

Extremal Trees with Respect to Some Versions of Zagreb Indices Via Majorization

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ABSTRACT

The objective of this article is to apply majorization theory to identify the classes of trees with extremal (minimal or maximal) values of some topological indices among all trees of order $n \geq 12$.

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1. INTRODUCTION

Throughout this article, only finite, undirected and simple graphs without loops and multiple edges are considered. Let G be such a graph and $V(G)$ and $E(G)$ be its vertex and edge set, respectively. The degree of a vertex v in G is the number of edges assigned to it, denoted by $d_G(v)$. The number of vertices of degree i will be denoted by n_i or $n_i(G)$. Evidently, $\sum_{i=1}^{\Delta(G)} n_i = |V(G)|$, where $\Delta(G)$ is the maximum degree of G . Assume that $V(G) = \{v_1, \dots, v_n\}$ and $d_k \geq d_{k+1}$, for $k = 1, \dots, n-1$, where $d_k := d_G(v_k)$. Then $D(G) = (d_1, d_2, \dots, d_n)$ is called the degree sequence of G . If the emphasis is on G , sometimes $d_k(D(G))$ is applied instead of d_k .

For an edge uv of $E(G)$, the $G - uv$ defines the subgraph of G obtained by deleting uv . In a similar manner, for any two nonadjacent vertices x and y of G , $G + xy$ is a graph obtained from G by adding the edge xy . A pendant vertex is a vertex with degree one and a tree is a connected acyclic graph. A star of order n , denoted by S_n , is the tree with $n-1$ pendant vertices and the path P_n is the tree of order n with exactly two pendant vertices. The symbol $\tau(n)$ represents the class of trees with n vertices.

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A topological index is a number related to a graph, which is invariant under each graph isomorphism. Topological indices play a significant role in mathematical chemistry, especially in the QSPR/QSAR assessments (See [6, 15]).

The first Zagreb index, introduced by Gutman and Trinajstić [14], is an important topological index in mathematical chemistry. This index is used by various researchers in QSPR/ QSAR studies [1, 20, 22]. In addition, the first Zagreb index has been subjected to a great number of mathematical studies [2, 3, 5, 12, 13]. The first Zagreb index of a graph G is defined as $M_1(G) = \sum_{v \in V(G)} d_G(v)^2 = \sum_{uv \in E(G)} [d_G(u) + d_G(v)]$. Recently, for an arbitrary real number α , except from 0 and 1, Li and Zheng [16] introduced the first general Zagreb index M_1^α of G as follows $M_1^\alpha(G) = \sum_{v \in V(G)} d_G(v)^\alpha$. Li and Zhao [17] characterized all trees with the first three smallest and largest values of the first general Zagreb index, where α is an integer or a fraction $1/k$ for a nonzero integer k . Todeschini et al. [22, 23] proposed the multiplicative versions of additive topological indices, applied to the first Zagreb index as $\pi_1(G) = \prod_{v \in V(G)} d_G(v)^2$, $\pi_1^*(G) = \prod_{uv \in E(G)} [d_G(u) + d_G(v)]$ and $\pi_2(G) = \prod_{uv \in E(G)} [d_G(u)d_G(v)]$. The symbols π_1 and π_2 are referred to as the multiplicative Zagreb indices.

In [11], Gutman showed that among all trees with $n \geq 5$ vertices, the extremal (minimal and maximal) trees regarding the multiplicative Zagreb indices are the path P_n and star S_n . Eliasi [7] identified thirteen trees with the first through ninth greatest multiplicative Zagreb index among all trees of order n . In the same line, Eliasi and Ghalavand [10] introduced a graph transformation, which decreases π_2 . By applying this operation, they identified the eight classes of trees with the first through eighth smallest π_2 among all trees of order $n \geq 12$. Also the effects on the first general Zagreb index were observed when some operations including edge moving, edge separating and edge switching were applied to the graphs [18]. Moreover, by using majorization theory, the authors [18] obtained the largest or smallest first general Zagreb indices among some classes of connected graphs. Some more outstanding mathematical studies on multiplicative Zagreb indices are [4, 8, 9, 19, 21, 24].

This paper is an attempt to investigate into the first general Zagreb index and the multiplicative Zagreb indices of trees via applying a new graph operation plus majorization theory, in particular, Schur-Convex function theory. Furthermore, some hands-on techniques and concluding remarks which complement the previous studies concerning aforementioned topological indices are introduced.

