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Extremal chemical trees with given number of vertices of maximum degree for degree-based topological indices

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Abstract

We define the general sum index for a graph G as follows:

$$GS_{\ell,\gamma}(G) = \sum_{ab \in E(G)} \gamma\,(d_G(a)^{2/\gamma} + d_G(b)^{2/\gamma})^{\ell}$$

where $d_G(a)$ is the degree of a vertex a and, ℓ and γ are non-zero real numbers. In this paper, we consider a class $\mathcal{CT}(n, k)$ of chemical trees with given order n and k vertices of maximum degree. We find those graphs in $\mathcal{CT}(n, k)$ which has extremal values of $\mathcal{CT}_{\ell,\gamma}$ when [$\gamma = 1$, $-1/2 \le \ell < 0$] or [$\gamma = 2$, $-1 \le \ell < 0$] or [$\gamma \in \{1,2\}$ and $0 < \ell \le 1/2$]. Given different values of ℓ and γ within the mentioned brackets, the $GS_{\ell,\gamma}$ coincides with the Sombor index (SO), modified Sombor index (SO_m), general sum-connectivity index (X_ℓ) and harmonic index (H). Furthermore, our findings reveal that in the class $\mathcal{CT}(n, k)$, specific chemical trees with maximum values of SO_m, H and X_ℓ ($-1 \le \ell < 0$) simultaneously attain minimum values of SO and X_ℓ ($0 < \ell \le 1/2$).

Subject Classification: *05C09, 05C35, 05C92.*

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1. Introduction

Throughout this paper, we consider a graph G of order n, where $\mathcal{V}(G)$ and $\mathcal{E}(G)$ denote its vertex and edge sets, respectively. For any vertex $a \in \mathcal{V}(G)$, its degree in G, denoted by $d_G(a)$, is defined as the number of edges that are incident to a. The set $N_G(a)$ is the set of vertices that are adjacent to a. A chemical tree is a tree where the degree of each vertex does not exceed 4. A chemical tree is called an extremal chemical tree if it has either a maximum or minimum value with respect to an index. The notation $G - ab$ indicates the graph formed by removing the edge ab from the graph G. Similarly, $G + ab$ refers to the graph formed by adding an edge ab between two non-adjacent vertices a and b in G. In notation $m_{ij}(G)$ counts the edges whose endpoints have degrees i and j in G. The notation $n_i(G)$ represents the number of vertices of degree i in G. When there is no risk of confusion, we write m_{ij} and n_i instead of $m_{ij}(G)$ and $n_i(G)$, respectively.

There are molecular descriptors in chemical graph theory that are called topological indices and are used to quantify the chemical properties of the molecules. The first ever topological index was introduced by Harry Wiener in 1947 to analyze the properties of alkanes [1]. In literature, several vertex-degree-based topological indices have been introduced and extensively studied [2-16]. Table 1 provides some degree-based topological indices. A degree-based topological index (TI) of a graph G can be represented as

$$\mathrm{T}I(G) = \sum_{ab \in E(G)} F(d_G(a), d_G(b)), \tag{1.1}$$

where $F(d_G(a), d_G(b))$ is a function with property $F(d_G(a), d_G(b)) = F(d_G(b), d_G(a))$.

Table 1

Certain vertex-degree-based indices outlined in this paper of the form (1.1). The parameter ℓ is a non-zero real number.

$F(d_G(a), d_G(b))$	Name	Symbol
$\sqrt{d_G(a)^2 + d_G(b)^2}$	Sombor index [3]	SO
$\frac{1}{\sqrt{d_G(a)^2+d_G(b)^2}}$	Modified Sombor index [5]	SO_m
$(d_G(a) + d_G(b))^{\ell}$	General sum-connectivity index [4]	X_ℓ
$\frac{2}{d_G(a)+d_G(b)}$	Harmonic index [2]	H

This paper introduces the general sum index, and our motivation for defining this index is its role in deriving some vertex-degree-based topological indices by assigning specific values to ℓ and γ. We now define the general sum index for graph G as follows:

$$GS_{\ell,\gamma}(G) = \sum_{ab \in E(G)} \gamma\,(d_G(a)^{2/\gamma} + d_G(b)^{2/\gamma})^{\ell}, \tag{1.2}$$

where ℓ and γ are non-zero real numbers. An important direction is to find trees with a maximum or minimum index in the class of trees. Several results on

extremal graphs with respect to indices have been documented in the literature [13, 16-25]. However, chemical trees with the given number of vertices of maximum degree received minimal attention in the literature. Let $\mathcal{CT}(n,k)$ denotes the set of chemical trees over order n with given k vertices of degree 4, where $k \geq 1$. For recent studies on tree class with k vertices of maximum degree and particularly the class $\mathcal{CT}(n,k)$, we refer readers to [12, 15]

In this paper, we obtain trees in $\mathcal{CT}(n,k)$ with extremal values of $GS_{\ell,\gamma}$ for certain values of ℓ and γ. In particular, if $[\gamma = 1, -1/2 \leq \ell < 0]$ or $[\gamma = 2, -1 \leq \ell < 0]$, then we find maximum value of $GS_{\ell,\gamma}$ among trees in $\mathcal{CT}(n,k)$. Similarly, if $[\gamma \in \{1,2\} and\ 0 < \ell \leq 1/2]$, then we find minimum value of $GS_{\ell,\gamma}$ among trees in $\mathcal{CT}(n,k)$. Given different values of ℓ and γ within the mentioned brackets, the $GS_{\ell,\gamma}$ coincides with the SO, SO_m, general sum-connectivity index and harmonic index. This enables us to easily find the extremal values of these indices within $\mathcal{CT}(n,k)$. Furthermore, we construct these extremal chemical trees.

For convenience, we define the following sets:

$A = \{\ell,\gamma| -1/2 \leq \ell < 0 \text{ and } \gamma = 1\} \cup \{\ell,\gamma| -1 \leq \ell < 0 \text{ and } \gamma = 2\}$
$B = \{\ell,\gamma|0 < \ell \leq 1/2 \text{ and } \gamma \in \{1,2\}\}$.

For $n < 3k+2$, there can be no graphs in $\mathcal{CT}(n,k)$. Therefore, throughout the paper, we assume that $n \geq 3k+2$.

