

## Trees with Extreme Values of Second Zagreb Index and Coindex

Reza Rasi, Seyed Mahmoud Sheikholeslami and Afshin Behmaram\*

### Abstract

The second Zagreb index  $M_2(G)$  is equal to the sum of the products of the degrees of pairs of adjacent vertices and the second Zagreb coindex  $\overline{M}_2(G)$  is equal to the sum of the products of the degrees of pairs of non-adjacent vertices. Kovijanić Vukićević and Popivoda (*Iranian J. Math. Chem.* **5** (2014) 19–29) prove that for any chemical tree of order  $n \geq 5$ ,

$$M_2(T) \leq \begin{cases} 8n - 26 & n \equiv 0, 1 \pmod{3} \\ 8n - 24 & \text{otherwise.} \end{cases}$$

In this paper we present a generalization of the aforementioned bound for all trees in terms of the order and maximum degree. We also give a lower bound on the second Zagreb coindex of trees.

Keywords: Zagreb index, second Zagreb index, second Zagreb coindex, tree.

2010 Mathematics Subject Classification: 05C30.

---

### How to cite this article

R. Rasi, S. M. Sheikholeslami and A. Behmaram, Trees with extreme values of second Zagreb index and coindex, *Math. Interdisc. Res.* **4** (2019) 227–238.

---

## 1. Introduction

In this paper,  $G$  is a simple connected graph with vertex set  $V = V(G)$  and edge set  $E = E(G)$ . The order  $|V|$  of  $G$  is denoted by  $n = n(G)$ . For every vertex  $v \in V$ , the *open neighborhood*  $N(v)$  is the set  $\{u \in V(G) \mid uv \in E(G)\}$  and the *closed neighborhood* of  $v$  is the set  $N[v] = N(v) \cup \{v\}$ . The *degree* of a vertex  $v \in V$  is  $d_v = |N(v)|$ . The *minimum* and *maximum degree* of a graph  $G$  are denoted by

---

\*Corresponding author (E-mail: behmaram@tabrizu.ac.ir)

Academic Editor: Tomislav Došlić

Received 11 May 2018, Accepted 21 June 2018

DOI: 10.22052/mir.2018.130441.1100

$\delta = \delta(G)$  and  $\Delta = \Delta(G)$ , respectively. A *leaf* of a tree is a vertex of degree 1 and a pendant edge is an edge adjacent to a leaf. Trees with the property  $\Delta \leq 4$  are called chemical trees.

The Zagreb indices have been investigated more than forty years ago by Gutman and Trinajstić in [6]. These parameters are important molecular descriptors and have been closely correlated with many chemical properties [6,8]. Hence, they attracted more and more attention from chemists and mathematicians [2–4,11,12].

The first Zagreb index,  $M_1 = M_1(G)$ , is equal to the sum of squares of the degrees of the vertices. Consult [9] for a good survey on this subject. Also, in [10] we found some lower bound for first Zagreb index of trees.

The second Zagreb index  $M_2 = M_2(G)$  is equal to the sum of the products of the degrees of pairs of adjacent vertices of the graph  $G$ , that is,

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v) = \sum_{uv \in E(G)} d_u d_v.$$

Došlić in [5] introduced two new graph invariants, the first and the second Zagreb coindices, defined as follows:

$$\overline{M}_1(G) = \sum_{uv \notin E(G)} (d_u + d_v),$$

$$\overline{M}_2(G) = \sum_{uv \notin E(G)} d_u d_v.$$

Let  $T$  be a tree of order  $n$  and let  $n_i$  be the number of vertices of degree  $i$  for each  $i = 1, 2, \dots, \Delta$ . Clearly

$$n_1 + n_2 + \dots + n_\Delta = n \tag{1}$$

and

$$n_1 + 2n_2 + \dots + \Delta n_\Delta = 2n - 2. \tag{2}$$

By (1) and (2), we have

$$n_2 + 2n_3 + \dots + (\Delta - 1)n_\Delta = n - 2. \tag{3}$$

Trees with the property  $\Delta \leq 4$  are called chemical trees. The following family of trees was introduced in [7]. For  $n = (\Delta - 1)k + r$  ( $k \geq 2$ ), let  $\tilde{\mathcal{T}}_n$  be the family of trees  $T$  of order  $n$  with maximum degree  $\Delta$  such that:

- If  $r = 0$ , then  $T$  has  $k - 1$  vertices of degree  $\Delta$  and one vertex of degree  $\Delta - 2$ , and the remaining vertices are pendant.