2. PRELIMINARY RESULTS

Let $x = (x_1, x_2, \dots, x_n)$ and $y = (y_1, y_2, \dots, y_n)$ be two non-increasing sequences of real numbers. If they meet the conditions $\sum_{i=1}^k x_i \leq \sum_{i=1}^k y_i$, for $1 \leq k \leq n - 1$ and

$\sum_{i=1}^k x_i = \sum_{i=1}^k y_i$, then it is deduced that x is **majorized** by y , thus $x \preceq y$. Furthermore, $x \prec y$ means that $x \preceq y$ and $x \neq y$. A real-valued function φ defined on a set $\Omega \subseteq \mathbb{R}^n$ is said to be Schur-convex on Ω if $x \preceq y$ implies $\varphi(x) \leq \varphi(y)$. It is called strictly Schur-convex on Ω if the inequality is strict. The following theorems are supposed to be utilized in the next sections.

Theorem 1. Let G and G' be two connected graphs with degree sequences $D(G)$ and $D(G')$, respectively. If $D(G) \preceq D(G')$, then (I) $\pi_1(G) \geq \pi_1(G')$. This equality holds if and only if $D(G) = D(G')$. (II) $\pi_2(G) \leq \pi_2(G')$, where equality holds if and only if $D(G) = D(G')$ (See [7]).

Theorem 2. Let G be a connected graph with degree sequence $D(G)$ and G' be a connected graph with degree sequence $D(G')$. (I) If $D(G) \preceq D(G')$, $\alpha < 0$ or $\alpha > 1$, then $M_\alpha(G) \leq M_\alpha(G')$; equality holds if and only if $D(G) = D(G')$. (II) If $D(G) \preceq D(G')$, $0 < \alpha < 1$, then $M_\alpha(G) \geq M_\alpha(G')$; equality holds if and only if $D(G) = D(G')$ (See [18]).

For positive integers x_1, x_2, \dots, x_m and y_1, y_2, \dots, y_m , let

$$T(x_1^{(y_1)}, x_2^{(y_2)}, \dots, x_m^{(y_m)})$$

be the class of trees with x_i vertices of the degree y_i , $i = 1, \dots, m$. This class may be empty. It is easy to see that if $G \in T(x_1^{(y_1)}, x_2^{(y_2)}, \dots, x_m^{(y_m)})$, then $\pi_1(G) = \prod_{i=1}^m y_i^{2x_i}$, $\pi_2(G) = \prod_{i=1}^m y_i^{x_i y_i}$ and $M_\alpha(G) = \sum_{i=1}^m x_i y_i^\alpha$.

Lemma 1. There is a tree of order $n (>2)$ in $T(x_1^{(y_1)}, x_2^{(y_2)}, \dots, x_m^{(y_m)})$ if and only if $\sum_{i=1}^m x_i y_i = 2n - 2$.

Proof. It is well-known that if a_1, a_2, \dots, a_n are positive integers with $n > 2$, then there exists a tree with degree sequence of a_1, a_2, \dots, a_n if and only if $\sum_{i=1}^n a_i = 2n - 2$. Hence there exists a tree $T \in T(x_1^{(y_1)}, x_2^{(y_2)}, \dots, x_m^{(y_m)})$ if and only if $\sum_{i=1}^m x_i y_i = 2n - 2$, as desired.

Remark 1. Let $n \geq 12$. According to Lemma 1, the class of trees in Table 1 are nonempty.

Lemma 2. Let T be a tree with n vertices. Then $n_1(T) = 2 + \sum_{i=3}^{\Delta(T)} n_i(i - 2)$ and $n_2(T) = n - 2 - \sum_{i=3}^{\Delta(T)} n_i(i - 1)$.

Proof. The above equations are obtained using $n_1 + n_2 + \sum_{i=3}^{\Delta(T)} n_i = n$ and $n_1 + 2n_2 + \sum_{i=3}^{\Delta(T)} i n_i = 2(n - 1)$.

3. A GRAPH TRANSFORMATION

A graph transformation that decreases the degree sequences of trees regarding the majorization is illustrated in this section.

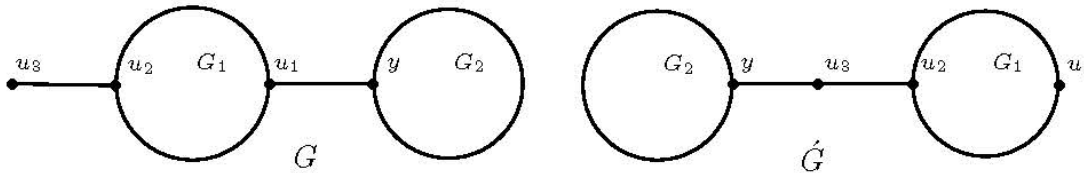


Figure 1. The Trees G_1, G_2, G and G' in Lemma 3.

