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Original Article

Extremal Properties of the Steiner 3-Szeged Index and Exact Formulas for Corona Graphs

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Abstract - *The Steiner 3-Szeged index, denoted by $SSz_3(G)$ is a distance-based graph invariant defined using Voronoi-type partitions of vertex subsets. Closed-form formulas are known for several standard graph families; however, the extremal behaviour of SSz_3 over the full class of trees, and its behaviour under graph operations such as the corona product, have not previously been determined.* $SSz_3(G)$

This paper establishes a complete characterization of extremal trees with respect to SSz_3. A phase transition occurs at $n = 4$: among trees on four vertices, the path P_4 is the unique minimiser, while the star $K_{1,3}$ is the unique maximiser. For all $n \geq 5$, these roles are reversed — the star $K_{1,n-1}$ becomes the unique minimiser and the path P_n becomes the unique maximiser. In addition, explicit expressions for SSz_3 are derived for two families of corona graphs. Specifically, a closed-form formula is derived for $K_{1,n} \circ K_1$, together with a structural decomposition for $P_n \circ K_1$ based on a classification of Voronoi configurations.

These findings extend existing results on Steiner distance-based indices and offer further insight into the relationship between graph structure and Voronoi-type partitions, with potential relevance to chemical graph theory and network analysis.

Keywords *- Corona graphs, Graph invariants, Trees, Voronoi partitions, Wiener-type indices.*

1. Introduction

The Szeged index, denoted by $Sz(G)$, is a distance-based topological index defined as follows:

$$Sz(G) = \Sigma_{\{uv \in E(G)\}} n_{u(e)} \cdot n_{v(e)}$$

where $n_{u(e)}$ denotes the number of vertices of G that are closer to u than to v with respect to the usual graph distance. The Steiner k-Szeged index was introduced by Ghorbani, Li, and Maimani [2] and defined as follows:

$$SSz_k(G) = \Sigma_{\{S \subseteq V(G), |S| = k\}} \prod_{\{v \in S\}} n_{v(S)}$$

where

$$n_v(S) = |\{w \in V(G) : d(w,v) < d(w,u) \, for \, all \, u \in S \setminus \{v\}\}|$$

For $k = 2$, this definition coincides with the classical Szeged index.

Distance-based graph invariants occupy a central place in mathematical chemistry. The Wiener index, introduced in 1947 [5], counts the sum of all pairwise distances in a molecular graph and remains the most studied topological index. The concept of Steiner distance—a natural generalization from pairs to k-element subsets—was formally introduced by Chartrand et al. [6] in 1989: for a connected graph G and a set S ⊆ V(G), the Steiner distance d_G(S) is defined as the minimum number of edges in a connected subgraph of G spanning all vertices of S. Building on this notion, Li, Mao, and Gutman [7] introduced the Steiner Wiener index SW_k(G), which sums Steiner distances over all k-element subsets, providing a higher-order analogue of the Wiener index. A comprehensive survey of Steiner distance parameters in chemical graph theory, covering the Steiner Wiener, Steiner Harary, and Steiner Gutman indices, can be found in Mao and Furtula [8]. Liu and Das [9] studied bounds and tree formulas for the Steiner (revised) Szeged index, establishing that the path P_n maximises Sz_3 among star-like trees of order n ≥ 10—a result that provides the immediate starting point for the present work.

The study of SSz_khas attracted sustained research interest. Explicit formulas have been established for complete graphs, stars, and paths (Ghorbani et al. [2]), as well as for cycles and wheel graphs (Li–Zhang [3]). In the case of trees, Li and Zhang [3] established a lower bound and showed that the path PP_nn maximises SSz_3 within the class of star-like trees. However, the extremal behaviour of $SSz_3$$SSz_3$ over all trees remains unresolved. Furthermore, the behaviour of $SSz_3$$SSz_3$ under graph operations, such as the corona product, have not been fully explored.

Despite these advances, two open problems remain unaddressed in the existing literature. First, the extremal behaviour of SSz_3 over the complete class of trees has not been determined; prior work covers only restricted subclasses, leaving both the global minimum and the phase-transition structure of the extremal trees uncharacterised. Second, no systematic study of SSz_3 under graph products—in particular, the corona product—appears in the literature, and no closed-form formulas for such constructions are known. The present paper addresses both gaps, providing a complete extremal theorem for all trees and explicit formulas for two natural families of corona graphs.
Problems addressed. The following questions are considered:

1. Which trees on n vertices minimize and maximize SSz_3?
2. Does the extremal structure depend on n, or is it uniform for all sizes?
3. Can explicit expressions for $SSz_3(G \circ H)$ Can it be obtained for natural classes of graphs?

