Filomat 33:14 (2019), 4673–4685
https://doi.org/10.2298/FIL1914673W

Published by Faculty of Sciences and Mathematics, University of Niš, Serbia
Available at: http://www.pmf.ni.ac.rs/filomat

Sharp Bounds for the Modified Multiplicative Zagreb Indices of Graphs with Vertex Connectivity at Most k

Haiying Wang*[a], Shaohui Wang[b], Bing Wei[c]

[a] *School of Science, China University of Geosciences(Beijing), Beijing 100083, China*
[b] *Department of Mathematics, Louisiana College, Pineville, LA 71359, USA*
[c] *Department of Mathematics, University of Mississippi,University 38677, USA*

Abstract. Zagreb indices and their modified versions of a molecular graph originate from many practical problems such as two dimensional quantitative structure-activity (2D QSAR) and molecular chirality. Nowadays, they have become important invariants which can be used to characterize the properties of graphs from different aspects.

Let $\mathbb{V}_n^k$ (or $\mathbb{E}_n^k$ respectively) be a set of graphs of n vertices with vertex connectivity (or edge connectivity respectively) at most k. In this paper, we explore some properties of the modified first and second multiplicative Zagreb indices of graphs in $\mathbb{V}_n^k$ and $\mathbb{E}_n^k$. By using analytic and combinatorial tools, we obtain some sharp lower and upper bounds for these indices of graphs in $\mathbb{V}_n^k$ and $\mathbb{E}_n^k$. In addition, the corresponding extremal graphs which attain the lower or upper bounds are characterized. Our results enrich outcomes on studying Zagreb indices and the methods developed in this paper may provide some new tools for investigating the values on modified multiplicative Zagreb indices of other classes of graphs.

1. Introduction

In many fields like Physics, Chemistry and Electric Network, the boiling point, the melting point, the chemical bonds and the bond energy are all important quantifiable parameters in their fields.

To understand physic-chemical properties of chemical compounds or network structures and practical problems, mathematical modelings, such as graphs, have been built.

A molecular structured graph is a simple finite connected graph which represents the carbon-atom skeleton of an organic molecule of a hydrocarbon. The vertices of a molecular graph represent the carbon atoms while their undirected edges represent the carbon bounds. Studying graphs is a constant focus in chemical graph theory and its applications in the effort to better understand molecular structures.

Secondly, many abstract concepts were defined based on degree or distance, and collectively named *topological descriptors* or *topological indices* after mathematical modelings. Different indices represent their corresponding chemical structures in graph-theoretical terms via arbitrary molecular graphs. Large number

2010 *Mathematics Subject Classification*. Primary 05C40; Secondary 05C75, 05C90
Keywords. Vertex connectivity, Edge connectivity, Extremal bounds, Modified multiplicative Zagreb indices
Received: 09 July 2018; Accepted: 27 August 2019
Communicated by Paola Bonacini
Research supported by NSFC of China (No.11701530) and Fundamental Research Funds for the Central Universities (No.2652017146)
Email addresses: whycht@126.com (Haiying Wang*), shaohuiwang@yahoo.com (Shaohui Wang), bwei@olemiss.edu (Bing Wei)

of articles about related all *topological indices* are proposed and based on edges or vertices in a molecular graph ([11-28]).

In the last decades, as a powerful approach, these two dimensional topological indices have been used to design or discover many new drugs such as Anticonvulsants, Anineoplastics, Antimalarials or Antiallergics and Silico generation ([4, 11-13, 26]). These topological indices play a key role in the process of drug discovery and other research areas ([5-8, 21]).

Among degree-based topological indices, Zagreb indices are the oldest ones and the most studied. Large numbers of articles about Zagreb indices and related indices have been published in the last decades (see for example [1, 3, 9, 10, 18, 19]). Recently, Gutman, Eliasi and Iranmanesh, respectively ([3, 9]) introduced the modified first multiplicative Zagreb index of a graph defined as follows:

$$\prod_1^*(G) = \prod_{uv\in E(G)} [d(u) + d(v)].$$

In 2016, Basavanagoud et al.([1]) studied several derived graphs and introduced another multiplicative version called the modified second multiplicative Zagreb index and defined as

$$\prod_2^*(G) = \prod_{uv\in E(G)} [d(u) + d(v)]^{[d(u)+d(v)]}.$$

With respect to Zagreb indices and modified versions, researchers are interested in finding upper and lower bounds for these indices of graphs and characterizing the graphs in which the maximal (respectively minimal) index values are attained (see [10, 15, 20, 23, 27, 28]). And mathematical and computational properties on Zagreb indices have also been considered. Furthermore, other directions include studies of relation between multiplicative Zagreb indices and the corresponding invariants of elements of the graph G (vertices, pendent vertices, diameter, maximum degree, girth, cut edge, cut vertex, perfect matching, connectivity). For example, Li and Zhou [16] found the maximum and minimum Zagreb indices of graphs with vertex connectivity at most k. Wang [25] extended the results and obtained the maximum and minimum multiplicative Zagreb indices of graphs under the same condition.

Since the modified multiplicative Zagreb indices are relatively new concepts and involve the sum of degrees of both vertices of every edge, their values are usually more difficult to determine. Thus, we need to search for new tools to deal with these kind of indices. For this purpose, in this paper we study properties of modified multiplicative Zagreb indices of graphs with vertex connectivity or edge connectivity at most k. We manage to use some basic analytic functions to find the upper and lower bounds for the modified first and second multiplicative Zagreb indices and characterize their extremal graphs:

Theorem 1.1. *Given $n, k \in \mathbb{N}$, $n \geq 3$ and $k \geq 1$, let G be a graph with n vertices and vertex connectivity at most k and K_n^k be a graph obtained by adding a vertex to a clique K_{n-1} and joining the vertex to exactly $k \leq n-1$ vertices of K_{n-1}. Then*

$$\prod_1^*(G) \leq \prod_1^*(K_n^k)$$

and

$$\prod_2^*(G) \leq \prod_2^*(K_n^k)$$

where the equalities hold if and only if $G \cong K_n^k$, where

$$\prod_1^*(K_n^k) = 2^{\frac{k(k-1)+(n-k-1)(n-k-2)}{2}} \cdot (n-1)^{\frac{k(k-1)}{2}} \cdot (n-2)^{\frac{(n-k-1)(n-k-2)}{2}} \cdot (2n-3)^{k(n-k-1)} \cdot (n+k-1)^k,$$

$$\prod_2^*(K_n^k) = 2^{(n-1)k(k-1)+(n-2)(n-k-1)(n-k-2)} \cdot (n-1)^{(n-1)k(k-1)} \cdot (n-2)^{(n-2)(n-k-1)(n-k-2)} \cdot (2n-3)^{(2n-3)k(n-k-1)} \cdot (n+k-1)^{(n+k-1)k}.$$

On the lower bounds for the modified first and second multiplicative Zagreb indices, we obtain the following:

Theorem 1.2. *Let G be a graph with n vertices and vertex connectivity at most k, where $n \geq 3$ and $k \geq 1$. Then $\prod_1^*(G) \geq 9 \cdot 4^{n-3}$ and $\prod_2^*(G) \geq 729 \cdot 256^{n-3}$, and the equalities hold if and only if $G \cong P_n$, where P_n is a path on n vertices.*

The methods we develop in this paper are expected to be used to study the properties of other indices of graphs. We first give some notations and graph operation properties of the modified first and second multiplicative Zagreb indices in Section 2 and then we prove our main results in Section 3.