2. Extremal chemical trees in $\boldsymbol{CT(n,k)}$

In this section, we find the chemical trees in $\mathcal{CT}(n,k)$ with maximum (or minimum) values of $GS_{\ell,\gamma}$ when $\ell,\gamma \in A$ (or $\ell,\gamma \in B$). Let

$$S = \{(i,j) \in \mathbb{N} \times \mathbb{N} \backslash (1,1) | 1 \leq i \leq j \leq 4\},$$

where $\mathbb{N}$ is the set of natural numbers. General sum index for a chemical tree $T \in \mathcal{CT}(n,k)$ can also be expressed as

$$GS_{\ell,\gamma}(T) = \sum_{(i,j)\in S} m_{ij}\, \gamma\, (i^{2/\gamma} + j^{2/\gamma})^{\ell}. \tag{2.1}$$

In [24], following relations are given for a chemical tree T:

$$n_1 = 2\, m_{1\,1} + m_{1\,2} + m_{1\,3} + m_{1\,4} \tag{2.2}$$

$$2n_2 = m_{1\,2} + 2\, m_{2\,2} + m_{2\,3} + m_{2\,4} \tag{2.3}$$

$$3n_3 = m_{1\,3} + m_{2\,3} + 2\, m_{3\,3} + m_{3\,4} \tag{2.4}$$

$$4\, n_4 = m_{1\,4} + m_{2\,4} + m_{3\,4} + 2\, m_{4\,4}. \tag{2.5}$$

Clearly,

$$n_1 + n_2 + n_3 + n_4 = n. \tag{2.6}$$

By handshaking lemma, we obtain

$$2(n-1) = n_1 + 2n_2 + 3n_3 + 4n_4. \tag{2.7}$$

To establish the theorem and its corollaries, the following lemmas are needed:

Lemma 2.1: *Let* $z \geq 1$ *and* $\gamma \geq 1$. *The function*

(i) $f_1(z) = (2^{2/\gamma} + z^{2/\gamma})^{\ell} - (3^{2/\gamma} + z^{2/\gamma})^{\ell}$ *is strictly decreasing if* $\ell < 0$, *and it is strictly increasing if* $0 < \ell \leq 1/2$

(ii) $f_2(z) = (2^{\frac{2}{\gamma}} + z^{\frac{2}{\gamma}}) - (1 + z^{\frac{2}{\gamma}})^{\ell}$ *is strictly increasing* (*or strictly decreasing*) *if* $\ell < 0$ (*or* $0 < \ell \leq 1/2$).

Proof:

(i) Note that $(2^{\frac{2}{\gamma}} + z^{\frac{2}{\gamma}})^{\ell-1} - (3^{\frac{2}{\gamma}} + z^{\frac{2}{\gamma}})^{\ell-1} > 0$ if $\ell < 0$ or $0 < \ell \leq 1/2$. We have

$$f_1'(z) = z^{2/\gamma-1}\left(\frac{2\ell}{\gamma}\right)\left((2^{2/\gamma} + z^{2/\gamma})^{\ell-1} - (3^{2/\gamma} + z^{2/\gamma})^{\ell-1}\right)$$

If $\ell < 0$, then $(2^{\frac{2}{\gamma}} + z^{\frac{2}{\gamma}})^{\ell-1} > (3^{\frac{2}{\gamma}} + z^{\frac{2}{\gamma}})^{\ell-1}$ and $z^{(\frac{2}{\gamma})-1} > 0$. Therefore, $f'_1(z) < 0$ and $f_1(z)$ is strictly decreasing. If $0 < \ell \leq 1/2$, then $(2^{\frac{2}{\gamma}} + z^{\frac{2}{\gamma}})^{\ell-1} < (3^{\frac{2}{\gamma}} + z^{\frac{2}{\gamma}})^{\ell-1}$ and $z^{(2/\gamma)-1} > 0$. Hence, $f'_1(z) < 0$ and $f_1(z)$ is strictly increasing.

(ii) The proof is similar to (i).

Lemma 2.2: *Suppose that* $T \in \mathcal{CT}(n,k)$ *is a tree such that* $GS_{\ell,\gamma}$ *attains maximum* (*or minimum*) *value in* $\mathcal{CT}(n,k)$ *when* $\ell, \gamma \in A$ $(or \ell, \gamma \in B)$. *Then*

(i) $n_3 = 0$.

(ii) $n_1 = 2k + 2$ *and* $n_2 = n - 3k - 2$.

Proof:

(i) In contrast, assume that there is a vertex u of degree 3 in T. Let $N_T(u) = \{u_1, u_2, u_3\}$, $x \notin N_T(u)$ be a pendant vertex of T and P be a u,x-path. Let $N_T(x) = \{x'\}$. Clearly, $2 \leq d_T(x') \leq 4$. We discuss two cases:

Case 1: When at most one neighbor of u has degree 4.

In this case, WLOG, we can assume that $1 \leq d_T(u_1), d_T(u_2) \leq 3$, $1 \leq d_T(u_3) \leq 4$ and u_1 do not lie on P. We obtain a tree T' as follows:

$$T' = T - u_1u + u_1x.$$

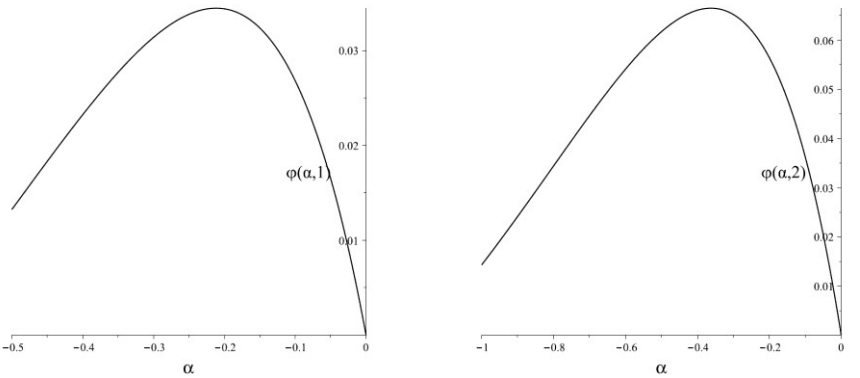
Then $d_{T'}(u) = 2$, $d_{T'}(x) = 2$ and $d_{T'}(v) = d_T(v)$ for all $v \in V(T)\backslash\{u,x\}$. Obviously, $T' \in \mathcal{CT}(n,k)$. We get

$$\begin{aligned} GS_{\ell,\gamma}(T') - GS_{\ell,\gamma}(T) &= \gamma\,[(2^{\frac{2}{\gamma}} + d_T(u_1)^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + d_T(u_1)^{\frac{2}{\gamma}})^{\ell} \\ &+ (2^{\frac{2}{\gamma}} + d_T(x')^{\frac{2}{\gamma}})^{\ell} - (1 + d_T(x')^{\frac{2}{\gamma}})^{\ell} \\ &+ (2^{\frac{2}{\gamma}} + d_T(u_2)^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + d_T(u_2)^{\frac{2}{\gamma}})^{\ell} \\ &+ (2^{\frac{2}{\gamma}} + d_T(u_3)^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + d_T(u_3)^{\frac{2}{\gamma}})^{\ell}]. \end{aligned} \tag{2.8}$$

Firstly, let $\ell, \gamma \in A$. We show that $GS_{\ell,\gamma}(T') - GS_{\ell,\gamma}(T) > 0$ to obtain a contradiction that T has maximum value of $GS_{\ell,\gamma}$. By using the Lemma 2.1 (i) for $\ell < 0$, Equation (2.8) yields

$$GS_{\ell,\gamma}(T') - GS_{\ell,\gamma}(T) > \gamma\,[(2^{\frac{2}{\gamma}} + 3^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + 3^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 2^{\frac{2}{\gamma}})^{\ell} - (1^{\frac{2}{\gamma}} + 2^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 3^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + 3^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell}].$$

Let



(a) $\varphi(\ell, 1)$ (b) $\varphi(\ell, 2)$

Figure 1
The function $\boldsymbol{\varphi(\ell, \gamma)}$ when $\boldsymbol{\ell, \gamma \in A}$

$$\varphi(\ell,\gamma) = \gamma\,[2(2^{\frac{2}{\gamma}} + 3^{\frac{2}{\gamma}})^{\ell} - 2(3^{\frac{2}{\gamma}} + 3^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 2^{\frac{2}{\gamma}})^{\ell} - (1^{\frac{2}{\gamma}} + 2^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell}],$$

where $\ell, \gamma \in A$. By computational software, we can see that $\varphi(\ell, \gamma) > 0$, as depicted in Figure 1. Therefore, $GS_{\ell,\gamma}(T') - GS_{\ell,\gamma}(T) > 0$, which is a contradiction.

