MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **96** (2026) 1015–1052
ISSN: 0340–6253
doi: 10.46793/match.96-3.26525

Comparative Study on Sombor and Elliptic Sombor Indices for Trees and Unicyclic Graphs with Fixed Number of Leaves

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(Received October 12, 2025)

Abstract

The Sombor index and the elliptic Sombor index of a graph G are defined, respectively, as:

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2},$$

$$ESO(G) = \sum_{uv \in E(G)} (d_u + d_v)\sqrt{d_u^2 + d_v^2},$$

where $E(G)$ denotes the edge set of G and d_u is the degree of the vertex u. Since their algebraic forms are closely related, it is natural to ask: Do they share the same extremal graphs? If not, what are the structural differences?

In order to address these questions, we investigate n-vertex trees, chemical trees, and unicyclic graphs, having a fixed number of leaves. For each considered class, the extremal graphs for SO and ESO do not always coincide, thereby revealing subtle yet significant structural distinctions between the two indices.

We also point out errors in the recent papers [11] and [19], and offer corrections.

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1 Introduction

We use $|X|$ to denote the cardinality of a set X. Throughout this study, all graphs are assumed to be finite and simple. Let $G(V, E)$ be such a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ and $|E(G)| = m$. A connected graph G is a tree if and only if $m = n - 1$, and a unicyclic graph if and only if $m = n$. For any vertex $v_i \in V(G)$, its neighborhood is defined as $N_G(v_i) = \{v_k \in V(G) : v_iv_k \in E(G)\}$, and its degree is given by $d_{v_i}(G) = |N_G(v_i)|$. By Δ we denote the maximum degree of a graph G. Two non-adjacent vertices v_i and v_j in G can be joined by an edge to obtain a new graph, denoted by $G + v_iv_j$. As usual, C_n, P_n, and S_n denote the cycle, the path, and the star on n vertices, respectively. The double star graph $DS_{s,t}$ is a tree with exactly two non-pendent vertices, where one has degree s and the other has degree t, such that $s+t = n$. A graph G is said to be a chemical graph if $\Delta(G) \leq 4$. A vertex of degree one is called a leaf (or pendent vertex), and a vertex of degree at least three a branching vertex. An edge that joins a leaf to a branching vertex is called a pendent edge. Denote by ℓ the total number of leafs. The degree sequence of an n-vertex graph G is the non-increasing sequence of the degrees of its vertices, denoted by $\pi(G)$.

A path $P = v_1v_2 \ldots v_k$ is called a pendent path if its one endpoint is a pendent vertex and the other is a branching vertex, and an internal path if its both endpoints are branching vertices. In either case, the internal vertices $v_2, \ldots, v_{k-1}$ (if they exist) have degree two. We denote by $\mathcal{P}(T)$ and $\mathcal{I}(T)(= T - \mathcal{P}(T))$ the sets of all pendent paths and internal paths, respectively. In a graph G, the distance between two vertices $v_i, v_j \in V(G)$, denoted by $d_G(v_i, v_j)$, is the number of edges in a shortest path connecting them. An edge whose end vertices have degrees i and j is referred to as an (i, j)-edge.

Let $n_i(G)$ denote the number of vertices in G of degree i, and let $e_{ij}(G) = |(i, j)|$ be the number of (i, j)-edges in G. Furthermore, define $E_k(G) = \{v_iv_j \in E(G) : d_{v_i}(G) = d_{v_j}(G) = k\}$. Note that $n_1(G) = \ell$.

A star-like tree is one that contains a unique branching vertex. Let I_k denote the tree formed by attaching k pendent paths of length 2 to a branching vertex, and I'_k the tree where one pendent path has length ≥ 3 and the others have length ≥ 2.

The symbol "(G)" will be omitted when the underlying graph is clear from the context. For notations used that are not defined here, see [6].

A topological index is a numerical invariant associated with a molecular graph, reflecting some of its structural features, expected to have some chemical, pharmacological or other applicative value. Scores of such topological indices depend only on the degrees of the vertices of the underlying graph. One recently introduced such vertex-degree-based graph invariant is the Sombor index [17], defined as:

$$SO(G) = \sum_{v_i v_j \in E(G)} \sqrt{d_{v_i}^2 + d_{v_j}^2}.$$

In a short time, it attracted considerable attention, leading to a flood of studies exploring its chemical applications, see for instance [32, 35, 36, 41] and mathematical properties, see for instance [7, 21, 25, 26, 29, 34, 39, 40]; see also the reviews [20, 31].

More recently, a variant of the original Sombor index was put forward, under the name elliptic Sombor index (ESO) [18], defined as:

$$ESO(G) = \sum_{v_i v_j \in E(G)} (d_{v_i} + d_{v_j}) \sqrt{d_{v_i}^2 + d_{v_j}^2}.$$

For its investigations in both chemical and mathematical directions, see for instance [2, 3, 5, 8, 14, 27, 28, 30, 33, 38].

Because of the closely related definitions of the Sombor index and its elliptic variant, the following question naturally arises.

Question 1. *Do the Sombor index and the elliptic Sombor index exhibit the same extremal graphs and related mathematical properties?*

In order to address this question, we investigated the families of n-vertex trees $\mathcal{T}_{n,\ell}$ and chemical trees $\mathcal{T}^c_{n,\ell}$, along with unicyclic graphs $\mathcal{U}_{n,\ell}$, having exactly ℓ pendent vertices. Our findings demonstrate that, within each class, the extremal graphs for SO and ESO do not always coincide, thereby uncovering subtle yet significant structural differences between the two indices.

For some recent research on pendent-vertex-containing molecular graphs, see [1, 9–13, 15, 16, 19, 22–24, 37].

We now present two elementary lemmas that serve as a foundation for the considerations in the subsequent sections.

Lemma 1. [2] *Let* $f(x) = (x+a)\sqrt{x^2+a^2} - (x+b)\sqrt{x^2+b^2}$, *where* $x \geq 1$, $a > b > 0$. *Then the function* $f(x)$ *is strictly increasing in* x.

Lemma 2. [2] *Let* $g(x,y) = (2+x)\sqrt{4+x^2} + (2+y)\sqrt{4+y^2} - (x+y)\sqrt{x^2+y^2}$, *where* $x, y \geq 2$. *Then* $g(x,y)$ *is a decreasing function in* $x \geq 2$ *and* $y \geq 2$.

The organization of the paper is as follows. Section 2 compares the ESO and SO indices in $\mathcal{T}_{n,\ell}$ and $\mathcal{T}^c_{n,\ell}$, while Section 3 addresses their comparison in $\mathcal{U}_{n,\ell}$. Finally, concluding remarks are given in Section 4.

2 Comparing the SO and ESO indices in $\mathcal{T}_{n,\ell}$ and $\mathcal{T}^c_{n,\ell}$

This section focuses on comparing the SO and ESO indices in the classes $\mathcal{T}_{n,\ell}$ and $\mathcal{T}^c_{n,\ell}$. The tree T is a path when $\ell = 2$, and a star when $\ell = n-1$. Therefore we restrict our attention to the case $3 \leq \ell \leq n-2$. Since $n_1 = \ell$, for every tree T the following equations satisfies:

$$\left.\begin{aligned} n &= \ell + n_2 + \cdots + n_\Delta \\ 2(n-1) &= \ell + 2n_2 + \cdots + \Delta n_\Delta \end{aligned}\right\} \tag{1}$$

and

$$i \times n_i = e_{1i} + e_{2i} + \cdots + e_{\Delta i} + e_{ii}, \ \ \forall \ \ i \in \{1, 2, \ldots, \Delta\}. \tag{2}$$

From (1), we obtain

$$\ell = 2 + n_3 + 2n_4 + \cdots + (\Delta - 2)\, n_\Delta. \tag{3}$$

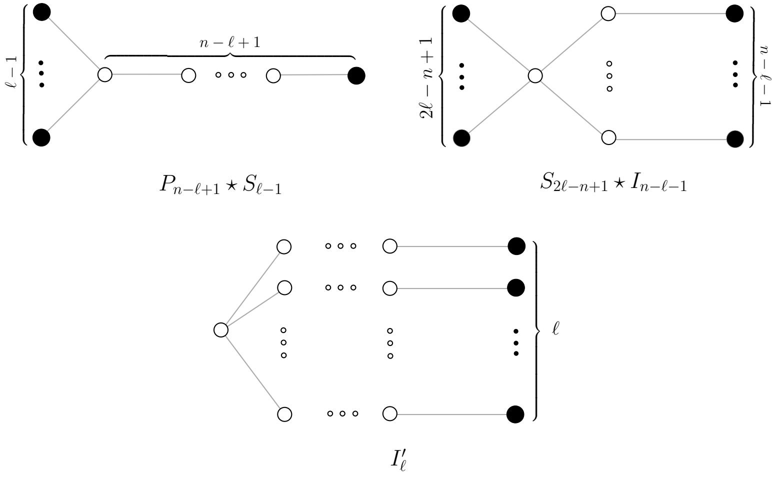
We first introduce some special trees that will be necessary for our results:

- A tree T is called an $(\ell, 3)$-regular tree if it has exactly ℓ leaves, and each of the remaining $n-\ell$ vertices has degree 3.

- Let $P_{n-\ell+1} \star S_{\ell-1}$ denote the star-like tree constructed by identifying the central vertex of the star $S_{\ell-1}$ with an end vertex of the path $P_{n-\ell+1}$; see Figure 1.

- Let $S_{2\ell-n+1} \star I_{n-\ell-1}$ denote the star-like tree obtained by identifying $n-\ell-1$ pendent paths of length 2 with the central vertex of the star $S_{2\ell-n+1}$; see Figure 1.

- Let I'_ℓ denote the star-like tree constructed by attaching ℓ pendent paths to a unique branching vertex; see Figure 1.



$P_{n-\ell+1} \star S_{\ell-1}$ $S_{2\ell-n+1} \star I_{n-\ell-1}$

I'_ℓ

Figure 1. The three star-like trees are $P_{n-\ell+1} \star S_{\ell-1}$, $S_{2\ell-n+1} \star I_{n-\ell-1}$ and I'_ℓ.

Lemma 3. *Let $T \in \mathcal{T}_{n,\ell}$ be a tree with $n \geq 3\ell - 5$ and $E_2(T) \subseteq E(\mathcal{I}(T))$. Then T satisfies*

$$|E_2(T)| \geq 2n_4 + 4n_5 + \cdots + 2(\Delta - 3)n_\Delta.$$

Proof. Since $E_2(T) \subseteq E(\mathcal{I}(T))$, it follows that $|E(\mathcal{P}(T))| = \ell$. One can observe that

$$|E(T)| = |E(\mathcal{I}(T))| + |E(\mathcal{P}(T))| = |E(\mathcal{I}(T))| + \ell. \tag{4}$$

Since $E_2(T) \subseteq E(\mathcal{I}(T))$, this implies that each internal path contains at most two edges that are not in $E_2(T)$. It follows

$$|E(\mathcal{I}(T))| - |E_2(T)| \leq 2\,[(n_3 + n_4 + \cdots + n_\Delta) - 1]$$

that is,

$$|E_2(T)| \geq |E(\mathcal{I}(T))| - 2\,[(n_3 + n_4 + \cdots + n_\Delta) - 1].$$

Together with (4), it implies that

$$\begin{aligned} |E_2(T)| &\geq |E(T)| - \ell - 2\,[(n_3 + n_4 + \cdots + n_\Delta) - 1] \\ &= n - 1 - \ell - 2\,[(n_3 + n_4 + \cdots + n_\Delta) - 1]. \end{aligned}$$

Since $n \geq 3\ell - 5$ and $\ell = 2 + n_3 + 2n_4 + \cdots + (\Delta - 2)n_\Delta$ (by (3)), it follows that

$$\begin{aligned} |E_2(T)| &\geq 2\ell - 6 - 2\,[n_3 + n_4 + \cdots + n_\Delta - 1] \\ &= 2\Big(2 + n_3 + 2n_4 + \cdots + (\Delta - 2)\,n_\Delta\Big) - 6 - 2\,[n_3 + \cdots + n_\Delta - 1] \\ &\geq 2n_4 + 4n_5 + \cdots + 2(\Delta - 3)\,n_\Delta. \end{aligned}$$

This completes the result. ■

2.1 Minimizing SO and ESO in classes $\mathcal{T}_{n,\ell}$ and $\mathcal{T}^c_{n,\ell}$

In this subsection, we investigate the structural differences between the SO and ESO indices by determining minimal graphs within the classes $\mathcal{T}_{n,\ell}$ and $\mathcal{T}^c_{n,\ell}$. The primary aim is to identify trees and to highlight how minimizers may differ in structural properties despite sharing the same degree sequence.

