

On the Extremal Zagreb Indices of n -Vertex Chemical Trees with Fixed Number of Segments or Branching Vertices

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Abstract

Let $\mathcal{CT}_{n,k}$ and $\mathcal{CT}_{n,b}^*$ be the classes of all n -vertex chemical trees with k segments and b branching vertices, respectively, where $3 \leq k \leq n - 1$ and $1 \leq b < \frac{n}{2} - 1$. The solution of the problem of finding trees from the class $\mathcal{CT}_{n,k}$ or $\mathcal{CT}_{n,b}^*$ with the minimum first Zagreb index or minimum second Zagreb index follows directly from the main results of [*MATCH Commun. Math. Comput. Chem.* **72** (2014) 825–834] or [*MATCH Commun. Math. Comput. Chem.* **74** (2015) 57–79]. In this paper, the chemical trees with the maximum first/second Zagreb index are characterized from each of the aforementioned graph classes. Along the way, some similar results concerning the reduced second Zagreb index are also discussed at the end of this paper.

1 Introduction

All the graphs discussed in this paper are simple and connected. Chemical compounds can be represented by graphs, known as chemical graphs, in which vertices correspond to atoms and edges represent the bonds of the considered chemical compound. Let G be

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a graph with vertex set $V(G)$ and edge set $E(G)$. If two vertices u and v of the graph G are adjacent, then the edge connecting them will be denoted by uv . The number of vertices adjacent to the vertex $u \in V(G)$ is its degree, and it will be denoted by $d_u(G)$. In a chemical graph, every vertex has degree at most 4. Let $n_i(T)$ be the number of vertices of degree i in a graph G . Let $N_G(u)$ be the set of all those vertices of G that are adjacent to the vertex $u \in V(G)$. A vertex of degree one is called a *pendent* vertex. A vertex of degree more than two is known as a *branching* vertex. A pendent vertex adjacent to a branching vertex is called a *starlike pendent* vertex. A graph with n vertices is called n -vertex graph. When the graph under consideration is clear, we drop “ G ” from the graph theoretical notations – for example, we write d_u , n_i and $N(u)$ instead of $d_u(G)$, $n_i(G)$ and $N_G(u)$, respectively. If $V(G) = \{v_1, v_2, \dots, v_n\}$ then the sequence $(d_{v_1}, d_{v_2}, \dots, d_{v_n})$ is called the degree sequence of G and it is usually assumed that $d_{v_1} \geq d_{v_2} \geq \dots \geq d_{v_n}$. Undefined terminology and notations from (chemical) graph theory can be found in books [7, 19, 26].

In chemical graph theory, the graph invariants (that found some chemical applications in chemistry) are called *topological indices*. Long time ago, a pair of topological indices were appeared within the study of the dependence of total π -electron energy of molecular structures [17, 18]. Nowadays, the members of this pair are known as the *first Zagreb* index, which is denoted by M_1 , and the *second Zagreb* index, which is denoted by M_2 . For a (molecular) graph G , these Zagreb indices are defined as

$$M_1(G) = \sum_{v \in V(G)} (d_v)^2 \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

These indices were given different names in the literature, such as the Zagreb Group indices [18], the Zagreb group parameters [10] and the Zagreb indices [27]. The Zagreb indices attracted much interest from mathematical chemists and mathematicians, and as a result a plethora of their mathematical properties were reported – detail about the mathematical theory and applications of these indices can be found in the recent surveys [3, 4, 8, 9, 16], recent papers [1, 2, 5, 11, 13, 20, 22–24, 29–32] and related references listed therein.

Let $P : u_0 u_1 u_2 \dots u_r$ be a path of length $r \geq 2$ in a graph. The vertices u_0 and u_r are called end vertices of P . If $r \geq 3$ then the vertices u_1, u_2, \dots, u_{r-1} are called internal vertices of P . A *pendent path* in a graph is a path in which one of the end vertices is pendent and the other is branching, and all the internal vertices (if exist) have degree 2. An *internal path* in a graph is a path in which both the end vertices are branching and all the internal vertices (if exist) have degree 2. A *segment* of a tree T is a non-trivial path

P' in T with the property that neither of the end vertices of P' has degree 2 and that all the internal vertices (if exist) of P' have degree 2.

Denote by $\mathcal{CT}_{n,k}$ and $\mathcal{CT}_{n,b}^*$ the classes of all n -vertex chemical trees with k segments and b branching vertices, respectively, where $1 \leq k \leq n - 1$ and $0 \leq b \leq \frac{n}{2} - 1$. The solution of the problem of finding trees from the class $\mathcal{CT}_{n,k}$ or $\mathcal{CT}_{n,b}^*$, with the minimal first Zagreb index or minimal second Zagreb index follows directly from the main results of [6] or [21]. The main purpose of the present paper is to solve the following chemical extremal graph theoretical problem.

Problem 1. *Characterize all the trees attaining the maximal first Zagreb index or maximal second Zagreb index from the class $\mathcal{CT}_{n,k}$ or $\mathcal{CT}_{n,b}^*$.*

Clearly, the classes $\mathcal{CT}_{n,1}$ and $\mathcal{CT}_{n,0}^*$ consist of only the path graph and the class $\mathcal{CT}_{n,2}$ is empty. It is mentioned in the papers [6, 21] that the n -vertex star graph is the unique tree with $n - 1$ segments – however, this is not the case because every n -vertex tree containing no vertex of degree 2 has $n - 1$ segments. Also, if $T \in \mathcal{CT}_{n, \frac{n}{2}-1}^*$ then T consists of the vertices only of degrees 1 and 3, and hence $M_1(T) = 5n - 8$, $M_2(T) = 6n - 15$, where $n \geq 4$. Thus, we solve Problem 1 under the constraints $3 \leq k \leq n - 1$ and $1 \leq b < \frac{n}{2} - 1$. Moreover, if $k = 3, 4$, the solution of the problem of characterizing trees from the class $\mathcal{CT}_{n,k}$ with the maximal first Zagreb index or maximal second Zagreb index follows directly from Theorem 1 of [21] or Theorem 3.1 of [6], respectively. However, for the sake of completeness, we state our main results, concerning segments, with the condition $3 \leq k \leq n - 1$ instead of $5 \leq k \leq n - 1$.

Let G' be a graph obtained from another graph G by applying some graph transformation such that $V(G) = V(G')$. In this paper, whenever such two graphs are under discussion, by the vertex degree d_u , we always mean that it is the degree of the vertex u in G .

2 Statements of the Main Results

This section is concerned with the statements of our main results, which give the solution of Problem 1. In order to state the first two of these results, we need the following elementary lemma.

Lemma 1. *For any tree $T \in \mathcal{CT}_{n,k}$, with $3 \leq k \leq n - 1$, the following results hold.*

a) $n_3 = 0$ if and only if $k \equiv 1 \pmod{3}$, $n_1 = \frac{2k+4}{3}$, $n_2 = n - k - 1$ and $n_4 = \frac{k-1}{3}$.

b) $n_3 = 1$ if and only if $k \equiv 0 \pmod{3}$, $n_1 = \frac{2k+3}{3}$, $n_2 = n - k - 1$ and $n_4 = \frac{k-3}{3}$.

c) $n_3 = 2$ if and only if $k \equiv 2 \pmod{3}$, $n_1 = \frac{2k+2}{3}$, $n_2 = n - k - 1$ and $n_4 = \frac{k-5}{3}$.

