

On the Minimum Multiplicative Sum Zagreb Indices of Connected Graphs and Tetracyclic (Molecular) Graphs

Xiaoling Sun and Jianwei Du*

Abstract—As one of the modified versions of the well-known Zagreb indices, the multiplicative sum Zagreb index of a graph is defined as the product of the sums of degrees over all pairs of adjacent vertices. In this article, we establish a sufficient condition for the multiplicative sum Zagreb index of graphs to attain its minimum value. Furthermore, we classify the tetracyclic (molecular) graphs without pendant vertices based on the values of the multiplicative sum Zagreb index, and we present a sharp lower bound for this index among all tetracyclic (molecular) graphs.

Index Terms—Multiplicative sum Zagreb index, Connected graph, Tetracyclic (molecular) graphs.

I. INTRODUCTION

THE topological indices are mathematical descriptors reflecting some structural properties and characteristics of organic compounds through their chemical graphs, and they play a significant role in chemistry and pharmacology (see [1]–[3]). The first and second Zagreb indices are two of the most renowned and extensively studied topological indices, which were originally used to examine the structure dependence of total π -electron energy on molecular orbital [4]. The first and second Zagreb indices of a graph G (denoted by M_1 and M_2) are defined as follows:

$$M_1(G) = \sum_{x \in V(G)} d(x)^2, \quad M_2(G) = \sum_{xy \in E(G)} d(x)d(y),$$

where $d(x)$ stands for the degree of vertex x in G .

The first and second Zagreb indices (M_1 and M_2) and their modified variants have been applied to explore diverse chemical properties, including ZE-isomerism, heterosystems, complexity and chirality of compounds, etc. [5]–[7]. Among these variants, the first and second multiplicative Zagreb indices (denoted by Π_1 and Π_2) [8], and the multiplicative sum Zagreb index (denoted by Π_1^*) [9] have garnered significant attention from researchers (such as recent works [10]–[19]). The indices Π_1 and Π_2 are defined as below:

$$\Pi_1(G) = \prod_{x \in V(G)} d(x)^2, \quad \Pi_2(G) = \prod_{xy \in E(G)} d(x)d(y),$$

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while the index Π_1^* is defined as follows:

$$\Pi_1^*(G) = \prod_{xy \in E(G)} (d(x) + d(y)).$$

Xu and Das [20] determined the minimal and maximal values of Π_1^* for trees, unicyclic graphs and bicyclic graphs. Eliasi et al. [9] showed that the connected graph with the minimum Π_1^* is a path, and determined the second minimum Π_1^* of trees. Božović et al. [21] derived the maximum value of Π_1^* for molecular trees and identified the corresponding extremal trees. Two authors of this article [12], [14] obtained the minimal and maximal values of Π_1^* on trees with a given domination number, and determined the maximum value of Π_1^* among all connected graphs with given number of cut edges, cut vertices, edge connectivity, or vertex connectivity. For further details on the multiplicative sum Zagreb index, we refer the readers to recent papers [15]–[19] and the references therein.

In this article, just simple connected graphs are taken into account. For such a graph G , the sets of vertices and edges are represented by $V(G)$ and $E(G)$, respectively. The neighborhood of a vertex $x \in V(G)$ is denoted by $N_G(x)$. For a graph G , let $n_i(G)$ (n_i for short) represent the number of vertices of degree i , and $m_{i,j}(G)$ (or simply $m_{i,j}$) denote the number of edges connecting the vertices of degree i and j . The minimum and maximum degrees of G are denoted by $\delta(G)$ and $\Delta(G)$ (δ and Δ for short), respectively. Let $G - uv$ and $G + uv$ be the graph arisen from G by deleting the edge $uv \in E(G)$ and by connecting the vertex u and v in G ($uv \notin E(G)$), respectively. A graph G of order n is called a tetracyclic graph if $|E(G)| = n + 3$. One can refer to [22] for other terminologies and notations.

The molecular (or chemical) graphs are graphs with maximum degree at most 4. In recent years, it is an important research focus to study the extremal values of topological indices for molecular (or chemical) graphs [23]–[33]. In this work, we establish sufficient a condition for Π_1^* of graphs to attain its minimum value. Furthermore, we classify the tetracyclic (molecular) graphs without pendant vertices according to the values of Π_1^* , and we obtain a sharp lower bound for Π_1^* among all tetracyclic (molecular) graphs.

II. SOME LEMMAS

Lemma 2.1: [13] The function $h(x) = \frac{x+c}{x}$ ($c \geq 1$ is an integer) is strictly decreasing with respect to $x \geq 1$.

Lemma 2.2: Let

$$l_1(\Delta, \delta) = \left(\frac{2\Delta}{2\Delta-1}\right)^\Delta \left(\frac{2\delta}{2\delta+1}\right)^\delta,$$

where Δ and δ are positive integers with $\delta + 2 \leq \Delta \leq n - 1$ ($n \geq 4$ is a finite positive integer). Then $l_1(\Delta, \delta) > 1$.

Proof: We first prove that $\ln(1+t) > \frac{t}{1+t}$ for $t > 0$. Let $\psi(t) = \ln(1+t) - \frac{t}{1+t}$, where $t > 0$. Then

$$\frac{d\psi(t)}{dt} = \frac{1}{t+1} - \frac{1}{(t+1)^2} > 0.$$

Thus $\psi(t) > \psi(0) = 0$ for $t > 0$, that is, $\ln(1+t) > \frac{t}{1+t}$.

