 2.3. *If $T \in \Omega(n,1)$, then*

$$n^{n-1} \geq \Pi_1^*(T) \geq \begin{cases} 3^k 4^{n-1-2k}(k+2)^k & \text{if } n \geq 2k+1, \\ (k+1)^{2k+1-n}[3(k+2)]^{n-1-k} & \text{if } k+1 \leq n < 2k+1 \end{cases}$$

with the right equality holds if and only if $T \cong S(n_1, n_2, \ldots, n_k)$ and the left equality holds if and only if $T \cong S_n$, where $n_i \geq 2,\ 1 \leq i \leq k$.

We now consider the extremal values for trees with exactly two branch vertices. Write

$$\Omega(n,2) = \{S(a_1, \ldots, a_r; \mathbf{x}; b_1, \ldots, b_s) : a_i \geq 0, b_j \geq 0, 1 \leq i \leq r, 1 \leq j \leq s, \mathbf{x} \geq 1, r, s \geq 2\}.$$

Lemma 2.4 ([18])**.** *Let uv be a non-pendant cut edge of graph G. Denote by $G' = G \cdot (uv) + uv$ the graph obtained by the contraction of uv onto the vertex u and adding a new pendant vertex v to u (see, Fig. 2). Then $\Pi_1^*(G) < \Pi_1^*(G')$.*

By repeatedly applying Lemma 2.4 to $T \in \Omega(n,2)$, the maximal Π_1^*-value is attained when T is isomorphic to some double star $\mathrm{DS}(p,q)$, where $p \geq q \geq 2$. Therefore, to determine the maximal Π_1^*-value in $\Omega(n,2)$, it is sufficient to find the maximum Π_1^*-value among all double stars $\mathrm{DS}(p,q)$. Let d denote the *diameter* of the graph G.

Theorem 2.5. *If $T \in \mathcal{T}_n$ $(T \notin \{S_n, \mathrm{DS}(n-3,1)\})$, then $\Pi_1^*(T) \leq 4^2 n(n-2)^{n-4}$ with equality if and only if $T \cong \mathrm{DS}(n-4,2)$.*

Proof. Note that for a double star $\mathrm{DS}(p,q)$, $(p+1)+(q+1)=n$. Then $\lceil \frac{n-2}{2} \rceil \leq p \leq n-4$ as $T \notin \{S_n, \mathrm{DS}(n-3,1)\}$.

If $d=3$, then T is isomorphic to a double star $\mathrm{DS}(p,q)$. By the definition of multiplicative sum Zagreb index,

$$\Pi_1^*(\mathrm{DS}(p,q)) = n(p+2)^p(q+2)^q.$$

Now we consider a function

$$f(x) = (x+2)^x(n-x)^{n-x-2}, \quad \left\lceil \frac{n-2}{2} \right\rceil \leq x \leq n-4.$$

Since $x+2 \geq n-x$,

$$f'(x) = f(x)\left[\ln(x+2) + \frac{x}{x+2} - \ln(n-x) - \frac{n-x-2}{n-x}\right] > 0,$$

which means $f(x)$ is increasing for $\lceil \frac{n-2}{2} \rceil \leq x \leq n-4$. It is deduced that $f(x)$ attain maximum value when $x=n-4$, that is, $f(x)_{\max} = f(n-4) = 4^2(n-2)^{n-4}$. Therefore, for any $T \in \mathcal{T}_n$, if $T \notin \{S_n, \mathrm{DS}(n-3,1)\}$, then

$$\Pi_1^*(T) \leq \Pi_1^*(\mathrm{DS}(p,q)) \leq \Pi_1^*(\mathrm{DS}(n-4,2)) = 4^2 n(n-2)^{n-4}.$$

FIGURE 3. Graph G and G' in Lemma 2.9.

If $d \geq 3$, then by repeatedly applying Lemma 2.4, the maximum Π_1^*-value is attained if and only if T is isomorphic to a double star $\mathrm{DS}(p,q)$ with $d(\mathrm{DS}(p,q)) = 3$. Therefore, we complete the proof of this theorem. □

By Theorem 2.5, we can completely determine the maximum Π_1^*-value for trees with two branch vertices.

Corollary 2.6. *For any $T \in \Omega(n,2)$, $\Pi_1^*(T) \leq 4^2 n(n-2)^{n-4}$ with equality if and only if $T \cong \mathrm{DS}(n-4,2)$.*

Let $P = uu_1u_2\ldots u_k$ be a path in G such that $d_G(u) \geq 3$, $d_G(u_k) = 1$ and $d_G(u_i) = 2$ for $1 \leq i < k$. Then it is called a *pendant path* in G, vertex u is called the *origin* and k is the length of P. We now look the minimum Π_1^*-value among the trees in $\Omega(n,2)$. For this purpose, the following lemma is necessary.

Lemma 2.7 ([18])**.** *Suppose that P and Q are two pendant paths at origin u and v in G. Let $ux \in E(P)$, and let y be the pendant vertex in Q. If $G' = G - ux + yx$, then:*

(i) *If $d_G(u) \geq 4$, then $\Pi_1^*(G') < \Pi_1^*(G)$.*
(ii) *If there exists a vertex $u_i \in N_G(u)$ such that $u_i \neq x$ and $d_G(u) + d_G(u_i) \leq 16$, then $\Pi_1^*(G') < \Pi_1^*(G)$.*

Theorem 2.8. *If $T \in \Omega(n,2)$ has the minimum Π_1^*-value, then T is isomorphic to a tree of the form $S(a,b;\mathbf{x};c,d)$, where $a,b,c,d \geq 0$.*

Proof. Assume that $S = S(a_1,\ldots,a_r;\mathbf{x};b_1,\ldots,b_s)$ has the minimum Π_1^*-value, where $r \geq 3$ or $s \geq 3$. Without loss of generality, we assume that $r \geq 3$. Then by Lemma 2.7(i), one can obtain $S' = S(a_1 + a_2,\ldots,a_r;\mathbf{x};b_1,\ldots,b_s)$ such that $\Pi_1^*(S') < \Pi_1^*(S)$. Therefore, by repeatedly using Lemma 2.7(i), if $T \in \Omega(n,2)$ has the minimum Π_1^*-value, then T is isomorphic to a tree of the form $S(a,b;\mathbf{x};c,d)$, where $a,b,c,d \geq 0$. □

By Theorem 2.8, to find the minimum Π_1^*-value in $\Omega(n,2)$, it is sufficient to determine the minimum Π_1^*-value among trees of the form $S(a,b;\mathbf{x};c,d)$.

Lemma 2.9. *Let G and G' be the graphs depicted in* Fig. 3*, where $d_G(u) \geq 2$. Then $\Pi_1^*(G') \leq \Pi_1^*(G)$.*

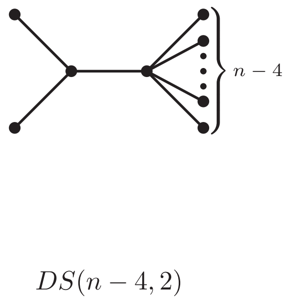
Proof. By the definition of Π_1^*,

$$\frac{\Pi_1^*(G)}{\Pi_1^*(G')} = \frac{3 \times 4 \times (d_G(u)+1)(d_G(v)+2)}{3^2(d_G(u)+2)(d_G(v)+2)} = \frac{4d_G(u)+4}{3d_G(u)+6} \geq 1$$

as $d_G(u) \geq 2$. Hence, $\Pi_1^*(G') \leq \Pi_1^*(G)$. □

By Lemma 2.9, the minimum Π_1^*-value is attained when $T \in \Omega(n,2)$ is of the form $S(a,b;\mathbf{x};c,d)$, where $a,b,c,d \geq 2$.

