Hindawi
Discrete Dynamics in Nature and Society
Volume 2020, Article ID 3295342, 6 pages
https://doi.org/10.1155/2020/3295342

Research Article

Extremum Modified First Zagreb Connection Index of *n*-Vertex Trees with Fixed Number of Pendent Vertices

Sadia Noureen,[1] Akhlaq Ahmad Bhatti ,[1] and Akbar Ali [2,3]

[1]*Department of Mathematics, National University of Computer and Emerging Sciences, Lahore, Pakistan*
[2]*Department of Mathematics, Faculty of Science, University of Ha'il, Ha'il, Saudi Arabia*
[3]*Knowledge Unit of Science, University of Management and Technology, Sialkot, Pakistan*

Correspondence should be addressed to Akbar Ali; akbarali.maths@gmail.com

Received 28 November 2019; Revised 26 January 2020; Accepted 19 February 2020; Published 27 April 2020

Academic Editor: Xiaohua Ding

The modified first Zagreb connection index ZC_1^* is a graph invariant that appeared about fifty years ago within a study of molecular modeling, and after a long time, it has been revisited in two papers ((Ali and Trinajstić, 2018) and (Naji et al., 2017)) independently. For a graph G, this graph invariant 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). In this paper, the graphs with maximum/minimum ZC_1^* value are characterized from the class of all n-vertex trees with fixed number of pendent vertices (that are the vertices of degree 1).

1. Introduction

Throughout this paper, we consider only simple and connected graphs. The vertex set and edge set of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The degree of a vertex $v \in V(G)$ is the number of edges incident to v and is denoted by $d_v(G)$ or simply by d_v if the graph under consideration is clear.

Let Ω be the collection of all graphs. A mapping $f\colon \Omega \longrightarrow \mathbb{R}$ is called a graph invariant or a topological index, if for every graph H isomorphic to G, it holds that $f(G) = f(H)$, where $\mathbb{R}$ is the set of all real numbers. In chemical graph theory, there are many topological indices having different applications in isomer discrimination, QSAR/QSPR investigation, pharmaceutical drug design, etc. There are various topological indices that are extensively studied by a number of researchers. The first Zagreb index M_1 and the second Zagreb index M_2 are among these much studied topological indices. These Zagreb indices for a graph G are defined as

$$M_1(G) = \sum_{v\in V(G)} (d_v)^2,$$
$$M_2(G) = \sum_{uv\in E(G)} d_u d_v. \qquad (1)$$

To the best of our knowledge, the first Zagreb index firstly appeared in a formula derived in [1] and the second Zagreb index was firstly introduced in [2]. These two Zagreb indices have several chemical applications, for example, see the recent papers [3, 4]. Detail about the mathematical properties of the indices M_1 and M_2 can be found in the recent survey papers [5–8], recent papers [9–22], and related references listed therein.

The following topological index ZC_1^* is known as the modified first Zagreb connection index [23]:

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

where τ_v is the connection number of the vertex v (that is, the number of vertices having distance 2 from v, see [24]).

Actually, this index initially appeared within a certain formula, derived by Gutman and Trinajstić [1]. The index ZC_1^* was referred as the third leap Zagreb index in [25]. After the publications of the papers [23, 25], the modified first Zagreb connection index has attracted a considerable attention from researchers, for example, see [25–39].

The main idea of the present paper comes from [40]. In the present paper, the sharp lower and upper bounds on the modified first Zagreb connection index of trees in terms of order and number of pendent vertices are derived and the corresponding extremal trees are characterized.

2. Some Definitions and Notations

For $s \geq 1$, let $P = v_0v_1, \ldots, v_s$ be a path in a graph G with $d_{v_1} = \cdots = d_{v_{s-1}} = 2$ unless $s = 1$. If $d_{v_0} = 1$ and $d_{v_s} \geq 3$, then P is called a pendent path of G and s is called the length of this pendent path. If $d_{v_0}, d_{v_s} \geq 3$, then P is called an internal path of G. A tree containing exactly one vertex of degree greater than 2 is called a starlike tree. $K_{1,n_1}(p_1, p_2, \ldots, p_{n_1})$ is used to denote the starlike tree of order n which is obtained by attaching paths of lengths $p_1, p_2, \ldots, p_{n_1}$ to the pendent vertices of the star K_{1,n_1} where $n = n_1 + 1 + \sum_{i=1}^{n_1} p_i$ and $p_i \geq 0$ for all $1 \leq i \leq n_1$.

