MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **68** (2012) 217-230

ISSN 0340 - 6253

Multiplicative Versions of First Zagreb Index

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(Received August 27, 2011)

Abstract

The first Zagreb index of a graph G, with vertex set $V(G)$ and edge set $E(G)$, is defined as $M_1(G) = \sum_{u \in V(G)} d(u)^2$ where $d(u)$ denotes the degree of the vertex v. An alternative expression for $M_1(G)$ is $\sum_{uv \in E(G)} [d(u) + d(v)]$. We consider a multiplicative version of M_1 defined as $\Pi_1^*(G) = \prod_{uv \in E(G)} [d(u) + d(v)]$. We prove that among all connected graphs with a given number of vertices, the path has minimal Π_1^*. We also determine the trees with the second–minimal Π_1^*.

1 Introduction

In this paper, we are concerned with finite graphs without loops, multiple, or directed edges. Let G be such a graph. Throughout this paper, n stands for the number of vertices of G.

Denote by uv the edge of G, connecting the vertices u and v. For any vertex u of G, the degree of u is denoted by $d(u)$. Numbers reflecting certain structural features of organic molecules that are obtained from the molecular graph are usually called molecular structure descriptors or, more commonly, topological indices. Topological indices play a

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significant role in chemistry, pharmacology, etc. (see [2, 3, 7–9, 13, 16, 17]). Many of the topological indices of current interest in mathematical chemistry are defined in terms of vertex degrees of the molecular graph. For example, the first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ are defined as [11, 12]:

$$\begin{aligned} M_1(G) &= \sum_{u \in V(G)} d(u)^2 \\ M_2(G) &= \sum_{uv \in E(G)} d(u)\, d(v) \ . \end{aligned}$$

The Zagreb indices and their variants have been used to study molecular complexity, chirality, ZE-isomerism, heterosystems, etc. We encourage the reader to consult [1, 6, 15, 18, 20–22] for historical background, computational techniques, and mathematical properties of Zagreb indices. A detailed bibliography on recent research of Zagreb indices is found in [4, 19].

The first Zagreb index can also be expressed as a sum over the edges of G [4, 12]:

$$M_1(G) = \sum_{uv \in E(G)} [d(u) + d(v)] \ . \tag{1}$$

Following an earlier idea of Narumi and Katayama [14], who put forward what nowadays is referred to as the Narumi–Katayama index,

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

one of the present authors [5] introduced the multiplicative version of the Zagreb indices. In particular he put forward

$$\begin{aligned} \Pi_1 = \Pi_1(G) &= \prod_{u \in V(G)} d(u)^2 \\ \Pi_2 = \Pi_2(G) &= \prod_{uv \in E(G)} d(u)\, d(v) \end{aligned}$$

where, of course, $\Pi_1 = (NK)^2$. In [5, 10], the graphs for which NK (and therefore also Π_1) assumes an extremal (minimal or maximal) value where characterized.

Bearing in mind the identity (1), we now consider a further multiplicative version of the first Zagreb index, namely:

$$\Pi_1^* = \Pi_1^*(G) = \prod_{uv \in E(G)} [d(u) + d(v)] \ . \tag{2}$$

It should be immediately noted that in the general case, the indices $\Pi_1(G)$ and $\Pi_1^*(G)$ assume different values. For instance, already for the 3-vertex graph P_3, their values are 4 and 9, respectively. It is easy to see that if the graph G is regular, then $\Pi_1(G) = \Pi_1^*(G)$.

The right–hand side of Eq. (2) is meaningful only if the graph G possesses edges. If $E(G) = \emptyset$, then we may, conventionally, assume that either $\Pi_1^*(G) = 0$ or, better, $\Pi_1^*(G) = 1$. In the case of connected graphs with more than one vertex, such a difficulty cannot be encountered.

In this paper we prove that among all connected graphs with a given number of vertices, the path has the minimal Π_1^* index. In addition, we characterize a class of trees that among all trees with $n \geq 7$ vertices, have the second–minimal Π_1^*-value.

2 Some notations

A tree is a connected acyclic graph. The path of order n is denoted by P_n, and the star of order n is denoted by S_n. A pendent vertex or leaf of a graph is a vertex of degree 1.

Suppose that $n_1 \geq 1$ and $2 \leq t \leq n - n_1 - 1$. Denote by $T(n, n_1, t)$ the tree of order n with the set of vertices $\{v_1, v_2, \ldots, v_n\}$, obtained from the path $v_1 v_2 v_3 \ldots v_{t+n_1}$ by appending the path $v_{t+n_1+1} v_{t+n_1+2} \ldots v_n$ to vertex v_t.

