



*Research article***On trees with a given number of segments and their maximum general Z-type index****Hicham Saber¹, Zahid Raza², Abdulaziz M. Alanazi³, Adel A. Attiya¹ and Akbar Ali^{1,*}**¹ Department of Mathematics, College of Science, University of Ha'il, Ha'il, Saudi Arabia² Department of Mathematics, College of Sciences, University of Sharjah, Sharjah, UAE³ Department of Mathematics, Faculty of Sciences, University of Tabuk, Tabuk, Saudi Arabia* **Correspondence:** Email: akbarali.maths@gmail.com.

Abstract: The general Z-type index is a molecular descriptor, introduced recently by Chen and Lin [*Discrete Optim.*, **50** (2023), 100808], which generalizes several well-known molecular descriptors, including the (general) sum-connectivity index and (general) Platt index. The primary objective of the current paper is to study the largest value of the general Z-type index of graphs in the class of all fixed-order trees (and chemical trees) with a particular number of segments.

Keywords: topological index; extremal graphs; general Platt index; segment; molecular descriptors**Mathematics Subject Classification:** 05C05, 05C07; 05C09; 05C35; 05C92

1. Introduction

Molecular descriptors are the numerical values that describe certain characteristics of molecules. These numbers are essential to the creation of a number of mathematical chemistry models, such as the QSAR/QSPR (quantitative structure activity/property relationship) models, which help forecast the physicochemical properties and biological activities of new compounds. One specific class of these descriptors is the class of topological indices; such descriptors depend on the graph of the structure of the compound under consideration. There are various such indices in the literature on mathematical chemistry, most of which are studied in relation to chemical graphs. The general Z-type index—a topological index introduced recently by Chen and Lin [5]—is the subject of this study.

To avoid trivialities, we are explicitly only taking connected graphs into account in this study. The notation $E(G)$ is used to represent the edge set of a graph G , while $V(G)$ is used to represent G 's vertex set. To express the degree of a vertex $u \in V(G)$, we use $d_u(G)$ (or just d_u , where there is no possibility of misunderstanding regarding the considered graph). As stated in [22], the sum-connectivity index $\chi_{-\frac{1}{2}}$ of a graph G is the sum of the values $(d_u + d_v)^{-1/2}$ across all of G 's edges uv .

In [21], the index $\chi_{-\frac{1}{2}}$ was generalized under the term “general sum-connectivity index” by substituting α for “ $-1/2$,” that is, χ_α , where α is a real number that differs from zero. The relationship between a graph's χ_α and its line graph was examined by Chen [4]. Milovanović et al. [12] examined a number of inequalities for χ_α . The extremum values of χ_α for trees with a certain maximum degree were examined by Swartz and Vetrík [16]. For graphs with a fixed cyclomatic number, Ali et al. [3] addressed a problem about extremum values of χ_α . Zhong and Qian [20] investigated a problem involving trees with a given matching number and minimum χ_α . By fixing the diameter and girth of unicyclic networks, Vetrík [19] investigated this index. Further information about certain extremal results involving χ_α can be found in [17, 18]. The indices χ_1, χ_2 , and $2\chi_{-1}$ are equivalent to the well-known first Zagreb index [15], hyper Zagreb index [10], and harmonic index [7], respectively.

The platt index [8, 14] is defined as

$$Pl(G) = \sum_{uv \in E(G)} (d_u + d_v - 2).$$

The general platt index [2] is defined as

$$Pl_\alpha(G) = \sum_{uv \in E(G)} (d_u + d_v - 2)^\alpha.$$

Additional detail on the general Platt index can be found in [1, 3].

The general Z-type index [5] is defined as

$$Z_{\alpha,\beta}(G) = \sum_{uv \in E(G)} (d_u + d_v - \beta)^\alpha,$$

where β is a nonzero real number different from 0. Certainly, $Z_{\alpha,\beta}$ generalizes all the abovementioned indices, namely, the sum-connectivity index, general sum-connectivity index (and hence the first Zagreb index, hyper Zagreb index, and harmonic index), Platt index, general Platt index (and hence the reformulated first Zagreb index [11]).

A tree is said to be a chemical tree if the degree of each vertex is less than 5. A graph with n vertices is called an n -order graph. A segment in a tree T is defined [6, 9] as a non-trivial path of T , indicated by $P : x_1 x_2 \dots x_r$ such that $d_{x_1}(T), d_{x_r}(T) \notin \{2\}$, and $d_{x_i}(T) = 2$ whenever $2 \leq i \leq r - 1$; in addition, if $\min\{d_{x_1}(T), d_{x_r}(T)\} = 1$ and $\max\{d_{x_1}(T), d_{x_r}(T)\} \geq 3$ then P is called a pendent path of T ; however, if $\min\{d_{x_1}(T), d_{x_r}(T)\} \geq 3$ and $\max\{d_{x_1}(T), d_{x_r}(T)\} \geq 3$ then P is called an internal path of T .

In the present paper, our main aim is to study the general Z-type index (and hence the abovementioned particular cases of this index, including the general Platt index) of n -order trees and chemical trees with a given number of segments. Particularly, the main goal of the present paper is to study the greatest value of $Z_{\alpha,\beta}$ of fixed-order chemical trees with a fixed number of segments for $1 < \alpha \leq 3$ and $\beta \leq 2$. Similar results for general trees are also established for $\alpha > 1$ and $\beta \leq 2$.

2. Main results

A vertex u in a tree T with $d_u(T) = 1$ or $d_u(T) > 2$ is called a pendent vertex of T or a branching vertex of T , respectively. A star-like tree is a tree containing only one branching vertex. To avoid trivialities, throughout this section, we consider trees containing not less than three segments.

Define $\Theta_{i,j}(T) := |\{uv \in E(T) : d_u(T) = i, d_v(T) = j\}|$ and $m_i(T) := |\{u \in V(T) : d_u(T) = i\}|$. For $2 \leq j \leq 4$ and $n \geq 3$, we have the following system of equations for an n -order chemical tree T :

$$\sum_{\substack{i=1 \\ i \neq j}}^4 \Theta_{j,i}(T) + 2\Theta_{j,j}(T) = j \cdot m_j(T). \tag{2.1}$$

$$\sum_{1 \leq i \leq j \leq 4} \Theta_{i,j}(T) = n - 1. \tag{2.2}$$

For $u \in V(T)$, we define $N_T(u) = \{u' \in V(T) : u'u \in E(T)\}$. Let ${}^1\mathcal{T}_{n,r}$ denote the set of n -order trees having r segments, provided that the chain of inequalities $3 \leq r \leq n - 1$ holds. We denote by ${}^1T_{max}$ a tree having the greatest value of $Z_{\alpha,\beta}$ in the set ${}^1\mathcal{T}_{n,r}$ for $\beta \leq 2$ and $\alpha > 1$.