$\mathscr{PT}_{n,n_1}$ is used to denote the set of all trees of order $n \geq 5$ and with n_1 pendent vertices. Since the path graph is the only member of $\mathscr{PT}_{n,2}$ and the star graph is the unique element of $\mathscr{PT}_{n,n-1}$, we assume $3 \leq n_1 \leq n-2$ in the remaining part of the paper. For any $T \in \mathscr{PT}_{n,n_1}$, we assume $V_1(T) := \{v\colon v$ is a pendent vertex of $T\}$, $V_2(T) := \cup_{v \in V_1(T)} N(v)$, and $V_3(T) := V(T) \backslash [V_1(T) \cup V_2(T)]$. Taking $S_{n_1}^n := K_{1,n_1}(0, 0, \ldots, n - n_1 - 1)$ and $K_{n_1}^n := K_{1,n_1}(0, 0, \ldots, 0, \underbrace{1, 1, \ldots, 1}_{n-n_1-1})$, we assume that $\mathscr{T}_{n_1}^n := \{K_{1,n_1}(p_1, p_2, \ldots, p_{n_1})\colon p_i \geq 1, 1 \leq i \leq n_1\}$. Then, $K_{n_1}^n \subseteq \mathscr{PT}_{n,n_1}$, $S_{n_1}^n \subseteq \mathscr{PT}_{n,n_1}$, and $\mathscr{T}_{n_1}^n \subseteq \mathscr{PT}_{n,n_1}$ (see Figure 1).

Let $\mathscr{T}_{n_1}^*\colon = \{T \in \mathscr{PT}_{2n_1-2,n_1}\colon T$ has $n_1 - 2$ vertices of degree 3, where $n_1 \geq 4\}$, further $E^*(T)\colon = \{uv \in E(T)\colon d_u = d_v = 3\}$. Let $\mathscr{T}_{n,n_1}^*$ be a set of trees of order n obtained from $T \in \mathscr{T}_{n_1}^*$ by replacing each edge of $E^*(T)$ by a path with length at least 2.

3. On the Minimum Modified First Zagreb Connection Index of Trees with Fixed Number of Pendent Vertices

Lemma 1 (see [41]). *Let $T \in \mathscr{PT}_{n,n_1}$ and $v \in V(T)$, then*

(i) $d_v \leq n_1$,

(ii) $d_v = n_1 > 2$ which implies that T is a starlike tree.

Lemma 2. *Let $T \in \mathscr{PT}_{n,n_1}$ and $P = v_0v_1, \ldots, v_s$ be considered as a suspended path of T such that $v_0 \in V_1(T)$ and $d_{v_s} = t \geq 3$. Considering $|N(v_s) \cap V_1(T)| = q$ and $N(v_s) \backslash (V_1(T) \cup \{v_{s-1}\}) = \{x_1, x_2, \ldots, x_{t-q}\}$ for $s = 1$ and $N(v_s) \backslash (V_1(T) \cup \{v_{s-1}\}) = \{x_1, x_2, \ldots, x_{t-q-1}\}$ for $s \geq 2$ and let $d_{x_i} = d_i \geq 2$ for $1 \leq i \leq t - q$, then*

(a) If $s \geq 2$, then (i) $\sum_{i=1}^{t-q-1}(d_i) \leq n_1 + t - 2q - 2$ and (ii) $q \geq max\{0, 2t - n\}$.

(b) If $s = 1$, then (i) $\sum_{i=1}^{t-q}(d_i) \leq n_1 + t - 2q$ and (ii) $\geq \max\{1, 2t - n + 1\}$.

Proof.

(a) See [41].

(b) (i) As $T \backslash \{v_0, v_1\}$ contains $t - q$ subtrees $T_{x_1}, T_{x_2}, \ldots, T_{x_{t-q}}$ containing $x_1, x_2, \ldots, x_{t-q}$, respectively, where each T_{x_i} has at least $d_i - 1$ pendent vertices of T. Therefore, $\sum_{i=1}^{t-q}(d_i - 1) \leq n_1 - q$ or $\sum_{i=1}^{t-q}(d_i - 1) \leq n_1 + t - 2q$.

(ii) Since for $n \geq 2t$ the result is obvious, so let $n < 2t$, and we observe that $\sum_{i=1}^{t-q-1}(d_i) \leq n - (t+1)$ and also $\sum_{i=1}^{t-q-1}(d_i) \geq t - q$ as $d_i \geq 2$.

Hence, $t - q \leq n - t - 1$ or $q \geq 2t - n + 1$. □

Lemma 3. *If $T \in \mathscr{PT}_{n,n_1}$ is a tree such that $ZC_1^*(T)$ is as small as possible, then T contains at most one pendent path of length greater than 1.*

Proof. We contrarily assume that $P = v_0v_1, \ldots, v_s$ and $P' = v_0'v_1', \ldots, v_l'(l, s \geq 2)$ are two pendent paths of T such that $v_0, v_0' \in V_1(T)$ and $d_{v_s}, d_{v_l'} \geq 3$. If $T' = T - v_{s-1}v_{s-2} + v_{s-2}v_0'$, then $T' \in \mathscr{PT}_{n,n_1}$ and we have

$$\begin{aligned} ZC_1^*(T') - ZC_1^*(T) &= (d_{v_s} - 1) - (3d_{v_s} - 2) + 4 - 1 \\ &= 2(2 - d_{v_s}) < 0, \end{aligned} \tag{3}$$

which is a contradiction to the choice of T.

