Iranian J. Math. Chem. 8(1) March (2017) 71−82

Iranian Journal of Mathematical Chemistry

Journal homepage: www.ijmc.kashanu.ac.ir

An Upper Bound on the First Zagreb Index in Trees

R. RASI[1], S. M. SHEIKHOLESLAMI[1,•] AND A. BEHMARAM[2]

[1] Department of Mathematics, Azarbaijan Shahid Madani University, Tabriz, I. R. Iran
[2] Faculty of Mathematical Sciences, University of Tabriz, Tabriz, I. R. Iran

ARTICLE INFO

Article History:

Received: 1 March, 2016
Accepted: 10 June 2016
Published online 6 February 2017
Academic Editor: Tomislav Došlić

Keywords:

first Zagreb index
first Zagreb coindex
tree
Chemical tree

ABSTRACT

The first Zagreb index $M_1(G)$ is equal to the sum of squares of the degrees of the vertices and the first Zagreb coindex $\overline{M_1}(G)$ is equal to the sum of sums of vertex degrees of the pairs of non-adjacent vertices. Kovijanić Vukićević and G. Popivoda (Iran. J. Math. Chem. **5** (2014) 19–29) proved that for any chemical tree of order n, $n \geq 5$,

$$M_1(T) \leq \begin{cases} 6n-12 & n \equiv 0,1 \pmod 3 \\ 6n-10 & \text{otherwise.} \end{cases}$$

In this paper, we generalize the aforementioned bound for all trees in terms of their order and maximum degree. Moreover, we give a lower bound on the first Zagreb coindex of trees.

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 $\delta = \delta(G)$ and $\Delta = \Delta(G)$, respectively. Trees with the property $\Delta \leq 4$ are called chemical trees.

The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajestić in [6]. They are important molecular descriptors and have been closely correlated with many chemical properties [6, 7]. Thus, it attracted more and more attention from chemists and mathematicians [2, 3, 4, 8, 10, 11].

The *first Zagreb index* $M_1(G)$ is defined as follows:

• Corresponding Author: (Email address: (m.sheikholeslami@azaruniv.edu)
DOI: 10.22052/ijmc.2017.42995

$$M_1(G) = \sum_{v \in V} d_v^2.$$

The first Zagreb index can be also expressed as the sum of vertex degree over edges of G, that is, $M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$. Došlić in [5] introduced a new graph invariant called the *first Zagreb coindex*, as $\overline{M}_1(G) = \sum_{uv \notin E(G)} (d_u + d_v)$. Next we introduce a family of trees. For $n = (\Delta - 1)k + p$ $(k \geq 2)$, let T_n be the family of trees of order n with maximum degree Δ such that:

- If $p = 0$, $k-1$ vertices have degree Δ, 1 vertex has degree $\Delta - 2$ and remaining vertices are pendant.
- If $p = 1$, $k-1$ vertices have degree Δ, 1 vertex has degree $\Delta - 1$ and remaining vertices are pendant.
- If $p = 2$, k vertices have degree Δ and remaining vertices are pendant.
- If $p \geq 3$, k vertices have degree Δ, 1 vertex has degree $p-1$, and $n-k-1$ remaining vertices are pendant.

Kovijanić Vukićević and Popivoda [9] proved the following upper bound on the first Zagreb index of chemical trees and characterized all extreme chemical trees.

Theorem 1. Let T be a chemical tree with $n \geq 5$ vertices. Then

$$M_1(T) \leq \begin{cases} 6n - 12 & n \equiv 0,1 \,(\mathrm{m}od\ 3) \\ 6n - 10 & \mathrm{o}therwise, \end{cases}$$

with equality if and only if $G \in \mathsf{T}_n$.

In this paper, we establish an upper bound on the first Zagreb index of trees in terms of the order and maximum degree, as a generalization of aforementioned bound. As a consequence, we obtain a lower bound on the first Zagreb coindex for trees.

2. MAIN RESULTS

In this section, we prove the following result:

Theorem 2. Let T be a tree of order n and maximum degree Δ. If $n \equiv p$ (mod $\Delta - 1$), then

$$M_1(T) \le \begin{cases} (\Delta+2)n-4\Delta+4 & p=0 \\ (\Delta+2)n-3\Delta & p=1 \\ (\Delta+2)n-2\Delta-2 & p=2 \\ (\Delta+2)n-2\Delta-3+p(p-2) & p\ge 3, \end{cases}$$

with equality if and only if $G \in \mathrm{T}_n$.

