Iranian J. Math. Chem. 12 (3) September (2021) 127 – 138

IRANIAN JOURNAL OF
Mathematical Chemistry
Journal homepage: ijmc.kashanu.ac.ir

Original Scientific Paper

On the Trees with Given Matching Number and the Modified First Zagreb Connection Index

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ARTICLE INFO

Article History:

Received: 29 March 2021
Accepted: 31 July 2021
Published online: 30 September 2021
Academic Editor: Petra Žigert Pleteršek

Keywords:

Extremal graph theory
Modified first Zagreb connection index
Matching number
Trees

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 denotes the connection number of v (that is, the number of vertices at the distance 2 from the vertex v). Let $\mathbb{T}_{n,\alpha}$ be the class of trees with order n and matching number α such that $n > 2\alpha - 1$. In this paper, we obtain the lower bounds on the modified first Zagreb connection index of trees belonging to the class $\mathbb{T}_{n,\alpha}$, for $2\alpha - 1 < n < 3\alpha + 2$.

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1. INTRODUCTION

In this paper, all the considered graphs are simple and connected. For a graph G, $V(G)$ and $E(G)$ denote the vertex set and edge set of G, respectively. The edge connecting the vertices u and v in the graph G is denoted by uv. The degree of a vertex $u \in V(G)$ is the number of vertices adjacent to u, and it will be denoted by $d_u(G)$. Let $N_G(u)$ denotes the set of all those vertices of a graph G that are adjacent to the vertex $u \in V(G)$, and $\Delta(G)$ denotes the maximum degree in a graph G. A graph with n vertices is the graph of order n.

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DOI: 10.22052/IJMC.2021.242169.1554

A graph with no cycles is called a tree. The trees S_n and P_n denote, respectively, the star and path on n vertices. Undefined terminologies and notations from graph theory can be found in books [3, 14].

In the interdisciplinary area where physics, chemistry and mathematics meet, molecular-graph-based structure descriptors, that are usually referred to as topological indices, have significant importance [9, 8, 26]. Among the oldest and most important such structure descriptors are the classical two Zagreb indices [11, 12] defined as:

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

For more details about the theory of Zagreb indices see the recent papers [1, 15, 27, 28, 19], and the survey article [4] and the references cited therein.

In the literature, various novel variants of the first and second Zagreb indices have been introduced and studied. The first Zagreb connection index ZC_1 and the second Zagreb connection index ZC_2 are recently reported as connection–number–based version of the Zagreb indices [2, 18]. These indices are defined as:

$$ZC_1(G) = \sum_{v \in V(G)} \tau_v^2 ,$$

$$ZC_2(G) = \sum_{vu \in E(G)} \tau_v \tau_u ,$$

where τ_v is the connection number of the vertex v (that is, the number of vertices having distance 2 from v, see in [25]).

The *modified first Zagreb connection index* ZC_1^* for a graph G is defined [2] as:

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

This topological index was initially introduced within a certain formula, derived by Gutman and Trinajstić [11]. In recent years, it attracted the attention of the researchers and appeared as the *third leap Zagreb index* [18]. Ali et al. reported that the above mentioned index has more precise values of the correlation coefficients of various octane isomers and referred it as the *modified first Zagreb connection index* [2]. Du et al. [7], Ducoffe et al. [6], and Shao et al. [23] determined extremal alkanes and cycloalkanes with different conditions using this index. Zhu et al. [29] established the lower bound by using the modified first Zagreb connection index of acyclic graphs with a given order and maximum degree. Tang et al. [24] computed the first and second Zagreb connection indices and modified first Zagreb connection index of the S-sum graphs. More detail about the mathematical properties of the modified first Zagreb connection index ZC_1^* can be found in [18, 16, 5, 21, 17, 10, 20, 22]. It was proved [2] that the modified first Zagreb connection index also can be presented as:

$$ZC_1^*(G) = \sum_{1 <= i < j <= n} x_{ij}(2ij - i - j),$$

where x_{ij} is the number of those edges of the graph G in which one end vertex has degree i and the other end vertex has degree j.