Proof. From the well known identities

$$n = n_1 + n_2 + n_3 + n_4 \tag{1}$$

and

$$n_1 + 2n_2 + 3n_3 + 4n_4 = 2(n - 1), \tag{2}$$

it follows that

$$n_1 = n_3 + 2n_4 + 2. \tag{3}$$

By using (3) in the equation $k = (n_1 + n_3 + n_4) - 1$, we get

$$k \equiv 2n_3 + 1 \pmod{3}. \tag{4}$$

Now, by using the identity $n_2 = n - k - 1$ (see [21] for details) in (2), we have

$$n_1 + 4n_4 = 2k - 3n_3. \tag{5}$$

By solving (3) and (5) for the unknowns n_1 and n_4 , we get

$$n_1 = \frac{2k - n_3 + 4}{3} \tag{6}$$

and

$$n_4 = \frac{k - 2n_3 - 1}{3}. \tag{7}$$

From (4), (6) and (7), the desired results follow. ■

Let $\mathcal{CT}_0(n, k)$, $\mathcal{CT}_1(n, k)$ and $\mathcal{CT}_2(n, k)$ be the subclasses of $\mathcal{CT}_{n,k}$ consisting of the trees that contain no vertex of degree 3, contain one vertex of degree 3 and contain two vertices of degree 3, respectively. Then, by Lemma 1, every member of $\mathcal{CT}_0(n, k)$, $\mathcal{CT}_1(n, k)$ or $\mathcal{CT}_2(n, k)$ satisfies $k \equiv 1 \pmod{3}$, $k \equiv 0 \pmod{3}$ or $k \equiv 2 \pmod{3}$, respectively, and also that member has the degree sequence

$$\underbrace{(4, 4, \dots, 4)}_{\frac{k-1}{3}}, \underbrace{(2, 2, \dots, 2)}_{n-k-1}, \underbrace{(1, 1, \dots, 1)}_{\frac{2k+4}{3}},$$

$$\underbrace{(4, 4, \dots, 4)}_{\frac{k-3}{3}}, \underbrace{(3, 2, 2, \dots, 2)}_{n-k-1}, \underbrace{(1, 1, \dots, 1)}_{\frac{2k+3}{3}}$$

or

$$\underbrace{(4, 4, \dots, 4)}_{\frac{k-5}{3}}, \underbrace{(3, 3, 2, 2, \dots, 2)}_{n-k-1}, \underbrace{(1, 1, \dots, 1)}_{\frac{2k+2}{3}},$$

respectively.

Theorem 1. *If $3 \leq k \leq n - 1$ and $CT \in \mathcal{CT}_{n,k}$, then*

$$M_1(CT) \leq \begin{cases} 4n + 2k - 10 & \text{if } k \equiv 0 \pmod{3}, \\ 4n + 2k - 8 & \text{if } k \equiv 1 \pmod{3}, \\ 4n + 2k - 12 & \text{if } k \equiv 2 \pmod{3}. \end{cases}$$

The equality holds if and only if $CT \in \mathcal{CT}'_1(n, k)$ for $k \equiv 0 \pmod{3}$, $CT \in \mathcal{CT}'_0(n, k)$ for $k \equiv 1 \pmod{3}$, and $CT \in \mathcal{CT}'_2(n, k)$ for $k \equiv 2 \pmod{3}$.

Let $\mathcal{CT}'_0(n, k)$, $\mathcal{CT}'_1(n, k)$ and $\mathcal{CT}'_2(n, k)$ be the subclasses of $\mathcal{CT}_0(n, k)$, $\mathcal{CT}_1(n, k)$ and $\mathcal{CT}_2(n, k)$, respectively, consisting of the trees that satisfy the following properties:

- every internal path (if exists) has length 1,
- if there is at least one starlike pendent vertex then there is no pendent path of length greater than 2,
- every vertex of degree 3 (if exists) does not have more than one branching neighbor,
- if there is a pendent neighbor of a vertex of degree 4 then there is no vertex of degree 3 having any neighbor of degree 2,
- if $n_4 > 0$ then the graph induced by the vertices of degree 4 is a tree.

Theorem 2. *If $CT \in \mathcal{CT}_{n,k}$, with $3 \leq k \leq n - 1$, then it holds that*

$$M_2(CT) \leq \begin{cases} 6n + 2k - 24 & \text{if } n < \frac{5k}{3} + 1 \text{ and } k \equiv 0 \pmod{3}, \\ \frac{30n-14k-87}{3} & \text{if } n = \frac{5k}{3} + 1 \text{ and } k \equiv 0 \pmod{3}, \\ \frac{12n+16k-66}{3} & \text{if } n > \frac{5k}{3} + 1 \text{ and } k \equiv 0 \pmod{3}, \\ 6n + 2k - 22 & \text{if } n < \frac{5k+7}{3} \text{ and } k \equiv 1 \pmod{3}, \\ \frac{12n+16k-52}{3} & \text{if } n \geq \frac{5k+7}{3} \text{ and } k \equiv 1 \pmod{3}, \\ 6n + 2k - 26 & \text{if } n < \frac{5k-4}{3}, k \equiv 2 \pmod{3} \text{ and } k \neq 5, \\ \frac{15n+11k-85}{3} & \text{if } \frac{5k-4}{3} \leq n \leq \frac{5k+2}{3}, k \equiv 2 \pmod{3} \text{ and } k \neq 5, \\ \frac{12n+16k-80}{3} & \text{if } n > \frac{5k+2}{3}, k \equiv 2 \pmod{3} \text{ and } k \neq 5, \\ 5n - 9 & \text{if } n < 10 \text{ and } k = 5, \\ 4n + 1 & \text{if } n \geq 10 \text{ and } k = 5. \end{cases}$$

with equality if and only if $CT \in \mathcal{CT}'_1(n, k)$ for $k \equiv 0 \pmod{3}$, $CT \in \mathcal{CT}'_0(n, k)$ for $k \equiv 1 \pmod{3}$, and $CT \in \mathcal{CT}'_2(n, k)$ for $k \equiv 2 \pmod{3}$.

Since $n_2 = n - k - 1$ (see [21] for details), we remark that the solution of the problem of finding trees from the class of all n -vertex chemical trees having n_2 number of vertices

of degree 2, with the maximal first Zagreb index or maximal second Zagreb index, follows from Theorem 1 or Theorem 2, respectively, where $0 \leq n_2 \leq n - 4$.

For $1 \leq b < \frac{n-2}{3}$ and for $\frac{n-2}{3} \leq b < \frac{n}{2} - 1$, denote by $\mathcal{BT}_1(n, b)$ and by $\mathcal{BT}_2(n, b)$ the subclasses of $\mathcal{CT}_{n,b}^*$ consisting of the trees with the degree sequences

$$\left(\underbrace{4, 4, \dots, 4}_b, \underbrace{2, 2, \dots, 2}_{n-3b-2}, \underbrace{1, 1, \dots, 1}_{2b+2} \right)$$

and

$$\left(\underbrace{4, 4, \dots, 4}_{n-2b-2}, \underbrace{3, 3, \dots, 3}_{3b-n+2}, \underbrace{1, 1, \dots, 1}_{n-b} \right)$$

respectively.

Theorem 3. *If $BT \in \mathcal{CT}_{n,b}^*$ then*

$$M_1(BT) \leq \begin{cases} 2(2n + 3b - 3) & \text{if } 1 \leq b < \frac{n-2}{3}, \\ 2(4n - 3b - 7) & \text{if } \frac{n-2}{3} \leq b < \frac{n}{2} - 1. \end{cases}$$

The equality sign in the inequality $M_1(BT) \leq 2(2n + 3b - 3)$ holds if and only if $BT \in \mathcal{BT}_1(n, b)$ for $1 \leq b < \frac{n-2}{3}$ and the equality sign in the inequality $M_1(BT) \leq 2(4n - 3b - 7)$ holds if and only if $BT \in \mathcal{BT}_2(n, b)$ for $\frac{n-2}{3} \leq b < \frac{n}{2} - 1$.

For $1 \leq b < \frac{n-2}{3}$ and for $\frac{n-2}{3} \leq b < \frac{n}{2} - 1$, denote by $\mathcal{BT}'_1(n, b)$ and by $\mathcal{BT}'_2(n, b)$ the subclasses of $\mathcal{BT}_1(n, b)$ and $\mathcal{BT}_2(n, b)$, respectively, consisting of the trees that satisfy the following constraints:

- every internal path (if exists) has length 1,
- if there is a pendent vertex adjacent to a vertex of degree 4, then there is no adjacent vertices of degree 3,
- if there is a pendent vertex adjacent to a branching vertex, then there is no pendent path of length greater than 2,
- every vertex of degree 3 (if exists) has at most one neighbor of degree 4,
- $n_4 > 0$ and the graph induced by the vertices of degree 4 is a tree.