To prove Theorem 2, we proceed with some definitions and lemmas. If n is a positive integer, then an integer partition of n is a non-increasing sequence of positive integers $(a_1, a_2, \ldots, a_t)$ whose sum is n. If $1 \le a_1 \le a_2 \le \ldots \le a_t \le a$, then $(a_1, a_2, \ldots, a_t)$ is called an integer partition of n on $N_a = \{1, 2, \ldots, a\}$. An integer partition $(a_1, a_2, \ldots, a_t)$ of n on N_a is called an integer a-partition if the number of a in this partition is as large as possible. In other words, if $n = ka$, then $(a, \ldots, a)$ is the integer a–partition and if $n = ka + b$ where $0 < b < a$ then $(b, a, \ldots, a)$ is the integer a–partition. The proof of the next result is straightforward and therefore omitted.

Lemma 3. *For positive integers* n, t *and* a_i *(*$1 \le i \le t$*), we have*

a) If $n = a_1 + a_2 + \ldots + a_t$ and $t > 1$, then $n^2 > a_1^2 + a_2^2 + \cdots + a_t^2$.

b) If $a_i \le a_j$, then $(a_i - 1)^2 + (a_j + 1)^2 \ge a_i^2 + a_j^2 + 2$.

Lemma 4. *If* $(a_1, a_2, \ldots, a_t)$ *is an integer partition of* $n = ka + b$ $(0 \le b < a)$ *on* N_a*, then*

$$\sum_{i=1}^{t} a_i^2 < ka^2 + b^2.$$

Proof. Let $(a_1, a_2, \ldots, a_t)$ be an partition of n on N_a. If $a_i \le a_j < a$ for some $1 \le i \ne j \le t$, then by switching (a_i, a_j) to $(a_i - 1, a_j + 1)$, we get a new integer partition of n on N_a Note that if $a_i - 1 = 0$, then we will remove $a_i - 1$ from the new partition. Applying Lemma 3 (a), we obtain

$$\sum_{i=1}^{t} a_i^2 < a_1^2 + \cdots + (a_i - 1)^2 + \cdots + (a_j + 1)^2 + \cdots + a_t^2.$$

By repeating this process, we arrive at an integer a–partition of n on N_a. It follows from Lemma 2 that $\sum_{i=1}^{t} a_i^2 < ka^2 + b^2$ and the proof is complete.

Lemma 5. Let $n=ka+b$ where $0\le b<a$ and let $(a_1,a_2,\ldots,a_t)$ be an integer partition of n on N_a which is not a–partition. Then the following statements holds:

a. If $b>0$, then $\sum_{i=1}^{t}(a_i+1)^2<k(a+1)^2+(b+1)^2$.

b. If $b=0$, then $\sum_{i=1}^{t}(a_i+1)^2<k(a+1)^2$.

Proof. (a) Since $n=a_1+\cdots+a_t=b+\underbrace{a+\cdots+a}_{k}=ka+b$, we have $t\ge k+1$. First let $t=k+1$. Then we have

$$\begin{aligned}(a_1+1)^2+\cdots+(a_t+1)^2 &= (a_1^2+\cdots+a_t^2)+t+2(ka+b)\\ &< (ka^2+b^2)+t+2(ka+b) \qquad \text{(by Lemma3)}\\ &= k(a+1)^2+(b+1)^2+t-(k+1)\\ &= k(a+1)^2+(b+1)^2,\end{aligned}$$

as desired. Now let $t>k+1$. Repeating the switching process described in the proof of Lemma 4, i.e. for any pair (a_i,a_j) where $1\le a_i<a_j<a$ and using the fact that $a_i^2+a_j^2\le(a_i-1)^2+(a_j+1)^2-2$, we get $a_i=0$ or $a_j=a$. To achieving an integer a–partition, we need to apply the switching process at least $t-(k+1)$ times. This implies that

$$a_1^2+\cdots+a_t^2\le ka^2+b^2-2(t-(k+1)). \qquad (1)$$

Thus

$$\begin{aligned}(a_1+1)^2+\ldots+(a_t+1)^2 &= (a_1^2+\ldots+a_t^2)+t+2(ka+b)\\ &\le ka^2+b^2-2(t-(k+1))+t+2(ka+b) \quad \text{(by } \textit{inequality } (1))\\ &= k(a+1)^2+(b+1)^2-(t-(k+1))\\ &< k(a+1)^2+(b+1)^2.\end{aligned}$$