Lemma 4. *Let $T \in \mathcal{T}_{n,\ell}$ contain a vertex v of degree $r \geq 4$ and $|E_2(T)| \geq r-3$. Then there exists another tree $T' \in \mathcal{T}_{n,\ell}$ such that $d_v(T') = 3$ and $ESO(T') < ESO(T)$.*

Proof. Suppose that $v \in V(T)$ such that $d_v = r \geq 4$ and $|E_2(T)| \geq r-3$. Let $v_i \in N_T(v)$, for $1 \leq i \leq r$, such that $d_{v_i} \geq 1$. Construct a tree T' by replacing the vertex v by an $(r,3)$-regular tree. In this process, we contract $r-3$ edges from $E_2(T)$ and each vertex in $N_T(v)$ is individually identified with the corresponding leaves in the $(r,3)$-regular tree. Clearly, one can see that $T' \in \mathcal{T}_{n,\ell}$. Then

$$\begin{aligned} ESO(T) - ESO(T') = &\sum_{i=1}^{r} \left((r + d_{v_i}) \sqrt{r^2 + d_{v_i}^2} - (3 + d_{v_i}) \sqrt{9 + d_{v_i}^2} \right) \\ &+ (r-3) \left(4\sqrt{8} - 6\sqrt{18} \right). \end{aligned}$$

Since $d_{v_i} \geq 1$, then by Lemma 1, we obtain $f(d_{v_i}) \geq f(1)$ with $a = r \geq 4$ and $b = 3$. Then

$$\begin{aligned} ESO(T) - ESO(T') \geq\, & r \left((r+1)\sqrt{r^2+1} - (3+1)\sqrt{9+1} \right) \\ &+ (r-3)\left(8\sqrt{2} - 18\sqrt{2} \right) \\ \geq\, & r\,(r+1)\sqrt{r^2+1} - 4r\,\sqrt{10} - 10\,\sqrt{2}\,(r-3). \end{aligned}$$

Since $r \geq 4$, it follows that $r(r+1)\sqrt{r^2+1} + 30\sqrt{2} > r(10\sqrt{2} + 4\sqrt{10})$. This means $ESO(T) > ESO(T')$, which completes the proof. ■

Lemma 5. *Let T be an ESO-minimal tree in $\mathcal{T}_{n,\ell}$ $(\ell \geq 3)$. Then T does not simultaneously contain internal paths of length 1 and length greater than or equal to 3.*

Proof. Suppose, to the contrary, that T contains an internal path $u - v$ of length $r_1 = 1$, together with another internal path of length $r_2 \geq 3$. Construct a tree $T' \in \mathcal{T}_{n,\ell}$ from T by modifying these paths so that r_1 is increased to 2 and r_2 is decreased by 1. Consequently, $d_z(T') = d_z(T)$ for all $z \in V(T)$. Then

$$ESO(T) - ESO(T') = 4\sqrt{8} + (d_u + d_v)\sqrt{d_u^2 + d_v^2} - (2 + d_v)\sqrt{4 + d_v^2} \\ - (2 + d_u)\sqrt{4 + d_u^2}.$$

Since $d_u, d_v \geq 3$, then by Lemma 2, we obtain $-g(d_u, d_v) \geq -g(3,3)$. Thus

$$ESO(T) - ESO(T') \geq 4\sqrt{8} + (3+3)\sqrt{9+9} - 2(2+3)\sqrt{4+9} \\ \approx 0.714 \ > 0,$$

which contradicts the choice of T, thereby completing the proof. ■

We define $\mathcal{F}_1$ and $\mathcal{F}_2$ as two distinct subsets of the class $\mathcal{T}_{n,\ell}$ that share the same degree sequence $\pi_1 = (\overbrace{3,\dots,3}^{\ell-2}, \overbrace{2,\dots,2}^{n-2\ell+2}, \overbrace{1,\dots,1}^{\ell})$, with $\mathcal{F}_1$ existing for $n \geq 3\ell - 2$ and $\mathcal{F}_2$ for $n \geq 3\ell - 5$, but differing in their structural properties as summarized in Table 1.

$\mathcal{F}_1$ & $\mathcal{F}_2$	π	n & ℓ	e_{33}	e_{13}	e_{22}	e_{23}	e_{12}
$\mathcal{F}_1 \subseteq \mathcal{T}_{n,\ell}$	π_1	$n \geq 3\ell - 2$	$\ell - 3$	0	$n + 2 - 3\ell$	ℓ	ℓ
$\mathcal{F}_2 \subseteq \mathcal{T}_{n,\ell}$		$n \geq 3\ell - 5$	0	ℓ	$n - 3\ell + 5$	$2(\ell - 3)$	0

Table 1. Structural properties (i.e., the values of e_{ij}) of trees in $\mathcal{F}_1, \mathcal{F}_2 \subseteq \mathcal{T}_{n,\ell}$, both having the same degree sequence π_1.

Having developed the necessary preliminaries, we are now ready to present our main results.

Theorem 1. *Let $T \in \mathcal{T}_{n,\ell}$ be a tree with $\ell \geq 3$.*

(i) [23] *If $n \geq 3\ell - 2$, then we have*

$$SO(T) \geq \ell(\sqrt{5} + \sqrt{13}) + (n - 3\ell + 2)\sqrt{8} + (\ell - 3)\sqrt{18}.$$

The equality holds if and only if $T \in \mathcal{F}_1$.

(ii) If $n \geq 3\ell - 5$, then we have

$$ESO(T) \geq \begin{cases} ESO(S_4) & \text{if } \ell = 3 \text{ and } n = 4, \\ ESO(P_{n-2} \star S_2) & \text{if } \ell = 3 \text{ and } n \geq 5, \\ 4\ell\sqrt{10} + 10(\ell-3)\sqrt{13} + 4(n-3\ell+5)\sqrt{8} & \\ & \text{if } 4 \leq \ell \leq \lfloor \frac{n+5}{3} \rfloor. \end{cases}$$

The equality holds for $\ell = 3$ and $n = 4$ if and only if $T \cong S_4$, for $\ell = 3$ and $n \geq 5$ if and only if $T \cong P_{n-2} \star S_2$, and for $4 \leq \ell \leq \lfloor \frac{n+5}{3} \rfloor$ if and only if $T \in \mathcal{F}_2$.

Proof. The proof of Part (*i*) is given in [23].

(*ii*) Let $T^* \in \mathcal{T}_{n,\ell}$ be an ESO-minimal tree among all trees in $\mathcal{T}_{n,\ell}$ with $3 \leq \ell \leq \lfloor \frac{n+5}{3} \rfloor$. We have to distinguish between two cases:

Case 1. $\ell = 3$.

This case implies that T^* contains a unique branching vertex of degree 3. It is evident that $\mathcal{T}_{4,3} = \{S_4\}$ and $\mathcal{T}_{5,3} = \{P_3 \star S_2\}$. Thus we consider $n \geq 6$. We claim that $T^* \cong P_{n-2} \star S_2$ for $n \geq 6$. For otherwise, T^* contains two pendent paths, each of length $r_1 \geq 2$ and $r_2 \geq 2$. Construct a tree T_1 from T^* by shortening the length of r_1 to 1 and increasing the length of r_2 by $r_2 + r_1 - 1 \geq 3$. Then $T_1 \in \mathcal{T}_{n,\ell}$ and $d_z(T_1) = d_z(T^*)$ for all $z \in V(T^*)$. We obtain

$$ESO(T^*) - ESO(T_1) = 5\sqrt{13} + 3\sqrt{5} - 4(\sqrt{8} + \sqrt{10}) \approx 0.7731 > 0.$$

This contradicts to the choice of T^*. So $T^* \cong P_{n-2} \star S_2$, and hence

$$ESO(T^*) = 3\sqrt{5} + 5\sqrt{13} + 8\sqrt{10} + 4(n-5)\sqrt{8}.$$

Case 2. $4 \leq \ell \leq \lfloor \frac{n+5}{3} \rfloor$.

In order to prove this case, we consider the following claims:

Claim 1. $e_{12} = 0$.

Proof of Claim 1. Since $n \geq 3\ell - 5$ and $\ell \geq 4$, it is obvious that $n_2 > 0$. Suppose opposite to our claim that $e_{12} \geq 1$. Then T^* contains a pendent path $x - y$ of length $r_1 \geq 2$, where x is a pendent vertex. If $\ell = 4$, then either $n_4 = 1$ or $n_3 = 2$. First we consider $n_4 = 1$ for $\ell = 4$ with $n_2 > 0$. Then one can easily obtain two branching vertices of degree 3 by construction of $T_2 \in \mathcal{T}_{n,\ell}\,(\ell = 4)$ from T^* with $ESO(T_2) < ESO(T^*)$. Thus we suppose that T^* contains an internal path $u - v$ of length $r_2 \geq 1$. Construct a tree $T_3 \in \mathcal{T}_{n,\ell}$ from T^* by modifying these paths so that $r_1(T_3) = 1$ and $r_2(T_3) = r_2(T^*) + r_1(T^*) - 1 \geq 2$. Consequently, $d_z(T_3) = d_z(T^*)$ for all $z \in V(T^*)$. We now discuss the possible two cases.

Case 1. The length of the internal path $u - v$ is 1. Then

$$\begin{aligned} & ESO(T^*) - ESO(T_3) \\ & \quad = (2 + d_y)\sqrt{4 + d_y^2} - (1 + d_y)\sqrt{1 + d_y^2} + (d_u + d_v)\sqrt{d_u^2 + d_v^2} \\ & \quad - (2 + d_v)\sqrt{4 + d_v^2} - (2 + d_u)\sqrt{4 + d_u^2} + 3\sqrt{5}. \end{aligned}$$

Since $d_y, d_u, d_v \geq 3$, then by Lemmas 1 and 2, we obtain $f(d_y) \geq f(3)$ with $a = 2$ and $b = 1$, and $-g(d_u, d_v) \geq -g(3, 3)$, respectively. Therefore

$$ESO(T^*) - ESO(T_3) \geq 3\sqrt{5} - 4\sqrt{10} + 6\sqrt{18} - 5\sqrt{13} \approx 1.487 \;\; > 0,$$

a contradiction.

Case 2. The length of the internal path $u - v$ is greater than 2. Then

$$ESO(T^*) - ESO(T_3) = (2 + d_y)\,\sqrt{4 + d_y^2} - (1 + d_y)\,\sqrt{1 + d_y^2} + 3\sqrt{5} - 4\sqrt{8}.$$

Since $d_y \geq 3$, by Lemma 1 we obtain $f(d_y) \geq f(3)$. Thus

$$ESO(T^*) - ESO(T_3) \geq 5\sqrt{13} - 4\sqrt{10} + 3\sqrt{5} - 4\sqrt{8} \approx 0.773 \;\; > 0,$$

which contradicts to the choice of T^*.

In each case, we obtain a contradiction, thereby completing **Claim 1.** ■

From Claim 1, it is clear that $E_2(T^*) \subseteq E(\mathcal{I}(T^*))$.