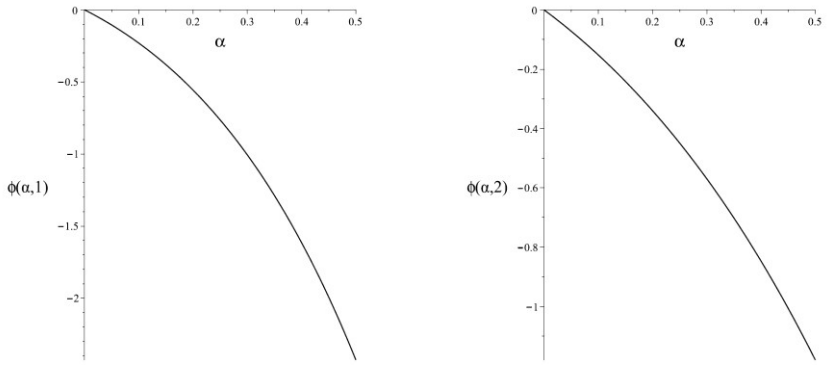
Secondly, let $\ell, \gamma \in B$. We show that $GS_{\ell,\gamma}(T') - GS_{\ell,\gamma}(T) < 0$ to obtain a contradiction that T has minimum value of $GS_{\ell,\gamma}$. By using the Lemma 2.1 (ii) for $0 < \ell \leq 1/2$, Equation (2.8) yields

$$GS_{\ell,\gamma}(T') - GS_{\ell,\gamma}(T) < \gamma\,[(2^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} - (1^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell}].$$

Let

$$\phi(\ell,\gamma) = \gamma\,[3(2^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} - 3(3^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} - (1^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell}],$$

where $\ell, \gamma \in B$. By utilizing computational software, we can see that $\phi(\ell, \gamma) < 0$, as depicted in Figure 2. Therefore, $GS_{\ell,\gamma}(T') - GS_{\ell,\gamma}(T) < 0$, which is a contradiction.



(a) $\phi(\ell, 1)$ (b) $\phi(\ell, 2)$

Figure 2
The function $\phi(\ell, \gamma)$ when $\ell, \gamma \in B$

Case 2: When at least two neighbors of u have degree 4.

In this case, WLOG, we can assume that $d_T(u_2) = d_T(u_3) = 4$, $1 \leq d_T(u_1) \leq 4$ and path P contains u_3. Define a tree T'' from T such that $T'' = T - u_2u - u_3u + ux + u_2u_3$. Then $d_{T'}(u) = 2$, $d_{T''}(x) = 2$ and $d_{T''}(t) = d_T(t)$ for all $t \in V(T)\backslash\{u, x\}$. Obviously, $T'' \in \mathcal{CT}(n, k)$. We get

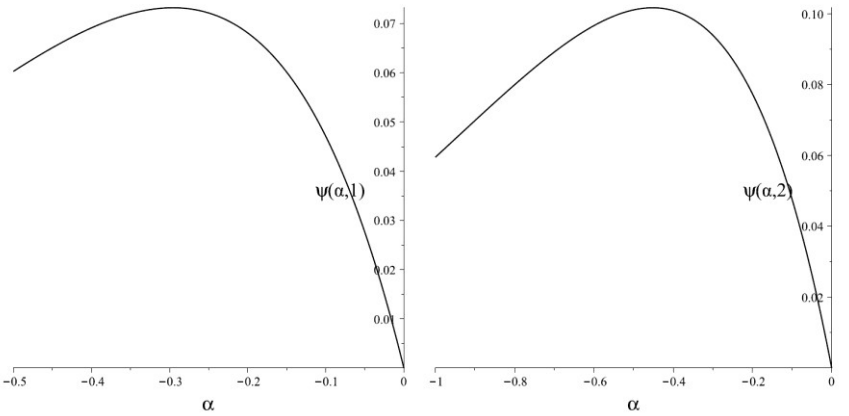
$$\begin{aligned} GS_{\ell,\gamma}(T'') - GS_{\ell,\gamma}(T) &= \gamma\,[(2^{\frac{2}{\gamma}} + d_T(u_1)^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 2^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + d_T(x')^{\frac{2}{\gamma}})^{\ell} \\ &\quad -(1 + d_T(x')^{\frac{2}{\gamma}})^{\ell} + (4^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} \\ &\quad -(3^{\frac{2}{\gamma}} + d_T(u_1)^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell}]. \end{aligned} \tag{2.9}$$

Firstly, let $\ell, \gamma \in A$. By applying software tools for analysis, we show that $GS_{\ell,\gamma}(T'') - GS_{\ell,\gamma}(T) > 0$ to obtain a contradiction that T has maximum value of $GS_{\ell,\gamma}$. By using the Lemma 2.1 (i) for $\ell < 0$, Equation (2.9) yields

$$\begin{aligned} GS_{\ell,\gamma}(T'') - GS_{\ell,\gamma}(T) &> \gamma\,[(2^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 2^{\frac{2}{\gamma}})^{\ell} \\ &\quad -(1^{\frac{2}{\gamma}} + 2^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 2^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} + (4^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell}]. \end{aligned}$$

Let

$$\begin{aligned} \Psi(\ell, \gamma) &= \gamma\,[(2^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} - 3(3^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} + 2(2^{\frac{2}{\gamma}} + 2^{\frac{2}{\gamma}})^{\ell} - (1^{\frac{2}{\gamma}} + 2^{\frac{2}{\gamma}})^{\ell} \\ &\quad +(4^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell}], \end{aligned}$$



(a) $\Psi(\ell, 1)$ (b) $\Psi(\ell, 2)$

Figure 3
The function $\Psi(\ell, \gamma)$ when $\ell, \gamma \in A$

where $\ell, \gamma \in A$. Through the use of numerical software, we can see that $\Psi(\ell, \gamma) > 0$, as depicted in Figure 3. Therefore, $GS_{\ell,\gamma}(T'') - GS_{\ell,\gamma}(T) > 0$, which is a contradiction.