(b) If $b=0$,then $n=a_1+\cdots+a_t=\underbrace{a+\cdots+a}_{k}=ka$. Since $(a_1,\ldots,a_t)$ is not a–partition, we have $t>k$. Applying (1), we obtain

$$\begin{aligned}(a_1+1)^2+\cdots+(a_t+1)^2 &= (a_1^2+\cdots+a_t^2)+t+2ka\\ &\le ka^2-2(t-k)+t+2ka\\ &= k(a+1)^2+k-t\\ &< k(a+1)^2.\end{aligned}$$

This completes the proof.

Remark 6. Let T be a tree of order n and maximum degree Δ. For each $i \in \{1,2,\ldots,\Delta\}$, let n_i denote the number of vertices of degree i. Then

$$n_1 + n_2 + \ldots + n_\Delta = n \tag{2}$$

and

$$n_1 + 2n_2 + \ldots + \Delta n_\Delta = 2n - 2. \tag{3}$$

Subtracting (2) from (3), yields

$$n_2 + 2n_3 + \ldots + (\Delta - 1)n_\Delta = n - 2. \tag{4}$$

By (4), we obtain the following integer partition

$$(\underbrace{1,\ldots,1}_{n_2}, \underbrace{2,\ldots,2}_{n_3}, \ldots, \underbrace{\Delta-1,\ldots,\Delta-1}_{n_\Delta}), \tag{5}$$

of $n-2$ on $N_{\Delta-1} = \{1,2,\ldots,\Delta-1\}$. It follows from Lemma 4 that $2^2 n_2 + 3^2 n_3 + \ldots + \Delta^2 n_\Delta$ is maximum if and only if the partition (5) obtained from (4), is an $(\Delta-1)-$partition of $n-2$ on $N_{\Delta-1}$. In that case, n_1 (the number of leaves) will be maximum.

Next result is an immediate consequence of above discussion.

Corollary 7. For any tree T of order n with maximum degree Δ, the first Zagreb index $M_1(T) = n_1 + 2^2 n_2 + \cdots + \Delta^2 n_\Delta$ is maximum if and only if the integer partition (5) is an $(\Delta-1)$–partition of $n-2$ on $N_{\Delta-1}$. In that case, the integer partition $(n_1, n_2, \ldots, n_\Delta)$ is called an optimal solution of (4).

Theorem 8. Let T be a tree of order n and maximum degree Δ with $n \equiv 0 \pmod{\Delta-1}$. Then $M_1(T) \le (\Delta+2)n - 4\Delta + 4$, with equality if and only if $T \in \mathsf{T}_n$.

Proof. Assume that $n = (\Delta-1)k$. By (4),

$$n_\Delta = k - \left(\frac{n_2 + 2n_3 + \cdots + (\Delta-2)n_{\Delta-1} + 2}{\Delta - 1}\right) = k - r,$$

where $r = \dfrac{n_2 + 2n_3 + \cdots + (\Delta-2)n_{\Delta-1} + 2}{\Delta - 1}$. Then $1 \le r \le k-1$ and $1 \le n_\Delta \le k-1$. We consider three cases as follows:

Case 1. $r = 1$. Then clearly $n_\Delta = k-1$. It follows that

$$n_2 + 2n_3 + \cdots + (\Delta-2)n_{\Delta-1} + (\Delta-1)(k-1) = (\Delta-1)k - 2$$

and so

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

Thus $n_{\Delta-1} = 0$ and so

$$n_2 + 2n_3 + \cdots + (\Delta - 3).n_{\Delta-2} = \Delta - 3. \tag{6}$$

According to Corollary 6, the optimal solution of (6) is $n_2 = n_3 = \cdots = n_{\Delta-3} = 0$ and $n_{\Delta-2} = 1$. Since $n_1 + n_2 + \cdots + n_\Delta = n$, we conclude that $n_1 = (\Delta - 2)k$. By Corollary 7,

$$(n_1, n_2, \ldots, n_{\Delta-3}, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta - 2)k, 0, \ldots, 0, 1, 0, k - 1)$$