Let $h_1(x) = \left(\frac{2x}{2x+1}\right)^x$, where $x \geq 1$. Then $\ln h_1(x) = x[\ln(2x) - \ln(2x+1)]$. Thus, by the above inequality proved, for $x \geq 1$, we get

$$\begin{aligned} \frac{d \ln h_1(x)}{dx} &= \frac{1}{2x+1} + \ln \frac{2x}{2x+1} \\ &= \frac{1}{2x+1} - \ln\left(1 + \frac{1}{2x}\right) \\ &< \frac{1}{2x+1} - \frac{\frac{1}{2x}}{1 + \frac{1}{2x}} = 0. \end{aligned}$$

So $h_1(x)$ is decreasing with respect to $x \geq 1$.

Let $h_2(x) = \left(\frac{2x}{2x-1}\right)^x \left(\frac{2x-4}{2x-3}\right)^{x-2}$, where $x \geq 3$. Then $\ln h_2(x) = x[\ln(2x) - \ln(2x-1)] + (x-2)[\ln(2x-4) - \ln(2x-3)]$. Therefore, for $x \geq 3$, we have

$$\begin{aligned} \frac{d \ln h_2(x)}{dx} &= \frac{1}{2x-3} - \frac{1}{2x-1} + \ln \frac{2x-4}{2x-3} + \ln \frac{2x}{2x-1} \\ &= \frac{2}{(2x-1)(2x-3)} - \ln\left(1 + \frac{3}{4x^2-8x}\right) \\ &< \frac{2}{(2x-1)(2x-3)} - \frac{\frac{3}{4x^2-8x}}{1 + \frac{3}{4x^2-8x}} \\ &= -\frac{1}{(2x-1)(2x-3)} < 0. \end{aligned}$$

So $h_2(x)$ is decreasing for $x \geq 3$.

Since $\delta \leq \Delta - 2$ and $\Delta \leq n - 1$, by the monotonicity of $h_1(x)$ and $h_2(x)$, we obtain

$$\begin{aligned} l_1(\Delta, \delta) &= \left(\frac{2\Delta}{2\Delta-1}\right)^\Delta \left(\frac{2\delta}{2\delta+1}\right)^\delta \\ &\geq \left(\frac{2\Delta}{2\Delta-1}\right)^\Delta \left(\frac{2(\Delta-2)}{2(\Delta-2)+1}\right)^{\Delta-2} \\ &\geq \left(\frac{2n-2}{2n-3}\right)^{n-1} \left(\frac{2n-6}{2n-5}\right)^{n-3}. \end{aligned}$$

Let $g(n) = \left(\frac{2n-2}{2n-3}\right)^{n-1} \left(\frac{2n-6}{2n-5}\right)^{n-3}$, where $n \geq 4$. Similar as $h_2(x)$, we can check that $g(n)$ is decreasing for $n \geq 4$. Since

$$\begin{aligned} &\lim_{n \rightarrow +\infty} \left(\frac{2n-2}{2n-3}\right)^{n-1} \left(\frac{2n-6}{2n-5}\right)^{n-3} \\ &= \lim_{n \rightarrow +\infty} \left(1 + \frac{1}{2n-3}\right)^{\frac{1}{2}} \cdot \left[\left(1 + \frac{1}{2n-3}\right)^{2n-3}\right]^{\frac{1}{2}} \\ &\quad \times \lim_{n \rightarrow +\infty} \left(1 - \frac{1}{2n-5}\right)^{-\frac{1}{2}} \cdot \left[\left(1 - \frac{1}{2n-5}\right)^{-(2n-5)}\right]^{-\frac{1}{2}} \\ &= e^{\frac{1}{2}} \cdot e^{-\frac{1}{2}} = 1, \end{aligned}$$

then $g = 1$ is the horizontal asymptote of $g(n)$. Furthermore, since n is a finite positive integer, $g(4) = 1.152 > 1$ and $g(n)$ is decreasing with respect to n , we deduce that $g(n) > 1$. Therefore, $l_1(\Delta, \delta) \geq g(n) > 1$.

We complete the proof. ■

Lemma 2.3: Let

$$l_2(\Delta, \delta) = \left(\frac{2\Delta}{2\Delta-1}\right)^{\Delta-1} \left(\frac{2\delta}{2\delta+1}\right)^{\delta-1},$$

where Δ and δ are positive integers with $\delta + 2 \leq \Delta \leq n - 1$ ($n \geq 4$ is a finite positive integer). Then $l_2(\Delta, \delta) > 1$.

Proof: According to Lemma 2.2, one has

$$\begin{aligned} l_2(\Delta, \delta) &= \left(\frac{2\Delta}{2\Delta-1}\right)^\Delta \left(\frac{2\delta}{2\delta+1}\right)^\delta \left(\frac{2\Delta}{2\Delta-1}\right)^{-1} \left(\frac{2\delta}{2\delta+1}\right)^{-1} \\ &= l_1(\Delta, \delta) \cdot \left(1 + \frac{2\Delta-2\delta-1}{4\Delta\delta}\right) \\ &\geq l_1(\Delta, \delta) \cdot \left(1 + \frac{2(\delta+2)-2\delta-1}{4\Delta\delta}\right) \\ &> l_1(\Delta, \delta) > 1. \end{aligned}$$

This completes the proof. ■

III. GRAPHS WITH MINIMUM MULTIPLICATIVE SUM ZAGREB INDEX

Theorem 3.1: Let G be a graph with n vertices and m edges. If G has the minimum multiplicative sum Zagreb index, then $\Delta - \delta \leq 1$.