2. Preliminaries and properties

Let $G = (V(G), E(G))$ be a simple connected graph with vertex set $V = V(G)$ and edge set $E = E(G)$. If a vertex $v \in V(G)$, then the neighborhood of v denotes the set $N(v) = N_G(v) = \{w \in V(G), vw \in E(G)\}$, and the degree of v is $d_G(v) = |N(v)|$, also denoted by $d(v)$. Let n_i denote the number of vertices of degree $i \geq 0$.

Given $V_1, V_2 \subseteq V(G)$, denote $E[V_1, V_2] = \{uv \in E(G) : u \in V_1, v \in V_2\}$. Given $S \subseteq V(G)$ and $F \subseteq E(G)$, we denote by $G[S]$ the subgraph of G induced by S, $G[F]$ the subgraph induced by F, $G - S$ the subgraph induced by $V(G) - S$ and $G - F$ for the subgraph of G obtained by deleting F. If $G - S$ contains at least 2 components, then S is said to be a vertex cut set of G. Similarly, if $G - F$ contains at least 2 components, then E is called an edge cut set. In our exposition we will use the terminology and notations of (chemical) graph theory (see [2, 22]).

A graph G is said to be k-connected with $k \geq 1$, if either G is complete graph K_{k+1}, or it has at least $k + 2$ vertices and contains no $(k - 1)$-vertex cut. The vertex connectivity of G, denoted by $\kappa(G)$, is defined as the maximal value of k for which a connected graph G is k-connected. Similarly, for $k \geq 1$, a graph G is called k-edge-connected if it has at least two vertices and does not contain a $(k - 1)$-edge cut. The maximal value of k for which a connected graph G is k-edge-connected is said to be the edge connectivity of G, denoted by $\kappa'(G)$. By the definitions, the following proposition is obtained.

Proposition 2.1. *Let G be a graph with n vertices. Then*
(i) $\kappa(G) \leq \kappa'(G) \leq n - 1$,
(ii) $\kappa(G) = n - 1, \kappa'(G) = n - 1$ *and* $G \cong K_n$ *are equivalent.*

Let $\mathbb{V}_n^k$ be a set of connected graphs with n vertices and vertex connectivity at most k, $\kappa(G) \leq k \leq n - 1$. Denote by $\mathbb{E}_n^k$ a set of connected graphs with n vertices and edge connectivity at most k, $\kappa'(G) \leq k \leq n - 1$. Let P_n and S_n be, respectively, a path and a star of n vertices. Let K_n denote a complete graph. The graph K_n^k is obtained by joining k vertices of K_{n-1} to an isolated vertex (see Figure 1). Then $K_n^k \in \mathbb{E}_n^k \subset \mathbb{V}_n^k$.

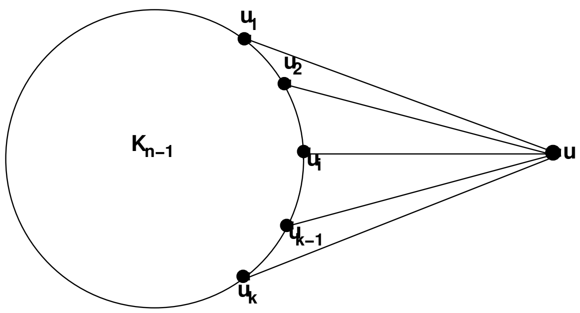

Figure 1.

According to the definitions of $\prod_1^*(G)$ and $\prod_2^*(G)$, the following proposition is routinely obtained.

Proposition 2.2. *Let e be an edge of a graph $G \in \mathbb{V}_n^k$ ($\mathbb{E}_n^k$ respectively). Then*
(i) $G - e \in \mathbb{V}_n^k$ *($\mathbb{E}_n^k$ respectively),*
(ii) $\prod_i^*(G - e) < \prod_i^*(G)$, $i = 1, 2$.

In addition, by elementary calculations, we have

Proposition 2.3. *If $m > 0$ and $b < a$, then $\frac{b}{a} < \frac{b+m}{a+m}$.*

Proposition 2.4. *If M is an integer with $M \geq 2$, then $(M+5)^M < (M+3)^{M+2}$.*

Proof. It is easy to verify that this proposition holds for $M = 2, 3$. Below we may assume that $M \geq 4$. By the fact $\frac{2^i}{i!} < 1$ for any $i = 4, \cdots, M$, we have

$$\begin{aligned} C_M^i (M+3)^{M-i} \cdot 2^i &= \tfrac{M(M-1)\cdots(M-i+1)}{i!} \cdot (M+3)^{M-i} \cdot 2^i \\ &< (M+3)^i \cdot (M+3)^{M-i} \\ &= (M+3)^M. \end{aligned}$$

By Binomial Theorem, we obtain

$$\begin{aligned} &(M+5)^M \\ &= [(M+3)+2]^M \\ &= (M+3)^M + 2M \cdot (M+3)^{M-1} + 2M(M-1) \cdot (M+3)^{M-2} + \tfrac{4}{3}M(M-1)(M-2) \cdot (M+3)^{M-3} + \sum_{i=4}^{M} C_M^i (M+3)^{M-i} \cdot 2^i \\ &< (M+3)^M + 2(M+3)^M + 2(M+3)^M + \tfrac{4}{3}(M+3)^M + (M-3) \cdot (M+3)^M \\ &= (M+3)^M [1 + 2 + 2 + \tfrac{4}{3} + (M-3)] \\ &< (M+3)^{M+2}. \end{aligned}$$

Thus,

$$(M+5)^M < (M+3)^{M+2}. \quad \square$$

We first provide some lemmas, which will play very important roles in the proofs of our main results. According to the definitions of $\prod_1^*(G)$ and $\prod_2^*(G)$, we have the following lemmas.

Lemma 2.5. *Let $u, v \in V(G)$ and $uv \notin E(G)$. Then*

$$\textstyle\prod_1^*(G) < \prod_1^*(G+uv), \quad \prod_2^*(G) < \prod_2^*(G+uv).$$

Given two graphs G_1 and G_2, if $V(G_1) \cap V(G_2) = \emptyset$, then the join graph $G_1 \oplus G_2$ is a graph with vertex set $V(G_1) \cup V(G_2)$ and edge set $E(G_1) \cup E(G_2) \cup \{uv, u \in V(G_1), v \in V(G_2)\}$.

Let $G(j, H_k, n-k-j) = K_j \oplus H_k \oplus K_{n-k-j}$ be a graph with $n \geq 3$ vertices, in which K_j and K_{n-k-j} are cliques, and H_k is a graph with k vertices (see Figure 2). Specially, $G(j, K_k, n-k-j)$ plays a key bridge role in this paper.