Lemma 2.1. *If $\Theta_{1,k}({}^1T_{max}) \neq 0$ for some k with $k \geq 3$, then every vertex of degree 2 (if exists) in ${}^1T_{max}$ has a pendent neighbor.*

Proof. We chose $t_1, t_2 \in V({}^1T_{max})$ in such a way that $t_1t_2 \in E({}^1T_{max})$, $d_{t_2}({}^1T_{max}) \geq 3$ and $d_{t_1}({}^1T_{max}) = 1$. Also, we assume contrarily that $x, x_1, x_2 \in V({}^1T_{max})$, such that $x_1x, x_2x \in E({}^1T_{max})$, $d_x({}^1T_{max}) = 2$ and $d_{x_i}({}^1T_{max}) \geq 2$ for $i = 1, 2$. If T^* denotes the tree formed from ${}^1T_{max}$ by dropping the edges t_1t_2, xx_1, xx_2 and adding the edges t_1x, t_2x, x_1x_2 , then certainly $T^* \in {}^1\mathcal{T}_{n,r}$. In the following, we assume $d_p({}^1T_{max}) = d_p$ for every $p \in V({}^1T_{max}) = V(T^*)$. The, we have

$$\begin{aligned} Z_{\alpha,\beta}({}^1T_{max}) - Z_{\alpha,\beta}(T^*) &= (d_{t_2} - \beta + 1)^\alpha + (d_{x_1} - \beta + 2)^\alpha + (d_{x_2} - \beta + 2)^\alpha \\ &\quad - (3 - \beta)^\alpha - (d_{t_2} - \beta + 2)^\alpha - (d_{x_1} + d_{x_2} - \beta)^\alpha. \end{aligned} \tag{2.3}$$

Let us define a function f of real variables a, b, c , with fixed real numbers α and β as

$$f(a, b, c) = (a - \beta + 1)^\alpha + (b - \beta + 2)^\alpha + (c - \beta + 2)^\alpha - (a - \beta + 2)^\alpha - (b + c - \beta)^\alpha - (3 - \beta)^\alpha,$$

where $\alpha > 1, \beta \leq 2, a \geq 3, b \geq 2$ and $c \geq 2$. We note that the function f is strictly decreasing in each of its variables a, b, c . Hence, (2.3) gives

$$Z_{\alpha,\beta}({}^1T_{max}) - Z_{\alpha,\beta}(T^*) \leq (4 - \beta)^\alpha - (3 - \beta)^\alpha - ((5 - \beta)^\alpha - (4 - \beta)^\alpha) < 0,$$

a contradiction to the definition of the tree ${}^1T_{max}$. □

Lemma 2.2. *The tree ${}^1T_{max}$ must be a star-like tree.*

Proof. Since ${}^1T_{max}$ has at least three segments, its number of branching vertices must be nonzero. We chose a vertex $t' \in V({}^1T_{max})$ of maximum degree. Contrarily, assume that the number of branching vertices of the tree ${}^1T_{max}$ is at least 2. Among all the branching vertices of ${}^1T_{max}$ different from t' , we pick a branching vertex $t \in V({}^1T_{max}) \setminus \{t'\}$ such that the vertices t' and t have the minimum distance between them. two distinct branching vertices. Let $d_{t'}({}^1T_{max}) = \tau'$ and $d_t({}^1T_{max}) = \tau$. Furthermore, we assume that $N_{{}^1T_{max}}(t) = \{v_l, t_1, \dots, t_{\tau-1}\}$ and $N_{{}^1T_{max}}(t') = \{y, t'_1, \dots, t'_{\tau'-1}\}$, where the vertices v_l and y lie on the unique path connecting t and t' . Let T^* be the tree obtained from ${}^1T_{max}$ by removing $t_1t, t_2t, \dots, t_{\tau-1}t$ and adding $t_1t', t_2t', \dots, t_{\tau-1}t'$. In the remaining proof, we assume that $d_\gamma = d_\gamma({}^1T_{max})$ for every $\gamma \in V({}^1T_{max}) = V(T^*)$.

Case 1: $t' t \notin E({}^1T_{max})$.

We note in the present case that $d_y = d_{v_l} = 2$ and hence

$$\begin{aligned} Z_{\alpha,\beta}({}^1T_{max}) - Z_{\alpha,\beta}(T^*) &= \sum_{i=1}^{\tau'-1} (\tau' + d_{t'_i} - \beta)^\alpha + (\tau' + 2 - \beta)^\alpha + \sum_{j=1}^{\tau-1} (\tau + d_{t_j} - \beta)^\alpha + (\tau + 2 - \beta)^\alpha \\ &\quad - \sum_{i=1}^{\tau'-1} ((\tau' + \tau - 1) - \beta + d_{t'_i})^\alpha - \sum_{j=1}^{\tau-1} ((\tau' + \tau - 1) - \beta + d_{t_j})^\alpha \\ &\quad - (\tau' + \tau - \beta + 1)^\alpha - (3 - \beta)^\alpha \\ &< (\tau' - \beta + 2)^\alpha + (\tau - \beta + 2)^\alpha - (\tau' + \tau - \beta + 1)^\alpha - (3 - \beta)^\alpha. \end{aligned} \quad (2.4)$$

We note that there are two real numbers τ_1 and τ_2 satisfying the inequalities $3 - \beta < \tau_1 < \tau - \beta + 2$ and $\tau' - \beta + 2 < \tau_2 < \tau' + \tau - \beta + 1$ such that

$$(\tau' - \beta + 2)^\alpha + (\tau - \beta + 2)^\alpha - (\tau' + \tau - \beta + 1)^\alpha - (3 - \beta)^\alpha = \alpha(\tau - 1) (\tau_1^{\alpha-1} - \tau_2^{\alpha-1}). \quad (2.5)$$

As $\tau' \geq \tau$, we have $\tau_1 < \tau_2$ and hence from (2.4) and (2.5), we arrive at $Z_{\alpha,\beta}({}^1T_{max}) - Z_{\alpha,\beta}(T^*) < 0$, a contradiction.