A vertex of degree 1 is called a *pendent* vertex and a vertex of degree greater than 2 is called a *branching* vertex. Let T be a tree and $P(s) = v_0 v_1 \dots v_s$ a sequence of vertices in T with $d_{v_1} = d_{v_2} = \dots = d_{v_{s-1}} = 2$ (unless $s = 1$). Then $P(s)$ is called a *pendent path* (*internal path*, respectively) of length s, if each two consecutive vertices in $P(s)$ are adjacent in T, one of the two vertices v_0, v_s is pendent and the other is branching (both the vertices v_0, v_s are branching, respectively). A pendent edge is an edge incident to a pendent vertex. Let V_1 denotes the set of pendent vertices of T. A matching M in a graph G is a set of pairwise non-adjacent edges from the graph G. A maximum matching in G is a matching that contains the largest possible number of edges. The matching number α in G, is the cardinality of a maximum matching of G. A vertex that is incident with an edge of a matching M, is an M-matched vertex, and a vertex is said to be an M-unmatched vertex if it is incident with no edges of M. A matching M in a graph G is called a perfect matching if every vertex of G is M-matched. Denote by $\mathbb{T}_{n,\alpha}$ the set of trees with order n and matching number α such that $n > 2\alpha - 1$. Let $\mathbb{T}'_{n,\alpha} = \{T\colon T$ in an n-vertex tree with matching number α, $\Delta(T) = 3$, $n - 2\alpha + 1$ pendent vertices having neighbors of degree 3 only and the lengths of internal paths are even with their sum equals to $2(\alpha - 1)\}$.

2. LEMMAS

Hou et al. [13] established following lemmas for the class of trees, which will be useful in proving our main results.

Lemma 1. [13] *Let T be a tree of order n having a perfect matching. Then T contains at least two pendent vertices such that they are adjacent to vertices of degree* 2, *respectively.*

Lemma 2. [13] *Let T be a tree with order n and matching number α. If $n - 1 = 2\alpha$, T contains a pendent vertex which is adjacent to a vertex of degree* 2.

Lemma 3. [13] *Let T be a tree with order n and matching number α, where $n \geq 2\alpha + 1$. Then there is a pendent vertex v and a matching M with $|M| = \alpha$ such that v is M-unmatched.*

Ducoffe et al. [6] proved the following result:

Lemma 4. [6] *Among trees with n $(n \geq 5)$ vertices, the path P_n has the minimum modified first Zagreb connection index.*

Let $V_1(T)$ denotes the set of pendent vertices in a graph T. The proof of the following lemma is trivial, so we will overlook it here.

Lemma 5. *Let T be an tree with n vertices and a perfect matching such that $n = 2\alpha$. For any vertex $u \in V(T)$, $|N_T(u) \cap V_1(T)| < 2$.*

Lemma 6. *If* $T \in \mathbb{T}'_{n,\alpha}$ $(\alpha > 1)$, $2\alpha + 2 < n < 3\alpha + 2$, *$T$ has a matching M with* $|M| = \alpha$ *and* $ZC_1^*(T) = 8n - 8\alpha - 18$.

Proof. If $\alpha = 2$, $T \cong \mathbb{T}_{7,2}$ by $T \in \mathbb{T}'_{n,\alpha}$. It is quite simple to check that the lemma is true for $\alpha = 2$. Now, we assume that $\alpha > 2$ and proceed by using induction on α. Let $P(l)\colon v_0v_1v_2 \cdots v_l$ be the longest path in T. Then $|N_T(v_1) \cap V_1(T)| = 2$.

