Malaya J. Mat. 5(3)(2017) 524–530

Malaya Journal of Matematik

MJM
an international journal of mathematical sciences with computer applications...

www.malayajournal.org

ISSN : 2319-3786

Extremal trees with respect to the first and second reformulated Zagreb index

Ali Ghalavand and Ali Reza Ashrafi*

Department of Pure Mathematics, Faculty of Mathematical Sciences, University of Kashan, Kashan 87317−51116, I. R. Iran.

Abstract

Let G be a graph with edge set $E(G)$. The first and second reformulated Zagreb indices of G are defined as $EM_1(G) = \sum_{e\in E(G)} deg(e)^2$ and $EM_2(G) = \sum_{e\sim f} deg(e)deg(f)$,respectively, where $deg(e)$ denotes the degree of the edge e, and $e \sim f$ means that the edges e and f are incident. In this paper, the extremal trees with respect to the first and second reformulated Zagreb indices are presented.

Keywords: Tree, first reformulated Zagreb, second reformulated Zagreb, graph operation.

2010 MSC: 05C07, 05C35, 05C76.

1 Basic Definitions

Throughout this paper we consider undirected finite graphs without loops and multiple edges. The vertex and edge sets of a G will be denoted by $V(G)$ and $E(G)$, respectively. For a vertex v in G, the degree of v, $deg(v)$, is the number of edges incident to v and $N[v,G]$ is the set of all vertices adjacent to v. A vertex with degree one is called a pendent and $\Delta = \Delta(G)$ denotes the maximum degree of G. The number of vertices of degree i and the number of edges of G connecting a vertex of degree i with a vertex of degree j are denoted by $n_i = n_i(G)$ and $m_{i,j}(G)$, respectively. One can easily see that $\sum_{i=1}^{\Delta(G)} n_i = |V(G)|$.

Suppose $V(G) = \{v_1, \ldots, v_n\}$ and $d_k = deg(v_k)$, $1 \leq k \leq n$. The sequence $D(G) = (d_1, d_2, \ldots, d_n)$ is called the **degree sequence** of G and for simplicity of our argument, we usually write $D(G) = (x_1^{a_1}, x_2^{a_2}, ..., x_t^{a_t})$, when

$$D(G) = (\overbrace{x_1, ..., x_1}^{a_1\ times}, \overbrace{x_2, ..., x_2}^{a_2\ times}, ..., \overbrace{x_t, ..., x_t}^{a_t\ times}),$$

$x_1 > x_2 > ... > x_t$ and $a_1, ..., a_t$ are positive integers with $a_1 + a_2 + ... + a_t = n$.

Suppose $W \subset V(G)$ and $L \subseteq E(G)$. The notations $G \setminus W$ and $G \setminus L$ stand for the subgraphs of G obtained by deleting the vertices of W and the subgraph obtained by deleting the edges of L, respectively. If $W = \{v\}$ or $L = \{xy\}$, then the subgraphs $G \setminus W$ and $G \setminus L$ will be written as $G - v$ and $G - xy$ for short, respectively. Moreover, for any two nonadjacent vertices x and y of G, let $G + xy$ be the graph obtained from G by adding an edge xy.

A tree is a connected acyclic graph. It is well-known that any tree with at least two vertices has at least two pendent vertices. The set of all $n-$vertex trees will be denoted by $\tau(n)$. We denote the $n-$vertex path, cycle and the star graphs with P_n, C_n and S_n, respectively.

2 Preliminaries

The well-known Zagreb indices are among the oldest and most important degree-based molecular structure-descriptors. The first and second Zagreb indices are defined as the sum of squares of the degrees of

*Corresponding author.
E-mail address: ashrafi@kashanu.ac.ir (A. R. Ashrafi), ali797ghalavand@gmail.com (A. Ghalavand).

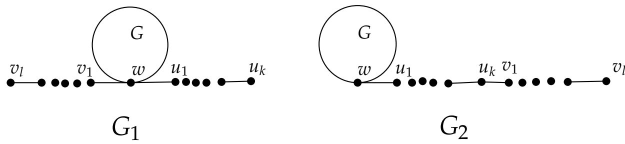

Figure 1: The Graphs G, P, Q, G_1 and G_2 in Transformation A.

the vertices and the sum of product of the degrees of adjacent vertices, respectively. These graph invariant was introduced many years ago by Gutman and Trinajesti/c [3]. We refer to [2, 9], for the history of these graph invariants and their role in QSAR and QSPR studies.