Secondly, let $\ell, \gamma \in B$. We show that $GS_{\ell,\gamma}(T'') - GS_{\ell,\gamma}(T) < 0$ to obtain a contradiction that T has minimum value of $GS_{\ell,\gamma}$. By using the Lemma 2.1 (ii) for $0 < \ell \leq 1/2$, Equation (2.9) yields

$$S_{\ell,\gamma}(T'') - GS_{\ell,\gamma}(T) < \gamma\,[(2^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell}$$
$$G - (1^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 2^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} + (4^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell}].$$

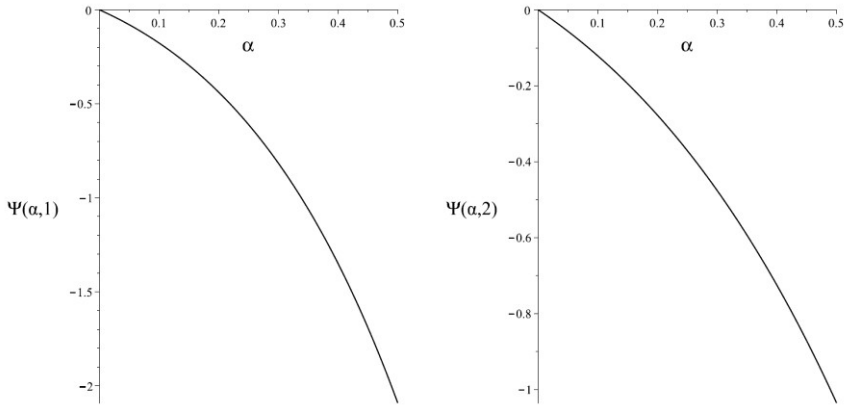
Let

$$\psi(\ell, \gamma) = \gamma\,[(2^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} - (3^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} - (1^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell}$$
$$-2(3^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 2^{\frac{2}{\gamma}})^{\ell} + (4^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell}],$$

where $\ell, \gamma \in B$. Using computational tools, we can obtain that $\psi(\ell, \gamma) < 0$, as depicted in Figure 4. This yields $GS_{\ell,\gamma}(T'') - GS_{\ell,\gamma}(T) < 0$, which contradicts the assumption. Hence, T has maximum (minimum) value of $GS_{\ell,\gamma}$ for $\ell, \gamma \in A$ $(\ell, \gamma \in B)$ with $n_3 = 0$.

(ii) Using Equations (2.6) and (2.7) and the fact that $n_3(T) = 0$ (by Part (i)), we get

$$\begin{aligned} n_1 + 2n_2 &= 2n - 2 - 4k, \\ n_1 + n_2 &= n - k. \end{aligned} \tag{2.10}$$



(a) $\psi(\ell, 1)$ (b) $\psi(\ell, 2)$

Figure 4
The function $\boldsymbol{\psi(\ell,\gamma)}$ when $\boldsymbol{\ell,\gamma \in B}$

The solution of system (2.10) is $n_1(T) = 2k + 2$ and $n_2(T) = n - 3k - 2$. This completes the proof.

Lemma 2.3: *Suppose $T \in \mathcal{CT}(n,k)$ is such that $GS_{\ell,\gamma}$ attains maximum (or minimum) value in $\mathcal{CT}(n,k)$ when $\ell,\gamma \in A$ $(or \ell,\gamma \in B)$. Let $x,w \in V(T)$ such that $d_T(x) = d_T(w) = 4$. Let z be an internal vertex on x,w-path. Then $d_T(z) = 4$.*

Proof: On the contrary, assume that $d_T(z) \neq 4$. Clearly, $d_T(z) \neq 1$. By Lemma 2.2(i), $d_T(z) \neq 3$. Therefore, we only need to prove that $d_T(z) \neq 2$. If $d_T(z) = 2$, then T possesses two vertices u and v of degree 4 on x,w-path such that u,v-path contains z and all its internal vertices have degree 2. Let y be a pendant vertex in T and y' be its neighbor with $2 \leq d_T(y') \leq 4$. Now, we consider two cases.

Case 1: $d_T(u,v) = 2$.

Clearly, $d_T(u,v) = 2$ implies that $N_T(z) = \{u,v\}$. WLOG, assume that zy-path contains v. We derive a tree T' as follows:

$$T' = T - uz - vz + uv + zy.$$

Then $d_{T'}(y) = d_T(y) + 1 = 2$, $d_{T'}(z) = d_T(z) - 1 = 1$ and $d_{T'}(t) = d_T(t)$ for all $t \in V(T)\backslash\{y,z\}$. Obviously, $T' \in \mathcal{CT}(n,k)$. We get

$$\begin{aligned} GS_{\ell,\gamma}(T') - GS_{\ell,\gamma}(T) \quad &= \gamma\,[(4^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} + (d_T(y')^{\frac{2}{\gamma}} + 2^{\frac{2}{\gamma}})^{\ell} \\ &\quad -(d_T(y')^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} - (2^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} - (2^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell}]. \end{aligned} \tag{2.11}$$

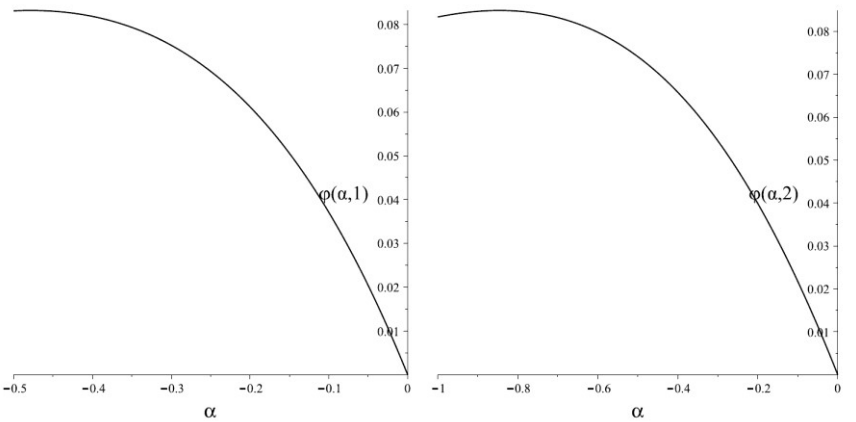
Firstly, let $\ell, \gamma \in A$. We show that $GS_{\ell,\gamma}(T') - GS_{\ell,\gamma}(T) > 0$ to obtain a contradiction that T has maximum value of $GS_{\ell,\gamma}$. By using the Lemma 2.1 (i) for $\ell < 0$, Equation (2.11) yields

$$GS_{\ell,\gamma}(T') - GS_{\ell,\gamma}(T) > \gamma\,[(4^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 2^{\frac{2}{\gamma}})^{\ell} - (1^{\frac{2}{\gamma}} + 2^{\frac{2}{\gamma}})^{\ell} - (2^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} - (2^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell}].$$

Let

$$\varphi(\ell, \gamma) = \gamma\,[(4^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 2^{\frac{2}{\gamma}})^{\ell} - (2^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} - (2^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell}].$$

where $\ell, \gamma \in A$. By mathematical tools, we can see that $\varphi(\ell, \gamma) > 0$, as depicted in Figure 5. Therefore, $GS_{\ell,\gamma}(T') - GS_{\ell,\gamma}(T) > 0$, which is a contradiction.