Let us denote $\mathscr{T}_{n_1} = \{T\colon T \in \mathscr{PT}_{n,n_1}$ and T is a generalized star$\}$. □

Lemma 4. *For any tree $T \in \mathscr{T}_{n_1}$,*

$$\{ZC_1^*(T) \geq 4n + n_1^2 - 3n_1 - 8\}. \tag{4}$$

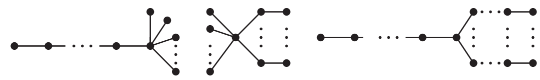
Equality in the above expression holds if and only if $T \cong S_{n_1}^n$.

Proof. Let $T\prime \in \mathscr{T}_{n_1}$ be the tree with minimal ZC_1^* among all the members of $\mathscr{T}_{n_1}$. Since $T\prime \cong K_{1,n_1}$, therefore it contains at least one pendent path of length greater than 1. By using Lemma 4, we conclude that $T\prime$ contains exactly one pendent path of length greater than 1. Therefore, $T\prime \cong S_{n_1}^n$. Since $T\prime$ is a starlike tree, and for any $T \in \mathscr{T}_{n_1}$,

$$ZC_1^*(T) \geq ZC_1^*(T\prime) = 4n + n_1^2 - 3n_1 - 8, \tag{5}$$

□

and equality in the above expression holds if and only if $T \cong S_{n_1}^n$.



(a) (b) (c)

Figure 1: The elements of the class $\mathscr{PT}_{n,n_1}$. (a) $T \in S^n_{n_1}$. (b) $T \in K^n_{n_1}$. (c) $T \in \mathscr{T}^n_{n_1}$.

Lemma 5. *If $T \in (\mathscr{PT}_{n,n_1} \backslash \mathscr{T}_{n_1})$ is a tree such that $ZC^*_1(T)$ is as small as possible, then T does not contain a pendent path of length greater than 1.*

Proof. We contrarily assume that $P = v_0 v_1, \ldots, v_s\ (s \geq 2)$ be a pendent path of T such that $v_0 \in V_1(T)$ and $d_{v_s} = q \geq 3$. As $T \in (\mathscr{PT}_{n,n_1} \backslash \mathscr{T}_{n_1})$, so there must be a vertex $v \in V(T) \backslash \{v_s\}$, with $v \in V(T) \backslash \{v_s\}$. Also, there must be a path between v and v_s. Let u be a vertex in this path, adjacent to v_s, and also, let $d_u = t \geq 2$. If $T' = T - \{v_s u, v_0 v_1\} + \{v_0 v_s, v_1 u\}$, then $T' \in \mathscr{PT}_{n,n_1} \backslash \mathscr{T}_{n_1}$ and we have

$$\begin{aligned} \mathrm{ZC}^*_1(T') - \mathrm{ZC}^*_1(T) &= 3t - 4 + q - 2tq + t + q \\ &= 2(q-2)(1-t) < 0, \end{aligned} \tag{6}$$

which is a contradiction to the minimality of T. □

Theorem 1. *If $T \in \mathscr{PT}_{n,n_1}$ for $3 \leq n_1 \leq n-2$, then*

$$\mathrm{ZC}^*_1(T) \geq 4n - 8, \quad \text{if } n_1 = 3, \text{ and } n \geq 5, \tag{7}$$

$$\mathrm{ZC}^*_1(T) \geq 4n + 4n_1 - 22, \quad \text{if } 4 \leq n_1 \leq n-2. \tag{8}$$

In the above inequality (7), equality holds if and only if $T \cong S^n_3$. In (8), equality holds if and only if $n \geq 3n_1 - 5$ and $T \in \mathscr{T}^*_{n,n_1}$.

Proof. Let we denote $\phi(n, n_1) = 4n + 4n_1 - 22$. If we take $T \in \mathscr{T}_{n_1}$, then by Lemma 4, $\mathrm{ZC}^*_1(T) \geq 4n + n_1^2 - 3n_1 - 8$ and the equality holds if and only if $T \cong S^n_3$. So, the above theorem holds. Now, we assume that $T \in \mathscr{PT}_{n,n_1} \backslash \mathscr{T}_{n_1}$ and $4 \leq n_1 \leq n-2$. We observe that if $T \in \mathscr{T}^*_{n,n_1}$, then $n \geq 3n_1 - 5$ and equality in equation (8) can be obtained by a simple elementary calculation. Now, by applying induction on n_1, we show that if $T \in \mathscr{PT}_{n,n_1} \backslash \mathscr{T}_{n_1}$, then (8) holds and the equality in (8) holds only if $T \in \mathscr{T}^*_{n,n_1}$. Let us choose T such that $\mathrm{ZC}^*_1(T)$ is as small as possible.

If $n_1 = 4$, then by Lemma 5 $T \in \mathscr{T}^*_4$ when $n = 6$, or $T \in \mathscr{T}^*_{n,4}$ if $n \geq 7$. Hence, $\mathrm{ZC}^*_1(T) = 20 > \phi(n, n_1)$ if $n = 6$ and $\mathrm{ZC}^*_1(T) = 4n - 6 = \phi(n, n_1)$ if $n \geq 7$. Therefore, equality in (8) holds for $n_1 = 4$ only if $n \geq 7$ and $T \in \mathscr{T}^*_{n,4}$. We assume that $n_1 \geq 5$ and the result is true for all smaller values of n_1.