Milićević et al. [8], was introduced the first and second reformulated Zagreb indices of a graph G as edge counterpart of the first and second Zagreb indices, respectively. They are defined as $EM_1(G) = \sum_{e\in E(G)} deg(e)^2$ and $EM_2(G) = \sum_{e\sim f} deg(e)deg(f)$, where $deg(e)$ denotes the degree of the edge e, and $e \sim f$ means that the edges e and f are incident. In a recent paper, Milovanović et al. [7] obtained some relationship between Zagreb and reformulated Zagreb indices.

Zhou and Trinajestić [11], obtained sharp bounds for the reformed Zagreb indices. Ilić and Zhou [4] gave upper and lower bounds for the first reformulated Zagreb index and lower bounds for the second reformulated Zagreb index. They proved that if G is an $n-$vertex unicyclic graph then $EM_i(G) \geq EM_i(C_n)$, $i = 1, 2$, with equality if and only if $G \cong C_n$. Suppose $S_n^\star$ denotes the $n-$vertex unicyclic graph obtained by adding an edge to an $n-$vertex star, connecting two pendent vertices. They also proved that if G is an $n-$vertex unicyclic graph then $EM_i(G) \leq EM_i(S_n^\star)$, $i = 1, 2$, with equality if and only if $G \cong S_n'$.

Ji et al. [6] provided a shorter proof for results given by Ilić and Zhou and characterized the extremal properties of the first reformulated Zagreb index in the class of trees and bicyclic graphs by introducing some graph operations which increase or decrease this invariant. In [5], the authors applied a similar method as those given in [6] to find sharp bound for the first reformulated Zagreb index among all tricyclic graphs.

Su et al. [10], obtained the maximum and minimum of the first reformulated Zagreb index of graphs with connectivity at most k and characterized the corresponding extremal graphs. We encourage the interested readers to consult papers [1, 12] and references therein for more information on Zagreb and reformulated Zagreb indices of simple graphs.

3 Some Graph Transformations

In this section some graph operations are introduced which decreases the first and the second reformulated Zagreb index of graphs.

Transformation A. Suppose G is a graph with a given vertex w such that $deg(w) \geq 1$. We also assume that $P := v_1v_2...v_l$ and $Q := u_1u_2...u_k$ are two paths with l and k vertices, respectively. Define G_1 to be the graph obtained from G, P and Q by attaching vertices v_1w, wu_1, and $G_2 = G_1 - v_1w + u_kv_1$. The above referred graphs have been illustrated in Figure 1.

Lemma 3.1. *Let G_1 and G_2 be two graphs as shown in Figure 1. Then $EM_1(G_2) < EM_1(G_1)$ and $EM_2(G_2) < EM_2(G_1)$.*

Proof. Suppose $deg(w) = x$, $N[w, G] = \{l_1, \ldots l_x\}$ and $deg(l_i) = d_i$, for $i = 1, \ldots, x$. If $k, l \geq 2$ and $x \geq 1$, then

$$\begin{aligned} EM_1(G_1) - EM_1(G_2) &= 2(x+2)^2 + \sum_{i=1}^{x}(d_i + x)^2 \\ &- ((x+1)^2 + 8 + \sum_{i=1}^{x}(d_i + x - 1)^2) > (x+2)^2 - 8 > 0. \end{aligned}$$

If $k = l = 1$, or ($k = 1$ & $l \geq 2$), then a simple calculation shows the validity of $EM_1(G_2) < EM_1(G_1)$, as

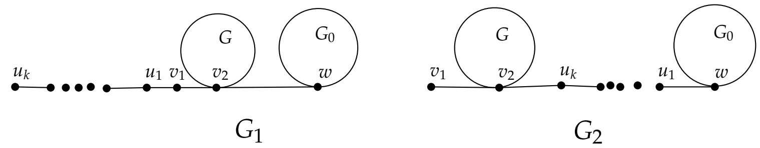

Figure 2: The Graphs G, G_0, P_k, G_1 and G_2 in Transformation B.