(a) $\varphi(\ell, 1)$ (b) $\varphi(\ell, 2)$

Figure 5
The function $\boldsymbol{\varphi(\ell, \gamma)}$ when $\boldsymbol{\ell, \gamma \in A}$

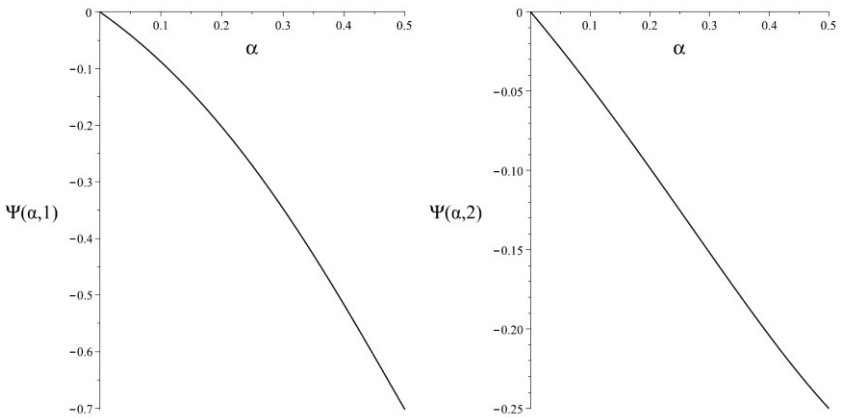
Secondly, let $\ell, \gamma \in B$. We show that $GS_{\ell,\gamma}(T') - GS_{\ell,\gamma}(T) < 0$ to obtain the contradiction that T has the minimum value of $GS_{\ell,\gamma}(T)$. By using the Lemma 2.1 (ii) for $0 < \ell \leq 1/2$, Equation (2.11) yields

$$GS_{\ell,\gamma}(T') - GS_{\ell,\gamma}(T) < \gamma\,[(4^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} + (4^{\frac{2}{\gamma}} + 2^{\frac{2}{\gamma}})^{\ell} - (4^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} - (2^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} - (2^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell}].$$

Let

$$\psi(\ell, \gamma) = \gamma\,[(4^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell} + (2^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} - (4^{\frac{2}{\gamma}} + 1^{\frac{2}{\gamma}})^{\ell} - (2^{\frac{2}{\gamma}} + 4^{\frac{2}{\gamma}})^{\ell}],$$

where $\ell, \gamma \in A$. By utilizing mathematical tools, we can see that $\psi(\ell, \gamma) < 0$, as depicted in Figure 6. Therefore, $GS_{\ell,\gamma}(T') - GS_{\ell,\gamma}(T) < 0$, which is a contradiction.



(a) $\psi(\ell, 1)$ (b) $\psi(\ell, 2)$

Figure 6
The function $\boldsymbol{\psi(\ell, \gamma)}$ when $\boldsymbol{\ell, \gamma \in B}$

Case 2: $d_T(u, v) \geq 3$.

Let $u_1 \in N_T(u)$ and $v_1 \in N_T(v)$ such that lying on u, v-path. Let v'_1 be the neighbor of v_1 other than v. Set T' such that

$$T'' = T - vv_1 - uu_1 + uv + u_1 y.$$

Then we see that $d_{T''}(y) = d_T(y) + 1 = 2$, $d_{T''}(v_1) = d_T(v_1) - 1 = 1$ and $d_{T''}(t) = d_T(t)$ for all $t \in V(T)\backslash\{y, v_1\}$. Obviously, $T'' \in \mathcal{CT}(n, k)$. Now, we show $GS_{\ell,\gamma}(T'') - GS_{\ell,\gamma}(T) > 0$ to obtain a contradiction. By using the similar calculations and argument used in Case 1, a contradiction arises that T has maximum $GS_{\ell,\gamma}$. Thus we conclude that $d_T(z) \neq 2$. Hence, $d_T(z) = 4$.

Lemma 2.4: *Suppose $T \in \mathcal{CT}(n, k)$ is a tree with $3k + 2 \leq n \leq 5k + 4$, such that $GS_{\ell,\gamma}$ attains maximum (or minimum) within $\mathcal{CT}(n, k)$ when $\ell, \gamma \in A$ $(or \ell, \gamma \in B)$. Then*

(i) $m_{13} = m_{23} = m_{33} = m_{34} = 0$.

(ii) $m_{44} = k - 1$.

(iii) $m_{22} = 0$.

(iv) $m_{12} = n - 3k - 2$, $m_{24} = n - 3k - 2$, $m_{14} = 5k + 4 - n$.

Proof:

(i) This part directly follows from part (i) of Lemma 2.2.

(ii) We derive this result directly from Lemma 2.3.

(iii) On the contrary, assume that T contains $uv \in E(T)$ such that $d_T(u) = 2 = d_T(v)$. We first show that there exists an edge $e' = xy$ with $d_T(x) = 1$ and $d_T(y) = 4$. If $m_{14} = 0$, then we use Lemma 2.2 and Parts (i) and (ii)

to solve the system in Equations (2.2)-(2.5) and obtain $m_{22} = n - 5k - 4$. This implies $m_{22} \leq 0$ since $3k + 2 \leq n \leq 5k + 4$, which is a contradiction. Therefore, the tree T possesses an edge $e' = xy \in E(T)$ with $d_T(x) = 1$ and $d_T(y) = 4$. Let $u_1 \in N_T(u)$ and $v_1 \in N_T(v)$. WLOG, let P be a u,x-path containing the vertex v. We transform a tree T' as follows:

$$T' = T - uu_1 + u_1x.$$

Then $d_{T'}(u) = 1$, $d_{T'}(x) = 2$ and $d_{T'}(t) = d_T(t)$ for all $t \in V(T)\backslash\{u, x\}$. Obviously, $T' \in \mathcal{CT}(n,k)$. We get

$$\begin{aligned} GS_{\ell,\gamma}(T') - GS_{\ell,\gamma}(T) &= \gamma\,[(d_T(u_1)^{2/\gamma} + 2^{2/\gamma})^{\ell} + (1^{2/\gamma} + 2^{2/\gamma})^{\ell} + (2^{2/\gamma} + 4^{2/\gamma})^{\ell} \\ &\quad -(d_T(u_1)^{2/\gamma} + 2^{2/\gamma})^{\ell} - (2^{2/\gamma} + 2^{2/\gamma})^{\ell} - (1^{2/\gamma} + 4^{2/\gamma})^{\ell}] \\ &= \gamma\,[(1^{2/\gamma} + 2^{2/\gamma})^{\ell} + (2^{2/\gamma} + 4^{2/\gamma})^{\ell} - (2^{2/\gamma} + 2^{2/\gamma})^{\ell} - (1^{2/\gamma} + 4^{2/\gamma})^{\ell}]. \end{aligned}$$

When $\ell, \gamma \in A$, we show that $GS_{\ell,\gamma}(T') - GS_{\ell,\gamma}(T) > 0$ to obtain a contradiction that T has maximum value of $GS_{\ell,\gamma}(T)$. Let

$$\begin{aligned} \varphi(\ell,\gamma) &= \gamma\,[(1^{2/\gamma} + 2^{2/\gamma})^{\ell} + (2^{2/\gamma} + 4^{2/\gamma})^{\ell} - (2^{2/\gamma} + 2^{2/\gamma})^{\ell} \\ &\quad -(1^{2/\gamma} + 4^{2/\gamma})^{\ell}]. \end{aligned}$$

where $\ell, \gamma \in A$. With the help of computational programs, one can see that $\varphi(\ell,\gamma) > 0$, as depicted in Figure 7 (a) and (b). Therefore, $GS_{\ell,\gamma}(T') > GS_{\ell,\gamma}(T)$, which is a contradiction. Similarly, we can see $GS_{\ell,\gamma}(T') < GS_{\ell,\gamma}(T)$ when $\ell, \gamma \in B$, as depicted in Figure 7(c) and (d). Therefore, $GS_{\ell,\gamma}(T') < GS_{\ell,\gamma}(T)$, which is a contradiction. Hence, $m_{22} = 0$ for $3k + 2 \leq n \leq 5k + 4$.