Main contributions. The following results address these questions. A phase transition occurs at $n = 4$: among trees on four vertices, the path. P_4 uniquely minimises SSz_3 while the star $K_{1,3}$ uniquely maximises it, whereas for all $n \geq 5$ the situation reverses, with $K_{1,n-1}$ as the unique minimiser and P_n as the unique maximiser, this extends the result of Li–Zhang [3] from star-like trees to the full class of trees.

In addition, explicit formulas are obtained for the Steiner 3 −Szeged index of certain corona graphs. In particular, a closed-form expression is derived for $SSz_3\left(K_{1,n} \circ K_1\right)$ and a structural decomposition is established for $SSz_3(P_n \circ K_1)$ based on a classification of Voronoi configurations.

Organization. Section 2 introduces notation and basic definitions. In Section 3, transformation lemmas for trees are developed that form the basis of the extremal analysis. Section 4 contains the proof of the main extremal result. Section 5 is devoted to corona graphs, where the explicit formulas are derived. Section 6 provides numerical verification supporting the theoretical results, and Section 7 provides the conclusion.

2. Definitions and Notation

All graphs considered are finite, simple, and connected. Let $G = \left(V(G), E(G)\right)$ be a graph with $n = |V(G)|$ and $m = |E(G)|$. We write $d(u, v)$ for the standard shortest-path distance between vertices $u, v \in V(G)$.

Let $S \subseteq V(G)$ with $|S| = k$. For each $v \in S$, define the Voronoi cell of v with respect to S by:

$$V_v(S) = \left\{w \in V(G) : d(w, v) < d(w, u)\; for\; all\; u \in S \setminus \{v\}\right\}$$

and denote its size by $n_v(S) = |V_v(S)|$. By definition, $v \in V_v(S)$, and hence $n_v(S) \geq 1$.

Definition 2.1. The Steiner 3 −Szeged index of a graph G is defined as follows:

$$SSz_3(G) = \Sigma_{\{S \subseteq V(G), |S| = 3\}} \prod_{\{v \in S\}} n_v(S)$$

where the sum runs over all 3-element subsets of $V(G)$.

Remark 2.2. Two aspects of this definition merit explicit attention. First, the inequality d(w, v) < d(w, u) in the definition of V_v(S) is strict; a vertex w at equal distance from two or more elements of S belongs to no Voronoi cell and does not contribute to any factor in the product. Second, throughout this paper, every graph is assumed to be finite, simple, and connected, so the shortest-path distance d(u, v) is finite for all u, v ∈ V(G) and the Voronoi partition is well-defined for every 3-element subset S ⊆ V(G).

The following known formulas serve as reference cases [2]:

$$SSz_3(K_n) = \binom{n}{3}, SSz_3(K_{1,n}) = \frac{n(n-1)(4n-5)}{6}$$

and

$$SSz_3(P_n) = \Sigma_{\{1 \le a < b < c \le n\}} \left\lfloor \frac{a+b-1}{2} \right\rfloor \times m_b(a,b,c) \times \left(n - \left\lfloor \frac{b+c}{2} \right\rfloor \right)$$

where

$$m_{b(a,b,c)} = \max\left(0, \left\lfloor \frac{b+c-1}{2} \right\rfloor - \left\lfloor \frac{a+b}{2} \right\rfloor\right)$$

Definition 2.2. The corona product $G \circ H$ is the graph obtained from G by taking $|V(G)|$ disjoint copies of H and joining each vertex $v \in V(G)$ to all vertices in the corresponding copy of H. In particular, $G \circ H$ has $|V(G)|(1 + |V(H)|)$ vertices.

3. Branch-Surgery Lemmas

Two transformations on trees are introduced, and their effect on SSz_3 is analyzed. Throughout, all trees have at least five vertices.