Lemma 3. Let G_1 be a tree and $u_1, u_2, u_3 \in V(G_1)$, where $d_{G_1}(u_1) \geq 2, d_{G_1}(u_2) \geq 2, d_{G_1}(u_3) = 1$, and $u_2u_3 \in E(G_1)$. In addition, assume that G_2 is another tree and y is a vertex in G_2 . As illustrated in Figure 1, let G be the graph obtained from G_1 and G_2 by attaching vertices y, u_1 and $G' = G - yu_1 + yu_3$. Then $D(G') < D(G)$.

Proof. Suppose that $d_{G_1}(u_1) = x$ and $D(G) = (d_1, d_2, \dots, d_i, d_{i+1} = x+1, d_{i+2}, \dots, d_m, 1, \dots, 1)$. Since $D(G') = (d_1, d_2, \dots, d_i, d_{i+1} = x, d_{i+2}, \dots, d_m, 2, 1, \dots, 1)$,

- (I) For each k ($1 \leq k \leq i$), $\sum_{j=1}^k d_j(D(G)) = \sum_{j=1}^k d_j(D(G'))$.
- (II) For each k ($i+1 \leq k \leq m$), $\sum_{j=1}^k d_j(D(G)) < \sum_{j=1}^k d_j(D(G'))$.
- (III) For each k ($m+1 \leq k \leq n$), $\sum_{j=1}^k d_j(D(G)) = \sum_{j=1}^k d_j(D(G'))$.

Thus $D(G') < D(G)$.

For a positive number $n \geq 12$, let $F(n) = \{T \in \tau(n) \mid \Delta(T) = 4\}$.

Theorem 3. Suppose that T' is a tree with $n \geq 12$ vertices such that $\Delta(T') = 3$ and that $n_3(T') \geq 6$. If $T \in T(5^{(3)}, (n-12)^{(2)}, 7^{(1)})$, then $D(T) < D(T')$.

Proof. We prove the theorem by induction on $n_3(T')$. If $n_3(T') = 6$, then by using Lemma 3 on a vertex of degree 3 in T' we obtain a tree, like T , with 5 vertices of degree 3. Since $\Delta(T) = 3$, Lemma 2 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 3, $D(T) < D(T')$. Now assume that $n_3(T') > 6$. Again, by using Lemma 3, we reduce the number of vertices of degree 3. Now we apply the induction hypothesis to $n_3(T')$ and obtain the result.

Theorem 4. Suppose that $T' \in F(n)$ and $T \in T(1^{(4)}, 2^{(3)}, (n-9)^{(2)}, 6^{(1)})$. If $n_4(T') = 1$ and $n_3(T') \geq 3$, then $D(T) < D(T')$.

Proof. The proof is by induction on $n_3(T')$. If $n_3(T') = 3$, then by applying Lemma 3 on a vertex of degree 3 in T' , we obtain a tree, say T , with two vertices of degree 3. Since $\Delta(T) = 4$ and $n_4(T) = 1$, Lemma 2 indicates that $n_1(T) = 6$ and $n_2(T) = n - 9$. Therefore, $T \in T(1^{(4)}, 2^{(3)}, (n-9)^{(2)}, 6^{(1)})$ and $D(T) < D(T')$ is obtained by Lemma 3. Now assume that $n_3(T') > 3$. Afterward, by using Lemma 3, we decrease the number of vertices of degree 3, and thus the proof can be verified by induction hypothesis.

Theorem 5. Suppose that $T' \in F(n)$ and $T \in T(2^{(4)}, (n-8)^{(2)}, 6^{(1)})$. If $n_4(T') \geq 2$ and $T' \notin T(2^{(4)}, (n-8)^{(2)}, 6^{(1)})$, then $D(T) < D(T')$.

Proof. By repeating application of Lemma 3 on vertices of degree 4 in T' , a tree T_t with $n_4(T_t) = 2$ in terms of adequate number of times (t -times) can be gained. By repeating application of Lemma 3 on vertices of degree 3 in T_t , adequate number of times (s -times), a tree T_s with $n_4(T_s) = 2$ and $n_3(T_s) = 0$ can again be obtained. Now, by Lemma 2, we conclude that $n_1(T_s) = 6$ and $n_2(T_s) = n - 8$. Consequently, $T_s \in T(2^{(4)}, (n-8)^{(2)}, 6^{(1)})$ and Lemma 3 gives $D(T) = D(T_s) < D(T')$.

Theorem 6. Suppose that T' is a tree with $n (\geq 12)$ vertices and $\Delta(T') \geq 5$. If $T' \notin T(1^{(5)}, (n-6)^{(2)}, 5^{(1)})$ and $T \in T(1^{(5)}, (n-6)^{(2)}, 5^{(1)})$, then $D(T) < D(T')$.

