Iranian J. Math. Chem. 11(4) December (2020) 213 − 226

Iranian Journal of Mathematical Chemistry

Journal homepage: ijmc.kashanu.ac.ir

On the Modified First Zagreb Connection Index of Trees of a Fixed Order and Number of Branching Vertices

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ARTICLE INFO

Article History:

Received: 30 August 2020
Accepted: 27 November 2020
Published online: December 2020
Academic Editor: Ali Reza Ashrafi

Keywords:

Topological index
First Zagreb connection index
Modified first Zagreb connection index
Branching vertex
Extremal problem

ABSTRACT

The modified first Zagreb connection index ZC_1^* for a graph G is defined as $ZC_1^*(G) = \sum_{v\in V(G)} d_v\tau_v$, where d_v is the degree of the vertex v and τ_v is the connection number of v (that is, the number of vertices having distance 2 from v). A branching vertex of a graph is a vertex with degree greater than 2. In this paper, graphs with the maximum and minimum ZC_1^* values are characterized from the class of all trees of a fixed order and having a fixed number of branching vertices.

1. INTRODUCTION

Throughout this paper, we are concerned with only simple and finite graphs. For a vertex $v \in V(G)$, the degree of v is denoted by d_v and is defined as the number of vertices adjacent to v. Let $N(v)$ be the neighborhood of the vertex $v \in V(G)$, and the maximum degree of a graph G is denoted by $\Delta(G)$. Let $n_i(G)$ (or simply n_i) be the number of vertices of degree i in a graph G and $x_{i,j}(G)$ (or $x_{i,j}$) denotes the number of edges connecting the vertices of degree i and j in a graph G. A vertex with degree 1 in a graph is said to be a *pendent vertex* and a vertex with degree 3 or more is called a *branching vertex*. 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

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DOI: 10.22052/ijmc.2020.240260.1514

is a path in which both the end vertices are branching and all the internal vertices (if exist) have degree 2. If G is a graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$, the sequence $(d_{v_1}, \dots, d_{v_n})$ is called a *degree sequence* of G. Undefined terminology and notation of (chemical) graph theory can be found in [12, 22, 35].

A *topological index* is a number that can be associated with chemical structures to predict their different properties [9]. Topological indices play an important role in mathematical chemistry particularly in the quantitative structure-property relationship and quantitative structure-activity relationship investigations. It is generally accepted fact that Wiener index [37] is one of the first topological indices that found applications in chemistry.

The first Zagreb index M_1 (appeared in [20]) and the second Zagreb index M_2 (devised in [21]) are among the oldest and the most studied degree-based topological indices. For a graph G, these indices are defined as:

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

where d_u, d_v are degrees of the vertices $u, v \in V(G)$, respectively, and $E(G)$ represents the edge set of G. Till now, many papers have been devoted to these Zagreb indices, for example, see the surveys [15, 18, 28], particularly the recent ones [1, 7, 10, 11], and the related references cited therein.

The paper [20], where the first Zagreb index was appeared, also contain another topological index, which did not gain explicit attention from researchers till 2016. Recently, this index was reconsidered in [6] and referred to as the *modified first Zagreb connection index*. It is denoted by ZC_1^* and for a graph G, it is defined as

$$ZC_1^*(G) = \sum_{v\in V(G)} d_v \tau_v$$

where τ_v is the connection number of v (that is, the number of vertices having distance 2 from v, see [36]). The topological index ZC_1^* was referred to as the *third leap Zagreb index* in [27]. Detail about the mathematical properties of the index ZC_1^* can be found in [2-5, 13, 14, 23, 26, 29-34, 38, 39]

The problem of finding (lower and upper) bounds on a topological index over the certain classs of graphs with fixed order and to characterize corresponding extremal graphs, is one of the most popular research problems in chemical graph theory. Detail about the research done on these lines can be found in [8, 15-19, 24, 25, 28, 31] and the related references cited therein.

In this paper, we contribute further in this direction by characterizing the graphs with the maximum and minimum ZC_1^* values from the class of all n-vertex trees with a fixed number of branching vertices. Denote by $\mathcal{T}^*_{n,b}$ the class of all n-vertex trees with exactly b branching vertices. Note that each tree different from the path graph contains at least one branching vertex, implying $b \geq 1$. Also, for an arbitrary tree $T \in \mathcal{T}^*_{n,b}$, Lin [25] proved that $b \leq \frac{n}{2} - 1$. Thus, we assume $1 \leq b \leq \frac{n}{2} - 1$.