- If  $r = 1$ , then  $T$  has  $k - 1$  vertices of degree  $\Delta$  and one vertex has degree  $\Delta - 1$ , and the remaining vertices are pendant.
- If  $r \geq 2$ , then  $T$  has  $k$  vertices of degree  $\Delta$  and one vertex has degree  $r - 1$ , and the remaining vertices are pendant.

**Theorem A.** [7] *If  $T$  is a chemical tree of order  $n \geq 5$ . Then*

$$M_2(T) \leq \begin{cases} 8n - 26, & n \equiv 0, 1 \pmod{3} \\ 8n - 24, & \text{otherwise} \end{cases}$$

*with equality if and only if  $T \in \tilde{\mathcal{T}}_n$ .*

In this paper we generalize the aforementioned upper bound and classify all extreme trees.

## 2. An Upper Bound on the Second Zagreb Index

In this section we present the following upper bound on the second Zagreb index of trees as a generalization of Theorem A.

**Theorem 2.1.** Let  $T$  be a tree of order  $n$  and maximum degree  $\Delta$ . If  $n \equiv r \pmod{\Delta - 1}$ , then

$$M_2(T) \leq \begin{cases} 2n\Delta - \Delta^2 - 4\Delta + 6 & r = 0 \\ 2n\Delta - \Delta^2 - 3\Delta + 2 & r = 1 \\ 2n\Delta - \Delta^2 - 2\Delta & r = 2 \\ 2n\Delta - \Delta^2 - r\Delta + 2 + r(r - 3) & r \geq 3 \end{cases}$$

*with equality if and only if  $T \in \tilde{\mathcal{T}}_n$ .*

We start with some lemmas.

**Lemma 2.2.** If  $T$  is a tree with at least two vertices of degree  $2 \leq \beta \leq \Delta - 1$ , then its second Zagreb index cannot be maximal.

*Proof.* Let  $x, y \in V(T)$  such that  $d(x) = d(y) = \beta$ ,  $2 \leq \beta \leq \Delta - 1$ .

Let  $N(x) = \{x_1, x_2, \dots, x_\beta\}$ ,  $N(y) = \{y_1, y_2, \dots, y_\beta\}$ ,  $e_i = xx_i$ ,  $g_i = yy_i$  and  $i = 1, 2, \dots, \beta$ .

We consider two cases.

**Case 1.**  $xy \notin E(T)$ , that is,  $x$  and  $y$  are not adjacent.

Without loss of generality, suppose that

$$d(x_1) + d(x_2) + \dots + d(x_\beta) \leq d(y_1) + d(y_2) + \dots + d(y_\beta)$$

and the unique path between  $x$  and  $y$  goes toward the vertices  $x_1$  and  $y_1$ . Let  $T'$  be a tree, such that from  $T$  obtained by remove edge  $e_\beta = xx_\beta$  and adding edge  $yx_\beta$ . i.e.  $T' = T - e_\beta + yx_\beta$  (see Figure 1).

We will show that  $M_2(T) < M_2(T')$ . To this end, let  $S = \{e_1, e_2, \dots, e_\beta, g_1, g_2, \dots, g_\beta\}$ . By definition we have

$$M_2(T) = \sum_{uv \notin S} d(u).d(v) + \beta(d(x_1) + \dots + d(x_\beta)) + \beta(d(y_1) + \dots + d(y_\beta)),$$

$$M_2(T') = \sum_{uv \notin S} d(u).d(v) + (\beta - 1)(d(x_1) + \dots + d(x_{\beta-1}))$$

$$+ (\beta + 1)(d(y_1) + \dots + d(y_\beta) + d(x_\beta)).$$

Thus

$$M_2(T) - M_2(T') = (d(x_1) + \dots + d(x_{\beta-1})) - d(x_\beta) - (d(y_1) + \dots + d(y_\beta))$$

$$= (d(x_1) + \dots + d(x_\beta)) - (d(y_1) + \dots + d(y_\beta)) - 2d(x_\beta)$$

$$< 0.$$

Therefore  $M_2(T) < M_2(T')$ , as desired.

