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ORDERING OF TREES BY MULTIPLICATIVE SECOND ZAGREB INDEX

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Abstract. For a graph G with edge set $E(G)$, the multiplicative second Zagreb index of G is defined as $\Pi_2(G) = \Pi_{uv\in E(G)}[d_G(u)d_G(v)]$, where $d_G(v)$ is the degree of vertex v in G. In this paper, we identify the eighth class of trees, with the first through eighth smallest multiplicative second Zagreb indices among all trees of order $n \geq 14$.

1. Introduction

Throughout the paper, $G = (V(G), E(G))$ is a connected undirected simple graph. The symbol uv is used to denoted an edge whose endpoints are the vertices u and v. The open neighborhood $n[v, G]$ of the vertex v consists of the set vertices adjacent to v, that is, $n[v, G] = \{w \in V(G) : vw \in E(G)\}$. The degree $d_G(v)$ of vertex v is the number of edges incident on v or equivalently, $d_G(v) = |n[v, G]|$. In particular, $\Delta = \Delta(G)$ is called the maximum degree of vertices of G, and a vertex of degree 1 is called a pendant vertex of G.

For an edge e in G, we denote by $G - e$ the subgraph of G obtained by deleting the edge e. For any two nonadjacent vertices u and v in G, let $G + uv$ be the graph obtained from G by adding an edge uv.

A tree is a connected acyclic graph. Any tree with at least two vertices has at least two pendant vertices. The set of all n-vertex trees will be denoted by $\tau(n)$. We denote the path graph and the star graph (both with n vertices) with P_n and S_n, respectively.

A graph invariant (topological index) is a real number related to a graph, which is invariant under graph isomorphism. For a graph G, the graph invariant

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

is called the second Zagreb index.

This index, in 1972, was found to occur within certain approximate expressions for the total $\pi-$electron energy of alternant hydrocarbons [7]. We encourage the reader to consult [1, 9, 15, 16] and [17] for historical background, computational techniques and mathematical properties of the second Zagreb index.

The problem of finding the graphs with extreme values of the second Zagreb index was studied by many researchers and the extreme values were gotten over some significant classes of graphs, see [2, 14].

Todeschini et al. [11, 12] have recently proposed to consider multiplicative variants of additive graph invariants. Gutman [5] applied this idea to the second Zagreb index and defined the multiplicative second Zagreb index as:

$$\Pi_2(G) = \prod_{uv \in E(G)} [d_G(u)d_G(v)].$$

The multiplicative second Zagreb index was subject to a large number of mathematical studies [3, 4, 6, 8, 10, 13].

In [6], Gutman determined that among all trees with $n \geq 5$ vertices, the extremal(minimal and maximal) trees with respect to the multiplicative second Zagreb index are path P_n and star S_n, respectively.

In [13] Xu and Hua introduced some graph transformations which increase the multiplicative second Zagreb index. As an application, they obtained a unified approach to characterize maximal trees, unicyclic graphs and bicyclic graphs with respect to multiplicative second Zagreb index, respectively. Also in [4] Eliasi, by theory of majorization, identified thirteen trees, with the first through ninth greatest multiplicative second Zagreb index among all trees of order n.

In this paper, we introduce a graph transformation, which decreases Π_2. By using this operation, we identify the eighth class of trees, with the first through eighth smallest multiplicative second Zagreb indices among all trees of order $n \geq 14$.

2. Notation and lemmas

Notation 1. *For positive integers $x_1, \ldots, x_m$, and $y_1, \ldots, y_m$, let $T(x_1^{(y_1)}, \ldots, x_m^{(y_m)})$ be the class of trees with x_i vertices of the degree y_i, $i = 1, \ldots, m$. Note that this class may be empty.*

Lemma 2.1. *There is a tree of order n (> 2) in $T(x_1^{(y_1)}, \ldots, x_m^{(y_m)})$ if and only if*

$$\sum_{i=1}^{m} x_i y_i = 2n - 2.$$

Proof. It is well-known that if $a_1, \ldots, a_n$ be positive integers, with $n > 2$, then there exists a tree with degree sequence $a_1, \ldots, a_n$ if and only if

$$\sum_{i=1}^{n} a_i = 2n - 2.$$

Hence there exists a tree $T \in T(x_1^{(y_1)}, \ldots, x_m^{(y_m)})$ if and only if