Claim 2. *The degree sequence of the tree T^* is*

$$\pi_1 = \big(\overbrace{3,\ldots,3}^{\ell-2},\overbrace{2,\ldots,2}^{n-2\ell+2},\overbrace{1,\ldots,1}^{\ell}\big).$$

Proof of Claim 2. Suppose that Claim 2 does not hold, i.e., that $\Delta(T^*) \geq 4$. Since $n \geq 3\ell - 5$ and $E_2(T^*) \subseteq E(\mathcal{I}(T^*))$, then from Lemma 3 we have

$$E_2(T^*) \geq 2n_4 + 4n_5 + \cdots + 2(\Delta - 3)n_\Delta \geq 2.$$

Let $v \in V(T^*)$ such that $d_v = r = \Delta \geq 4$. Since $E_2(T^*) \geq 2(r-3) > r-3$, then by Lemma 4 we obtain a contradiction to the choice of T^*. Hence $\Delta(T^*) = 3$. This with (1) implies that the degree sequence of T^* is $\big(\overbrace{3,\ldots,3}^{\ell-2},\overbrace{2,\ldots,2}^{n-2\ell+2},\overbrace{1,\ldots,1}^{\ell}\big)$. This completes **Claim 2**. ■

Claim 3. $e_{33} = 0$.

Proof of Claim 3. From Claim 2, it follows that $\Delta(T^*) = 3$. This means that the number of internal paths in T^* is $n_3 - 1$. Since $\Delta = 3$, then by using (3), we obtain $\ell = n_3 + 2$. This implies that $n_3 - 1 = (\ell - 2) - 1 = \ell - 3$. Since $n \geq 3\ell - 5$, then by π_1, we obtain $n_2 \geq \ell - 3$. Thus $n_2 \geq n_3 - 1$. Combining this with Claim 1 and Lemma 5, one conclude that $e_{33} = 0$. ■

By using Claims 1-3 in (2), we obtain $e_{13} = \ell$, $e_{22} = n - 3\ell + 5$ and $e_{23} = 2(\ell - 3)$. Thus $T^* \in \mathcal{F}_2$. As a result

$$ESO(T^*) = 4\ell\sqrt{10} + 10(\ell - 3)\sqrt{13} + 4(n - 3\ell + 5)\sqrt{8}.$$

This completes the proof. ■

Remark. Since $\mathcal{F}_1, \mathcal{F}_2 \subseteq \mathcal{T}^c_{n,\ell} \subseteq \mathcal{T}_{n,\ell}$, it follows directly that Theorem 1 also holds when the class $\mathcal{T}^c_{n,\ell}$ is considered in place of $\mathcal{T}_{n,\ell}$.

2.2 Maximizing SO and ESO in classes $\mathcal{T}_{n,\ell}$ and $\mathcal{T}^c_{n,\ell}$

In this subsection, we study the extremal behavior of the SO and ESO indices by identifying the maximizing trees within the classes $\mathcal{T}_{n,\ell}$ and $\mathcal{T}^c_{n,\ell}$. Our focus is on characterizing the structural properties that lead to the maximal values, with attention to how these properties manifest differently in general and chemical tree settings.

Theorem 2. *Let $T \in \mathcal{T}_{n,\ell}$ be a tree. Then*

$$(i) \qquad [7] \quad SO(T) \le SO(P_{n-\ell+1} \star S_{\ell-1}).$$

$$(ii) \qquad [38] \quad ESO(T) \le \begin{cases} I'_\ell & if \quad \ell < \lfloor \frac{n}{2} \rfloor, \\ S_{2\ell-n+1} \star I_{n-\ell-1} & if \quad \ell \ge \lfloor \frac{n}{2} \rfloor. \end{cases}$$

The equality holds in (i) if and only if $T \cong P_{n-\ell+1} \star S_{\ell-1}$, and in (ii) if and only if $T \cong I'_\ell$ for $\ell < \lfloor \frac{n}{2} \rfloor$ and $T \cong S_{2\ell-n+1} \star I_{n-\ell-1}$ for $\ell \ge \lfloor \frac{n}{2} \rfloor$.

From Theorem 2, star-like trees emerge as the extremal structures for both the SO and ESO indices in $\mathcal{T}_{n,\ell}$. Motivated by this, we now turn to the subclass of chemical trees $\mathcal{T}^c_{n,\ell}$ and characterize the extremal members that maximize these indices. For $\ell \in \{3, 4\}$, the result in $\mathcal{T}^c_{n,\ell}$ follows directly from Theorem 2. Note that $\mathcal{T}^c_{7,5} = \{DS_{4,3}\}$. Hence, we restrict to the case $\ell \ge 5$ and $n \ge 8$.

Lemma 6. *Let T be an ESO-maximal in $\mathcal{T}^c_{n,\ell}$. Then T contains at most one vertex of degree* 3.

Proof. Assume, to the contrary, that there exists $x, y \in V(T)$, such that $d_x = d_y = 3$. Let $N_T(y) = \{y_1, y_2, y_3\}$ and $N_T(x) = \{x_1, x_2, x_3\}$. Without loss of generality, we assume that y_3 and x_3 are located on the $x - y$ path. Therefore $d_{y_3}, d_{x_3} \ge 2$. Construct a tree T' as follows: $T' = T - \{yy_1\} + \{xy_1\}$. Then $T' \in \mathcal{T}^c_{n,\ell}$, $d_y(T') = 2$, $d_x(T') = 4$, and $d_w(T') = d_w(T)$ for all $w \in V(T) \setminus \{x, y\}$. Then

$$ESO(T') - ESO(T)$$

$$= (4 + d_{y_1})\sqrt{16 + d_{y_1}^2} - (3 + d_{y_1})\sqrt{9 + d_{y_1}^2} + \sum_{i=1}^{3}\Big((4 + d_{x_i})\sqrt{16 + d_{x_i}^2}$$

$$- (3 + d_{x_i})\sqrt{9 + d_{x_i}^2}\Big) + \sum_{j=2}^{3}\Big((2 + d_{y_j})\sqrt{4 + d_{y_j}^2} - (3 + d_{y_j})\sqrt{9 + d_{y_j}^2}\Big).$$

Since $1 \leq d_{y_j} \leq 4$, $d_{x_3} \geq 2$ and $d_{x_i} \geq 1$, for $i \in \{1, 2\}$, then by Lemma 1, we obtain $f(d_{y_1}) \geq f(1)$ with $a = 4$, $b = 3$, $-f(d_{y_j}) \leq -f(4)$ with $a = 2$, $b = 3$ for $i \in \{2, 3\}$. Similarly, we obtain $f(d_{x_3}) \geq f(2)$ and $f(d_{x_1}), f(d_{x_2}) \geq f(1)$ with $a = 4$ and $b = 3$. Then

$$ESO(T') - ESO(T)$$

$$\geq 5\sqrt{1 + 16} - 4\sqrt{1 + 9} + 2\Big(5\sqrt{16 + 1} - 4\sqrt{9 + 1}\Big) + 6\sqrt{16 + 4}$$

$$- 5\sqrt{9 + 4} + 2\,(6\sqrt{4 + 16} - 7\sqrt{9 + 16}) \approx 16.37 > 0.$$

This completes the proof. ■

Now take into account the following result.

Lemma 7. [1] *For any tree $T \in \mathcal{T}_{n,\ell}^c$, the following results hold:*

- (i) $n_3 = 0$ *if and only if ℓ is even. Moreover, the degree sequence of T is*

$$(\overbrace{4, \ldots, 4}^{\frac{\ell-2}{2}}, \overbrace{2, \ldots, 2}^{\frac{2n-3\ell+2}{2}}, \overbrace{1, \ldots, 1}^{\ell}).$$

- (ii) $n_3 = 1$ *if and only if ℓ is odd. Moreover, the degree sequence of T is*

$$(\overbrace{4, \ldots, 4}^{\frac{\ell-3}{2}}, 3, \overbrace{2, \ldots, 2}^{\frac{2n-3\ell+1}{2}}, \overbrace{1, \ldots, 1}^{\ell}).$$

Lemma 8. *Let $T \in \mathcal{T}_{n,\ell}^c$ be ESO-maximal, where $\ell \geq 5$ and $n \geq 8$. Then the following holds:*

- (i) *The length of every internal path in T is* 1.
- (ii) *If $e_{14} > 0$ in T, then $e_{23} = 0$.*

(*iii*) *The tree T cannot simultaneously contain a pendent path of length at least 3 and a pendent path of length 1.*

Proof. (*i*) Since $\ell \geq 5$ and $n \geq 8$, then by Lemma 7, it follows that T contains an internal path and $n_2 > 0$. Assume, to the contrary, that there exists an internal path: $u_1 u_2 \cdots u_s$ for $s \geq 3$, where $d_{u_1} = d_{u_s} \geq 3$ and $d_{u_2} = \cdots = d_{u_{s-1}} = 2$. Let $zz_1 \in E(T)$, where $d_z = 1$ and $d_{z_1} \geq 2$. Consider a tree $T_4 = T - \{u_1u_2, u_{s-1}u_s\} + \{u_1u_s, zu_2\}$. Then $T_4 \in \mathcal{T}^c_{n,\ell}$, $d_z(T_4) = 2$, $d_{u_{s-1}}(T_4) = 1$ and $d_v(T_4) = d_v(T)$ for all $v \in V(T) \setminus \{z, u_{s-1}\}$. This implies:

$$\begin{aligned}
&ESO(T_4) - ESO(T)\\
&= (d_{u_1} + d_{u_s})\sqrt{d_{u_1}^2 + d_{u_s}^2} - (2 + d_{u_1})\sqrt{4 + d_{u_1}^2} - (2 + d_{u_s})\sqrt{4 + d_{u_s}^2}\\
&+ (2 + d_{z_1})\sqrt{4 + d_{z_1}^2} - (1 + d_{z_1})\sqrt{1 + d_{z_1}^2} + 3\sqrt{5}.
\end{aligned}$$

Since $d_{u_1}, d_{u_s} \geq 3$ and $d_{z_1} \geq 2$, by Lemma 1 we obtain $f(d_{z_1}) \geq f(2)$ with $a = 2$ and $b = 1$, whereas by Lemma 2, we obtain $-g(d_{u_1}, d_{u_2}) \geq -g(3,3)$. Thus

$$\begin{aligned}
ESO(T_4) - ESO(T) &\geq (3+3)\sqrt{9+9} - (2+3)\sqrt{4+9} - (2+3)\sqrt{4+9}\\
&+ (2+2)\sqrt{4+4} - 3\sqrt{5} + 3\sqrt{5} \approx 0.714 > 0,
\end{aligned}$$

which is a contradiction. Thus (*i*) is satisfied.

(*ii*) On the contrary, suppose that $e_{14} > 0$ and $e_{23} > 0$ in T. Then T contains $u_1u_2, v_2v_3 \in E(T)$ such that $d_{u_1} = 1$, $d_{u_2} = 4$, $d_{v_2} = 2$ and $d_{v_3} = 3$. Let v_1 be another neighbor of v_2 with $d_{v_1} \geq 1$. Construct a tree $T_5 = T - \{v_1v_2, v_2v_3\} + \{v_1v_3, v_2u_1\}$. Then $T_5 \in \mathcal{T}^c_{n,\ell}$, $d_{u_1}(T_5) = 2$, $d_{v_2}(T_5) = 1$ and $d_v(T_5) = d_v(T)$ for all $v \in V(T) \setminus \{u_1, v_2\}$. This implies:

$$\begin{aligned}
&ESO(T_5) - ESO(T)\\
&= (3 + d_{v_1})\sqrt{9 + d_{v_1}^2} - (2 + d_{v_1})\sqrt{4 + d_{v_1}^2} + (1+2)\sqrt{1+4}\\
&+ (2+4)\sqrt{4+16} - (2+3)\sqrt{4+9} - (1+4)\sqrt{1+16}.
\end{aligned}$$

Since $d_{v_1} \geq 1$, then by Lemma 1, we obtain $f(d_{v_1}) \geq f(1)$, with $a = 3$ and $b = 2$. Thus

$$ESO(T_5) - ESO(T) \geq (3+1)\sqrt{9+1} - (2+1)\sqrt{4+1} + 3\sqrt{5} + 6\sqrt{20}$$
$$- 5\sqrt{13} - 3\sqrt{17} \approx 0.839 > 0.$$

This contradicts to the given T, so (ii) holds true.