Theorem 4. *If $BT \in \mathcal{CT}_{n,b}^*$, where $1 \leq b < \frac{n}{2} - 1$, then*

$$M_2(BT) \leq \begin{cases} 4n + 16b - 12 & \text{if } 1 \leq b \leq \frac{n-4}{5}, \\ 6n + 6b - 20 & \text{if } \frac{n-4}{5} < b < \frac{n-2}{3}, \\ 10n - 6b - 28 & \text{if } \frac{n-2}{3} \leq b < \frac{3n-4}{7}, \\ 16n - 20b - 36 & \text{if } \frac{3n-4}{7} \leq b < \frac{n}{2} - 1. \end{cases}$$

The equality holds if and only if $BT \in \mathcal{BT}'_1(n, b)$ for $1 \leq b < \frac{n-2}{3}$, and $BT \in \mathcal{BT}'_2(n, b)$ for $\frac{n-2}{3} \leq b < \frac{n}{2} - 1$.

3 Proofs of Theorems 1 and 2

Let CT_{max}^1 (respectively CT_{max}^2) be the tree with the maximal first Zagreb index (respectively, second Zagreb index) among all the members of the class $\mathcal{CT}_{n,k}$ where $3 \leq k \leq n-1$. In order to prove Theorems 1 and 2, we first establish some structural properties of the trees CT_{max}^1 and CT_{max}^2 .

Lemma 2. *The tree $CT_{max}^1 \in \mathcal{CT}_{n,k}$ (respectively $CT_{max}^2 \in \mathcal{CT}_{n,k}$) contains at most two vertices of degree 3 where $3 \leq k \leq n-1$.*

Proof. We give a proof by contradiction. Suppose that the tree CT_{max}^1 (respectively CT_{max}^2) contains the vertices u, v and w of degree 3. If the vertices u, v and w lie on the same path, then without loss of generality, we assume that the vertex v lies on the $u-w$ path. Whether the vertices u, v and w lie on the same path or not, we assume that w_1 and w_2 are the neighbors of w that do not lie on the $u-w$ path. Then, in either case, v must not be coincident with either of the vertices w_1 and w_2 . Let T' be the tree obtained from CT_{max}^1 (respectively CT_{max}^2) by deleting the edges ww_1, ww_2 and adding the edges uw_1, vw_2 , then it is clear that $T' \in \mathcal{CT}_{n,k}$. It can be easily checked that

$$M_1(CT_{max}^1) - M_1(T') < 0,$$

which is a contradiction to the definition of CT_{max}^1 .

Next, we show that $M_2(CT_{max}^2) - M_2(T') < 0$, which contradicts the definition of CT_{max}^2 . Let w_3 be the unique neighbor of w that lies on the path $u-w$. By definition of M_2 , it holds that

$$M_2(CT_{max}^2) - M_2(T') = 2d_{w_3} - d_{w_1} - d_{w_2} - \sum_{x \in N_G(u)} d_x - \sum_{y \in N_G(v)} d_y. \quad (8)$$

The right hand side of (8) is negative due to the facts that $\sum_{x \in N(u)} d_x \geq 4$, $\sum_{y \in N(v)} d_y \geq 4$ and $d_{w_3} \leq 4$. This completes the proof. ■

We can now prove Theorem 1.

Proof of Theorem 1. Recall that we have denoted by CT_{max}^1 the tree attaining the maximal first Zagreb index among all the members of $\mathcal{CT}_{n,k}$. By Lemma 2, CT_{max}^1 must have at most two vertices of degree 3 and hence by Lemma 1, we have

$$M_1(CT_{max}^1) = \begin{cases} 4n + 2k - 10 & \text{if } k \equiv 0 \pmod{3}, \\ 4n + 2k - 8 & \text{if } k \equiv 1 \pmod{3}, \\ 4n + 2k - 12 & \text{if } k \equiv 2 \pmod{3}. \end{cases}$$

Now, bearing in mind the definitions (see Section 2) of $\mathcal{CT}_0(n, k)$, $\mathcal{CT}_1(n, k)$ and $\mathcal{CT}_2(n, k)$, we get the desired result. ■

In order to prove Theorem 2, we need to establish some further structural properties of the tree CT_{max}^2 .

Lemma 3. *For $3 \leq k \leq n - 1$, the tree $CT_{max}^2 \in \mathcal{CT}_{n,k}$ does not contain any internal path of length greater than 1.*

Proof. Assume, on the contrary, that there is an internal path $v_0v_1 \cdots v_{r-1}v_r$ of length at least 2 in CT_{max}^2 where v_0 and v_r are branching vertices and $d_{v_1} = d_{v_2} = \cdots = d_{v_{r-1}} = 2$. Let u be a pendent vertex adjacent to some vertex $v \in V(CT_{max}^2)$. The vertex v may or may not be coincident with either of the vertices v_0 and v_r . If $CT' = CT_{max}^2 - \{uv, v_0v_1, v_{r-1}v_r\} + \{v_0v_r, uv_1, v_{r-1}v\}$, then $CT' \in \mathcal{CT}_{n,k}$. Whether the vertex v is coincident with either of the vertices v_0 and v_r , or not, in both cases we have

$$\begin{aligned} M_2(CT_{max}^2) - M_2(CT') &= 2d_{v_0} + 2d_{v_r} - d_{v_0}d_{v_r} - d_v - 2 \\ &\leq -4 + 2(d_{v_0} + d_{v_r}) - d_{v_0}d_{v_r}. \end{aligned} \tag{9}$$

The right hand side of (9) is negative because the function f defined by $f(x, y) = 2(x + y) - xy - 4$, with $3 \leq x, y \leq 4$, is decreasing in both x and y , and hence we have $M_2(CT_{max}^2) < M_2(CT')$, which is a contradiction to the choice of CT_{max}^2 . ■

Lemma 4. *If the tree $CT_{max}^2 \in \mathcal{CT}_{n,k}$ contains a pendent vertex adjacent to a branching vertex, then CT_{max}^2 does not contain a pendent path of length greater than 2 where $3 \leq k \leq n - 1$.*

Proof. Suppose, on the contrary, that $v_1v_2 \cdots v_r$ is a pendent path of length at least 3 and there is a pendent vertex $u \in V(CT_{max}^2)$ adjacent to some branching vertex $v \in V(CT_{max}^2)$, where v_1 is a pendent vertex and v_r is a branching vertex (the vertex v_r may coincides with the vertex v). Let $CT' = CT_{max}^2 - \{uv, v_1v_2, v_2v_3\} + \{uv_2, v_2v, v_1v_3\}$. Certainly, the tree CT' belongs to the class $\mathcal{CT}_{n,k}$ and from the fact $d_v \geq 3$, it follows that $M_2(CT_{max}^2) - M_2(CT') = -d_v + 2 < 0$, which is a contradiction to the choice of CT_{max}^2 . ■

Lemma 5. *If the tree $CT_{max}^2 \in \mathcal{CT}_{n,k}$ contains a pendent vertex adjacent to a vertex of degree 4 then CT_{max}^2 does not contain any vertex of degree 3 adjacent to a vertex of degree 2 where $3 \leq k \leq n - 1$.*

Proof. Suppose, on the contrary, that $v \in V(CT_{max}^2)$ is a vertex of degree 3 adjacent to a vertex u of degree 2 and $p \in V(CT_{max}^2)$ is a pendent vertex adjacent to some vertex w of degree 4. Let t be the neighbor of u different from v . Because of Lemmas 3 and 4, it holds that $d_t = 1$. If $CT' = CT_{max}^2 - \{tu, uv, pw\} + \{tv, pu, uw\}$ then we have $M_2(CT_{max}^2) - M_2(CT') = -1 < 0$, which is a contradiction to the definition of CT_{max}^2 .