$$\sum_{i=1}^{m} x_i y_i = 2n - 2,$$

which completes the proof. $\square$

Remark 2.2. *Let $n \geq 14$. By Lemma 2.1, the following classes of trees, that we use of them in this paper, are nonempty sets.*
$T((n-2)^{(2)}, 2^{(1)}), T(1^{(3)}, (n-4)^{(2)}, 3^{(1)}), T(2^{(3)}, (n-6)^{(2)}, 4^{(1)}), T(1^{(4)}, (n-5)^{(2)}, 4^{(1)}), T(3^{(3)}, (n-8)^{(2)}, 5^{(1)}), T(1^{(4)}, 1^{(3)}, (n-7)^{(2)}, 5^{(1)}), T(4^{(3)}, (n-10)^{(2)}, 6^{(1)}), T(1^{(4)}, 2^{(3)}, (n-9)^{(2)}, 6^{(1)}), T(1^{(5)}, (n-6)^{(2)}, 5^{(1)})$ *and* $T(5^{(3)}, (n-12)^{(2)}, 7^{(1)})$.

The following lemma give us a necessary and sufficient condition, that the
It was proved in [5]

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

So, if $T \in T(x_1^{(y_1)}, \ldots, x_m^{(y_m)})$, then $\Pi_2(T) = \prod_{i=1}^{m} y_i^{x_i y_i}$.

For a graph G, the number of vertices of degree i will be denoted by n_i. Then, evidently, $\sum_{i=1}^{\Delta(G)} n_i = |V(G)|$.

In the following lemma, we introduce a graph transformation which, decreases the multiplicative second Zagreb index of trees.

Lemma 2.3. *Suppose that G_0 is a tree with given vertices v_1,v_2 and v_3, such that $d_{G_0}(v_1) \geq 2$, $d_{G_0}(v_2) \geq 2$, $d_{G_0}(v_3) = 1$ and $v_2v_3 \in E(G_0)$. In addition, suppose that G is another tree and w is a vertex in G. As shown in Figure 1, let G_1 be the graph obtained from G_0 and G by attaching vertices w, v_1 and $G_2 = G_1 - wv_1 + wv_3$. Then $\Pi_2(G_2) < \Pi_2(G_1)$.*

Proof. Suppose that $d_{G_0}(v_1) = x$, $n[v_1, G_0] = \{l_1, \ldots, l_x\}$, $d_{G_0}(l_i) = d_i$, for $i = 1, \ldots, x$. Let $d_{G_0}(v_2) = m$ and $d_G(w) = k$. We consider the following cases:

(I) $x \geq 3$ and $v_1 \neq v_2$.
We have

$$\frac{\Pi_2(G_1)}{\Pi_2(G_2)} = \frac{(k+1)(x+1)m \prod_{i=1}^{x} d_i(x+1)}{2m(k+1)2 \prod_{i=1}^{x}(d_i x)} > \frac{(x+1)}{4} \geq 1.$$

(II) $x \geq 3$ and $v_1 = v_2$.
Without loss of generality, we may assume that $l_1 = v_3$. So,

$$\frac{\Pi_2(G_1)}{\Pi_2(G_2)} = \frac{(k+1)(x+1)(x+1)\prod_{i=2}^{x} d_i(x+1)}{2x(k+1)2\prod_{i=2}^{x} d_i x} > \frac{(x+1)}{4} \geq 1.$$

(III) $x = 2$ and $v_1 \neq v_2$.

In this case

$$\frac{\Pi_2(G_1)}{\Pi_2(G_2)} = \frac{(k+1)3m3d_1 3d_2}{2m(k+1)2d_1 2d_2} = \frac{27}{16} > 1.$$

(IV) $x = 2$ and $v_1 = v_2$.

We have

$$\frac{\Pi_2(G_1)}{\Pi_2(G_2)} = \frac{(k+1)3 \times 3 \times 3 \times 3d_1}{2 \times 2 \times 2(k+1)2d_1} = \frac{27}{16} > 1,$$

which completes the proof. □

For a positive number $n \geq 14$, let:

$$H(n) = \{T \in \tau(n) |\ \Delta(T) = 3\},\ F(n) = \{T \in \tau(n) |\ \Delta(T) = 4\}.$$

Lemma 2.4. *For each $T \in \tau(n)$, we have*

$$\begin{aligned} n_1(T) &= 2 + \sum_{i=3}^{\Delta(T)} n_i(i-2) \\ n_2(T) &= n - 2 - \sum_{i=3}^{\Delta(T)} n_i(i-1). \end{aligned}$$

Proof. We have $n_1 + n_2 + \sum_{i=3}^{\Delta(T)} n_i = n$ and $n_1 + 2n_2 + \sum_{i=3}^{\Delta(T)} n_i i = 2(n-1)$. These equations give use the result. □