Denote $N_T(v_1) \cap V_1(T) = \{v_0, u\}$. Let $P'(r)\colon v_1v_2 \ldots v_r$ $(r < l)$ be an internal path. Then r is odd and denote $r = 2z + 1$ $(z \geq 1)$. If $r = l - 1$, then $T \cong \mathbb{T}_{2(\alpha+1)+1,\alpha}$. It may be seen that lemma holds for this situation. Or else, $r \leq l - 3$. If T' is the tree constructed by deleting the set $\{u, v_0, v_1, \ldots, v_{2z-1}\}$ of vertices from T, observe that $T' \in \mathbb{T}'_{n-2z-1,\alpha-z}$ with $\alpha - z \geq 2$. By using induction, $2(\alpha - z + 1) \leq n - 1 - (2z + 1) \leq 3(\alpha - z)$, T' has $(\alpha - z)$-matching and $ZC_1^*(T') = 8(n - 2z - 1) - 8(\alpha - z) - 18$. It is easy to see that $2\alpha + 3 < n \leq 3\alpha + 2 - z < 3\alpha + 2$ and $ZC_1^*(T) - ZC_1^*(T') = 2(2(3) - 1 - 3) + 2(2(6) - 3 - 2) + (2z - 2)(2(4) - 2 - 2) - (2(3) - 1 - 3)$, which implies that $ZC_1^*(T) = ZC_1^*(T') + 8z + 8 = 8n - 8\alpha - 18$. Hence, the proof is complete. □

3. MAIN RESULTS

In this section, some lower bounds for the modified first Zagreb connection index among the class $\mathbb{T}_{n,\alpha}$ are determined, where $n < 3\alpha + 2$.

Denote $\psi_0(\alpha) = 8\alpha - 10$, $\psi_1(\alpha) = 8\alpha - 6$, $\psi_2(\alpha) = 8\alpha$ and $\psi_3(\alpha) = 8\alpha + 6$, where α is a positive integer. As usual, P_n denotes the path graph of order n. By Lemma 4, one can easily obtain Theorems 1 and 2 instantly.

Theorem 1. *Let T be a tree with matching number α and order 2α. Then*

$$ZC_1^*(T) \geq \psi_0(\alpha) \tag{1}$$

Equality (1) *holds for* $T \cong P_{2\alpha}$.

Theorem 2. *Let T be a tree with matching number α and order $2\alpha + 1$. Then*

$$ZC_1^*(T) \geq \psi_1(\alpha) \tag{2}$$

Equality (2) *holds for* $T \cong P_{2\alpha+1}$.

Denote $S_4^n (n \geq 4)$ by the graph constructed from S_4 by dividing only one edge $(n - 4)$ times (see Figure 1).

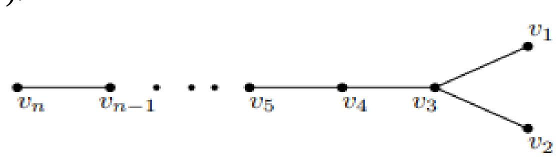

Figure 1: The tree S_4^n.

Theorem 3. *Let T be a tree with matching number α and order $2\alpha + 2$. Then*

$$ZC_1^*(T) \geq \psi_2(\alpha) \tag{3}$$

Equality (3) *holds for* $T \cong S_4^{2(\alpha+1)}$.

Proof. Note that if $T \cong S_4^{2(\alpha+1)}$ $(\alpha > 1)$, the Equality in (3) holds. We now show that if $T \cong \mathbb{T}_{2\alpha+2,\alpha}$ $(\alpha > 1)$, (3) holds and the Equality in (3) can be obtained only if $T \cong S_4^{2(\alpha+1)}$. If $\alpha = 2$, one can observe that there are only three trees T_3, T_4 and S_4^6 (see Figure 2), of order $2(\alpha + 1)$ with a matching having α elements. Also, $ZC_1^*(T_3) - ZC_1^*(S_4^6) > 0$ and $ZC_1^*(T_4) - ZC_1^*(S_4^6) > 0$ implies that Theorem 3 clearly holds for $\alpha = 2$.

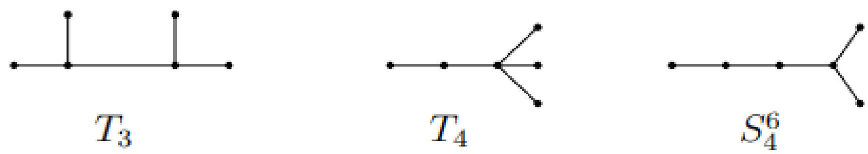

Figure 2: The trees for $\mathbb{T}_{6,2}$.