Case 2: $t' t \in E({}^1T_{max})$.

In the present case, we obtain

$$\begin{aligned} Z_{\alpha,\beta}({}^1T_{max}) - Z_{\alpha,\beta}(T^*) &= \sum_{i=1}^{\tau'-1} (\tau' + d_{t'_i} - \beta)^\alpha + \sum_{j=1}^{\tau-1} (\tau + d_{t_j} - \beta)^\alpha \\ &\quad - \sum_{i=1}^{\tau'-1} (\tau + \tau' - \beta + d_{t'_i} - 1)^\alpha - \sum_{j=1}^{\tau-1} (\tau + \tau' - \beta + d_{t_j} - 1)^\alpha < 0, \end{aligned}$$

again a contradiction.

In both possible cases, we arrive at a contradiction. Therefore, the tree ${}^1T_{max}$ contains exactly one branching vertex. \square

Theorem 1. *If the chain of inequalities $\lfloor (n-1)/2 \rfloor \leq r \leq n-1$ holds then the tree ${}^1T_{max}$ is star-like and $\Theta_{2,2}({}^1T_{max}) = 0$.*

Proof. Lemma 2.2 confirms that the tree ${}^1T_{max}$ is star-like. Hence, the number of segments r of ${}^1T_{max}$ is equal to its maximum degree. Suppose, contrarily, that $\Theta_{2,2}({}^1T_{max}) > 0$. Then, Lemma 2.1 confirms that $\Theta_{r,1}({}^1T_{max}) = 0$. Consequently, we have $2r = \Theta_{2,r}({}^1T_{max}) + \Theta_{1,2}({}^1T_{max}) \leq |E({}^1T_{max})| - 1 = n - 2$, a contradiction. \square

Theorem 2. *If the chain of inequalities $3 \leq r \leq \lfloor (n-1)/2 \rfloor$ holds then the tree ${}^1T_{max}$ is star-like and $\Theta_{r,1}({}^1T_{max}) = 0$.*

Proof. Lemma 2.2 confirms that the tree ${}^1T_{max}$ is star-like. Hence, the number of segments r of ${}^1T_{max}$ is equal to its maximum degree. Suppose, contrarily, that $\Theta_{r,1}({}^1T_{max}) > 0$. Then, Lemma 2.1 confirms that $\Theta_{2,2}({}^1T_{max}) = 0$. So, we have $2r > \Theta_{1,2}({}^1T_{max}) + r = |E({}^1T_{max})| = n - 1$, a contradiction. \square

In the rest of this section, we focus on chemical trees. Denote by $\mathcal{T}_{n,r}$ the set of all n -order chemical trees possessing r segments such that $3 \leq r \leq n - 1$. For $r \in \{3, 4\}$, the tree(s) maximizing $Z_{\alpha,\beta}$ in the set $\mathcal{T}_{n,r}$ for $\beta \leq 2$ and $\alpha > 1$ can be obtained directly by utilizing Theorem 1 and/or Theorem 2. Hence, in the remaining part of the present section, we assume that $5 \leq r \leq n - 1$. Denote by T_{max} a tree with the greatest value of $Z_{\alpha,\beta}$ in the set $\mathcal{T}_{n,r}$ with the conditions $1 < \alpha \leq 3$, $\beta \leq 2$ and $5 \leq r \leq n - 1$.

Lemma 2.3. *It holds that $m_3(T_{max}) \leq 2$.*

Proof. Contrarily, assume that $m_3(T_{max}) \geq 3$. We pick the vertices $x, y, z \in V(T_{max})$ of degree 3 in such a way that if all these three vertices lie on one path then the vertex y must lie on the path connecting x and z . Let $P : (x =)u_1u_2 \dots u_l(= z)$ be the path connecting z and x in T_{max} . Let $N_z(T_{max}) = \{z_1, z_2, z_3\}$, where $z_3 = u_{l-1}$. Certainly, x, y, z , must be pairwise nonadjacent when these vertices do not lie on one path. Let T' denote the tree constructed from T_{max} by deleting the edges zz_1, zz_2 and inserting xz_1, yz_2 . In the rest of the proof, we take $d_\gamma(T_{max}) = d_\gamma$ for $\gamma \in V(T') = V(T_{max})$. We may assume, without loss of generality, that $d_{z_2} \leq d_{z_1}$.

Case 1: The vertices x, y, z , are pairwise nonadjacent.

In this case, we obtain

$$\begin{aligned} & Z_{\alpha,\beta}(T_{max}) - Z_{\alpha,\beta}(T') \\ &= \sum_{x' \in N_{T_{max}}(x)} [(d_{x'} - \beta + 3)^\alpha - (d_{x'} - \beta + 4)^\alpha] + \sum_{y' \in N_{T_{max}}(y)} [(d_{y'} - \beta + 3)^\alpha - (d_{y'} - \beta + 4)^\alpha] \\ &+ \sum_{i=1}^2 [(d_{z_i} - \beta + 3)^\alpha - (d_{z_i} - \beta + 4)^\alpha] + (d_{z_3} - \beta + 3)^\alpha - (d_{z_3} - \beta + 1)^\alpha. \end{aligned} \quad (2.6)$$

We note that each of the vertices x, y, z , may have at most two pendent neighbors; if x, y, z , lie on one path then y may have at most one pendent neighbor. Thus, Equation (2.6) implies that

$$\begin{aligned} Z_{\alpha,\beta}(T_{max}) - Z_{\alpha,\beta}(T') &\leq 6[(4 - \beta)^\alpha - (5 - \beta)^\alpha] + 2[(5 - \beta)^\alpha - (6 - \beta)^\alpha] + (7 - \beta)^\alpha - (5 - \beta)^\alpha \\ &= 6[(4 - \beta)^\alpha - (5 - \beta)^\alpha] + [(5 - \beta)^\alpha - (6 - \beta)^\alpha] + (7 - \beta)^\alpha - (6 - \beta)^\alpha \\ &< 7[(4 - \beta)^\alpha - (5 - \beta)^\alpha] + (7 - \beta)^\alpha - (6 - \beta)^\alpha. \end{aligned} \quad (2.7)$$