desired. Suppose that $k, l \geq 3$. Then,

$$\begin{aligned} EM_2(G_1) - EM_2(G_2) &> 2(x+2) + (x+2)^2 + \sum_{i=1}^{x}(x+2)(x+d_i) + 2 - (4+4+4) \\ &> 0. \end{aligned}$$

If $k, l \in \{1,2\}$, or ($k = 1$ & $l \geq 3$) or ($k = 2$ & $l \geq 3$), then a simple calculation shows the validity of $EM_2(G_2) < EM_2(G_1)$, proving the lemma. □

Transformation B. Suppose G and G_0 are two graphs with given vertices $\{v_1, v_2\} \subseteq V(G)$ and $w \in V(G_0)$ such that $d_G(v_1) = 1$, $d_G(v_2) \geq 2$, $d_{G_0}(w) \geq 1$, and $v_1v_2 \in E(G)$. We also assume that $P_k := u_1u_2 \ldots u_k$ is a path with $k \geq 1$ vertices. Construct G_1 as the graph obtained from G, G_0 and P_k by adding the edges v_1u_1, v_2w, and $G_2 = G_1 - \{v_1u_1, v_2w\} + \{v_2u_k, u_1w\}$. The above referred graphs have been illustrated in Figure 2.

Lemma 3.2. *Let G_1 and G_2 be two graphs as shown in Figure 2. Then $EM_1(G_2) < EM_1(G_1)$ and $EM_2(G_2) < EM_2(G_1)$.*

Proof. Suppose $deg(v_2) = x$, $N[v_2, G] = \{l_1 := v_1, \ldots l_x\}$ and $deg(l_i) = d_i$, for $i = 2, \ldots, x$. In addition, suppose $deg(w) = h$, $N[w, G_0] = \{r_1, \ldots r_h\}$ and $deg(r_i) = b_i$, for $i = 1, \ldots, h$. If $x \geq 2$ and $h \geq 1$, then

$$\begin{aligned} EM_1(G_1) - EM_1(G_2) &= 1 + (x+1)^2 + (x+h)^2 - (x^2 + (x+1)^2 + (h+1)^2) \\ &= 2h(x-1) > 0, \end{aligned}$$

as desired. Suppose $k \geq 2$. Then,

$$\begin{aligned} EM_2(G_1) - EM_2(G_2) &= 2 + 2(x+1) + (x+1)(x+h) + \sum_{i=2}^{x}(x+1)(d_i + x - 1) \\ &+ \sum_{i=2}^{x}(x+h)(d_i + x - 1) + \sum_{i=1}^{h}(x+h)(b_i + h - 1) \\ &- \Big(x(x+1) + 2(x+1) + 2(h+1) + \sum_{i=2}^{x} x(d_i + x - 1) \\ &+ \sum_{i=2}^{x}(x+1)(d_i + x - 1) + \sum_{i=1}^{h}(h+1)(b_i + h - 1)\Big) \\ &> 2 + (x+1)(x+h) - x(x+1) - 2(h+1) = h(x-1) > 0. \end{aligned}$$

If $k = 1$, then a simple calculation shows the validity of $EM_2(G_2) < EM_2(G_1)$, proving the lemma. □

Transformation C. Suppose G, G_0 and G' are three graphs with given vertices $w \in V(G_0)$, $\{v_1, v_2\} \subseteq V(G)$ and $y \in V(G')$ such that $d_{G_0}(w) \geq 2$, $d_G(v_1) \geq 2$, $d_G(v_2) = 1$ and $d_{G'}(y) \geq 2$. In addition, we assume that $P_k := u_1u_2 \ldots u_k$ is a path with $k \geq 1$ vertices. Define G_1 to be the graph obtained from G, G_0, G' and P_k by adding the edges wv_1, v_2u_1, u_ky and $G_2 = G_1 - \{wv_1, v_2u_1, u_ky\} + \{wu_1, u_kv_1, v_2y\}$. The above referred graphs have been illustrated in Figure 3.