Now, we assume that $\alpha > 2$ and proceed by using induction on α. By Lemma 3, T contains a pendent vertex v and a matching M with $|M| = \alpha$ such that v is M-unmatched. Let uv be an edge in $E(T)$ and note, that $d_u = t > 1$. If we consider

$N_T(u) \cap V_1(T) = \{u_1, u_2, \dots, u_{s-1}, u_s = v\}$ and $N_T(u) \backslash V_1(T) = \{x_1, x_2, \dots, x_{t-s}\}$, $d_{x_j} = d_j > 1$ where $1 \leq j \leq t - s$.

We consider the following cases:

Case 1. If $t = 2$, there is a unique non–pendent vertex w different from the vertex v and adjacent to u. Let $d_w = r$. Denote $N_T(w) \cap V_1(T) = \{w_1, w_2, \dots, w_p\}$ and $N_T(w) \backslash V_1(T) = \{y_1, y_2, \dots, y_{r-p}\}$ which implies that $d_{y_j} = q_j > 1$. If $T' = T - \{u, v\}$, $T' \in \mathbb{T}_{2\alpha,\alpha-1}$ and keeping in mind the fact $r - p \geq 2$, we have

$$\begin{aligned} ZC_1^*(T) = ZC_1^*(T') &+ (2(2) - 2 - 1) + (2(2r) - 2 - r) + p(2(r) - 1 - r) \\ &+ \textstyle\sum_{j=1}^{r-p-1} (2(rq_j) - r - q_j) - p(2(r-1) - 1 - r + 1) \\ &- \textstyle\sum_{j=1}^{r-p-1} ((2(r-1)q_j) - r + 1 - q_j) \\ &= ZC_1^*(T') + 3r + p - 1 + \textstyle\sum_{j=1}^{r-p-1} (2q_j - 1) \\ &\geq ZC_1^*(T') + 3r + p - 1 + (r - p - 1)(3) = ZC_1^*(T') + 6r - 2p - 4 \\ &\geq \psi_2(\alpha - 1) + 6r - 2p - 4 \\ &= \psi_2(\alpha) + 2(r - p) + 4r - 12 \geq \psi_2(\alpha) + 4r - 8 \geq \psi_2(\alpha). \end{aligned}$$

To have the equality in the above expression, all the inequalities described above ought to be equalities. Thus we have $ZC_1^*(T') = \psi_2(\alpha - 1)$, $r = 2$ and $p = 0$. Therefore, by induction, $T' \cong S_4^{2\alpha}$ and $T \cong S_4^{2(\alpha+1)}$.

Case 2. If $t > 2$. If $T' = T - \{v\}$, $T' \in \mathbb{T}_{2\alpha+1,\alpha}$ and Theorem 2 gives that $ZC_1^*(T') \geq \psi_1(\alpha)$. Using the fact $t - s \geq 1$, we have

$$\begin{aligned} ZC_1^*(T) &= ZC_1^*(T') + s(t-1) + \\ &+ \sum_{i=1}^{t-s} [(2td_i - d_i - t) - (2d_i(t-1) - d_i - t + 1)] \\ &-(s-1)(t-2) \\ &\geq \psi_1(\alpha) + s + t - 2 + \sum_{i=1}^{t-s} (2d_i - 1) \\ &\geq 8\alpha + s + t - 8 + 3(t-s) = \psi_2(\alpha) + 2t + 2(t-s) - 8 \\ &\geq \psi_2(\alpha) + 2t + 2 - 8 = \psi_2(\alpha) + 2t - 6 \geq \psi_2(\alpha). \end{aligned}$$

To have the equality in the above expression, all the inequalities ought to be equalities. Thus, $ZC_1^*(T') = \psi_1(\alpha)$, $t = 3$ and $s = 2$. By induction, $T' \cong P_{2\alpha+1}$, so $T \cong S_4^{2(\alpha+1)}$, which completes the proof. □

Denote $\mathcal{T}_{2\alpha+3,\alpha}$ by a tree that is obtained from a path $P_{2\alpha+1} = v_1 v_2 \cdots v_{2\alpha} v_{2\alpha+1}$ by attaching a new pendant edge to v_2 and $v_{2\alpha}$, respectively. $\mathcal{T}_{11,4}$ is shown in Figure 3.