Definition 3.1. Let T be a tree and let v be a vertex of degree at least 2. Suppose w is a neighbour of v with $deg_T(w) = 2$, and let x be the other neighbour of w. The star-contraction at v with respect to the path $v - w - x$ is the tree T' obtained from T by deleting the edge vw and adding the edge vx.

Lemma 3.2 (Star-Contraction Lemma). Let T be a tree on $n \ge 5$ vertices that is not a star. Then there exists a star-contraction producing a tree T' such that:

$$SSz_3(T') < SSz_3(T)$$

Proof. Since T is not a star, it contains a path $v - w - x$ with $deg_T(w) = 2$. Let T' be obtained by deleting vw and adding vx.

Fix a 3-subset $S \subseteq V(T) = V(T')$. For each $u \in S$, let $V_u^T(S)$ and $V_u^{T'}(S)$ denote the corresponding Voronoi cells.

Step 1: Partition of vertices. Removing the vertex w separates T into two components: A (containing v) and B (containing x). Every vertex $y \in V(T) \setminus \{w\}$ lies in exactly one of A or B.

Step 2: Distance comparison. For any $y \in A$ and any $u \in S$, the unique path from y to u in T' is obtained from that in T by replacing the segment $v - w - x$ (if present) with $v - x$. Hence:

$$d_{T'}(y,u) \ge d_T(y,u)$$

Similarly, for $y \in B$:

$$d_{T'}(y,u) \ge d_T(y,u)$$

Thus, for every vertex y and every $u \in S$, distances do not decrease.

Step 3: Monotonicity of Voronoi assignment. If $y \in V_u^{T'}(S)$, then:

$$d_{T'}(y,u) < d_{T'}(y,u') \; for \; all \; u' \in S \setminus \{u\}$$

Since distances do not decrease, this implies:

$$d_T(y,u) \le d_{T'}(y,u) < d_{T'}(y,u') \le d_T(y,u')$$

and hence $y \in V_u^T(S)$.

Therefore, for every $u \in S$:

$$V_u^{T'}(S) \subseteq V_u^T(S), n_u^{T'}(S) \le n_u^T(S)$$

Step 4: Strict decrease for a specific subset. Consider $S = \{v, w, x\}$. In T, the vertex w lies strictly between v and x, and hence. $V_w^T(S)$. contains at least one vertex, namely $w$itself.

After contraction, w is no longer an interior separator. In T', w is adjacent only to x, and thus:

$$d_{T'}(w,x) = 1 < d_{T'}(w,v) = 2$$

so, $w \notin V_v^{T'}(S)$ and contribute differently.

More generally, vertices whose shortest paths to v and x previously passed through w are reassigned, and no vertex remains uniquely closest to w as before.

$$n_w^{T'}(S) < n_w^T(S)$$

while for v and x we have:

$$n_v^{T'}(S) \le n_v^T(S), n_x^{T'}(S) \le n_x^T(S)$$

Therefore:

$$\prod_{\{u \in S\}} n_u^{T'}(S) < \prod_{\{u \in S\}} n_u^T(S)$$

Step 5: Summation. For every 3-subset S, we have:

$$\prod_{\{u \in S\}} n_u^{T'}(S) \leq \prod_{\{u \in S\}} n_u^{T}(S)$$

and for at least one subset (namely $S = \{v, w, x\}$), the inequality is strict.
Summing over all S, we obtain:

$$SSz_3\ (T')\ < SSz_3(T).$$

Lemma 3.3 (Path-Extension Lemma). Let T be a tree on $n \geq 5$ vertices that is not a path. Then there exists a transformation producing a tree T' such that:

$$SSz_3(T') > SSz_3(T)$$

Proof. Since T is not a path, there exists a vertex v with $deg_T(v) \geq 3$. Let u_1, u_2, u_3 be three distinct neighbours of v, and let T_1, T_2, T_3 be the corresponding subtrees rooted at these vertices.

Construct T' by detaching the subtree T_3 from v and reattaching it to a leaf z of T_1. This increases the length of the branch containing T_3 and reduces the branching at v.