(iv). Using Lemma 2.2 and Parts (i)-(iii) in Equations (2.2)-(2.5), we obtain $m_{12} = n - 3k - 2 = m_{24} = n - 3k - 2$ and $m_{14} = 5k + 4 - n$. This finishes the proof.

Lemma 2.5: *Let $T \in \mathcal{CT}(n,k)$ with $n > 5k + 4$ be such that $GS_{\ell,\gamma}$ achieves maximum (or minimum) value in $\mathcal{CT}(n,k)$ when $\ell, \gamma \in A$ $(or \ell, \gamma \in B)$. Then*

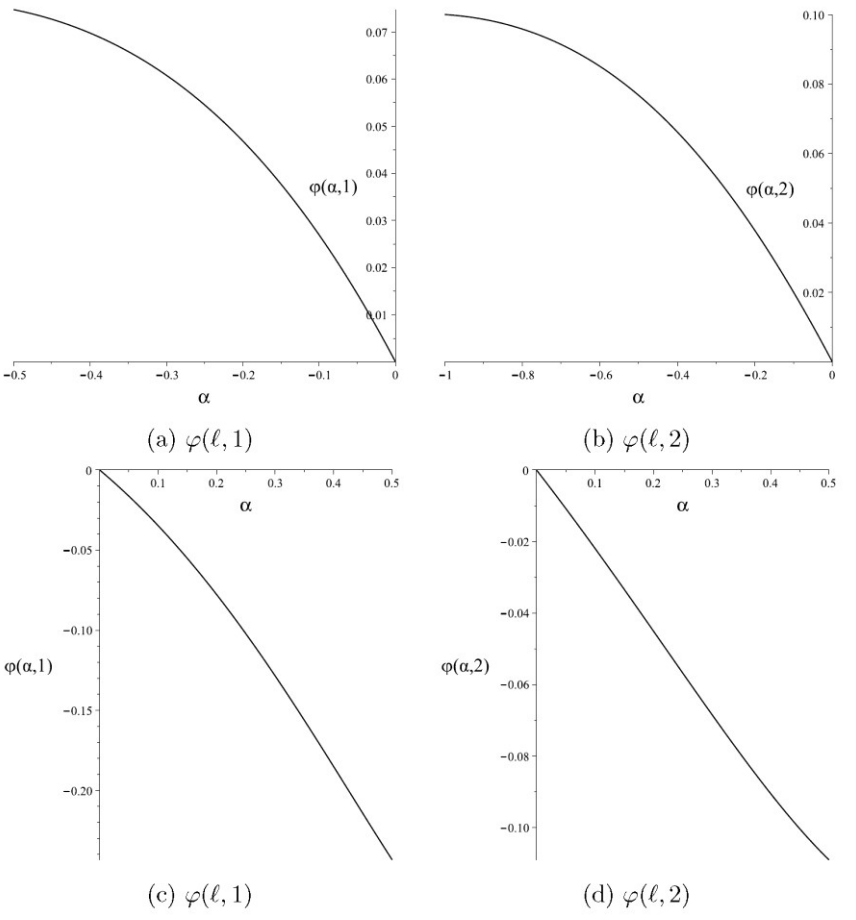
(i) $m_{13} = m_{23} = m_{33} = m_{34} = 0$.
(ii) $m_{44} = k - 1$.
(iii) $m_{14} = 0$.
(iv) $m_{12} = 2k + 2$, $m_{24} = 2k + 2$, $m_{22} = n - 5k - 4$.

Proof:

(i) It follows from Lemma 2.2 (i) that this result holds.
(ii) This result is a direct consequence of Lemma 2.3.
(iii) On the contrary, assume that T has an edge $e = xy$ with $d_T(x) = 1, d_T(y) = 4$. We first show that there exists an edge $uv \in E(T)$ with $d_T(u) = 2 = d_T(v)$. If $m_{22} = 0$, then we use Lemma 2.2 and Parts (i) and

(ii) to solve the system in Equations (2.2)-(2.5) and obtain $m_{14} = 5k + 4 - n$. This implies $m_{14} < 0$ since $n > 5k + 4$, which is a contradiction. Thus $m_{22} \neq 0$. Now, by using the same argument and transformation used in Lemma 2.4 (iii), we can conclude that $m_{14} = 0$ for $n > 5k + 4$.

(iv). Using Lemma 2.2 and Parts (i)-(iii) in Equations (2.2)-(2.5), we obtain $m_{12} = 2k + 2 = m_{24}$ and $m_{22} = n - 5k - 4$. This finishes the proof.



(a) $\varphi(\ell, 1)$ (b) $\varphi(\ell, 2)$

(c) $\varphi(\ell, 1)$ (d) $\varphi(\ell, 2)$

Figure 7

The function $\varphi(\ell, \gamma)$. When $\ell, \gamma \in A$, the graphs are given in (a) and (b). When $\ell, \gamma \in B$, the graphs are given in (c) and (d)

Let $\Lambda(n, k)$ denote the class of chemical trees within $\mathcal{CT}(n, k)$ that satisfy:

- Each tree in $\Lambda(n, k)$ has a degree sequence $(\underbrace{4, \dots, 4}_{k}, \underbrace{2, \dots, 2}_{n-3k-2}, \underbrace{1, \dots, 1}_{2k+2})$.

- If $3k+2 \le n \le 5k+4$, then the tree $T \in \Lambda(n,k)$ holds $m_{44} = k-1$, $m_{22} = 0$, $m_{12} = n-3k-2 = m_{24}$ and $m_{14} = 5k+4-n$.
- If $3k+2 \le n \le 5k+4$, then the tree $T \in \Lambda(n,k)$ holds $m_{44} = k-1$, $m_{14} = 0$, $m_{12} = 2k+2 = m_{24}$ and $m_{14} = n-5k-4$.

Theorem 2.6: *Assume that T is a chemical tree within $\mathcal{CT}(n,k)$, where $n \ge 3k+2$.*

(i) *If $\ell, \gamma \in A$, then*

$$GS_{\ell,\gamma}(T) \le \begin{cases} (n-3k-2)(1^{2/\gamma}+2^{2/\gamma})^{\ell} + (n-3k-2)(2^{2/\gamma}+4^{2/\gamma})^{\ell} \\ +(k-1)(4^{2/\gamma}+4^{2/\gamma})^{\ell} + (5k-n+4)(1^{2/\gamma}+4^{2/\gamma})^{\ell} \\ \text{if } 3k+2 \le n \le 5k+4, \\ (2k+2)(1^{2/\gamma}+2^{2/\gamma})^{\ell} + (2k+2)(2^{2/\gamma}+4^{2/\gamma})^{\ell} \\ +(k-1)(4^{2/\gamma}+4^{2/\gamma})^{\ell} + (n-5k-4)(2^{2/\gamma}+2^{2/\gamma})^{\ell} \\ if\ n > 5k+4. \end{cases}$$

(ii) *If $\ell, \gamma \in B$, then*

$$GS_{\ell,\gamma}(T) \ge \begin{cases} (n-3k-2)(1^{2/\gamma}+2^{2/\gamma})^{\ell} + (n-3k-2)(2^{2/\gamma}+4^{2/\gamma})^{\ell} \\ +(k-1)(4^{2/\gamma}+4^{2/\gamma})^{\ell} + (5k-n+4)(1^{2/\gamma}+4^{2/\gamma})^{\ell} \\ if\ 3k+2 \le n \le 5k+4, \\ (2k+2)(1^{2/\gamma}+2^{2/\gamma})^{\ell} + (2k+2)(2^{2/\gamma}+4^{2/\gamma})^{\ell} \\ +(k-1)(4^{2/\gamma}+4^{2/\gamma})^{\ell} + (n-5k-4)(2^{2/\gamma}+2^{2/\gamma})^{\ell} \\ if\ n > 5k+4. \end{cases}$$

The equality holds in each part iff $T \in \Lambda(n,k)$.