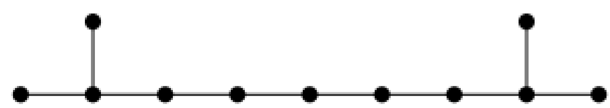

Figure 3: The tree $\mathcal{T}_{11,4}$.

Theorem 4. *Let T be a tree with matching number α and order $2\alpha + 3$. Then*

$$ZC_1^*(T) \geq \psi_3(\alpha). \tag{4}$$

The Equality in (4) *holds for $T \cong \mathcal{T}_{2\alpha+3,\alpha}$.*

Proof. The equality in (4) holds if $T \cong \mathcal{T}_{n,\alpha}$ $(\alpha > 1)$, where $n = 2\alpha + 3$. Further, it is needed to show that for $T \in \mathbb{T}_{2\alpha+3,\alpha}$ $(\alpha > 1)$, (4) holds and for the equality the only condition is $T \cong \mathcal{T}_{2\alpha+3,\alpha}$.

For $\alpha = 2$, there exist only four trees T_5, T_6, T_7 and $\mathcal{T}_{7,2}$ (see Figure 4), of order $2\alpha + 3$ with a matching having α elements.

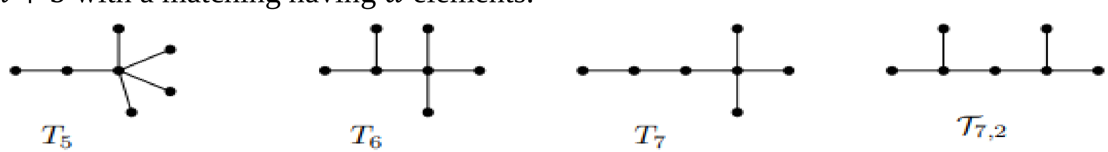

Figure 4: The trees $\mathbb{T}_{2m+3,m}$ for $m = 2$.

It holds that $ZC_1^*(T_5) - ZC_1^*(\mathcal{T}_{7,2}) = 8 > 0$, $ZC_1^*(T_6) - ZC_1^*(\mathcal{T}_{7,2}) = 8 > 0$ and $ZC_1^*(T_7) - ZC_1^*(\mathcal{T}_{7,2}) = 2 > 0$. Thus, for $\alpha = 2$, result is obtained.

We now assume that $\alpha > 2$ and use induction on α. By Lemma 3, T contains a pendent vertex v and a matching M with $|M| = \alpha$ such that v is M-unmatched. Let uv is the member of $E(T)$ with $d_u = t > 1$. If $N_T(u) \cap V_1(T) = \{u_1 u_2, \cdots, u_{s-1}, u_s = v\}$ and $N_T(u) \backslash V_1(T) = \{x_1, x_2, \dots, x_{t-s}\}$, $d_{xj} = d_j > 1$, where $1 \le j \le t - s$.

Consider the following possible cases:

Case 1. If $t = 2$, there exists a unique vertex w ($w \ne v$) adjacent to u with $d_w = r > 1$. Denote $N_T(w) \cap V_1(T) = \{w_1, w_2, \dots, w_p\}$ and $N_T(w) \backslash V_1(T) = \{y_1, y_2, \dots, y_{r-p}\}$ which implies that $d_{y_j} = q_j > 1$. If $T' = T - \{u, v\}$, $T' \in \mathbb{T}_{2\alpha+1,\alpha-1}$ and using the fact $r - p \ge 2$, we have

$$\begin{aligned} ZC_1^*(T) &= ZC_1^*(T') + 3r + p - 1 + \textstyle\sum_{j=1}^{r-p-1} (2q_j - 1) \\ &\ge ZC_1^*(T') + 3r + p - 1 + (r - p - 1)(3) \\ &= ZC_1^*(T') + 6r - 2p - 4 \\ &\ge \psi_3(\alpha - 1) + 6r - 2p - 4 \\ &= \psi_3(\alpha) + 6r - 2p - 12 = \psi_3(\alpha) + 2(r - p) + 4r - 12 \ge \psi_3(\alpha). \end{aligned}$$

To have the equality, the inequalities described above ought to be equalities. Thus, we have $ZC_1^*(T') = \psi_3(\alpha - 1)$, $r = 2$, $p = 0$ and $q_1 = 2$. Therefore, by induction hypothesis, $T' \cong \mathcal{T}_{2\alpha+1,\alpha-1}$ and it is easy to see that $T \cong \mathcal{T}_{2\alpha+3,\alpha}$.