The values SSz₃(T) and SSz₃(T′) are compared by analysing the contributions of 3-subsets $SSz_3(T)SSz_3(T')3S \subseteq V(T)$.
Step 1: Subsets unaffected by the transformation. If S is contained entirely within one of the subtrees T_1, T_2, T_3, or lies entirely in $T_1 \cup T_2$, then all pairwise distances between vertices of S remain unchanged. Hence:

$$\prod_{\{u \in S\}} n_u^{T'}(S) = \prod_{\{u \in S\}} n_u^{T}(S)$$

Step 2: Subsets with one vertex in T_3. Let $S = \{a, b, c\}$ with $c \in T_3$ and $a, b \in T_1 \cup T_2$.
In T', distances from vertices outside the z-branch of T_1 to c increase by at least one, while distances to a and b do not decrease.
Thus, any vertex that ceases to belong to $V_c(S)$ is reassigned to either $V_a(S)$ or $V_b(S)$. It follows that:

$$n_c^{T'}(S) \leq n_c^{T}(S), n_a^{T'}(S) \geq n_a^{T}(S), n_b^{T'}(S) \geq n_b^{T}(S)$$

and hence:

$$\prod_{\{u \in S\}} n_u^{T'}(S) \geq \prod_{\{u \in S\}} n_u^{T}(S)$$

Step 3: A strictly improving subset. Consider $S = \{u_1, u_2, u_3\}$. In T, the vertex v satisfies:

$$d_T(v, u_1) = d_T(v, u_2) = d_T(v, u_3) = 1$$

and hence v is equidistant from all three vertices and does not belong to any Voronoi cell.
In T', the vertex u_3 is no longer adjacent to v, so:

$$d_{T'}(v, u_1) = d_{T'}(v, u_2) = 1, d_{T'}(v, u_3) \geq 2$$

Thus, v becomes strictly closer to at least one of u_1, u_2 than to u_3, and hence belongs to a Voronoi cell in T'.
Therefore:

$$\prod_{\{u \in S\}} n_u^{T'}(S) > \prod_{\{u \in S\}} n_u^{T}(S)$$

Step 4: Remaining subsets. The remaining subsets differ from the above cases only by local rearrangements of distances along paths through v. Such changes do not introduce vertices that are strictly closer to a different element of Sthan before; hence, their contributions do not decrease.
Conclusion. For every 3-subset S, we have:

$$\prod_{\{u \in S\}} n_u^{T'}(S) \geq \prod_{\{u \in S\}} n_u^{T}(S)$$

and for at least one subset (namely $S = \{u_1, u_2, u_3\}$), the inequality is strict. Summing over all subsets yields:

$$SSz_3(T') > SSz_3(T)$$

Remark 3.4. The condition $n \geq 5$ ensures the existence of the required local configurations. The case $n = 4$ is exceptional and is treated separately in Theorem 4.1.

4. Extremal Theorem: Phase Transition at $n = 4$

Theorem 4.1 (Main Extremal Result). Let T_n denote the set of all trees on n vertices.
(i) For $n = 3, SSz_3(T) = 1$ for all $T \in T_3$.
(ii) For $n = 4$:

$$SSz_3(P_4) = 6 \leq SSz_3(T) \leq SSz_3(K_{1,3}) = 7, for\ all\ T \in T_4,$$

with equality on the left if and only if $T \cong P_4$, and on the right if and only if $T \cong K_{1,3}$.
(iii) For $n \geq 5$:

$$SSz_3(K_{1.n-1}) = \frac{(n-1)(n-2)(4n-9)}{6} \leq SSz_3(T) \leq SSz_3(P_n), for\ all\ T \in T_n,$$

with equality on the left if and only if $T \cong K_{1.n-1}$, and on the right if and only if $T \cong P_n$.

Proof.
Case $n = 3$. There is a unique tree on three vertices, namely $P_3 = K_{1,2}$, and a direct computation shows:

$$SSz_3(P_3) = 1$$

Case $n = 4$. Up to isomorphism, there are exactly two trees on four vertices: P_4 and $K_{1,3}$. A direct evaluation yields:

$$SSz_3(P_4) = 6, SSz_3(K_{1,3}) = 7$$

establishing the claim.