■

Lemma 6. *If the tree $CT_{max}^2 \in \mathcal{CT}_{n,k}$ contains a vertex u of degree 3 then u does not have more than one branching neighbor where $3 \leq k \leq n - 1$.*

Proof. Suppose, on the contrary, that v and w are two branching neighbors of u . Let $P = v_1v_2 \cdots v_{i-1}v_iv_{i+1} \cdots v_r$ be the longest path containing u, v and w , where $v_{i-1} = v, v_i = u$ and $v_{i+1} = w$. By Lemma 2, P contains at most two vertices of degree 3 including u . If P has two vertices of degree 3 including u then, without loss of generality, we assume that $d_{v_j} = 3$ for some j , where $1 \leq j \leq i - 1$. Thus, there exists some l with $i + 1 \leq l \leq r - 1$ such that v_l has exactly one branching neighbor and $d_{v_l} = 4$. If $CT' = CT_{max}^2 - \{v_{i-1}v_i, v_iv_{i+1}, v_lv_{l+1}\} + \{v_{i-1}v_{i+1}, v_lv_i, v_lv_{l+1}\}$ then bearing in mind the facts $d_{v_{i+1}} \leq 2, d_{v_{i+1}} = 4$ and $d_{v_{i-1}} = 3$ or 4 , we have

$$M_2(CT_{max}^2) - M_2(CT') = -d_{v_{i-1}} + d_{v_{l+1}} < 0,$$

a contradiction to the definition of CT_{max}^2 . ■

The next corollary follows directly from Lemmas 3 and 6.

Corollary 1. *If the maximum degree of the tree $CT_{max}^2 \in \mathcal{CT}_{n,k}$ is 4 then the graph induced by the vertices of degree 4 of CT_{max}^2 is a tree where $3 \leq k \leq n - 1$.*

Denote by $x_{i,j}(G)$ (or simply by $x_{i,j}$) the number of edges in a graph G connecting the vertices of degrees i and j . The following system of equations holds for any chemical tree T :

$$\sum_{\substack{1 \leq i \leq 4 \\ i \neq j}} x_{j,i} + 2x_{j,j} = j \cdot n_j \tag{10}$$

where $j = 1, 2, 3, 4$.

We are now in position to prove Theorem 2.

Proof of Theorem 2. Recall that we have denoted by CT_{max}^2 the tree attaining the maximal second Zagreb index among all the members of $\mathcal{CT}_{n,k}$. Thus, $M_2(CT) \leq M_2(CT_{max}^2)$

with equality if and only if $CT \cong CT_{max}^2$. If $k = 3, 4$, the desired result follows from Theorem 3.1 of [6]. In what follows, we determine $M_2(CT_{max}^2)$ under the assumption $5 \leq k \leq n - 1$.

By Lemma 2, the tree CT_{max}^2 contains at most two vertices of degree 3 and hence by Lemma 1, the degree sequence $DS(CT_{max}^2)$ of CT_{max}^2 is

$$DS(CT_{max}^2) = \begin{cases} \left(\underbrace{4, 4, \dots, 4}_{\frac{k-3}{3}}, 3, \underbrace{2, 2, \dots, 2}_{n-k-1}, \underbrace{1, 1, \dots, 1}_{\frac{2k+3}{3}} \right) & \text{if } k \equiv 0 \pmod{3}, \\ \left(\underbrace{4, 4, \dots, 4}_{\frac{k-1}{3}}, 2, \underbrace{2, \dots, 2}_{n-k-1}, \underbrace{1, 1, \dots, 1}_{\frac{2k+4}{3}} \right) & \text{if } k \equiv 1 \pmod{3}, \\ \left(\underbrace{4, 4, \dots, 4}_{\frac{k-5}{3}}, 3, 3, \underbrace{2, 2, \dots, 2}_{n-k-1}, \underbrace{1, 1, \dots, 1}_{\frac{2k+2}{3}} \right) & \text{if } k \equiv 2 \pmod{3}. \end{cases}$$

Thus, by Lemmas 3–6 and Corollary 1 one can conclude that the tree CT_{max}^2 belongs to $CT'_0(n, k)$, $CT'_1(n, k)$ or $CT'_2(n, k)$.

Case 1. The tree CT_{max}^2 is a member of $CT'_0(n, k)$.

We note that CT_{max}^2 has the degree sequence

$$\left(\underbrace{4, 4, \dots, 4}_{\frac{k-1}{3}}, \underbrace{2, 2, \dots, 2}_{n-k-1}, \underbrace{1, 1, \dots, 1}_{\frac{2k+4}{3}} \right)$$

and the congruence $k \equiv 1 \pmod{3}$ holds. Because of the assumption $k \geq 5$, we have $n_4 \geq 1$. By Corollary 1, it holds that

$$x_{4,4} = n_4 - 1 = \frac{k-4}{3}. \tag{11}$$

Subcase 1.1. The inequality $n < \frac{5k+7}{3}$ holds.

From the inequality $n < \frac{5k+7}{3}$, we have $n_1 > n_2$ and thus (by Lemmas 3 and 4), it holds that

$$x_{2,2} = 0. \tag{12}$$

From (10), (11) and (12), it follows that $x_{1,2} = x_{2,4} = n - k - 1$, $x_{1,4} = \frac{5k-3n+7}{3}$.

Hence

$$M_2(CT_{max}^2) = 6n + 2k - 22.$$

Subcase 1.2. $n \geq \frac{5k+7}{3}$.

In this subcase, it holds that $n_1 \leq n_2$ and hence (by using Lemmas 3 and 4) we have

$$x_{1,4} = 0. \tag{13}$$

From (10), (11) and (13), it follows that $x_{1,2} = x_{2,4} = \frac{2k+4}{3}$, $x_{2,2} = \frac{3n-5k-7}{3}$, therefore we have

$$M_2(CT_{max}^2) = \frac{12n + 16k - 52}{3}.$$

Case 2. $CT_{max}^2 \in CT_1'(n, k)$.

In this case, the tree CT_{max}^2 has the degree sequence

$$\underbrace{(4, 4, \dots, 4)}_{\frac{k-3}{3}}, \underbrace{3, 2, 2, \dots, 2}_{n-k-1}, \underbrace{1, 1, \dots, 1}_{\frac{2k+3}{3}}$$

and the congruence $k \equiv 0 \pmod{3}$ holds, which implies that $k \geq 6$ (because of the assumption $k \geq 5$). Thus, $n_4 \geq 1$ and hence by Corollary 1, it holds that

$$x_{4,4} = n_4 - 1 = \frac{k - 6}{3}. \tag{14}$$

Also, it holds that

$$x_{3,3} = 0. \tag{15}$$

By Lemmas 3 and 6, we have

$$x_{3,4} = 1. \tag{16}$$

We note that $x_{2,2} = 0$ and $x_{1,4} \neq 0$ if $n_2 < 2n_4 + 2$; $x_{2,2} = x_{1,4} = 0$ if $n_2 = 2n_4 + 2$; $x_{1,4} = 0$ and $x_{2,2} \neq 0$ if $n_2 > 2n_4 + 2$. We discuss these three cases in the following.

Subcase 2.1. $n < \frac{5k}{3} + 1$.

The inequality $n < \frac{5k}{3} + 1$ implies that $n_2 < 2n_4 + 2$ and hence, it holds that

$$x_{2,2} = 0 \tag{17}$$

and $x_{1,4} \neq 0$, and hence (by Lemma 5)

$$x_{2,3} = 0. \tag{18}$$

From (10), (14), (15), (16), (17) and (18), it follows that $x_{2,4} = x_{1,2} = n - k - 1$, $x_{1,3} = 2$, $x_{1,4} = \frac{5k-3n}{3}$ and hence

$$M_2(CT_{max}^2) = 6n + 2k - 24.$$

Subcase 2.2. $n = \frac{5k}{3} + 1$.