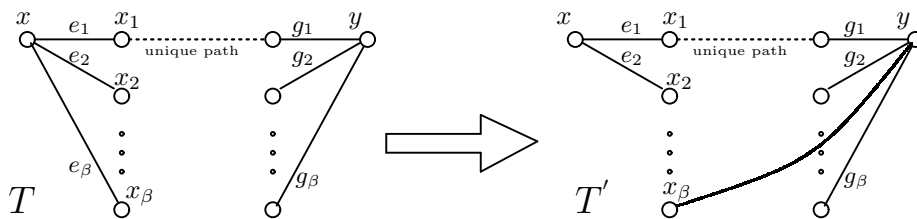


Figure 1: Case 1 - Lemma 2.2.

**Case 2.**  $xy \in E(T)$ , that is,  $x$  and  $y$  are adjacent.

The vertices  $x_1$  and  $y_1$  from the above construction are the vertices  $y$  and  $x$ , respectively, and the edges  $e_1$  and  $g_1$  are one and the same edge  $xy$ . Similar to the proof of case 1, we suppose that

$$d(x_2) + \dots + d(x_\beta) \leq d(y_2) + \dots + d(y_\beta).$$

Let  $S = \{e_1 = g_1, e_2, \dots, e_\beta, g_2, \dots, g_\beta\}$  (see Figure 2). By definition we have

$$M_2(T) = \sum_{uv \notin S} d(u).d(v) + \beta(d(x_2) + \dots + d(x_\beta)) + \beta^2 + \beta(d(y_2) + \dots + d(y_\beta)),$$

$$M_2(T') = \sum_{uv \notin S} d(u).d(v) + (\beta - 1)(d(x_2) + \dots + d(x_{\beta-1})) + (\beta - 1)(\beta + 1) + (\beta + 1)(d(y_2) + \dots + d(y_\beta) + d(x_\beta)).$$

Thus

$$M_2(T) - M_2(T') = (d(x_2) + \dots + d(x_{\beta-1})) - d(x_\beta) + 1 - (d(y_2) + \dots + d(y_\beta)) = (d(x_1) + \dots + d(x_\beta)) - (d(y_1) + \dots + d(y_\beta)) - 2d(x_\beta) + 1 < 0.$$

Since  $d(x_\beta) \geq 1$ ,  $-2d(x_\beta) + 1 < 0$ . This completes the proof. □

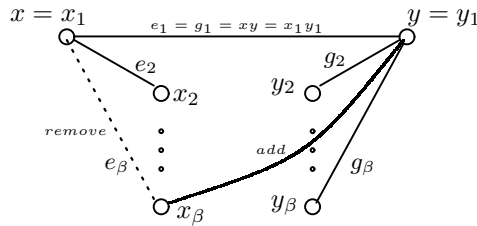


Figure 2: Case 2 - Lemma 2.2.

**Lemma 2.3.** If  $T$  be a tree with at least one vertex of degree  $\alpha$  and one vertex of degree  $\beta$ ,  $2 \leq \alpha < \beta \leq \Delta - 1$ , then its second Zagreb index cannot be maximal.

*Proof.* Let  $x, y \in V(T)$  such that  $d(x) = \alpha$  and  $d(y) = \beta$ ,  $2 \leq \alpha < \beta \leq \Delta - 1$ . Let  $N(x) = \{x_1, x_2, \dots, x_\alpha\}$ ,  $N(y) = \{y_1, y_2, \dots, y_\beta\}$  and  $e_i = xx_i$  and  $g_j = yy_j$  be the appropriate edges for each  $i = 1, 2, \dots, \alpha$  and  $j = 1, 2, \dots, \beta$ .