Proof: Assume to the contrary that $\Delta - \delta \geq 2$. Let x, y be two vertices with $d(x) = \Delta$ and $d(y) = \delta$ in G . Since $d(x) > d(y)$, there exists a neighbor of x , say z , such that $z \notin N_G(y)$. Set $G' = G - xz + yz$. Next, we discuss the following two cases.

Case 1. $xy \notin E(G)$.

Let $a_1, a_2, \dots, a_\Delta$ and $b_1, b_2, \dots, b_\delta$ be the degree of vertices in $N_G(x)$ and $N_G(y)$, respectively. Without loss of generality, we suppose that $d(z) = a_\Delta$. Note that for $i \in \{1, 2, \dots, \Delta\}$ and $j \in \{1, 2, \dots, \delta\}$, $\delta \leq a_i, b_j \leq \Delta$ and $\Delta - 1 \geq \delta + 1$, by the definition of multiplicative sum Zagreb index and Lemmas 2.1, 2.2, we have

$$\begin{aligned} &\frac{\Pi_1^*(G)}{\Pi_1^*(G')} \\ &= \frac{\prod_{i=1}^{\Delta} (\Delta + a_i) \prod_{j=1}^{\delta} (\delta + b_j)}{(\delta + 1 + a_\Delta) \prod_{i=1}^{\Delta-1} (\Delta - 1 + a_i) \prod_{j=1}^{\delta} (\delta + 1 + b_j)} \\ &= \frac{\prod_{i=1}^{\Delta} (\Delta + a_i) \prod_{j=1}^{\delta} (\delta + b_j)}{\prod_{i=1}^{\Delta} (\Delta - 1 + a_i) \prod_{j=1}^{\delta} (\delta + 1 + b_j)} \cdot \frac{\Delta - 1 + a_\Delta}{\delta + 1 + a_\Delta} \\ &\geq \prod_{i=1}^{\Delta} \frac{\Delta + a_i}{\Delta - 1 + a_i} \cdot \prod_{j=1}^{\delta} \frac{\delta + b_j}{\delta + 1 + b_j} \\ &\geq \left(\frac{2\Delta}{2\Delta-1}\right)^\Delta \cdot \left(\frac{2\delta}{2\delta+1}\right)^\delta > 1. \end{aligned}$$

Hence, $\Pi_1^*(G) > \Pi_1^*(G')$, a contradiction.

Case 2. $xy \in E(G)$.

Let $a_1, a_2, \dots, a_{\Delta-1}$ and $b_1, b_2, \dots, b_{\delta-1}$ be the degree of vertices in $N_G(x) \setminus \{y\}$ and $N_G(y) \setminus \{x\}$, respectively. Without loss of generality, we assume that $d(z) = a_{\Delta-1}$. By the definition of multiplicative sum Zagreb index and

Lemmas 2.1, 2.3, we derive

$$\begin{aligned}
 & \frac{\Pi_1^*(G)}{\Pi_1^*(G')} \\
 &= \frac{(\Delta + \delta) \prod_{i=1}^{\Delta-1} (\Delta + a_i) \prod_{j=1}^{\delta-1} (\delta + b_j)}{(\delta + 1 + a_{\Delta-1}) (\Delta - 1 + \delta + 1) \prod_{i=1}^{\Delta-2} (\Delta - 1 + a_i) \prod_{j=1}^{\delta-1} (\delta + 1 + b_j)} \\
 &= \frac{\prod_{i=1}^{\Delta-1} (\Delta + a_i) \prod_{j=1}^{\delta-1} (\delta + b_j)}{\prod_{i=1}^{\Delta-1} (\Delta - 1 + a_i) \prod_{j=1}^{\delta-1} (\delta + 1 + b_j)} \cdot \frac{\Delta - 1 + a_{\Delta-1}}{\delta + 1 + a_{\Delta-1}} \\
 &\geq \prod_{i=1}^{\Delta-1} \frac{\Delta + a_i}{\Delta - 1 + a_i} \cdot \prod_{j=1}^{\delta-1} \frac{\delta + b_j}{\delta + 1 + b_j} \\
 &\geq \left(\frac{2\Delta}{2\Delta - 1} \right)^{\Delta-1} \cdot \left(\frac{2\delta}{2\delta + 1} \right)^{\delta-1} > 1.
 \end{aligned}$$

Thus $\Pi_1^*(G) > \Pi_1^*(G')$, which is a contradiction again. We complete the proof. ■

By Theorem 3.1, one can derive Corollary 3.2 and Corollary 3.3 below immediately.

Corollary 3.2: [20] Suppose T is a tree with n ($n \geq 3$) vertices having the minimum Π_1^* , then T is a path.