Let $u \in V_2(T)$ and denote the degree of vertex u by t. Considering $v_1, v_2, \ldots, v_q$ and $v_{q+1}, v_{q+2}, \ldots, v_t$ as the pendent and nonpendent neighbors of u, respectively, then $t - q \geq 1$ (because $T \ncong K_{1,n-1}$). Lemma 5 ensures that (HTML translation failed), and we consider the following cases:

Case I: $t \geq 4$.

Let $T' = T - v_1$. So, $T' \in \mathscr{PT}_{n-1,n_1-1}$ and we have

$$\begin{aligned} \mathrm{ZC}^*_1(T) &= \mathrm{ZC}^*_1(T') + 2q - 2 + 2\sum_{i=q+1}^{t} d_{v_i} \\ &\geq \phi(n-1, n_1-1) + 2(q-1) + 2(2(t-q)) \\ &= \phi(n, n_1) + 2t + 2(t-q) - 10 \geq \phi(n, n_1). \end{aligned} \tag{9}$$

Case II: $t = 3$.

If $q = 1$, then we take $N(u) \backslash \{v_1\} = \{x_1, x_2\}$ and let $d_{x_i} = d_i$ for $i = 1, 2$.

If $T' = T - \{v_1\}$, then $T' \in \mathscr{PT}_{n-1,n_1-1}$ and

$$\begin{aligned} \mathrm{ZC}^*_1(T) &= \mathrm{ZC}^*_1(T') + 2d_1 + 2d_2 \\ &\geq \phi(n-1, n_1-1) + 8 = \phi(n, n_1), \end{aligned} \tag{10}$$

and equality holds only if $d_1 = d_2 = 2$ and $\mathrm{ZC}^*_1(T') = \phi(n-1, n_1-1)$. Further, by induction hypothesis, $T' \in \mathscr{T}^*_{n-1,n_1-1}$. As $d_1 = d_2 = 2$, so there must be an internal path of length at least 4, connecting x_1 and x_2 in T' and $|V(T')| \geq 3(n_1 - 1) - 3$. Hence, $n = |V(T')| + 1 \geq 3n_1 - 5$ and T belongs to $\mathscr{T}^*_{n,n_1}$. If we take $q = 2$, then $N(u) \backslash \{v_1, v_2\} = \{x_1\}$ and let $d_{x_1} = d_1$. Assuming that P: $u_0 (= u) u_1 (= x_1) u_2, \ldots, u_l$ be an internal path of T with $d_u = 3$ and $d_{u_l} = s \geq 3$, having $l \geq 1$, we consider the following cases:

Subcase I. If $l = 1$,
we consider $T' = T - \{v_1, v_2\}$, then $T' \in \mathscr{PT}_{n-2,n_1-1}$ and

$$\begin{aligned} \mathrm{ZC}^*_1(T) &= \mathrm{ZC}^*_1(T') + 2 + 4d_1 \\ &\geq \phi(n-2, n_1-1) + 2 + 4d_1 \\ &= \phi(n, n_1) + 4d_1 - 10 > \phi(n, n_1). \end{aligned} \tag{11}$$

$$\begin{aligned} \mathrm{ZC}^*_1(T) &= \mathrm{ZC}^*_1(T') + 2s + 4l + 2 \\ &\geq \phi(n-l-1, n_1-1) + 2s + 4l + 2 \\ &= \phi(n, n_1) + 2s - 6 \geq \phi(n, n_1). \end{aligned} \tag{12}$$

Subcase II. If $l \geq 2$,

we can obtain a tree $T' = T - \{v_1, v_2, u_0, \ldots, u_{l-2}\}$ such as $T' \in \mathscr{PT}_{n-l-1,n_1-1}$ and

To get equality, all the relations considered above should be reduced to equalities. So, we get $\mathrm{ZC}^*_1(T) = \phi(n-l-1, n_1-1)$, $s = 3$, and $l \geq 2$.

Further, by induction hypothesis, $T' \in \mathscr{T}^*_{n-l-1,n_1-1}$ and $|V(T')| \geq 3(n_1 - 1) - 3 - l$. Therefore,

$n = |V(T\prime)| + (l+1) \geq 3n_1 - 5$ and $T \in \mathcal{T}^*_{n,n_1}$ which completes the proof. □

4. On the Maximum Modified First Zagreb Connection Index of Trees with Fixed Number of Pendent Vertices

Lemma 6. *Let $T \in \mathcal{PT}_{n,n_1}$ be a tree that maximizes ZC_1^*, then*

(a) *For $n \geq 2n_1 + 1$, T contains at least one pendent path of length greater than 1,*

(b) *For $n \leq 2n_1$, T contains at least one pendent path of length 1.*

Proof.

(a) Let $n \geq 2n_1 + 1$, and we assume that every pendent path of T has length at most 1, so we have $d_u \geq 3$ for all $u \in V_2(T)$. Now, we show that $d_w \geq 3$ for all $w \in V_3(T)$. Otherwise, there would be a path $P = w_0 w_1 w_2, \ldots, w_q w_{q+1}$, such that for some l, $1 < l < q$, $w_l \in V_3(T)$, and $d_{w_l} = 2$, where $w_0, w_{q+1} \in V_1(T)$. Let $d_{w_i} = d_i$, $0 \leq i \leq q+1$. Then, $d_1, d_q \geq 3$ and $d_i \geq 2$ for $2 \leq i \leq q-1$.