(iii) Suppose, to the contrary, that there exists a pendent path $u - v$ of length 1, with $d_v \geq 3$, and another pendent path of length $t \geq 3$. Construct a tree T_6 from T by reducing the pendent path of length t to $t-1$ and increasing the length of path $u - v$ by one. As a result, $T_6 \in \mathcal{T}^c_{n,\ell}$, and $d_z(T_6) = d_z(T)$ for all $z \in V(T)$. Then

$$ESO(T_6) - ESO(T) = (2 + d_v)\sqrt{4 + d_v^2} - (1 + d_v)\sqrt{1 + d_v^2} + 3\sqrt{5} - 4\sqrt{8}.$$

Since $d_v \geq 3$, then by Lemma 1, we obtain $f(d_v) \geq f(3)$ with $a = 2$ and $b = 1$. Thus

$$ESO(T_6) - ESO(T) \geq (2+3)\sqrt{4+9} - (1+3)\sqrt{1+9} + 3\sqrt{5} - 8\sqrt{2}$$
$$\approx 0.773 > 0,$$

which is a contradiction to the choice of T. ■

We define the following two degree sequences:

$$\pi_2(T) = (\overbrace{4, \ldots, 4}^{\frac{\ell-2}{2}}, \overbrace{2, \ldots, 2}^{\frac{2n-3\ell+2}{2}}, \overbrace{1, \ldots, 1}^{\ell}),$$

and

$$\pi_3(T) = (\overbrace{4, \ldots, 4}^{\frac{\ell-3}{2}}, 3, \overbrace{2, \ldots, 2}^{\frac{2n-3\ell+1}{2}}, \overbrace{1, \ldots, 1}^{\ell}).$$

Let $\mathcal{F}_3, \mathcal{F}_5 \subseteq \mathcal{T}^c_{n,\ell}$ be families of trees with degree sequence π_2, and $\mathcal{F}_4, \mathcal{F}_6 \subseteq \mathcal{T}^c_{n,\ell}$ be families with degree sequence π_3, where the subsets differ only in their structural properties as summarized in Tables 2 and 3.

Sets	π	n & ℓ	e_{44}	e_{34}	e_{14}	e_{33}	e_{13}	e_{24}	e_{23}	e_{12}	e_{22}
$\mathcal{F}_3$	π_2	$n < 2\ell - 3$	$2\ell - n - 3$	0	ℓ	0	0	$2n - 3\ell + 2$	0	0	0
		$n \geq 2\ell - 3$	0	0	ℓ	0	0	$\ell - 4$	0	0	$n - 2\ell + 3$
$\mathcal{F}_4$	π_3	$\ell = 5, n \geq 8$	0	0	3	0	1	1	0	0	$n - 8$
		$\ell = 7, n = 10$	0	2	6	0	1	0	0	0	0
		$\ell = 7, n = 11$	0	1	6	0	1	1	1	0	0
		$\ell = 7, n \geq 12$	0	0	6	0	1	2	2	0	$n - 12$
		$\ell = 9, 13 \leq n \leq 15$	0	$16 - n$	9	0	0	$n - 13$	$n - 13$	0	0
		$\ell = 9, n \geq 16$	0	0	9	0	0	3	3	0	$n - 16$
		$\ell \geq 11, n \leq 2\ell - 6$	$2\ell - n - 5$	3	ℓ	0	0	$2n - 3\ell + 1$	0	0	0
		$\ell \geq 11,\ 2\ell - 5 \leq n \leq 2\ell - 3$	‘ 0	$2\ell - 2 - n$	ℓ	0	0	$n - \ell - 4$	$n - 2\ell + 5$	0	0
		$\ell \geq 11,\ n \geq 2\ell - 2$	0	0	ℓ	0	0	$\ell - 6$	3	0	$n - 2\ell + 2$

Table 2. Structural properties (*i.e.*, the values of e_{ij}) for trees in $\mathcal{F}_3, \mathcal{F}_4 \subseteq \mathcal{T}^c_{n,\ell}$.

Sets	π	n & ℓ	e_{44}	e_{34}	e_{14}	e_{33}	e_{13}	e_{24}	e_{23}	e_{12}	e_{22}
$\mathcal{F}_5$	π_2	$8 \leq n \leq \frac{5\ell-2}{2}$	$\frac{\ell-4}{2}$	0	$\frac{5\ell-2n-2}{2}$	0	0	$\frac{2n-3\ell+2}{2}$	0	$\frac{2n-3\ell+2}{2}$	0
		$n > \frac{5\ell-2}{2}$	$\frac{\ell-4}{2}$	0	0	0	0	ℓ	0	ℓ	$\frac{2n-5\ell+2}{2}$
$\mathcal{F}_6$	π_3	$8 \leq n \leq \frac{5\ell-7}{2}$	$\frac{\ell-5}{2}$	1	$\frac{5\ell-2n-5}{2}$	0	2	$\frac{2n-3\ell+1}{2}$	0	$\frac{2n-3\ell+1}{2}$	0
		$\frac{5\ell-5}{2} \leq n \leq \frac{5\ell-3}{2}$	$\frac{\ell-5}{2}$	1	0	0	$\frac{5\ell-2n-1}{2}$	$\ell - 2$	$\frac{2n-5\ell+5}{2}$	$\frac{2n-3\ell+1}{2}$	0
		$n \geq \frac{5\ell-1}{2}$	$\frac{\ell-5}{2}$	1	0	0	0	$\ell - 2$	2	ℓ	$\frac{2n-5\ell+1}{2}$

Table 3. Structural properties (*i.e.*, the values of e_{ij}) for trees in $\mathcal{F}_5, \mathcal{F}_6 \subseteq \mathcal{T}^c_{n,\ell}$.

Theorem 3. [1] *Let $T \in \mathcal{T}^c_{n,\ell}$ be a tree with $\ell \geq 5$.*

(i) If ℓ is even, then each tree in $\mathcal{F}_3$ maximizes the SO index.

(ii) If ℓ is odd, then each tree in $\mathcal{F}_4$ maximizes the SO index.

Theorem 4. *Let $T \in \mathcal{T}^c_{n,\ell}$ be a tree with $\ell \geq 5$ and $n \geq 8$.*

(i) If $\ell (\geq 6)$ is even, then

$$ESO(T) \leq 16\,(\ell - 4)\sqrt{2} + \begin{cases} 5\left(\frac{5\ell-2n-2}{2}\right)\sqrt{17} + 15\left(\frac{2n-3\ell+2}{2}\right)\sqrt{5} \\ \qquad\qquad\qquad \text{if } \ell \geq 6 \text{ and } 8 \leq n \leq \frac{5\ell-2}{2}, \\ 4\,(2n - 5\ell + 2)\sqrt{2} + 15\,\ell\sqrt{5} \\ \qquad\qquad\qquad \text{if } \ell \geq 6 \text{ and } n > \frac{5\ell-2}{2}. \end{cases}$$

The equality holds if and only if $T \in \mathcal{F}_5$.

(ii) If $\ell (\geq 5)$ is odd, then

$$ESO(T) \leq 16\,(\ell - 5)\sqrt{2}$$

$$+\begin{cases} 15\left(\frac{2n-3\ell+1}{2}\right)\sqrt{5}+5\left(\frac{5\ell-5-2n}{2}\right)\sqrt{17}+7\sqrt{25}+8\sqrt{10} \\ \qquad\qquad\qquad\qquad \textit{if } \ell \geq 5 \textit{ and } 8 \leq n \leq \frac{5\ell-7}{2}, \\ \\ 3\left(\frac{2n-3\ell+1}{2}\right)\sqrt{5}+12\,(\ell-2)\sqrt{5}+5\left(\frac{2n-5\ell+5}{2}\right)\sqrt{13}+7\sqrt{25} \\ +2\,(5\ell-1-2n)\sqrt{10} \qquad \textit{if } \ell \geq 5 \textit{ and } \frac{5\ell-5}{2} \leq n \leq \frac{5\ell-3}{2}, \\ \\ 3\,\ell\sqrt{5}+12\,(\ell-2)\sqrt{5}+10\sqrt{13}+7\sqrt{25}+4\,(2n-5\ell+1)\sqrt{2} \\ \qquad\qquad\qquad\qquad \textit{if } \ell \geq 5 \textit{ and } n \geq \frac{5\ell-1}{2}. \end{cases}$$

The equality holds if and only if $T \in \mathcal{F}_6$.

Proof. Let T^* be an ESO-maximal tree in $\mathcal{T}^c_{n,\ell}$ for $\ell \geq 5$ and $n \geq 8$. By Lemma 6, the tree T^* contains at most one vertex of degree 3, and hence by Lemma 7, the degree sequence of T^* is as follows:

$$\pi = \begin{cases} \pi_2 = (\overbrace{4,\ldots,4}^{\frac{\ell-2}{2}},\overbrace{2,\ldots,2}^{\frac{2n-3\ell+2}{2}},\overbrace{1,\ldots,1}^{\ell}) & \text{if } \ell \text{ is even,} \\ \pi_3(T) = (\overbrace{4,\ldots,4}^{\frac{\ell-3}{2}},3,\overbrace{2,\ldots,2}^{\frac{2n-3\ell+1}{2}},\overbrace{1,\ldots,1}^{\ell}) & \text{if } \ell \text{ is odd.} \end{cases} \tag{5}$$

We divide the proof into two cases:

(i) First we assume that ℓ is even. From (5), we have

$$\pi_2 = (\overbrace{4,\ldots,4}^{\frac{\ell-2}{2}},\overbrace{2,\ldots,2}^{\frac{2n-3\ell+2}{2}},\overbrace{1,\ldots,1}^{\ell}).$$

Since $n_3 = 0$, it follows that $e_{3i} = 0$ for $1 \leq i \leq 4$. Moreover, by Lemma 8 (i), we obtain that $e_{44} = n_4 - 1 = \dfrac{\ell-4}{2}$. Substituting these relations together with (2) yields

$$\left.\begin{aligned} &e_{12}+e_{14}=\ell, \\ &e_{12}+2\,e_{22}+e_{24}=2n-3\ell+2, \\ &e_{14}+e_{24}=\ell. \end{aligned}\right\} \tag{6}$$

By simultaneously solving (6), we obtain

$$e_{22} - e_{14} = n - \frac{5\ell - 2}{2}. \tag{7}$$

We now consider our two cases:

Case 1. $8 \le n \le \frac{5\ell-2}{2}$.

In this case, we claim that $e_{22} = 0$. Otherwise, suppose that $e_{22} \ge 1$. Since $n \le \frac{5\ell-2}{2}$, then by (7), we obtain $1 \le e_{22} \le e_{14}$. Since $e_{44} = n_4 - 1$ and $e_{14} \ge e_{22} \ge 1$, the situation is similar to Lemma 8 (*iii*), which implies a contradiction. Hence $e_{22} = 0$. Substituting this into (6), we obtain $e_{14} = \frac{5\ell-2n-2}{2}$ and $e_{12} = e_{24} = \frac{2n-3\ell+2}{2}$. Thus T^* satisfies π_2, $e_{44} = \frac{\ell-4}{2}$, $e_{3i} = 0$ for $1 \le i \le 4$, $e_{14} = \frac{5\ell-2n-2}{2}$, $e_{24} = e_{12} = \frac{2n-3\ell+2}{2}$ and $e_{22} = 0$, and hence $T^* \in \mathcal{F}_5$. Therefore

$$ESO(T^*) = 16\,(\ell - 4)\sqrt{2} + 5\left(\frac{5\ell - 2n - 2}{2}\right)\sqrt{17} + 15\left(\frac{2n - 3\ell + 2}{2}\right)\sqrt{5}.$$

Case 2. $n > \frac{5\ell-2}{2}$.