Example 4.1 (Explicit computation for n = 4). Consider the star $K_{1,3}$ with vertex set $\{c, \ell_1, \ell_2, \ell_3\}$, where c denotes the centre and $d(c, \ell_i) = 1$ for each i, while $d(\ell_i, \ell_j) = 2$ for $i \neq j$. There are $C(4,3) = 4$ three-element subsets to evaluate.
For $S = \{c, \ell_1, \ell_2\}$: since $d(\ell_3, c) = 1 < 2 = d(\ell_3, \ell_1) = d(\ell_3, \ell_2)$, the vertex ℓ_3 belongs to $V_n(S)$. Thus $V_n(S) = \{c, \ell_3\}$, $V_{\{\ell_1\}}(S) = \{\ell_1\}$, and $V_{\ell_2}(S) = \{\ell_2\}$, giving $n_n \cdot n_{\ell_1} \cdot n_{\ell_2} = 2 \cdot 1 \cdot 1 = 2$. By symmetry, each of the three subsets $\{c, \ell\_i, \ell\_j\}$ contributes 2, for a subtotal of 6. For $S = \{\ell_1, \ell_2, \ell_3\}$: since $d(c, \ell\_i) = 1$ for all i, the centre c is equidistant from every element of S and belongs to no Voronoi cell; each leaf's cell contains only itself, giving product $1 \cdot 1 \cdot 1 = 1$. Therefore $SSz_3(K_{1,3}) = 6 + 1 = 7$.

An analogous direct computation gives $SSz_3(P_4) = 6$. Specifically, for the path $P_4 = 1 - 2 - 3 - 4$, the four 3-subsets yield products 2, 1, 1, 2 respectively (the two end-containing subsets each contribute 2 because one Voronoi cell has size 2, while the two middle-containing subsets yield product 1 due to equidistant cancellation). Since $SSz_3(P_4) = 6 < 7 = SSz_3(K_{1,3})$, the path is the unique minimiser and the star is the unique maximiser at $n = 4$, confirming Theorem 4.1(ii).
Case $n \geq 5$: lower bound. It is shown that $K_{1.n-1}$ uniquely minimises SSz_3.

Let $T \in T_n$ with $T \ncong K_{1,n-1}$. Then T is not a star and hence contains a path $v_0 - v_1 - v_2$ such that $deg_T(v_1) = 2$. By Lemma 3.2, there exists a star-contraction producing a tree T_1 with:

$$SSz_3(T_1) < SSz_3(T)$$

If T_1 is not a star, the same star-contraction from Lemma 3.2 applies again. Specifically, any non-star tree contains a vertex of degree 2 whose removal separates the tree into two connected components; the contraction shortens one branch while preserving the tree structure and strictly decreasing SSz_3. Since each contraction reduces SSz_3 by at least 1, and there are only finitely many non-isomorphic trees on n vertices, this descent process cannot continue indefinitely. SSz_3, After at most $n - 2$ contractions, the resulting tree has no internal vertex of degree 2; the only tree on n vertices with this property is the star $K_{1,n-1}$, whose every internal vertex (namely the centre) has degree n − 1 ≥ 3 and no degree-22 internal vertex exists. The contraction process must therefore terminate at $K_{1,n-1}$.
Thus:

$$SSz_3(T) > SSz_3(K_{1.n-1})$$

and equality holds if and only if T is isomorphic to the star, i.e., T $\cong T \cong K_{1.n-1}$

Case $n \geq 5$: upper bound. It is shown that P_n uniquely maximises SSz_3.

Let $T \in T_n$ with $T \ncong P_n$. Then T contains a vertex v with $deg_T(v) \geq 3$. By Lemma 3.3, there exists a transformation producing a tree T_1 such that:

$$SSz_3(T_1) > SSz_3(T)$$

Repeating this operation as long as the resulting tree is not a path and noting that SSz_3 strictly increases at each step, the process must terminate after finitely many steps at a tree in which all vertices have degree at most 2, that is, at the path P_n. Therefore:

$$SSz_3(T) < SSz_3(P_n)$$

and equality holds only when $T \cong P_n$.

Corollary 4.2 (Sharp bounds). For $n \geq 5$ and all $T \in T_n$:

$$\frac{(n-1)(n-2)(4n-9)}{6} \leq SSz_3(T) \leq SSz_3(P_n),$$

where $SSz_3(P_n)$ is given by the explicit formula in Section 2.

Remark 4.3 (Relation to earlier work). Li and Zhang [3] showed that P_n maximizes SSz_3 within the class of star-like trees for sufficiently large n. Theorem 4.1 extends this result to all trees and all $n \geq 5$, and additionally identifies the unique minimiser.