Lemma 3.3. *Let G_1 and G_2 be two graphs as shown in Figure 3. Then $EM_1(G_2) < EM_1(G_1)$.*

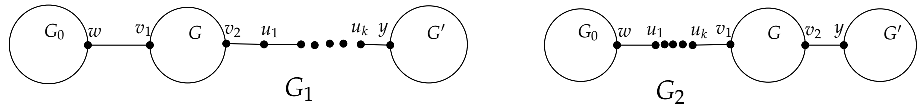

Figure 3: The Graphs G_0, G,G', P_k, G_1 and G_2 in Transformation C.

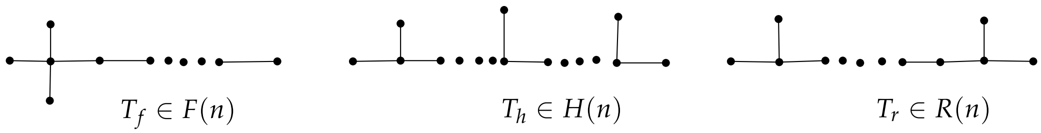

Figure 4: The trees in $F(n)$, $H(n)$ and $R(n)$.

Proof. Suppose that $d_{G_0}(w) = x$, $d_G(v_1) = k$ and $k, x \geq 2$. Then,

$$\begin{aligned} EM_1(G_1) - EM_1(G_2) &= (x+k)^2 + 4 - ((x+1)^2 + (k+1)^2) \\ &= 2kx + 2 - (2(x+k)) > 0, \end{aligned}$$

proving the lemma. □

4 Main Results

The aim of this section is to apply Transformations A-C to obtain an ordering of trees with respect to the first and second reformulated Zagreb indices. For simplicity of our argument, we first introduce a notation. Set

$$F(n) = \{T \in (4^1, 2^{n-5}, 1^4)|\ m_{1,2}(T) = 1,\ m_{1,4}(T) = 3,\ m_{2,4}(T) = 1 \textit{ and } m_{2,2}(T) = n-6\},$$

where $n \geq 7$ is a positive integer. It is easy to see that for each $T \in F(n)$,

$$EM_1(T) = 4n + 20 \quad , \quad EM_2(T) = 4n + 45. \tag{4.1}$$

Theorem 4.1. *Let T' be a tree with $\Delta(T') \geq 4$. If $T' \notin F(n)$, then for each $T \in F(n)$, we have $EM_1(T) < EM_1(T')$ and $EM_2(T) < EM_2(T')$.*

Proof. We first assume that $T' \in (4^1, 2^{n-5}, 1^4)$. Since $T' \notin F(n)$, $m_{1,2}(T) \neq 1$, $m_{1,4}(T) \neq 3$, $m_{2,4}(T) \neq 1$ or $m_{2,2}(T) \neq n-6$. We now apply a repeated application of Transformation B to obtain a tree $Q \in F(n)$. By Lemma 3.2, $EM_1(T) = EM_1(Q) < EM_1(T')$ and $EM_2(T) = EM_2(Q) < EM_2(T')$, as desired.

Next suppose $T' \notin (4^1, 2^{n-5}, 1^4)$. Then by a repeated application of Transformation A, we obtain a tree $G \in (4^1, 2^{n-5}, 1^4)$. If $G \in F(n)$, then by Lemma 3.1, $EM_1(T) = EM_1(G) < EM_1(T')$ and $EM_2(T) = EM_2(G) < EM_2(T')$. In other cases, we obtain the result by replacing T' with G in the first case. □

Suppose $n \geq 10$ and define $H(n) = \{T \in (3^3, 2^{n-8}, 1^5)|m_{1,2}(T) = 0, m_{1,3}(T) = 5, m_{2,3}(T) = 4, m_{3,3}(T) = 0 \textit{ and } m_{2,2}(T) = n-10\}$. It is easy to see that for each $T \in H(n)$,

$$EM_1(T) = 4n + 16. \tag{4.2}$$

Theorem 4.2. *Let T' be a tree with $n \geq 10$ vertices and $\Delta(T') = 3$ such that $n_3(T') \geq 3$. If $T' \notin H(n)$, then for each $T \in H(n)$, $EM_1(T) < EM_1(T')$.*