In this case, we claim that $e_{14} = 0$. For otherwise, let $e_{14} \ge 1$. Since $n > \frac{5\ell-2}{2}$, then by (7), we obtain $e_{22} > e_{14} \ge 1$. Since $e_{44} = n_4 - 1$ and $e_{22} > e_{14} \ge 1$, the situation is similar to Lemma 8 (*iii*), which gives a contradiction. Hence $e_{14} = 0$. Substituting this into (6), we obtain $e_{22} = \frac{2n-5\ell+2}{2}$ and $e_{12} = e_{24} = \ell$. Thus T^* satisfies π_2, $e_{44} = \frac{\ell-4}{2}$, $e_{3i} = 0$ for $1 \le i \le 4$, $e_{24} = e_{12} = \ell$ and $e_{22} = \frac{2n-5\ell+2}{2}$, hence $T^* \in \mathcal{F}_5$. Therefore

$$ESO(T^*) = 16\,(\ell - 4)\sqrt{2} + 4\,(2n - 5\ell + 2)\sqrt{2} + 15\,\ell\,\sqrt{15}.$$

This completes the proof of Part (*i*).

(*ii*) We now assume that ℓ is odd. From (5), we have

$$\pi_3(T) = (\overbrace{4, \ldots, 4}^{\frac{\ell-3}{2}}, 3, \overbrace{2, \ldots, 2}^{\frac{2n-3\ell+1}{2}}, \overbrace{1, \ldots, 1}^{\ell}).$$

We now state the following claim.

Claim 4. $e_{34} = 1$.

Proof of Claim 4. If $\ell = 5$, then by π_3, we have $n_4 = 1 = n_3$, and hence by Lemma 8 (i), we conclude $e_{34} = 1$. For $\ell \geq 7$, by π_3, we have $n_4 \geq 2$ and $n_3 = 1$. We have to prove $e_{34} = 1$. Suppose oppositely that $e_{34} \geq 2$. Then T^* contain edges $w_1w, ww_2 \in E(T^*)$ such that $d_w = 3$, $d_{w_1} = 4 = d_{w_2}$. Let us consider a $v_1 - v_S$ pendent path such that $v_1v_2\ldots v_s$ $(s \geq 2)$, where $d_{v_1} = 4$ and $d_{v_s} = 1$ (v_1 may coincides either with w_1 or w_2). Let

$$T_4 = T^* - \{w_1w, ww_2, v_1v_2\} + \{w_1w_2, v_1w, wv_2\}.$$

As a result $T_4 \in \mathcal{T}^c_{n,\ell}$ and $d_z(T_4) = d_z(T^*)$ for all $z \in V(T^*)$. Then

$$\begin{aligned} ESO(T_4) - ESO(T^*) &= (3 + d_{v_2})\sqrt{9 + d_{v_2}^2} - (4 + d_{v_2})\sqrt{16 + d_{v_2}^2} \\ &\quad + 8\sqrt{32} - 7\sqrt{25}. \end{aligned}$$

Since $d_{v_2} \leq 2$, by Lemma 1 we obtain $-f(d_{v_2}) \geq -f(2)$ with $a = 3$ and $b = 4$. Thus

$$\begin{aligned} ESO(T_4) - ESO(T^*) &= (3 + 2)\sqrt{9 + 4} - (4 + 2)\sqrt{16 + 4} + 8\sqrt{32} - 7\sqrt{25} \\ &\approx 1.449 > 0, \end{aligned}$$

which contradicts to our assumption, so the claim holds true. ■

By combining Claim 4 and Lemma 8 (i), we obtain

$$e_{44} = n_4 - 1 = \frac{\ell - 5}{2} \text{ and } e_{34} = 1. \tag{8}$$

By substituting the degree sequence π_3 and expression (8) in (2), we obtain

$$\left.\begin{aligned} &e_{12} + e_{13} + e_{14} = \ell, \\ &e_{12} + 2\,e_{22} + e_{23} + e_{24} = 2n - 3\ell + 1, \\ &e_{13} + e_{23} = 2, \\ &e_{14} + e_{24} + \ell - 4 = 2\,(\ell - 3). \end{aligned}\right\} \tag{9}$$

We now consider three cases:

Case 1. $8 \leq n \leq \frac{5\ell-7}{2}$.

This case implies $n_2 \leq \ell - 3$. Since $n_3 = 1$, $e_{34} = 1$, $e_{44} = n_4 - 1$ and $n_2 \leq \ell - 3$, by Lemma 8 (ii) & (iii) one can conclude easily that $e_{23} = 0$ and $e_{22} = 0$, respectively. Substituting these values into (9), we obtain $e_{13} = 2$, $e_{12} = e_{24} = \frac{2n-3\ell+1}{2}$ and $e_{14} = \frac{5\ell-2n-5}{2}$. Thus T^* holds π_3, $e_{44} = \frac{\ell-5}{2}$, $e_{34} = 1$, $e_{14} = \frac{5\ell-2n-5}{2}$, $e_{33} = 0$, $e_{13} = 2$, $e_{24} = e_{12} = \frac{2n-3\ell+1}{2}$, and $e_{22} = 0$. Therefore we conclude that $T^* \in \mathcal{F}_6$, and therefore

$$ESO(T^*) = 16\,(\ell-5)\,\sqrt{2} + 15\left(\frac{2n-3\ell+1}{2}\right)\sqrt{5} + 5\left(\frac{5\ell-5-2n}{2}\right)\sqrt{17} + 7\,\sqrt{25} + 8\,\sqrt{10}.$$

Case 2. $\frac{5\ell-5}{2} \leq n \leq \frac{5\ell-3}{2}$.

This case implies $\ell - 2 \leq n_2 \leq \ell - 1$. Since $n_3 = 1 = e_{34}$, $e_{44} = n_4 - 1$ and $\ell - 2 \leq n_2 \leq \ell - 1$,by Lemma 8 (ii) & (iii), one concludes that $e_{14} = 0$ and $e_{22} = 0$. Substituting these values into (9), we obtain $e_{24} = \ell - 2$, $e_{23} = \frac{2n-5\ell+5}{2}$, $e_{13} = \frac{5\ell-2n-1}{2}$ and $e_{12} = \frac{2n-3\ell+1}{2}$. Thus T^* holds π_3, $e_{44} = \frac{\ell-5}{2}$, $e_{34} = 1$, $e_{14} = 0$, $e_{33} = 0$, $e_{13} = \frac{5\ell-2n-1}{2}$, $e_{24} = \ell - 2$, $e_{23} = \frac{2n-5\ell+5}{2}$, $e_{12} = \frac{2n-3\ell+1}{2}$ and $e_{22} = 0$. Therefore we conclude that $T^* \in \mathcal{F}_6$, and hence

$$ESO(T^*) = 16\,(\ell-5)\,\sqrt{2} + 3\left(\frac{2n-3\ell+1}{2}\right)\sqrt{5} + 12\,(\ell-2)\,\sqrt{5} + 5\left(\frac{2n-5\ell+5}{2}\right)\sqrt{13} + 7\,\sqrt{25} + 2\,(5\ell-2n-1)\,\sqrt{10}.$$

Case 3. $n \geq \frac{5\ell-1}{2}$.

This case yields $n_2 \geq \ell$. Since $n_3 = 1 = e_{34}$, $e_{44} = n_4 - 1$ and $\ell - 2 \leq n_2 \leq \ell - 1$, by Lemma 8 (ii) & (iii) one concludes that $e_{14} = e_{13} = 0$. Substituting these values in (9), we obtain $e_{12} = \ell$, $e_{23} = 2$, $e_{24} = \ell - 2$ and $e_{22} = \frac{2n-5\ell+1}{2}$. Thus T^* holds π_3, $e_{44} = \frac{\ell-5}{2}$, $e_{34} = 2$, $e_{14} = 0$, $e_{33} = 0$, $e_{13} = 0$, $e_{24} = \ell - 2$, $e_{23} = 2$, $e_{12} = \ell$ and $e_{22} = \frac{2n-5\ell+1}{2}$. Therefore,

$T^* \in \mathcal{F}_6$ and

$$ESO(T^*) = 16\,(\ell-5)\,\sqrt{2} + 3\,\ell\,\sqrt{5} + 12\,(\ell-2)\,\sqrt{5} + 10\,\sqrt{13} + 7\,\sqrt{25} + 4\,(2n-5\ell+1)\,\sqrt{2}.$$

This completes the proof of this theorem. ■

3 Comparing SO and ESO indices in $\mathcal{U}_{n,\ell}$

In this section, we study the SO and ESO indices within the class $\mathcal{U}_{n,\ell}$ of unicyclic graphs for $0 \le \ell \le n-3$, with particular focus on characterizing the maximizing structures. Since $\mathcal{U}_{n,0} = \{C_n\}$, we restrict our attention to the case $1 \le \ell \le n-3$.

Denote by C_k the cycle of length $k \ge 3$ contained as subgraph in a unicyclic graph U, and by $U\backslash\{C_k\}$ the trees attached to this cycle. A unicyclic star-like graph is a unicyclic graph containing exactly one branching vertex. We now introduce several special unicyclic star-like graphs that play a central role in our results:

- $C_{n-\ell} \star S_\ell$, obtained by identifying the central vertex of the star S_ℓ with a branching vertex of the cycle $C_{n-\ell}$; see Figure 2.

- $S_{2\ell-n+3} \star C_3 \star I_{n-\ell-3}$, obtained by attaching the star $S_{2\ell-n+3}$ and the graph $I_{n-\ell-3}$ to a single vertex of the cycle C_3; see Figure 2.

- $C_k \star I'_\ell$, obtained by attaching I'_ℓ to a vertex of the cycle C_k, where $k \ge 3$; see Figure 2.

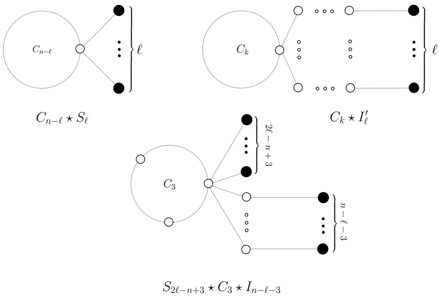


Figure 2. The three unicyclic star-like graphs are $C_{n-\ell} \star S_\ell$, $S_{2\ell-n+3} \star C_3 \star I_{n-\ell-3}$ and $C_k \star I'_\ell$.

Lemma 9. *Let G be a graph containing a vertex w of degree 2, with neighbors w_1 and w_2, such that $d_{w_1}, d_{w_2} \geq 2$. Let $vv_1 \in E(G)$ with $d_{v_1} = 1$ and $d_v \geq 3$. Construct a graph*

$$G_1 = G - \{w_1w, ww_2\} + \{w_1w_2, v_1w\}.$$

Then $ESO(G_1) > ESO(G)$.