From $n = \frac{5k}{3} + 1$, it follows that $n_2 = 2n_4 + 2$ and hence we have

$$x_{2,2} = x_{1,4} = 0. \tag{19}$$

From (10), (14), (15), (16) and (19), it follows that $x_{1,2} = n - k - 1$, $x_{1,3} = 1$, $x_{2,3} = 1$, $x_{2,4} = n - k - 2$, and hence

$$M_2(CT_{max}^2) = \frac{30n - 14k - 87}{3}.$$

Subcase 2.3. $n > \frac{5k}{3} + 1$.

The inequality $n > \frac{5k}{3} + 1$ yields $n_2 > 2n_4 + 2$, which further implies that

$$x_{1,4} = 0. \tag{20}$$

and $x_{2,2} \neq 0$, and hence (by Lemmas 3 and 4)

$$x_{1,3} = 0. \tag{21}$$

From (10), (14), (15), (16), (20) and (21), it follows that $x_{1,2} = \frac{2k+3}{3}$, $x_{2,2} = \frac{3n-5k-6}{3}$, $x_{2,3} = 2$, $x_{2,4} = \frac{2k-3}{3}$ and hence

$$M_2(CT_{max}^2) = \frac{12n + 16k - 66}{3}.$$

Case 3. $CT_{max}^2 \in CT_2'(n, k)$.

In this case, the tree CT_{max}^2 has the degree sequence

$$\underbrace{(4, 4, \dots, 4, 3, 3)}_{\frac{k-5}{3}}, \underbrace{(2, 2, \dots, 2, 1, 1, \dots, 1)}_{n-k-1}, \underbrace{(1, 1, \dots, 1)}_{\frac{2k+2}{3}}$$

and the congruence $k \equiv 2 \pmod{3}$ holds. If $k = 5$ then $n_4 = 0$, $x_{3,3} = 1$ and hence

$$M_2(CT_{max}^2) = \begin{cases} 5n - 9 & \text{if } 6 \leq n \leq 10, \\ 4n + 1 & \text{if } n > 10. \end{cases}$$

Next, in what follows, we assume $k \geq 8$, which implies that $n_4 \geq 1$. By Corollary 1, it holds that

$$x_{4,4} = n_4 - 1 = \frac{k - 8}{3}. \tag{22}$$

By Lemmas 3 and 6, we have

$$x_{3,3} = 0 \quad \text{and} \quad x_{3,4} = 2. \tag{23}$$

Subcase 3.1. $n \leq \frac{5k-7}{3}$.

The inequality $n \leq \frac{5k-7}{3}$ implies that $n_2 \leq 2n_4$ and hence, it holds that

$$x_{2,2} = 0 \tag{24}$$

and $x_{1,4} \neq 0$, and hence (by Lemma 5)

$$x_{2,3} = 0. \tag{25}$$

From (10), (22), (23), (24) and (25), it follows that $x_{1,2} = x_{2,4} = n - k - 1$, $x_{1,3} = 4$, $x_{1,4} = \frac{5k-3n-7}{3}$ and hence

$$M_2(CT_{max}^2) = 6n + 2k - 26.$$

Subcase 3.2. $\frac{5k-4}{3} \leq n \leq \frac{5k+2}{3}$.

From $\frac{5k-4}{3} \leq n \leq \frac{5k+2}{3}$, it follows that $2n_4 + 1 \leq n_2 \leq 2n_4 + 3$ and hence we have

$$x_{2,2} = x_{1,4} = 0. \tag{26}$$

From (10), (22), (23) and (26), it follows that $x_{1,2} = n - k - 1$, $x_{2,3} = \frac{3n-5k+7}{3}$, $x_{2,4} = 2(\frac{k-5}{3})$, $x_{1,3} = \frac{5k-3n+5}{3}$ and hence

$$M_2(CT_{max}^2) = \frac{15n + 11k - 85}{3}.$$

Subcase 3.3. $n > \frac{5k+2}{3}$.

The inequality $n > \frac{5k+2}{3}$ yields $n_2 > 2n_4 + 3$, which further implies that

$$x_{1,4} = 0. \tag{27}$$

and $x_{2,2} \neq 0$, and hence (by Lemmas 3 and 4)

$$x_{1,3} = 0. \tag{28}$$

From (10), (22), (23), (27) and (28), it follows that $x_{1,2} = \frac{2k+2}{3}$, $x_{2,2} = \frac{3n-5k-5}{3}$, $x_{2,3} = 4$, $x_{2,4} = 2(\frac{k-5}{3})$ and hence

$$M_2(CT_{max}^2) = \frac{12n + 16k - 80}{3}.$$

This completes the proof. ■

4 Proofs of Theorems 3 and 4

Let $C'T_{max}^1$ (respectively $C'T_{max}^2$) be the tree with the maximal M_1 (respectively, M_2) value among all members of $\mathcal{CT}_{n,b}^*$ for $1 \leq b < \frac{n}{2} - 1$. We need to prove some lemmas first, to prove Theorems 3 and 4.

Lemma 7. *For $1 \leq b < \frac{n}{2} - 1$, the tree $C'T_{max}^2 \in \mathcal{CT}_{n,b}^*$ does not contain any internal path of length greater than 1.*

Proof. The proof is fully analogous to that of Lemma 3. ■

Lemma 8. *If the tree $C'T_{max}^2 \in \mathcal{CT}_{n,b}^*$ contains a pendent vertex adjacent to a branching vertex, then it does not contain any pendent path of length greater than 2 where $1 \leq b < \frac{n}{2} - 1$.*

Proof. The proof is fully analogous to that of Lemma 4. ■

Lemma 9. *Let $1 \leq b < \frac{n}{2} - 1$. If the tree $C'T_{max}^1 \in \mathcal{CT}_{n,b}^*$ (respectively $C'T_{max}^2 \in \mathcal{CT}_{n,b}^*$) contains some vertex/vertices of degree 2, then it does not contain any vertex of degree 3. That is, the tree $C'T_{max}^1 \in \mathcal{CT}_{n,b}^*$ (respectively $C'T_{max}^2 \in \mathcal{CT}_{n,b}^*$) does not contain the vertices of degrees 2 and 3 simultaneously.*

Proof. On the contrary, we assume that the conclusion of the lemma is wrong and that the hypothesis of the lemma is true. Let z be a vertex of degree 3 in $C'T_{max}^1$ (respectively $C'T_{max}^2$). We take a vertex v of degree 2 with neighbors u and w . Take $N(z) = \{z_1, z_2, z_3\}$. Without loss of generality, we assume that the vertices z_3 and u lie on the unique $v - z$ path (it is possible that the vertex z or z_3 is coincident with u ; also, $z = u$ if and only if $z_3 = v$). If T' is the tree obtained from $C'T_{max}^1$ (respectively $C'T_{max}^2$) by deleting the edges z_1z, z_2z and adding the edges vz_1, vz_2 , then it can be observed that $T' \in \mathcal{CT}_{n,b}^*$, and that

$$M_1(C'T_{max}^1) - M_1(T') = -4 < 0$$

which is a contradiction to the choice of $C'T_{max}^1$.

For the tree $C'T_{max}^2$, it holds that $d_u \geq 2$ and $d_w = 1$ or 2, because of Lemma 7. After simple calculations, we have

$$M_2(C'T_{max}^2) - M_2(T') = 2d_{z_3} - 2d_u - 2d_w - d_{z_1} - d_{z_2}. \tag{29}$$

If $d_{z_1} \geq 2, d_{z_2} \geq 2$, then keeping in mind the inequalities $d_u \geq 2$ and $d_{z_3} \leq 4$, from Equation (29) we get $M_2(C'T_{max}^2) - M_2(T') \leq -2d_w < 0$ which is a contradiction to the definition of $C'T_{max}^2$. If $d_{z_1} = 1$ or $d_{z_2} = 1$, then by Lemmas 7 and 8 it holds that $d_u \geq 3, d_w = 1$ and hence from Equation (29) it follows that $M_2(C'T_{max}^2) - M_2(T') < 0$, which is again a contradiction. ■

Lemma 10. *Let $1 \leq b < \frac{n}{2} - 1$. For the tree $C'T_{max}^1 \in \mathcal{CT}_{n,b}^*$ (respectively $C'T_{max}^2 \in \mathcal{CT}_{n,b}^*$), the following statements hold:*

- a) if $n_2 > 0$ then $n_1 = 2b + 2, n_2 = n - 3b - 2, n_3 = 0$ and $n_4 = b$;
- b) $n_2 = 0$ if and only if $n_1 = n - b, n_3 = 3b - n + 2$ and $n_4 = n - 2b - 2$.