Corollary 3.3: [20] Suppose G is a unicyclic with n ($n \geq 3$) vertices having the minimum Π_1^* , then G is a cycle.

Corollary 3.4: Let G be a graph having n vertices and m edges. If G has the minimum Π_1^* , then G contains $n - 2m + n \lfloor \frac{2m}{n} \rfloor$ vertices with degree $\lfloor \frac{2m}{n} \rfloor$ and $2m - n \lfloor \frac{2m}{n} \rfloor$ vertices with degree $\lfloor \frac{2m}{n} \rfloor + 1$.

Proof: If $\delta = \Delta$, then $n\Delta = 2m$ and it is not difficult to check that the result is true. So one can assume that $\delta \neq \Delta$. By Theorem 3.1, we have $\Delta = \delta + 1$. Now we can suppose that G contains r vertices degree δ and s vertices degree $\Delta = \delta + 1$. Thus one can derive that $r\delta + s(\delta + 1) = 2m$, that is, $(r + s)\delta + s = 2m$. Furthermore, $r + s = n$, it follows that $n\delta + s = 2m$. We have $\delta + \frac{s}{n} = \frac{2m}{n}$ by dividing both sides by n . Since $s < n$, one has

$$\delta = \lfloor \frac{2m}{n} \rfloor, \Delta = \lfloor \frac{2m}{n} \rfloor + 1.$$

Moreover, from $s = 2m - n\delta$, we derive that

$$r = n + n \lfloor \frac{2m}{n} \rfloor - 2m, \quad s = 2m - n \lfloor \frac{2m}{n} \rfloor.$$

The proof is complete. ■

According to Corollary 3.4, we have an immediate Corollary 3.5.

Corollary 3.5: Let G be a graph having n vertices and m edges. If G has the minimum Π_1^* and $n \mid 2m$, then $\Pi_1^*(G) = (\frac{4m}{n})^m$ and G is a $\frac{2m}{n}$ -regular graph.

IV. TETRACYCLIC (MOLECULAR) GRAPHS WITH MINIMUM MULTIPLICATIVE SUM ZAGREB INDEX

Let TMG_n and TG_n be the collections of n -vertex tetracyclic molecular graphs and tetracyclic graphs, respectively.

Lemma 4.1: [26] G belongs to one of equivalence classes given in Table I if and only if $G \in TG_n$ with $n_1(G) = 0$.

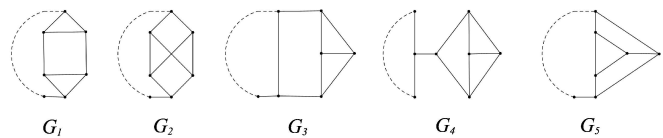


Fig. 1. Five extremal tetracyclic graphs G_1, G_2, \dots, G_5 with minimum Π_1^*

The edge degree and vertex degree divisions for tetracyclic graphs satisfying $n_1(G) = 0$ in A_i , along with their values of Π_1^* , all displayed in Tables I-V, where $1 \leq i \leq 11$. It is worth noting that except the values of Π_1^* , the related data in Tables II-V comes from [33] (also used in [32] recently).

Let $\Phi = \Phi_1 \cup \Phi_2$, where $\Phi_1 = \{G \mid G \in TG_n \text{ with } n_1(G) = 0\}$ and $\Phi_2 = \{G \mid G \in TG_n \text{ with } n_1(G) \geq 1\}$. Thus $\Phi_1 = \cup_{i=1}^{11} A_i = \cup_{i=1}^{95} \epsilon_i$, which can be seen in Tables I-V. Notice that $\epsilon_7 = \{G \mid G \in \Phi_1 \text{ with } m_{3,3} = 8, m_{3,2} = 2, m_{2,2} = n - 7\}$. It can be easily seen that $\epsilon_7 = \{G_1, G_2, \dots, G_5\}$, see Fig. 1. In what follows, we shall prove that the graphs belonging to ϵ_7 are the extremal graphs having the minimum Π_1^* among TG_n or TMG_n .

By a simple calculation, one can get the following Lemma 4.2.

Lemma 4.2: Let $G \in \epsilon_7$. Then $\Pi_1^*(G) = 5^2 6^8 4^{n-7} \approx 4^n \cdot 2562.89$.

Theorem 4.3: Suppose $G \in TG_n$, where $n \geq 9$, then

$$\Pi_1^*(G) \geq 5^2 6^8 4^{n-7}.$$

The equality occurs if and only if $G \in \epsilon_7$, that is, $G \cong G_i$, where $1 \leq i \leq 5$ (see Fig. 1).

Proof: Choose $G \in TG_n$ such that G has the minimal value of Π_1^* , where $n \geq 9$. If $n_1 \geq 1$, we have $\Delta - \delta \geq 2$, which contradicts the result of Theorem 3.1. Hence $n_1(G) = 0$. For all $G \in TG_n$ with $n_1(G) = 0$ in A_i and their Π_1^* are displayed in Tables II-V, where $1 \leq i \leq 11$. We compare the values of Π_1^* in Tables II-V, one can get the expected conclusions. ■

It is easy to see that the tetracyclic graphs G_1, G_2, \dots, G_5 in Fig. 1 are all molecular graphs, so we have

Theorem 4.4: Suppose $G \in TMG_n$, where $n \geq 9$, then

$$\Pi_1^*(G) \geq 5^2 6^8 4^{n-7}.$$

The equality holds if and only if $G \in \epsilon_7$, that is, $G \cong G_i$, where $1 \leq i \leq 5$ (see Fig. 1).