Theorem 2.5. *Let $\acute{T}$ be a tree with $n \geq 14$ vertices and $\Delta(\acute{T}) = 3$, such that $n_3(\acute{T}) \geq 6$. Then for each $T \in T(5^{(3)}, (n-12)^{(2)}, 7^{(1)})$, we have $\Pi_2(T) < \Pi_2(T')$.*

Proof. The proof is by induction on $n_3(\acute{T})$. If $n_3(\acute{T}) = 6$, then by using Lemma 2.3 on a vertex of degree 3 in $\acute{T}$, we obtain a tree, as T, with 5 vertices of degree 3. Since $\Delta(T) = 3$, Lemma 2.4 shows that $n_1(T) = 7$ and $n_2(T) = n - 12$. Therefore $T \in T(5^{(3)}, (n-12)^{(2)}, 7^{(1)})$ and by Lemma 2.3, $\Pi_2(T) < \Pi_2(T')$.

Now suppose that $n_3(\acute{T}) > 6$. Again by using Lemma 2.3, we decrease the number of vertices of degree 3 and complete the proof by the hypothesis of induction. □

It is easy to see that for each $T \in T \in T(5^{(3)}, (n-12)^{(2)}, 7^{(1)})$ and $H \in T(1^{(5)}, (n-6)^{(2)}, 5^{(1)})$ we have

$$\Pi_2(T) = 3^{15} \times 2^{2(n-12)}, \tag{2.1}$$

$$\Pi_2(H) = 5^5 \times 2^{2(n-6)}, \tag{2.2}$$

Theorem 2.6. *Let $\acute{T}$ be a tree in $F(n)$, where $n \geq 14$. If $n_4(\acute{T}) \geq 2$ or ($n_4(\acute{T}) = 1$ and $n_3(\acute{T}) \geq 3$), then for each $T \in T(1^{(4)}, 2^{(3)}, (n-9)^{(2)}, 6^{(1)})$, we have $\Pi_2(T) < \Pi_2(T')$.*

Proof. At first suppose that $n_4(\acute{T}) \geq 2$. We consider the following cases:

(I) $n_4(\acute{T}) = 2$ and $n_3(\acute{T}) = 0$. In this case Lemma 2.4, shows that $n_1(\acute{T}) = 6$ and $n_2(\acute{T}) = n-8$, hence $\acute{T} \in T(2^{(4)}, (n-8)^{(2)}, 6^{(1)})$, and $\Pi_2(\acute{T}) = 4^8 \times 2^{2(n-8)}$. Therefore if $T \in T(1^{(4)}, 2^{(3)}, (n-9)^{(2)}, 6^{(1)})$, then $\frac{\Pi_2(T')}{\Pi_2(T)} = \frac{4^8 \times 2^{2(n-8)}}{4^4 \times 3^6 \times 2^{2(n-9)}} > 1$.

(II) $n_4(\acute{T}) = 2$ and $n_3(\acute{T}) = 1$. By using Lemma 2.3 on a vertex of degree 4 in $\acute{T}$, we arrive at a tree T, with $n_4(T) = 1$, $n_3(T) = 2$. Also by Lemma 2.4, we have $n_1(T) = 6$ and $n_2(T) = n-9$. Therefore $T \in T(1^{(4)}, 2^{(3)}, (n-9)^{(2)}, 6^{(1)})$ and by Lemma 2.3, $\Pi_2(T) < \Pi_2(T')$.

(III) $n_4(\acute{T}) = 2$ and $n_3(\acute{T}) \geq 2$. By repeated application of Lemma 2.3 on vertices of degree 3 in $\acute{T}$, sufficient number of times (s-times), we arrive at a tree T_s, with $n_4(T_s) = 2$ and $n_3(T_s) = 1$. By choosing $\acute{T} = T_s$ in *(II)*, we obtain the result.

(IV) $n_4(\acute{T}) \geq 3$ and $n_3(\acute{T}) \geq 0$. By repeated application of Lemma 2.3 on vertices of degree 3 in $\acute{T}$, sufficient number of times (s-times), we arrive at a tree $T_s \in F(n)$, with $n_4(T_s) \geq 3$ and $n_3(T_s) = 0$. Also by repeated application of Lemma 2.3 on vertices of degree 4 in T_s, sufficient number of times (t-times), we arrive at a tree T_t, with $n_3(T_t) = 0$ and $n_4(T_t) = 2$. By choosing $\acute{T} = T_t$ in *(I)*, we obtain the result.