Proof. a) We note that

$$n_3 + n_4 = b. \tag{30}$$

Since $n_2 > 0$, by Lemma 9, it holds that

$$n_3 = 0. \tag{31}$$

From Equations (1), (2), (30) and (31), it follows that $n_1 = 2b + 2$, $n_2 = n - 3b - 2$ and $n_4 = b$.

b) If $n_1 = n - b$, $n_3 = 3b - n + 2$ and $n_4 = n - 2b - 2$ then Equation (1) yields $n_2 = 0$. Conversely, suppose that $n_2 = 0$. Bearing in mind the assumption $n_2 = 0$ and by solving Equations (1), (2), (30), we get $n_1 = n - b$, $n_3 = 3b - n + 2$ and $n_4 = n - 2b - 2$. ■

Lemma 11. For the tree $C'T_{max}^1 \in \mathcal{CT}_{n,b}^*$ (respectively $C'T_{max}^2 \in \mathcal{CT}_{n,b}^*$), the inequality $n_2 > 0$ holds if and only if $1 \leq b < \frac{n-2}{3}$ where $1 \leq b < \frac{n}{2} - 1$.

Proof. If $n_2 > 0$, then by using Lemma 10(a) we have $n_2 = n - 3b - 2$ and hence $b < \frac{n-2}{3}$. Conversely, suppose that $1 \leq b < \frac{n-2}{3}$, that is $n \geq 3b + 3$ with $b \geq 1$. We have to show that $n_2 > 0$ and we will prove it by induction on b . For $b = 1$, we have $n \geq 6$ and the graph in this case is the starlike tree with maximum degree at most 4, and hence the result is true for $b = 1$. Assume that every chemical tree of order at least $3k + 3$ with exactly k branching vertices contains at least one vertex of degree 2, where $k \geq 1$. Let $C'T_{max}^1$ (respectively $C'T_{max}^2$) be the chemical tree of order $n \geq 3(k + 1) + 3$ with exactly $k + 1$ branching vertices. Let $P : u_1 u_2 \cdots u_{r-1} u_r$ be the longest path in $C'T_{max}^1$ (respectively $C'T_{max}^2$). We note that u_2 is a branching vertex and that its every neighbor different from u_3 is pendent. Let T' be the tree obtained from $C'T_{max}^1$ (respectively $C'T_{max}^2$) by removing all the pendent neighbors of u_2 . Clearly, the tree T' has order at least $3k + 3$ and has exactly k branching vertices. Hence, by inductive hypothesis T' contains at least one vertex of degree 2. Thus, the tree $C'T_{max}^1$ (respectively $C'T_{max}^2$) has also at least one vertex of degree 2. This completes the induction and hence the proof. ■

Proof of Theorem 3. Recall that we have denoted by $C'T_{max}^1$ the tree attaining the maximal first Zagreb index among all the members of $\mathcal{CT}_{n,b}^*$. By Lemma 9, $C'T_{max}^1$ cannot contain the vertices of degrees 2 and 3 simultaneously and hence by Lemmas 10 and 11, we have

$$M_1(C'T_{max}^1) = \begin{cases} 4n + 6b - 6 & \text{if } 1 \leq b < \frac{n-2}{3}, \\ 8n - 6b - 14 & \text{if } \frac{n-2}{3} \leq b \leq \frac{n}{2} - 1. \end{cases}$$

Now, bearing in mind the definitions of $\mathcal{BT}_1(n, b)$ and $\mathcal{BT}_2(n, b)$ (see Section 2), we get the desired result. \blacksquare

In what follows, we prove some further structural properties of the tree $C'T_{max}^2$, which are needed to prove Theorem 4.

Lemma 12. *If the tree $C'T_{max}^2 \in \mathcal{CT}_{n,b}^*$ contains a pendent vertex adjacent to a vertex of degree 4, then $C'T_{max}^2$ does not contain adjacent vertices of degree 3 where $1 \leq b < \frac{n}{2} - 1$.*

Proof. Assume, on the contrary, that $w, z \in V(C'T_{max}^2)$ are the adjacent vertices of degree 3 and that $u \in V(C'T_{max}^2)$ is a pendent vertex adjacent to a vertex $v \in V(C'T_{max}^2)$ of degree 4. Without loss of generality, we assume that z lies on the unique $u-w$ path. Let w_1 and w_2 be the neighbors of w different from z . If $T' = C'T_{max}^2 - \{w_1w, w_2w\} + \{uw_1, uw_2\}$, then it can easily be observed that $T' \in \mathcal{CT}_{n,b}^*$ and $M_2(C'T_{max}^2) - M_2(T') = -2 < 0$, which is a contradiction to the choice of $C'T_{max}^2$. \blacksquare

Lemma 13. *For $1 \leq b < \frac{n}{2} - 1$, each vertex of degree 3 (if exists) of the tree $C'T_{max}^2 \in \mathcal{CT}_{n,b}^*$ has at most one neighbor of degree 4.*

Proof. Suppose, on the contrary, that $z \in V(C'T_{max}^2)$ is a vertex of degree 3 and that the vertices $x, y \in N(z)$ have degree 4. Then, by Lemma 9, the tree $C'T_{max}^2$ does not contain any vertex of degree 2. Let $u \in V(C'T_{max}^2)$ be a pendent vertex adjacent to a branching vertex $v \neq z$ (it is possible that the vertex v is coincident with x or y). If $T' = C'T_{max}^2 - \{xz, zy, uv\} + \{xy, uz, zv\}$, then $T' \in \mathcal{CT}_{n,b}^*$ and $M_2(C'T_{max}^2) - M_2(T') = 5 - 2d_v < 0$, which is a contradiction to the definition of $C'T_{max}^2$. \blacksquare

Lemma 14. *For $1 \leq b < \frac{n}{2} - 1$, the tree $C'T_{max}^2 \in \mathcal{CT}_{n,b}^*$ has at least one vertex of degree 4 and the graph induced by the vertices of degree 4 of $C'T_{max}^2$ is a tree.*

Proof. If $1 \leq b < \frac{n-2}{3}$ then by using Lemmas 10 and 11, we have $n_3 = 0$ and the inequality $b \geq 1$ implies that $n_4 > 0$. Hence, by Lemma 7, the graph induced by the vertices of degree 4 of $C'T_{max}^2$ is a tree. In what follows, we assume that $\frac{n-2}{3} \leq b < \frac{n}{2} - 1$. By Lemmas 10 and 11, it holds that $n_2 = 0$ and $n_4 = n - 2b - 2 > 0$. By Lemma 7, every internal path of $C'T_{max}^2$ has length 1. Suppose contrarily that the graph induced by the vertices of degree 4 of $C'T_{max}^2$ is not a tree. Let $u_0u_1u_2 \cdots u_r$ be a path of length at least 2 in $C'T_{max}^2$ such that $d_{u_0} = d_{u_r} = 4$ and $d_{u_1} = d_{u_2} = \cdots = d_{u_{r-1}} = 3$. Let $v \in V(C'T_{max}^2)$ be a pendent vertex adjacent to a branching vertex w . If $T' = C'T_{max}^2 - \{u_0u_1, u_{r-1}u_r, vw\} + \{u_0u_r, u_1v, u_{r-1}w\}$, then $T' \in \mathcal{CT}_{n,b}^*$ and $M_2(C'T_{max}^2) - M_2(T') = 5 - 2d_w < 0$, which is a contradiction to the definition of $C'T_{max}^2$. This completes the proof. \blacksquare

Finally, we are now able to give the proof of Theorem 4.