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

Table 1. Classes of Trees and their Multiplicative Version of Zagreb Indices.

Class	π_1	π_2
$T((n-2)^{(2)}, 2^{(1)})$	$2^{2(n-2)}$	$2^{2(n-2)}$
$T(1^{(3)}, (n-4)^{(2)}, 3^{(1)})$	$3^2 \times 2^{2(n-4)}$	$3^3 \times 2^{2(n-4)}$
$T(2^{(3)}, (n-6)^{(2)}, 4^{(1)})$	$3^4 \times 2^{2(n-6)}$	$3^6 \times 2^{2(n-6)}$
$T(3^{(3)}, (n-8)^{(2)}, 5^{(1)})$	$3^6 \times 2^{2(n-8)}$	$3^9 \times 2^{2(n-8)}$
$T(4^{(3)}, (n-10)^{(2)}, 6^{(1)})$	$3^8 \times 2^{2(n-10)}$	$3^{12} \times 2^{2(n-10)}$
$T(5^{(3)}, (n-12)^{(2)}, 7^{(1)})$	$3^{10} \times 2^{2(n-12)}$	$3^{15} \times 2^{2(n-12)}$
$T(1^{(4)}, (n-5)^{(2)}, 4^{(1)})$	$4^2 \times 2^{2(n-5)}$	$4^4 \times 2^{2(n-5)}$
$T(1^{(4)}, 1^{(3)}, (n-7)^{(2)}, 5^{(1)})$	$4^2 \times 3^2 \times 2^{2(n-7)}$	$4^4 \times 3^4 \times 2^{2(n-7)}$
$T(1^{(4)}, 2^{(3)}, (n-9)^{(2)}, 6^{(1)})$	$4^2 \times 3^4 \times 2^{2(n-9)}$	$4^4 \times 3^6 \times 2^{2(n-9)}$
$T(2^{(4)}, (n-8)^{(2)}, 6^{(1)})$	$4^4 \times 2^{2(n-8)}$	$4^8 \times 2^{2(n-8)}$
$T(1^{(5)}, (n-6)^{(2)}, 5^{(1)})$	$5^2 \times 2^{2(n-6)}$	$5^5 \times 2^{2(n-6)}$

Table 2. Classes of Trees and their General First Zagreb Indices.

Class	M_1^α
$T((n-2)^{(2)}, 2^{(1)})$	$(n-2)2^\alpha + 2$
$T(1^{(3)}, (n-4)^{(2)}, 3^{(1)})$	$3^\alpha + (n-4)2^\alpha + 3$
$T(2^{(3)}, (n-6)^{(2)}, 4^{(1)})$	$2 \times 3^\alpha + (n-6)2^\alpha + 4$
$T(3^{(3)}, (n-8)^{(2)}, 5^{(1)})$	$3 \times 3^\alpha + (n-8)2^\alpha + 5$
$T(4^{(3)}, (n-10)^{(2)}, 6^{(1)})$	$4 \times 3^\alpha + (n-10)2^\alpha + 6$
$T(5^{(3)}, (n-12)^{(2)}, 7^{(1)})$	$5 \times 3^\alpha + (n-12)2^\alpha + 7$
$T(1^{(4)}, (n-5)^{(2)}, 4^{(1)})$	$4^\alpha + (n-5)2^\alpha + 4$
$T(1^{(4)}, 1^{(3)}, (n-7)^{(2)}, 5^{(1)})$	$4^\alpha + 3^\alpha + (n-7)2^\alpha + 5$
$T(1^{(4)}, 2^{(3)}, (n-9)^{(2)}, 6^{(1)})$	$4^\alpha + 2 \times 3^\alpha + (n-9)2^\alpha + 6$
$T(2^{(4)}, (n-8)^{(2)}, 6^{(1)})$	$2 \times 4^\alpha + (n-8)2^\alpha + 6$
$T(1^{(5)}, (n-6)^{(2)}, 5^{(1)})$	$5^\alpha + (n-6)2^\alpha + 5$

4. MAIN THEOREMS

Based on Tables 1 and 2 and the transformations in Section 3, the main theorems are discussed below.

Remark 2. For $n \geq 12$, we assume that $T_1 := P_n$, $T_2 \in T(1^{(3)}, (n-4)^{(2)}, 3^{(1)})$, $T_3 \in T(2^{(3)}, (n-6)^{(2)}, 4^{(1)})$, $T_4 \in T(1^{(4)}, (n-5)^{(2)}, 4^{(1)})$, $T_5 \in T(3^{(3)}, (n-8)^{(2)}, 5^{(1)})$, $T_6 \in T(1^{(4)}, 1^{(3)}, (n-7)^{(2)}, 5^{(1)})$, $T_7 \in T(4^{(3)}, (n-10)^{(2)}, 6^{(1)})$, $T_8 \in T(1^{(5)}, (n-6)^{(2)}, 5^{(1)})$, $T_9 \in T(1^{(4)}, 2^{(3)}, (n-9)^{(2)}, 6^{(1)})$, $T_{10} \in T(2^{(4)}, (n-8)^{(2)}, 6^{(1)})$ and $T_{11} \in T(5^{(3)}, (n-12)^{(2)}, 7^{(1)})$.