Without loss of generality, suppose that the unique path between  $x$  and  $y$  goes toward the vertices  $x_1$  and  $y_1$ . (see Figure 3).

Let  $S = \{e_1, e_2, \dots, e_\alpha, g_1, g_2, \dots, g_\beta\}$ . We consider two cases.

**Case 1.**  $xy \notin E(T)$ , that is,  $x$  and  $y$  are not adjacent.

**Subcase 1.1**  $d(x_1) > d(y_1)$ . Let  $T' = T - \{e_1, g_1\} + \{yx_1, xy_1\}$ . So

$$M_2(T) = \sum_{uv \notin S} d(u).d(v) + \alpha(d(x_1) + \dots + d(x_\alpha)) + \beta(d(y_1) + \dots + d(y_\beta)),$$

$$M_2(T') = \sum_{uv \notin S} d(u).d(v) + \alpha(d(y_1) + d(x_2) + \dots + d(x_\alpha)) + \beta(d(x_1) + d(y_2) + \dots + d(y_\beta)).$$

Therefore

$$\begin{aligned} M_2(T) - M_2(T') &= d(x_1)(\alpha - \beta) + d(y_1)(\beta - \alpha) \\ &= (d(x_1) - d(y_1))(\alpha - \beta) \\ &< 0. \end{aligned}$$

Because, by hypothesis,  $\alpha < \beta$  and  $d(y_1) < d(x_1)$ .

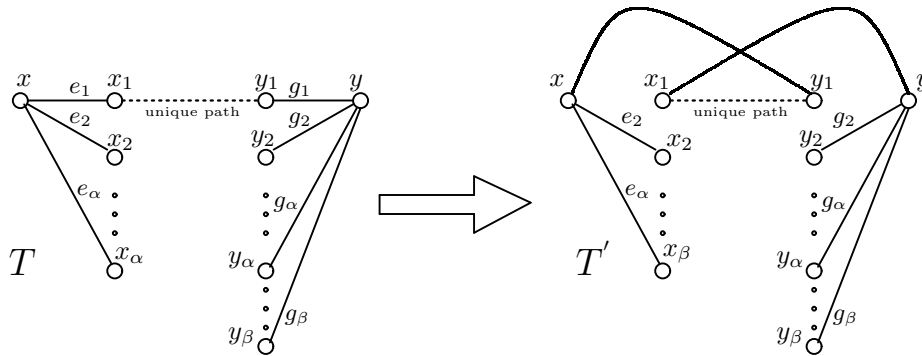


Figure 3: Case 1 - Lemma 2.3.

**Subcase 1.2**  $d(x_1) \leq d(y_1)$  and for some  $i, j$ ,  $d(x_i) > d(y_j)$  ( $2 \leq i \leq \alpha$ ,  $2 \leq j \leq \beta$ ). Let  $T' = T - \{e_i, g_j\} + \{yx_i, xy_j\}$ . So

$$M_2(T) = \sum_{uv \notin S} d(u).d(v) + \alpha(d(x_1) + \dots + d(x_\alpha)) + \beta(d(y_1) + \dots + d(y_\beta)),$$

$$M_2(T') = \sum_{uv \notin S} d(u).d(v) + \alpha(d(x_1) + \dots + d(x_\alpha)) + \beta(d(y_1) + \dots + d(y_\beta)) + (\beta d(x_i) - \alpha d(x_i)) + (\alpha d(y_j) - \beta d(y_j)).$$

Therefore

$$\begin{aligned} M_2(T) - M_2(T') &= d(x_i)(\alpha - \beta) + d(y_j)(\beta - \alpha) \\ &= (d(x_i) - d(y_j))(\alpha - \beta) \\ &< 0. \end{aligned}$$

Because, by hypothesis,  $\alpha < \beta$  and  $d(y_j) < d(x_i)$ .