Proof of Theorem 4. Recall that we have denoted by $C'T_{max}^2$ the tree attaining the maximal second Zagreb index among all the members of $\mathcal{CT}_{n,b}^*$. Thus, $M_2(BT) \leq M_2(C'T_{max}^2)$ with equality if and only if $BT \cong C'T_{max}^2$. In what follows, we determine $M_2(C'T_{max}^2)$.

By Lemmas 10 and 11, the degree sequence $DS(C'T_{max}^2)$ of $C'T_{max}^2$ is

$$DS(C'T_{max}^2) = \begin{cases} \left(\underbrace{4, 4, \dots, 4}_b, \underbrace{2, 2, \dots, 2}_{n-3b-2}, \underbrace{1, 1, \dots, 1}_{2b+2} \right) & \text{if } 1 \leq b < \frac{n-2}{3}, \\ \left(\underbrace{4, 4, \dots, 4}_{n-2b-2}, \underbrace{3, 3, \dots, 3}_{3b-n+2}, \underbrace{1, 1, \dots, 1}_{n-b} \right) & \text{if } \frac{n-2}{3} \leq b \leq \frac{n}{2} - 1. \end{cases}$$

Now, by Lemmas 7 – 14 one can conclude that the tree $C'T_{max}^2$ belongs to $\mathcal{BT}'_1(n, b)$ or $\mathcal{BT}'_2(n, b)$.

Case 1. $1 \leq b < \frac{n-2}{3}$.

In this case, we have $n_1 = 2b + 2$, $n_2 = n - 3b - 2$, $n_3 = 0$, $n_4 = b$ and hence (by Lemma 14), it holds that

$$x_{4,4} = n_4 - 1 = b - 1. \tag{32}$$

Subcase 1.1 $1 \leq b \leq \frac{n-4}{5}$.

In this subcase, it holds that $x_{1,4} = 0$ and hence from (10) and (32), it follows that $x_{1,2} = x_{2,4} = 2b + 2$ and $x_{2,2} = n - 5b - 4$. Thus,

$$M_2(C'T_{max}^2) = 4n + 16b - 12.$$

Subcase 1.2 $\frac{n-4}{5} < b < \frac{n-2}{3}$.

In this subcase, we have $x_{1,4} \neq 0$. Thus, it holds that $x_{2,2} = 0$ (by Lemmas 7 and 8) and hence from (10) and (32), it follows that $x_{1,2} = x_{2,4} = n - 3b - 2$, $x_{1,4} = 5b - n + 4$. Thereby,

$$M_2(C'T_{max}^2) = 6n + 6b - 20.$$

Case 2. $\frac{n-2}{3} \leq b < \frac{n}{2} - 1$.

In this case, it holds that $n_1 = n - b$, $n_2 = 0$, $n_3 = 3b - n + 2$, $n_4 = n - 2b - 2 > 0$ and hence (by Lemma 14), it holds that

$$x_{4,4} = n_4 - 1 = n - 2b - 3. \tag{33}$$

Subcase 2.1 $\frac{n-2}{3} \leq b < \frac{3n-4}{7}$.

In this subcase, we have $x_{1,4} \neq 0$, which forces that $x_{3,3} = 0$ (by Lemma 12) and hence

from (10) and (33), we get $x_{1,4} = 3n - 7b - 4$, $x_{1,3} = 6b - 2n + 4$, $x_{3,4} = 3b - n + 2$. Thus,

$$M_2(C'T_{max}^2) = 10n - 6b - 28.$$

Subcase 2.2 $\frac{3n-4}{7} \leq b < \frac{n}{2} - 1$. We note that $x_{1,4} = 0$ in this subcase and thereby from (10) and (33), it follows that $x_{1,3} = n - b$, $x_{3,4} = 2n - 4b - 2$, $x_{3,3} = 7b - 3n + 4$. Hence,

$$M_2(C'T_{max}^2) = 16n - 20b - 36.$$

This completes the proof. ■

5 Closing Remarks

Let us consider the Wiener polarity index [12] which was firstly appeared in a linear formula, derived for the prediction of the boiling points of paraffins [28]. Du et al. [12] showed that Wiener polarity index W_p of a tree T can be written as:

$$W_p(T) = \sum_{uv \in E(T)} (d_u - 1)(d_v - 1). \tag{34}$$

We remark here that the right hand side of Equation (34) actually coincides with the definition of the reduced second Zagreb index [14, 15, 25] of T .

Because of the similarity between the definitions of M_2 and W_p for trees, at first sight, we thought that among all the members of the class $\mathcal{CT}_{n,b}^*$, for $1 \leq b < \frac{n}{2} - 1$, the classes of trees having the maximal M_2 value and those having the maximal W_p value would be same. However, this is not the case – for example, both the trees T_1 and T_2 depicted in Figure 1 have the maximal W_p value in the class $\mathcal{CT}_{7,1}^*$ but $M_2(T_1) < M_2(T_2)$. Also, the trees T_3 and T_4 shown in Figure 1 attains the maximal W_p value in the class $\mathcal{CT}_{14,4}^*$ but $M_2(T_3) < M_2(T_4)$.

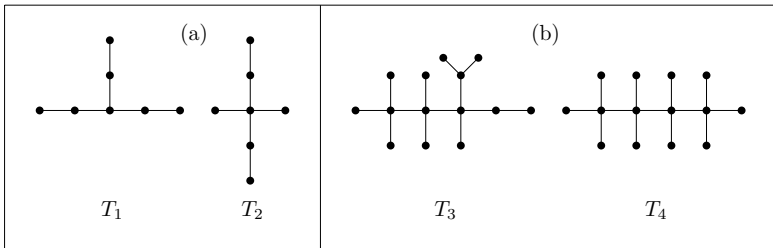


Figure 1. (a) Two trees in the class $\mathcal{CT}_{7,1}^*$ (b) Two trees in the class $\mathcal{CT}_{14,4}^*$.

Although, among all the members of the class $\mathcal{CT}_{n,b}^*$, for $1 \leq b < \frac{n}{2} - 1$, the classes of trees having the maximal M_2 value and those having the maximal W_p value are not same. We still believe that the extremal trees belonging to these two classes have several common structural properties. Let BT_{max} be the tree with the maximal W_p value among all the members of $\mathcal{CT}_{n,b}^*$ for $1 \leq b < \frac{n}{2} - 1$. We state the results concerning the structural properties of BT_{max} whose proofs are very similar to some of the results proved in this paper.

Lemma 15. *The tree $BT_{max} \in \mathcal{CT}_{n,b}^*$ does not contain any internal path of length greater than 1, where $1 \leq b < \frac{n}{2} - 1$.*

Proof. The proof is fully analogous to that of Lemma 3. ■

Lemma 16. *If the tree $BT_{max} \in \mathcal{CT}_{n,b}^*$ contains a pendent vertex adjacent to a vertex of degree 4, then $C'T_{max}^2$ does not contain adjacent vertices of degree 3, where $1 \leq b < \frac{n}{2} - 1$.*

Proof. The proof is fully analogous to that of Lemma 12. ■

Lemma 17. *If the tree $BT_{max} \in \mathcal{CT}_{n,b}^*$ contains a pendent vertex adjacent to a branching vertex, then it does not contain any pendent path of length greater than 2, where $1 \leq b < \frac{n}{2} - 1$.*

Proof. The proof is fully analogous to that of Lemma 4. ■

If T' is the tree obtained from BT_{max} by applying the transformation used in the proof of Lemma 9, then we have

$$W_p(BT_{max}) - W_p(T') = 2(d_{z_3} - 1) - 2(d_u - 1) - 2(d_w - 1) - (d_{z_1} - 1) - (d_{z_2} - 1). \quad (35)$$

If $d_{z_1} = d_{z_2} = d_u = 2$, $d_w = 1$ and $d_{z_3} = 4$, then from Equation (35) we get $W_p(BT_{max}) - W_p(T') > 0$ and hence we conclude that the technique adopted in proving Lemma 9 does not work for the following result – nevertheless, we believe that the following result is true and hence it needs to be proved in some other way.