is the optimal solution and so $M_1(T)$ is maximum. Therefore,

$$\begin{aligned} M_1(T) &\le n_1 + 2^2 n_2 + \ldots + (\Delta - 2)^2.n_{\Delta-2} + (\Delta - 1)^2.n_{\Delta-1} + \Delta^2.n_\Delta \\ &= (\Delta - 2)k + (\Delta - 2)^2 + \Delta^2(k - 1) \\ &= (\Delta + 2)(\Delta - 1)k - 4\Delta + 4 \\ &= (\Delta + 2)n - 4\Delta + 4. \end{aligned}$$

Case 2. $2 \le r < \Delta$. Then $n_2 + 2n_3 + \ldots + (\Delta - 2)n_{\Delta-1} = (\Delta - 2)r + (r - 2)$. Since $r - 2 < \Delta - 2$, it follows from Corollary 7 that

$$(n_1, n_2, \ldots, n_{r-2}, n_{r-1}, n_r, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta - 2)k - 1, 0, \ldots, 0, 1, 0, \ldots, 0, r, k - r)$$

is an optimal solution in this case. Since $2 \le r < \Delta$ and $4 \le \Delta$, we have $r(r - 2\Delta - 1) < -4\Delta + 4$ and so

$$\begin{aligned} M_1(T) &\le (\Delta - 2)k - 1 + (r - 1)^2 + (\Delta - 1)^2 r + \Delta^2(k - r) \\ &= (\Delta + 2)(\Delta - 1)k + r(r - 2\Delta - 1) \\ &< (\Delta + 2)n - 4\Delta + 4. \end{aligned}$$

Case 3. $\Delta \le r \le k - 1$. Then $n_2 + 2n_3 + \ldots + (\Delta - 2).n_{\Delta-1} = (\Delta - 2)r + (r - 2)$. There are non-negative integers t, s such that $(r - 2) = t(\Delta - 2) + s$ and $0 \le s < \Delta - 2$. Hence $n_2 + 2n_3 + \ldots + (\Delta - 2).n_{\Delta-1} = (\Delta - 2)(r + t) + s.$ If $0 < s < \Delta - 2$, then

$$(n_1, n_2, \ldots, n_s, n_{s+1}, n_{s+2}, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta - 2)k - (t + 1), 0, \ldots, 0, 1, 0, \ldots, 0, r + t, k - r)$$

is the optimal solution and since $(s - \Delta) < 0$ and $4 \le \Delta \le r$, we obtain

$$\begin{aligned} M_1(T) &\le (\Delta - 2)k - (t + 1) + (s + 1)^2 + (\Delta - 1)^2(r + t) + \Delta^2(k - r) \\ &= (\Delta + 2)(\Delta - 1)k + s(s + 2) + r(1 - 2\Delta) + t\Delta(\Delta - 2) \\ &= (\Delta + 2)n + (s - \Delta)(s + 2) - r\Delta + r \\ &< (\Delta + 2)n + (s - \Delta)(s + 2) - r\Delta + r \\ &< (\Delta + 2)n - 4\Delta + 4. \end{aligned}$$

If $s = 0$, then the optimal solution is

$$(n_1, n_2, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta - 2)k - t, 0, \ldots, 0, r + t, k - r).$$

Since $t(\Delta-2)=r-2-s$, $(s+2)>0$ and $4\le\Delta\le r$, we conclude that

$$\begin{aligned} M_1(T) &\le n_1+4n_2+9n_3+\ldots+\Delta^2.n_\Delta \\ &= ((\Delta-2)k-t)+(\Delta-1)^2(r+t)+\Delta^2(k-r) \\ &= \Delta k-2k-t+\Delta^2 r-2\Delta r+r+\Delta^2 t-2\Delta t+t+\Delta^2 k-\Delta^2 r \\ &= (\Delta+2)n-(s+2)-r\Delta+r \\ &< (\Delta+2)n-r\Delta+r \\ &< (\Delta+2)n-4\Delta+4. \end{aligned}$$

Therefore, in all cases $M_1(T)\le(\Delta+2)n-4\Delta+4$. If $T\in\mathsf{T}_n$, then clearly $M_1(T)=(\Delta+2)n-4\Delta+4$. Conversely, let T be a tree of order n with $n\equiv 0 \pmod{\Delta-1}$ and $M_1(T)=(\Delta+2)n-4\Delta+4$. This occurs only in Case 1, that is, T has $k-1=\frac{n-\Delta+1}{\Delta-1}$ vertices of degree Δ, one vertex of degree $\Delta-2$ and $(\Delta-2)k$ leaves. Hence $T\in\mathsf{T}_n$ and the proof is complete.