For $n \geq 7$, we define the sets

$$T^*(n, n_1) = \{T(n, n_1, t) \mid 3 \leq t \leq n-3\} \quad \text{and} \quad T^*(n) = \bigcup_{n_1} T^*(n, n_1) \ .$$

For an illustrative example see Figure 1.

The comet P_{n,n_1}, of order n and with n_1 pendent vertices, is obtained by appending a path with $n - n_1 - 1$ edges to a pendent vertex of the star S_{n_1+1}. By our notation, $T(n, 1, n-2) \cong P_{n,3}$, cf. Figure 2.

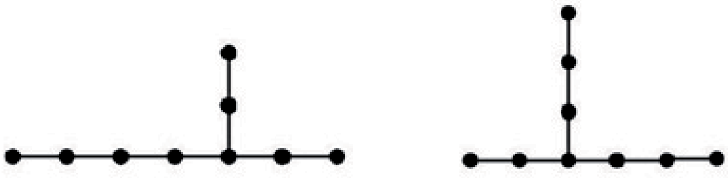

Fig. 1. The trees forming the class $T^*(9) = \{\text{T(9,2,5)} \ \ \text{(left)}, \text{T(9,3,3)} \ \ \text{(right)}\}$.

Fig. 2. The broom $P_{n,3} \cong T(n, 1, n-2)$.

3 Bounds for the Π_1^* index

Theorem 1 *Among all connected graphs with a fixed number of vertices, the path has minimal* Π_1^* *index.*

Proof: For a graph G with $n \geq 3$ vertices and m edges, denote by x_i the number of vertices with degree i for $i = 1, 2, \ldots, n-1$. Let $x_{i,j}$ be the number of edges of G connecting vertices of degree i and j, where $1 \leq i \leq j \leq n-1$. Then

$$\begin{aligned}
n &= x_1 + x_2 + \cdots + x_{n-1} \\
2m &= x_1 + 2x_2 + \cdots + (n-1)x_{n-1} \\
x_1 &= x_{1,2} + x_{1,3} + \cdots + x_{1,n-1} \\
2x_2 &= x_{1,2} + 2x_{2,2} + \cdots + x_{2,n-1} \\
&\vdots \\
(n-1)x_{n-1} &= x_{1,n-1} + x_{2,n-1} + \cdots + 2x_{n-1,n-1} \ .
\end{aligned}$$

Using the abbreviations

$$\begin{aligned} f_1 &= x_{1,3} + x_{1,4} + \cdots + x_{1,n-1} \\ f_2 &= x_{2,3} + x_{2,4} + \cdots + x_{2,n-1} \\ f_3 &= x_{1,3} + x_{2,3} + 3x_{3,3} \cdots + x_{3,n-1} \\ &\vdots \\ f_{n-1} &= x_{1,n-1} + x_{2,n-1} + \cdots + 2x_{n-1,n-1} \end{aligned}$$

i. e.,

$$\begin{aligned} f_1 &= x_1 - x_{1,2} \\ f_2 &= 2x_2 - x_{1,2} - 2x_{2,2} \\ f_3 &= 3x_3 \\ &\vdots \\ f_{n-1} &= (n-1)x_{n-1} \end{aligned}$$

we have:

$$\begin{aligned} \sum_{i=1}^{n-1} f_i &= 2m - 2x_{1,2} - 2x_{2,2} \\ \sum_{i=1}^{n-1} \frac{1}{i} f_i &= n - \frac{3}{2} x_{1,2} - x_{2,2} \ . \end{aligned}$$

This implies

$$\begin{aligned} x_{1,2} &= 2n - 2m + \sum_{i=1}^{n-1} \left(1 - \frac{2}{i}\right) f_i \\ &= 2n - 2m + \sum_{*} \left(2 - \frac{2}{i} - \frac{2}{j}\right) x_{i,j} \qquad (3) \\ x_{2,2} &= 3m - 2n + \sum_{i=1}^{n-1} \left(\frac{2}{i} - \frac{3}{2}\right) f_i \\ &= 2n - 2m + \sum_{*} \left(\frac{2}{i} + \frac{2}{j} - 3\right) x_{i,j} \qquad (4) \end{aligned}$$

where $\sum_{*}$ indicates summation goes over all (i, j) satisfying $1 \leq i \leq j \leq n-1$, except