TABLE I
VERTEX DEGREE DIVISIONS (VDD) OF TG_n WITH $n_1 = 0$

VDD	n_1	n_2	n_3	n_4	n_5	n_6	n_7	n_8	$n_i (i \geq 9)$
A_1	0	$n - 1$	0	0	0	0	0	1	0
A_2	0	$n - 2$	1	0	0	0	1	0	0
A_3	0	$n - 2$	0	1	0	1	0	0	0
A_4	0	$n - 3$	2	0	0	1	0	0	0
A_5	0	$n - 2$	0	0	2	0	0	0	0
A_6	0	$n - 3$	1	1	1	0	0	0	0
A_7	0	$n - 4$	3	0	1	0	0	0	0
A_8	0	$n - 3$	0	3	0	0	0	0	0
A_9	0	$n - 4$	2	2	0	0	0	0	0
A_{10}	0	$n - 5$	4	1	0	0	0	0	0
A_{11}	0	$n - 6$	6	0	0	0	0	0	0

TABLE II
EDGE DEGREE DIVISIONS (EDD) OF TG_n WITH $n_1 = 0, \Delta = 3$ AND THEIR Π_1^*

EDD	VDD	$m_{3,3}$	$m_{3,2}$	$m_{2,2}$	Π_1^*
ϵ_1	A_{11}	3	12	$n - 12$	$4^n \cdot 3143.21$
ϵ_2	A_{11}	2	14	$n - 13$	$4^n \cdot 3274.18$
ϵ_3	A_{11}	5	8	$n - 10$	$4^n \cdot 2896.79$
ϵ_4	A_{11}	4	10	$n - 11$	$4^n \cdot 3017.49$
ϵ_5	A_{11}	7	4	$n - 8$	$4^n \cdot 2669.68$
ϵ_6	A_{11}	6	6	$n - 9$	$4^n \cdot 2780.91$
ϵ_7	A_{11}	8	2	$n - 7$	$4^n \cdot 2562.89$