Now suppose that $n_4(\acute{T}) = 1$ and $n_3(\acute{T}) \geq 3$. By repeated application of Lemma 2.3 on vertices of degree 3 in $\acute{T}$. sufficient number of times (t-times), we arrive at a tree T_t, with $n_3(T_t) = 2$ and $n_4(T_t) = 1$. In addition, by Lemma 2.4 we have $n_1(T_t) = 6$ and $n_2(T_t) = n-9$. Therefore $T_t \in T(1^{(4)}, 2^{(3)}, (n-9)^{(2)}, 6^{(1)})$ and by Lemma 2.3, $\Pi_2(T_t) < \Pi_2(T')$. □

Theorem 2.7. *Let $\acute{T}$ be a tree with $n(\geq 14)$ vertices and $\Delta(\acute{T}) \geq 5$. Then for each $T \in T(1^{(5)}, (n-6)^{(2)}, 5^{(1)})$, we have $\Pi_2(T) < \Pi_2(T')$.*

Proof. Suppose that $v_1 \in V(\acute{T})$ and $d_{\acute{T}}(v_1) = \Delta(\acute{T})$. Let $U = \{v \in V(\acute{T}) \mid v \neq v_1,\ d_{\acute{T}}(v) \geq 3\}$. By repeated application of Lemma 2.3 on vertices in U, sufficient number of times, we arrive at a tree T_m, with only one vertex v_1 of degree $(\Delta(\acute{T})$ and the degree of other vertices is 1 or 2. In addition, by repeated application of Lemma 2.3 on v_1, $(\Delta(\acute{T})-5)$-times, we arrive at a tree T, such that $n_5(T) = 1$ and $n_i = 0$, for $i \geq 3$. On the other hand, by Lemma 2.4 we have $n_1(T) = 5$ and $n_2(T) = n-6$. Therefore $T \in T(1^{(5)}, (n-6)^{(2)}, 5^{(1)})$ and by Lemma 2.3, $\Pi_2(T) < \Pi_2(T')$. □

Table 1. Trees with smallest values of Π_2

Class	Π_2
$T((n-2)^{(2)}, 2^{(1)})$	$2^{2(n-2)}$
$T(1^{(3)}, (n-4)^{(2)}, 3^{(1)})$	$3^3 \times 2^{2(n-4)}$
$T(2^{(3)}, (n-6)^{(2)}, 4^{(1)})$	$3^6 \times 2^{2(n-6)}$
$T(1^{(4)}, (n-5)^{(2)}, 4^{(1)})$	$4^4 \times 2^{2(n-5)}$
$T(3^{(3)}, (n-8)^{(2)}, 5^{(1)})$	$3^9 \times 2^{2(n-8)}$
$T(1^{(4)}, 1^{(3)}, (n-7)^{(2)}, 5^{(1)})$	$4^4 \times 3^3 \times 2^{2(n-7)}$
$T(4^{(3)}, (n-10)^{(2)}, 6^{(1)})$	$3^{12} \times 2^{2(n-10)}$
$T(1^{(4)}, 2^{(3)}, (n-9)^{(2)}, 6^{(1)})$	$4^4 \times 3^6 \times 2^{2(n-9)}$

3. Main Theorems

Theorem 3.1. *If $n \geq 14$ and $T_1 := P_n, T_2 \in T(1^{(3)}, (n-4)^{(2)}, 3^{(1)}), T_3 \in T(2^{(3)}, (n-6)^{(2)}, 4^{(1)}), T_4 \in T(1^{(4)}, (n-5)^{(2)}, 4^{(1)}), T_5 \in T(3^{(3)}, (n-8)^{(2)}, 5^{(1)}), T_6 \in T(1^{(4)}, 1^{(3)}, (n-7)^{(2)}, 5^{(1)}), T_7 \in T(4^{(3)}, (n-10)^{(2)}, 6^{(1)}), T_8 \in T(1^{(4)}, 2^{(3)}, (n-9)^{(2)}, 6^{(1)}), T_9 \in T(1^{(5)}, (n-6)^{(2)}, 5^{(1)})$ and $T_{10} \in T(5^{(3)}, (n-12)^{(2)}, 7^{(1)})$ then we have*
$\Pi_2(T_1) < \Pi_2(T_2) < \Pi_2(T_3) < \Pi_2(T_4) < \Pi_2(T_5) < \Pi_2(T_6) < \Pi_2(T_7) < \Pi_2(T_8) < \Pi_2(T_9) < \Pi_2(T_{10})$.