$(i,j) = (1,2)$ and $(i,j) = (2,2)$. On the other hand,

$$\ln(\Pi_1^*(G)) = \sum_{uv \in E(G)} \ln(d(u)+d(v)) = \sum_{1 \le i \le j \le n-1} \ln(i+j) x_{i,j} \ . \tag{5}$$

By substituting Eqs. (3) and (4) back into Eq. (5) we readily arrive at:

$$\begin{aligned} \ln(\Pi_1^*(G)) &= x_{1,2} \ln 3 + x_{2,2} \ln 4 + \sum_* \ln(i+j)\, x_{i,j} \\ &= (2n-2m) \ln 3 + (3m-2n) \ln 4 \\ &+ \sum_* \left[\ln(i+j) + \left(2 - \frac{2}{i} - \frac{2}{j}\right) \ln 3 + \left(\frac{2}{i} + \frac{2}{j} - 3\right) \ln 4 \right] x_{i,j} \ . \end{aligned} \tag{6}$$

Let

$$f(i,j) = \ln(i+j) + \left(2 - \frac{2}{i} - \frac{2}{j}\right) \ln 3 + \left(\frac{2}{i} + \frac{2}{j} - 3\right) \ln 4 \ .$$

Then it is easy to see that

$$f(i,j) = \ln(i+j) + 2(\ln 4 - \ln 3) \left(\frac{1}{i} + \frac{1}{j}\right) + 2 \ln 3 - 3 \ln 4 \ . \tag{7}$$

Since $-2 < 2\ln 3 - 3\ln 4 < 0$, so if $i + j \ge [e^2] + 1 = 8$, then $f(i,j) > 0$. In Table 1, we calculated the values of $f(i,j)$ for (i,j) when $i+j \le 7$, $1 \le i \le j \le n-1$ and $(i,j) \ne (1,2)$ and $(i,j) \ne (2,2)$.

Table 1: Values of $f(i,j)$ for all possible degree pairs

i	j	$f(i,j)$	i	j	$f(i,j)$
1	3	0.19179	1	4	0.36699
1	5	0.52054	1	6	0.65551
2	3	0.12725	2	4	0.26162
2	5	0.38701	3	4	0.31988
3	3	0.21368			

So we have $f(i,j) > 0$, for $1 \le i \le j \le n-1$, except for $(i,j) = (1,2)$ and $(i,j) = (2,2)$. Therefore

$$\ln(\Pi_1^*(G)) \ge (2n-2m) \ln 3 + (3m-2n) \ln 4$$

with the equality if and only if all parameters $x_{i,j}$ are equal to zero, except $x_{1,2}$ and $x_{2,2}$. If the graph G is assumed to be connected, then this requirement implies that G it the path P_n or the cycle C_n with n vertices. It is easy to see that $\ln(\Pi_1^*(P_n)) \le \ln(\Pi_1^*(C_n))$ which completes the proof. $\square$

Corollary 1 *Let G be a connected graph with $n \geq 3$ vertices and m edges. Then*

$$3^{2n-2m}\,4^{3m-2n} \leq \Pi_1^*(G) \leq (2n-2)^m$$

with the left–hand side equality if and only $G \cong P_n$ and the right–hand side equality if and only if $G \cong K_n$.

Theorem 2 [10] *Among all connected graphs with a fixed number of vertices, the star has minimal Narumi–Katayama index.*

Corollary 2 *Let G be a connected graph with $n \geq 3$ vertices and m edges. Then*

$$n-1 \leq NK(G) \leq (n-1)^m \ .$$

The equality on the left–hand side holds if and only if G is the star and the equality on the right–hand side holds if and only if G is the complete graph.

Corollary 3 [5] *Among all connected graphs with a fixed number of vertices, the star has the minimal Π_1 index.*

Corollary 4 *Let G be a connected graph with $n \geq 3$ vertices and m edges. Then*

$$(n-1)^2 \leq \Pi_1(G) \leq (n-1)^{2m}$$

with the left–hand side equality if and only $G \cong S_n$ and the right–hand side equality if and only if $G \cong K_n$.

4 Trees with second–minimal Π_1^* index

We start with the following elementary result:

Lemma 5 *(a) Let T be a graph in the class of $T^*(n)$, where $n \geq 7$. Then*

$$\Pi_1^*(T) = 3^3 \times 5^3 \times 4^{n-7} \ .$$

(b) Suppose that U_n, a tree of order $n \geq 7$ and $V(U_n) = \{v_1, v_2, \ldots, v_n\}$, is obtained from the path $v_1v_2v_3 \ldots v_{n-1}$ by appending the edge $v_{n-3}v_n$. Then for each $T \in T^*(n)$, we have $\Pi_1^*(U_n) > \Pi_1^*(T)$.

