

Triplet Sombor Index of Graphs

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Abstract

In this paper, we introduce the Triplet Sombor Index (TSO), a new degree-based topological index defined over connected triples of vertices. We also establish several basic properties and bounds of the index in terms of graph parameters. In particular, we determine extremal trees with respect to TSO, and we prove that among all trees with n vertices, the star graph S_n achieves the maximum Triplet Sombor Index, while the path graph P_n attains the minimum value. Some structural properties and illustrative examples are also discussed.

1 Introduction

Topological indices are important tools in mathematical chemistry and graph theory for characterizing molecular structures and predicting physicochemical properties. These numerical invariants capture essential structural information of graphs that represent molecular frameworks, enabling correlations with physical and chemical properties. The past decade has

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significant advancements in developing novel topological indices with enhanced predictive capabilities and mathematical elegance.

Among recent studies, the Sombor index, introduced by Gutman [2] in 2021, has attracted considerable attention due to its geometric foundations and strong correlation performance. Defined as the sum of Euclidean distances of degree vectors associated with edges, the Sombor index provides an intuitive geometric interpretation and demonstrates remarkable performance in quantitative structure-property relationship (QSPR) studies. Its success has inspired numerous extensions and variants, each aiming to capture different aspects of molecular complexity.

In this work, we extend this geometric paradigm to higher-order connectivity patterns by introducing the *Triplet Sombor Index* (TSO), which generalizes the concept from edges to connected triples of vertices. This novel graph invariant captures local clustering and branching patterns that are often crucial in determining molecular properties but may be overlooked by edge-based indices. The TSO admits a natural geometric interpretation as the sum of Euclidean distances in three-dimensional space, where each connected triple corresponds to a point whose coordinates are the degrees of the constituent vertices.

Our investigation of the Triplet Sombor Index unfolds in several directions. First, we establish fundamental properties and derive explicit formulas for common graph families, including complete graphs, paths, cycles, and stars. We then develop general bounds for TSO in terms of graph parameters such as maximum and minimum degrees. The extremal behavior of TSO on trees receives special attention: we prove that among all trees with n vertices, the star graph maximizes TSO while the path graph minimizes it. Furthermore, we provide a detailed analysis of the isomer discrimination capability of TSO through a comprehensive case study of C_6H_{14} alkane isomers, comparing its performance with established indices including Wiener, Randić, Balaban J, and Zagreb indices.

This paper is organized as follows. Section 2 presents the definition of TSO, its geometric interpretation, and explicit formulas for common graphs. Section 3 establishes bounds for TSO in general graphs and extremal results for trees. In Section 4, we analyze the isomer discrimination

capability of TSO with a detailed case study of hexane isomers. The paper concludes with a discussion of implications and future research directions.

2 Definition and basic properties

Ali, et al. in [4] provided foundational results on the Sombor index of various graph classes. Here, we introduce the concept "Triplet Sombor Index" as a new generalization of the Sombor Index and discuss its general properties.

Definition 1 (Triplet Sombor Index). Let $G = (V, E)$ be a simple graph. The *Triplet Sombor Index* (TSO) of G is defined as

$$\text{TSO}(G) = \sum_{\{u,v,w\} \in \mathcal{T}(G)} \sqrt{(\deg(u))^2 + (\deg(v))^2 + (\deg(w))^2},$$

where $\mathcal{T}(G)$ denotes the set of all unordered triples of distinct vertices $\{u, v, w\}$ such that the induced subgraph $G[\{u, v, w\}]$ is connected.

The Triplet Sombor Index can be reformulated as follows:

$$\text{TSO}(G) = \text{TSO}_{P_3}(G) + \text{TSO}_{K_3}(G),$$

where

$$\text{TSO}_{P_3}(G) = \sum_{P_3: u-v-w} \sqrt{(\deg(u))^2 + (\deg(v))^2 + (\deg(w))^2},$$

$$\text{TSO}_{K_3}(G) = \sum_{\Delta_{uvw}} \sqrt{(\deg(u))^2 + (\deg(v))^2 + (\deg(w))^2}.$$

Here, the first sum is over all 3-vertex paths $u - v - w$ (counted once per path), and the second sum is over all triangles Δ_{uvw} (counted once per triangle). Note that if G is triangle-free (in particular when G is a tree), then $\text{TSO}_{K_3}(G) = 0$.

For chemical graphs, the decomposition has the following interpretation:

- TSO_{P_3} captures contributions from paths of length two, which are present in all connected graphs. This term is particularly relevant for alkanes and branched molecular structures.
- TSO_{K_3} is nonzero only in graphs containing triangular subgraphs. In organic chemistry, such 3-cycles occur in molecules like cyclopropane and its derivatives. For most organic compounds (including alkanes, alkenes, alkynes, and aromatic compounds such as benzene), the molecular graph is triangle-free, hence $\text{TSO}_{K_3}(G) = 0$.