**Subcase 1.3**  $d(x_1) \leq d(y_1)$  and for all  $2 \leq i \leq \alpha$  and  $2 \leq j \leq \beta$ , we have  $d(x_i) \leq d(y_j)$ . Let  $T' = T - e_\alpha + yx_\alpha$ . So

$$M_2(T) = \sum_{uv \notin S} d(u).d(v) + \alpha(d(x_1) + \dots + d(x_\alpha)) + \beta(d(y_1) + \dots + d(y_\beta)),$$

$$M_2(T') = \sum_{uv \notin S} d(u).d(v) + (\alpha - 1)(d(x_1) + \dots + d(x_{\alpha-1}))$$

$$+ (\beta + 1)(d(y_1) + \dots + d(y_\beta) + d(x_\alpha)).$$

Therefore

$$M_2(T) - M_2(T') = (d(x_1) + \dots + d(x_{\alpha-1})) + (\alpha - \beta - 1)d(x_\alpha)$$

$$- (d(y_1) + \dots + d(y_\beta))$$

$$= (d(x_1) + \dots + d(x_\alpha)) + (\alpha - \beta - 2)d(x_\alpha)$$

$$- (d(y_1) + \dots + d(y_\beta))$$

$$< 0.$$

Because, by hypothesis and  $\alpha < \beta$ .

**Case 2.**  $xy \in E(T)$ , that is,  $x$  and  $y$  are adjacent. The vertices  $x_1$  and  $y_1$  from the above construction are the vertices  $y$  and  $x$ , respectively, and the edges  $e_1$  and  $g_1$  are one and the same edge  $xy$ . Let  $S = \{e_2, \dots, e_\alpha, g_2, \dots, g_\beta\}$ . We consider two subcases.

**Subcase 2.1** There exist  $2 \leq i \leq \alpha$  and  $2 \leq j \leq \beta$ , such that  $d(x_i) > d(y_j)$ . Let  $T' = T - \{e_i, g_j\} + \{x_iy, xy_j\}$ . So

$$M_2(T) = \sum_{uv \notin S} d(u).d(v) + \alpha(d(x_2) + \dots + d(x_\alpha)) + \beta(d(y_2) + \dots + d(y_\beta)),$$

$$M_2(T') = \sum_{uv \notin S} d(u).d(v) + \alpha(d(x_2) + \dots + d(x_\alpha)) + \beta(d(y_2) + \dots + d(y_\beta))$$

$$- \alpha d(x_i) + \beta d(x_i) - \beta d(y_j) + \alpha d(y_j).$$

It follows that

$$M_2(T) - M_2(T') = (\alpha - \beta)d(x_i) + (\beta - \alpha)d(y_j) = (\alpha - \beta)(d(x_i) - d(y_j)) < 0.$$

Because, by hypothesis  $\alpha - \beta < 0$  and  $d(x_i) - d(y_j) > 0$ .

**Subcase 2.2** For all  $2 \leq i \leq \alpha$  and  $2 \leq j \leq \beta$ , we have  $d(x_i) \leq d(y_j)$ .

In this case, we suppose that  $S = \{e_2, \dots, e_\alpha, g_2, \dots, g_\beta, e_1 = g_1 = xy\}$  and  $T' = T - e_\alpha + yx_\alpha$ . We deduce that

$$\begin{aligned} M_2(T) &= \sum_{uv \notin S} d(u).d(v) + \alpha(d(x_1 = y) + \dots + d(x_\alpha)) \\ &\quad + \beta(d(y_1 = x) + \dots + d(y_\beta)), \\ M_2(T') &= \sum_{uv \notin S} d(u).d(v) + (\alpha - 1)(d(x_1 = y) + \dots + d(x_{\alpha-1})) \\ &\quad + (\beta + 1)(d(y_1 = x) + \dots + d(y_\beta) + d(x_\alpha)). \end{aligned}$$

Therefore

$$\begin{aligned} M_2(T) - M_2(T') &= (d(y) + d(x_2) + \dots + d(x_{\alpha-1})) + (\alpha - \beta - 1)d(x_\alpha) \\ &\quad - (d(x) + d(y_2) + \dots + d(y_\beta)) \\ &= (\alpha - \beta - 1)d(x_\alpha) + (d(y) - d(x)) - (d(y_2) + \dots + d(y_\beta)) \\ &\quad + (d(x_2) + \dots + d(x_{\alpha-1})) \\ &= (\alpha - \beta - 1)d(x_\alpha) + (\beta - \alpha) - (d(y_2) + \dots + d(y_{\beta-\alpha+2})) \\ &\quad - (d(y_{\beta-\alpha+3}) + \dots + d(y_\beta)) + (d(x_2) + \dots + d(x_{\alpha-1})) \\ &< 0. \end{aligned}$$