Proof: (a) The proof is straightforward.

(b) It suffices to observe that

$$\frac{\Pi_1^*(U_n)}{\Pi_1^*(T)} = \frac{4^{n-5} \times 3^2 \times 5^2}{3^3 \times 5^3 \times 4^{n-7}} > 1 \ .$$

□

Theorem 3 *Among all trees with $n \geq 7$ vertices, those belonging to the class $T^*(n)$ have the second–minimal Π_1^* index.*

Proof: From Theorem 1, we know that P_n has the minimal Π_1^* index and $\Pi_1^*(P_n) = 3^2 \times 4^{n-3}$. Suppose that T is a tree with the second–minimal Π_1^* index. Since $\Pi_1^*(P_{n,3}) = 3 \times 5 \times 4^{n-3} > 3^3 \times 5^3 \times 4^{n-7}$ (see Lemma 5(a)), so T is neither a path nor $P_{n,3}$. Suppose that $P = v_1 v_2 \cdots, v_{k-1} v_k$ is a longest path of T. Then $d(v_1) = d(v_k) = 1$. We show that $d(v_{k-1}) = d(v_2) = 2$. We have to distinguish between the following two cases:

Case 1. $d(v_2) \geq 4$ or $d(v_{k-1}) \geq 4$. Without loss of generality, we may assume that $d(v_{k-1}) = d \geq 4$. Since P is a longest path of T, all vertices adjacent to v_{k-1}, other than v_{k-2}, must be leaves. Let $u_1, u_2, \ldots, u_{d-2}$ be the neighbors of v_{k-1} other than v_{k-2} and v_k. By deleting the edges $v_{k-1}u_1,\ v_{k-1}u_2, \ldots, v_{k-1}u_{d-2}$ from T and adding edges $v_k u_1,\ v_k u_2, \ldots, v_k u_{d-2}$, we get a new tree T', which is not a path, as shown in the Figure 3.

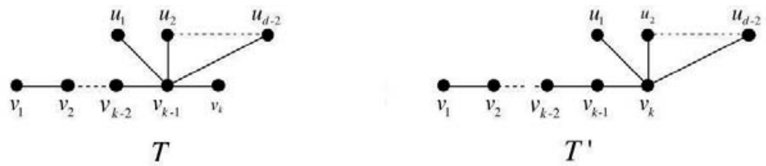

Fig. 3. Diagrams pertaining to the proof of Theorem 3, Case 1.

If $d(v_{k-2}) = 1$, then T is the star. Then $\Pi_1^*(T) = \Pi_1^*(S_n) = n^{n-1}$. For $n \geq 5$, we have

$$\frac{\Pi_1^*(S_n)}{\Pi_1^*(P_{n,3})} = \frac{n^{n-1}}{3 \times 5 \times 4^{n-3}} > 1$$

which contradicts to the second–minimality of T.

Now we can assume that $d(v_{k-2}) \geq 2$. So we have

$$\frac{\Pi_1^*(T)}{\Pi_1^*(T')} = \frac{(d(v_{k-2})+d)(d+1)^{d-1}}{(d(v_{k-2})+2)(d+1)d^{d-2}} > 1$$

which contradicts to the choice of T.

Case 2. $d(v_{k-1}) = 3$ or $d(v_2) = 3$. Without loss of generality, we may assume that $d(v_{k-1}) = 3$. Since the tree T is neither the path P_n nor $P_{n,3}$, there exists a vertex v_i such that $d(v_i) \geq 3$ for some $i \in \{3, 4, \ldots, k-2\}$. Since $d(v_{k-1}) = 3$, let u be the neighbor of v_{k-1}, other than v_{k-2} and v_k. Since u is a leaf, therefore $d(u) = 1$. By deleting the edge uv_{k-1} from T and adding a new edge uv_k, we get a new tree T' as shown in the Figure 4, and T' is not the path. Consequently,

$$\frac{\Pi_1^*(T)}{\Pi_1^*(T')} = \frac{(d(v_{k-2})+3)(1+3)^2}{(d(v_{k-2})+2)(2+2)(1+2)} > 1 \ .$$

Hence, we get $\Pi_1^*(T) > \Pi_1^*(T')$, which is a contradiction. Therefore $d(v_{k-1}) = d(v_2) = 2$.