Proof. Suppose $T' \in (3^3, 2^{n-8}, 1^5)$. Since $T' \notin H(n)$, $m_{1,2}(T) \neq 0$, $m_{1,3}(T) \neq 5$, $m_{2,3}(T) \neq 4$, $m_{3,3}(T) \neq 0$ or $m_{2,2}(T) \neq n-10$. Again a repeated application of Transformations B and C, will result a tree $Q \in H(n)$. Now by Lemmas 3.2 and 3.3, $EM_1(T) = EM_1(Q) < EM_1(T')$. Suppose $n_3(T') \geq 4$. Since $n_3(T') \geq 4$, by a repeated application of Transformation A we obtain a tree $G \in (3^3, 2^{n-8}, 1^5)$. If $G \in H(n)$, then by Lemma 3.1, $EM_1(T) = EM_1(G) < EM_1(T')$. In other cases, we obtain the result by replacing T' with G in the first case. □

Table 1: The Trees with $\Delta \leq 3$ and $n_3 \leq 2$.

Notation	$m_{3,3}$	$m_{2,3}$	$m_{1,2}$	$m_{1,3}$	$m_{2,2}$	EM_1
A_1	0	0	2	0	n-3	4n-10
A_2	0	1	1	2	n-5	4n-2
A_3	0	2	2	1	n-6	4n
A_4	0	3	3	0	n-7	4n+2
A_5	0	2	0	4	n-7	4n+6
A_6	0	3	1	3	n-8	4n+8
A_7	0	4	2	2	n-9	4n+10
A_8	1	1	1	3	n-7	4n+10
A_9	0	5	3	1	n-10	4n+12
A_{10}	1	2	2	2	n-8	4n+12
A_{11}	0	6	4	0	n-11	4n+14
A_{12}	1	3	3	1	n-9	4n+14
A_{13}	1	4	4	0	n-10	4n+16

Suppose $n \geq 8$ and define:
$R(n) = \{T \in (3^2, 2^{n-6}, 1^4) |\ m_{1,2}(T) = 0,\ m_{1,3}(T) = 4,\ m_{2,3}(T) = 2,\ m_{3,3}(T) = 0\ \textit{and}\ m_{2,2}(T) = n-7\}$.
It is easy to see that for each $T \in R(n)$,

$$EM_2(T) = 4n + 12. \tag{4.3}$$

Theorem 4.3. *Let T' be a tree with $n \geq 8$ vertices and $\Delta(T') = 3$ such that $n_3(T') \geq 2$. If $T' \notin R(n)$, then for each $T \in R(n)$, $EM_2(T) < EM_2(T')$.*

Proof. Suppose $T' \in (3^2, 2^{n-6}, 1^4)$. Since $T' \notin R(n)$, $m_{1,2}(T) \neq 0$, $m_{1,3}(T) \neq 4$, $m_{2,3}(T) \neq 2$, $m_{3,3}(T) \neq 0$ or $m_{2,2}(T) \neq n-7$. Again a repeated application of Transformation B, will result a tree $Q \in R(n)$. Now by Lemma 3.2, $EM_2(T) = EM_2(Q) < EM_2(T')$. Suppose $n_3(T') \geq 3$. Since $n_3(T') \geq 3$, by a repeated application of Transformation A we obtain a tree $G \in (3^2, 2^{n-6}, 1^4)$. If $G \in R(n)$, then by Lemma 3.1, $EM_1(T) = EM_1(G) < EM_1(T')$. In other case, we obtain the result by replacing T' with G in the first case. □