We note that there exist two real numbers a_1 and a_2 which satisfy the inequalities $6 - \beta < a_1 < 7 - \beta$ and $4 - \beta < a_2 < 5 - \beta$ such that

$$7[(4 - \beta)^\alpha - (5 - \beta)^\alpha] + (7 - \beta)^\alpha - (6 - \beta)^\alpha = \alpha(a_1^{\alpha-1} - 7a_2^{\alpha-1}). \quad (2.8)$$

Since

$$\frac{7 - \beta}{4 - \beta} \leq \frac{5}{2},$$

we have

$$\left(\frac{7 - \beta}{4 - \beta}\right)^{\alpha-1} \leq \left(\frac{5}{2}\right)^{\alpha-1} \leq 7,$$

and hence

$$a_1^{\alpha-1} < (7 - \beta)^{\alpha-1} \leq 7(4 - \beta)^{\alpha-1} < 7a_2^{\alpha-1},$$

which confirms that the right-hand side of Eq (2.8) is negative; thus, (2.7) yields $Z_{\alpha,\beta}(T_{max}) < Z_{\alpha,\beta}(T')$, a contradiction.

Case 2: Vertices x, y, z , lie on one path, and only one of x, z , is a neighbor of y .

We suppose, without loss of generality, that $xy \notin E(T_{max})$ and $yz \in E(T_{max})$. Then $y = z_3$. Thus, we obtain

$$\begin{aligned}
 & Z_{\alpha,\beta}(T_{max}) - Z_{\alpha,\beta}(T') \\
 &= \sum_{x' \in N_{T_{max}}(x)} (d_{x'} - \beta + 3)^\alpha + \sum_{y' \in N_{T_{max}}(y) \setminus \{z\}} (d_{y'} - \beta + 3)^\alpha + \sum_{z_i \in N_{T_{max}}(z) \setminus \{y\}} (d_{z_i} - \beta + 3)^\alpha \\
 &+ (6 - \beta)^\alpha - \sum_{x' \in N_{T_{max}}(x)} (d_{x'} - \beta + 4)^\alpha - \sum_{y' \in N_{T_{max}}(y) \setminus \{z\}} (d_{y'} - \beta + 4)^\alpha \\
 &- (d_{z_1} - \beta + 4)^\alpha - (d_{z_2} - \beta + 4)^\alpha - (5 - \beta)^\alpha, \\
 &< \sum_{i=1}^2 [(d_{z_i} - \beta + 3)^\alpha - (d_{z_i} - \beta + 4)^\alpha] + (6 - \beta)^\alpha - (5 - \beta)^\alpha + [(d_{u_2} - \beta + 3)^\alpha - (d_{u_2} - \beta + 4)^\alpha] \\
 &< (6 - \beta)^\alpha - (5 - \beta)^\alpha + (d_{u_2} - \beta + 3)^\alpha - (d_{u_2} - \beta + 4)^\alpha \leq 0, \tag{2.9}
 \end{aligned}$$

a contradiction.

Case 3: Vertices x, y, z , lie on one path provided that $xy \in E(T_{max})$ and $yz \in E(T_{max})$.

In this case, we obtain

$$\begin{aligned}
 & Z_{\alpha,\beta}(T_{max}) - Z_{\alpha,\beta}(T') \\
 &= \sum_{x' \in N_{T_{max}}(x) \setminus \{y\}} (d_{x'} - \beta + 3)^\alpha + \sum_{y' \in N_{T_{max}}(y) \setminus \{x,z\}} (d_{y'} - \beta + 3)^\alpha + \sum_{z_i \in N_{T_{max}}(z) \setminus \{y\}} (d_{z_i} - \beta + 3)^\alpha \\
 &+ 2(6 - \beta)^\alpha - \sum_{x' \in N_{T_{max}}(x) \setminus \{y\}} (d_{x'} - \beta + 4)^\alpha - \sum_{y' \in N_{T_{max}}(y) \setminus \{x,z\}} (d_{y'} - \beta + 4)^\alpha - (8 - \beta)^\alpha \\
 &- (d_{z_1} - \beta + 4)^\alpha - (d_{z_2} - \beta + 4)^\alpha - (5 - \beta)^\alpha \\
 &< \sum_{i=1}^2 [(d_{z_i} - \beta + 3)^\alpha - (d_{z_i} - \beta + 4)^\alpha] + (6 - \beta)^\alpha - (5 - \beta)^\alpha + (6 - \beta)^\alpha - (8 - \beta)^\alpha \\
 &< (6 - \beta)^\alpha - (5 - \beta)^\alpha - [(8 - \beta)^\alpha - (6 - \beta)^\alpha] < 0.
 \end{aligned}$$

Thus, we arrive at $Z_{\alpha,\beta}(T_{max}) < Z_{\alpha,\beta}(T')$, a contradiction. \square

Lemma 2.4. Every internal path of the tree T_{max} has length 1.

Proof. Assume to the contrary that $P : t_1 \dots t_k$ is an internal path of length $k - 1 \geq 2$ in T_{max} . Let $x \in V(T_{max})$ be a pendent vertex, and let t be its unique neighbor. Let T' be the tree deduced from T_{max} by dropping $tx, t_1 t_2, t_{k-1} t_k$ and adding $t_1 t_k, t_2 x, t_{k-1} t$. In the following, we use d_γ to represent the degree of a vertex γ in T_{max} . It is clear that $T' \in \mathcal{T}_{n,r}$. On the other hand, we have

$$Z_{\alpha,\beta}(T_{max}) - Z_{\alpha,\beta}(T') = (d_{t_1} - \beta + 2)^\alpha + (d_t - \beta + 1)^\alpha + (d_{t_k} - \beta + 2)^\alpha - (d_{t_1} + d_{t_k} - \beta)^\alpha$$

$$\begin{aligned}
& -(d_t - \beta + 2)^\alpha - (3 - \beta)^\alpha \\
& \leq (d_{t_1} - \beta + 2)^\alpha + (3 - \beta)^\alpha + (5 - \beta)^\alpha - (d_{t_1} + 3 - \beta)^\alpha - (4 - \beta)^\alpha - (3 - \beta)^\alpha \\
& \leq (5 - \beta)^\alpha - (4 - \beta)^\alpha - [(6 - \beta)^\alpha - (5 - \beta)^\alpha] < 0,
\end{aligned}$$

a contradiction. \square

Lemma 2.5. *If $\Theta_{1,s}(T_{max}) \neq 0$ for some s with $s \geq 3$, then T_{max} contains no pendent path of length larger than 2.*