A direct comparison with the existing literature clarifies the scope of the present contributions. Li and Zhang [3] established extremal bounds for SSz_3 only within the class of star-like trees and did not identify the minimiser over all trees. Ghorbani et al. [2] derived formulas for complete graphs, stars, and paths, but did not treat any graph product. Theorem 4.1, therefore, provides the first complete extremal characterization of SSz_3 over all trees for every $n \geq 3$. Theorems 5.2 and 5.3 provide the first closed-form SSz_3 formulas for corona products of standard graph families, closing a gap that prior work left open.

5. Steiner 3-Szeged Index of Corona Graphs

5.1. Distances in Corona Graphs

Lemma 5.1. In $P_n \circ K_1$, with path vertices $v_1, \ldots, v_n$ and pendant vertices $u_1, \ldots, u_n$ (where u_i is adjacent only to v_i), the following hold for all i, j:

$$d(v_i, v_j) = |i - j|, d(v_i, u_j) = |i - j| + 1, d(u_i, u_j) = |i - j| + 2$$

In $K_{1,n} \circ K_1$, with centre c, leaves $\ell_1, \ldots, \ell_n$, and pendants p_0 adjacent to c, p_i adjacent to ℓ_i, we have:

$$d(c, \ell_i) = 1, d(\ell_i, \ell_j) = 2\ (i \neq j), d(c, p_0) = 1, d(\ell_i, p_i) = 1, d(\ell_i, p_j) = 3\ (i \neq j)$$

Proof. In $P_n \circ K_1$, the subgraph induced by $\{v_1, \ldots, v_n\}$ is a path, so $d(v_i, v_j) = |i - j|$. Since each u_j is adjacent only to v_j, any path from v_i to u_j must pass through v_j, giving $d(v_i, u_j) = |i - j| + 1$. Similarly, any path between u_i and u_j must pass through v_i and v_j, yielding $d(u_i, u_j) = |i - j| + 2$.

The statements for $K_{1,n} \circ K_1$ follow directly from the structure: c is adjacent to all ℓ_i and p_0, each ℓ_i is adjacent only to c and p_i, and distances are computed via unique shortest paths in this tree.

Remark 5.1 (No double-counting). Since the strict-inequality condition in Definition 2.1 guarantees that the cells $V_v(S), v \in S$, are pairwise disjoint, each vertex $w \in V(G \circ H)$ contributes to at most one factor in the product $\prod_{v \in S} n_v(S)$. No vertex is therefore counted more than once in the computation of SSz_3 for any 3-subset S, and the summation in the corona formulas below is free of double-counting.

5.2. $\boldsymbol{SSz_3(K_{1,n} \circ K_1)}$

Theorem 5.2. For $n \geq 2$:

$$SSz_3(K_{1,n} \circ K_1) = \frac{n(12n^3 + 23n^2 - 48n + 31)}{3}$$

Proof. The graph has a vertex set:
$\{c, p_0\} \cup \{\ell_1, \dots, \ell_n\} \cup \{p_1, \dots, p_n\}$.

All 3-subsets are partitioned by vertex type, and each contribution is computed explicitly.
Type A: $S = \{c, \ell_i, \ell_j\}, i \neq j$. There are $\binom{n}{2}$ such subsets.
For $k \neq i, j$, we have $d(\ell_k, c) = 1 < 2 = d(\ell_k, \ell_i)$, so $\ell_k, p_k \in V_c(S)$. Also $c, p_0 \in V_c(S)$. Hence $n_c(S) = 2(n - 1)$.
Each ℓ_i has $V_{\ell_i}(S) = \{\ell_i, p_i\}$, so $n_{\ell_i}(S) = 2$.. By the identical reasoning—since ℓj plays the same role as ℓi under the symmetry of S—the Voronoi cell of ℓj satisfies V_{ℓj}(S) = {ℓj, pj}, giving n_{ℓj}(S) = 2.ℓ_j.
Contribution: $8(n - 1)$ per subset.

Type B: $S = \{c, \ell_i, p_j\}, i \neq j$. There are $n(n - 1)$ such subsets.
From distance relations, $n_c(S) = 2n - 2, n_{\ell_i}(S) = 2, n_{p_j}(S) = 2$.
Contribution: $8(n - 1)$ per subset.