Because, by hypothesis  $(\alpha - \beta - 1)d(x_\alpha) < -1$ ,  $(\beta - \alpha) - (d(y_2) + \dots + d(y_{\beta-\alpha+2})) \leq \beta - \alpha - (\beta - \alpha + 1) \leq -1$  and  $(d(x_2) + \dots + d(x_{\alpha-1})) - (d(y_{\beta-\alpha+3}) + \dots + d(y_\beta)) \leq 0$ . Consequently, in any cases we have  $M_2(T) < M_2(T')$ , that is contradiction.  $\square$

From the Lemmas 2.2 and 2.3, we make the next conclusion.

**Corollary 2.4.** If  $T$  is tree of order  $n$  such that  $M_2(T) = \max\{M_2(T') \mid T' \text{ is a tree of order } n\}$ , then  $T$  satisfies exactly one of the next two conditions:

- (i) all vertices of the graph  $T$  have degrees 1 or  $\Delta$ ;
- (ii) in  $V(T)$  there is exactly one vertex of degree  $\beta$  ( $1 < \beta < \Delta$ ) and remaining vertices have degrees 1 or  $\Delta$ .

**Proof of Theorem 2.1.** By Theorem A, we may assume that  $\Delta \geq 5$ . Let  $T$  be a tree such that

$$M_2(T) = \max\{M_2(T') \mid T' \text{ is a tree of order } n \text{ with maximum degree } \Delta\}.$$

By Corollary 2.4,  $T$  has at most one vertex of degree  $t$  where  $2 \leq t \leq \Delta - 1$ . Let  $A$  be the set of all pendant edges of  $T$  and  $B = E(T) \setminus A$ . Define the function  $\omega$



on  $E(T)$  by  $w(uv) = d(u)d(v)$ . Then

$$M_2(T) = \sum_{e \in A} w(e) + \sum_{e \in B} w(e).$$

There are non-negative integers  $k, r$  such that  $n = (\Delta - 1)k + r$  and  $0 \leq r \leq \Delta - 2$ . By (3), we have

$$n_2 + 2n_3 + \dots + (\Delta - 2)n_{\Delta-1} = (\Delta - 1)(k - n_\Delta) + r - 2. \tag{4}$$

**Case 1.**  $n_t = 1$ .

It follows from (4) that  $t + 1 - r = (\Delta - 1)(k - n_\Delta)$  and so  $n_\Delta = k - \frac{t + 1 - r}{\Delta - 1}$ .

Since  $0 \leq r \leq \Delta - 2$  and  $2 \leq t \leq \Delta - 1$  and since  $\frac{t + 1 - r}{\Delta - 1}$  is an integer between 0 and 1, we deduce that one of the following statement holds.

- (a) if  $r = 0$ , then  $t = \Delta - 2$ ,  $n_\Delta = k - 1$ ,  $n_{\Delta-2} = 1$  and  $n_1 = n - k$ ,
- (b) if  $r = 1$ , then  $t = \Delta - 1$ ,  $n_\Delta = k - 1$ ,  $n_{\Delta-1} = 1$  and  $n_1 = n - k$ ,
- (c) if  $3 \leq r \leq \Delta - 2$ , then  $t = r - 1$ ,  $n_\Delta = k$ ,  $n_{r-1} = 1$  and  $n_1 = n - k - 1$ .