Case 2. If $t > 2$. If T' is the tree by deleting the vertex v from T, $T' \in \mathbb{T}_{2\alpha+2,\alpha}$. By Theorem 3, $ZC_1^*(T') \ge \psi_2(\alpha)$. Using the fact $t - s \ge 1$, we have

$$\begin{aligned} ZC_1^*(T) &= ZC_1^*(T') + s(t-1) \\ &\quad + \textstyle\sum_{i=1}^{t-s} [(2td_i - d_i - t) - (2d_i(t-1) - d_i - t + 1)] \\ &\quad - (s-1)(t-2) \\ &\ge \psi_2(\alpha) + s + t - 2 + \textstyle\sum_{i=1}^{t-s} (2d_i - 1) \\ &\ge \psi_2(\alpha) + s + t - 2 + 3(t - s) = \psi_3(\alpha) + 4t - 2s - 8 \\ &= \psi_3(\alpha) + 2t + 2(t - s) - 8 \ge \psi_3(\alpha) + 2t + 2 - 8 \\ &= \psi_3(\alpha) + 2t - 6 \ge \psi_3(\alpha), \end{aligned}$$

which completes the proof. □

Theorem 5. *Let* $T \in \mathbb{T}_{n,\alpha}$ $(2\alpha + 2 < n < 3\alpha + 2)$. *Then*

$$ZC_1^*(T) \ge 8n - 8\alpha - 18. \tag{5}$$

The Equality in (5) holds if and only if $T \in \mathbb{T}'_{n,\alpha}$.

Proof. Note that if $T \in \mathbb{T}'_{n,\alpha}$, the equality in (5) holds by Lemma 6. We apply induction on n to prove that if $T \in \mathbb{T}_{n,\alpha}$, (5) and the Equality in (5) holds for $T \in \mathbb{T}'_{n,\alpha}$. If $n-1 = 2\alpha + 2$, the result in the theorem is true by Theorem 4 and $\{\mathcal{T}_{2\alpha+3,\alpha}\} = \mathbb{T}'_{2\alpha+3,\alpha}$. Assume that $n-1 \geq 2\alpha+3$ and the result is true for the lesser values of n.

Lemma 3 ensures that T contains a matching M with α elements and an M-unmatched pendent vertex v. Let v is adjacent to a non–pendent vertex u of degree t. If we consider $N_T(u) \cap V_1(T) = \{u_1, u_2, \dots, u_{s-1}, u_s = v\}$ and $N_T(u) \backslash V_1(T) = \{y_1, y_2, \dots, y_{t-s}\}$, $d_{y_j} = d_j > 1$ where $1 \leq j \leq t-s$.

The following possible cases arise:

Case 1. If $t > 3$ and $T' = T - \{v\}$, it can be observed that $T' \in \mathbb{T}_{n-1,\alpha}$ and $n-1 \geq 2\alpha + 3$. Using induction as well as the fact $t - s \geq 1$, we have

$$\begin{aligned}
ZC_1^*(T) &= ZC_1^*(T') + s(2t-1-t) \\
&\quad + \textstyle\sum_{j=1}^{t-s} \left[(2td_j - d_j - t) - (2d_j(t-1) - d_j - t + 1)\right] \\
&\quad -(s-1)(2(t-1)-1-t+1) \\
&= ZC_1^*(T') + s(t-1) - (s-1)(t-2) + \textstyle\sum_{j=1}^{t-s} (2d_j - 1) \\
&\geq ZC_1^*(T') + s + t - 2 + (t-s)(3) = ZC_1^*(T') + 4t - 2s - 2 \\
&\geq 8(n-1) - 8\alpha - 18 + 4t - 2s - 2 \\
&= 8n - 8\alpha - 18 + 2(t-s) + 2t - 10 \\
&\geq 8n - 8\alpha - 18.
\end{aligned}$$

Case 2. If $t = 2$. The proof is fully analogous to that of Case 1 of Theorem 4.