If $T' = T - \{w_{l-1}w_l, w_l w_{l+1}, w_0 \quad w_1\} + \{w_{l-1}w_{l+1}, w_0 w_l, w_1 w_l\}$, then $T' \in \mathcal{PT}_{n,n_1}$ and we have

$$\begin{aligned} ZC_1^*(T') - ZC_1^*(T) &= 1 + 3d_1 - 2 + 2d_{l-1}d_{l+1} - d_{l-1} - d_{l+1} \\ &\quad - 2d_1 + 1 + d_1 - 4d_{l-1} + 2 + d_{l-1} \\ &\quad - 4d_{l+1} + 2 + d_{l+1} \\ &= 2d_1 - 4 + 2(d_{l-1} - 2)(d_{l+1} - 2) > 0, \end{aligned} \tag{13}$$

which is a contradiction to the choice of T. Hence, we have the result that $d_v \geq 3$ for all $v \in V(T)V_1(T)$. Therefore, $2(n-1) = \sum_{v \in V(T)} \geq \quad n_1 + 3(n - n_1)$ which gives $n \leq 2n_1 - 2$, a contradiction.

(b) Now for $n \leq 2n_1$, if we assume that each pendent vertex of T is adjacent to a vertex of degree 2, then $|V_2(T)| = n_1$. Since $T \ncong K_{1,n-1}$, we therefore have $|V(T) \setminus (V_1(T) \cup V_2(T))| \geq 1$. Hence, $n = |V_1(T)| + |V_2 \quad (T)| + |V(T) \setminus (V_1(T) \cup V_2(T))| \geq 2n_1 + 1$, a contradiction. □

Theorem 2. *Let T be a tree such that $T \in \mathcal{PT}_{n,n_1}$, and if $3 \leq n_1 \leq n-2$, then*

$$ZC_1^*(T) \leq 4n + 3n_1^2 - 9n_1 - 4, \quad \text{if } n \geq 2n_1 + 1, \tag{14}$$

$$ZC_1^*(T) \leq n_1(2n - n_1 - 3), \quad \text{if } n \leq 2n_1. \tag{15}$$

Equalities in (14) and (15) hold if and only if $T \in \mathcal{T}^n_{n_1}$ and $T \cong K^n_{n_1}$, respectively.

Proof. We observe that if $T \in \mathcal{T}^n_{n_1}$ and $T \cong K^n_{n_1}$, then, respectively, equalities (14) and (15) hold by using simple elementary calculation. □

Let us denote $\varphi_1(n, n_1) := 4n + 3n_1^2 - 9n_1 - 4$ and $\varphi_2(n, n_1) := n_1(2n - n_1 - 3)$. Now, by applying induction on n_1, we show that if $T \in \mathcal{T}_{n,n_1}$ for $n_1 \geq 3$, then (14) and (15) hold and the equalities in (14) and (15) hold only if $T \in \mathcal{T}^n_{n_1}$ and $T \cong K^n_{n_1}$, respectively. Let $n_1 = 3$, then T is a starlike tree and $n \geq 5$. It can be easily verified that $\mathcal{T}_{5,3} = \{T_1\}$ and $\mathcal{T}_{6,3} = \{T_2, T_3\}$ (see Figure 2).

Note that $ZC_1^*(T_1) = 12 = \varphi_2(5,3)$, $ZC_1^*(T_2) = 16 < \varphi_2(6,3)$, $ZC_1^*(T_3) = 18 = \varphi_2(6,3)$, and $T_1 \cong K^5_3$, $T_3 \cong K^6_3$. Therefore, Theorem 2 holds for $n = 5, 6$, so we assume that $n \geq 7$ or $n \geq 2n_1 + 1$, and we find the following results:

$$ZC_1^*(T) = \begin{cases} 4n - 4 = \varphi_1(n,3), & \text{if } T \in \mathcal{T}^n_3, \\ 4n - 8 < \varphi_1(n,3), & \text{if } T \cong S^n_3, \\ 4n - 6 < \varphi_1(n,3), & \text{if } T \in \mathcal{T}_{n,3} \setminus (\mathcal{T}^n_3 \cup \{S^n_3\}). \end{cases} \tag{16}$$

So, now we have to consider $n_1 \geq 4$, as the results hold for the smaller values of n_1. Let $T \in \mathcal{T}_{n,n_1}$ if $T \cong S^n_{n_1}$, then $ZC_1^*(T) = 4n + n_1^2 - 3n_1 - 8$. Therefore, $ZC_1^*(T) = \varphi_1(n, n_1) - 2(n_1 - 1)(n_1 - 2) < \varphi_1(n, n_1)$ and

$$ZC_1^*(T) = \varphi_2(n, n_1) - 2(n_1 - 2)(n - n_1 - 2) \leq \varphi_2(n, n_1). \tag{17}$$

We observe that equality in (17) holds if $n = n_1 + 2$. Also, if $n = n_1 + 2$, then $S^n_{n_1} \cong K^n_{n_1}$. Now, we consider the case that $T \ncong S^n_{n_1}$ and $T \ncong K^n_{n_1}$ for $4 \leq n_1 \leq n - 3$.