TABLE III
 EDD OF TG_n WITH $n_1 = 0, \Delta = 4$ AND THEIR Π_1^*

EDD	VDD	$m_{4,4}$	$m_{4,3}$	$m_{4,2}$	$m_{3,3}$	$m_{3,2}$	$m_{2,2}$	Π_1^*
ϵ_8	A_8	1	0	10	0	0	$n - 8$	$4^n \cdot 7381.13$
ϵ_9	A_8	0	0	12	0	0	$n - 9$	$4^n \cdot 8303.77$
ϵ_{10}	A_8	3	0	6	0	0	$n - 6$	$4^n \cdot 5832.00$
ϵ_{11}	A_8	2	0	8	0	0	$n - 7$	$4^n \cdot 6561.00$
ϵ_{12}	A_9	0	0	8	1	4	$n - 10$	$4^n \cdot 6006.77$
ϵ_{13}	A_9	0	0	8	0	6	$n - 11$	$4^n \cdot 6257.06$
ϵ_{14}	A_9	0	1	7	1	3	$n - 9$	$4^n \cdot 5606.32$
ϵ_{15}	A_9	0	1	7	0	5	$n - 10$	$4^n \cdot 5839.92$
ϵ_{16}	A_9	0	2	6	0	4	$n - 9$	$4^n \cdot 5450.59$
ϵ_{17}	A_9	1	0	6	0	6	$n - 10$	$4^n \cdot 5561.83$
ϵ_{18}	A_9	0	2	6	1	2	$n - 8$	$4^n \cdot 5232.57$
ϵ_{19}	A_9	1	0	6	1	4	$n - 9$	$4^n \cdot 5339.36$
ϵ_{20}	A_9	0	3	5	0	3	$n - 8$	$4^n \cdot 5087.22$
ϵ_{21}	A_9	1	1	5	0	5	$n - 9$	$4^n \cdot 5191.04$
ϵ_{22}	A_9	0	3	5	1	1	$n - 7$	$4^n \cdot 4883.73$
ϵ_{23}	A_9	1	1	5	1	3	$n - 8$	$4^n \cdot 4983.40$
ϵ_{24}	A_9	0	4	4	0	2	$n - 7$	$4^n \cdot 4748.07$
ϵ_{25}	A_9	1	2	4	0	4	$n - 8$	$4^n \cdot 4884.97$
ϵ_{26}	A_9	0	4	4	1	0	$n - 6$	$4^n \cdot 4558.15$
ϵ_{27}	A_9	1	2	4	1	2	$n - 7$	$4^n \cdot 4651.17$
ϵ_{28}	A_9	1	3	3	1	1	$n - 6$	$4^n \cdot 4341.10$
ϵ_{29}	A_9	1	3	3	0	3	$n - 7$	$4^n \cdot 4521.97$
ϵ_{30}	A_9	1	4	2	0	2	$n - 6$	$4^n \cdot 4220.51$
ϵ_{31}	A_9	1	4	2	1	0	$n - 5$	$4^n \cdot 4051.69$
ϵ_{32}	A_{10}	0	0	4	0	12	$n - 13$	$4^n \cdot 4714.82$
ϵ_{33}	A_{10}	0	1	3	0	11	$n - 12$	$4^n \cdot 4400.50$
ϵ_{34}	A_{10}	0	0	4	1	10	$n - 12$	$4^n \cdot 4526.23$
ϵ_{35}	A_{10}	0	1	3	1	9	$n - 11$	$4^n \cdot 4224.48$
ϵ_{36}	A_{10}	0	0	4	2	8	$n - 11$	$4^n \cdot 4345.18$
ϵ_{37}	A_{10}	0	2	2	0	10	$n - 11$	$4^n \cdot 4107.13$
ϵ_{38}	A_{10}	0	0	4	3	6	$n - 10$	$4^n \cdot 4171.37$
ϵ_{39}	A_{10}	0	0	4	4	4	$n - 9$	$4^n \cdot 4004.52$
ϵ_{40}	A_{10}	0	1	3	2	7	$n - 10$	$4^n \cdot 4055.50$
ϵ_{41}	A_{10}	0	1	3	3	5	$n - 9$	$4^n \cdot 3893.28$
ϵ_{42}	A_{10}	0	2	2	1	8	$n - 10$	$4^n \cdot 3942.85$
ϵ_{43}	A_{10}	0	0	4	5	2	$n - 8$	$4^n \cdot 3844.34$
ϵ_{44}	A_{10}	0	3	1	0	9	$n - 10$	$4^n \cdot 3833.32$
ϵ_{45}	A_{10}	0	1	3	4	3	$n - 8$	$4^n \cdot 3737.55$
ϵ_{46}	A_{10}	0	2	2	2	6	$n - 9$	$4^n \cdot 3785.13$
ϵ_{47}	A_{10}	0	2	2	3	4	$n - 8$	$4^n \cdot 3633.73$
ϵ_{48}	A_{10}	0	3	1	1	7	$n - 9$	$4^n \cdot 3679.99$
ϵ_{49}	A_{10}	0	1	3	5	1	$n - 7$	$4^n \cdot 3588.05$
ϵ_{50}	A_{10}	0	4	0	0	8	$n - 9$	$4^n \cdot 3577.77$
ϵ_{51}	A_{10}	0	2	2	4	2	$n - 7$	$4^n \cdot 3488.38$
ϵ_{52}	A_{10}	0	3	1	2	5	$n - 8$	$4^n \cdot 3532.79$
ϵ_{53}	A_{10}	0	3	1	3	3	$n - 7$	$4^n \cdot 3391.48$
ϵ_{54}	A_{10}	0	4	0	1	6	$n - 8$	$4^n \cdot 3434.66$
ϵ_{55}	A_{10}	0	4	0	2	4	$n - 7$	$4^n \cdot 3297.27$
ϵ_{56}	A_{10}	0	2	2	5	0	$n - 6$	$4^n \cdot 3348.84$
ϵ_{57}	A_{10}	0	4	0	3	2	$n - 6$	$4^n \cdot 3165.38$
ϵ_{58}	A_{10}	0	3	1	4	1	$n - 6$	$4^n \cdot 3255.82$

TABLE IV
EDD OF TG_n WITH $n_1 = 0, \Delta = 5$ AND THEIR Π_1^*

EDD	VDD	$m_{5,5}$	$m_{5,4}$	$m_{5,3}$	$m_{5,2}$	$m_{4,3}$	$m_{4,2}$	$m_{3,3}$	$m_{3,2}$	$m_{2,2}$	Π_1^*
ϵ_{59}	A_5	1	0	0	8	0	0	0	0	$n-6$	$4^n \cdot 14074.22$
ϵ_{60}	A_5	0	0	0	10	0	0	0	0	$n-7$	$4^n \cdot 17240.92$
ϵ_{61}	A_6	0	0	0	5	1	3	0	2	$n-8$	$4^n \cdot 9693.98$
ϵ_{62}	A_6	0	0	0	5	0	4	0	3	$n-9$	$4^n \cdot 10386.41$
ϵ_{63}	A_6	0	1	0	4	0	3	0	3	$n-8$	$4^n \cdot 8902.63$
ϵ_{64}	A_6	0	0	1	4	0	4	0	2	$n-8$	$4^n \cdot 9496.14$
ϵ_{65}	A_6	0	1	0	4	1	2	0	2	$n-7$	$4^n \cdot 8309.12$
ϵ_{66}	A_6	0	0	1	4	1	3	0	1	$n-7$	$4^n \cdot 8863.07$
ϵ_{67}	A_6	0	1	1	3	1	2	0	1	$n-6$	$4^n \cdot 7596.91$
ϵ_{68}	A_6	0	1	1	3	0	3	0	2	$n-7$	$4^n \cdot 8139.55$
ϵ_{69}	A_7	0	0	0	5	0	0	1	7	$n-10$	$4^n \cdot 7513.31$
ϵ_{70}	A_7	0	0	0	5	0	0	0	9	$n-11$	$4^n \cdot 7826.37$
ϵ_{71}	A_7	0	0	1	4	0	0	0	8	$n-10$	$4^n \cdot 7155.54$
ϵ_{72}	A_7	0	0	0	5	0	0	2	5	$n-9$	$4^n \cdot 7212.78$
ϵ_{73}	A_7	0	0	1	4	0	0	1	6	$n-9$	$4^n \cdot 6869.32$
ϵ_{74}	A_7	0	0	0	5	0	0	3	3	$n-8$	$4^n \cdot 6924.27$
ϵ_{75}	A_7	0	0	2	3	0	0	0	7	$n-9$	$4^n \cdot 6542.21$
ϵ_{76}	A_7	0	0	1	4	0	0	2	4	$n-8$	$4^n \cdot 6594.54$
ϵ_{77}	A_7	0	0	2	3	0	0	1	5	$n-8$	$4^n \cdot 6280.52$
ϵ_{78}	A_7	0	0	1	4	0	0	3	2	$n-7$	$4^n \cdot 6330.76$
ϵ_{79}	A_7	0	0	3	2	0	0	0	6	$n-8$	$4^n \cdot 5981.45$
ϵ_{80}	A_7	0	0	2	3	0	0	2	3	$n-7$	$4^n \cdot 6029.30$
ϵ_{81}	A_7	0	0	3	2	0	0	1	4	$n-7$	$4^n \cdot 5742.19$
ϵ_{82}	A_7	0	0	2	3	0	0	3	1	$n-6$	$4^n \cdot 5788.13$
ϵ_{83}	A_7	0	0	3	2	0	0	3	0	$n-5$	$4^n \cdot 5292.00$
ϵ_{84}	A_7	0	0	3	2	0	0	2	2	$n-6$	$4^n \cdot 5512.50$