Theorem 7. $\pi_1(T_1) > \pi_1(T_2) > \pi_1(T_3) > \pi_1(T_4) > \pi_1(T_5) > \pi_1(T_6) > \pi_1(T_7) > \pi_1(T_8) > \pi_1(T_9) > \pi_1(T_{10}) > \pi_1(T_{11})$.

Proof. Make use of Table 1.

Theorem 8. If $n \geq 12$ and $T \in \tau(n) \setminus \{T_1, T_2, \dots, T_8\}$, then $\pi_1(T_1) > \pi_1(T_2) > \pi_1(T_3) > \pi_1(T_4) > \pi_1(T_5) > \pi_1(T_6) > \pi_1(T_7) > \pi_1(T_8) > \pi_1(T)$.

Proof. Theorem 7 shows that $\pi_1(T_1) > \pi_1(T_2) > \pi_1(T_3) > \pi_1(T_4) > \pi_1(T_5) > \pi_1(T_6) > \pi_1(T_7) > \pi_1(T_8)$. If $T \in \{T_9, T_{10}, T_{11}\}$, then the result follows from Theorem 7. If $\Delta(T) = 3$ and $n_3(T) \geq 6$, then $\pi_1(T_{11}) > \pi_1(T)$, by Theorems 3 and 1(I), and thus Theorem 7 implies $\pi_1(T_8) > \pi_1(T)$. Assume that $\Delta(T) = 4$. If $n_4(T) = 1$ and $n_3(T) \geq 3$, then by Theorems 4 and 1(I) we derive that $\pi_1(T_9) > \pi_1(T)$. Therefore, the result is an immediate consequence of Theorem 7. If $n_4(T) \geq 2$, then by Theorems 5 and 1(I) the $\pi_1(T_{10}) > \pi_1(T)$ will be yielded. If $\Delta(T) \geq 5$, then by Theorems 6 and 1(I) the $\pi_1(T_8) > \pi_1(T)$ can be obtained and again Theorem 7 gives the result. Ultimately, otherwise, $T \in \{T_1, T_2, \dots, T_8\}$.

Theorem 9. $\pi_2(T_1) < \pi_2(T_2) < \pi_2(T_3) < \pi_2(T_4) < \pi_2(T_5) < \pi_2(T_6) < \pi_2(T_7) < \pi_2(T_8) < \pi_2(T_9) < \pi_2(T_{11}) < \pi_2(T_{10})$.

Proof. Apply Table 1.

Theorem 10. If $n \geq 12$ and $T \in \tau(n) \setminus \{T_1, T_2, \dots, T_7, T_9\}$, then $\pi_2(T_1) < \pi_2(T_2) < \pi_2(T_3) < \pi_2(T_4) < \pi_2(T_5) < \pi_2(T_6) < \pi_2(T_7) < \pi_2(T_9) < \pi_2(T)$.

Proof. We get $\pi_2(T_1) < \pi_2(T_2) < \pi_2(T_3) < \pi_2(T_4) < \pi_2(T_5) < \pi_2(T_6) < \pi_2(T_7) < \pi_2(T_9)$ from Theorem 9. If $T \in \{T_8, T_{10}, T_{11}\}$, then Theorem 9 implies $\pi_2(T_9) < \pi_2(T)$. If $\Delta(T) = 3$ and $n_3(T) \geq 6$, then by Theorems 3, 1(II) and 9, $\pi_2(T_9) < \pi_2(T)$. Assume that $\Delta(T) = 4$. If $n_4(T) = 1$ and $n_3(T) \geq 3$, then by using Theorems 4, 1(II) and 9, $\pi_2(T_9) < \pi_2(T)$. If $n_4(T) \geq 2$, then by Theorems 5 and 1(II) we have $\pi_2(T_{10}) < \pi_2(T)$. Hence, Theorem 9 yields the result. If $\Delta(T) \geq 5$, then by Theorems 6 and 1(II) we have $\pi_2(T_8) < \pi_2(T)$ and Theorem 9 implies $\pi_2(T_9) < \pi_2(T)$. Eventually, otherwise, $T \in \{T_1, T_2, \dots, T_7, T_9\}$.

Theorem11.