Lemma 2.10. *Suppose S and S' are two trees in $\Omega(n,2)$, where $S = S(a,b;\mathbf{x};c,d)$, $S' = S(a+1,b;\mathbf{x}-1;c,d)$, $a,b,c,d \geq 2$, $\mathbf{x} \geq 2$. Then $\Pi_1^*(S) \geq \Pi_1^*(S')$.*



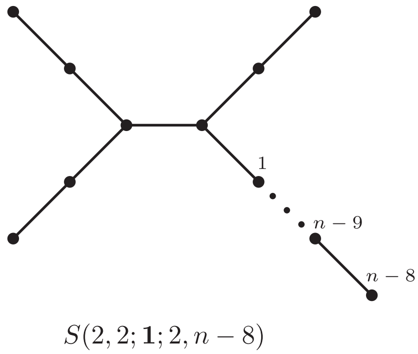


FIGURE 4. Double star DS$(n-4,2)$ and a tree $S(2,2;\mathbf{1};2,n-8)$ with extremal Π_1^*-values.

Proof. One can easily see that if $\mathbf{x}=2$, then

$$x_{12}(S)=4,\ x_{13}(S)=0,\ x_{22}(S)=n-11,\ x_{23}(S)=6,\ x_{33}(S)=0,$$
$$x_{12}(S')=4,\ x_{13}(S')=0,\ x_{22}(S')=n-10,\ x_{23}(S')=4,\ x_{33}(S')=1.$$

By the definition of Π_1^*,

$$\frac{\Pi_1^*(S)}{\Pi_1^*(S')}=\frac{3^4 4^{n-11}5^6}{3^4 4^{n-10}5^4 6}=\frac{25}{24}>1.$$

If $\mathbf{x}\geq 3$, then by the direct calculation, we obtain $\Pi_1^*(S)=\Pi_1^*(S')$. Hence, $\Pi_1^*(S)\geq\Pi_1^*(S')$ (Fig. 4). □

Now by Lemma 2.10, we can completely determine the minimum Π_1^*-value for the trees in $\Omega(n,2)$ in the following theorem.

Theorem 2.11. *If $T\in\Omega(n,2)$, then $\Pi_1^*(T)\geq 3^4 4^{n-10}5^4 6$ with equality if and only if T is isomorphic to a tree of the form $S(a,b;\mathbf{1};c,d)$, where $a,b,c,d\geq 1$.*

3. EXTREMAL TREES ON MULTIPLICATIVE SUM ZAGREB INDEX WITH THREE BRANCH VERTICES

In this section, we investigate for the extremal Π_1^*-values in $\Omega(n,3)$. At the beginning of this section, we denote by $S(a_1,\dots,a_r;\mathbf{x};b_1,\dots,b_s;\mathbf{y};c_1,\dots,c_t)$ the tree with three branch vertices, as depicted in Figure 5. Then we define:

$$\Omega(n,3)=\{S(a_1,\dots,a_r;\mathbf{x};b_1,\dots,b_s;\mathbf{y};c_1,\dots,c_t):a_i,b_j,c_l\geq 0,1\leq i\leq r,1\leq j\leq s,1\leq l\leq t,r,s,t\geq 2\}.$$

In particular, if $a_1=a_2=\cdots=a_r$, then tree $S(a_1,\dots,a_r;\mathbf{x};b_1,\dots,b_s;\mathbf{y};c_1,\dots,c_t)$ can be simply written as $S(a^r;\mathbf{x};b_1,\dots,b_s;\mathbf{y};c_1,\dots,c_t)$. Similar simplifications apply when $b_1=b_2=\cdots=b_s$ and $c_1=c_2=\cdots=c_t$.

By repeatedly applying Lemma 2.4, if necessary, one can construct a Π_1^*-value sequence for any $T\in\Omega(n,3)$ as follows:

$$\Pi_1^*(T)<\Pi_1^*(T_1)<\Pi_1^*(T_2)<\cdots<\Pi_1^*(U),$$

where $U=S(1^x;\mathbf{1};1^y;\mathbf{1};1^z)$. Therefore, the maximum Π_1^*-value is attained when T is isomorphic to a tree of the form $U=S(1^x;\mathbf{1};1^y;\mathbf{1};1^z)$.

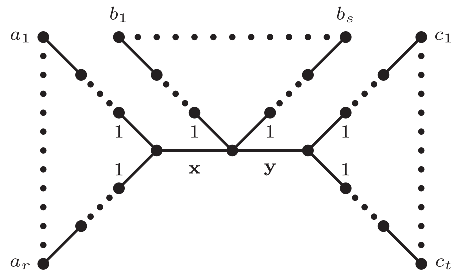


FIGURE 5. Tree $S(a_1, \cdots, a_r; \mathbf{x}; b_1, \cdots, b_s; \mathbf{y}; c_1, \cdots, c_t)$.

Lemma 3.1. *Let* $T = S(1^x; \mathbf{1}; 1^y; \mathbf{1}; 1^z)$ *and* $T' = S(1^{x-1}; \mathbf{1}; 1^y; \mathbf{1}; 1^{z+1})$ *be two trees in* $\Omega(n, 3)$*. If* $3 \le x < z+1$*, then* $\Pi_1^*(T) < \Pi_1^*(T')$*.*

Proof. Let us now consider two functions

$$f(x) = (x+2)^x(x+y+3), \ x \ge 0, \ y \ge 0,$$
$$g(x) = \ln f(x) = x\ln(x+2) + \ln(x+y+3), x \ge 0, \ y \ge 0.$$

Then

$$g''(x) = [\ln f(x)]'' = \frac{x+4}{(x+2)^2} - \frac{1}{(x+y+3)^2} > 0.$$

Thus, $[\ln f(x)]'$ is increasing. It follows that $[\ln f(x+1) - \ln f(x)]' > 0$. Hence, $\ln f(z+1) - \ln f(z) > \ln f(x) - \ln f(x-1)$ as $3 \le x < z+1$, that is, $f(x-1)f(z+1) > f(x)f(z)$. Hence, by the definition of Π_1^*,

$$\frac{\Pi_1^*(T')}{\Pi_1^*(T)} = \frac{(x+1)^{x-1}(x+y+2)(z+3)^{z+1}(z+y+4)}{(x+2)^x(x+y+3)(z+2)^z(z+y+3)} = \frac{f(x-1)f(z+1)}{f(x)f(z)} > 1.$$

Hence, $\Pi_1^*(T) < \Pi_1^*(T')$. □

Lemma 3.2. *Let* $T = S(1^2; \mathbf{1}; 1^y; \mathbf{1}; 1^z)$*,* $T' = S(1^2; \mathbf{1}; 1^{y-1}; \mathbf{1}; 1^{z+1})$*, and* $A = S(1^2; \mathbf{1}; 1^{n-7}; \mathbf{1}; 1^2)$*. Then:*

(i) *If* $3 \le y \le z$*, then* $\Pi_1^*(T) < \Pi_1^*(T')$*.*
(ii) *If* $y > z \ge 2$*, then* $\Pi_1^*(T) \le \Pi_1^*(A)$*.*

Proof. Let $f(x) = \dfrac{(x+2)^x}{(x+1)^{x-1}}$, where $x \ge 3$. We obtain

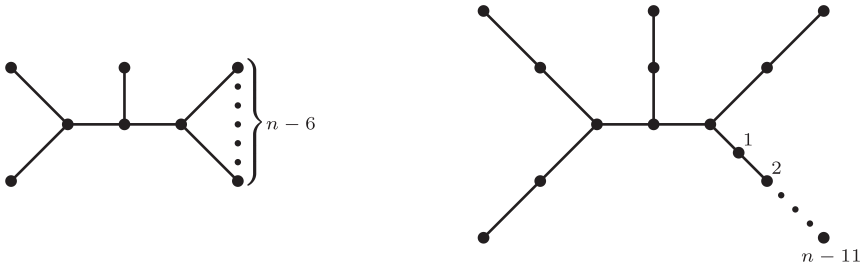
$$f'(x) = f(x)\left[\ln(x+2) + \frac{x}{x+2} - \ln(x+1) - \frac{x-1}{x+1}\right] > 0. \tag{2}$$

Thus $f(x)$ is an increasing function.