Proof. Let $t_1, t_2 \in V(T_{max})$ be two adjacent vertices such that $d_{t_1}(T_{max}) = 1$ and $d_{t_2}(T_{max}) \geq 3$. Contrarily, we assume that $P : x_1 \dots x_k$ is a pendent path having length $k \geq 3$ in T_{max} , where $d_{x_k}(T_{max}) = 1$ and $d_{x_1}(T_{max}) \geq 3$. Let T^* be the tree formed from T_{max} by deleting $t_1 t_2, x x_1, x x_2$ and adding $t_1 x, t_2 x, x_1 x_2$. Clearly, $T^* \in \mathcal{T}_{n,r}$. But,

$$\begin{aligned}
Z_{\alpha,\beta}(T_{max}) - Z_{\alpha,\beta}(T^*) &= (d_{t_2}(T_{max}) - \beta + 1)^\alpha + (4 - \beta)^\alpha - (3 - \beta)^\alpha - (d_{t_2}(T_{max}) - \beta + 2)^\alpha \\
&\leq (4 - \beta)^\alpha - (3 - \beta)^\alpha - [(5 - \beta)^\alpha - (4 - \beta)^\alpha] < 0,
\end{aligned}$$

which is a contradiction. \square

Lemma 2.6. *If $\Theta_{1,4}(T_{max}) \neq 0$ then $\Theta_{2,3}(T_{max}) = 0$.*

Proof. We assume to the contrary that $\Theta_{2,3}(T_{max}) \neq 0$ as well as $\Theta_{1,4}(T_{max}) \neq 0$. We consider four vertices t_2, t_3, t_4, t_5 of T_{max} such that $t_4 t_5, t_2 t_3 \in E(T_{max})$ and $(d_{t_2}(T_{max}), d_{t_3}(T_{max}), d_{t_4}(T_{max}), d_{t_5}(T_{max})) = (2, 3, 4, 1)$. Let $N_{T_{max}}(t_2) = \{t_1, t_3\}$. Then Lemmas 2.4 and 2.5 confirm that $d_{t_1}(T_{max}) = 1$. Let T' be the graph generated from T_{max} by removing $t_1 t_2, t_2 t_3, t_4 t_5$ and inserting $t_1 t_3, t_2 t_4, t_2 t_5$. Clearly, we have $T' \in \mathcal{T}_{n,r}$. So, we have

$$Z_{\alpha,\beta}(T_{max}) - Z_{\alpha,\beta}(T') = 2 \cdot (5 - \beta)^\alpha - (4 - \beta)^\alpha - (6 - \beta)^\alpha < 0,$$

a contradiction. \square

Lemma 2.7. *If $t_j \in V(T_{max})$ is a vertex of degree three, then t_j has at most one branching neighbor.*

Proof. Contrarily, suppose that $t_{j-1}, t_{j+1} \in V(T_{max})$ are any two branching vertices adjacent to t_j . Let $P : t_1 t_2 \dots t_{j-1} t_j t_{j+1} \dots t_l$ be the largest path in T_{max} containing the aforementioned branching vertices. Because of Lemma 2.3, the path P contains not more than two vertices having degree 3 (in T_{max}) including t_j . In the case when the path P has two vertices having degree 3 (in T_{max}) then without loss of generality, we suppose that $t_i \in V(P)$ is a vertex with degree 3 (in T_{max}) for some i with $1 \leq i < j$. Thus, there is a vertex $t_k \in V(P)$ of degree 4 for some k with $j + 1 \leq k \leq l - 1$, which has only one branching neighbor. So, $d_{t_{k+1}}(T_{max}) = 1$ or 2, $d_{t_{j-1}}(T_{max}) = 3$ or 4, and $d_{t_{j+1}}(T_{max}) = 4$. If T^* is the tree constructed from T_{max} by dropping $t_{j-1} t_j, t_j t_{j+1}, t_k t_{k+1}$ and inserting $t_{j-1} t_{j+1}, t_k t_j, t_j t_{k+1}$, then $T^* \in \mathcal{T}_{n,r}$ and

$$\begin{aligned}
Z_{\alpha,\beta}(T_{max}) - Z_{\alpha,\beta}(T^*) &= (d_{t_{j-1}} - \beta + 3)^\alpha + (d_{t_{k+1}} - \beta + 4)^\alpha - (d_{t_{j-1}} - \beta + 4)^\alpha - (d_{t_{k+1}} - \beta + 3)^\alpha \\
&\leq 2 \cdot 6^\alpha - 7^\alpha - 5^\alpha < 0.
\end{aligned}$$

which is a contradiction, where $d_{t_{j-1}} = d_{t_{j-1}}(T_{max})$ and $d_{t_{k+1}} = d_{t_{k+1}}(T_{max})$. \square

From Lemmas 2.4 and 2.7, next result follows.

Corollary 1. *The induced subgraph of T_{\max} formed by its vertices of degree 4 is a tree.*

For every $\ell \in \{2, 3, 4\}$, denote by ${}^\ell\mathcal{T}_{n,r}$ the set of those n -order chemical trees having r segments that has/have $\ell - 2$ vertex/vertices of degree 3; so, because of [13], it holds that $r \equiv 2\ell \pmod{3}$.