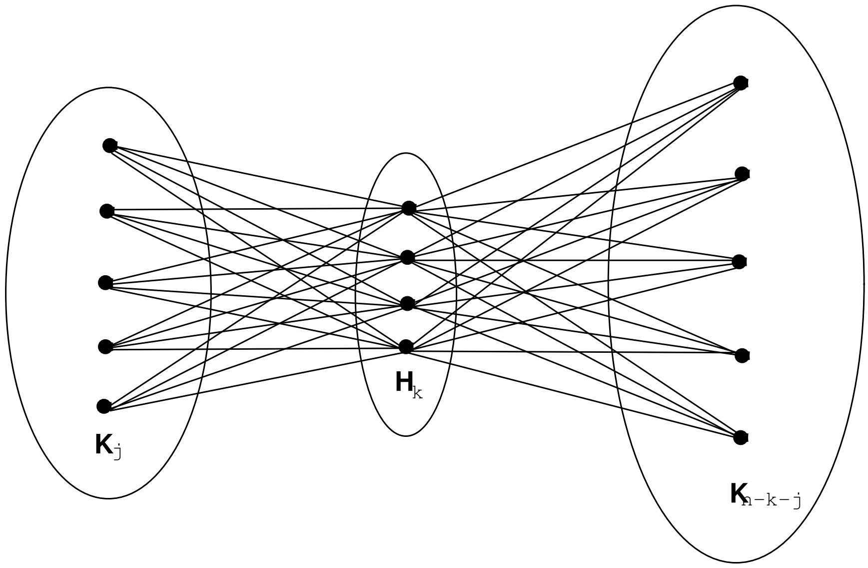

Figure 2. $G(j, H_k, n-k-j)$

Lemma 2.6. *For any $G(j, H_k, n-k-j) = K_j \oplus H_k \oplus K_{n-k-j}$ with $n \geq 3$, $k \geq 1$ and $1 \leq j \leq \frac{n-k}{2}$, we have*

$$d_{G(j,H_k,n-k-j)}(v) = \begin{cases} k+j-1, & \text{if } v \in V(K_j), \\ d_{H_k}(v)+n-k, & \text{if } v \in V(H_k), \\ n-j-1, & \text{if } v \in V(K_{n-k-j}). \end{cases}$$

The next lemma is a key lemma in the proofs for upper bounds of our main results.

Lemma 2.7. *Let $G(j, K_k, n-k-j) = K_j \oplus K_k \oplus K_{n-k-j}$ be a graph with n vertices, in which K_j, K_k and K_{n-k-j} are cliques. If $n \geq 3$, $k \geq 1$ and $2 \leq j \leq \frac{n-k}{2}$, then*

$$\prod\nolimits_1^*(G(j, K_k, n-k-j)) < \prod\nolimits_1^*(G(1, K_k, n-k-1))$$

and

$$\prod\nolimits_2^*(G(j, K_k, n-k-j)) < \prod\nolimits_2^*(G(1, K_k, n-k-1)).$$

Proof. Let the graph $G = G(j, K_k, n-k-j)$ for any $n \geq 3$, $k \geq 1$ and $1 \leq j \leq \frac{n-k}{2}$. By Lemma 2.6, we know that

$$d_G(v) = \begin{cases} k+j-1, & \text{if } v \in V(K_j), \\ n-1, & \text{if } v \in V(K_k), \\ n-j-1, & \text{if } v \in V(K_{n-k-j}). \end{cases}$$

Let $E_1 = E[V(K_j)] \cap E(G)$, $E_2 = E[V(K_k)] \cap E(G)$, $E_3 = E[V(K_{n-k-j})] \cap E(G)$, $B_1 = E[V(K_j), V(K_k)] \cap E(G)$, $B_2 = E[V(K_k), V(K_{n-k-j})] \cap E(G)$. Then

$$|E_1| = \frac{j(j-1)}{2},$$

$$|E_2| = \frac{k(k-1)}{2},$$

$$|E_3| = \frac{(n-k-j)(n-k-j-1)}{2},$$

$$|B_1| = jk,$$

$$|B_2| = k(n-k-j).$$

Let $f(x,y)$ be the unified function of $\prod_1^*$ and $\prod_2^*$. By the concepts of $\prod_1^*$, $\prod_2^*$ and the structure of the class of the graph $G = G(j, K_k, n-k-j)$, we have

$$\prod_i^*(G) = \prod_{\forall uv \in E(G)} f(d(u), d(v))$$

$$= \prod_{\forall uv \in E_1} f(d(u), d(v)) \cdot \prod_{\forall uv \in E_2} f(d(u), d(v)) \cdot \prod_{\forall uv \in E_3} f(d(u), d(v)) \cdot \prod_{\forall uv \in B_1} f(d(u), d(v)) \cdot \prod_{\forall uv \in B_2} f(d(u), d(v))$$

$$= [f(k+j-1, k+j-1)]^{|E_1|} \cdot [f(n-1, n-1)]^{|E_2|} \cdot [f(n-j-1, n-j-1)]^{|E_3|} \cdot [f(k+j-1, n-1)]^{|B_1|} \cdot [f(n-1, n-j-1)]^{|B_2|},$$

where $i = 1, 2$.

With respect to $\prod_1^*(G)$, its corresponding function is $f(x,y) = x + y$. After calculations, we have

$$\prod_1^*(G) = \prod_{\forall uv \in E(G)} [d_G(u) + d_G(v)]$$

$$= [2(k+j-1)]^{\frac{j(j-1)}{2}} \cdot [2(n-1)]^{\frac{k(k-1)}{2}} \cdot [2(n-j-1)]^{\frac{(n-k-j)(n-k-j-1)}{2}} \cdot [n+k+j-2]^{jk} \cdot [2n-j-2]^{k(n-k-j)}. \tag{*1}$$

Claim 1. Let $G = G(j, K_k, n-k-j)$ with given $n \geq 3$ and $k \geq 1$. Then $\prod_1^*(G)$ is a strictly decreasing discrete function with respect to the variable j, where $1 \leq j < \frac{n-k}{2}$.

Furthermore, if $\frac{n-k}{2} \geq 2$ is an integer, then

$$\prod_1^*(G(\tfrac{n-k}{2}, K_k, \tfrac{n-k}{2})) < \prod_1^*(G(1, K_k, n-k-1)).$$

Proof of Claim 1.

Since $\prod_1^*(G) > 0$ for $1 \leq j \leq \frac{n-k}{2}$, $\ln[\prod_1^*(G)]$ has the same monotonicity as $\prod_1^*(G)$.

Define the corresponding real function

$$\prod_1^*(x) = [2(k+x-1)]^{\frac{x(x-1)}{2}} \cdot [2(n-1)]^{\frac{k(k-1)}{2}} \cdot [2(n-x-1)]^{\frac{(n-k-x)(n-k-x-1)}{2}} \cdot [n+k+ x-2]^{xk} \cdot [2n-x-2]^{k(n-k-x)} \qquad (\star 1)$$

with respect to one variable x in the interval $[1, \frac{n-k}{2})$.