(i) If $3 \le y \le z$, then $f(z+1) \ge f(y+1)$. By the definition of Π_1^*,

$$\begin{aligned}\frac{\Pi_1^*(T')}{\Pi_1^*(T)} &= \frac{(y+4)(y+z+3)(y+2)^{y-1}(z+3)^{z+1}}{(y+5)(y+z+3)(y+3)^y(z+2)^z} = \frac{(y+4)(y+2)^{y-1}(z+3)^{z+1}}{(y+5)(y+3)^y(z+2)^z} \\ &= \frac{f(z+1)(y+4)(y+2)^{y-1}}{(y+5)(y+3)^y} \ge \frac{f(y+1)(y+4)(y+2)^{y-1}}{(y+5)(y+3)^y} \\ &= \frac{(y+3)^{y+1}}{(y+2)^y} \cdot \frac{(y+4)(y+2)^{y-1}}{(y+5)(y+3)^y} = \frac{y^2+7y+12}{y^2+7y+10} > 1.\end{aligned}$$

Hence, $\Pi_1^*(T) < \Pi_1^*(T')$.



$S(1^2;\mathbf{1};1;\mathbf{1};1^{n-6})$ $S(2^2;\mathbf{1};2;\mathbf{1};2,n-11)$

FIGURE 6. Trees with extremal Π_1^*-values in $\Omega(n,3)$.

(ii) Note that $y+z=n-5$ and $y>z\geq 2$. Then $\frac{n-5}{2}<y\leq n-7$. We now consider a function

$$f(y)=(y+3)^y(n-3-y)^{n-5-y},\ y\geq 3.$$

Then

$$f'(y)=f(y)\left[\ln(y+3)+\frac{y}{y+3}-\ln(n-3-y)-\frac{n-5-y}{n-3-y}\right]>0,$$

which means $f(y)$ is increasing when $y\geq 3$. Thus, $f(x)\leq f(n-7)=4^2(n-4)^{n-7}$. Therefore,

$$\begin{aligned}\Pi_1^*(T)&=4^2(y+5)(y+z+3)(y+3)^y(z+2)^z\\&=4^2(y+5)(n-2)(y+3)^y(n-3-y)^{n-5-y}\\&\leq 4^4(n-2)^2(n-4)^{n-7}=\Pi_1^*(A).\end{aligned}$$

We complete the proof of this lemma. □

Now we determine the maximum Π_1^*-value in $\Omega(n,3)$ in the following theorem (Fig. 6).

Theorem 3.3. *If* $T\in\Omega(n,3)$, *then* $\Pi_1^*(T)\leq 4^3 6(n-2)(n-4)^{n-6}$ *with equality if and only if* $T\cong S\left(1^2;\mathbf{1};1;\mathbf{1};1^{n-6}\right)$.

Proof. By Lemmas 3.1 and 3.2, it is sufficient to compare the Π_1^*-values for $A=S\left(1^2;\mathbf{1};1^{n-7};\mathbf{1};1^2\right)$ and $Z=S\left(1^2;\mathbf{1};1;\mathbf{1};1^{n-6}\right)$. Therefore,

$$\frac{\Pi_1^*(Z)}{\Pi_1^*(A)}=\frac{4^3 6(n-2)(n-4)^{n-6}}{4^4(n-2)^2(n-4)^{n-7}}=\frac{3(n-4)}{2(n-2)}\geq 1$$

as $n\geq 8$. Hence, for any $T\in\Omega(n,3)$, $\Pi_1^*(T)\leq 4^3 6(n-2)(n-4)^{n-6}$ and the equality holds if and only if $T\cong Z$. □

Lemma 3.4. *Let* $X_{n,1}$ *and* $X_{n,i}$ *be the graphs depicted in* Fig. 7, *where* $d_u\geq 3$. *Then* $\Pi_1^*(X_{n,1})<\Pi_1^*(X_{n,i})$ *for* $2\leq i\leq\lceil\frac{n}{2}\rceil$.

Proof. By the definition of Π_1^*, we obtain

$$\frac{\Pi_1^*(X_{n,i})}{\Pi_1^*(X_{n,1})}\geq\frac{3^2 4^{n-5}(d_u+1+1)(d_u+1+2)}{3\times 4^{n-3}(d_u+2)}\times\prod_{u_i\in N_H(u)}\frac{d_u+1+d_{u_i}}{d_u+d_{u_i}}>\frac{3(d_u+3)}{16}>1$$

as $d_u\geq 3$ and $2\leq i\leq\lceil\frac{n}{2}\rceil$. Hence $\Pi_1^*(X_{n,1})<\Pi_1^*(X_{n,i})$. □

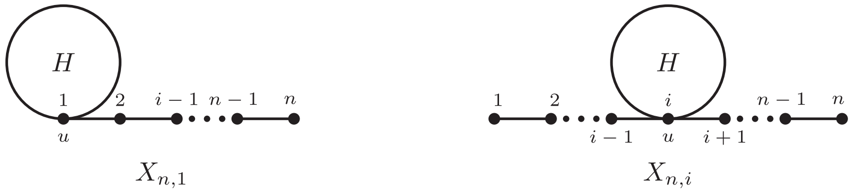


FIGURE 7. Graphs $X_{n,1}$ and $X_{n,i}$ in Lemma 3.4.

Lemma 3.5. *Let $n \geq 15$. If the tree $T = S(a, b; \mathbf{c}; d; \mathbf{e}; f, g) \in \Omega(n, 3)$ has minimum Π_1^*-value, then all pendant paths have length greater than one.*

Proof. Suppose that there is a pendant path of length one in T. Without loss of generality, assume that $a = 1$. Then by Lemma 2.9, $b, d, f, g \leq 2$. Hence $\mathbf{c} + \mathbf{e} = n - 1 - (1 + b + d + f + g) \geq n - 10 \geq 5$. It is deduced that one of $\mathbf{c}$ and $\mathbf{e}$ is strictly greater than 2. Assume that $\mathbf{c} \geq 3$, and $D = S(2, b; \mathbf{c} - \mathbf{1}; d; \mathbf{e}; f, g)$. Then we obtain

$$\frac{\Pi_1^*(T)}{\Pi_1^*(D)} = \frac{4^{\mathbf{c}-1}5^2}{3 \times 4^{\mathbf{c}-3}5^3} > 1.$$

It contradicts to the fact that T has minimum Π_1^*-value in $\Omega(n, 3)$. □

In light of Lemma 3.5, the minimum Π_1^*-value is attained when $T \in \Omega_{n,3}$ is of the form $S(a, b; \mathbf{c}; d; \mathbf{e}; f, g)$, where $a, b, d, f, g \geq 2$.

Lemma 3.6. *If $\mathbf{c} + \mathbf{e} \geq 3$, $T = S(a, b; \mathbf{c}; d; \mathbf{e}; f, g)$ and $T' = S(a, b; \mathbf{1}; d; \mathbf{c} + \mathbf{e} - 1; f, g)$, then $\Pi_1^*(T) \geq \Pi_1^*(T')$.*

Proof. It is not hard to see that if $\mathbf{c} + \mathbf{e} = 3$, then $\Pi_1^*(T) \geq \Pi_1^*(T')$. Now we can assume that $\mathbf{c} \geq 2$ and $\mathbf{e} \geq 2$. By the definition of Π_1^*, we obtain

$$\frac{\Pi_1^*(T)}{\Pi_1^*(T')} = \frac{4^{\mathbf{c}+\mathbf{e}-4}5^4}{4^{\mathbf{c}+\mathbf{e}-3}5^2 6} = \frac{25}{24} > 1.$$

Hence, $\Pi_1^*(T) \geq \Pi_1^*(T')$. □

Theorem 3.7. *Let $n \geq 15$. Then, for any $T \in \Omega(n, 3)$, $\Pi_1^*(T) \geq 3^5 4^{n-15} 5^7 6^2$ with equality if and only if T is isomorphic to a tree of the form $Y = S(a, b; \mathbf{1}; d; \mathbf{1}; f, g)$, where $a, b, d, f, g \geq 2$ and $a + b + d + f + g = n - 3$.*

Proof. For two trees $X = S(a', b', \mathbf{1}; d', \mathbf{e}; f', g')$ and $Y = S(a, b; \mathbf{1}; d; \mathbf{1}; f, g)$, it is easy to see that

$$x_{22}(X) = n - 14,\ x_{23}(X) = 7,\ x_{33}(X) = 1,\ x_{12}(X) = 5,$$
$$x_{22}(Y) = n - 13,\ x_{23}(Y) = 5,\ x_{33}(Y) = 2,\ x_{12}(Y) = 5.$$

By the definition of Π_1^*, we obtain

$$\frac{\Pi_1^*(X)}{\Pi_1^*(Y)} = \frac{3^5 4^{n-14} 5^7 6}{3^5 4^{n-13} 5^5 6^2} = \frac{25}{24} > 1.$$

Hence, $\Pi_1^*(X) > \Pi_1^*(Y)$. □

4. Upper Bounds of multiplicative sum Zagreb index

In this section, we investigate upper bounds for the multiplicative sum Zagreb index relative to some graph parameters. For any two nonadjacent vertices v_k and v_ℓ in a graph G, we use $G + v_k v_\ell$ to denote the graph obtained by adding the edge $v_k v_\ell$ to G.