Let  $V_i$  be the set consists of all vertices of degree  $i$  for each  $i = 1, 2, \dots, \Delta$ . Suppose  $E_{i,j}$  denotes the set of all edges with one end in  $V_i$  and the other end in  $V_j$ . Clearly,  $E = E_{1,t} \cup E_{1,\Delta} \cup E_{t,\Delta} \cup E_{\Delta,\Delta}$  and  $t = |E_{1,t}| + |E_{t,\Delta}|$ . Therefore

$$\begin{aligned} M_2(T) &= \sum_{e \in A} w(e) + \sum_{e \in B} w(e) \\ &= (|E_{1,t}| \cdot t + |E_{1,\Delta}| \cdot \Delta) + (|E_{t,\Delta}| \cdot t\Delta + |E_{\Delta,\Delta}| \cdot \Delta^2) \\ &= (|E_{1,t}| \cdot t + (n_1 - |E_{1,t}|)\Delta) + (|E_{t,\Delta}| \cdot t\Delta + (n - n_1 - |E_{t,\Delta}| - 1) \cdot \Delta^2) \\ &= (t - \Delta)(|E_{1,t}| + \Delta|E_{t,\Delta}|) + n_1\Delta - n_1\Delta^2 + (n - 1)\Delta^2. \end{aligned} \tag{**}$$

Since  $t - \Delta < 0$  and  $M_2(T)$  is maximum, we should minimize  $|E_{1,t}| + |E_{t,\Delta}|\Delta$ . It follows from  $t = |E_{1,t}| + |E_{t,\Delta}|$  that  $|E_{t,\Delta}| = 1$  and  $|E_{1,t}| = t - 1$ . Hence,

$$M_2(T) = t^2 - t - 2\Delta^2 + \Delta + n_1\Delta - n_1\Delta^2 + n\Delta^2. \tag{***}$$

If (a) holds, then  $n = (\Delta - 1)k$  and by (\*\*\*) we have

$$\begin{aligned} M_2(T) &= (\Delta - 2)^2 - (\Delta - 2) - 2\Delta^2 + \Delta + (\Delta - 2)k\Delta - (\Delta - 2)k\Delta^2 + (\Delta - 1)k\Delta^2 \\ &= -\Delta^2 - 4\Delta + 6 - 2k\Delta + 2k\Delta^2 \\ &= 2n\Delta - \Delta^2 - 4\Delta + 6. \end{aligned}$$

If (b) holds, then  $n = (\Delta - 1)k + 1$  and by (\*\*\*) we obtain

$$\begin{aligned} M_2(T) &= (\Delta - 1)^2 - (\Delta - 1) - 2\Delta^2 + \Delta + ((\Delta - 2)k + 1)\Delta - ((\Delta - 2)k + 1)\Delta^2 \\ &\quad + ((\Delta - 1)k + 1)\Delta^2 \\ &= -\Delta^2 - \Delta + 2 - 2k\Delta + 2k\Delta^2 \\ &= -\Delta^2 - \Delta + 2 + 2(n - 1)\Delta \\ &= 2n\Delta - \Delta^2 - 3\Delta + 2. \end{aligned}$$

If (c) holds, then  $n = (\Delta - 1)k + r$  and by (\*\*\*) we have

$$\begin{aligned} M_2(T) &= t^2 - t - 2\Delta^2 + \Delta + n_1\Delta - n_1\Delta^2 + n\Delta^2 \\ &= r^2 - 3r + 2 - \Delta^2 - 2k\Delta + r\Delta + 2k\Delta^2. \\ &= 2k(\Delta - 1)\Delta - \Delta^2 + r\Delta + 2 + r(r - 3) \\ &= 2n\Delta - \Delta^2 - r\Delta + 2 + r(r - 3). \end{aligned}$$

**Case 2.**  $n_t = 0$ .

By (4) we have  $(\Delta - 1)(k - n_\Delta) + r - 2 = 0$  that leads to  $r = 2$  and  $n_\Delta = k$ . It follows from (\*\*) that

$$\begin{aligned} M_{2_{max}}(T) &= n_1\Delta - n_1\Delta^2 + (n - 1)\Delta^2 \\ &= ((\Delta - 2)k + 2)\Delta - ((\Delta - 2)k + 2)\Delta^2 + ((\Delta - 1)k + 1)\Delta^2 \\ &= 2\Delta(\Delta - 1)k - \Delta^2 + 2\Delta \\ &= 2\Delta(n - 2) - \Delta^2 + 2\Delta \\ &= 2n\Delta - \Delta^2 - 2\Delta. \end{aligned}$$

This completes the proof.  $\square$

### 3. Lower Bound on the Second Zagreb Coindex among All Trees

In [1], Ashrafi and others proved that for any connected graph  $G$  with  $n$  vertices and  $m$  edges,

$$\overline{M}_2(G) = 2m^2 - M_2(G) - \frac{1}{2}M_1(G).$$

The next corollary is direct consequence this equality and Theorem 2.1.