By Derivative Theory of a function with one variable, we first need to prove that

$$\frac{d[\ln(\prod_1^*(x))]}{dx} < 0.$$

By $(\star 1)$, we have

$$\frac{d[\ln(\prod_1^*(x))]}{dx} = (2x+k-n) \cdot \ln 2 + \frac{1}{2}[(2x-1)\ln(k+x-1) - (2n-2k-2x-1)\ln(n-x-1)] +$$
$$[\frac{x(x-1)}{(k+x-1)} - \frac{(n-k-x)(n-k-x-1)}{(n-x-1)}] + k\Big\{[\ln(n+k+x-2) - \ln(2n-x-2)] + [\frac{x}{n+k+x-2} - \frac{n-k-x}{2n-x-2}]\Big\}.$$

Below, we need to prove that, given numbers $k \geq 1$ and $n \geq 3$, all of the following are negative for any $1 \leq x < \frac{n-k}{2}$:

$$\Delta_1 = (2x+k-n)\ln 2,$$

$$\Delta_2 = (2x-1)\ln(k+x-1) - (2n-2k-2x-1)\ln(n-x-1),$$

$\Delta_3 = \frac{x(x-1)}{(k+x-1)} - \frac{(n-k-x)(n-k-x-1)}{(n-x-1)}$,

$\Delta_4 = \ln(n+k+x-2) - \ln(2n-x-2)$,

$\Delta_5 = \frac{x}{n+k+x-2} - \frac{n-k-x}{2n-x-2}$.

(1) Since $1 \le x < \frac{n-k}{2}$, $2x+k-n < 0$. Then $\Delta_1 < 0$.

(2) Since $1 \le x < \frac{n-k}{2}$, $n-k > 2x$ and $n-x-1 > x+k-1$. Then

$$(n-x-1)^{2n-2k-2x-1} = (n-x-1)^{2(n-k)-2x-1} > (n-x-1)^{2\cdot 2x-2x-1} = (n-x-1)^{2x-1} > (x+k-1)^{2x-1}$$

which implies that $\frac{(x+k-1)^{2x-1}}{(n-x-1)^{2n-2k-2x-1}} < 1$, that is $\Delta_2 < 0$.

(3) Since $1 \le x < \frac{n-k}{2}$, $x < n-k-x$. Let us consider

$$f(x) = \frac{x(x-1)}{k+x-1}.$$

Then the function $f(x)$ is increasing for $1 \le x < \frac{n-k}{2}$ and $k \ge 1$. Thus,

$\Delta_3 = \frac{x(x-1)}{(k+x-1)} - \frac{(n-k-x)(n-k-x-1)}{(n-x-1)} = \frac{x(x-1)}{(k+x-1)} - \frac{(n-k-x)[(n-k-x)-1]}{k+(n-k-x)-1} = f(x) - f(n-k-x) < 0.$

(4) Since $1 \le x < \frac{n-k}{2}$, $n+k+x-2 < 2n-x-2$. Then $\frac{n+k+x-2}{2n-x-2} < 1$, which implies

$$\ln\frac{n+k+x-2}{2n-x-2} < 0,$$

that is,

$$\Delta_4 < 0.$$

(5) Since $1 \le x < \frac{n-k}{2}$, $n-k-2x > 0$. By Proposition 2.3,

$$\Delta_5 = \frac{x}{n+k+x-2} - \frac{n-k-x}{2n-x-2} = \frac{x}{n+k+x-2} - \frac{x+(n-k-2x)}{n+k+x-2+(n-k-2x)},$$

implying

$$\Delta_5 < 0.$$

Up to now, we have proved that for any $1 \le x < \frac{n-k}{2}$,

$$\frac{d[\ln(\prod_1^*(x))]}{dx} < 0.$$

Now we only need to clarify that for an integer $\frac{n-k}{2} \ge 2$,

$$\prod_1^*(G(\tfrac{n-k}{2}, K_k, \tfrac{n-k}{2})) < \prod_1^*(G(1, K_k, n-k-1)).$$

In fact, since $\frac{n-k}{2}$ is a positive integer, n, k have the same parity. Since $1 \le k \le n-4$, then $n+k-2 \le 2n-6$, $\frac{3n+k-4}{2} \le 2n-4$, $n+k-1 \le 2n-5$, and $2 \le n-k-2 \le n-3$. Since $n \ge 5$, $2n-4 \ge 6$.

By (*1), we have

$$\prod_1^*(G(1, K_k, n-k-1)) = [2(n-1)]^{\frac{k(k-1)}{2}} \cdot [2(n-2)]^{\frac{(n-k-1)(n-k-2)}{2}} \cdot [n+k-1]^k \cdot [2n-3]^{k(n-k-1)}$$

and

$$\prod_1^*(G(\tfrac{n-k}{2}, K_k, \tfrac{n-k}{2})) = [2(n-1)]^{\frac{k(k-1)}{2}} \cdot [n+k-2]^{\frac{(n-k)(n-k-2)}{4}} \cdot [\tfrac{3n+k-4}{2}]^{k(n-k)}.$$

Immediately, we have

$$\begin{aligned}
&\frac{\prod_1^*(G(1,K_k,n-k-1))}{\prod_1^*(G(\frac{n-k}{2},K_k,\frac{n-k}{2}))}\\
&=\frac{(2n-4)^{\frac{(n-k)(n-k-2)}{4}}}{(n+k-2)^{\frac{(n-k)(n-k-2)}{4}}}\cdot\frac{(2n-3)^{k(n-k)}}{(\frac{3n+k-4}{2})^{k(n-k)}}\cdot\frac{(n+k-1)^k}{(2n-3)^k}\cdot(2n-4)^{\frac{(n-k-2)^2}{4}}\\
&>\frac{(n+k-1)^k}{(2n-3)^k}\cdot(2n-4)^{\frac{(n-k-2)^2}{4}}
\end{aligned}$$

Now, we want to prove $\frac{(n+k-1)^k}{(2n-3)^k}\cdot(2n-4)^{\frac{(n-k-2)^2}{4}}>1$. Let

$$h(x)=\frac{(n+x-1)^x}{(2n-3)^x}\cdot(2n-4)^{\frac{(n-x-2)^2}{4}}$$

with $x\in[1,n-4]$ and $n\geq 5$. After a simple calculation, we have

$$\frac{d(\ln[h(x)])}{dx}=[\ln(n+x-1)-\ln(2n-3)]+[\frac{x}{x+(n-1)}-(n-x-2)\ln\sqrt{2n-4}].$$

Since $n\geq 5$ and $1\leq x\leq n-4$, we have

$$\ln(n+x-1)<\ln(2n-3),$$

$$\frac{x}{x+n-1}<1<2\cdot\ln\sqrt{6}<(n-x-2)\cdot\ln\sqrt{2n-4}.$$

Therefore, $\frac{d(\ln[h(x)])}{dx}<0$, implying that $h(x)$ is strictly decreasing in $1\leq x\leq n-4$. Then by Proposition 2.4, we have

$$\frac{\prod_1^*(G(1,K_k,n-k-1))}{\prod_1^*(G(\frac{n-k}{2},K_k,\frac{n-k}{2}))}>1.$$

Hence, Claim 1 holds. □

Similarly, with respect to $\prod_2^*(G)$, its corresponding function is $f(x,y)=(x+y)^{x+y}$. After calculation, we obtain that

$$\begin{aligned}
\prod_2^*(G)&=\prod_{\forall uv\in E(G)}[d_G(u)+d_G(v)]^{[d_G(u)+d_G(v)]}\\
&=[2(k+j-1)]^{2(k+j-1)\cdot\frac{j(j-1)}{2}}\cdot[2(n-1)]^{2(n-1)\cdot\frac{k(k-1)}{2}}\cdot[2(n-j-1)]^{2(n-j-1)\cdot\frac{(n-k-j)(n-k-j-1)}{2}}\cdot[n+\\
&\quad k+j-2]^{(n+k+j-2)\cdot jk}\cdot[2n-j-2]^{(2n-j-2)\cdot k(n-k-j)}
\end{aligned}\tag{*2}$$

Claim 2. For the class of the graphs $G=G(j,K_k,n-k-j)$ with given $n\geq 3$ and $k\geq 1$, we have $\prod_2^*(G)$ is a strictly decreasing discrete function with respect to the variable j, where $1\leq j<\frac{n-k}{2}$. Furthermore, if $\frac{n-k}{2}\geq 2$ is an integer, then $\prod_2^*(G(\frac{n-k}{2},K_k,\frac{n-k}{2}))<\prod_2^*(G(1,K_k,n-k-1))$.