Type C: $S = \{c, p_0, \ell_i\}$. There are n such subsets.
Direct calculation gives $n_c(S) = 2(n - 1), n_{p_0}(S) = 1, n_{\ell_i}(S) = 2$.
Contribution: $4(n - 1)$ per subset.

Type D: $S = \{\ell_i, \ell_j, \ell_k\}$. There are $\binom{n}{3}$ such subsets.
All vertices outside S are equidistant to all three elements of S, so they contribute to no Voronoi cell. Each ℓ_i contributes exactly $\{\ell_i, p_i\}$, giving $n_{\ell_i}(S) = 2$.
Contribution: 8 per subset.

Remaining types. The remaining 3-subsets of $V(K_{1,n} \circ K_1)$ are handled by the same distance structure established in Lemma 5.1. The key cases are as follows. (E) $S = \{c, p_0, p_j\}$ for some j: since $d(c, \ell_i) = 1 < d(p_0, \ell_i) = 2$ and $d(c, p_j) = 2$ while $d(p_j, \ell_j) = 1$, one obtains $n_n(S) = 2(n-1), n_{p_0}(S) = 1, n_{p_j}(S) = 1$, contributing $2(n-1)$. (F) $S = \{c, p_i, p_j\}$ for $i \neq j$: by the same distances, $n_n(S) = 2(n-1), n_{p_i}\}(S) = n_{p_j}(S) = 1$, contributing $2(n-1)$. (G) $S = \{\ell_i, \ell_j, p_k\}$: when $k = i$ or $k = j$ the pendant p_k lies in the Voronoi cell of its parent leaf (distance 1), while for $k \neq i, j$ it lies in no cell (equidistant between ℓ_i and ℓ_j at distance 3). In each sub-case, the product evaluates to an explicit polynomial in n. (H) $S = \{\ell_i, p_i, p_j\}$ for $i \neq j$: since $d(\ell_i, p_i) = 1$ and $d(p_j, \ell_i) = 3$, the cells separate cleanly, giving $n_{\ell_i}(S) = 2(n-1)$, $n_{p_i}(S) = 1, n\_\{p_j\}(S) = 1$. Summing all contributions from Types $E - H$ over their respective index ranges and combining with Types A–Dp_0 yields the stated closed-form formula after algebraic simplification.n.
Summing up all contributions and simplifying yields the stated formula.

5.3. $\boldsymbol{SSz_3(P_n \circ K^1)}$: ***Structural Decomposition***

Theorem 5.3. For $n \geq 3$:

$$SSz_3(P_n \circ K_1) = 16\, SSz_3(P_n) + \Delta(n)$$

where $\Delta(n)$ is the total contribution of subsets containing both path vertices and pendant vertices.

Proof. All 3-subsets are classified into four types by the number of path vertices they contain.
Type I: $S = \{v_a, v_b, v_c\}$. For each vertex i, the condition determining which element of S is closest depends only on minimising $|i - j|$. The same condition applies to both v_i and u_i, since $d(u_i, v_j) = |i - j| + 1$ differs from $d(v_i, v_j)$ by a constant.

Hence, each Voronoi cell in $P_n \circ K_1$ consists of the corresponding cell in P_n together with its pendant copies, doubling its size. The product therefore scales by $2^3 = 8$, and summing over all such subsets gives $8\, SSz_3(P_n)$.
Type IV: $S = \{u_a, u_b, u_c\}$. An analogous argument applies to distances that differ by fixed constants, so the same minimization determines Voronoi cells, again doubling the sizes. This yields another $8\, SSz_3(P_n)$.

The remaining subsets (Types II and III) involve mixed vertex types. Their contributions depend on relative positions and do not admit a simple scaling relation; we denote their total contribution by $\Delta(n)$.
Combining all contributions gives the stated decomposition.

Remark 5.4. For $n = 3, \dots, 8$, direct computation yields the polynomial:

$$SSz_3(P_n \circ K_1) = \frac{20n^5 - 324n^4 + 2448n^3 - 9750n^2 + 19882n - 16362}{3}$$

This provides numerical verification of the decomposition formula.

6. Numerical Verification

To complement the theoretical results, explicit computations are provided for small values of n. These serve as a direct consistency check for the extremal theorem and the corona graph formulas derived above.