TABLE V
EDD OF TG_n WITH $n_1 = 0, \Delta = 6, 7, 8$ AND THEIR Π_1^*

EDD	VDD	$m_{8,2}$	$m_{7,3}$	$m_{7,2}$	$m_{6,4}$	$m_{6,3}$	$m_{6,2}$	$m_{4,2}$	$m_{3,3}$	$m_{3,2}$	$m_{2,2}$	Π_1^*
ϵ_{85}	A_4	0	0	0	0	0	6	0	1	4	$n-8$	$4^n \cdot 15000.0$
ϵ_{86}	A_4	0	0	0	0	0	6	0	0	6	$n-9$	$4^n \cdot 15625.0$
ϵ_{87}	A_4	0	0	0	0	1	5	0	1	3	$n-7$	$4^n \cdot 13500.0$
ϵ_{88}	A_4	0	0	0	0	1	5	0	0	5	$n-8$	$4^n \cdot 14062.5$
ϵ_{89}	A_4	0	0	0	0	2	4	0	1	2	$n-6$	$4^n \cdot 12150.0$
ϵ_{90}	A_4	0	0	0	0	2	4	0	0	4	$n-7$	$4^n \cdot 12656.3$
ϵ_{91}	A_3	0	0	0	1	0	5	3	0	0	$n-6$	$4^n \cdot 17280.0$
ϵ_{92}	A_3	0	0	0	0	0	6	4	0	0	$n-7$	$4^n \cdot 20736.0$
ϵ_{93}	A_2	0	1	6	0	0	0	0	0	2	$n-6$	$4^n \cdot 32436.6$
ϵ_{94}	A_2	0	0	7	0	0	0	0	0	3	$n-7$	$4^n \cdot 36491.2$
ϵ_{95}	A_1	8	0	0	0	0	0	0	0	0	$n-5$	$4^n \cdot 97656.3$