Proof: (i). Assume that $T \in \mathcal{CT}(n,k)$ is a tree with maximum $GS_{\ell,\gamma}$ index when $\ell, \gamma \in A$. By Lemmas 2.2-2.3, the tree T holds the degree sequence $(\underbrace{4,\dots,4}_{k}, \underbrace{2,\dots,2}_{n-3k-2}, \underbrace{1,\dots,1}_{2k+2})$ and $m_{44} = k-1$, respectively. We now consider two cases:

Case 1: $3k+2 \le n \le 5k+4$. From Lemma 2.4, we obtain $T \in \Lambda(n,k)$, and hence the Equation (2.1) yields

$$\begin{aligned} GS_{\ell,\gamma}(T) &= (n-3k-2)(1^{2/\gamma}+2^{2/\gamma})^{\ell} + (n-3k-2)(2^{2/\gamma}+4^{2/\gamma})^{\ell} \\ &\quad +(k-1)(4^{2/\gamma}+4^{2/\gamma})^{\ell} + (5k-n+4)(1^{2/\gamma}+4^{2/\gamma})^{\ell}. \end{aligned}$$

Case 2: $n > 5k+4$. From Lemma 2.5, we obtain $T \in \Lambda(n,k)$, and hence the Equation (2.1) yields

$$\begin{aligned} GS_{\ell,\gamma}(T) &= (2k+2)(1^{2/\gamma}+2^{2/\gamma})^{\ell} + (2k+2)(2^{2/\gamma}+4^{2/\gamma})^{\ell} \\ &\quad +(k-1)(4^{2/\gamma}+4^{2/\gamma})^{\ell} + (n-5k-4)(2^{2/\gamma}+2^{2/\gamma})^{\ell}. \end{aligned}$$

(ii). Similarly, if $\ell, \gamma \in B$, then the required result holds by Lemmas 2.2-2.5. This finishes the proof.

For a chemical tree $T \in \mathcal{CT}(n,k)$, degree-based indices given in Table can be obtained from the general sum index as follows:

$$GS_{\ell,\gamma}(T) = \begin{cases} SO(T) \ when \ \gamma = 1 \ \ and \ \ \ell = 1/2, \\ SO_m(T) \ \ when \ \gamma = 1 \ \ and \ \ \ell = -1/2, \\ 2X_\ell(T) \ \ when \ \gamma = 2 \ \ and \ \ [-1 \le \ell < 0 \ or \ 0 < \ell \le 1/2]. \end{cases} \quad (2.12)$$

Theorem provides a general statement, determining the maximum value of $GS_{\ell,\gamma}(T)$ when $\ell, \gamma \in A$ and the minimum value of $GS_{\ell,\gamma}(T)$ when $\ell, \gamma \in B$ among trees in $\mathcal{CT}(n,k)$. Subsequently, for specific values of ℓ and γ, we present the following corollaries, which readily follow from Theorem and Equation (2.12).

Corollary 2.7: *Let $T \in \mathcal{CT}(n,k)$ be a chemical tree. Then*

$$SO(T) \ge \begin{cases} (n-3k-2)(\sqrt{5}+\sqrt{20}) + (k-1)\sqrt{32} + (5k-n+4)\sqrt{17} \\ \qquad if \ 3k+2 \le n \le 5k+4, \\ (2k+2)(\sqrt{5}+\sqrt{20}) + (k-1)\sqrt{32} + (n-5k-4)\sqrt{8} \\ \qquad if \ n > 5k+4. \end{cases}$$

The inequality turns into equality iff $T \in \Lambda(n,k)$.

Corollary 2.8: *Let $T \in \mathcal{CT}(n,k)$ be a chemical tree. Then we have*

$$SO_m(T) \le \begin{cases} (n-3k-2)(\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{20}}) + (k-1)\frac{1}{\sqrt{32}} + (5k-n+4)\frac{1}{\sqrt{17}} \\ \qquad if \ 3k+2 \le n \le 5k+4, \\ (2k+2)(\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{20}}) + (k-1)\frac{1}{\sqrt{32}} + (n-5k-4)\frac{1}{\sqrt{8}} \\ \qquad if \ n > 5k+4. \end{cases}$$

The inequality becomes equality iff $T \in \Lambda(n,k)$.

Corollary 2.9: *Let $T \in \mathcal{CT}(n,k)$ be a chemical tree. Then*

$$H(T) \le \begin{cases} (\frac{1}{3}+\frac{1}{6})(n-3k-2) + \frac{1}{8}(k-1) + \frac{1}{5}(5k-n+4) \\ \qquad if \ 3k+2 \le n \le 5k+4, \\ (\frac{1}{3}+\frac{1}{6})(2k+2) + \frac{1}{8}(k-1) + \frac{1}{4}(n-5k-4) \ \ if \ n > 5k+4. \end{cases}$$

The inequality changes into equality iff $T \in \Lambda(n,k)$.

Corollary 2.10: *Let $T \in \mathcal{CT}(n,k)$ be a chemical tree.*

(i) If $-1 \le \ell < 0$, then

$$X_\ell(T) \le \begin{cases} (n-3k-2)(3^\ell + 6^\ell) + (k-1)8^\ell + (5k-n+4)5^\ell \\ \qquad if \ 3k+2 \le n \le 5k+4, \\ (2k+2)(3^\ell + 6^\ell) + (k-1)8^\ell + (n-5k-4)4^\ell \\ \qquad if \ n > 5k+4. \end{cases}$$

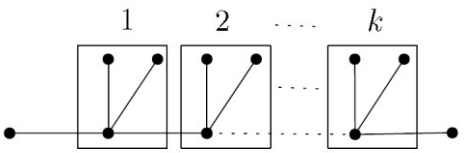
(ii) If $0 < \ell \le 1/2$, then

$$X_\ell(T) \geq \begin{cases} (n-3k-2)(3^\ell+6^\ell)+(k-1)8^\ell+(5k-n+4)5^\ell \\ \quad if\ 3k+2 \leq n \leq 5\,k+4, \\ (2k+2)(3^\ell+6^\ell)+(k-1)8^\ell+(n-5k-4)4^\ell \\ \quad if\ n > 5k+4. \end{cases}$$

The equality holds in each part iff $T \in \Lambda(n,k)$.