Proof of Claim 2.
Since $\prod_2^*(G)>0$ for $1\leq j\leq\frac{n-k}{2}$, $\ln[\prod_2^*(G)]$ has the same monotonicity as $\prod_2^*(G)$.

Define the corresponding real function

$\prod_2^*(x)=[2(k+x-1)]^{2(k+x-1)\cdot\frac{x(x-1)}{2}}\cdot[2(n-1)]^{2(n-1)\cdot\frac{k(k-1)}{2}}\cdot[2(n-x-1)]^{2(n-x-1)\cdot\frac{(n-k-x)(n-k-x-1)}{2}}\cdot[n+$

$$k+x-2]^{(n+k+x-2)\cdot xk}\cdot[2n-x-2]^{(2n-x-2)\cdot k(n-k-x)} \qquad (\star 2)$$

with respect to one variable x in the interval $[1, \frac{n-k}{2})$. By Derivative Theory of a function with one variable, we only need to prove that

$$\frac{d[\ln(\prod_2^*(x))]}{dx}<0.$$

By ($\star$2) we have

$$\begin{aligned}
&\frac{d[\ln(\prod_2^*(x))]}{dx}\\
&=\ln 2\cdot\Big\{[x(x-1)-(n-k-x)(n-k-x-1)]+[(2x-1)(k+x-1)-(n-x-1)(2n-2k-2x-1)]\Big\}+\\
&\quad[(2x-1)(k+x-1)\ln(k+x-1)-(2n-2k-2x-1)(n-x-1)\ln(n-x-1)]+\\
&\quad\Big\{x(x-1)[1+\ln(k+x-1)]-(n-k-x)(n-k-x-1)[1+\ln(n-x-1)]\Big\}+\\
&\quad k\Big\{[(n+k+x-2)\ln(n+k+x-2)-(2n-x-2)\ln(2n-x-2)]+\\
&\qquad[x(1+\ln(n+k+x-2))-(n-k-x)(1+\ln(2n-x-2))]\Big\}.
\end{aligned}$$

Below, we need to prove all of the following are non-positive for any $1\le x<\frac{n-k}{2}$ and given numbers $k\ge 1$ and $n\ge 2$ as follows.

$\Delta_{11}=x(x-1)-(n-k-x)(n-k-x-1)$,
$\Delta_{12}=(2x-1)(k+x-1)-(n-x-1)(2n-2k-2x-1)$,
$\Delta_2=(2x-1)(k+x-1)\ln(k+x-1)-(2n-2k-2x-1)(n-x-1)\ln(n-x-1)$,
$\Delta_3=x(x-1)[1+\ln(k+x-1)]-(n-k-x)(n-k-x-1)[1+\ln(n-x-1)]$,
$\Delta_4=(n+k+x-2)\ln(n+k+x-2)-(2n-x-2)\ln(2n-x-2)$,
$\Delta_5=x[1+\ln(n+k+x-2)]-(n-k-x)[1+\ln(2n-x-2)]$.

(1) Let us consider $f(x)=x(x-1)-(n-k-x)(n-k-x-1)$ and $g(x)=(2x-1)(k+x-1)$ with respect to x. They are both increasing functions for $1\le x\le\frac{n-k}{2}$ and $k\ge 1$. Since $1\le x<\frac{n-k}{2}$, $n-k-x>x$. Then

$\Delta_{11}=x(x-1)-(n-k-x)(n-k-x-1)=f(x)-f(n-k-x)<0$,
$\Delta_{12}=(2x-1)(k+x-1)-[2(n-k-x)-1][k+(n-k-x)-1]=g(x)-g(n-k-x)<0$.

(2) Since $1\le x<\frac{n-k}{2}$, $x<n-k-x$. Consider a function

$$f(x)=(2x-1)(k+x-1)\ln(k+x-1).$$

It is obvious that $f(x)$ is strictly increasing for $1\le x<\frac{n-k}{2}$ and $k\ge 1$. Thus,

$$\begin{aligned}\Delta_2&=(2x-1)(k+x-1)\ln(k+x-1)-[2(n-k-x)-1]\cdot[k+(n-k-x)-1]\cdot\ln[k+(n-k-x)-1]\\&=f(x)-f(n-k-x)<0.\end{aligned}$$

(3) Let $f(x)=x(x-1)[1+\ln(k+x-1)]$. It is obvious that $f(x)$ is strictly increasing for $1\le x<\frac{n-k}{2}$ and $k\ge 1$. Since $1\le x<\frac{n-k}{2}$, $x<n-k-x$. Thus,

$\Delta_3=x(x-1)[1+\ln(k+x-1)]-(n-k-x)(n-k-x-1)[1+\ln(n-x-1)]=f(x)-f(n-k-x)<0$.

(4) Since $1\le x<\frac{n-k}{2}$, $k+x<n-x$. Let

$$f(x)=(n+k+x-2)\ln(n+k+x-2).$$

It is obvious that $f(x)$ is increasing for $1\le x<\frac{n-k}{2}$. Then
$\Delta_4=(n+k+x-2)\ln(n+k+x-2)-(2n-x-2)\ln(2n-x-2)=f(k+x)-f(n-x)<0$.

(5) Since $1\le x<\frac{n-k}{2}$, we have $2x<n-k$ and $k+x<n-x$. Then

$$\begin{aligned}\Delta_5 &= x[1+\ln(n+k+x-2)] - (n-k-x)[1+\ln(2n-x-2)]\\ &< x[1+\ln(n+k+x-2)] - (2x-x)[1+\ln(x+k+n-2)] = 0.\end{aligned}$$

Up to now, we have proved that for any $1 \le x < \frac{n-k}{2}$,

$$\frac{d[\ln(\prod_2^*(x))]}{dx} < 0.$$

Now we only need to clarify that for an integer $\frac{n-k}{2} \ge 2$,

$$\textstyle\prod_2^*(G(\frac{n-k}{2}, K_k, \frac{n-k}{2})) < \prod_2^*(G(1, K_k, n-k-1)).$$

In fact, since n, k have the same parity, $\frac{n-k}{2}$ is a positive integer. Since $1 \le k \le n-4$, $4 \le n-k \le n-1$, $3 \le n-k-1 \le n-2$, $2 \le n-k-2 \le n-3$, $n \le n+k-1 \le 2n-5$, $n-1 \le n+k-2 \le 2n-6$, $\frac{3n-3}{2} \le \frac{3n+k-4}{2} \le 2n-4$.