Lemma 4.1 ([29]). *Let G be a graph with $v_i v_j \in E(G)$ and $v_k v_\ell \notin E(G)$. Then $\Pi_1^*(G) > \Pi_1^*(G - v_i v_j)$, and $\Pi_1^*(G) < \Pi_1^*(G + v_k v_\ell)$.*

The number of vertices in the largest independent set of a graph is called the *independence number*, denoted by α. If a graph on n vertices contains a clique of $n-\alpha$ vertices and the rest α vertices is a stable set, where every vertex within the clique is linked to every vertex in the stable set, then the graph is called a *complete split graph* and is denoted by $\mathrm{CS}(n,\alpha)$, $1 \le \alpha \le n-1$. We now give an upper bound on $\Pi_1^*(G)$ in terms of order n and independence number α of any graph G, and characterize the extremal graphs.

Theorem 4.2. *Let G be a graph of order n with independence number α. Then*

$$\Pi_1^*(G) \le 2^a\,(n-1)^a\,(2n-\alpha-1)^{\alpha\,(n-\alpha)},$$

where $a = \binom{n-\alpha}{2}$. Moreover, the equality holds if and only if $G \cong \mathrm{CS}(n,\alpha)$.

Proof. If $G \cong \mathrm{CS}(n,\alpha)$, then the equality holds. Otherwise, $G \ncong \mathrm{CS}(n,\alpha)$. Let G' be a graph of order n with independence number α such that $G' = G + e$, where e is not an edge in G. By Lemma 4.1, one can easily see that

$$\Pi_1^*(G) < \Pi_1^*(G') < \cdots < \Pi_1^*(\mathrm{CS}(n,\alpha)).$$

This completes the proof of the theorem. □

Let m_u be the average degree of the adjacent vertices of the vertex u in G. Then

$$m_u = \frac{\sum_{v:uv\in E(G)} d_v}{d_u}, \quad \text{that is,} \quad d_u m_u = \sum_{v:uv\in E(G)} d_v.$$

Lemma 4.3 ([7]). *Let G be a connected graph. Then $d_u + m_u = d_v + m_v$ for any u, $v \in V(G)$ if and only if G is a regular graph or a bipartite semiregular graph.*

We now give an upper bound on $\Pi_1^*(G)$ of any graph G, and characterize the extremal graphs.

Theorem 4.4. *Let G be a graph with m edges. Then*

$$\Pi_1^*(G) \le \max_{u\in V(G)} (d_u + m_u)^m, \tag{3}$$

where d_u is the degree of the vertex $u \in V(G)$, and m_u is the average degree of the adjacent vertices of the vertex $u \in V(G)$. If G is connected, then the equality holds in (3) if and only if G is a regular graph or G is a bipartite semiregular graph.

Proof. Since m_u is the average degree of the adjacent vertices of the vertex u, one can easily see that $\sum_{v:uv\in E(G)} (d_u + d_v) = d_u^2 + d_u\, m_u$. Using this, from the arithmetic-geometric-mean inequality, we obtain

$$\prod_{v:\,uv\in E(G)} (d_u + d_v) \le \left(\frac{\sum_{v:uv\in E(G)} (d_u + d_v)}{d_u}\right)^{d_u} = (d_u + m_u)^{d_u}$$

with equality if and only if $d_v = d_w$ for every $v,\, w \in N_G(u)$.

From the definition, we obtain

$$\Pi_1^*(G)^2 = \left(\prod_{uv\in E(G)} (d_u + d_v)\right)^2 = \prod_{u\in V(G)} \prod_{v:\, uv\in E(G)} (d_u + d_v) \le \prod_{u\in V(G)} (d_u + m_u)^{d_u}. \tag{4}$$

Let $d_r + m_r = \max\limits_{u\in V(G)} (d_u + m_u)$. Then we have $d_u + m_u \le d_r + m_r$ for any $u \in V(G)$. From (4), we obtain

$$\Pi_1^*(G)^2 \le \prod_{u\in V(G)} (d_r + m_r)^{d_u} = (d_r + m_r)^{\sum\limits_{u\in V(G)} d_u} = (d_r + m_r)^{2m},$$

that is,

$$\Pi_1^*(G) \le (d_r + m_r)^m = \max_{u\in V(G)} (d_u + m_u)^m$$

with equality if and only if $d_u + m_u = d_v + m_v$ for any $u,\, v \in V(G)$.

Moreover, the equality holds in (3) if and only if $d_u + m_u = d_v + m_v$ for any $u,\, v \in V(G)$, that is, by Lemma 4.3, the equality holds in (3) if and only if G is a regular graph or a bipartite semiregular graph as G is connected. □

Corollary 4.5. *Let G be a graph with m edges and maximum degree Δ. Then*

$$\Pi_1^*(G) \le (2\Delta)^m. \tag{5}$$

If G is a connected graph, then the equality holds in (5) if and only if G is a regular graph.

Proof. Since $d_u \le \Delta$ for all $u \in V(G)$, we have $m_u \le \Delta$ for all $u \in V(G)$. Using this, from (3), we obtain the result. By Theorem 4.4, the equality holds in (5) if and only if each connected component of G is a Δ-regular graph, that is, if and only if G is a regular graph. □

The *chromatic number* of a graph G, denoted by r, is the minimum number of colors such that G can be colored with these colors such that no two adjacent vertices have the same color. We denote by $K_{n_1,n_2,\ldots,n_r}$ the complete r-partite graph of order n, with partition sets of sizes $n_1,\, n_2, \ldots,\, n_r$, respectively. Recall that the *Turán graph* $T_n(r)$ is a special r-partite graph of order n, where the partition sets differ in size by at most 1. We obtain

$$\Pi_1^*(T_n(r)) = \left(\sqrt{2(n-p)}\right)^{p^2\,(r-q)\,(r-q-1)} \left(\sqrt{2(n-p-1)}\right)^{(p+1)^2\,q\,(q-1)} \times (2n-2p-1)^{pq\,(p+1)\,(r-q)},$$

where $p = \lfloor \frac{n}{r} \rfloor$, and $q = n - r \lfloor \frac{n}{r} \rfloor$. We now give an upper bound on $\Pi_1^*(G)$ of graph G in terms of n and chromatic number r, and characterize the extremal graphs.

Theorem 4.6. *Let G be a graph of order n with chromatic number r. Then*

$$\Pi_1^*(G) \le \left(\sqrt{2(n-p)}\right)^{p^2\,(r-q)\,(r-q-1)} \left(\sqrt{2(n-p-1)}\right)^{(p+1)^2\,q\,(q-1)} \times (2n-2p-1)^{pq\,(p+1)\,(r-q)}, \tag{6}$$

where $p = \lfloor \frac{n}{r} \rfloor$, and $q = n - r \lfloor \frac{n}{r} \rfloor$. Moreover, the equality holds if and only if $G \cong T_n(r)$.