2. MAIN RESULTS

Problem. Characterize all the trees with maximum and minimum modified first Zagreb connection index from the class $\mathcal{T}^*{}_{n,b}$ for $1 \le b \le \frac{n}{2} - 1$.

Since $\mathcal{T}^*{}_{4,1}$ contains a unique tree T_1 whereas $\mathcal{T}^*{}_{5,1}$ contains only two trees T_2 and T_3 given in Figure 1, such that $ZC_1^*(T_2) = ZC_1^*(T_3)$; therefore, we will proceed with $n \ge 6$.

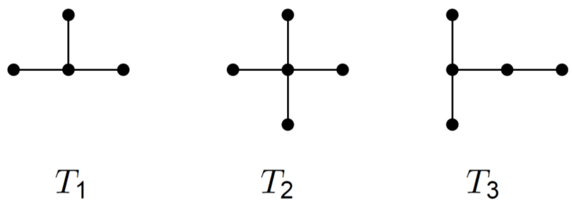

Figure 1: Trees for $\mathcal{T}^*{}_{4,1}$ and $\mathcal{T}^*{}_{5,1}$.

Theorem 1. Let $T \in \mathcal{T}^*{}_{n,b}$, where $n \ge 6$ and $1 \le b \le \frac{n}{2} - 1$, then

$$ZC_1^*(T) \ge \begin{cases} 4n + 4b - 14 & if \;\; n \ge 3b + 1\,, \\ 2n + 10b - 12 & if \;\; n < 3b + 1\,, \end{cases}$$

with equality if and only if $T \in \mathcal{B}^*{}_{min}(n, b)$, where $\mathcal{B}^*{}_{min}(n, b)$ is the family of all n-vertex trees with the degree sequence $(\underbrace{3,3,\ldots,3}_{b}, \underbrace{2,2,\ldots,2}_{n-2b-2}, \underbrace{1,1,\ldots,1}_{b+2})$, and the vertices of degree 2 are placed between the vertices of degree 3 so that there is at least one vertex of degree 2 between any two vertices of degree 3 (if we have enough vertices of degree 2, i.e., $n_2 \ge n_3 - 1$ implying $n \ge 3b + 1$), and then the remaining vertices of degree 2 (if they exist) are placed arbitrarily between any two vertices of degree 2 or one vertex of degree 2 and one vertex of degree 3.

Ducoffe in [16] proved that the trees with $n \ge 4$ vertices having the maximum value of modified first Zagreb connection index are the trees with a diameter at most 3, that is for $b = 1$ (respectively $b = 2$), the star graph (respectively double star graph) gives the maximum value $(n - 2)(n - 1)$ to ZC_1^*.

Theorem 2. Let $T \in \mathcal{T}^*{}_{\mathrm{n,b}}$, where $n \ge 6$ and $3 \le b \le \frac{n}{2} - 1$, then

$$ZC_1^*(T) \le \begin{cases} n^2 - 3n - 4b^2 + 12b - 6 & if \;\; 3 \le b \le \frac{n+2}{3}\,, \\ 5n^2 + 20b^2 - 20nb - 3n + 20b - 22 & if \;\; \frac{n+2}{3} < b \le \frac{n}{2} - 1, \end{cases}$$

and the equality holds if and only if $T \cong B_1^*$ for $3 \le b \le \frac{n+2}{3}$, where B_1^* is a tree with degree sequence $(n-2b+1, \underbrace{3,3,\ldots,3}_{b-1}, \underbrace{1,1,\ldots,1}_{n-b})$ given in Figure 2, and $T \in T_1^*(n,b)$ for $\frac{n+2}{3} < b \le \frac{n}{2} - 1$, where $T_1^*(n,b)$ is the set of n-vertex trees with the degree sequence $(n-2b+1, \underbrace{3,3,\ldots,3}_{b-1}, \underbrace{1,1,\ldots,1}_{n-b})$ such that the vertex of degree $n-2b+1$ has only branching neighbors.

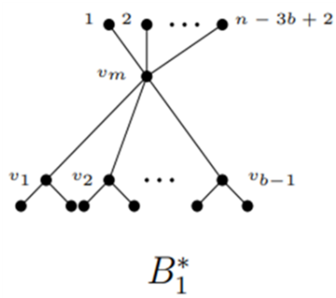

Figure 2: Maximum Tree for $3 \le b \le \frac{n+2}{3}$.