Let P: $v_0 v_1, \ldots, v_s$ be a pendent path of T such that $v_0 \in V_1(T)$ and $d_{v_s} = t \geq 3$. Considering $|N(v_s) \cap V_1(T)| = q$ and $N(v_s) \setminus (V_1(T)) \cup \{v_{s-1}\} = \{x_1, x_2, \ldots, x_{t-q-1}\}$. Then, $q \geq 0$, $t - q \geq 2$ (Since $T \ncong K^n_{n_1}$ and $d_{x_i} = d_i \geq 2$). Now, we consider the following two cases:

Case I. $n \geq 2n_1 + 1$.

Here, we choose T such that $ZC_1^*(T)$ is as large as possible. Therefore, by Lemma 6, T contains at least one pendent path (say) P of length greater than 1. Let us consider $T' = T - \{v_0, v_1, \ldots, v_{s-1}\}$, so $T' \in \mathcal{PT}_{n-s, n_1-1}$. Now, for $n - s \geq 2(n_1 - 1) + 1$, Lemma 2 implies that $\sum_{i=1}^{t-q-1} (d_i) \leq n_1 + t - 2q - 2$ and

$$\begin{aligned} ZC_1^*(T) &= ZC_1^*(T\prime) + 1 + 4(s-2) + 3t - 2 + q \\ &\quad - (t - q - 1) + 2\sum_{i=1}^{t-q-1} d_i \\ &\leq \varphi_1(n - s, n_1 - 1) + 1 + 4(s-2) + 3t - 2 \\ &\quad + q - (t - q - 1) + 2(n_1 + t - 2q - 2) \\ &= \varphi_1(n, n_1) - 4n_1 + 4t - 2q \\ &\leq \varphi_1(n, n_1), \end{aligned} \tag{18}$$

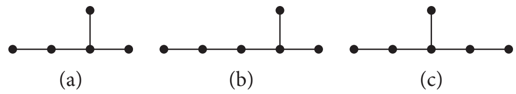


Figure 2: The trees (a) T1, (b) T_2, and (c) T_3.

where the equality holds if all the inequalities mentioned in the above argument turn into equalities. Thus, we have $ZC_1^*(T') = \varphi_1(n-s, n_1-1)$, if $q=0$ and $n_1 = t$.

By the induction hypothesis, $T' \in \mathcal{T}_{n_1-1}^{n-s}$. Here, $T\prime$ contains a unique vertex of degree greater than 2, and hence $T \in \mathcal{T}_{n_1}^{n}$.

Now if $n - s \leq 2(n_1 - 1)$, then

$$\begin{aligned} ZC_1^*(T) = {} & ZC_1^*(T\prime) + 1 + 4(s-2) + 3t - 2 + q \\ & - (t-q-1) + 2\sum_{i=1}^{t-q-1} d_i \\ & \varphi_2(n-s, n_1-1) + 1 + 4(s-2) + 3t - 2 \\ & + q - (t-q-1) + 2(n_1 + t - 2q - 2) \\ & \varphi_1(n, n_1) + (2n_1 - 6)(n-s) - 4n_1^2 + 10n_1 \\ & - 6 + 4t - 2q \\ & \varphi_1(n, n_1) + 2(n_1 - 1)(2n_1 - 6) - 4n_1^2 + 10n_1 \\ & - 6 + 4t - 2q \\ & \varphi_1(n, n_1) - 4n_1 + 4t - 2n_1 - 6 - 2q < \varphi_1(n, n_1). \end{aligned} \tag{19}$$

Case II: $n \leq 2n_1$

By using Lemma 2, we may choose P with $s = 1$. Let $T' = T - v_0$, then $T' \in \mathcal{PT}_{n-1, n_1-1}$. So.

$$\begin{aligned} ZC_1^*(T) &= ZC_1^*(T') + 2q - 2 + 2\sum_{i=1}^{t-q} d_i \\ &\leq ZC_1^*(T') + 2n_1 + 2t - 2q - 2. \end{aligned} \tag{20}$$

Now if $n = 2n_1$, then $n - 1 = 2n_1 - 1$ and we get

$$\begin{aligned} ZC_1^*(T) &\leq \varphi_1(2n_1 - 1, n_1 - 1) + 2n_1 + 2t - 2q - 2 \\ &= \varphi_2(2n_1, n_1) - 2n_1 + 2t - 2q + 2 \\ &\leq \varphi_2(2n_1, n_1), \end{aligned} \tag{21}$$

where the equality holds only if $ZC_1^*(T') = \varphi_1(2n_1 - 1, n_1 - 1)$, $q = 1$, and $n_1 = t$. As $T' \cong K_{n_1-1}^{2n_1-1}$ and $K_{n_1-1}^{2n_1-1}$ contain a unique vertex with degree greater than 2, so we have $T \cong K_{n_1}^{2n_1}$.