Theorem 4.4. *If $n \geq 11$, $T_1 \in A_1$, $T_2 \in A_2$, $T_3 \in A_3$, $T_4 \in A_4$, $T_5 \in A_5$, $T_6 \in A_6$, $T_7 \in A_7$, $T_8 \in A_8$, $T_9 \in A_9$, $T_{10} \in A_{10}$, $T_{11} \in A_{11}$, $T_{12} \in A_{12}$, $T_{13} \in A_{13}$, $T_{14} \in H(n)$ and $T \in \tau(n) \diagdown \{T_1, T_2, ..., T_{14}\}$, then $EM_1(T_1) < EM_1(T_2) < EM_1(T_3) < EM_1(T_4) < EM_1(T_5) < EM_1(T_6) < EM_1(T_7) = EM_1(T_8) < EM_1(T_9) = EM_1(T_{10}) < EM_1(T_{11}) = EM_1(T_{12}) < EM_1(T_{13}) = EM_1(T_{14}) < EM_1(T)$.*

Proof. From Table 1 and Equation 4.2, we have $EM_1(T_1) < EM_1(T_2) < EM_1(T_3) < EM_1(T_4) < EM_1(T_5) < EM_1(T_6) < EM_1(T_7) = EM_1(T_8) < EM_1(T_9) = EM_1(T_{10}) < EM_1(T_{11}) = EM_1(T_{12}) < EM_1(T_{13}) = EM_1(T_{14})$. If $\Delta(T) = 3$ and $n_3(T) \geq 3$ then the proof is completed by applying Theorem 4.2. If $\Delta(T) \geq 4$, then Theorem 4.1 and Equation 4.1, gives the result. Otherwise, $T \in \{T_1, T_2, ..., T_{14}\}$. □

Theorem 4.5. *Suppose that T is a tree with $n(\geq 10)$ vertices, except $T'_1, T'_2, \ldots, T'_8$, illustrated in Figure 6. Then we have $EM_2(T'_1) < EM_2(T'_2) < EM_2(T'_3) < EM_2(T'_4) < EM_2(T'_5) < EM_2(T'_6) < EM_2(T'_7) < EM_2(T'_8) < EM_2(T)$.*

Proof. Let $T' \in F(n)$ and $n \geq 10$. We consider the following cases:

Case 1. $\Delta(T) = 3$. If $n_3(T) \geq 2$, then Theorem 4.3 shows that $EM_2(T'_8) < M_2(T)$. Now suppose that $n_3(T) = 1$. Clearly, $T'_2, T'_3, \ldots, T'_7$ are all trees with $n_3(T) = 1$. It is easy to see that $EM_2(T'_2) = 4n$, $EM_2(T'_3) = 4n+4$, $EM_2(T'_4) = 4n+5$, $EM_2(T'_5) = 4n+9$, $EM_2(T'_6) = 4n+10$ and $EM_2(T'_7) = 4n+11$.

Case 2. $\Delta(T) \geq 4$. Then by Theorem 4.1, $EM_2(T') < M_2(T)$. Since $EM_2(T'_8) = 4n+12 < 4n+45 = EM_2(T')$, $EM_2(T'_8) < EM_2(T)$.

Case 3. $\Delta(T) = 2$. Then $T \cong P_n$ and $M_2(T) = 4n - 12$.