For the convenience of writing, let $F(x) = x^x$. It is a strictly increasing function on $x \in [5, +\infty)$ and $F'(x) = (1+x)F(x)$. By (*2), we have

$$\begin{aligned}&\textstyle\prod_2^*(G(1, K_k, n-k-1))\\ &= [F(2(n-1))]^{\frac{k(k-1)}{2}} \cdot [F(2(n-2))]^{\frac{(n-k-1)(n-k-2)}{2}} \cdot [F(n+k-1)]^k \cdot [F(2n-3)]^{k(n-k-1)}.\end{aligned}$$

and

$$\begin{aligned}&\textstyle\prod_2^*(G(\frac{n-k}{2}, K_k, \frac{n-k}{2}))\\ &= [F(2(n-1))]^{\frac{k(k-1)}{2}} \cdot [F(n+k-2)]^{\frac{(n-k)(n-k-2)}{4}} \cdot [F(\tfrac{3n+k-4}{2})]^{k(n-k)}.\end{aligned}$$

Immediately, we have

$$\begin{aligned}&\frac{\prod_2^*(G(1, K_k, n-k-1))}{\prod_2^*(G(\frac{n-k}{2}, K_k, \frac{n-k}{2}))}\\ &= \frac{[F(2(n-2))]^{\frac{(n-k-1)(n-k-2)}{2}}}{[F(\frac{3n+k-4}{2})]^{k(n-k)}} \cdot \frac{[F(n+k-1)]^k}{[F(n+k-2)]^{\frac{(n-k)(n-k-2)}{4}}} \cdot [F(2n-3)]^{k(n-k-1)}\\ &> [F(2n-4)]^{\frac{(n-k-1)(n-k-2)}{2} - k(n-k)} \cdot [F(n+k-2)]^{k - \frac{(n-k)(n-k-2)}{4}} \cdot [F(2n-3)]^{k(n-k-1)}\\ &= [F(2n-4)]^{\frac{1}{2}[n^2-4nk+3k^2-3(n-k)+2]} \cdot [F(n+k-2)]^{\frac{1}{4}[2k-n^2-k^2+2nk+2n]} \cdot [F(2n-3)]^{k(n-k-1)}.\end{aligned}$$

Now, we want to prove that

$$[F(2n-4)]^{\frac{1}{2}[n^2-4nk+3k^2-3(n-k)+2]} \cdot [F(n+k-2)]^{\frac{1}{4}[2k-n^2-k^2+2nk+2n]} \cdot [F(2n-3)]^{k(n-k-1)} > 1.$$

Let

$$g(x) = [F(2n-4)]^{\frac{1}{2}[n^2-4nx+3x^2-3(n-x)+2]} \cdot [F(n+x-2)]^{\frac{1}{4}[2x-n^2-x^2+2nx+2n]} \cdot [F(2n-3)]^{x(n-x-1)}$$

with $x \in [1, n-4]$ and $n \ge 5$. After a simple calculation, we have

$$\begin{aligned}&\frac{d[\ln g(x)]}{dx}\\ &= \frac{-4n+6x+3}{2} \cdot \ln F(2n-4) + \frac{n-x+1}{2} \cdot \ln F(n+x-2) + \frac{1}{4}[2(x+n) - (n-x)^2] \cdot [1+\ln(n+x-2)] +\\ &\qquad (n-2x-1) \cdot \ln F(2n-3)\\ &< \frac{(-4n+6x+3)+(n-x+1)+(n-2x-1)}{2} \cdot \ln F(2n-3) + \frac{2(x+n)-(n-x)^2}{4}[1+\ln(n+x-2)]\\ &= \frac{-(n-x-2)}{2} \cdot \ln F(2n-3) + \frac{(x+n)}{2}[1+\ln(n+x-2)] - \frac{(n-x)^2}{4}[1+\ln(n+x-2)]\\ &< -\frac{(n-x-2)(2n-3)}{2}\ln(2n-3) + \frac{x+n-2}{2}\ln(n+x-2) + \frac{2(x+n)-(n-x)^2}{4}\end{aligned}$$

$= -\frac{n-x-2}{2}\ln F(2n-3) + \frac{1}{2}\ln F(n+x-2) + \frac{2(x+n)-(n-x)^2}{4}$
$< -\frac{n-x-2}{2}\ln F(2n-3) + \frac{1}{2}\ln F(2n-3) + (n-6)$
$= \frac{-n+x+3}{2}\ln F(2n-3) + (n-6) < 0$

as $\frac{2(x+n)-(n-x)^2}{4}$ is strictly increasing in $[1, n-4]$, and $-n+x+3 < -1$ and $\ln F(2n-3) > n-6$ when $n \geq 5$.

Therefore, $\frac{d[\ln g(x)]}{dx} < 0$, implying that $g(x)$ is strictly decreasing in $1 \leq x \leq n-4$. Then

$$[F(2n-4)]^{\frac{1}{2}[n^2-4nk+3k^2-3(n-k)+2]} \cdot [F(n+k-2)]^{\frac{1}{4}[2k-n^2-k^2+2nk+2n]} \cdot [F(2n-3)]^{k(n-k-1)}$$

$$> g(n-4) = [F(2n-4)]^{\frac{(3n-5)^2+13}{2}} \cdot [F(3n-6)]^{n-2} \cdot [F(2n-3)]^{n-2} > 1.$$

Hence, Claim 2 holds. □

By Claims 1 and 2, we can recursively use this process from j to $j-1$, and obtain that

$$\prod_i^*(G(j, K_k, n-k-j)) < \prod_i^*(G(j-1, K_k, n-k-j+1)) < \prod_i^*(G(j-2, K_k, n-k-j+2)) < \cdots < \prod_i^*(G(1, K_k, n-k-1)).$$

Therefore, $\prod_i^*(G(j, K_k, n-k-j)) < \prod_i^*(G(1, K_k, n-k-1))$ for any $2 \leq j \leq \frac{n-k}{2}$ and $i = 1, 2$.
Thus, we complete the proof. □

Now, we give a lemma related to the minimum values of the modified Zagreb indices of graphs.

Lemma 2.8. *Let G be a connected graph with $u \in V(G)$ such that $d_G(u) = 1$ and $uv \in E(G)$. If $d_G(v) \geq 3$, then we can find a connected graph G' such that $\prod_i^*(G') < \prod_i^*(G)$ with $i = 1, 2$.*

Proof. Choose a vertex w in $N(v) - \{u\}$ and construct a connected graph G' by deleting vw and adding uw. Then it is easy to check that $\prod_i^*(G') < \prod_i^*(G)$ with $i = 1, 2$ holds. □

3. Proofs of the main results

We now turn to prove our main results in this section.