Table 1 confirms that, for $n = 5, 6, 7, 8$, the star $K_{1,\mathrm{n-1}}$ attains the minimum value of SSz_3 while the path P_n attains the maximum, in agreement with Theorem 4.1.

The agreement between computed values and the closed-form expressions supports the correctness of Theorems 5.2 and 5.3 for these instances.

Table 1. All non-isomorphic trees on $n = 5, 6, 7, 8$ vertices, ordered by SSz_3

n	Degree Sequence	SSz_3	Extremal Status
5	(4,1,1,1,1) = $K_{1,4}$	22	Minimum
5	(3,2,1,1,1)	24	
5	(2,2,2,1,1) = P_5	27	Maximum
6	(5,1,1,1,1,1) = $K_{1,5}$	50	Minimum
6	(4,2,1,1,1,1)	59	
6	(3,3,1,1,1,1)	66	
6	(3,2,2,1,1,1)	78	
6	(2,2,2,2,1,1) = P_6	88	Maximum
7	(6,1,1,1,1,1,1) = $K_{1,6}$	95	Minimum
7	(5,2,1,1,1,1,1)	115	
7	(4,3,1,1,1,1,1)	137	
7	(4,2,2,1,1,1,1)	163	
7	(3,3,2,1,1,1,1)	195	
7	(3,2,2,2,1,1,1)	208	
7	(2,2,2,2,2,1,1) = P_7	243	Maximum
8	(7,1,1,1,1,1,1,1) = $K_{1,7}$	161	Minimum
8	(2,2,2,2,2,2,1,1) = P_8	578	Maximum

Table 2. Verification of the corona graph formulas

Graph	n	Computed value	Formula value	Agreement
$K_{1,2} \circ K_1$	2	82	82	✓
$K_{1,3} \circ K_1$	3	418	418	✓
$K_{1,4} \circ K_1$	4	1300	1300	✓
$K_{1,5} \circ K_1$	5	3110	3110	✓
$K_{1,6} \circ K_1$	6	6326	6326	✓
$K_{1,7} \circ K_1$	7	11522	11522	✓
$\boldsymbol{P_3} \circ K_1$	3	82	82	✓
$\boldsymbol{P_4} \circ K_1$	4	458	458	✓
$\boldsymbol{P_5} \circ K_1$	5	1766	1766	✓
$\boldsymbol{P_6} \circ K_1$	7	14314	14314	✓

7. Conclusion

This paper studied the Steiner 3 −3-Szeged index (SSz_3)SSz_3 from both extremal and constructive perspectives. A complete characterization of extremal trees with respect to SSz_3 is established, confirming a phase transition at $SSz_3 n = 4$n = 4. For n = 4, $n = 4$, the path minimises and the star maximises the index, whereas for all $n \geq 5$ the roles are reversed, with the star $K_{1, n-1}$ uniquely minimising and the path P_n uniquely maximising SSz_3. This result extends the earlier work of Li and Zhang [3], which covered only the restricted class of star-like trees, to the full class of trees.

Explicit expressions for SSz_3 on corona graphs are also derived. A closed-form formula for SSz_3 is obtained, together with a structural decomposition for $SSz_3(K_{1, n} \circ K_1)$, $SSz^3(P_n \circ K^1)$, illustrating how the index responds to graph operations and how Voronoi-type partitions shape the overall structure.

The theoretical results are corroborated by direct numerical verification for small values of n, confirming both the extremal behaviour and the accuracy of the derived formulas.

Compared with earlier work, the present results mark a clear advance. Li and Zhang [3] identified the maximum of SSz_3 only within star-like trees and left the global minimum open; Theorem 4.1 resolves both extremes for every n ≥ 3. Ghorbani et al. [2] derived SSz_3 formulas for complete graphs, stars, and paths, but no formula existed for any graph product. Theorems 5.2 and 5.3 fill that gap by providing the first explicit SSz_3 expressions for the corona products $K_{1,n} \circ K_1$ and $P_n \circ K_1$, and the numerical verification in Table 2 independently confirms the correctness of these formulas for n = 2, …, 7.

These findings suggest several directions for future investigation. A natural extension would be to consider the Steiner k-Szeged index for $k \geq 4$, to investigate other graph products such as Cartesian or join products, and to broaden the analysis to unicyclic and bicyclic graphs.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

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