Conjecture 18. *Let $1 \leq b < \frac{n}{2} - 1$. If the tree $BT_{max} \in \mathcal{CT}_{n,b}^*$ contains some vertex/vertices of degree 2, then it does not contain any vertex of degree 3. That is, the tree $BT_{max} \in \mathcal{CT}_{n,b}^*$ does not contain the vertices of degrees 2 and 3 simultaneously.*

Let us now consider the question: among all the members of the class $\mathcal{CT}_{n,k}$, for $3 \leq k \leq n - 1$, are the classes of trees having the maximal M_2 value and those having the

maximal W_p value same? The answer of this question is not positive – it can be easily verified that both the trees T_5 and T_6 shown in Figure 2 attains the maximal W_p value in the class $\mathcal{CT}_{16,15}$ but $M_2(T_5) < M_2(T_6)$.

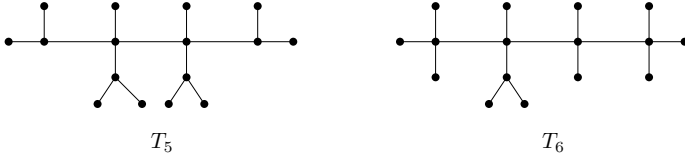


Figure 2. Two trees in the class $\mathcal{CT}_{16,15}$.

Although, among all the members of the class $\mathcal{CT}_{n,k}$, for $3 \leq k \leq n - 1$, the classes of trees having the maximal M_2 value and those having the maximal W_p value are not same. We still believe that the extremal trees belonging to these two classes have several common structural properties. Let ST_{max} be the tree with the maximal W_p value among all the members of $\mathcal{CT}_{n,k}$ for $3 \leq k \leq n - 1$. In what follows, we give the results concerning the structural properties of ST_{max} whose proofs are very similar to some of the results proved in this paper.

Lemma 19. *The tree $ST_{max} \in \mathcal{CT}_{n,k}$ does not contain any internal path of length greater than 1, where $3 \leq k \leq n - 1$.*

Proof. The proof is fully analogous to that of Lemma 3. ■

Lemma 20. *If the tree $ST_{max} \in \mathcal{CT}_{n,k}$ contains a pendent vertex adjacent to a branching vertex, then ST_{max} does not contain a pendent path of length greater than 2, where $3 \leq k \leq n - 1$.*

Proof. The proof is fully analogous to that of Lemma 4. ■

Lemma 21. *If the tree $ST_{max} \in \mathcal{CT}_{n,k}$ contains a pendent vertex adjacent to a vertex of degree 4 then ST_{max} does not contain any vertex of degree 3 adjacent to a vertex of degree 2 where $3 \leq k \leq n - 1$.*

Proof. The proof is fully analogous to that of Lemma 5. ■

At this point, we left finding the complete structure of the trees BT_{max} and ST_{max} as an open problem.

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References

- [1] A. Ali, Tetracyclic graphs with maximum second Zagreb index: a simple approach, *Asian Eur. J. Math.* **11** (2018) #1850064.
- [2] A. Ali, K. C. Das, S. Akhter, On the extremal graphs for second Zagreb index with fixed number of vertices and cyclomatic number, *Miskolc Math. Notes*, in press.
- [3] A. Ali, I. Gutman, E. Milovanović, I. Milovanović, Sum of powers of the degrees of graphs: extremal results and bounds, *MATCH Commun. Math. Comput. Chem.* **80** (2018) 5–84.
- [4] A. Ali, L. Zhong, I. Gutman, Harmonic index and its generalizations: extremal results and bounds, *MATCH Commun. Math. Comput. Chem.* **81** (2019) 249–311.
- [5] A. R. Ashrafi, M. Eliasi, A. Ghalavand, Laplacian coefficients and Zagreb indices of trees, *Lin. Multilin. Algebra* **67** (2019) 1736–1749.
- [6] B. Borovičanin, On the extremal Zagreb indices of trees with given number of segments or given number of branching vertices, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 57–79.
- [7] J. A. Bondy, U. S. R. Murty, *Graph Theory with Applications*, Elsevier, New York, 1976.
- [8] B. Borovičanin, K. C. Das, B. Furtula, I. Gutman, Bounds for Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 17–100.
- [9] B. Borovičanin, K. C. Das, B. Furtula, I. Gutman, Zagreb indices: Bounds and extremal graphs, in: I. Gutman, B. Furtula, K. C. Das, E. Milovanović, I. Milovanović (Eds.), *Bounds in Chemical Graph Theory Basics*, Univ. Kragujevac, Kragujevac, 2017, pp. 67–153.
- [10] A. T. Balaban, I. Motoc, D. Bonchev, O. Mekenyan, Topological indices for structure-activity correlations, *Topics Curr. Chem.* **114** (1983) 21–55.
- [11] K. C. Das, A. Ali, On a conjecture about the second Zagreb index, *Discr. Math. Lett.* **2** (2019) 38–43.
- [12] W. Du, X. Li, Y. Shi, Algorithms and extremal problem on Wiener polarity index, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 235–244.
- [13] M. Eliasi, A. Ghalavand, Trees with minimal second Zagreb index, *Kragujevac J. Math.* **42** (2018) 325–333.
- [14] B. Furtula, I. Gutman, S. Ediz, On the difference of Zagreb indices, *Disc. Appl. Math.* **178** (2014) 83–88.
- [15] I. Gutman, B. Furtula, C. Elphick, Three new/old vertex-degree-based topological indices, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 617–632.
- [16] I. Gutman, E. Milovanović, I. Milovanović, Beyond the Zagreb indices, *AKCE. Int. J. Graph. Comb.*, in press.

- [17] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π -electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.
- [18] I. Gutman, B. Rušić, N. Trinajstić, C. F. Wilcox, Graph theory and molecular orbitals. XII. Acyclic polyenes, *J. Chem. Phys.* **62** (1975) 3399–3405.
- [19] F. Harary, *Graph Theory*, Addison-Wesley, Reading, 1969.
- [20] F. Javaid, M. K. Jamil, I. Tomescu, Extremal k -generalized quasi unicyclic graphs with respect to first and second Zagreb indices, *Discr. Appl. Math.* **270** (2019) 153–158
- [21] H. Lin, On segments, vertices of degree two and the first Zagreb index of trees, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 825–834.
- [22] E. Milovanović, I. Milovanović, M. Jamil, Some properties of the Zagreb indices, *Filomat* **32** (2018) 2667–2675.
- [23] D. A. Mojdeh, M. Habibi, L. Badakhshian, Y. Rao, Zagreb indices of trees, unicyclic and bicyclic graphs with given (total) domination, *IEEE Access* **99** (2019) 94143–94149.
- [24] L. Pei, X. Pan, Extremal values on Zagreb indices of trees with given distance k -domination number, *J. Ineq. Appl.* **2018** (2018) #16.
- [25] S. Shafique, A. Ali, On the reduced second Zagreb index of trees, *Asian Eur. J. Math.* **10** (2017) #1750084.
- [26] N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, 1993.
- [27] R. Todeschini, V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2000.
- [28] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.
- [29] A. Yurtas, M. Togan, V. Lokeshia, I. N. Cangul, I. Gutman, Inverse problem for Zagreb indices, *J. Math. Chem.* **57** (2019) 609–615.
- [30] F. Zhan, Y. Qiao, J. Cai, Relations between the first Zagreb index and spectral moment of graphs, *MATCH Commun. Math. Comput. Chem.* **81** (2019) 383–392.
- [31] A. B. Zakharov, A. V. Dyachenko, V. V. Ivanov, Topological characteristics of iterated line graphs in QSAR problem: Octane numbers of saturated hydrocarbons, *J. Chemom.* **33** (2019) #e3169.
- [32] A. B. Zakharov, V. V. Ivanov, A new approach in topological descriptors usage. Iterated line graphs in the theoretical prediction of physico-chemical properties of saturated hydrocarbons, *Kharkov Univ. Bull. Chem. Ser.* **32** (2019) 38–45.