If we have $n < 2n_1$, then

$$\begin{aligned} ZC_1^*(T) &\leq \varphi_2(n-1, n_1-1) + 2n_1 + 2t - 2q - 2 \\ &= \varphi_2(n, n_1) - 2n + 2n_1 + 2t - 2q + 2 \\ &\leq \varphi_2(n, n_1). \end{aligned} \tag{22}$$

The above inequality follows from Lemma 2. Equality $ZC_1^*(T) = \varphi_2(n, n_1)$ shows that all the above relations are also equalities. Particularly $ZC_1^*(T') = \varphi_2(n-1, n_1-1)$. Therefore, by induction hypothesis, $T' \cong K_{n_1-1}^{n-1}$. We observe that $K_{n_1-1}^{n-1}$ contains a unique vertex of degree greater than 2 and $d_{v_s} \geq 3$, hence $T \cong K_{n_1}^{n}$. By this result the proof of Theorem 2 is complete.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

This work was supported by the National University of Computer and Emerging Sciences, Lahore, Pakistan.

References

[1] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. Total φ-electron energy of alternant hydrocarbons," *Chemical Physics Letters*, vol. 17, no. 4, pp. 535–538, 1972.

[2] I. Gutman, B. Ruščić, N. Trinajstić, and C. F. Wilcox, "Graph theory and molecular orbitals. XII. Acyclic polyenes," *The Journal of Chemical Physics*, vol. 62, no. 9, pp. 3399–3405, 1975.

[3] A. B. Zakharov, A. V. Dyachenko, and V. V. Ivanov, "Topological characteristics of iterated line graphs in QSAR problem: octane numbers of saturated hydrocarbons," *Journal of Chemometrics*, vol. 33, no. 9, Article ID e3169, 2019.

[4] A. B. Zakharov and 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 University Bulletin Chemical Series*, vol. 32, no. 55, pp. 38–45, 2019.

[5] A. Ali, I. Gutman, E. Milovanović, and I. Milovanović, "Sum of powers of the degrees of graphs: extremal results and bounds," *Communications in Mathematical and in Computer Chemistry*, vol. 80, pp. 5–84, 2018.

[6] A. Ali, L. Zhong, and I. Gutman, "Harmonic index and its generalizations: extremal results and bounds," *Communications in Mathematical and in Computer Chemistry*, vol. 81, no. 2, pp. 249–311, 2019.

[7] B. Borovićanin, K. C. Das, B. Furtula, and I. Gutman, "Bounds for Zagreb indices," *Communications in Mathematical and in Computer Chemistry*, vol. 78, pp. 17–10, 2017.

[8] I. Gutman, E. Milovanović, and I. Milovanović, "Beyond the Zagreb indices," *AKCE International Journal of Graphs and Combinatorics*, 2018, In press.

[9] A. Ali, "Tetracyclic graphs with maximum second Zagreb index: a simple approach," *Asian-European Journal of Mathematics*, vol. 11, no. 5, Article ID 1850064, 2018.

[10] A. Ali, K. C. Das, and S. Akhter, "On the extremal graphs for second Zagreb index with fixed number of vertices and cyclomatic number," *Miskolc Mathematical Notes*, 2019, In press.

[11] A. R. Ashrafi, M. Eliasi, and A. Ghalavand, "Laplacian coefficients and Zagreb indices of trees," *Linear and Multilinear Algebra*, vol. 67, no. 9, pp. 1736–1749, 2019.

[12] M. Azari, "Generalized Zagreb index of product graphs," *Transactions on Combinatorics*, vol. 8, no. 4, pp. 35–48, 2019.

[13] K. C. Das and A. Ali, "On a conjecture about the second Zagreb index," *Discrete Mathematics Letters*, vol. 2, pp. 38–43, 2019.

[14] M. Eliasi and A. Ghalavand, "Trees with the minimal second Zagreb index," *Kragujevac Journal of Mathematics*, vol. 42, no. 3, pp. 325–333, 2018.

[15] F. Javaid, M. K. Jamil, and I. Tomescu, "Extremal k-generalized quasi unicyclic graphs with respect to first and second Zagreb indices," *Discrete Applied Mathematics*, vol. 270, pp. 153–158, 2019.

[16] J.-B. Liu, C. Wang, S. Wang, and B. Wei, "Zagreb indices and multiplicative Zagreb indices of eulerian graphs," *Bulletin of the Malaysian Mathematical Sciences Society*, vol. 42, no. 1, pp. 67–78, 2019.

[17] E. Milovanović, I. Milovanović, and M. Jamil, "Some properties of the Zagreb indices," *Filomat*, vol. 32, no. 7, pp. 2667–2675, 2018.

[18] D. A. Mojdeh, M. Habibi, L. Badakhshian, and Y. Rao, "Zagreb indices of trees, unicyclic and bicyclic graphs with given (total) domination," *IEEE Access*, vol. 7, pp. 94143–94149, 2019.