Proof. Since G has n vertices with chromatic number r, we can assume that $V(G) = V_1 \cup V_2 \cup \cdots \cup V_r$, where $V_i \cap V_j = \emptyset\,(1 \le i \ne j \le r)$ and $|V_i| = n_i\,(1 \le i \le r)$, $n_1 \ge n_2 \ge \cdots \ge n_r$, $n_1 + n_2 + \cdots + n_r = n$. By Lemma 4.1, we obtain $\Pi_1^*(G) \le \Pi_1^*(K_{n_1,n_2,\ldots,n_r})$ with equality if and only if $G \cong K_{n_1,n_2,\ldots,n_r}$. If $n_1 - n_r \le 1$, then $K_{n_1,n_2,\ldots,n_r} \cong T_n(r)$, and hence $\Pi_1^*(G) \le \Pi_1^*(K_{n_1,n_2,\ldots,n_r}) = \Pi_1^*(T_n(r))$. Moreover, the equality holds in (6) if and only if $G \cong T_n(r)$. Otherwise, $n_1 - n_r \ge 2$.

Claim 1.

$$\Pi_1^*(K_{n_1,n_2,\ldots,n_r}) < \Pi_1^*(K_{n_1-1,n_2,\ldots,n_r+1}).$$

Proof Claim 1. Since $n_1 - n_r \ge 2$, one can easily see that

$$\begin{aligned}(2n - n_1 - n_i + 1)(2n - n_r - n_i - 1) &= (2n - n_1 - n_i)\,(2n - n_r - n_i) + n_1 - n_r - 1 \\ &> (2n - n_1 - n_i)\,(2n - n_r - n_i),\end{aligned}$$

that is,

$$\frac{(2n - n_1 - n_i + 1)\,(2n - n_r - n_i - 1)}{(2n - n_1 - n_i)\,(2n - n_r - n_i)} > 1.$$

Moreover,

$$\frac{2n - n_1 - n_i + 1}{2n - n_1 - n_i} > 1 \quad \text{and} \quad \frac{2n - n_r - n_i - 1}{2n - n_1 - n_i + 1} \ge 1.$$

Thus we obtain

$$\begin{aligned}\frac{(2n - n_1 - n_i + 1)^{(n_1-1)}\,(2n - n_r - n_i - 1)^{(n_r+1)}}{(2n - n_1 - n_i)^{n_1}\,(2n - n_r - n_i)^{n_r}} &= \left(\frac{(2n - n_1 - n_i + 1)\,(2n - n_r - n_i - 1)}{(2n - n_1 - n_i)\,(2n - n_r - n_i)}\right)^{n_r} \\ &\quad \times \left(\frac{2n - n_1 - n_i + 1}{2n - n_1 - n_i}\right)^{n_1 - n_r} \times \left(\frac{2n - n_r - n_i - 1}{2n - n_1 - n_i + 1}\right) > 1.\end{aligned}$$

Using the above result, we obtain

$$\begin{aligned}\frac{\Pi_1^*(K_{n_1-1,n_2,\ldots,n_r+1})}{\Pi_1^*(K_{n_1,n_2,\ldots,n_r})} &= \frac{\prod_{i=2}^{r-1}\left((2n - n_1 - n_i + 1)^{(n_1-1)\,n_i}\,(2n - n_r - n_i - 1)^{(n_r+1)\,n_i}\right)}{\prod_{i=2}^{r-1}\left((2n - n_1 - n_i)^{n_1\,n_i}\,(2n - n_r - n_i)^{n_r\,n_i}\right)} \\ &\quad \times \frac{(2n - n_1 - n_r)^{(n_1-1)\,(n_r+1)}}{(2n - n_1 - n_r)^{n_1\,n_r}} \\ &= \prod_{i=2}^{r-1}\left(\frac{\left((2n - n_1 - n_i + 1)^{(n_1-1)}\,(2n - n_r - n_i - 1)^{(n_r+1)}\right)}{\left((2n - n_1 - n_i)^{n_1}\,(2n - n_r - n_i)^{n_r}\right)}\right)^{n_i} \\ &\quad \times (2n - n_1 - n_r)^{(n_1 - n_r - 1)} > 1.\end{aligned}$$

This proves the Claim 1. □

By applying Claim 1 several times if necessary, we obtain

$$\Pi_1^*(G) \le \Pi_1^*(K_{n_1,n_2,\ldots,n_k}) < \Pi_1^*(K_{n_1-1,n_2,\ldots,n_k+1}) < \cdots < \Pi_1^*(T_n(r)).$$

This completes the proof of the theorem. □

5. Multiplicative Sombor index for chemical graphs

This section considers the extremal values of the multiplicative Sombor index for chemical graphs. We recall that a chemical graph is a graph with maximum degree $\Delta \leq 4$. Denoted by $\mathcal{CG}_n$ the class of all chemical graphs of order n. Denoted by n_i the number of vertices with degree i. Then one can easily get

$$\begin{cases} n_1 + n_2 + n_3 + n_4 + \cdots + n_{n-1} = n, \\ 2x_{11} + x_{12} + x_{13} + \cdots + x_{1,n-1} = n_1, \\ x_{12} + 2x_{22} + x_{23} + \cdots + x_{2,n-1} = 2n_2, \\ x_{13} + x_{23} + 2x_{33} + \cdots + x_{3,n-1} = 3n_3, \\ \qquad \cdots\cdots\cdots\cdots \\ x_{1,n-1} + x_{2,n-1} + \cdots + 2x_{n-1,n-1} = (n-1)n_{n-1}. \end{cases}$$

Therefore,

$$n = \sum_{1 \leq i \leq j \leq n-1} \frac{i+j}{ij} x_{ij}.$$

For the sake of simplicity, write

$$\Omega = \{(i,j) : 1 \leq i \leq j \leq 4\},\ \Omega_1 = \{(i,j) \in \Omega : (i,j) \neq (4,4)\}.$$

Theorem 5.1. *For any graph $G \in \mathcal{CG}_n$, $\Pi_{\mathrm{SO}}(G) \leq 1024^{\frac{n}{2}}$ with equality if and only if G is isomorphic to 4-regular graph.*

Proof. By the definition of Π_{SO}, we obtain

$$\begin{aligned} \Pi_{\mathrm{SO}}(G)^2 &= \prod_{(i,j)\in\Omega} (i^2+j^2)^{x_{ij}} = (4^2+4^2)^{x_{44}} \prod_{(i,j)\in\Omega_1} (i^2+j^2)^{x_{ij}} \\ &= 32^{2n-2\sum_{(i,j)\in\Omega_1} \frac{i+j}{ij}x_{ij}} \prod_{(i,j)\in\Omega_1} (i^2+j^2)^{x_{ij}} = \frac{1024^n \prod_{(i,j)\in\Omega_1}(i^2+j^2)^{x_{ij}}}{1024^{\sum_{(i,j)\in\Omega_1} \frac{i+j}{ij}x_{ij}}} \leq 1024^n \end{aligned} \tag{7}$$

as for all $(i,j) \in \Omega_1$, $i^2+j^2 < 1024^{\frac{i+j}{ij}}$. The equality holds in (7) if and only if for any $(i,j) \in \Omega_1$, $x_{ij} = 0$, that is, G is isomorphic to a 4-regular graph. □

Theorem 5.2. *If n is even, then $\Pi_{\mathrm{SO}}(G) \geq 2^{\frac{n}{4}}$ with equality if and only if $G \cong \frac{n}{2}P_2$.*

Proof. Write

$$\Omega_2 = \{(i,j) \in \Omega : (i,j) \neq (1,1)\}.$$

By the definition of Π_{SO}, we obtain

$$\begin{aligned} \Pi_{\mathrm{SO}}(G)^2 &= \prod_{(i,j)\in\Omega} (i^2+j^2)^{x_{ij}} = (1^2+1^2)^{x_{11}} \prod_{(i,j)\in\Omega_2} (i^2+j^2)^{x_{ij}} \\ &= 2^{\frac{n}{2}-\frac{1}{2}\sum_{(i,j)\in\Omega_2} \frac{i+j}{ij}x_{ij}} \prod_{(i,j)\in\Omega_2} (i^2+j^2)^{x_{ij}} = \frac{2^{\frac{n}{2}} \prod_{(i,j)\in\Omega_2}(i^2+j^2)^{x_{ij}}}{2^{\frac{1}{2}\sum_{(i,j)\in\Omega_2} \frac{i+j}{ij}x_{ij}}} \geq 2^{\frac{n}{2}} \end{aligned}$$

as for any $(i,j) \in \Omega_2$, $i^2+j^2 \geq 2^{\frac{1}{2}\frac{i+j}{ij}}$. The equality holds if and only if for any $(i,j) \in \Omega_2$, $x_{ij} = 0$, that is, $G \cong \frac{n}{2}P_2$. □