Proof of Theorem 1.1

Note that the degree sequence of K_n^k is $k, \underbrace{n-2, n-2, \cdots, n-2}_{n-k-1}, \underbrace{n-1, n-1, \cdots, n-1}_{k}$. By the definitions of $\prod_1^*(G)$, $\prod_2^*(G)$ and routine calculations, we have

$$\prod_1^*(K_n^k) = 2^{\frac{k(k-1)+(n-k-1)(n-k-2)}{2}} \cdot (n-1)^{\frac{k(k-1)}{2}} \cdot (n-2)^{\frac{(n-k-1)(n-k-2)}{2}} \cdot (2n-3)^{k(n-k-1)} \cdot (n+k-1)^k,$$

$$\prod_2^*(K_n^k) = 2^{(n-1)k(k-1)+(n-2)(n-k-1)(n-k-2)} \cdot (n-1)^{(n-1)k(k-1)} \cdot (n-2)^{(n-2)(n-k-1)(n-k-2)} \cdot (2n-3)^{(2n-3)k(n-k-1)} \cdot (n+k-1)^{(n+k-1)k}.$$

It suffices to prove that $\prod_1^*(G) \leq \prod_1^*(K_n^k)$ and $\prod_2^*(G) \leq \prod_2^*(K_n^k)$, and the equalities hold if and only if $G \cong K_n^k$.

If $k = n-1$, then $G \cong K_n^{n-1} \cong K_n$, and the theorem is true. Below, we assume $1 \leq k \leq n-2$ and then choose a graph $\overline{G}_1$ ($\overline{G}_2$ respectively) in $\mathbb{V}_n^k$ such that $\prod_1^*(\overline{G}_1)$ ($\prod_2^*(\overline{G}_2)$ respectively) is maximal.

Since $\overline{G}_i \ncong K_n$ for $i = 1, 2$, then $\overline{G}_i$ has a vertex cut set of size k. Let $V_i = \{v_{i1}, v_{i2}, \cdots, v_{ik}\}$ be the cut vertex set of $\overline{G}_i$. Let $\omega(\overline{G}_i - V_i)$ denote the number of components of $\overline{G}_i - V_i$. By Lemma 2.5 and the choice of $\overline{G}_i$, it is very easy to check that $\omega(\overline{G}_i - V_i) = 2$ and the induced subgraphs of $V(G_{i1}) \cup V_i$ and $V(G_{i2}) \cup V_i$ in $\overline{G}_i$ are complete subgraphs for $i = 1,2$. Thus, we obtain that G_{i1}, $\overline{G}_i[V_i]$ and G_{i2} are complete subgraphs of $\overline{G}_i$. Let $G_{i1} = K_{n'}$ and $G_{i2} = K_{n''}$. Then we have $\overline{G}_i = K_{n'} \oplus K_k \oplus K_{n''}$ which is a type of $G(j, K_k, n-k-j)$. Without loss of generality, assume that $n' \leq n''$. Then $1 \leq n' \leq \frac{n-k}{2}$. By Lemma 2.7, we have a new graph $\overline{G'}_i = K_1 \oplus K_k \oplus K_{n-k-1}$ in $\mathbb{V}_n^k$ such that $\prod_i^*(\overline{G'}_i) \geq \prod_i^*(\overline{G}_i)$ and equality holds if and only if $\overline{G}_i = K_1 \oplus K_k \oplus K_{n-k-1} = K_n^k$ for $i = 1,2$. Hence the proof of Theorem 1.1 is complete.

Since $K_n^k \in \mathbb{E}_n^k \subset \mathbb{V}_n^k$, then the following result is an immediate consequence.

Theorem 3.1. *Let G be a graph in $\mathbb{E}_n^k$. Then*

$$\textstyle\prod_1^*(G) \leq \prod_1^*(K_n^k) \quad \textit{and} \quad \prod_2^*(G) \leq \prod_2^*(K_n^k),$$

where the equalities hold if and only if $G \cong K_n^k$, and

$$\textstyle\prod_1^*(K_n^k) = 2^{\frac{k(k-1)+(n-k-1)(n-k-2)}{2}} \cdot (n-1)^{\frac{k(k-1)}{2}} \cdot (n-2)^{\frac{(n-k-1)(n-k-2)}{2}} \cdot (2n-3)^{k(n-k-1)} \cdot (n+k-1)^k,$$

$$\textstyle\prod_2^*(K_n^k) = 2^{(n-1)k(k-1)+(n-2)(n-k-1)(n-k-2)} \cdot (n-1)^{(n-1)k(k-1)} \cdot (n-2)^{(n-2)(n-k-1)(n-k-2)} \cdot (2n-3)^{(2n-3)k(n-k-1)} \cdot (n+k-1)^{(n+k-1)k}.$$

Proof of Theorem 1.2

Since we consider the minimal values of the modified first and second Zagreb indices of graphs G in $\mathbb{V}_n^k$, by Proposition 2.2(ii), $k = 1$ and G contains no cycles. Thus G must be a tree with n vertices. By Lemma 2.6 and routine calculations, we have

$$\textstyle\prod_1^*(P_n) = 9 \cdot 4^{n-3} \quad \text{and} \quad \prod_2^*(P_n) = 729 \cdot 256^{n-3}.$$

We only need to prove that for any tree T_n in $\mathbb{V}_n^1$, if $T_n \neq P_n$ then there exists a tree T_n' such that $\prod_i^*(T_n') < \prod_i^*(T_n)$ for $i = 1,2$. Since $T_n \neq P_n$, then there exists a vertex w in T_n such that $d_{T_n}(w) \geq 3$ and T_n has at least three vertices, x_1, y_1, z_1 such that $d_{T_n}(x_1) = d_{T_n}(y_1) = d_{T_n}(z_1) = 1$. Let x_1x_2, y_1y_2 and z_1z_2 be three edges of T_n. Applying Lemma 2.8, we may assume that $d_{T_n}(x_2) = d_{T_n}(y_2) = d_{T_n}(z_2) = 2$.

Choose a path $P = x_1x_2 \cdots x_k$ in T_n such that $d_{T_n}(x_i) = 2$ for $2 \leq i \leq k-1$ and $d_{T_n}(x_k) \geq 3$. If $d_{T_n}(x_k) \geq 4$, then set $T_n' = T - x_{k-1}x_k + x_{k-1}y_1$ and we can get $d_{T_n}(x_{k-1}) + d_{T_n}(x_k) \geq 6$, $d_{T_n}(y_1) + d_{T_n}(y_2) = 3$, $d_{T_n'}(x_{k-1}) + d_{T_n'}(y_1) = 4$ and $d_{T_n'}(y_1) + d_{T_n'}(y_2) = 4$. Noting that $d_{T_n'}(w) \leq d_{T_n}(w)$ for any $w \in V(T_n) - \{x_{k-1}, x_k, y_1, y_2\}$, we can easily check that that $\prod_i^*(T_n') < \prod_i^*(T_n)$ for $i = 1,2$. Hence, we may assume that $d_{T_n}(x_k) = 3$.