This completes the proof. □

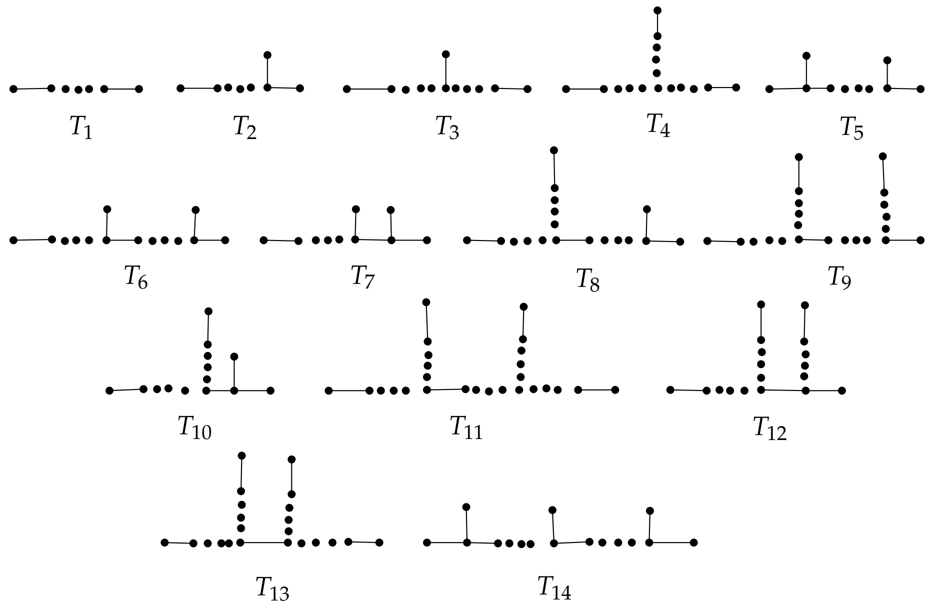

Figure 5: The Trees in Theorem 4.4.

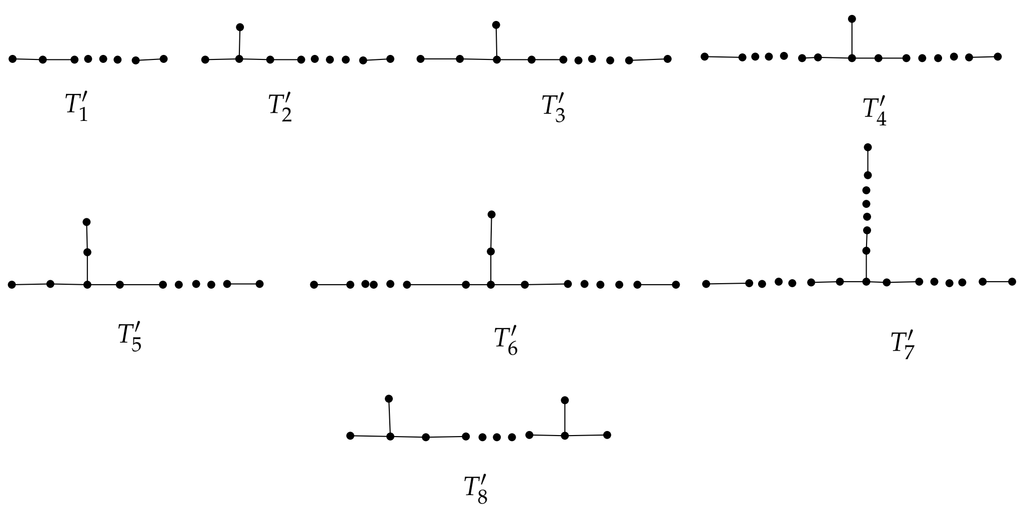

Figure 6: The Trees in Theorem 4.5.

5 Acknowledgment

The research of the authors are partially supported by the University of Kashan under grant no 572760/3.

References

[1] N. De, Some bounds of reformulated Zagreb indices, *Appl. Math. Sci.* (*Ruse*), 6 (101-104) (2012), 5005–5012.

[2] I. Gutman and K.C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.*, 50 (2004), 83–92.

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

[4] A. Ilić and B. Zhou, On reformulated Zagreb indices, *Discrete Appl. Math.*, 160 (3) (2012), 204–209.

[5] S. Ji, Y. Qu and X. Li, The reformulated Zagreb indices of tricyclic graphs, *Appl. Math. Comput.*, 268 (2015), 590–595.

[6] S. Ji, X. Li and B. Huo, On reformulated Zagreb indices with respect to acyclic, unicyclic and bicyclic graphs, *MATCH Commun. Math. Comput. Chem.*, 72 (3)(2014), 723–732.

[7] E. I. Milovanović, I. Ž. Milovanović, E. Ć. Dolićanin and E. Glogić, A note on the first reformulated Zagreb index, *Appl. Math. Comput.*, 273 (2016), 16–20.

[8] A. Milićević, S. Nikolić and N. Trinajstić, On reformulated Zagreb indices, *Mol. Divers.*, 8 (2004), 393–399.

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

[10] 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(4) (2011), 75–83.

[11] B. Zhou and N. Trinajstić, Some properties of the reformulated Zagreb indices, *J. Math. Chem.*, 48(3) (2010), 714–719.

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

Received: October 11, 2016; *Accepted*: April 23, 2017

UNIVERSITY PRESS

Website: http://www.malayajournal.org/