Proof. See Tables 1, equation 2.1 and 2.2. □

Theorem 3.2. *Let G be a tree with n vertices, except the trees given in Table 1. If $n \geq 14$ and $T_1 := P_n, T_2 \in T(1^{(3)}, (n-4)^{(2)}, 3^{(1)}), T_3 \in T(2^{(3)}, (n-6)^{(2)}, 4^{(1)}), T_4 \in T(1^{(4)}, (n-5)^{(2)}, 4^{(1)}), T_5 \in T(3^{(3)}, (n-8)^{(2)}, 5^{(1)}), T_6 \in T(1^{(4)}, 1^{(3)}, (n-7)^{(2)}, 5^{(1)}), T_7 \in T(4^{(3)}, (n-10)^{(2)}, 6^{(1)})$ and $T_8 \in T(1^{(4)}, 2^{(3)}, (n-9)^{(2)}, 6^{(1)})$, then we have*
$\Pi_2(T_1) < \Pi_2(T_2) < \Pi_2(T_3) < \Pi_2(T_4) < \Pi_2(T_5) < \Pi_2(T_6) < \Pi_2(T_7) < \Pi_2(T_8) < \Pi_2(G)$.

Proof. Of Theorem 3.1 we have
$\Pi_2(T_1) < \Pi_2(T_2) < \Pi_2(T_3) < \Pi_2(T_4) < \Pi_2(T_5) < \Pi_2(T_6) < \Pi_2(T_7) < \Pi_2(T_8)$. Now, if $\Delta(G) = 3$ and $n_3(G) = 5$ then Theorem 3.1 gives us the result. If $\Delta(G) = 3$ and $n_3(G) \geq 6$ then Theorem 2.5 and 3.1 completes the proof. Suppose that $\Delta(G) = 4$. If $n_4(G) \geq 2$ or ($n_4(G) = 1$ and $n_3(G) \geq 3$), then Theorem 2.6, completes the proof. If $\Delta(G) \geq 5$ then Theorem 2.7 and 3.1 gives us the result. Otherwise, G is included in Table 1. □

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References

[1] 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.*, **54** (2005) 163–176.

[2] D. Vukievi, S. M. Rajtmajer and N. Trinajsti, Trees with maximal second Zagreb index and prescribed number of vertices of the given degree, *MATCH Commun. Math. Comput. Chem.*, **60** (2008) 65–70.

[3] K. C. Kinkar, A. Yurttas, M. Togan, A. S. Cevik and I. N. Cangu, The multiplicative Zagreb indices of graph operations, *J. Inequal. Appl.*, **90** (2013) 1–14.

[4] M. Eliasi, A simple approach to orther the multiplicative Zagreb indices of connected graphs, *Trans. Comb.*, **1** no. 4 (2012) 17–24.

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

[6] I. Gutman, Multiplicative Zagreb indices of trees, *Bull. Int. Math. Virtual Inst.*, **1** (2011) 13–19.

[7] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals Total p-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.*, **17** (1972) 535–538.

[8] J. Liu and Q. Zhang, Sharp upper bounds for multiplicative Zagreb indices, *MATCH Commun. Math. Comput. Chem.*, **68** (2012) 231–240.

[9] S. Nikolić, G. Kovacević, A. Milićević and N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta*, **76** (2003) 113–124.

[10] T. Reti and I. Gutman, Relation between ordinary and multiplicative zagreb indices, *Bull. Int. Math. Virtual Inst.*, **2** (2012) 133–140.

[11] 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.

[12] R. Todeschini, D. Ballabio and V. Consonni, *Novel molecular descriptors based on functions of new vertex degrees*, in: I. Gutman and B. Furtula (Eds.), Novel Molecular Structure Descriptors-Theory and Applications I, Univ. Kragujevac, Kragujevac, 2010 73–100.

[13] K. Xu and H. Hua, A unified approach to extremal multiplicative Zagreb indices for trees, Unicyclic and Bicyclic Graphs, *MATCH Commun. Math. Comput. Chem.*, **68** (2012) 241–256.

[14] Z. Yan, Huiqing Liu and Heguo Liu, Sharp bounds for the second Zagreb index of unicyclic graphs, *J. Math. Chem.*, **42** (2007) 565–574.

[15] B. Zhou and I. Gutman, Relations between Wiener, hyper-Wiener and Zagreb indices, *Chem. Phys. Lett.*, **394** (2004) 93–95.

[16] B. Zhou, Zagreb indices, *MATCH Commun. Math. Comput. Chem.*, **52** (2004) 113–118.

[17] B. Zhou and I. Gutman, Further properties of Zagreb indices, *MATCH Commun. Math. Comput. Chem.*, **54** (2005) 233–239.

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