Let $\{w_1, w_2\} = N_{T_n}(x_k) - \{x_{k-1}\}$. We now show that $d_{T_n}(w_i) = 2$ for $i = 1,2$. In fact, by Lemma 2.8, we may assume that $d_{T_n}(w_i) \geq 2$ for $i = 1,2$. If $d_{T_n}(w_i) \geq 3$, let $T_n' = T_n - x_kw_1 + x_1z_1$, where x_1 and z_1 are in the different components of $T_n - x_kw_1$. Then T_n' is a tree and $d_{T_n}(x_1) + d_{T_n}(x_2) = d_{T_n}(z_1) + d_{T_n}(z_2) = 3$, $d_{T_n}(w_1) + d_{T_n}(x_k) \geq 6$, $d_{T_n}(x_{k-1}) + d_{T_n}(x_k) = 5$, and $d_{T_n'}(x_1) + d_{T_n'}(x_2) = d_{T_n'}(z_1) + d_{T_n'}(z_2) = d_{T_n'}(x_1) + d_{T_n'}(z_1) = d_{T_n'}(x_{k-1}) + d_{T_n'}(x_k) = 4$. Noting that $d_{T_n'}(w) \leq d_{T_n}(w)$ for any $w \in V(T_n) - \{x_1, x_2, z_1, z_2, w_1, x_{k-1}, x_k\}$, we can deduce that $\prod_i^*(T_n') < \prod_i^*(T_n)$ for $i = 1,2$. Hence we may assume that $d_{T_n}(w_i) = 2$ for $i = 1,2$.

Now, let $T_n' = T_n - x_kw_1 + x_1w_1$. Then T_n' is a tree and $d_{T_n}(x_1) + d_{T_n}(x_2) = 3$, $d_{T_n}(x_{k-1}) + d_{T_n}(x_k) = d_{T_n}(w_1) + d_{T_n}(x_k) = 5$, and $d_{T_n'}(x_1) + d_{T_n'}(x_2) = d_{T_n'}(x_{k-1}) + d_{T_n'}(x_k) = d_{T_n'}(x_1) + d_{T_n'}(w_1) = 4$. Noting that $d_{T_n'}(w) \leq d_{T_n}(w)$ for any $w \in V(T_n) - \{x_1, x_2, x_{k-1}, w_1, x_k\}$, we can deduce that $\prod_i^*(T_n') < \prod_i^*(T_n)$ for $i = 1,2$.

Hence, the proof of Theorem 1.2 is complete.

Note that $P_n \in \mathbb{E}_n^k \subset \mathbb{V}_n^k$, then the following theorem is obvious.

Theorem 3.2. *Let G be a graph in $\mathbb{E}_n^k$. Then*

$$\textstyle\prod_1^*(G) \geq 9 \cdot 4^{n-3} \textit{ and } \prod_2^*(G) \geq 729 \cdot 256^{n-3},$$

where the equalities hold if and only if $G \cong P_n$.

4. Acknowledgments

The authors would like to thank Editor Paola Bonacini and the referees for providing their valuable comments and suggestions, which lead to great improvements in writing of this paper.

References

[1] B. Basavanagoud, S. Patil, Multiplicative Zagreb indices and coindices of some derived graphs, Opuscula Math. 36 (2016) 287-299.
[2] B. Bollob*á*s, Modern Graph Theory, Springer-Verlag, 1998.
[3] M. Eliasi, A. Iranmanesh, I. Gutman, Multiplicative versions of first Zagreb index, MATCH Commun. Math. Comput. Chem. 68 (2012) 217-230.
[4] E. Estrada, G. Patlewicz, E. Uriarte, From Molecular graphs to Drugs. A Review on the use of topological indices in drug design and discovery, Indian Journal of Chemistry 42 (2003) 1315-1329.
[5] I. Gutman, in Advances in the Theory of Benzenoid Hydrocarbons 2, Topics in Current Chemistry, Springer, Berlin, 162 (1992).
[6] I. Gutman, Extremal hexagonal chains. J. Math. Chem. 12 (1993) 197-210.
[7] I. Gutman, S.J. Cyvin, Introduction to the Theory of Benzenoid Hydrocarbons, Springer, Berlin, 1989.
[8] I. Gutman, S.J. Cyvin, in Advances in the Theory of Benzenoid Hydrocarbons, Topics in Current Chemistry, Springer, Berlin, 153 (1990).
[9] I. Gutman, Degree-based topological indices, Croat. Chem. Acta 86 (2013) 351-361.
[10] S. Ji, X. Li, B. Huo, On Reformulated Zagreb Indices with respect to Acyclic, Unicyclic and Bicyclic Graphs, MATCH:Communications in Mathematical and in Computer Chemistry 72 (2014) 723-732.
[11] L.B. Kier, L.H. Hall, Molecular Connectivity in Chemistry and Drug Research, Academic Press, New York, 1976.
[12] L.B. Kier, L.H. Hall, Molecular Connectivity in Structure-Activity Analysis, Wiley, New York, 1986.
[13] L.B. Kier L.H. Hall, W.J. Murray and M. Randić, Molecular connectivity V.: The connectivity concept applied to density, J. Pharm. Sci. 65(1976) 1226-1230.
[14] F. Li, M. Lu, On the zeroth-order general Randić index of unicycle graphs with k pendant vertices, Ars Combinatoria 109 (2013) 229-237.
[15] B. Liu, I. Gutman, Estimating the Zagreb and the general Randić indices, MATCH Commun. Math. Comput. Chem. 57 (2007) 617-632.
[16] S. Li, H. Zhou, On the maximum and minimum Zagreb indices of graphs with connectivity at most k, Applied Mathematics Letters 23 (2010) 128-132.
[17] M. Lu, etc., On the Randic index of cacti, MATCH-Communications in Mathematical and in Computer Chemistry 56 (2006) 551-556.
[18] M. Randić, On characterization of molecular branching. J. Am. Chem. Soc. 97 (1975) 6609-6615.
[19] M. Randić, The connectivity index 25 years after, J. Mol. Graph. Modell. 20(2001) 19-35.
[20] G. Su, L. Xiong, L. Xu and B. Ma, On the maximum and minimum first reformulated Zagreb index of graphs with connectivity at most k, Filomat 25 (2011) 75-83.
[21] R. Todeschini, D. Ballabio, V. Consonni, Novel molecular descriptors based on functions of new vertex degrees, in: I. Gutman, B. Furtula (Eds.), Novel Molecular Structure Descriptors Theory and Applications I, Univ. Kragujevac, Kragujevac (2010) 73-100.
[22] N. Trinajstić, Chemical Graph Theory, CRC Press, 1992.
[23] A. Vasilyev, R. Darda, D. Stevanović, Trees of given order and independence number with minimal First Zagreb Index, MATCH Commu. Math. Comput. Chem. 72 (2014) 775-782.
[24] S. Wang, B. Wei, Multiplicative Zagreb Indices of k-Trees, Discrete Applied Math. 180 (2015) 168-175.
[25] S. Wang, On the sharp upper and lower bounds of multiplicative Zagreb indices of graphs with connectivity at most k, arXiv:1704.06943 [math.CO].
[26] R. Zanni, M. Galvez-LIompart, R. G-Domenech, J. Galvez, Latest advances in molecular topology applications for drug discovery, Expert opinion on drug discovery 10 (2015) 945-957.
[27] Q. Zhao, S. Li, On the maximum Zagreb indices of graphs with k cut vertices, Acta Appl. Math. 111 (2010) 93-106.
[28] B. Zhou, Remarks on Zagreb indices, MATCH Commun. Math. Comput. Chem. 57 (2007) 591-596.