2.1. PROOF OF THEOREM 1

Denote by T_{min}^* the tree with minimum modified first Zagreb connection index among all the members of $\mathcal{T}^*_{n,b}$ for $n \ge 6$ and $1 \le b \le \frac{n}{2} - 1$. Then the following properties hold for T_{min}^*:

Lemma 1. A branching vertex in the tree $T_{min}^* \in \mathcal{T}^*_{n,b}$ contains at least one non-pendent neighbor.

Proof. It can easily be observed that for $b \ge 2$ the result is obvious, so we prove the result for $b = 1$. Contrarily, suppose T_{min}^* is a star graph that is, the branching vertex v of T_{min}^* contains pendent neighbors only. Let $N(v) = \{v_1, v_2, \ldots, v_{d_v}\}$ be the set of neighbors of v. The assumption $n \ge 6$ ensures that $d_v \ge 5$. If a tree T' is obtained from T_{min}^* as $T' = T_{min}^* - \{vv_4, vv_5\} + \{v_1v_4, v_4v_5\}$, $T' \in \mathcal{T}^*_{n,b}$ and

$$\begin{aligned} ZC_1^*(T') - ZC_1^*(T_{min}^*) &= (d_v - 3)(2(d_v - 2) - 1 - d_v + 2) + (4(d_v - 2) - 2 - d_v + 2) \\ &\quad + (4) + (1) - d_v(2d_v - 1 - d_v) \\ &= 6 - 2d_v < 0, \end{aligned}$$

which is a contradiction to the minimality of T_{min}^*. □

Lemma 2. Every branching vertex in the tree $T^*_{min} \in \mathcal{T^*}_{n,b}$ has degree 3.

Proof. Contrarily, we assume that the tree T^*_{min} contains a branching vertex v of degree greater than 3 such that the degree of v in T^*_{min} is maximum. Suppose $N(v) = \{v_1, v_2, v_3, v_4, \ldots, v_{d_v}\}$ such that

$$d_{v_1} = min\{d_{v_1}, d_{v_2}, \ldots, d_{v_{d_v}}\} \text{ and } d_{v_2} = max\{d_{v_1}, d_{v_2}, \ldots, d_{v_{d_v}}\}.$$

Let z_1 denotes a pendent vertex connected to v via v_1 and z_2 be the neighbor of z_1 (z_1 may coincide with v_1 or $z_2 = v$ if $d(v_1) = 1$).

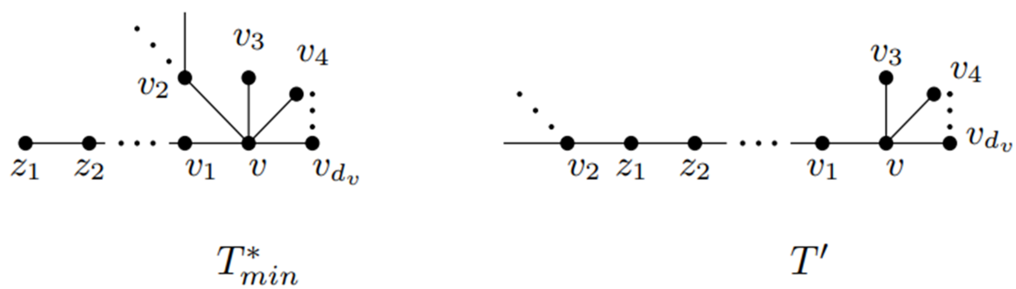

Figure 3: T^*_{min} and T'.

Let T' be the tree obtained from T^*_{min} by deleting the edge vv_2 and adding the new edge z_1v_2 (see Figure 3). We note that $T' \in \mathcal{T^*}_{n,b}$ and the only vertices whose degrees differ in T^*_{min} and T' are v and z_1. If $v_1 \neq z_1$ or $d_{v_1} > 1$, $d_{v_i} \geq 2$ for $2 \leq i \leq d_v$. Also, by keeping in mind the facts $d_{z_2} \leq d_v$ and $\sum_{i=1,i\neq 2}^{d_v} (2d_{v_i} - 1)) \geq 9$, we have