Case 3. If $t = 3$, the following subcases arise:

Subcase 3.1. $s = 1$, let $N_T(u) \backslash \{v\} = \{y_1, y_2\}$. If $T' = T - \{v\}$, $T' \in \mathbb{T}_{n-1,\alpha}$ and $n - 1 \geq 2\alpha + 3$. Therefore, using induction, we have

$$\begin{aligned}
ZC_1^*(T) &= ZC_1^*(T') + (2(3)-3-1) + (2(3d_1)-3-d_1) + (2(3d_2)-3-d_2) \\
&\quad -(2(2d_1)-2-d_1) - (2(2d_2)-2-d_2) = ZC_1^*(T') + 2d_1 + 2d_2 \\
&\geq 8(n-1) - 8\alpha - 18 + 2d_1 + 2d_2 = 8n - 8\alpha - 18 + 2d_1 + 2d_2 - 8 \\
&\geq 8n - 8\alpha - 18
\end{aligned}$$

and the equality holds only if $d_1 = d_2 = 2$ and $ZC_1^*(T') = \psi(n-1, \alpha)$. Induction hypothesis implies that $T' \in \mathbb{T}'_{n-1,\alpha}$. Thus, there is a vertex v' in T' with $|N_T(v') \cap V_1(T)| = 2$. By replacing u with v', theorem holds by a contention like that in the following case.

Subcase 3.2. $s = 2$. For this subcase, $N_T(u) \cap V_1(T) = \{u_1, u_2\}$. Let $P(l): x'_0(= u)x'_1(= x_1)x'_2 \dots x'_l$ be an internal path of T with $d_{x'_l} = d$, where $l \geq 1$. Let $|N_T(x'_l) \cap V_1(T)| = q$.

Subcase 3.2.1. If $l = 1$ and $T' = T - \{u, u_1, u_2\}$, $T' \in \mathbb{T}_{n-3,\alpha-1}$ and $n - 3 \geq 2(\alpha - 1) + 3$. Therefore, using induction and the fact $d \geq 3$, we have

$$\begin{aligned} ZC_1^*(T) &= ZC_1^*(T') + 2(2(3) - 1 - 3) + (2(3d) - 3 - d) + q(2d - 1 - d) \\ &\quad -q(2(d-1) - 1 - d + 1) + \textstyle\sum_{y \in N_T(x'_1) \setminus (V_1 \cup \{u\})} (2d_y - 1) \\ &= ZC_1^*(T') + 5d + q + 1 + \textstyle\sum_{y \in N_T(x'_1) \setminus (V_1 \cup \{u\})} (2d_y - 1) \\ &\geq 8(n-3) - 8(\alpha - 1) - 18 + 5d + q + 1 \\ &\quad + \textstyle\sum_{y \in N_T(x'_1) \setminus (V_1 \cup \{u\})} (2d_y - 1) \\ &\geq 8n - 8\alpha - 8 + 5d + q - 15 + \textstyle\sum_{y \in N_T(x'_1) \setminus (V_1 \cup \{u\})} (2d_y - 1) \\ &\geq 8n - 8\alpha - 18 + q + \textstyle\sum_{y \in N_T(x'_1) \setminus (V_1 \cup \{u\})} (2d_y - 1) > 8n - 8\alpha - 18. \end{aligned}$$

Subcase 3.2.2. $l = 2z$, where $z \geq 1$. For this subcase, $z \leq \alpha - 2$. If $T' = T - \{u_1, u_2, x'_0, \dots, x'_{2z-3}, x'_{2z-2}\}$, it can be easily observed that $T' \in \mathbb{T}_{n-2z-1,\alpha-z}$ with $n - 2z - 1 \geq 2(\alpha - z) + 3$ and $\alpha - z \geq 2$. Thus, we have

$$\begin{aligned} ZC_1^*(T) &= ZC_1^*(T') + 2(2(3) - 1 - 3) + (2(3)(2) - 3 - 2) \\ &\quad +(2z - 2)(2(4) - 2 - 2) + (2(2d) - 2 - d) - (2(d) - 1 - d) \\ &\geq 8(n - 2z - 1) - 8(\alpha - z) - 18 + 4 + 7 + 4(2z - 2) + 2d - 1 \\ &\geq 8n - 8\alpha - 18 + 2d - 6 \geq 8n - 8\alpha - 18. \end{aligned}$$