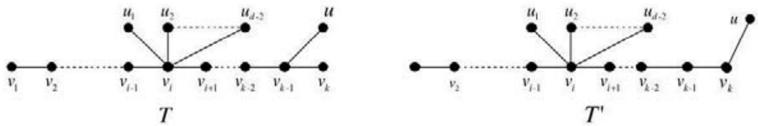

Fig. 4. Diagrams pertaining to the proof of Theorem 3, Case 2.

In what follows, we prove that T must be in $T^*(n)$. By considering Lemma 5(a), without loss of generality, we may assume that $d = d(v_{k-2}) \geq 3$. We prove that $T \in T(n, 2, n-4) \in T^*(n)$. Since P is a longest path of T, each vertex adjacent to v_{k-2}, other than v_{k-3}, must be a leaf or has only a neighbor other than v_{k-2}. Let $u_1, u_2, \ldots, u_{d-2}$ be the neighbors of v_{k-2} other than v_{k-3} and v_{k-1}. Now we consider the following three subcases.

Subcase 3.1. For each i, $d(u_i) = 1$. If $d = 3$, then the neighbors of v_{k-2} are v_{k-3}, u_1 and v_{k-1}. Since by Lemma 5(b) $T \notin U(n)$, so by deleting the edge $v_{k-2}u_1$ from T and adding the edge $v_k u_1$ we get a new tree T', which is not the path, see Figure 5. Therefore

$$\frac{\Pi_1^*(T)}{\Pi_1^*(T')} = \frac{(d(v_{k-3})+3)(1+3)(2+3)(1+2)}{(d(v_{k-3})+2)(1+2)(2+2)(2+2)} > 1$$

which is a contradiction.

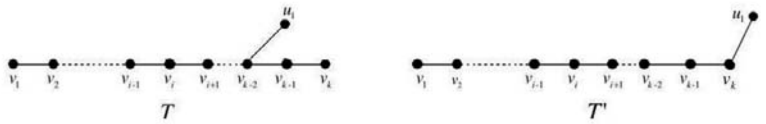

Fig. 5. Diagrams pertaining to the proof of Theorem 3, Subcase 3.1, $d = 3$.

If $d \geq 4$, then by deleting the edges $v_{k-2}u_1,\ v_{k-2}u_2, \ldots, v_{k-2}u_{d-3}$ from T and adding the edges $v_1u_1,\ u_1u_2, \ldots, u_{d-4}u_{d-3}$ we get a new tree T' (see Figure 6), which is not the path and

$$\frac{\Pi_1^*(T)}{\Pi_1^*(T')} = \frac{(1+2)(d(v_{k-3})+d)(1+d)^{d-2}(d+2)}{(2+2)(d(v_{k-3})+3)(2+2)^{d-4}(1+2)(1+3)(3+2)}$$

$$> \frac{(1+d)^2(d+2)}{(2+2)(1+3)(3+2)} > 1$$

which is a contradiction.

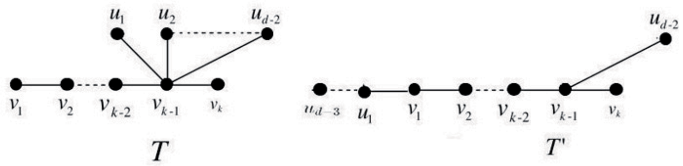

Fig. 6. Diagrams pertaining to the proof of Theorem 3, Subcase 3.1, $d \geq 4$.

Subcase 3.2. There is $\ell \in N$ such that $d(u_1) = \cdots = d(u_\ell) = 1$, $d(u_{\ell+1}) = \cdots = d(u_{d-2}) = 2$ and $\ell \neq d-2$. Since $\ell \neq d-2$ and $d \geq 3$, it must be $d \geq 4$. Since P is a longest path of T, there are leaves $w_{\ell+1}, \ldots, w_{d-2}$ in T, such that for each $i \in \{\ell+1, \ldots, d-2\}$, the only neighbors of u_i other than v_{k-2} is w_i. By deleting the edges $v_{k-2}u_1,\ v_{k-2}u_2, \ldots, v_{k-2}u_\ell$ from T and adding the edges $v_1u_1, u_1u_2, \ldots, u_{\ell-1}u_\ell$ we get a new tree T', which is not the path (see Figure 7) and