Proof. Note that $d_{v_1}(G_1) = 2$, $d_w(G_1) = 1$ and $d_z(G_1) = d_z(G)$ for all $z \in V(G)$. We obtain

$$\begin{aligned} &ESO(G_1) - ESO(G) \\ &\quad = (d_{w_1} + d_{w_2})\sqrt{d_{w_1}^2 + d_{w_2}^2} - (2 + d_{w_1})\sqrt{4 + d_{w_1}^2} - (2 + d_{w_2})\sqrt{4 + d_{w_2}^2} \\ &\quad + (2 + d_v)\sqrt{4 + d_v^2} - (1 + d_v)\sqrt{1 + d_v^2} + 3\sqrt{5}. \end{aligned}$$

Since $d_{w_1}, d_{w_2} \geq 2$ and $d_v \geq 3$, by Lemma 1 we obtain $f(d_v) \geq f(3)$ with $a = 2$ and $b = 1$, whereas by Lemma 2, we obtain $-g(d_{w_1}, d_{w_2}) \geq -g(2, 2)$.

$$\begin{aligned} ESO(G_1) - ESO(G) &\geq 4\sqrt{8} - 2(4\sqrt{8}) + 5\sqrt{13} - 4\sqrt{10} + 3\sqrt{5} \\ &\approx 0.773 > 0. \end{aligned}$$ ■

Lemma 10. *Let $U \in \mathcal{U}_{n,\ell}$ be an ESO-maximal graph. Then all the branching vertices lie on C_k.*

Proof. Suppose to the opposite, that $v \in V(U \backslash \{C_k\})$ satisfies $d_v \geq 3$. Choose $u \in V(C_k)$ with $d_u \geq 3$ such that the distance $d_U(u, v)$ is minimum. Let $d_u = r + 1$ and $d_v = s + 1$, where $r \geq 2$ and $s \geq 2$. Let $zz_1 \in E(U)$ such that $d_z = 1$ and $d_{z_1} \geq 2$. We now distinguish two cases with regards to $d_U(u, v)$:

Case 1. $d_U(u, v) = 1$.

Let $N_U(v) = \{u, v_1, \ldots, v_s\}$, $N_U(u) = \{v, u_1, u_2, \ldots, u_r\}$, where $u_1, u_2 \in V(C_k)$. Construct a graph $U_1 \in \mathcal{U}_{n,\ell}$ from U as:

$$U_1 = U - \{uv, vv_1, \ldots, vv_s\} + \{uv_1, \ldots, uv_s, zv\}.$$

Then $d_u(U_1) = r + s$, $d_v(U_1) = 1$, $d_z(U_1) = 2$ and $d_w(U_1) = d_w(U)$ for all $w \in V(U)$. We have

$$\begin{aligned}
&ESO(U_1) - ESO(U)\\
&= 3\sqrt{5} - (r+s+2)\sqrt{(r+1)^2+(s+1)^2}\\
&+ (2+d_{z_1})\sqrt{4+d_{z_1}^2} - (1+d_{z_1})\sqrt{1+d_{z_1}^2}\\
&+ \sum_{i=1}^{s}\Big((d_{v_i}+r+s)\sqrt{d_{v_i}^2+(r+s)^2} - (d_{v_i}+s+1)\sqrt{d_{v_i}^2+(s+1)^2}\Big)\\
&+ \sum_{j=1}^{r}\Big((d_{u_j}+r+s)\sqrt{d_{u_j}^2+(r+s)^2} - (d_{u_j}+r+1)\sqrt{d_{u_j}^2+(r+1)^2}\Big)\\
&> 3\sqrt{5} - (r+s+2)\sqrt{(r+1)^2+(s+1)^2}\\
&+ \sum_{i=1}^{s}\Big((d_{v_i}+r+s)\sqrt{d_{v_i}^2+(r+s)^2} - (d_{v_i}+s+1)\sqrt{d_{v_i}^2+(s+1)^2}\Big)\\
&+ \sum_{j=1}^{2}\Big((d_{u_j}+r+s)\sqrt{d_{u_j}^2+(r+s)^2} - (d_{u_j}+r+1)\sqrt{d_{u_j}^2+(r+1)^2}\Big).
\end{aligned}$$

Since $d_{v_i} \geq 1$, $d_{u_j} \geq 2$ (as $u_1, u_2 \in V(C_k)$), and $r, s \geq 2$, by Lemma 1 we obtain $f(d_{v_i}) \geq f(1)$ with $a = r + s$ and $b = s + 1$, whereas $f(d_{u_j}) \geq f(2)$ with $a = r + s$ and $b = r + 1$. This yields

$$\begin{aligned}
&ESO(U_1) - ESO(U)\\
&> 3\sqrt{5} - (r+s+2)\sqrt{(r+1)^2+(s+1)^2}\\
&+ s\Big((r+s+1)\sqrt{1+(r+s)^2} - (s+2)\sqrt{1+(s+1)^2}\Big)\\
&+ 2\Big((r+s+2)\sqrt{4+(r+s)^2} - (r+3)\sqrt{4+(r+1)^2}\Big).
\end{aligned}$$

Since $r \geq 2$ and $s \geq 2$, it follows that $(rs - r - s + 1) > 0$, that is,

$$(r+s+2)\sqrt{4+(r+s)^2} > (r+s+2)\sqrt{(r+1)^2+(s+1)^2}.$$

Then

$$\begin{aligned}&ESO(U_1) - ESO(U)\\ &\qquad > 3\sqrt{5} + s\,(r+s+1)\,\sqrt{1+(r+s)^2} - s\,(s+2)\,\sqrt{1+(s+1)^2}\\ &\qquad + (r+s+2)\,\sqrt{4+(r+s)^2} - 2\,(r+3)\,\sqrt{4+(r+1)^2}.\end{aligned}$$

Claim 5.

$$\left.\begin{array}{c}3\sqrt{5} + s\,(r+s+1)\,\sqrt{1+(r+s)^2} - s\,(s+2)\,\sqrt{1+(s+1)^2}\\ +(r+s+2)\,\sqrt{4+(r+s)^2} - 2\,(r+3)\,\sqrt{4+(r+1)^2}\end{array}\right\} > 0.$$

Proof of Claim 5. Consider the function

$$\begin{aligned}h(x) &= 3\,\sqrt{5} + s\,(x+s+1)\,\sqrt{1+(x+s)^2} - s\,(s+2)\,\sqrt{1+(s+1)^2}\\ &+ (x+s+2)\,\sqrt{4+(x+s)^2} - 2\,(x+3)\,\sqrt{4+(x+1)^2},\end{aligned}$$

where $x \geq 2$ and $s \geq 2$. Then we obtain

$$\begin{aligned}h'(x) &= s\,\sqrt{1+(x+s)^2} + \frac{s\,(x+s+1)\,(x+s)}{\sqrt{1+(x+s)^2}} + \sqrt{4+(x+s)^2}\\ &+ \frac{(x+s+2)\,(x+s)}{\sqrt{4+(x+s)^2}} - 2\Big(\sqrt{4+(x+1)^2} + \frac{(x+3)\,(x+1)}{\sqrt{4+(x+1)^2}}\Big).\end{aligned}$$

Since $s \geq 2$ and $r \geq 2$, it follows that

$$x^2\,(s^2-2) + s^2\,(s^4+2) - 10 + 2x\,(s^3-2) > 0,$$

that is,

$$s\,\sqrt{1+(x+s)^2} > 2\,\sqrt{4+(x+1)^2}\,.$$

Then

$$h'(x) > \frac{s\,(x+s+1)\,(x+s)}{\sqrt{1+(x+s)^2}} + \frac{(x+s+2)\,(x+s)}{\sqrt{4+(x+s)^2}} - \frac{2\,(x+3)\,(x+1)}{\sqrt{4+(x+1)^2}}. \tag{10}$$

Since $\min\{s,x\} \geq 2$, it follows that $s^2+x^2\,(s^2-3+2s) > 0$, $xs\,(2s-4) \geq 0$ and $2\,(x+5s)-11 > 0$. Combining these, we obtain

$$s^2 + x^2\,(s^2-3+2s) + xs\,(2s-4) + 2\,(x+5s) - 11 > 0,$$

that is,

$$(x+s+1)(x+s)(s+1)\sqrt{4+(x+1)^2} > 2(x+3)(x+1)\sqrt{4+(x+s)^2},$$

that is,

$$\frac{s(x+s+1)(x+s)}{\sqrt{4+(x+s)^2}} + \frac{(x+s+2)(x+s)}{\sqrt{4+(x+s)^2}} > \frac{2(x+3)(x+1)}{\sqrt{4+(x+1)^2}}.$$

Now one can see that

$$\begin{aligned} &\frac{s\,(x+s+2)\,(x+s)}{\sqrt{1+(x+s)^2}} + \frac{(x+s+2)\,(x+s)}{\sqrt{4+(x+s)^2}} \\ &\qquad > \frac{s\,(x+s+1)\,(x+s)}{\sqrt{4+(x+s)^2}} + \frac{(x+s+2)\,(x+s)}{\sqrt{4+(x+s)^2}} > \frac{2\,(x+3)\,(x+1)}{\sqrt{4+(x+1)^2}}. \end{aligned}$$

This with (10) implies $h'(x) > 0$, which means that $h(x)$ is a strictly increasing function on $x \geq 2$. Now it is evident that

$$\begin{aligned} h(x) \geq h(2) &= 3\sqrt{5} + s\,(s+3)\,\sqrt{1+(s+2)^2} - s\,(s+2)\,\sqrt{1+(s+1)^2} \\ &\quad + (s+4)\,\sqrt{4+(s+2)^2} - 10\,\sqrt{13} \\ &> 3\sqrt{5} + s\,\sqrt{1+(s+2)^2} + (s+4)\,\sqrt{4+(s+2)^2} - 10\,\sqrt{13} \\ &\geq 3\sqrt{5} + 2\,\sqrt{17} + 6\,\sqrt{20} - 10\,\sqrt{13} \approx 5.65 > 0. \end{aligned}$$

This proves **Claim 5**. ■

By **Claim 5**, we obtain $ESO(U_1) - ESO(U) > 0$, which contradicts our assumption.

Case 2. $d_U(u,v) \geq 2$.

Let $uw_1 \ldots w_t v\ (t \geq 1)$ be an internal path, where $d_{w_1} = \cdots = d_{w_l} = 2$.

Let $N_U(u) = \{w_1, u_1, u_2, \ldots, u_r\}$ and $N_U(v) = \{w_t, v_1, \ldots, v_s\}$, where $u_1, u_2 \in V(C_k)$. Construct a graph $U_2 \in \mathcal{U}_{n,\ell}$ from U as:

$$U_2 = U - \{uw_1, vv_1, \ldots, vv_s\} + \{uv_1, \ldots, uv_s, zw_1\}.$$

Then $d_u(U_2) = r + s$, $d_v(U_2) = 1$, $d_z(U_2) = 2$ and $d_q(U_2) = d_q(U)$ for all $q \in V(U)$. We obtain

$$\begin{aligned}
&ESO(U_2) - ESO(U)\\
&= 3\sqrt{5} - (s+3)\sqrt{4+(s+1)^2} + 4\sqrt{8} - (r+3)\sqrt{4+(r+1)^2}\\
&+ (2+d_{z_1})\sqrt{4+d_{z_1}^2} - (1+d_{z_1})\sqrt{1+d_{z_1}^2}\\
&+ \sum_{i=1}^{s}\left((d_{v_i}+r+s)\sqrt{d_{v_i}^2+(r+s)^2} - (d_{v_i}+s+1)\sqrt{d_{v_i}^2+(s+1)^2}\right)\\
&+ \sum_{j=1}^{r}\left((d_{u_j}+r+s)\sqrt{d_{u_j}^2+(r+s)^2} - (d_{u_j}+r+1)\sqrt{d_{u_j}^2+(r+1)^2}\right)\\
&> 3\sqrt{5} - (s+3)\sqrt{4+(s+1)^2} + 4\sqrt{8} - (r+3)\sqrt{4+(r+1)^2}\\
&+ \sum_{i=1}^{s}\left((d_{v_i}+r+s)\sqrt{d_{v_i}^2+(r+s)^2} - (d_{v_i}+s+1)\sqrt{d_{v_i}^2+(s+1)^2}\right)\\
&+ \sum_{j=1}^{2}\left((d_{u_j}+r+s)\sqrt{d_{u_j}^2+(r+s)^2} - (d_{u_j}+r+1)\sqrt{d_{u_j}^2+(r+1)^2}\right).
\end{aligned}$$