REFERENCES

- [1] I. Gutman, and B. Furtula (Eds.), "Novel Molecular Structure Descriptors - Theory and Applications I," Univ. Kragujevac, Kragujevac, 2010.
- [2] I. Gutman, and B. Furtula (Eds.), "Novel Molecular Structure Descriptors - Theory and Applications II," Univ. Kragujevac, Kragujevac, 2010.
- [3] R. Todeschini, and V. Consonni, "Handbook of Molecular Descriptors," Wiley-VCH, Weinheim, 2000.
- [4] I. Gutman, and N. Trinajstić, "Graph theory and molecular orbitals. III. Total π -electron energy of alternant hydrocarbons," *Chem. Phys. Lett.*, vol. 17, no.4, pp535-538, 1972.
- [5] J. Braun, A. Kerber, M. Meringer, and C. Rucker, "Similarity of molecular descriptors: The equivalence of Zagreb indices and walk counts," *MATCH Commun. Math. Comput. Chem.*, vol. 54, no.1, pp163-176, 2005.
- [6] S. Nikolić, G. Kovačević, A. Milicević, and N. Trinajstić, "The Zagreb indices 30 years after," *Croat. Chem. Acta*, vol. 76, no.2, pp113-124, 2003.
- [7] S. Nikolić, I. M. Tolić, N. Trinajstić, and I. Baučić, "On the Zagreb indices as complexity indices," *Croat. Chem. Acta*, vol. 73, no.4, pp909-921, 2000.
- [8] R. Todeschini, and V. Consonni, "New local vertex invariants and molecular descriptors based on functions of the vertex degrees," *MATCH Commun. Math. Comput. Chem.*, vol. 64, no.2, pp359-372, 2010.
- [9] M. Eliasi, A. Iranmanesh, and I. Gutman, "Multiplicative versions of first Zagreb index," *MATCH Commun. Math. Comput. Chem.*, vol. 68, no.1, pp217-230, 2012.
- [10] J. Du, and X. Sun, "Extremal quasi-unicyclic graphs with respect to the general multiplicative Zagreb indices," *Discr. Appl. Math.*, vol. 325, pp200-211, 2023.
- [11] X. Sun, and J. Du, "Extremal (chemical) graphs with respect to the general multiplicative Zagreb indices," *IAENG International Journal of Applied Mathematics*, vol. 54, no.12, pp2792-2798, 2024.
- [12] J. Du, and X. Sun, "On the multiplicative sum Zagreb index of graphs with some given parameters," *J. Math. Inequal.*, vol. 14, no.4, pp1165-1181, 2020.
- [13] J. Du, and X. Sun, "Quasi-tree graphs with extremal general multiplicative Zagreb indices," *IEEE Access*, vol. 8, pp194676-194684, 2020.
- [14] X. Sun, Y. Gao, and J. Du, "On multiplicative sum Zagreb index of trees with fixed domination number," *J. Math. Inequal.*, vol. 17, no.1, pp83-98, 2023.
- [15] C. Xu, B. Horoldagva, and L. Buyantogtokh, "Cactus graphs with maximal multiplicative sum Zagreb index," *Symmetry*, vol. 13, no.5, p.913, 2021.
- [16] M. Azari, and A. Iranmanesh, "Some inequalities for the multiplicative sum Zagreb index of graph operations," *J. Math. Inequal.*, vol. 9, no.3, pp727-738, 2015.
- [17] V. Božović, Ž. K. Kovijanić, and G. Popivoda, "Chemical trees with extreme values of a few types of multiplicative Zagreb indices," *MATCH Commun. Math. Comput. Chem.*, vol. 76, no.1, pp207-220, 2016.
- [18] B. Horoldagva, C. Xu, L. Buyantogtokh, and S. Dorjsembe, "Extremal graphs with respect to the multiplicative sum Zagreb index," *MATCH Commun. Math. Comput. Chem.*, vol. 84, no.3, pp773-786, 2020.
- [19] X. Sun, and J. Du, "The multiplicative sum Zagreb indices of graphs with given clique number," *J. Comb. Math. Comb. Comput.*, vol. 122, pp343-350, 2024.
- [20] K. Xu, and K. C. Das, "Trees, unicyclic, and bicyclic graphs extremal with respect to multiplicative sum Zagreb index," *MATCH Commun. Math. Comput. Chem.*, vol. 68, no.1, pp257-272, 2012.
- [21] V. Božović, Ž. K. Kovijanić, and G. Popivoda, "Chemical trees with extreme values of a few types of multiplicative Zagreb indices," *MATCH Commun. Math. Comput. Chem.*, vol. 76, no.1, pp207-220, 2016.
- [22] J. A. Bondy, and U. S. R. Murty, "Graph Theory with Applications," Elsevier, New York, 1976.
- [23] X. Zuo, A. Jahanbani and H. Shooshtari, "On the atom-bond sum-connectivity index of chemical graphs," *J. Mol. Struct.*, vol. 1296, p.136849, 2024.
- [24] H. Liu, L. You, and Y. Huang, "Ordering chemical graphs by Sombor indices and its applications," *MATCH Commun. Math. Comput. Chem.*, vol. 87, no.1, pp5-22, 2022.
- [25] A. Ghalavand, and A. R. Ashrafi, "Ordering chemical graphs by Randić and sum-connectivity numbers," *Appl. Math. Comput.*, vol. 331, pp160-168, 2018.
- [26] I. Gutman, A. Ghalavand, T. Dehghan-Zadeh, and A. R. Ashrafi, "Graphs with smallest forgotten index," *Iran. J. Math. Chem.*, vol. 8, no.3, pp259-273, 2017.
- [27] A. R. Ashrafi, and A. Ghalavand, "Ordering chemical trees by Wiener polarity index," *Appl. Math. Comput.*, vol. 313, pp301-312, 2017.
- [28] A. Ghalavand, and A. R. Ashrafi, "Ordering of c -cyclic graphs with respect to total irregularity," *J. Appl. Math. Comput.*, vol. 63, no.1-2, pp707-715, 2020.
- [29] A. Ali, Z. Du, and M. Ali, "A note on chemical trees with minimum Wiener polarity index," *Appl. Math. Comput.*, vol. 335, pp231-236, 2018.
- [30] Y. Jiang, X. Chen, and W. Lin, "A note on chemical trees with maximal inverse sum indeg index," *MATCH Commun. Math. Comput. Chem.*, vol. 86, no.1, pp29-38, 2021.
- [31] A. Ghalavand, and A. R. Ashrafi, "Extremal graphs with respect to variable sum exdeg index via majorization," *Appl. Math. Comput.*, vol. 303, pp.19-23, 2017.
- [32] H. Liu, L. You, and Y. Huang, "Extremal Sombor indices of tetracyclic (chemical) graphs," *MATCH Commun. Math. Comput. Chem.*, vol. 88, no.3, pp573-581, 2022.
- [33] S. Balachandran, H. Deng, S. Elumalai, and T. Mansour, "Extremal graphs on geometri-arithmetic index of tetracyclic chemical graphs," *Int. J. Quantum Chem.*, vol. 121, p.e26516, 2021.