Theorem 9. Let T be a tree of order n with maximum degree Δ and $n\equiv 1 \,(\mathrm{mod}\ \Delta-1)$. Then $M_1(T)\le(\Delta+2)n-3\Delta,$ with equality if and only if $T\in\mathsf{T}_n$.

Proof. Let $n=(\Delta-1)k+1$. Set $r=\frac{n_2+2n_3+\ldots+(\Delta-2)n_{\Delta-1}+1}{\Delta-1}$. By (4),

$$n_\Delta = k-\left(\frac{n_2+2n_3+\ldots+(\Delta-2)n_{\Delta-1}+1}{\Delta-1}\right)=k-r.$$

Then clearly $1\le r\le k-1$ and $1\le n_\Delta\le k-1$. We consider three cases.

Case 1. $r=1$. Since $n_\Delta=k-1$, it follows from (4) that $n_2+\ldots+(\Delta-2).n_{\Delta-1}=(\Delta-2)$ and by Corollary 7

$$(n_1,n_2,\ldots,n_{\Delta-2},n_{\Delta-1},n_\Delta)=((\Delta-2)k+1,0,\ldots,0,1,k-1)$$

is the optimal solution. Thus

$$\begin{aligned} M_1(T) &\le n_1+2^2 n_2+\ldots+(\Delta-2)^2.n_{\Delta-2}+(\Delta-1)^2.n_{\Delta-1}+\Delta^2.n_\Delta \\ &= ((\Delta-2)k+1)+(\Delta-1)^2(1)+\Delta^2(k-1) \\ &= (\Delta+2)n-3\Delta. \end{aligned}$$

Case 2. $2\le r<\Delta-1$. As above, $n_2+\ldots+(\Delta-2).n_{\Delta-1}=(\Delta-2)r+(r-1)$. Since $r-1<\Delta-2$, it follows from Corollary 7 that

$$(n_1, n_2, \ldots, n_{r-1}, n_r, n_{r+1}, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta-2)k, 0, \ldots, 0, 1, 0, \ldots, 0, r, k-r)$$

is the optimal soloution. Since $2 \le r < \Delta - 1$, it is easy to see that $2\Delta(1-r) + (r^2 + r - 2) < 0$ and we have

$$\begin{aligned} M_1(T) &= n_1 + 4n_2 + \ldots + (\Delta-2)^2 . n_{\Delta-2} + (\Delta-1)^2 . n_{\Delta-1} + \Delta^2 . n_\Delta \\ &= (\Delta-2)k + r^2(1) + (\Delta-1)^2 r + \Delta^2(k-r) \\ &= (\Delta+2)(\Delta-1)k + r^2 + r - 2r\Delta \\ &= (\Delta+2)n - 3\Delta + 2\Delta(1-r) + (r^2 + r - 2) \\ &< (\Delta+2)n - 3\Delta. \end{aligned}$$

Case 3. $\Delta - 1 \le r \le k - 1$. There are non-negative integers t, s such that $r - 1 = t(\Delta-2) + s$, $t \ge 1$ and $s < \Delta - 1$. By substituting in (4), we have $n_2 + 2n_3 + \ldots + (\Delta-2)n_{\Delta-1} = (\Delta-2)(r+t) + s$. First let $0 < s$. Since $s \le \Delta - 2$, it follows from Corollary 7 that

$$(n_1, n_2, \ldots, n_s, n_{s+1}, n_{s+2}, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta-2)k - t, 0, \ldots, 0, 1, 0, \ldots, 0, 0, r+t, k-r)$$

is the optimal solution. Thus

$$\begin{aligned} M_1(T) &\le (\Delta-2)k - t + (s+1)^2 + (\Delta-1)^2(r+t) + \Delta^2(k-r) \\ &= (\Delta+2)(\Delta-1)k + (s+1)^2 + r(1-2\Delta) + t\Delta(\Delta-2) \\ &= (\Delta+2)n - 3\Delta - s(\Delta-s-2) - (r-1)(\Delta-1) \\ &< (\Delta+2)n - 3\Delta. \end{aligned}$$