Since $d_{v_i} \geq 1$, $d_{u_j} \geq 2$ (as $u_1, u_2 \in V(C_k)$), and $r, s \geq 2$, by Lemma 1 we obtain $f(d_{v_i}) \geq f(1)$ with $a = r + s$ and $b = s + 1$, whereas $f(d_{u_j}) \geq f(2)$ with $a = r + s$ and $b = r + 1$. This results in

$$\begin{aligned}
&ESO(U_3) - ESO(U)\\
&> 3\sqrt{5} + 4\sqrt{8} - (r+3)\sqrt{4+(r+1)^2} - (s+3)\sqrt{4+(s+1)^2}\\
&+ s\left((r+s+1)\sqrt{1+(r+s)^2} - (s+2)\sqrt{1+(s+1)^2}\right)
\end{aligned}$$

$$+\,2\left((r+s+2)\sqrt{4+(r+s)^2}-(r+3)\sqrt{4+(r+1)^2}\right)$$
$$>3\sqrt{5}+4\sqrt{8}-3\,(r+3)\sqrt{4+(r+1)^2}-(s+3)\sqrt{4+(s+1)^2}$$
$$+\,s\,(1+r+s)\sqrt{1+(r+s)^2}-s\,(s+2)\sqrt{1+(s+1)^2}$$
$$+\,2\,(2+r+s)\sqrt{4+(r+s)^2}.$$

Claim 6.

$$\left.\begin{array}{c} 3\sqrt{5}+4\sqrt{8}-3\,(r+3)\sqrt{4+(r+1)^2}-(s+3)\sqrt{4+(s+1)^2} \\ +s(1+r+s)\sqrt{1+(r+s)^2}-s\,(s+2)\sqrt{1+(s+1)^2} \\ +2\,(2+r+s)\sqrt{4+(r+s)^2} \end{array}\right\} > 0.$$

Proof of Claim 6. Consider the function

$$\phi(x)=3\sqrt{5}+4\sqrt{8}-3\,(x+3)\sqrt{4+(x+1)^2}-(s+3)\sqrt{4+(s+1)^2}$$
$$+\,s\,(1+x+s)\sqrt{1+(x+s)^2}-s\,(s+2)\sqrt{1+(s+1)^2}$$
$$+\,2(2+x+s)\sqrt{4+(x+s)^2},$$

where $x \geq 2$ and $s \geq 2$. Then we obtain

$$\phi'(x)=s\sqrt{1+(x+s)^2}+\frac{s\,(1+x+s)\,(x+s)}{\sqrt{1+(x+s)^2}}+2\sqrt{4+(x+s)^2}$$
$$+\,\frac{2(2+x+s)\,(x+s)}{\sqrt{4+(x+s)^2}}-3\sqrt{4+(x+1)^2}-\frac{3\,(x+3)\,(x+1)}{\sqrt{4+(x+1)^2}}.$$

Since $\min\{x,s\}\geq 2$, then it follows that

$$s\sqrt{1+(x+s)^2}+2\sqrt{4+(x+s)^2}\geq 2\sqrt{1+(x+2)^2}+2\sqrt{4+(x+2)^2}$$
$$>-3\sqrt{4+(x+1)^2}.$$

Similarly, one can see that

$$\frac{s\,(1+x+s)\,(x+s)}{\sqrt{1+(x+s)^2}}+\frac{2\,(2+x+s)\,(x+s)}{\sqrt{4+(x+s)^2}}\geq\frac{2\,(1+x+2)\,(x+2)}{\sqrt{1+(x+2)^2}}$$

$$+\frac{2\,(2+x+2)\,(x+2)}{\sqrt{4+(x+2)^2}} > \frac{3\,(x+3)\,(x+1)}{\sqrt{4+(x+1)^2}}.$$

The above two relations imply that $\phi'(x)$ is a strictly increasing function on $x \geq 2$. Thus $\phi(x) \geq \phi(2)$, which implies

$$\phi(x) \geq \phi(2) = 3\sqrt{5} + 4\sqrt{8} - 15\sqrt{13} - (s+3)\sqrt{4+(s+1)^2} + s\,(s+3)$$
$$\times \sqrt{1+(s+2)^2} - s\,(s+2)\sqrt{1+(s+1)^2} + 2\,(s+4)\sqrt{4+(s+2)^2}$$
$$> 3\sqrt{5} + 4\sqrt{8} - 15\sqrt{13} + (s+5)\sqrt{4+(s+2)^2} + s\sqrt{1+(s+2)^2}$$
$$\geq 3\sqrt{5} + 4\sqrt{8} - 15\sqrt{13} + 7\sqrt{20} + 2\sqrt{17} \approx 3.35 > 0.$$

This proves **Claim 6**. ■

By **Claim 6**, we obtain $ESO(U_2) - ESO(U) > 0$, which contradicts to our assumption. In each case, we obtained a contradiction. This completes the proof. ■

Lemma 11. *Let $U \in \mathcal{U}_{n,\ell}$ be an ESO-maximal graph. Then U contains a unique branching vertex.*

Proof. From Lemma 10, bearing in mind that all the branching vertices lie on the cycle C_k. Without loss of generality, we assume that $u \in V(C_k)$ such that $\Delta = d_u \geq d_w$ for all $w \in V(C_k)$. Suppose to the contrary that U contains u and v vertices such that $\Delta = d_u \geq d_v \geq 3$. Now consider the following cases:

Case 1. $d_U(u,v) = 1$

Let $N_U(u) = \{v, u_1, \ldots, u_r\}$ and $N_U(v) = \{u, v_1, \ldots, v_s\}$, where $u_1, v_1 \in V(C_k)$, $r = d_u - 1 = \Delta - 1 \geq 2$ and $s = d_v - 1 \geq 2$. Construct a graph $U_3 \in \mathcal{U}_{n,\ell}$ from U as:

$$U_3 = U - \{vv_2, vv_3, \ldots, vv_s\} + \{uv_2, uv_3, \ldots, uv_s\}.$$

Then $d_u(U_3) = r + s$, $d_v(U_3) = 2$, and $d_w(U) = d_w(U_3)$ for all $w \in$

$V(U)\backslash\{u,v\}$. Then

$$\begin{aligned}
&ESO(U_3) - ESO(U)\\
&= (r+s+2)\sqrt{4+(r+s)^2} - (r+s+2)\sqrt{(r+1)^2+(s+1)^2}\\
&+ (d_{v_1}+2)\sqrt{4+d_{v_1}^2} - (d_{v_1}+s+1)\sqrt{d_{v_1}^2+(s+1)^2}\\
&+ (d_{u_1}+r+s)\sqrt{d_{u_1}^2+(r+s)^2} - (d_{u_1}+r+1)\sqrt{d_{u_1}^2+(r+1)^2}\\
&+ \sum_{i=2}^{s}\Big((d_{v_i}+r+s)\sqrt{d_{v_i}^2+(r+s)^2} - (d_{v_i}+s+1)\sqrt{d_{v_i}^2+(s+1)^2}\,\Big)\\
&+ \sum_{j=2}^{r}\Big((d_{u_j}+r+s)\sqrt{d_{u_j}^2+(r+s)^2} - (d_{u_j}+r+1)\sqrt{d_{u_j}^2+(r+1)^2}\,\Big)\\
&> (r+s+2)\sqrt{4+(r+s)^2} - (r+s+2)\sqrt{(r+1)^2+(s+1)^2}\\
&+ (d_{v_1}+2)\sqrt{4+d_{v_1}^2} - (d_{v_1}+s+1)\sqrt{d_{v_1}^2+(s+1)^2}\\
&+ (d_{u_1}+r+s)\sqrt{d_{u_1}^2+(r+s)^2} - (d_{u_1}+r+1)\sqrt{d_{u_1}^2+(r+1)^2}.
\end{aligned}$$

Since $d_{u_1} \geq 2$ and $d_{v_1} \leq d_u \leq r+1$, from Lemma 1 we obtain $-f(d_{v_1}) \geq -f(r+1)$ with $a=2$ and $b=s+1$, and $f(d_{u_1}) \geq f(2)$ with $a=r+s$ and $b=r+1$. Then

$$\begin{aligned}
&ESO(U_3) - ESO(U)\\
&\quad > (r+s+2)\,\sqrt{4+(r+s)^2} - (r+s+2)\sqrt{(r+1)^2+(s+1)^2}\\
&\quad + (r+3)\,\sqrt{4+(r+1)^2} - (r+s+2)\,\sqrt{(r+1)^2+(s+1)^2}\\
&\quad + (r+s+2)\,\sqrt{4+(r+s)^2} - (r+3)\,\sqrt{4+(r+1)^2}\\
&\quad > 2\,(r+s+2)\,\Big(\sqrt{4+(r+s)^2} - \sqrt{(r+1)^2+(s+1)^2}\,\Big).
\end{aligned}$$

Since $\min\{r,s\} \geq 2$, it follows that $(rs - r - s + 1) > 0$, that is, $\sqrt{4+(r+s)^2} > (r+s+2)\,\sqrt{(r+1)^2+(s+1)^2}$. Therefore $ESO(U_3) > ESO(U)$, which is a contradiction to the choice of U.

Case 2. $d_U(u,v) \geq 2$.

Let $N_U(u) = \{u_1, u_2, \dots, u_r\}$ and $N_U(v) = \{v_1, v_2, \dots, v_s\}$, where $u_1, u_2, v_1, v_2 \in V(C_k)$, $r = \Delta = d_u \geq 3$, $s = d_v \geq 3$. From the previous case, it is evident that $d_{u_1} = d_{u_2} = d_{v_1} = d_{v_2} = 2$. Define $U_4 \in \mathcal{U}_{n,\ell}$ as:

$$U_4 = U - \{vv_3, \dots, vv_s\} + \{uv_3, \dots, uv_s\}.$$

Then $d_u(U_4) = r + s - 2$, $d_v(U_4) = 2$ and $d_w(U) = d_w(U_4)$ for all $w \in V(U) \backslash \{u, v\}$. We obtain

$$\begin{aligned}
&ESO(U_4) - ESO(U) \\
&= 2\left(4\sqrt{8} - (s+2)\sqrt{4+s^2}\right) \\
&+ 2\left((r+s)\sqrt{4+(r+s-2)^2} - (r+2)\sqrt{4+r^2}\right) \\
&+ \sum_{i=3}^{s}\left((d_{v_i}+r+s-2)\sqrt{d_{v_i}^2+(r+s-2)^2} - (d_{v_i}+s)\sqrt{d_{v_i}^2+s^2}\right) \\
&+ \sum_{j=3}^{r}\left((d_{u_j}+r+s-2)\sqrt{d_{u_j}^2+(r+s-2)^2} - (d_{u_j}+r)\sqrt{d_{u_j}^2+r^2}\right).
\end{aligned}$$

Since $1 \leq d_{u_i}, d_{v_i} \leq 2$ (by Lemma 10), then by Lemma 1, we obtain $f(d_{v_i}) \geq f(1)$ with $a = r + s - 2 \geq 4$ and $b = s \geq 3$, and $f(d_{u_j}) \geq f(1)$ with $a = r + s - 2 \geq 4$ and $b = r \geq 3$. Then

$$\begin{aligned}
&ESO(U_4) - ESO(U) \\
&> 16\sqrt{2} - 2(s+2)\sqrt{4+s^2} + 2(r+s)\sqrt{4+(r+s-2)^2} \\
&- 2(r+2)\sqrt{4+r^2} + (r+s-1)\sqrt{1+(r+s-2)^2} - (s+1)\sqrt{1+s^2} \\
&+ (r+s-1)\sqrt{1+(r+s-2)^2} - (r+1)\sqrt{1+r^2} \\
&> 16\sqrt{2} - 2(s+2)\sqrt{4+s^2} + 2(s-2)\sqrt{4+(r+s-2)^2} \\
&+ (r-2)\sqrt{1+(r+s-2)^2} + (s-2)\sqrt{1+(r+s-2)^2}.
\end{aligned}$$

Consider the function

$$\psi(x) = 16\sqrt{2} - 2\,(x+2)\,\sqrt{4+x^2} + 2\,(x-2)\,\sqrt{4+(r+x-2)^2}$$
$$+\,(r-2)\,\sqrt{1+(r+x-2)^2} + (x-2)\,\sqrt{1+(r+x-2)^2},$$

where $r \geq x \geq 3$. One can easily see that $\psi(x)$ is strictly increasing. Thus

$$\begin{aligned} \psi(x) &\geq \psi(3) = 16\sqrt{2} - 10\sqrt{13} + 2\sqrt{4+(r+1)^2} \\ &+ (r-1)\sqrt{1+(r+1)^2} \approx 3.75 > 0\,(\text{as } r \geq 3). \end{aligned}$$

This implies that $ESO(U_4) > ESO(U)$, which is a contradiction.