$$\begin{aligned} ZC_1^*(T') - ZC_1^*(T^*_{min}) = &\sum_{i=1,i\neq 2}^{d_v} (2(d_v - 1)d_{v_i} - d_{v_i} - d_v + 1) + (4d_{z_2} - 2 - d_{z_2}) \\ &+(4d_{v_2} - 2 - d_{v_2}) - \textstyle\sum_{i=1,i\neq 2}^{d_v} (2d_v d_{v_i} - d_{v_i} - d_v) \\ &-(2d_{z_2} - 1 - d_{z_2}) - (2d_v d_{v_2} - d_v - d_{v_2}) \\ &= -\textstyle\sum_{i=1,i\neq 2}^{d_v} (2d_{v_i} - 1)) + 2d_{z_2} + 4d_{v_2} - 2d_v d_{v_2} + d_v - 3 \\ &\leq 4d_{v_2} - 2d_v d_{v_2} + 3d_v - 12, \end{aligned}$$

which is negative because the function f defined by $f(a, b) = 4a - 2ab + 3b - 12$, with $a \geq 2$ and $b \geq 4$, is negative, and hence we have $ZC_1^*(T') < ZC_1^*(T^*_{min})$, a contradiction to the choice of T^*_{min}.

Also, in a special case when $v_1 = z_1$ (i.e., $z_2 = v$), Lemma 1 ensures that $d_{v_2} \geq 2$ and $\sum_{i=3}^{d_v} (2d_{v_i} - 1)) \geq 2$ we have,

$$\begin{aligned} ZC_1^*(T') - ZC_1^*(T^*_{min}) = &\textstyle\sum_{i=3}^{d_v} (2(d_v - 1)d_{v_i} - d_{v_i} - d_v + 1) + (4d_{v_2} - 2 - d_{v_2}) \\ &+(4(d_v - 1) - 2 - d_v + 1) - \textstyle\sum_{i=3}^{d_v} (2(d_v)d_{v_i} - d_{v_i} - d_v) \end{aligned}$$

$$-(2d_v - 1 - d_v) - (2d_v d_{v_2} - d_v - d_{v_2})$$
$$= -\sum_{i=3}^{d_v} (2d_{v_i} - 1)) + 4d_{v_2} - 2d_v d_{v_2} + d_v - 6$$
$$\leq 4d_{v_2} - 2d_v d_{v_2} + 3d_v - 8$$

which is negative because the function f defined by $f(a, b) = 4a - 2ab + 3b - 8$ with $a \geq 2$ and $b \geq 4$, is negative, and hence a contradiction. □

Consequently, in the tree T^*_{min} there are only vertices of degree 1, 2, or 3. Now keeping in mind $n_i = 0$ for $i \geq 4$ and using the facts $\sum_i in_i = 2(n-1)$ and $\sum_i n_i = n$, we arrive at $n_1 = n_3 + 2$. Also, it holds that $n_1 = b + 2$ and $n_2 = n - 2b - 2$ since $n_3 = b$. Now we prove some more lemmas to obtain the structure of T^*_{min}.

Lemma 3. If a branching vertex v in the tree $T^*_{min} \in \mathcal{T}^*{}_{n,b}$ contains a non-pendent neighbor (say) w, then T^*_{min} does not contain any pendent path of length greater than 1 adjacent to the vertex v via a neighbor different from w.

Proof. Contrarily, assume that there is a path $P: u_0 u_1 u_2 \ldots u_{t-1} u_t v$ with $t \geq 1$ in T^*_{min} where $d_{u_0} = 1$, $d_{u_1} = d_{u_2} = \cdots = d_{u_t} = 2$ and $v_t \neq w$.

Let $T' = T^*_{min} - \{u_0 u_1, u_t v, vw\} + \{u_0 v, v u_1, u_t w\}$. We can observe that $T' \in \mathcal{T}^*{}_{n,b}$. As Lemma 2 ensures that $d_v = 3$, also using $d_w \geq 2$, we have

$$ZC_1^*(T^*_{min}) - ZC_1^*(T') = 2(d_w - 1) > 0,$$

which implies that $ZC_1^*(T') < ZC_1^*(T^*_{min})$, hence a contradiction to the choice of T^*_{min}. □

Lemma 4. If the tree $T^*_{min} \in \mathcal{T}^*{}_{n,b}$ contains any pair of adjacent branching vertices then it does not contain any internal path of length greater than 2.