$$\frac{\Pi_1^*(T)}{\Pi_1^*(T')} = \frac{(1+2)(d(v_{k-3})+d)(2+d)^{d-2-\ell}\,(1+d)^{\ell}\,(2+d)}{(2+2)(d(v_{k-3})+d-\ell)(2+d-\ell)^{d-2-\ell}\,(2+d-\ell)(1+2)4^{\ell-1}}$$

$$> \frac{(1+d)^{\ell}}{(2+2)4^{\ell-1}} = \frac{(1+d)^{\ell}}{4^{\ell}} > 1$$

w

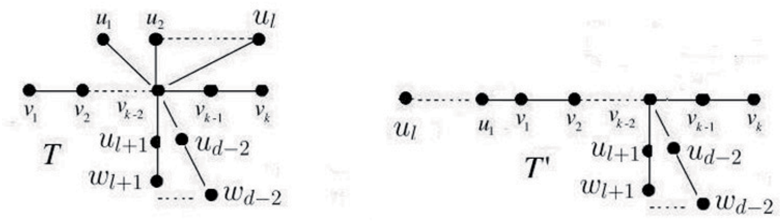

Fig. 7. Diagrams pertaining to the proof of Theorem 3, Subcase 3.2.

Subcase 3.3. $d(u_1) = \cdots = d(u_{d-2}) = 2$. If $d \geq 4$, then since P is a longest path of T, there are leaves $w_\ell, \ldots, w_{d-2}$ in T, such that for each $i \in \{1, \ldots, d-2\}$, the only neighbor of u_i other than v_{k-2} is w_i. By deleting the edges $v_{k-2}u_1, v_{k-2}u_2, \ldots, v_{k-2}u_{d-3}$, $u_1w_1, u_2w_2, \ldots u_{d-3}w_{d-3}$ from T and adding the edges $v_1u_1, u_1w_1, w_1u_2, u_2w_2, w_2u_3 \ldots$, $w_{d-4}u_{d-3}, u_{d-3}w_{d-4}$, we get a new tree T', which is not the path and

$$\frac{\Pi_1^*(T)}{\Pi_1^*(T')} = \frac{(1+2)(d(v_{k-3})+d)(1+2)^{d-2}\,(2+d)^{d-2}\,(2+d)}{(2+2)(d(v_{k-3})+3)(1+2)(2+3)(2+3)4^{2d-7}\,(1+2)}$$

$$> \frac{3^{d-3}(2+d)^{d-1}}{25 \times 4^{2d-6}} .$$

Let

$$f(d) = \frac{3^{d-3}(2+d)^{d-1}}{25 \times 4^{2d-6}} .$$

Then for $d > 3$, the function f monotonically increases. Therefore, $f(d) > f(3) = 1$. This implies $\Pi_1^*(T) > \Pi_1^*(T')$, which is a contradiction.

If $d = 3$, then $d(u_1) = 2$ and w_1 in T is the only neighbor of u_1 other than v_{k-2}. If $T \notin T(n, 2, n-4)$, then there is $i \in \{3, \ldots, n-3\}$ such that $d(v_i) \geq 3$. By deleting the edges $v_{k-2}u_1, u_1w_1$ and adding the edges v_1u_1, u_1w_1 we get a new tree T', which is not the path and

$$\begin{aligned}\frac{\Pi_1^*(T)}{\Pi_1^*(T')} &= \frac{(d(v_{k-3})+3)(2+3)(2+3)(1+2)}{(d(v_{k-3})+2)(2+2)(2+2)(2+2)} \\ &> \frac{5\times 5\times 3}{4\times 4\times 4} > 1\ .\end{aligned}$$

This is a contradiction and the proof is thus completed. □

Corollary 6 *Let G be a connected graph with $n \geq 7$ vertices, such that no one of its spanning tree is isomorphic to P_n. Then $\Pi_1^*(G) \geq 3^3 \times 5^3 \times 4^{n-7}$ and the equality holds if and only $G \in T^*(n)$.*

For $n \geq 7$, suppose that $U(n,t)$, $2 < t < n-2$, is a tree with vertex set $\{v_1, v_2, \ldots, v_n\}$, obtained from the path $v_1v_2v_3\ldots v_{n-1}$ by appending the edge v_tv_n. Also let $U^*(n) = \{U(n,t) \mid t < n\}$. Then we conjecture that among all trees with $n \geq 7$ vertices, the trees belonging to $U^*(n)$ have the third–minimal Π_1^* index.

Acknowledgement. I. G. thanks for support by the Serbian Ministry of Science (Grant No. 174033).

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