Lemma 2.8. [13] *The degree sequence of $T \in \mathcal{T}_{n,r}$ having no more than 2 vertices of degree 3, with $5 \leq r \leq n - 1$, is as follow:*

$$DS(T) = \begin{cases} \left(\underbrace{(4, \dots, 4)}_{\frac{r-1}{3}}, \underbrace{(2, \dots, 2)}_{n-r-1}, \underbrace{(1, \dots, 1)}_{\frac{2(r+2)}{3}} \right) = DS_2 & \text{when } r \equiv 1 \pmod{3}, \\ \left(\underbrace{(4, \dots, 4)}_{\frac{r-3}{3}}, \underbrace{(3, 2, \dots, 2)}_{n-r-1}, \underbrace{(1, \dots, 1)}_{\frac{2r+3}{3}} \right) = DS_3 & \text{when } r \equiv 0 \pmod{3}, \\ \left(\underbrace{(4, \dots, 4)}_{\frac{r-5}{3}}, \underbrace{(3, 3, 2, \dots, 2)}_{n-r-1}, \underbrace{(1, \dots, 1)}_{\frac{2(r+1)}{3}} \right) = DS_4 & \text{when } r \equiv 2 \pmod{3}. \end{cases}$$

Theorem 3. *If $T \in \mathcal{T}_{n,r}$ with $7 \leq r < n < \frac{5r+7}{3}$ and $r \equiv 1 \pmod{3}$, then*

$$\begin{aligned} Z_{\alpha,\beta}(T) &\leq n((3-\beta)^\alpha - (5-\beta)^\alpha + (6-\beta)^\alpha) \\ &\quad + r\left(- (3-\beta)^\alpha + \frac{5}{3}(5-\beta)^\alpha - (6-\beta)^\alpha + \frac{1}{3}(8-\beta)^\alpha\right) \\ &\quad - (3-\beta)^\alpha - \frac{7}{3}(5-\beta)^\alpha - (6-\beta)^\alpha - \frac{4}{3}(8-\beta)^\alpha. \end{aligned}$$

Proof. We assume that ${}^2T_{\max}$ is a tree having the maximum value of $Z_{\alpha,\beta}$ over the set $\mathcal{T}_{n,r}$ provided that $7 \leq r < n < \frac{5r+7}{3}$ and $r \equiv 1 \pmod{3}$. Lemmas 2.3 and 2.8 confirm that DS_2 is the degree sequence of the tree ${}^2T_{\max}$. Thus, $\Theta_{3,k}({}^2T_{\max}) = 0$ for every $k \in \{1, 2, 3, 4\}$. The condition $r \geq 7$ confirms that $m_4({}^2T_{\max}) \geq 2$. Now, because of Corollary 1, it holds that $\Theta_{4,4}({}^2T_{\max}) = m_4 - 1$ and so $\Theta_{4,4}({}^2T_{\max}) = \frac{r-4}{3}$. Also, the constraint $n < \frac{5r+7}{3}$ implies that $m_1 > m_2$; hence, Lemmas 2.4 and 2.5 confirm that $\Theta_{2,2}({}^2T_{\max}) = 0$. Finally, Eq (2.1) gives

$$\Theta_{1,4}({}^2T_{\max}) = \frac{5r - 3n + 7}{3}, \Theta_{2,4}({}^2T_{\max}) = \Theta_{1,2}({}^2T_{\max}) = n - r - 1.$$

Hence, we calculate $Z_{\alpha,\beta}({}^2T_{\max})$, which is the same as the right-hand side of the desired inequality. \square

Theorem 4. *If $T \in \mathcal{T}_{n,r}$ with $7 \leq r$ and $n \geq \frac{5r+7}{3}$ and $r \equiv 1 \pmod{3}$, then*

$$\begin{aligned} Z_{\alpha,\beta}(T) &\leq n(4-\beta)^\alpha + r\left(\frac{2}{3}(3-\beta)^\alpha - \frac{5}{3}(4-\beta)^\alpha + \frac{2}{3}(6-\beta)^\alpha + \frac{1}{3}(8-\beta)^\alpha\right) \\ &\quad + \frac{4}{3}(3-\beta)^\alpha - \frac{7}{3}(4-\beta)^\alpha + \frac{4}{3}(6-\beta)^\alpha - \frac{4}{3}(8-\beta)^\alpha. \end{aligned}$$

Proof. We assume that ${}^2T_{\max}$ is a tree having the maximum value of $Z_{\alpha,\beta}$ over the set $\mathcal{T}_{n,r}$ under the given constraints. Lemmas 2.3 and 2.8 confirm that DS_2 is the degree sequence of the tree ${}^2T_{\max}$.

Thus, $\Theta_{3,k}(^2T_{\max}) = 0$ for every $k \in \{1, 2, 3, 4\}$. Now, by using Corollary 1, we obtain $\Theta_{4,4}(^2T_{\max}) = \frac{r-4}{3}$. Lemmas 2.4 and 2.5 confirm that $\Theta_{1,4}(^2T_{\max}) = 0$. Finally, by utilizing Eq (2.1), we obtain

$$\Theta_{1,2}(^2T_{\max}) = \frac{2r+4}{3} = \Theta_{4,2}(^2T_{\max}), \Theta_{2,2}(^2T_{\max}) = \frac{3n-5r-7}{3}.$$

Hence, we calculate $Z_{\alpha,\beta}(^2T_{\max})$, which is the same as the right-hand side of the desired inequality. \square

Theorem 5. If $T \in \mathcal{T}_{n,r}$ with $6 \leq r < n < \frac{5r+3}{3}$ and $r \equiv 0 \pmod{3}$, then

$$\begin{aligned} Z_{\alpha,\beta}(T) \leq & n((3-\beta)^\alpha - (5-\beta)^\alpha + (6-\beta)^\alpha) \\ & + r\left(- (3-\beta)^\alpha + \frac{5}{3}(5-\beta)^\alpha - (6-\beta)^\alpha + \frac{1}{3}(8-\beta)^\alpha\right) \\ & - (3-\beta)^\alpha + 2(4-\beta)^\alpha - (6-\beta)^\alpha + (7-\beta)^\alpha - 2(8-\beta)^\alpha \end{aligned}$$

Proof. We assume that ${}^3T_{\max}$ is a tree having the maximum value of $Z_{\alpha,\beta}$ over the set $\mathcal{T}_{n,r}$ under the given constraints. Lemmas 2.3 and 2.8 confirm that DS_3 is the degree sequence of ${}^3T_{\max}$; hence, $\Theta_{3,3}(^3T_{\max}) = 0$. By using Corollary 1, we have $\Theta_{4,4}(^3T_{\max}) = \frac{r}{3} - 2$. Lemmas 2.4 and 2.7 confirm that $\Theta_{3,4}(^3T_{\max}) = 1$. Also, note that $\Theta_{2,2}(^3T_{\max}) = 0$ and $\Theta_{1,4}(^3T_{\max}) \neq 0$; so, by utilizing Lemma 2.6, we obtain $\Theta_{2,3}(^3T_{\max}) = 0$. Finally, by using Eq (2.1), we obtain $\Theta_{1,4}(^3T_{\max}) = \frac{5r}{3} - n$, $\Theta_{1,2}(^3T_{\max}) = \Theta_{2,4}(^3T_{\max}) = n - r - 1$, $\Theta_{3,1}(^3T_{\max}) = 2$. Hence, we calculate $Z_{\alpha,\beta}(^3T_{\max})$, which is the same as the right-hand side of the desired inequality. \square