Now let $s = 0$. Then the optimal solution is

$$(n_1, n_2, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta-2)k - t + 1, 0, \ldots, 0, r+t, k-r)$$

and we have

$$\begin{aligned} M_1(T) &\le (\Delta-2)k - t + 1 + (\Delta-1)^2(r+t) + \Delta^2(k-r) \\ &= (\Delta+2)(\Delta-1)k - r(2\Delta-1) + 1 + t\Delta(\Delta-2) \\ &= (\Delta+2)n - 3\Delta - (\Delta-1)(r-1) \\ &< (\Delta+2)n - 3\Delta. \end{aligned}$$

As in the proof of Theorem 8 we can see that $M_1(T) = (\Delta+2)n - 3\Delta$ if and only if $T \in \mathrm{T}_n$.

Theorem 10. Let T be a tree of order n with maximum degree Δ and $n \equiv p \pmod{\Delta - 1}$ where $2 \le p \le \Delta - 2$. Then

$$M_1(T) \le \begin{cases} (\Delta+2)n - 2\Delta - 2 & p = 2 \\ (\Delta+2)n - 2\Delta - 3 + p(p-2) & p \ge 3, \end{cases}$$

with equality if and only if $T \in \mathsf{T}_n$.

Proof. Let $n = (\Delta-1)k + p$. Suppose that $r = \dfrac{n_2 + 2n_3 + \ldots + (\Delta-2)n_{\Delta-1} + (2-p)}{\Delta-1}$. By (4), we have

$$n_\Delta = k - \left(\frac{n_2 + 2n_3 + \ldots + (\Delta-2)n_{\Delta-1} + (2-p)}{\Delta-1}\right) = k - r.$$

Then clearly $0 \le r \le k-1$ and $1 \le n_\Delta \le k$. We consider four cases.

Case 1. $r = 0$. Then $n_\Delta = k$ and by (4) we have

$$n_2 + 2n_3 + \cdots + (\Delta-2).n_{\Delta-1} = (n-2) - ((\Delta-1).n_\Delta) = ((\Delta-1)k + p - 2) - (\Delta-1)k = p - 2.$$

If $p = 2$, then $n_2 + 2n_3 + \ldots(\Delta-2).n_{\Delta-1} = 0$. This implies that $n_2 = n_3 = \ldots = n_{\Delta-1} = 0$ and $n_1 = n - k$ by (2). Thus

$$\begin{aligned} M_1(T) &\le n_1 + 2^2 n_2 + \cdots + (\Delta-1)^2.n_{\Delta-1} + \Delta^2.n_\Delta \\ &= (n-k) + \Delta^2 k \\ &= n + (\Delta+1)(\Delta-1)k \\ &= n + (\Delta+1)(n-2) \\ &= (\Delta+2)n - 2\Delta - 2. \end{aligned}$$

Now let $2 < p \le \Delta - 2$. Since $1 \le p - 2 \le \Delta - 4$ and $n_2 + 2n_3 + \ldots(\Delta-2).n_{\Delta-1} = p - 2$, it follows from Corollary 7 that

$$(n_1, n_2, \ldots, n_{p-2}, n_{p-1} n_p, \ldots, n_{\Delta-1}, n_\Delta) = (n-k-1, 0, \ldots, 0, 1, 0, \ldots, 0, k)$$

is the optimal solution and so

$$\begin{aligned} M_{1_{max}}(T) &\le n_1 + 4n_2 + \ldots + (\Delta-1)^2.n_{\Delta-1} + \Delta^2.n_\Delta \\ &= (n-k-1) + (p-1)^2(1) + \Delta^2(k) \\ &= (\Delta+1)(\Delta-1)k + n + p^2 - 2p \\ &= (\Delta+1)(n-p) + n + p^2 - 2p \\ &= (\Delta+2)n - p\Delta + p^2 - 3p. \end{aligned}$$