For the equality, the inequalities described above ought to be equalities. Thus, $ZC_1^*(T') = 8(n - 2z - 1) - 8(\alpha - z) - 18$, $s = 2$ and $d = 3$. So the induction hypothesis implies that $T' \in \mathbb{T}'_{n-2z-1,\alpha-z}$ and $T \in \mathbb{T}'_{n,\alpha}$.

Subcase 3.2.3. $l = 2z + 1$, where $z \geq 1$.In this particular subcase, $z \leq \alpha - 3$ with T having a matching with α elements and $n \geq 2\alpha + 4$. Let T' be a tree obtained from T such that $T' = T - \{u_1, u_2, x'_0, \dots, x'_{2z-2}, x'_{2z-1}\}$, it is not difficult to observe that either $T' \in \mathbb{T}_{n-2z-2,\alpha-z-1}$ or $T' \in \mathbb{T}_{n-2z-2,\alpha-z}$ with $n - 2z - 2 \geq 2(\alpha - z - 1) + 4$. If $T' \in \mathbb{T}_{n-2z-2,\alpha-z-1}$, we have

$$\begin{aligned} ZC_1^*(T) &= ZC_1^*(T') + 2(2(3) - 1 - 3) + (2(6) - 3 - 2) \\ &\quad + (2z - 1)(2(4) - 2 - 2) + (2(2d) - 2 - d) - (2(d) - 1 - d) \\ &\geq \psi(n - 2z - 2, \alpha - z - 1) + 8z + 2d + 6 \\ &= \psi(n, \alpha) + 2d - 2 > \psi(n, \alpha). \end{aligned}$$

Now, if $T' \in \mathbb{T}_{n-2z-2,\alpha-z}$, x'_{2z} is M-matched for every matching M with α elements in T'. Hence, $N_T(x'_{2z+1}) \cap V_1(T) = \emptyset$. If $T^* = T' - \{x'_{2z}\}$, $T^* \in \mathbb{T}_{n-2z-3,\alpha-z-1}$ and we have

$$\begin{aligned} ZC_1^*(T) &= ZC_1^*(T^*) + 2(2(3) - 1 - 3) + (2(6) - 3 - 2) \\ &\quad +(2z-1)(2(4) - 2 - 2) + (2(2d) - 2 - d) \\ &\quad + \textstyle\sum_{x \in N_T(x'_{2z+1}) \setminus \{x'_{2z}\}} (2d_x - 1) \\ &\geq 8(n - 2z - 3) - 8(\alpha - z - 1) - 18 + 8h \\ &\quad +3d + 5 + \textstyle\sum_{x \in N_T(x'_{2z+1}) \setminus \{x'_{2z}\}} (2d_x - 1) \\ &= 8n - 8\alpha - 18 + 3d - 11 + \textstyle\sum_{x \in N_T(x'_{2z+1}) \{x'_{2z}\}} (2d_x - 1) \\ &> 8n - 8\alpha - 18, \end{aligned}$$

due to the fact that $d \geq 3$ and $\sum_{x \in N_T(x'_{2z+1}) \setminus \{x'_{2z}\}} (2d_x - 1) \geq 3$. Hence the proof of the Theorem is complete. □

4. CONCLUSION

One of the most studied problems in chemical graph theory is the problem to characterize the extremal elements, with respect to some certain topological indices along with some particular conditions, in the collection of all n-vertex trees. In the present study, we give the sharp lower bounds for the modified first Zagreb connection index among the trees with a given order n and matching number α, where $2\alpha - 1 < n < 3\alpha + 2$.

ACKNOWLEDGMENTS. The authors are thankful to the anonymous referees and the handling editor for their valuable comments and suggestions which improve the previous version of the paper.

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