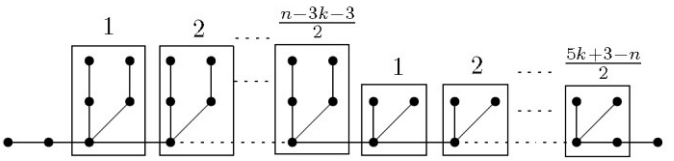
2.1 *Construction of extremal chemical trees in* $\mathcal{CT}(n,k)$

Corollaries and give chemical trees attaining minimum values of SO and X_ℓ $(0 < \ell \leq 1/2)$ among the class $\mathcal{CT}(n,k)$, while Corollaries 2.8-2.10 give trees attaining maximum values of SO_m, H, and X_ℓ $(-1 \leq \ell < 0)$ among the class $\mathcal{CT}(n,k)$. These corollaries straightforwardly result from Theorem when specific values of ℓ and γ are considered. Therefore, it is evident from Theorem that the trees with minimum values of SO and X_ℓ $(0 < \ell \leq 1/2)$ and maximum values of SO_m, H, and X_ℓ $(-1 \leq \ell < 0)$ are the same. These extremal trees are depicted in Figures 8-11. One can construct these extremal chemical trees by using Lemmas 2.4 and 2.5.



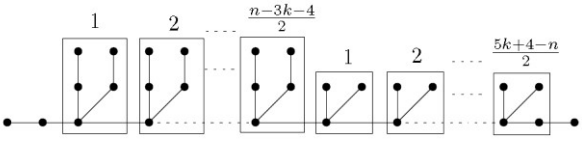
T_1

Figure 8
$n = 3k + 2$.



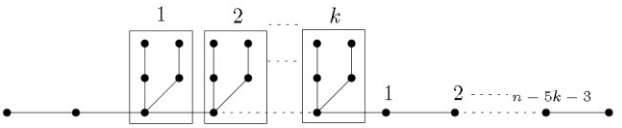
T_2

Figure 9
$3k + 2 \leq n \leq 5k + 4$ and $n - 3k - 2$ is odd.



T_3

Figure 10
$3k + 2 < n \leq 5k + 4$ and $n - 3k - 2$ is even.



T_4

Figure 11
$n > 5k + 4$.

3. Conclusion

In this paper, we find the extremal chemical trees for $GS_{\ell,\gamma}$ among all trees in $\mathcal{CT}(n,k)$, when $\ell, \gamma \in A$ or B. By giving specific values to ℓ and γ, $GS_{\ell,\gamma}$ coincides with the SO index, SO_m index, harmonic index and general sum-connectivity index. In the class $\mathcal{CT}(n,k)$, we successfully find trees with maximum values of SO_m, H and X_ℓ $(-1 \leq \ell < 0)$ and these same trees simultaneously attain minimum values of SO and X_ℓ $(0 < \ell \leq 1/2)$.

References

[1] H. Wiener, "Structural determination of paraffin boiling points," *Journal of American Chemical Society,* vol. 69, no. 1, pp. 17–20 (1947).

[2] S. Fajtlowicz, "On conjectures of graffiti-ii," *Congressus Numerantium,* vol. 60, pp. 187–197 (1987).

[3] I. Gutman, "Geometric approach to degree-based topological indices: Sombor indices," *MATCH Communications in Mathematical and in Computer Chemistry,* vol. 86, no. 1, pp. 11–16 (2021).

[4] B. Zhou and N. Trinajstić, "On general sum-connectivity index," *Journal of Mathematical Chemistry,* vol. 47, pp. 210–218 (2010).

[5] V. Kulli and I. Gutman, "Computation of Sombor indices of certain networks," *SSRG International Journal of Applied Chemistry*, vol. 8, no. 1, pp. 1–5 (2021).

[6] R. Cruz, J. Monsalve, and J. Rada, "On chemical trees that maximize atom-bond connectivity index, its exponential version, and minimize exponential geometric-arithmetic index," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 84, pp. 691–718 (2020).

[7] F. Li, H. Broersma, J. Rada, and Y. Sun, "Extremal benzenoid systems for two modified versions of the Randić index," *Applied Mathematics and Computation,* vol. 337, pp. 14–24 (2018).

[8] C. Betancur, R. Cruz, and J. Rada, "Vertex-degree-based topological indices over starlike trees," *Discrete Applied Mathematics*, vol. 185, pp. 18–25 (2015).

[9] W. Gao and M. R. Farahani, "The Zagreb topological indices for a type of benzenoid systems jagged-rectangle," *Journal of Interdisciplinary Mathematics,* vol. 20, no. 5, pp. 1341–1348 (2017).

[10] J. Kok and M. K. Jamil, "A note on the harmonic index and harmonic polynomial of graphs with weighted vertex degrees," *Journal of Information and Optimization Sciences*, vol. 40, no. 1, pp. 13–21 (2019).

[11] S. Kazi, "Consecutive chemical trees with respect to energy of graph," *Journal of Discrete Mathematical Sciences and Cryptography,* vol. 24, no. 3, pp. 827–841 (2021).

[12] I. Jahangir, M. Ahmad, S. Ahmad, and R. Farooq, "The Sombor index and harmonic index of chemical trees with a given number of vertices of maximum degree," *Journal of Discrete Mathematical Sciences and Cryptography*, in press.

[13] S. Ahmad, R. Farooq, and K. C. Das, "The general Sombor index of extremal trees with a given maximum degree," *MATCH Communications in Mathematical and in Computer Chemistry,* vol. 94, no. 3, pp. 825–853 (2025).

[14] K. C. Das, M. Imran, and T. Vetrík, "General Somborombor index of graphs and trees," *Journal of Discrete Mathematical Sciences and Cryptography,* vol. 28, no. 1, pp. 101–111 (2025).

[15] H. Faheem, S. Ahmad, and R. Farooq, "Maximal and minimal Zagreb indices of trees with fixed number of vertices of maximum degree," *MATCH Communications in Mathematical and in Computer Chemistry*, Vol. 95, no. 1, pp. 233–264 (2026).

[16] S. Ahmad and K. C. Das, "A complete solution for maximizing the general Sombor index of chemical trees with given number of pendant vertices," *Applied Mathematics and Computation,* vol. 505, p. 129532 (2025).

[17] Q. Cui and L. Zhong, "On the general sum-connectivity index of trees with given number of pendent vertices," *Discrete Applied Mathematics*, vol. 222, pp. 213–221 (2017).

[18] Z. Du, B. Zhou, and N. Trinajstić, "On the general sum-connectivity index of trees," *Applied Mathematics Letters*, vol. 24, no. 3, pp. 402–405 (2011).

[19] R. Xing, B. Zhou, and N. Trinajstić, "Sum-connectivity index of molecular trees," *Journal of Mathematical Chemistry,* vol. 48, pp. 583–591 (2010).

[20] K. C. Das and I. Gutman, "On Sombor index of trees," *Applied Mathematics and Computation,* vol. 412, p. 126575 (2022).

[21] Ž. K. Vukićević, "On the Sombor index of chemical trees," *Mathematica Montisnigri,* vol. 50, pp. 5–14 (2021).

[22] S. Liu and J. Li, "Some properties on the harmonic index of molecular trees," *International Scholarly Research Notices*, vol. 781668 (2014).

[23] H. Deng, S. Balachandran, Y. Venkatakrishnan, and S. R. Balachandar, "Trees with smaller harmonic indices," *Filomat,* vol. 30, no. 11, pp. 2955–2963 (2016).

[24] R. Cruz, I. Gutman, and J. Rada, "Sombor index of chemical graphs," *Applied Mathematics and Computation,* vol. 399, p. 126018 (2021).

[25] R. Cruz, J. Monsalve, and J. Rada, "Extremal values of vertex-degree-based topological indices of chemical trees," *Applied Mathematics and Computation*, vol. 380, p. 125281 (2020).

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