In both cases, we obtain a contradiction to the choice of U. Therefore our lemma holds. ■

Theorem 5. *Let U be a unicyclic graph in $\mathcal{U}_{n,\ell}$. Then*

(*i*) [4,11,19] $SO(U) \leq SO(C_{n-\ell} \star S_\ell)$.

(*ii*) $ESO(U) \leq \begin{cases} S_{2\ell-n+3} \star C_3 \star I_{n-\ell-3} & \text{if } n \leq 2\ell+2, \\ C_k \star I'_\ell & \text{if } n \geq 2\ell+3. \end{cases}$

Equality in (*i*) *holds if and only if $U \cong C_{n-\ell} \star S_\ell$. Equality in* (*ii*) *is attained if and only if $U \cong S_{2\ell-n+3} \star C_3 \star I_{n-\ell-3}$ for $n \leq 2\ell+2$ and $U \cong C_k \star I'_\ell$ for $n \geq 2\ell+3$.*

Proof. The proof of Part (*i*) is provided in Refs. [4] (see Remark 2 therein), [19], and [11]. It is important to note that in [11], the authors claimed that the unicyclic graph $S_{\ell-1} \star C_3 \star I'_1$ (constructed by attaching a star $S_{\ell-1}$ and a pendent path I'_1 of length at least two to the same vertex of the cycle C_3) maximizes the SO-index. However, this claim is incorrect. As a counterexample, one can transform $S_{\ell-1} \star C_3 \star I'_1$ into $C_{n-\ell} \star S_\ell$, which yields a contradiction.

(*ii*) Let $U' \in \mathcal{U}_{n,\ell}$ be an ESO-maximal graph. Lemmas 10 and 11 imply that U' is a unicyclic star-like graph. Denote by v the unique branching vertex of U'. We then show that $U' \cong S_{2\ell-n+3} \star C_3 \star I_{n-\ell-3}$ for $n \leq 2\ell+2$ and $U' \cong C_k \star I'_\ell$ for $n \geq 2\ell+3$. Accordingly, we divide the proof into the following two cases:

Case 1. $n \leq 2\ell+2$.

This case implies that U' contains a pendent edge $vv_1 \in E(U')$ such that $d_{v_1} = 1$. Otherwise, suppose that U' has no pendent edges. Then $d_{U'}(v,z) \geq 2$ for all $z \in V(U \backslash \{C_k\})$. Hence U' contains ℓ pendent paths, each of length at least 2. This together with the fact $|V(C_k)| \geq 3$ implies that $n \geq 2\ell+3$. This contradicts to the assumption $n \leq 2\ell+2$. Thus there exists $vv_1 \in E(U')$ with $d_{v_1} = 1$. We now consider the following claims:

Claim 7. *The unique cycle C_k of the star-like graph U' is a triangle; that is, $|C_k| = 3$.*

Proof of Claim 7. Suppose the opposite, i.e., that $|C_k| \geq 4$. Then in the star-like graph U', the cycle C_k contains three consecutive vertices w, w_1, w_2 such that $d_w = d_{w_1} = d_{w_2} = 2$. Since U' contains a pendent edge vv_1, by applying the transformation and the calculations from Lemma 9, we obtain a contradiction to the maximality of U'. Hence $|C_k| = 3$, which completes the proof of **Claim 7**.

Claim 8. *For every vertex $z \in V(U' \setminus \{C_k\})$, it holds $d_{U'}(v,z) \leq 2$.*

Proof of Claim 8. By Claim 7, we have $|C_k| = 3$. To derive a contradiction to our assumption, suppose that there exists a vertex $z \in V(U')$ such that $d_{U'}(v,z) \geq 3$. Then the unicyclic star-like graph U' contains a pendent path of length at least 3, which must contain three consecutive vertices w, w_1, w_2 satisfying $d_w = d_{w_1} = d_{w_2} = 2$. Since U' also contains a pendent edge vv_1, by applying the transformation and calculations from Lemma 9, we obtain a contradiction to the maximality of U'. Therefore every vertex $z \in V(U')$ must satisfy $d_{U'}(v,z) \leq 2$, which completes the proof of **Claim 8**.

By **Claims 7** and **8**, it follows that $U' \cong S_{2\ell-n+3} \star C_3 \star I_{n-\ell-3}$. Hence

$$ESO(S_{2\ell-n+3} \star C_3 \star I_{n-\ell-3}) = 4\sqrt{8} + (n-\ell-1)(\ell+4)\sqrt{(\ell+2)^2+4}$$

$$+ 3\,(n-\ell-3)\,\sqrt{5} + (2\ell-n+3)\,(\ell+3)\,\sqrt{(\ell+2)^2+1}.$$

Case 2. $n \geq 2\ell + 3$.

In this case, we claim that $U' \cong C_k \star I'_\ell$. We prove this claim by contradiction. Therefore, suppose the opposite, namely that the unicyclic star-like graph U' is not isomorphic to $C_k \star I'_\ell$. Then the unicyclic star-like graph U' contains a pendent edge vv_1, such that $d_{v_1} = 1$. Since $n \geq 2\ell + 3$ and $vv_1 \in E(U')$, it follows that U' contain three consecutive vertices w, w_1, w_2 satisfying $d_w = d_{w_1} = d_{w_2} = 2$. Otherwise, $U' \cong S_{2\ell-n+3} \star C_3 \star I_{n-\ell-3}$, contradicting the assumption $n \geq 2\ell+3$. Thus U' necessarily contains edges $ww_1, ww_2 \in E(U')$ with $d_w = d_{w_1} = d_{w_2} = 2$. By applying the transformation and calculations from Lemma 9, we then reach a contradiction to the maximality of U'. Hence $U' \cong C_k \star I'_\ell$. As a result

$$ESO(C_k \star I'_\ell) = (\ell+2)(\ell+4)\,\sqrt{(\ell+2)^2+4} + 3\ell\,\sqrt{5} + 4\sqrt{8}\,(n-2\ell-2).$$

This completes the proof. ■

4 Concluding remarks

In this paper, we presented a comparative study of the Sombor index and the elliptic Sombor index for three important classes of graphs: trees $\mathcal{T}_{n,\ell}$, chemical trees $\mathcal{T}^c_{n,\ell}$, and unicyclic graphs $\mathcal{U}_{n,\ell}$ with exactly ℓ leaves. This study was motivated by the naturally arising Question 1, inspired by the close algebraic similarity in the definitions of the two indices.

A comprehensive summary of our results is provided in Table 4, which offers a clear comparative overview of the extremal graphs optimizing the Sombor and elliptic Sombor indices in each class.

		$\mathcal{T}_{n,\ell}$	$\mathcal{T}^c_{n,\ell}$	$\mathcal{U}_{n,\ell}$
SO	max	[7] $P_{n-\ell+1} \star S_{\ell-1}$	[1] members of $\mathcal{F}_3$ for even ℓ members of $\mathcal{F}_4$ for odd ℓ	[4] $C_{n-\ell} \star S_\ell$
	min	[23] members of $\mathcal{F}_1$	[23] members of $\mathcal{F}_1$	?
ESO	max	[38] I'_ℓ for $\ell < \lfloor \frac{n}{2} \rfloor$ $S_{2\ell-n+1} \star I_{n-\ell-1}$ for $\ell \geq \lfloor \frac{n}{2} \rfloor$	members of $\mathcal{F}_5$ for even ℓ members of $\mathcal{F}_6$ for odd ℓ	$S_{2\ell-n+3} \star C_3 \star I_{n-\ell-1}$ for $n \leq 2\ell+2$ $C_k \star I'_\ell$ for $n \geq 2\ell+3$
	min	members of $\mathcal{F}_2$	members of $\mathcal{F}_2$	?

Table 4. Extremal graphs for SO and ESO within $\mathcal{T}_{n,\ell}$, $\mathcal{T}^c_{n,\ell}$ and $\mathcal{U}_{n,\ell}$.

From Table 4, it is evident that the extremal graphs for the Sombor index and the elliptic Sombor index do not generally coincide. This highlights subtle yet meaningful distinctions in structure-dependency of the two indices, even when studied within the same family of graphs. The question marks in Table 4 indicate unresolved cases.

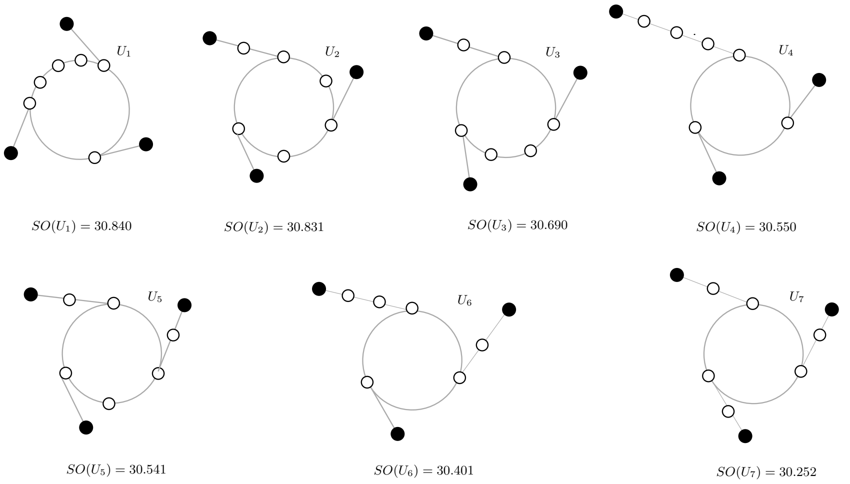


Figure 3. Counterexamples to the lower bound stated in Theorem 3 of [19] for $n = 9$ and $\ell = 3$.

It is worth noting that the unicyclic graphs in $\mathcal{U}_{n,\ell}$ corresponding to the lower bound of Theorem 3 in [19] are not the true minimizers of the Sombor index, as counterexamples exist. For instance, when $n = 9$ and $\ell = 3$, Theorem 3 of [19] identifies U_1 as the minimizer; however, six other graphs $U_2, \ldots, U_7$ of the same order and number of leaves yield smaller Sombor indices, with $SO(U_1) > SO(U_2) > SO(U_3) > SO(U_4) > SO(U_5) > SO(U_6) > SO(U_7)$, as illustrated in Figure 3. Thus the lower bound claim of Theorem 3 in [19] is invalid, and we leave question marks in Table 4 to indicate that the precise minimizers in $\mathcal{U}_{n,\ell}$ remain open.

We conclude by posing a natural question: "Are there graph classes, beyond the standard examples such as paths, stars, and complete graphs, in which the Sombor index and the elliptic Sombor index share the same extremal graphs, both maximal and minimal?"

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