Case 2. $r = 1$. Then $n_\Delta = k - 1$ and

$$(n_1, n_2, \ldots, n_{p-1}, n_p, n_{p+1}, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta-2)k + p - 1, 0, \ldots, 0, 1, 0, \ldots, 0, 1, k-1)$$

is the optimal solution and since $p \le \Delta - 2$ we have

$$\begin{aligned} M_1(T) &= n_1 + 4n_2 + \ldots + (\Delta-1)^2.n_{\Delta-1} + \Delta^2.n_\Delta \\ &= (\Delta-2)k + p - 1 + p^2 + (\Delta-1)^2 + \Delta^2(k-1) \\ &= \Delta k - 2k + p - 1 + p^2 + \Delta^2 - 2\Delta + 1 + \Delta^2 k - \Delta^2 \\ &= (\Delta+2)(\Delta-1)k + p + p^2 - 2\Delta \\ &= (\Delta+2)(n-p) + p + p^2 - 2\Delta \\ &< (\Delta+2)n - p\Delta + p^2 - 3p. \end{aligned}$$

Case 3. $2 \le r < \Delta - p$. By (4), we have $n_2 + 2n_3 + \ldots + (\Delta-2)n_{\Delta-1} = (\Delta-2)r + (p+r-2)$. Since $r-2 < \Delta-2$, it follows from Corollary 7 that
$(n_1, n_2, \ldots, n_{p+r-2}, n_{p+r-1}, n_{p+r}, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta-2)k + p - 1, 0, \ldots, 0, 1, 0, \ldots, 0, r, k-r)$
is the optimal solution. On the other hand, we deduce from $p \le \Delta - 2$ and $r < \Delta - p$ that $r - 1 + 2(p-\Delta) < \Delta - p - 1 + 2(p-\Delta) = p - \Delta - 1 < 0$ and so $r(r-1+2(p-\Delta)) < 0$. Thus

$$\begin{aligned} M_1(T) &\le n_1 + 4n_2 + \ldots + (\Delta-1)^2.n_{\Delta-1} + \Delta^2.n_\Delta \\ &= ((\Delta-2)k + p - 1) + (p+r-1)^2(1) + (\Delta-1)^2(r) + \Delta^2(k-r) \\ &= \Delta k - 2k + p - 1 + p^2 + r^2 + 1 + 2rp - 2p - 2r + r\Delta^2 - 2\Delta r + r + \Delta^2 k - r\Delta^2 \\ &= (\Delta+2)(\Delta-1)k + p^2 - p - 2\Delta r + r(r + 2p - 1) \\ &= (\Delta+2)(n-p) + p^2 - p - 2\Delta r + r(r+2p-1) \\ &= (\Delta+2)n - p\Delta + p^2 - 3p + r(r - 1 + 2(p-\Delta)) \\ &< (\Delta+2)n - p\Delta + p^2 - 3p = M_{1_{max}}(T). \end{aligned}$$

Case 4. $\Delta - p \le r \le k-1$. Let $p + r - 2 = t(\Delta-2) + s$. By substituting in (4), we have $n_2 + 2n_3 + \ldots + (\Delta-2)n_{\Delta-1} = (\Delta-2)(r+t) + s$. If $s = 0$ then by Corollary 7,

$$(n_1, n_2, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta-2)k + p - t, 0, \ldots, 0, r+t, k-r)$$

is the optimal solution. Since $\Delta - p \le r$ and $p \le \Delta - 2$, we have

$$\begin{aligned} (2p - p^2 + p\Delta - \Delta r - 2\Delta + r) &= p(\Delta - p + 2) - \Delta r - 2\Delta + r \\ &\le p(r+2) - \Delta r - 2\Delta + r \\ &= (p-\Delta)(r+2) + r \\ &< (p-\Delta)(r+2) + (r+2) \\ &= (p - \Delta + 1)(r+2) < 0. \end{aligned}$$

Thus

$$\begin{aligned} M_1(T) &= n_1 + 4n_2 + \ldots + (\Delta-1)^2.n_{\Delta-1} + \Delta^2.n_\Delta \\ &= ((\Delta-2)k + p - t) + (\Delta-1)^2(r+t) + \Delta^2(k-r) \\ &= (\Delta^2 k + \Delta k - 2k) + \Delta t(\Delta-2) + p - 2\Delta r + r \\ &= (\Delta+2)(n-p) + \Delta t(\Delta-2) + p - 2\Delta r + r \\ &= (\Delta+2)n - p\Delta - 2p + p\Delta + \Delta r + p - 2\Delta - 2\Delta r + r \\ &= (\Delta+2)n - p\Delta + p^2 - 3p + (2p - p^2 + p\Delta - \Delta r - 2\Delta + r) \\ &< (\Delta+2)n - p\Delta + p^2 - 3p. \end{aligned}$$