Proof. Suppose, on the contrary, that there is an internal path $P: u_1 u_2 \cdots u_s$ of length at least 3 in T^*_{min} provided that u_1 and u_s are branching vertices, let there also exists a pair of adjacent, branching vertices u and v in T^*_{min}. Lemma 2 confirms that $d_u = d_v = 3$. If $T' = T^*_{min} - \{u_1 u_2, u_2 u_3, uv\} + \{u_1 u_3, u u_2, u_2 v\}, T' \in \mathcal{T}^*{}_{n,b}$, and

$$ZC_1^*(T^*_{min}) - ZC_1^*(T') = 2 > 0$$

or $ZC_1^*(T') < ZC_1^*(T^*_{min})$, which is a contradiction to the choice of T^*_{min}. □

Now, we can prove Theorem 1.

Proof of Theorem 1. By Lemmas 1–4, one can conclude that the tree T^*_{min} from $\mathcal{T}^*{}_{n,b}$ must belong to $\mathcal{B}^*{}_{min}(n, b)$. We have further two cases:

For $n < 3b + 1$ we get $x_{1,2} = x_{2,2} = 0$, $x_{1,3} = b + 2$, $x_{2,3} = 2n - 4b - 4$ and $x_{3,3} = 3b - n + 1$. Therefore, $ZC_1^*(T_{min}^*) = x_{1,2} + 4x_{2,2} + 2x_{1,3} + 7x_{2,3} + 12x_{3,3} = 2n + 10b - 12$.

Similarly, for $n \geq 3b + 1$, we have $x_{1,2} = 0$, $x_{2,2} = n - 3b - 1$, $x_{1,3} = b + 2$, $x_{2,3} = 2b - 2$ and $x_{3,3} = 0$. Hence, $ZC_1^*(T_{min}^*) = x_{1,2} + 4x_{2,2} + 2x_{1,3} + 7x_{2,3} + 12x_{3,3} = 4n + 4b - 14$ which completes the proof. □

2.2. Proof of Theorem 2

We first find the structure of the tree that maximizes the modified first Zagreb connection index among all n-vertex trees with a fixed number of branching vertices. Now, let T_{max}^* be the tree with maximum ZC_1^* value among all the members of $\mathcal{T}^*_{n,b}$ for $3 \leq b \leq \frac{n}{2} - 1$. To prove the main result of this section, we need to establish some lemmas first.

Lemma 5. The tree $T_{max}^* \in \mathcal{T}^*_{n,b}$ does not contain any vertex of degree 2.

Proof. Recall that $b \geq 3$. Contrarily suppose T_{max}^* contains a vertex u of degree 2 adjacent to a branching vertex w. Let $N(u) = \{v, w\}$ and $N(w) = \{u, w_1, w_2, \ldots, w_{d_w-1}\}$. If T' is the tree obtained from T_{max}^* by deleting the edge uv and adding the new edge vw, $T' \in \mathcal{T}^*_{n,b}$ and keeping in mind the fact $b \geq 3$ which implies that if $d_v = 1$ then $\sum_{j=1}^{d_w-1} (2d_{w_j} - 1) \geq 4$, and if $d_v > 1$ then $\sum_{j=1}^{d_w-1} (2d_{w_j} - 1) \geq 2$, we have

$$\begin{aligned} ZC_1^*(T') - ZC_1^*(T_{max}^*) &= (2(d_w + 1) - 1 - d_w - 1) + (2(d_w + 1)d_v - d_w - 1 - d_v) \\ &+ \sum_{j=1}^{d_w-1} (2(d_w + 1)d_{w_j} - d_{w_j} - d_w - 1) \\ &- (4d_v - 2 - d_v) - (4d_w - 2 - d_w) \\ &- \sum_{j=1}^{d_w-1} (2d_w d_{w_j} - d_{w_j} - d_w) \\ &= (d_w - 1)(2d_v - 3) + \sum_{j=1}^{d_w-1} (2d_{w_j} - 1) \\ &\geq 2(2d_v - 3) + \sum_{j=1}^{d_w-1} (2d_{w_j} - 1) \\ &> 0, \end{aligned}$$

which is a contradiction. □

Consequently, Lemma 5 ensures that the tree T_{max}^* contains only pendent vertices and branching vertices. Denote by $\mu(x)$ the sum of the degrees of vertices adjacent to a vertex x in T_{max}^*. We also need the following result:

Lemma 6. If the tree T_{max}^* contains two vertices u and v with degrees at least 4 (i.e. $d_u \geq 4$ and $d_v \geq 4$) with assumptions $N(u) = \{u_1, u_2, \ldots, u_{d_u}\}$, $N(v) = \{v_1, v_2, \ldots, v_{d_v}\}$

and $\mu(v) \geq \mu(u)$ such that u is connected to v via u_1(it may be $u_1 = v$), then there is a tree $T' = T^*_{max} - \{uu_i: 4 \leq i \leq d_u\} + \{vu_i: 4 \leq i \leq d_u\}$ such that $T' \in \mathcal{T}^*{}_{n,b}$ (see Figure 6) and $ZC_1^*(T^*_{max}) < ZC_1^*(T')$.