(I) If $\alpha < 0$ or $\alpha > 1$, then

$$M_1^\alpha(T_1) < M_1^\alpha(T_2) < M_1^\alpha(T_3) < \min \{M_1^\alpha(T_4), M_1^\alpha(T_5), M_1^\alpha(T_6), M_1^\alpha(T_7), M_1^\alpha(T_8), M_1^\alpha(T_9), M_1^\alpha(T_{10}), M_1^\alpha(T_{11})\}.$$

(II) If $0 < \alpha < 1$, then

$$M_1^\alpha(T_1) > M_1^\alpha(T_2) > M_1^\alpha(T_3) > \max \{M_1^\alpha(T_4), M_1^\alpha(T_5), M_1^\alpha(T_6), M_1^\alpha(T_7), M_1^\alpha(T_8), M_1^\alpha(T_9), M_1^\alpha(T_{10}), M_1^\alpha(T_{11})\}.$$

(III) If $\alpha = 2$, then

$$M_1^\alpha(T_1) < M_1^\alpha(T_2) < M_1^\alpha(T_3) < M_1^\alpha(T_4) = M_1^\alpha(T_5) < M_1^\alpha(T_6) = M_1^\alpha(T_7) < M_1^\alpha(T_9) = M_1^\alpha(T_{11}) < M_1^\alpha(T_8) = M_1^\alpha(T_{10}).$$

(IV) If $\alpha = \frac{1}{2}$, then

$$M_1^\alpha(T_1) > M_1^\alpha(T_2) > M_1^\alpha(T_3) > M_1^\alpha(T_4) > M_1^\alpha(T_5) > M_1^\alpha(T_6) > M_1^\alpha(T_7) > M_1^\alpha(T_8) > M_1^\alpha(T_9) > M_1^\alpha(T_{11}) > M_1^\alpha(T_{10}).$$

Proof. (I) The proof of $M_1^\alpha(T_1) < M_1^\alpha(T_2)$ would suffice and other cases can be proved in a similar manner. For this purpose, the following equation is applied:

$$M_1^\alpha(T_1) - M_1^\alpha(T_2) = (2 \times 2^\alpha) - (3^\alpha + 1). \quad (1)$$

Let $X = (2,2)$ and $Y = (3,1)$, then $X < Y$. By Lemma 2 (I), the $(2 \times 2^\alpha) < (3^\alpha + 1)$ is yielded. Now, Equation (1) shows that $M_1^\alpha(T_1) < M_1^\alpha(T_2)$.

(II) Here, $M_1^\alpha(T_1) > M_1^\alpha(T_2)$ is proved. Other cases can be proved in a similar manner. It is easy to check that:

$$M_1^\alpha(T_1) - M_1^\alpha(T_2) = (2 \times 2^\alpha) - (3^\alpha + 1). \quad (2)$$

Let $X = (2,2)$ and $Y = (3,1)$, then $X < Y$. Thus, by Lemma 2(II) we have $(2 \times 2^\alpha) > (3^\alpha + 1)$. Therefore, Equation (2) implies $M_1^\alpha(T_1) > M_1^\alpha(T_2)$. To prove (III) and (IV), it is enough to apply Table 2.

Theorem 12.

- I.** If $\alpha < 0$ or $\alpha > 1$ and $T \in \tau(n) \setminus \{T_1, T_2, T_3\}$, then $M_1^\alpha(T_1) < M_1^\alpha(T_2) < M_1^\alpha(T_3) < M_1^\alpha(T)$.
- II.** If $0 < \alpha < 1$ and $T \in \tau(n) \setminus \{T_1, T_2, T_3\}$, then $M_1^\alpha(T_1) > M_1^\alpha(T_2) > M_1^\alpha(T_3) > M_1^\alpha(T)$.
- III.** If $\alpha = 2$ and $T \in \tau(n) \setminus \{T_1, T_2, \dots, T_7, T_9\}$, then $M_1^\alpha(T_1) < M_1^\alpha(T_2) < (T_3) < M_1^\alpha(T_4) = M_1^\alpha(T_5) < M_1^\alpha(T_6) = M_1^\alpha(T_7) < M_1^\alpha(T_9) = M_1^\alpha(T_{11}) < M_1^\alpha(T)$.
- IV.** If $\alpha = \frac{1}{2}$ and $T \in \tau(n) \setminus \{T_1, T_2, \dots, T_8\}$, then $M_1^\alpha(T_1) > M_1^\alpha(T_2) > M_1^\alpha(T_3) > M_1^\alpha(T_4) > M_1^\alpha(T_5) > M_1^\alpha(T_6) > M_1^\alpha(T_7) > M_1^\alpha(T_8) > M_1^\alpha(T)$.