Theorem 5.3. *If n is odd, then $\Pi_{\mathrm{SO}}(G) \geq 2^{\frac{n-3}{4}}5$, where G is isomorphic to $\frac{n-3}{2}P_2 \cup P_3$.*

Proof. Since n is odd, then there is no isolated vertex in G. Then $x_{11} \leq \frac{n-3}{2}\cdot$ Write

$$\Omega_3 = \{(i,j) \in \Omega : (i,j) \neq (1,1), (i,j) \neq (1,2)\}.$$

Since

$$n = 2x_{11} + \frac{3}{2}x_{12} + \sum_{(i,j)\in\Omega_3} \frac{i+j}{ij}x_{ij},$$

we have

$$x_{12} = \frac{2}{3}n - \frac{4}{3}x_{11} - \frac{2}{3}\sum_{(i,j)\in\Omega_3} \frac{i+j}{ij}x_{ij}.$$

By the definition of Π_{SO} and for any $(i,j)\in\Omega_3$, $i^2+j^2 > \frac{i+j}{ij}$, and we obtain

$$\Pi_{\mathrm{SO}}(G)^2 = \prod_{(i,j)\in\Omega}(i^2+j^2)^{x_{ij}} = (1^2+1^2)^{x_{11}}(1^2+2^2)^{x_{12}}\prod_{(i,j)\in\Omega_3}(i^2+j^2)^{x_{ij}}$$

$$= 2^{x_{11}}5^{\frac{2}{3}n-\frac{4}{3}x_{11}-\frac{2}{3}\sum_{(i,j)\in\Omega_3}\frac{i+j}{ij}x_{ij}}\prod_{(i,j)\in\Omega_3}(i^2+j^2)^{x_{ij}} = \frac{2^{x_{11}}5^{\frac{2}{3}n}\prod_{(i,j)\in\Omega_3}(i^2+j^2)^{x_{ij}}}{5^{\frac{4}{3}x_{11}+\frac{2}{3}\sum_{(i,j)\in\Omega_3}\frac{i+j}{ij}x_{ij}}}$$

$$\geq \left(\frac{2}{5^{\frac{4}{3}}}\right)^{x_{11}} \times 5^{\frac{2n}{3}} \times \frac{\prod_{(i,j)\in\Omega_3}(i^2+j^2)^{x_{ij}}}{5^{\sum_{(i,j)\in\Omega_3}\frac{i+j}{ij}x_{ij}}} \geq \left(\frac{2}{5^{\frac{4}{3}}}\right)^{x_{11}} \times 5^{\frac{2n}{3}} \geq \left(\frac{2}{5^{\frac{4}{3}}}\right)^{\frac{n-3}{2}} \times 5^{\frac{2n}{3}} = 2^{\frac{n-3}{2}}5^2. \quad (8)$$

If the equality in (8) holds, then $x_{11} = \frac{n-3}{2}$ and for any $(i,j)\in\Omega_3$, $x_{ij}=0$, that is, $G \cong \frac{n-3}{2}P_2 \cup P_3$. □

Corollary 5.4. *If G is a connected chemical graph, then $5\times 8^{\frac{n-3}{2}} = \Pi_{\mathrm{SO}}(P_n) \leq \Pi_{\mathrm{SO}}(G) \leq 1024^{\frac{n}{2}}$, where the right equality holds if and only if G is isomorphic to a 4-regular graph.*

6. Multiplicative Sombor index for chemical trees

In this section, we consider the multiplicative Sombor index for chemical trees. The following lemma can be easily obtained from the definition of the multiplicative Sombor index.

Lemma 6.1. *For any tree $T\in\mathcal{T}_n$, $\Pi_{\mathrm{SO}}(T) \geq \Pi_{\mathrm{SO}}(P_n) = 5\times 8^{\frac{n-3}{2}}$.*

Note that P_n is a chemical tree, it follows that the minimal Π_{SO}-value is determined by Lemma 6.1. Write

$$\Omega_4 = \{(i,j)\in\Omega : (i,j)\neq(1,1),(i,j)\neq(1,4),(i,j)\neq(4,4)\}.$$

Denoted by $\mathcal{CT}_n$ the class of all chemical trees of order n. Obviously, for any chemical tree $T\in\mathcal{CT}_n$, $x_{11}(T)=0$. By the definition of chemical trees,

$$\frac{5}{4}x_{14} + \frac{1}{2}x_{44} + \sum_{(i,j)\in\Omega_4}\frac{i+j}{ij}x_{ij} = n,\ x_{14}+x_{44}+\sum_{(i,j)\in\Omega_4}x_{ij} = n-1.$$

Therefore,

$$x_{14} = \frac{2n+2}{3} - \frac{1}{3}\sum_{(i,j)\in\Omega_4}\left(4\frac{i+j}{ij}-2\right)x_{ij},\ x_{44} = \frac{n-5}{3} + \frac{1}{3}\sum_{(i,j)\in\Omega_4}\left(4\frac{i+j}{ij}-5\right)x_{ij}.$$

We denote

$$\mathcal{U}_1 = \{T\in\mathcal{CT}_n : n_2 = n_3 = 0\},$$
$$\mathcal{U}_2 = \{T\in\mathcal{CT}_n : n_2 = 1, n_3 = 0\},$$
$$\mathcal{U}_3 = \{T\in\mathcal{CT}_n : n_2 = 0, n_3 = 1\}.$$

Then the following theorem determine the maximal Π_{SO}-value for chemical trees (Fig. 8).

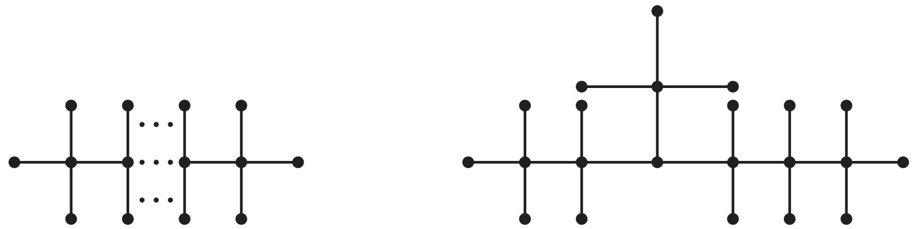


FIGURE 8. Tree in $\mathcal{U}_1$ and a chemical tree on 22 vertices in $\mathcal{U}_3$.

FIGURE 9. Two chemical trees with 18 vertices in $\mathcal{U}_2$.

Theorem 6.2. *For any chemical tree $T \in \mathcal{CT}_n$, $\Pi_{\mathrm{SO}}(T) \leq 17^{\frac{2n+2}{6}} 32^{\frac{n-5}{6}}$ with equality if and only if $T \in \mathcal{U}_1$.*

Proof. By the definition of Π_{SO}, we obtain

$$\begin{aligned}\Pi_{\mathrm{SO}}(T)^2 &= \prod_{(i,j)\in\Omega}(i^2+j^2) = (1^2+4^2)^{x_{14}}(4^2+4^2)^{x_{44}}\prod_{(i,j)\in\Omega_4}(i^2+j^2)^{x_{ij}}\\ &= 17^{\frac{2n+2}{3}-\frac{1}{3}\sum_{(i,j)\in\Omega_4}\left(4\frac{i+j}{ij}-2\right)x_{ij}}32^{\frac{n-5}{3}+\frac{1}{3}\sum_{(i,j)\in\Omega_4}\left(4\frac{i+j}{ij}-5\right)x_{ij}}\prod_{(i,j)\in\Omega_4}(i^2+j^2)^{x_{ij}}\\ &= 17^{\frac{2n+2}{3}}32^{\frac{n-5}{3}}\frac{32^{\frac{1}{3}\sum_{(i,j)\in\Omega_4}\left(4\frac{i+j}{ij}-5\right)x_{ij}}}{17^{\frac{1}{3}\sum_{(i,j)\in\Omega_4}\left(4\frac{i+j}{ij}-2\right)x_{ij}}}\prod_{(i,j)\in\Omega_4}(i^2+j^2)^{x_{ij}} \leq 17^{\frac{2n+2}{3}}32^{\frac{n-5}{3}} \qquad (9)\end{aligned}$$

as for any $(i,j)\in\Omega_4$,

$$\frac{32^{\frac{1}{3}\left(4\frac{i+j}{ij}-5\right)}}{17^{\frac{1}{3}\left(4\frac{i+j}{ij}-2\right)}}(i^2+j^2) \leq 1.$$