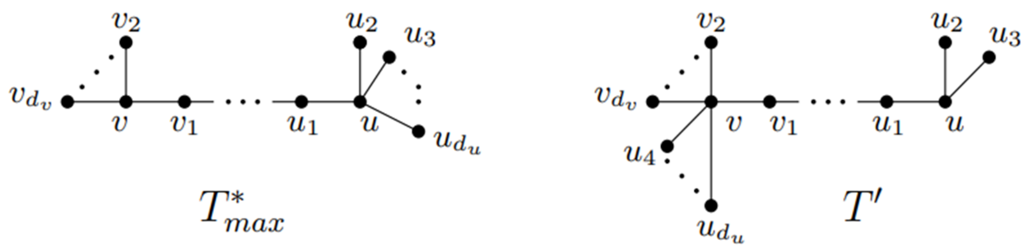

Figure 4: T^*_{max} and T'.

Proof. We consider the following cases:

Case 1. The vertices u and v are non-adjacent.

$$\begin{aligned} ZC_1^*(T') - ZC_1^*(T^*_{max}) &= \sum_{i=1}^{d_v} (2d_{v_i}(d_v + d_u - 3) - d_{v_i} - d_v - d_u + 3) \\ &+ \sum_{j=4}^{d_u} (2d_{u_j}(d_v + d_u - 3) - d_{u_j} - d_v - d_u + 3) \\ &+(6d_{u_1} - 3 - d_{u_1}) + (6d_{u_2} - 3 - d_{u_2}) \\ &+(6d_{u_3} - 3 - d_{u_3}) - \sum_{i=1}^{d_v} (2d_{v_i}d_v - d_{v_i} - d_v) \\ &- \sum_{j=4}^{d_u} (2d_{u_j}d_u - d_{u_j} - d_u) - (2d_{u_1}d_u - d_{u_1} - d_u) \\ &-(2d_{u_2}d_u - d_{u_2} - d_u) - (2d_{u_3}d_u - d_{u_3} - d_u) \\ &= (d_u - 3)(\sum_{i=1}^{d_v} (2d_{v_i} - 1) - \sum_{i=1}^{3} (2d_{u_i} - 1)) \\ &+(d_v - 3)\sum_{j=4}^{d_u} (2d_{u_j} - 1) \\ &> 0, \end{aligned}$$

which is a contradiction, where we have used the facts $\sum_{i=1}^{d_v} (2d_{v_i} - 1) \geq \sum_{i=1}^{3} (2d_{u_i} - 1)$, $\sum_{j=4}^{d_u} (2d_{u_j} - 1) \geq 1$, $d_u > 3$ and $d_v > 3$.

Case 2. The vertices u and v are adjacent, that is, $v_1 = u$ (and also $v = u_1$).
Denote by $\mu_{\neq u}(v)$ (respectively $\mu_{\neq v}(u)$) the sum of the degrees of vertices adjacent to v (respectively u), different from u (respectively v). Now, we compare $\mu_{\neq u}(v)$ and $\mu_{\neq v}(u)$. Suppose, without loss of generality, $\mu_{\neq v}(u) \leq \mu_{\neq u}(v)$. We can transform the tree T^*_{max} into the tree T', as described in Case I. It holds that

$$\begin{aligned} ZC_1^*(T') - ZC_1^*(T^*_{max}) &= \sum_{i=2}^{d_v} (2d_{v_i}(d_v + d_u - 3) - d_{v_i} - d_v - d_u + 3) \\ &+ \sum_{j=4}^{d_u} (2d_{u_j}(d_v + d_u - 3) - d_{u_j} - d_v - d_u + 3) \\ &+ (6d_{u_2} - 3 - d_{u_2}) + (6d_{u_3} - 3 - d_{u_3}) \end{aligned}$$