Proof. (I) Theorem 11(I) shows that $M_1^\alpha(T_1) < M_1^\alpha(T_2) < M_1^\alpha(T_3)$. Using Theorem 11(I), it suffices to prove that there exists $T_i \in \{T_4, T_5, \dots, T_{11}\}$ such that $M_1^\alpha(T_i) < M_1^\alpha(T)$. If $\Delta(T) = 3$ and $n_3(T) \geq 6$, then by Theorems 3 and 2(I), the $M_1^\alpha(T_{11}) < M_1^\alpha(T)$ is yielded. Assume that $\Delta(T) = 4$. If $n_4(T) = 1$ and $n_3(T) \geq 3$. Then by Theorems 4 and 2(I) we obtain $M_1^\alpha(T_9) < M_1^\alpha(T)$. If $n_4(T) \geq 2$, Theorems 5 and 2(I) imply that $M_1^\alpha(T_{10}) < M_1^\alpha(T)$. If $\Delta(T) \geq 5$, then Theorems 6 and 2(I) yields $M_1^\alpha(T_8) < M_1^\alpha(T)$. Finally, otherwise, $T \in \{T_4, T_5, \dots, T_{11}\}$ and therefore $M_1^\alpha(T_3) < M_1^\alpha(T)$ follows from Theorem 11(I).

(II) This case can be proved by the same procedure as mentioned in the proof (I). Instead of using Theorems 11(I) and 2(I) in the proof of (I), here we apply Theorems 11(II) and 2(II), respectively.

(III) Theorem 11 (III) yields $M_1^\alpha(T_1) < M_1^\alpha(T_2) < (T_3) < M_1^\alpha(T_4) = M_1^\alpha(T_5) < M_1^\alpha(T_6) = M_1^\alpha(T_7) < M_1^\alpha(T_9) = M_1^\alpha(T_{11})$. It will thus be sufficient to prove that there exists a $T_i \in \{T_8, T_{10}, T_{11}\}$, with $M_1^\alpha(T_i) < M_1^\alpha(T)$. If $\Delta(T) = 3$ and $n_3(T) \geq 6$, then by Theorems 3 and 2(I) we have $M_1^\alpha(T_{11}) < M_1^\alpha(T)$. Assume that $\Delta(T) = 4$. If $n_4(T) = 1$ and $n_3(T) \geq 3$. then Theorems 4 and 2(I) give $M_1^\alpha(T_9) < M_1^\alpha(T)$. If $n_4(T) \geq 2$, then by Theorems 5 and 2(I) we have $M_1^\alpha(T_{10}) < M_1^\alpha(T)$. If $\Delta(T) \geq 5$, then Theorems 6 and 2(I) yield $M_1^\alpha(T_8) < M_1^\alpha(T)$. Eventually, otherwise, $T \in \{T_8, T_{10}, T_{11}\}$ and again Theorem 11(III) gives the result.

(IV) This case can be proved by a similar argument as in the proof of (III). Instead of using Theorems 11(III) and 2(I) in the proof of (III), here we apply Theorems 11(IV) and 2(II), respectively.