Theorem 6. If $T \in \mathcal{T}_{n,r}$ with $6 \leq r < n = \frac{5r+3}{3}$ and $r \equiv 0 \pmod{3}$, then

$$\begin{aligned} Z_{\alpha,\beta}(T) \leq & n((3-\beta)^\alpha - (4-\beta)^\alpha + (5-\beta)^\alpha) - (3-\beta)^\alpha \\ & + 2(4-\beta)^\alpha - (6-\beta)^\alpha + (7-\beta)^\alpha - 2(8-\beta)^\alpha \\ & + r\left(- (3-\beta)^\alpha + \frac{5}{3}(4-\beta)^\alpha - \frac{5}{3}(5-\beta)^\alpha + \frac{2}{3}(6-\beta)^\alpha + \frac{1}{3}(8-\beta)^\alpha\right). \end{aligned}$$

Proof. We assume that ${}^3T_{\max}$ is a tree having the maximum value of $Z_{\alpha,\beta}$ over the set $\mathcal{T}_{n,r}$ under the given constraints. Lemmas 2.3 and 2.8 confirm that DS_3 is the degree sequence of ${}^3T_{\max}$; hence, $\Theta_{3,3} = 0$. Now, by using Corollary 1, Lemmas 2.4 and 2.7, and Eq (2.1), we obtain

$$\Theta_{4,4}(^3T_{\max}) = \frac{r}{3} - 2, \Theta_{3,4}(^3T_{\max}) = 1, \Theta_{2,2}(^3T_{\max}) = 0 = \Theta_{1,4}(^3T_{\max}), \Theta_{1,2}(^3T_{\max}) = n - r - 1 = \frac{2r}{3},$$

$$\Theta_{1,3}(^3T_{\max}) = \frac{5r}{3} - n + 2 = 1, \Theta_{2,3}(^3T_{\max}) = \frac{3n-5r}{3} = 1, \text{ and } \Theta_{2,4}(^3T_{\max}) = \frac{2r}{3} - 1.$$

Hence, we calculate $Z_{\alpha,\beta}(^3T_{\max})$, which is the same as the right-hand side of the desired inequality. \square

Theorem 7. If $T \in \mathcal{T}_{n,r}$ with $6 \leq r$ and $r \equiv 0 \pmod{3}$ and $n > \frac{5r+3}{3}$, then

$$\begin{aligned} Z_{\alpha,\beta}(T) \leq & n(4-\beta)^\alpha + r\left(\frac{2}{3}(3-\beta)^\alpha - \frac{5}{3}(4-\beta)^\alpha + \frac{2}{3}(6-\beta)^\alpha + \frac{1}{3}(8-\beta)^\alpha\right) \\ & + (3-\beta)^\alpha - 2(4-\beta)^\alpha + 2(5-\beta)^\alpha - (6-\beta)^\alpha + (7-\beta)^\alpha - 2(8-\beta)^\alpha. \end{aligned}$$

Proof. We assume that ${}^3T_{\max}$ is a tree having the maximum value of $Z_{\alpha,\beta}$ over the set $\mathcal{T}_{n,r}$ under the given constraints. Lemmas 2.3 and 2.8 confirm that DS_3 is the degree sequence of ${}^3T_{\max}$; hence, $\Theta_{3,3}({}^3T_{\max}) = 0$. Now, by using Corollary 1, Lemmas 2.4, 2.5 and 2.7, and Eq (2.1), we obtain

$$\Theta_{4,4}({}^3T_{\max}) = \frac{r}{3} - 2, \Theta_{3,4}({}^3T_{\max}) = 1, \Theta_{1,4}({}^3T_{\max}) = 0, \Theta_{1,3}({}^3T_{\max}) = 0,$$

$$\Theta_{1,2}({}^3T_{\max}) = \frac{2r}{3} + 1, \Theta_{2,2}({}^3T_{\max}) = -\frac{5r}{3} + n - 2, \Theta_{2,4}({}^3T_{\max}) = \frac{2r}{3} - 1, \text{ and } \Theta_{3,2}({}^3T_{\max}) = 2.$$

Hence, we calculate $Z_{\alpha,\beta}({}^3T_{\max})$, which is the same as the right-hand side of the desired inequality. \square

Theorem 8. *If $T \in \mathcal{T}_{n,r}$ with $8 \leq r < n < \frac{5r-4}{3}$ and $r \equiv 2 \pmod{3}$, then*

$$Z_{\alpha,\beta}(T) \leq n((3-\beta)^\alpha - (5-\beta)^\alpha + (6-\beta)^\alpha)$$

$$+ r\left(- (3-\beta)^\alpha + \frac{5}{3}(5-\beta)^\alpha - (6-\beta)^\alpha + \frac{1}{3}(8-\beta)^\alpha\right)$$

$$- (3-\beta)^\alpha + 4(4-\beta)^\alpha - \frac{7}{3}(5-\beta)^\alpha - (6-\beta)^\alpha + 2(7-\beta)^\alpha - \frac{8}{3}(8-\beta)^\alpha.$$

Proof. We assume that ${}^4T_{\max}$ is a tree having the maximum value of $Z_{\alpha,\beta}$ over the set $\mathcal{T}_{n,r}$ under the given constraints. Lemmas 2.3 and 2.8 confirm that DS_4 is the degree sequence of ${}^4T_{\max}$. By keeping in mind the given constraints, using Corollary 1, Lemmas 2.4, 2.6 and 2.7, and Eq (2.1), we obtain

$$\Theta_{4,4}({}^4T_{\max}) = \frac{r-8}{3}, \Theta_{3,4}({}^4T_{\max}) = 2, \Theta_{3,3}({}^4T_{\max}) = 0 = \Theta_{2,2}({}^4T_{\max}) = \Theta_{2,3}({}^4T_{\max}),$$

$$\Theta_{1,2}({}^4T_{\max}) = \Theta_{2,4}({}^4T_{\max}) = n - r - 1, \Theta_{1,4}({}^4T_{\max}) = \frac{5r - 3n - 7}{3}, \text{ and } \Theta_{3,1}({}^4T_{\max}) = 4.$$