$$
\begin{aligned}
&+\ (6(d_v + d_u - 3) - 3 - d_v - d_u + 3) \\
&-\textstyle\sum_{i=2}^{d_v} (2d_{v_i}d_v - d_{v_i} - d_v) - \sum_{j=4}^{d_u} (2d_{u_j}d_u - d_{u_j} - d_u) \\
&-(2d_u d_v - d_u - d_v) - (2d_u d_{u_2} - d_u - d_{u_2}) \\
&-(2d_u d_{u_2} - d_u - d_{u_2}) \\
&= (d_u - 3)(\textstyle\sum_{i=2}^{d_v} (2d_{v_i} - 1) - \sum_{i=2}^{3} (2d_{u_i} - 1) - (d_v - 3)) \\
&+(d_v - 3)(\textstyle\sum_{j=4}^{d_u} (2d_{u_j} - 1) - (d_u - 3)) \\
&> 0,
\end{aligned}
$$

which is again a contradiction to the choice of T^*_{max} due to the fact $b \geq 3$ implying that either $\sum_{i=1}^{d_v} (2d_{v_i} - 1) > \sum_{i=1}^{3} (2d_{u_i} - 1) - (d_v - 3)$ and $\sum_{j=4}^{d_u} (2d_{u_j} - 1) \geq (d_u - 3)$ or $\sum_{i=1}^{d_v} (2d_{v_i} - 1) \geq \sum_{i=1}^{3} (2d_{u_i} - 1) - (d_v - 3)$ and $\sum_{j=4}^{d_u} (2d_{u_j} - 1) > (d_u - 3)$. This completes the proof. □

Let $V_3(T^*_{max}) = \{v_m, v_1, v_2, \cdots, v_{b-1}\}$ denote the set of all branching vertices from T^*_{max} and Δ denote the maximum degree among the vertices of T^*_{max} then using Lemmas 5 and 6, one can conclude that there is at most one branching vertex in T^*_{max} of degree greater than 3. Let $d_{v_i} = 3$ for $1 \leq i \leq b-1$ and $d_{v_m} = \Delta$. Hence, $T^*_{max}(n, b)$ is the collection of trees with maximum ZC_1^* with $n_3 = b - 1$, $n_1 = n - b$ also the fact $\sum_i in_i = 2(n-1)$ implies that $\Delta = n - 2b + 1$. Now, we need to place the pendent vertices and the vertices in the set $V_3(T^*_{max})$ so that we may get the maximum tree T^*_{max}. For this purpose, we establish the following lemmas:

Lemma 7. If $n_3 \leq \Delta$, then every vertex of degree 3 in T^*_{max} is adjacent to the vertex v_m of degree Δ.

Proof. Suppose there exists a branching vertex v_i $(1 \leq i \leq b-1)$ non-adjacent to v_m, and $n_3 = b - 1 \leq \Delta$. So, there must be a pendent neighbor (say) w of v_m in T^*_{max}. Let $N(v_i) = \{v_j, z_1, z_2\}$ $(1 \leq j \leq b-1,\ j \neq i)$, where z_1 and z_2 are either pendent or branching vertices different from v_m and v_i is connected to v_m via d_{v_j}. Denote by T' the tree obtained from T^*_{max} as $T' = T^*_{max} - \{v_jv_i, wv_m\} + \{v_iv_m, wv_j\}$.

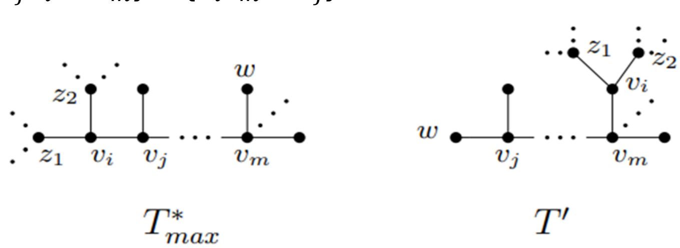

Figure 5: T^*_{max} and T'.

Clearly, the newly obtained tree T' belongs to $\mathcal{T}^*{}_{n,b}$ (see Figure 5) and $3 \leq b \leq \frac{n+2}{3}$. It holds

$$ZC_1^*(T') - ZC_1^*(T_{max}^*) = (2\Delta d_{v_i} - \Delta - d_{v_i}) + (2d_{v_i} - d_{v_i} - 1)$$
$$-(2d_{v_i}d_{v_j} - d_{v_i} - d_{v_j}) - (2\Delta - \Delta - 1)$$
$$= 4(\Delta - 3) > 0,$$

which is a contradiction. □

Note that, Lemma 7 ensures that the maximum tree T_{max}^* for $b - 1 \leq n - 2b + 1$ or $3 \leq b \leq \frac{n+2}{3}$ must be B_1^* given in Figure 2. Now, we consider the case if $n_3 > \Delta$ (i.e. $\frac{n+2}{3} < b \leq \frac{n}{2} - 1$), there is at least one vertex of degree 3 non-adjacent to v_m. Besides, the vertex v_m has only branching neighbors, so we have the following result:

Lemma 8. If a tree $T \in \mathcal{T}^*{}_{n,b}$ contains a vertex u of degree 3 with branching neighbors z, v and w, with $d_v \geq 3, d_z = d_w = 3$ and $N(w) = \{u, w_1, w_2\}$, then a tree $T' = T - \{zu, w_1w\} + \{w_1u, zw\}$ can be obtained from T(see Figure 8) such as $T' \in \mathcal{T}^*{}_{n,b}$, and $ZC_1^*(T') = ZC_1^*(T)$.

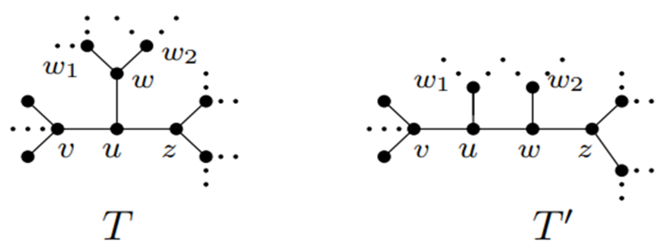

Figure 6: The Trees T and T'.

Proof. It is obvious that $T' \in \mathcal{T}^*{}_{n,b}$. Also, it holds that

$$ZC_1^*(T') - ZC_1^*(T) = (2d_u d_{w_1} - d_u - d_{w_1}) + (2d_z d_w - d_z - d_w)$$
$$-(2d_z d_u - d_z - d_u) - (2d_w d_{w_1} - d_w - d_{w_1}) = 0.$$

□

Consequently, using Lemmas 5-8, one can conclude that in order to maximize ZC_1^*, we place the vertices of degree 3 in the neighbors of v_m such that there is no pendent neighbor of v_m, then the remaining vertices of degree 3 can be placed arbitrarily in the neighbor of any pendent vertex adjacent to a vertex of degree 3.

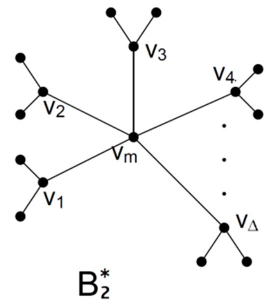

Figure 7: The base B_2^* of a tree with maximum ZC_1^* for $\frac{n+2}{3} < b \leq \frac{n}{2} - 1$.

Hence, T_{max}^* can be constructed, by starting from the tree B_2^* given in Figure 7, and then inserting the remaining vertices of degree 3 arbitrarily in the neighbor of any pendent vertex adjacent to a vertex of degree 3. So, the next result follows:

Proof of Theorem 2. Using Lemmas 5-7 one can conclude that the maximum tree $T_{max}^* \cong B_1^*$ for $2 \leq b \leq \frac{n+2}{3}$ given in Figure 2 which implies that $x_{1,3} = 2n_3 = 2b - 2$, $x_{1,\Delta} = \Delta - n_3 = n - 3b + 2$, $x_{3,\Delta} = n_3 = b - 1$ and $x_{3,3} = 0$. Hence, $ZC_1^*(T_{max}^*) = n^2 - 3n - 4b^2 + 12b - 6$ for $3 \leq b \leq \frac{n+2}{3}$.

Now, using the results in Lemmas 5-8 one can construct T_{max}^* for $\frac{n+2}{3} < b \leq \frac{n}{2} - 1$ by starting from the tree B_2^* given in Figure 7 and then inserting the remaining vertices of degree 3 arbitrarily in the neighbor of any pendent vertex adjacent to a vertex of degree 3 which implies that $T_{max}^* \in T_1^*(n, b)$ and $x_{1,3} = n_1 = n - b$, $x_{1,\Delta} = 0$, $x_{3,\Delta} = \Delta = n - 2b + 1$ and $x_{3,3} = n_3 - \Delta = 3b - n - 2$. Hence, $ZC_1^*(T_{max}^*) = 5n^2 + 20b^2 - 20nb - 3n + 20b - 22$ for $\frac{n+2}{3} < b \leq \frac{n}{2} - 1$ which completes the proof. □

ACKNOWLEDGMENTS. The authors are grateful to the anonymous referee for his/her valuable comments, which have considerably improved the presentation of this paper.

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