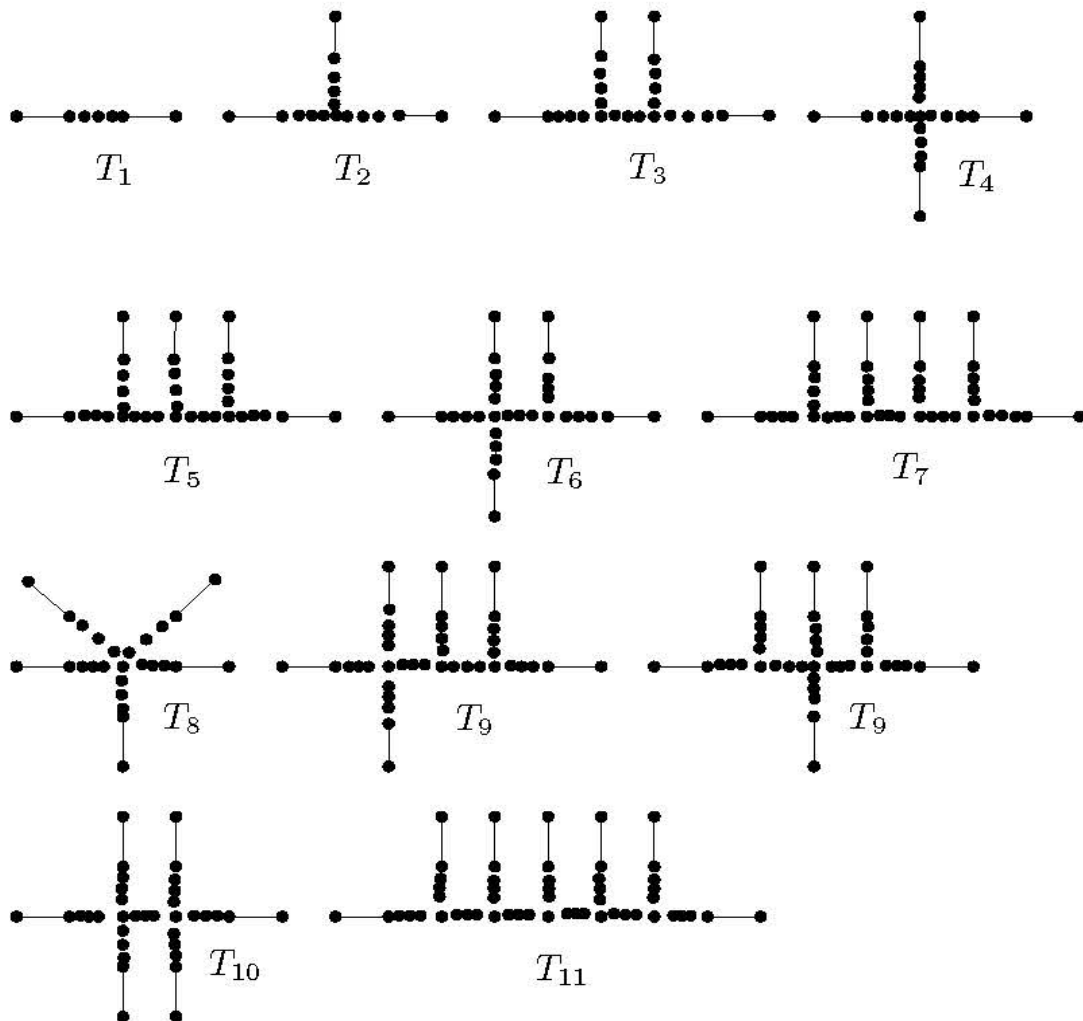


Figure 3. The Trees in Remark 2.

REFERENCES

1. A. T. Balaban, I. Motoc, D. Bonchev and O. Mekenyan, Topological indices for structure activity correlations, *Topics Curr. Chem.* **114** (1983) 21–55.
2. C. Bey, An upper bound on the sum of squares of degrees in a hypergraph, *Discrete Math.* **269** (2003) 259–263.
3. K. C. Das, Sharp bounds for the sum of the squares of the degrees of a graph, *Kragujevac J. Math.* **25** (2003) 31–49.
4. K. C. Das, 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.
5. D. de Caen, An upper bound on the sum of squares of degrees in a graph, *Discrete Math.* **185** (1998) 245–248.

6. J. Devillers and A. T. Balaban, *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon and Breach Science Publishers (1999).
7. M. Eliasi, A simple approach to order the multiplicative Zagreb indices of connected graphs, *Trans. Comb.* **1** (2012) 17–24.
8. M. Eliasi, A. Iranmanesh and I. Gutman, Multiplicative versions of first Zagreb index, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 217–230.
9. M. Eliasi and D. Vukicević, Comparing the multiplicative Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **69** (2013) 765–773.
10. M. Eliasi and A. Ghalavand, Ordering of trees by multiplicative second Zagreb index, *Trans. Comb.* **5** (1) (2016) 49–55.
11. I. Gutman, Multiplicative Zagreb indices of trees, *Bull. Int. Math. Virt. Inst.* **1** (2011) 13–19.
12. I. Gutman and K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.
13. I. Gutman, Graphs with smallest sum of squares of vertex degree, *Kragujevac J. Math.* **25** (2003) 51–54.
14. I. Gutman and N. Trinajstić, Graph theory and molecular orbital. Total π -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.
15. M. Karelson, *Molecular Descriptors in QSAR/QSPR*, Wiley, New York (2000).
16. X. Li and J. Zheng, A unified approach to the extremal trees for different indices, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 195–208.
17. X. Li and H. Zhao, Trees with the first three smallest and largest generalized topological indices, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 57–62.
18. M. Liu and B. Liu, Some properties of the first general Zagreb index, *Australas. J. Combin.* **47** (2010) 285–294.
19. J. Liu and Q. Zhang, Sharp upper bounds for multiplicative Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 231–240.
20. S. Nikolić, G. Kovacević, A. Miličević and N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta* **76** (2003) 113–124.
21. T. Rseti and I. Gutman, Relation between ordinary and multiplicative Zagreb indices, *Bull. Int. Math. Virt. Inst.* **2** (2012) 133–140.
22. R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley–VCH (2000).
23. 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.
24. 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.