Now let $0 < s$. Since $s < \Delta - 2$, it follows from Corollary 7 that $(n_1, n_2, \ldots, n_s, n_{s+1}, n_{s+2}, \ldots, n_{\Delta-2}, n_{\Delta-1}, n_\Delta) = ((\Delta-2)k + p - (t+1), 0, \ldots, 0, 1, 0, \ldots, 0, 0, r+t, k-r)$ is the optimal solution. Since $2 \le p \le \Delta - 2$ and $0 < s \le \Delta - 3$, it is straightforward to verify that $p\Delta - p^2 + 2p + s^2 + 2s - \Delta r + r - 2\Delta - \Delta s < 0$. Thus

$$\begin{aligned} M_1(T) &= n_1 + 4n_2 + \cdots + (\Delta-1)^2.n_{\Delta-1} + \Delta^2.n_\Delta \\ &= (\Delta-2)k + p - (t+1) + (s+1)^2 + (\Delta-1)^2(r+t) + \Delta^2(k-r) \\ &= (\Delta^2 k + \Delta k - 2k) + p + s^2 + 2s - 2\Delta r + r + \Delta^2 t - 2\Delta t \\ &= (\Delta+2)(\Delta-1)k + p + s^2 + 2s - 2\Delta r + r + \Delta t(\Delta-2) \\ &= (\Delta+2)(n-p) + p + s^2 + 2s - 2\Delta r + r + \Delta(p + r - 2 - s) \\ &= (\Delta+2)n - p + s^2 + 2s - \Delta r + r - 2\Delta - \Delta s \\ &= (\Delta+2)n - p\Delta + p^2 - 3p + (p\Delta - p^2 + 2p + s^2 + 2s - \Delta r + r - 2\Delta - \Delta s) \\ &< (\Delta+2)n - p\Delta + p^2 - 3p. \end{aligned}$$

Therefore, in all cases $M_1(T) \le \Delta + 2)n - p\Delta + p^2 - 3p$. As in the proof of Theorem 8, we can see that

$$M_1(T) = \begin{cases} (\Delta+2)n - 2\Delta - 2 & p = 2 \\ (\Delta+2)n - 2\Delta - 3 + p(p-2) & p \ge 3, \end{cases}$$

if and only if $T \in \mathsf{T}_n$. This completes the proof.

We now present a lower bound on the first Zagreb coindex among all trees. Ashrafi et al. [1] proved that for any conneted graph G of order n and size m

$$\overline{M}_1(G) = 2m(n-1) - M_1(G).$$

Next result is an immediate consequence of this equality and Theorem 1.

Corollary 11. Let T be a tree of order n with maximum degree Δ. If $n \equiv p \pmod{\Delta - 1}$, then

$$\overline{M}_1(T) \leq \begin{cases} -(\Delta+6)n + 2n^2 + 4\Delta - 2 & p = 0 \\ -(\Delta+6)n + 2n^2 + 3\Delta + 2 & p = 1 \\ -(\Delta+6)n + 2n^2 + 2\Delta + 4 & p = 2. \\ -(\Delta+6)n + 2n^2 + p\Delta + 2 - p(p-3) & p \geq 3. \end{cases}$$

REFERENCES

[1] A. R. Ashrafi, T. Došlić, A. Hamzeh, The Zagreb coindices of graph operations, *Discrete Appl. Math.* **158** (2010), 1571–1578.

[2] K. C. Das, Sharp bounds for the sum of the squares of the degrees of a graph, *Kragujevac J. Math*. **25** (2003), 31–49.

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

[7] X. L. Li, I. Gutman, Mathematical Aspects of Randić-Type Molecular Structure Descriptors, Mathematical Chemistry Monograph **1**, University of Kragujevac, 2006.

[8] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta* **76** (2003), 113–124.

[9] Ž. Kovijanić Vukićević, G. Popivoda, Chemical trees with extreme values of Zagreb indices and coindices, *Iranian. J. Math. Chem*. **5** (2014) 19–29.

[10] S. Zhang, W. Wang, 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.

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