Hence, we calculate $Z_{\alpha,\beta}({}^4T_{\max})$, which is the same as the right-hand side of the desired inequality. \square

Theorem 9. *If $T \in \mathcal{T}_{n,r}$ with $8 \leq r$ and $r \equiv 2 \pmod{3}$ and $\frac{5r-4}{3} \leq n \leq \frac{5r+2}{3}$, then*

$$Z_{\alpha,\beta}(T) \leq n((3-\beta)^\alpha - (4-\beta)^\alpha + (5-\beta)^\alpha)$$

$$+ r\left(- (3-\beta)^\alpha + \frac{5}{3}(4-\beta)^\alpha - \frac{5}{3}(5-\beta)^\alpha + \frac{2}{3}(6-\beta)^\alpha + \frac{1}{3}(8-\beta)^\alpha\right)$$

$$- (3-\beta)^\alpha + \frac{5}{3}(4-\beta)^\alpha + \frac{7}{3}(5-\beta)^\alpha - \frac{10}{3}(6-\beta)^\alpha + 2(7-\beta)^\alpha - \frac{8}{3}(8-\beta)^\alpha.$$

Proof. We assume that ${}^4T_{\max}$ is a tree having the maximum value of $Z_{\alpha,\beta}$ over the set $\mathcal{T}_{n,r}$ under the given constraints. Lemmas 2.3 and 2.8 confirm that DS_4 is the degree sequence of ${}^4T_{\max}$. By keeping in mind the given constraints, using Corollary 1, Lemmas 2.4 and 2.7, and Eq (2.1), we obtain

$$\Theta_{4,4}({}^4T_{\max}) = \frac{r-8}{3}, \Theta_{3,4}({}^4T_{\max}) = 2, \Theta_{3,3}({}^4T_{\max}) = \Theta_{1,4}({}^4T_{\max}) = 0 = \Theta_{2,2}({}^4T_{\max}), \Theta_{1,2}({}^4T_{\max}) = n-r-1,$$

$$\Theta_{1,3}({}^4T_{\max}) = \frac{5r-3n+5}{3}, \Theta_{2,3}({}^4T_{\max}) = \frac{3n-5r+7}{3} \text{ and } \Theta_{2,4}({}^4T_{\max}) = \frac{2(r-5)}{3}.$$

Hence, we calculate $Z_{\alpha,\beta}({}^4T_{\max})$, which is the same as the right-hand side of the desired inequality. \square

Theorem 10. If $T \in \mathcal{T}_{n,r}$ with $8 \leq r$ and $r \equiv 2 \pmod{3}$ and $n > \frac{5r+2}{3}$, then

$$Z_{\alpha,\beta}(T) \leq n(4-\beta)^\alpha + r \left(\frac{2}{3}(3-\beta)^\alpha - \frac{5}{3}(4-\beta)^\alpha + \frac{2}{3}(6-\beta)^\alpha + \frac{1}{3}(8-\beta)^\alpha \right) \\ + \frac{2}{3}(3-\beta)^\alpha - \frac{5}{3}(4-\beta)^\alpha + 4(5-\beta)^\alpha - \frac{10}{3}(6-\beta)^\alpha + 2(7-\beta)^\alpha - \frac{8}{3}(8-\beta)^\alpha.$$

Proof. We assume that ${}^4T_{\max}$ is a tree having the maximum value of $Z_{\alpha,\beta}$ over the set $\mathcal{T}_{n,r}$ under the given constraints. Lemmas 2.3 and 2.8 confirm that DS_4 is the degree sequence of ${}^4T_{\max}$. By keeping in mind the given constraints, using Corollary 1, Lemmas 2.4, 2.5 and 2.7, and Eq (2.1), we obtain

$$\Theta_{4,4}({}^4T_{\max}) = \frac{r-8}{3}, \Theta_{3,4}({}^4T_{\max}) = 2, \Theta_{3,3}({}^4T_{\max}) = \Theta_{1,4}({}^4T_{\max}) = 0 = \Theta_{1,3}({}^4T_{\max}), \\ \Theta_{1,2}({}^4T_{\max}) = \frac{2(r+1)}{3}, \Theta_{2,2}({}^4T_{\max}) = \frac{3n-5r-5}{3}, \Theta_{2,4}({}^4T_{\max}) = \frac{2(r-5)}{3} \text{ and } \Theta_{2,3}({}^4T_{\max}) = 4.$$

Hence, we calculate $Z_{\alpha,\beta}({}^4T_{\max})$, which is the same as the right-hand side of the desired inequality. \square

3. Conclusions

We have characterized graphs attaining the greatest value of $Z_{\alpha,\beta}$ in the set of all fixed-order trees with a fixed number of segments for $\alpha > 1$ and $\beta \leq 2$ (see Theorems 1 and 2). We have also found the largest value of $Z_{\alpha,\beta}$ trees belonging to the aforementioned set of trees for $1 < \alpha \leq 3$ and $\beta \leq 2$ (see Theorems 3–10). The obtained results also hold for the general Platt index Pl_α because $Z_{\alpha,\beta}$ is a generalized version of Pl_α .

All the results proved in this paper hold for $\alpha > 1$, except Lemma 2.3 (particularly, the desired inequality in its Case 1). It seems to be interesting to prove this lemma (particularly, the desired inequality in its Case 1) for $\alpha > 3$ and $\beta \leq 2$.

Author contributions

Hicham Saber: Writing-review & editing, Funding acquisition; Zahid Raza: Writing-original draft, Writing-review & editing; Abdalaziz M. Alanazi: Writing-original draft, Writing-review & editing; Adel A. Attiya: Writing-review & editing, Funding acquisition; Akbar Ali: Writing-review & editing, Funding acquisition. All authors have read and approved the final version of the manuscript for publication.

Use of Generative-AI tools declaration

The authors declare that they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

Authors have no conflict of interests to declare.

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