The equality holds in (9) if and only if for all $(i,j)\in\Omega_4$, $x_{ij}=0$, that is, $n_2=n_3=0$. □

Corollary 6.3. *Suppose $n \geq 5$ and $n \equiv 2 \pmod 3$. If the Π_{SO}-value attains its maximum in $\mathcal{CT}_n$, then $T \in \mathcal{U}_1$.*

Proof. Note that for any $T \in \mathcal{U}_1$, Π_{SO}-value is always a constant, that is, $\Pi_{\mathrm{SO}}(T) = 17^{\frac{2n+2}{6}}32^{\frac{n-5}{6}}$. □

Corollary 6.4. *Suppose $n \geq 9$ and $n \equiv 0 \pmod 3$. If the Π_{SO}-value attains its maximum in $\mathcal{CT}_n$, then $T \in \mathcal{U}_2$ and $x_{12} = 0$* (Fig. 9).

Proof. If $T \in \mathcal{U}_1 \cup \mathcal{U}_3$, then by the famous Handshaking Lemma, the following equations hold:

$$2(n-1) = n_1 + 4n_4 \quad \text{or} \quad 2(n-1) = n_1 + 3n_3 + 4n_4.$$

However, these equations are not valid if $n \equiv 0 \pmod 3$. It gives that $T \notin \mathcal{U}_1 \cup \mathcal{U}_3$. Assume that

$$\phi(i,j) = \frac{32^{\frac{1}{3}\left(4\frac{i+j}{ij}-5\right)}}{17^{\frac{1}{3}\left(4\frac{i+j}{ij}-2\right)}}(i^2+j^2).$$

Obviously, $\phi(1,3) < 1, \phi(3,3) < 1, \phi(3,4) < 1$, $\phi(1,2) < \phi(2,3) < \phi(2,4) < 1$ and $\phi(2,2) < \phi(2,4)^2$. Therefore, by the definition of Π_{SO}, we obtain

$$\begin{aligned}
\Pi_{\mathrm{SO}}(T)^2 &= \prod_{(i,j)\in\Omega}(i^2+j^2) = (1^2+4^2)^{x_{14}}(4^2+4^2)^{x_{44}}\prod_{(i,j)\in\Omega_4}(i^2+j^2)\\
&= 17^{\frac{2n+2}{3}}32^{\frac{n-5}{3}}\frac{32^{\frac{1}{3}\sum_{(i,j)\in\Omega_4}(4\frac{i+j}{ij}-5)x_{ij}}}{17^{\frac{1}{3}\sum_{(i,j)\in\Omega_4}(4\frac{i+j}{ij}-2)x_{ij}}}\prod_{(i,j)\in\Omega_4}(i^2+j^2)^{x_{ij}}\\
&= 17^{\frac{2n+2}{3}}32^{\frac{n-5}{3}}\times\prod_{(i,j)\in\Omega_4}\phi(i,j)^{x_{ij}}\\
&\le 17^{\frac{2n+2}{3}}32^{\frac{n-5}{3}}\times\phi(1,2)^{x_{12}}\phi(2,2)^{x_{22}}\phi(2,3)^{x_{23}}\phi(2,4)^{x_{24}}\\
&\le 17^{\frac{2n+2}{3}}32^{\frac{n-5}{3}}\times\phi(2,4)^{x_{12}+2x_{22}+x_{23}+x_{24}} = 17^{\frac{2n+2}{3}}32^{\frac{n-5}{3}}\times\phi(2,4)^{2n_2}.
\end{aligned}$$

If $n_2 = 0$, then $\Pi_{\mathrm{SO}}(T) \le 17^{\frac{2n+2}{6}}32^{\frac{n-5}{6}}$, where the equality holds if and only if $T\in\mathcal{U}_1$, which is impossible. Otherwise, $n_2 \ge 1$. Then by combining the fact $\phi(2,4) < 1$, we have

$$\Pi_{\mathrm{SO}}(T)^2 \le 17^{\frac{2n+2}{3}}32^{\frac{n-5}{3}}\times\phi(2,4)^{2n_2} \le 17^{\frac{2n+2}{3}}32^{\frac{n-5}{3}}\times\phi(2,4)^2,$$

where the equality holds if and only if $x_{24} = 2$ and $x_{12} = x_{22} = x_{13} = x_{23} = x_{33} = x_{34} = 0$. It follows that the Π_{SO}-value attains maximal if and only if $n_2 = 1$ and $n_3 = 0$. Therefore, if $n \equiv 0 \pmod 3$ and $n \ge 9$, the maximal Π_{SO}-value is attained when $T \in \mathcal{U}_2$ and $x_{12} = 0$. □

Corollary 6.5. *Suppose $n \ge 13$ and $n \equiv 1 \pmod 3$. If the Π_{SO}-value attains its maximum in $\mathcal{CT}_n$, then $T \in \mathcal{U}_3$ and $x_{13} = 0$.*

Proof. If $T \in \mathcal{U}_1\cup\mathcal{U}_2$, then by the famous Handshaking Lemma, the following equations hold:

$$2(n-1) = n_1 + 4n_4 \quad\text{or}\quad 2(n-1) = n_1 + 3n_3 + 4n_4.$$

However, these equations are not valid if $n \equiv 1 \pmod 3$. It gives that $T \notin \mathcal{U}_1\cup\mathcal{U}_2$. Assume that

$$\phi(i,j) = \frac{32^{\frac{1}{3}(4\frac{i+j}{ij}-5)}}{17^{\frac{1}{3}(4\frac{i+j}{ij}-2)}}(i^2+j^2).$$

Obviously, $\phi(1,3) < 1$, $\phi(3,3) < 1$, $\phi(2,2) < 1$, $\phi(2,4) < 1$, $\phi(1,2) < \phi(2,3) < \phi(3,4) < 1$, $\phi(3,3) < \phi(3,4)^2$. Therefore, by the definition of Π_{SO}, we obtain

$$\begin{aligned}
\Pi_{\mathrm{SO}}(T)^2 &= (1^2+4^2)^{\frac{2n+2}{3}}(4^2+4^2)^{\frac{n-5}{3}}\frac{32^{\frac{1}{3}\sum_{(i,j)\in\Omega_4}(4\frac{i+j}{ij}-5)x_{ij}}}{17^{\frac{1}{3}\sum_{(i,j)\in\Omega_4}(4\frac{i+j}{ij}-2)x_{ij}}}\prod_{(i,j)\in\Omega_4}(i^2+j^2)^{x_{ij}}\\
&= 17^{\frac{2n+2}{3}}32^{\frac{n-5}{3}}\times\prod_{(i,j)\in\Omega_4}\phi(i,j)^{x_{ij}}\\
&\le 17^{\frac{2n+2}{3}}32^{\frac{n-5}{3}}\times\phi(1,3)^{x_{13}}\phi(2,3)^{x_{23}}\phi(3,3)^{x_{33}}\phi(3,4)^{x_{34}}\\
&\le 17^{\frac{2n+2}{3}}32^{\frac{n-5}{3}}\times\phi(3,4)^{x_{13}+x_{23}+2x_{33}+x_{34}} = 17^{\frac{2n+2}{3}}32^{\frac{n-5}{3}}\times\phi(3,4)^{3n_3}.
\end{aligned}$$