**Corollary 3.1.** Let  $T$  be a tree of order  $n$  and maximum degree  $\Delta$ . If  $n \equiv r \pmod{\Delta - 1}$ , then

$$2\overline{M}_2(T) \geq \begin{cases} 4n^2 - 5n(\Delta + 2) + 2\Delta^2 + 12(\Delta - 1) & r = 0 \\ 4n^2 - 5n(\Delta + 2) + 2\Delta^2 + 9\Delta & r = 1 \\ 4n^2 - 5n(\Delta + 2) + 2\Delta^2 + 6(\Delta + 1) & r = 2 \\ 4n^2 - 5n(\Delta + 2) + 2\Delta^2 + (2 + 3r)\Delta + (7 - 3r)r & r \geq 3. \end{cases}$$

*Proof.* From Theorem 2.1, we conclude that  $2\overline{M}_2(G) = 4n^2 - 8n + 4 - (2M_2(T) + M_1(T))$ . Now by Theorem 2.1 and Corollary 2.1, the proof is straightforward.  $\square$

**Conflicts of Interests.** The authors declare that there are no conflicts of interest regarding the publication of this article.

## References

- [1] A. R. Ashrafi, T. Došlić and A. Hamzeh, The Zagreb coindices of graph operations, *Discrete Appl. Math.* **158** (2010) 1571–1578.
- [2] K. Ch. Das, Sharp bounds for the sum of the squares of the degrees of a graph, *Kragujevac J. Math.* **25** (2003) 31–49.
- [3] K. Ch. Das, Maximizing the sum of the squares of the degrees of a graph, *Discrete Math.* **285** (2004) 57–66.
- [4] D. de Caen, An upper bound on the sum of squares in a graph, *Discrete Math.* **185** (1998) 245–248.
- [5] T. Došlić, Vertex-weighted Wiener polynomials for composite graphs, *Ars Math. Contemp.* **1** (2008) 66–80.
- [6] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals, total  $\pi$ -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.
- [7] Ž. Kovijanić Vukićević and G. Popivoda, Chemical trees with extreme values of Zagreb indices and coindices, *Iranian J. Math. Chem.* **5** (2014) 19–29.
- [8] X. Li and I. Gutman, *Mathematical Aspects of Randić-Type Molecular Structure Descriptors*, Mathematical Chemistry Monograph 1, University of Kragujevac and Faculty of Science Kragujevac, Kragujevac, 2006.
- [9] S. Nikolić, G. Kovačević, A. Miličević and N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta* **76** (2003) 113–124.
- [10] R. Rasi, S. M. Sheikholeslami and A. Behmaram, An upper bound on the first Zagreb index in trees, *Iranian J. Math. Chem.* **8**(1) (2017) 71–82.

- [11] S. Zhang, W. Wang and T. C. E. Cheng, Bicyclic graphs with the first three smallest and largest values of the first general Zagreb index, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 579–592.
- [12] B. Zhou and I. Gutman, Relations between Wiener, hyper-Wiener and Zagreb indices, *Chem. Phys. Lett.* **394** (2004) 93–95.

Reza Rasi  
Department of Mathematics,  
Azarbaijan Shahid Madani University,  
Tabriz, I. R. Iran  
E-mail: r.raii@azaruniv.edu

Seyed Mahmoud Sheikholeslami  
Department of Mathematics,  
Azarbaijan Shahid Madani University,  
Tabriz, I. R. Iran  
E-mail: s.m.sheikholeslami@azaruniv.edu

Afshin Behmaram  
Faculty of Mathematical Sciences,  
University of Tabriz,  
Tabriz, I. R. Iran  
E-mail: behmaram@tabrizu.ac.ir