[19] L. Pei and X. Pan, "Extremal values on Zagreb indices of trees with given distance k-domination number," *Journal of Inequalities and Applications*, vol. 2018, Article ID 16, 2018.

[20] A. Yurtas, M. Togan, V. Lokesha, I. N. Cangul, and I. Gutman, "Inverse problem for Zagreb indices," *Journal of Mathematical Chemistry*, vol. 57, no. 2, pp. 609–615, 2019.

[21] F. Zhan, Y. Qiao, and J. Cai, "Relations between the first Zagreb index and spectral moment of graphs," *Communications in Mathematical and in Computer Chemistry*, vol. 81, pp. 383–392, 2019.

[22] T. Réti, A. Ali, P. Varga, and E. Bitay, "Some properties of the neighborhood first Zagreb index," *Discrete Mathematics Letters*, vol. 2, pp. 10–17, 2019.

[23] A. Ali and N. Trinajstić, "A novel/old modification of the first Zagreb index," *Molecular Informatics*, vol. 37, no. 6-7, Article ID 1800008, 2018.

[24] R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley VCH, Weinheim, Germany, 2000.

[25] A. M. Naji, N. D. Soner, and I. Gutman, "On leap Zagreb indices of graphs," *Communications in Combinatorics and Optimization*, vol. 2, pp. 99–117, 2017.

[26] B. Basavanagoud and E. Chitra, "On the leap Zagreb indices of generalized xyz-point-line transformation graphs $T^{xyz}(G)$ when $z = 1$," *International Journal of Mathematical Combinatorics*, vol. 2, pp. 44–66, 2018.

[27] Z. Du, A. Ali, and N. Trinajstić, "Alkanes with the first three maximal/minimal modified first Zagreb connection indices," *Molecular Informatics*, vol. 38, no. 4, Article ID 1800116, 2019.

[28] G. Ducoffe, R. Marinescu-Ghemeci, C. Obreja, A. Popa, and R. M. Tache, *Proceedings of the 16th Cologne-Twente Workshop on Graphs and Combinatorial Optimization*, CNAM, Paris, France, 2018.

[29] G. Ducoffe, R. Marinescu-Ghemeci, C. Obreja, A. Popa, and R. M. Tache, "Extremal graphs with respect to the modified first Zagreb connection index," in *Proceedings of the 20th International Symposium on Symbolic and Numeric Algorithms for Scientific Computing (SYNASC)*, pp. 141–148, Timisoara, Romania, 2018.

[30] N. Fatima, A. A. Bhatti, A. Ali, and W. Gao, "Zagreb connection indices of two dendrimer nanostars," *Acta Chemica Iasi*, vol. 27, no. 1, pp. 1–14, 2019.

[31] S. Khalid, J. Kok, A. Ali, and M. Bashir, "Zagreb connection indices of TiO_2 nanotubes," *Chemistry: Bulgarian Journal of Science Education*, vol. 27, pp. 86–92, 2018.

[32] S. Manzoor, N. Fatima, A. A. Bhatti, and A. Ali, "Zagreb connection indices of some nanostructures," *Acta Chemica Iasi*, vol. 26, no. 2, pp. 169–180, 2018.

[33] D. Maji and G. Ghorai, "A novel graph invariant: the third leap Zagreb index under several graph operations," *Discrete Mathematics, Algorithms and Applications*, vol. 11, no. 5, Article ID 1950054, 2019.

[34] A. M. Naji, B. Davvaz, S. S. Mahde, and N. D. Soner, "A study on some properties of leap graphs," *Communications in Combinatorics and Optimization*, vol. 5, no. 1, pp. 9–17, 2020.

[35] A. M. Naji and N. D. Soner, "The first leap Zagreb index of some graph operations," *International Journal of Applied Graph Theory*, vol. 2, pp. 7–18, 2018.

[36] S. Noureen, A. A. Bhatti, and A. Ali, "Extremal trees for the modified first Zagreb connection index with fixed number of segments or vertices of degree 2," *Journal of Taibah University for Science*, vol. 14, no. 1, pp. 31–37, 2019.

[37] Z. Shao, I. Gutman, Z. Li, S. Wang, and P. Wu, "Leap Zagreb indices of trees and unicyclic graphs," *Communications in Combinatorics and Optimization*, vol. 3, no. 2, pp. 179–194, 2018.

[38] J.-H. Tang, U. Ali, M. Javaid, and K. Shabbir, "Zagreb connection indices of subdivision and semi-total point operations on graphs," *Journal of Chemistry*, vol. 2019, Article ID 9846913, 14 pages, 2019.

[39] A. Ye, M. I. Qureshi, A. Fahad et al., "Zagreb connection number index of nanotubes and regular hexagonal lattice," *Open Chemistry*, vol. 17, no. 1, pp. 75–80, 2019.

[40] H. Liu, M. Lu, and F. Tian, "Trees of extremal connectivity index," *Discrete Applied Mathematics*, vol. 154, no. 1, pp. 106–119, 2006.

[41] I. Gutman and B. Furtula, *Recent Results in the Theory of Randic Index*, University of Kragujevac, Kragujevac, Serbia, 2008.