If $n_3 = 0$, then $\Pi_{\mathrm{SO}}(T) \le 17^{\frac{2n+2}{6}}32^{\frac{n-5}{6}}$, the equality holds if and only if $T \in \mathcal{U}_1$, which is impossible. Otherwise, $n_3 \ge 1$. Then by combining the fact $\phi(3,4) < 1$, we have

$$\Pi_{\mathrm{SO}}(T)^2 \le 17^{\frac{2n+2}{3}}32^{\frac{n-5}{3}}\times\phi(3,4)^{3n_3} \le 17^{\frac{2n+2}{3}}32^{\frac{n-5}{3}}\times\phi(3,4)^3,$$

where the equality holds if and only if $x_{34} = 3$ and $x_{12} = x_{22} = x_{13} = x_{23} = x_{24} = x_{33} = 0$. It follows that the Π_{SO}-value attains maximum if and only if $n_2 = 0$ and $n_3 = 1$. Therefore, if $n \equiv 1 \pmod 3$ and $n \geq 13$, the maximum Π_{SO}-value is attained when $T \in \mathcal{U}_3$ and $x_{13} = 0$. □

7. Conclusions

This paper focuses two multiplicative variants of topological indices. After giving a general formula for the multiplicative version of the topological index of graphs, we determine the extremal values of the multiplicative sum Zagreb indices for trees with at most three branch vertices, as well as the extremal values of the multiplicative Sombor index for chemical graphs and chemical trees. In addition, the bounds of the multiplicative sum Zagreb index in terms of various graph parameters are established. Furthermore, the graphs that achieve these extremal values and bounds are completely characterized.

Funding

Xu Chunlei is supported by the Doctoral Scientific Research Funds of Inner Mongolia Minzu University (BSZ013, BSZ014, BS643), the Natural Science Foundation of Inner Mongolia Autonomous Region (2025MS01023), and the Programs Foundation of Basic Scientific Research of Colleges and Universities directly under the Inner Mongolia Autonomous Region (GXKY22156, GXKY25Z014). Li Guanru is supported by the Inner Mongolia Minzu University Doctoral Research Funds (BS643, BSZ013, BSZ014) and Inner Mongolia Autonomous Region, and the Same Level of Public Institutions Introduced Talent Scientific Research Projects of 2021 (RCQD202204). Lei Yiming is supported by Ph.D. Research Start-up Foundation (0522bs006) and Research Foundation of Bohai University (0522xn031).

Conflicts of interest

The authors declare no conflict of interest.

Data availability statement

The research data associated with this article are included in the article.

References

[1] M.S. Abubakar, K.O. Aremu, M. Aphane and M.K. Siddiqui, Exploring topological indices of oligothiophene dendrimer via neighbourhood M-polynomial. *RAIRO-Oper. Res.* **59** (2025) 149–161.

[2] A. Ali, K.C. Das and S. Akhter, On the extremal graphs for second Zagreb index with fixed number of vertices and cyclomatic number. *Miskolc Math. Notes* **23** (2022) 41–50.

[3] M. An and K.C. Das, First Zagreb index, k-connectivity, beta-deficiency and k-hamiltonicity of graphs. *MATCH Commun. Math. Comput. Chem.* **80** (2018) 141–151.

[4] H. Aram, Expected value for the k-distance degree index of a graph. *RAIRO-Oper. Res.* **58** (2024) 5159–5166.

[5] B. Bollobás, P. Erdös and A. Sarkar, Extremal graphs for weights. *Discrete Math.* **200** (1999) 5–19.

[6] B. Borovicanin and T.A. Lampert, On the maximum and minimum Zagreb indices of trees with a given number of vertices of maximum degree. *MATCH Commun. Math. Comput. Chem.* **74** (2015) 81–96.

[7] K.C. Das, Maximizing the sum of the squares of the degrees of a graph. *Discrete Math.* **285** (2004) 57–66.

[8] K.C. Das and I. Gutman, Some properties of the second Zagreb index. *MATCH Commun. Math. Comput. Chem.* **52** (2004) 103–112.

[9] K.C. Das, N. Akgünes, M. Togan, A. Yurttas, I.N. Cangül and A.S. Çevik, On the first Zagreb index and multiplicative Zagreb coindices of graphs. *Analele Stiintifice ale Universitatii Ovidius Constanta* **24** (2016) 153–176.

[10] H. Deng, A unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs. *MATCH Commun. Math. Comput. Chem.* **57** (2007) 597–616.

[11] J. Du and X. Sun, On the multiplicative sum Zagreb index of graphs with some given parameters. *J. Math. Inequal.* **14** (2020) 1165–1181.

[12] M. Eliasi, A. Iranmanesh and I. Gutman, Multiplicative version of the first Zagreb index. *MATCH Commun. Math. Comput. Chem.* **68** (2012) 217–230.

[13] C. Elphick and T. Reti, On the relations between the Zagreb indices, clique numbers and walks in graphs. *MATCH Commun. Math. Comput. Chem.* **74** (2015) 19–34.
[14] I. Gutman, Multiplicative Zagreb indices of trees. *Bull. Int. Math. Virt. Inst.* **1** (2011) 13–19.
[15] I. Gutman and K.C. Das, The first Zagreb index 30 years after. *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.
[16] I. Gutman, B. Furtula and C. Elphick, Three new/old vertex degree-based topological indices. *MATCH Commun. Math. Comput. Chem.* **72** (2014) 617–682.
[17] B. Horoldagva and K.C. Das, On Zagreb indices of graphs, *MATCH Commun. Math. Comput. Chem.* **85** (2021) 295–301.
[18] B. Horoldagva, C. Xu, L. Buyantogtokh and L. Dorjsembe, Extremal graphs with respect to the multiplicative sum Zagreb index, *MATCH Commun. Math. Comput. Chem.* **84** (2020) 773–786.
[19] Y. Jin, S. Zhou, T. Tian and K.C. Das, Sufficient conditions for Hamiltonian properties of graphs based on the difference of Zagreb indices. *Comput. Appl. Math.* **43** (2024) 385.
[20] R. Kazemi, Note on the multiplicative Zagreb indices. *Discrete Appl. Math.* **198** (2016) 147–154.
[21] V.R. Kulli, Multiplicative Sombor indices of certain nanotubes. *Int. J. Math. Arch.* **12** (2021) 1–5.
[22] H. Liu, Multiplicative Sombor index of graphs. *Discrete Math. Lett.* **9** (2022) 80–85.
[23] B. Liu and Z. You, A survey on comparing Zagreb indices. *MATCH Commun. Math. Comput. Chem.* **65** (2011) 581–593.
[24] S. Nikolić, G. Kovačević, A. Miličević and N. Trinajstić, The Zagreb indices 30 years after. *Croat. Chem. Acta* **76** (2003) 113–124.
[25] Z. Raza, L. Saha and K.C. Das, On inverse symmetric division deg index of graphs. *RAIRO-Oper. Res.* **57** (2023) 3223–3236.
[26] T. Selenge and B. Horoldagva, Maximum Zagreb indices in the class of k-apex trees. *Korean J. Math.* **23** (2015) 401–408.
[27] R. Todeschini and V. Consonni, New local vertex invariants and molecular descriptors based on functions of the vertex degrees. *MATCH Commun. Math. Comput. Chem.* **64** (2010) 359–372.
[28] H. Wang and S. Yuan, On the sum of squares of degrees and products of adjacent degrees. *Discrete Math.* **339** (2016) 1212–1220.
[29] K. Xu and K.C. Das, Trees, unicyclic, and bicyclic graphs extremal with respect to multiplicative sum Zagreb index. *MATCH Commun. Math. Comput. Chem.* **68** (2012) 257–272.
[30] K. Xu, F. Gao, K.C. Das and N. Trinajstić, A formula with its applications on the difference of Zagreb indices of graphs. *J. Math. Chem.* **57** (2019) 1618–1626.
[31] C. Xu, B. Horoldagva and L. Buyantogtokh, Cactus graphs with maximal multiplicative sum Zagreb index. *Symmetry* **13** (2021) 913.
[32] C. Xu, B. Horoldagva, L. Buyantogtokh, K.C. Das and T.-A. Selenge, Multiplicative Sombor index of graphs. *Rocky Mt. Jour. Math.*, in press.