It is important to note that TSO_{K_3} does **not** capture aromaticity. Aromatic rings (e.g., benzene) are typically 6-membered cycles with delocalized π -electrons and contain no triangular substructures. Therefore, the term TSO_{K_3} is zero for all standard aromatic compounds.

The decomposition into TSO_{P_3} and TSO_{K_3} is mathematically convenient for analysis, but any chemical interpretation of TSO_{K_3} must be restricted to graphs that actually contain triangles.

Example 1. (i) For the complete graph K_n with $n \geq 3$:

$$\text{TSO}(K_n) = \binom{n}{3} \cdot (n-1)\sqrt{3} = \frac{n(n-1)^2(n-2)\sqrt{3}}{6}.$$

(ii) For the path graph P_n with $n \geq 3$:

$$\text{TSO}(P_n) = \sum_{i=2}^{n-1} \left(\sqrt{(\deg(i-1))^2 + (\deg(i))^2 + (\deg(i+1))^2} \right),$$

where $\deg(1) = 1$, $\deg(n) = 1$, and $\deg(i) = 2$ for $2 \leq i \leq n-1$. Evaluating this sum yields:

$$\text{TSO}(P_n) = 2\sqrt{1^2 + 2^2 + 2^2} + (n-4)\sqrt{2^2 + 2^2 + 2^2} \quad \text{for } n \geq 4,$$

which simplifies to $2\sqrt{9} + (n-4)\sqrt{12} = 6 + 2\sqrt{3}(n-4)$ for $n \geq 4$.

(iii) For the cycle graph C_n with $n \geq 3$:

$$\text{TSO}(C_n) = n \cdot \sqrt{2^2 + 2^2 + 2^2} = n\sqrt{12} = 2n\sqrt{3},$$

since every vertex has degree 2 and every triple of consecutive vertices forms a connected triple.

(iv) For the star graph S_n with $n \geq 3$:

$$\begin{aligned} \text{TSO}(S_n) &= \binom{n-1}{2} \cdot \sqrt{(n-1)^2 + 1^2 + 1^2} \\ &= \frac{(n-1)(n-2)}{2} \sqrt{n^2 - 2n + 3}. \end{aligned}$$

(v) For the complete bipartite graph $K_{a,b}$ with $a, b \geq 2$:

$$\text{TSO}(K_{a,b}) = a \binom{b}{2} \sqrt{a^2 + b^2 + b^2} + b \binom{a}{2} \sqrt{b^2 + a^2 + a^2}.$$

(vi) For an r -regular triangle-free graph G with n vertices:

$$\text{TSO}(G) = n \binom{r}{2} \cdot \sqrt{r^2 + r^2 + r^2} = n \binom{r}{2} r \sqrt{3}.$$

The numerical values of the Triplet Sombor index of the above graphs with $n = 3, 4, 5, 6$ are presented in the following tables.

Table 1. TSO values for standard graph families (Part 1: $n = 3, 4, 5$)

Graph	$n = 3$	$n = 4$	$n = 5$
K_n	$2\sqrt{3} \approx 3.464$	$12\sqrt{3} \approx 20.785$	$40\sqrt{3} \approx 69.282$
P_n	$\sqrt{6} \approx 2.449$	$6 + 2\sqrt{3} \approx 9.464$	$6 + 4\sqrt{3} \approx 12.928$
C_n	$2\sqrt{3} \approx 3.464$	$8\sqrt{3} \approx 13.856$	$10\sqrt{3} \approx 17.321$
S_n	$\sqrt{6} \approx 2.449$	$3\sqrt{11} \approx 9.949$	$6\sqrt{18} \approx 25.456$

Table 2. TSO values for standard graph families (Part 2: $n = 6, 7$)

Graph	$n = 6$	$n = 7$
K_n	$100\sqrt{3} \approx 173.205$	$210\sqrt{3} \approx 363.730$
P_n	$6 + 4\sqrt{3} \approx 12.928$	$6 + 4\sqrt{3} \approx 12.928$
C_n	$12\sqrt{3} \approx 20.785$	$14\sqrt{3} \approx 24.249$
S_n	$10\sqrt{27} \approx 51.962$	$15\sqrt{38} \approx 92.466$

In the following results, we determine the Triplet Sombor index for a graph operation.

Theorem 1. *Let G be a simple connected graph and let $R(G)$ denote its R -graph, obtained by replacing each edge $uv \in E(G)$ with a triangle whose vertices are u , v , and a new vertex w_{uv} . Then the Triplet Sombor Index of $R(G)$ satisfies*

$$\begin{aligned} \text{TSO}(R(G)) &= 2 \text{TSO}(G) + \sum_{uv \in E(G)} (\deg_G(u) + \deg_G(v) - 1) \times \\ &\quad \sqrt{4 \deg_G(u)^2 + 4 \deg_G(v)^2 + 4} \\ &\quad + \sum_{x \in V(G)} \binom{\deg_G(x)}{2} \sqrt{4 \deg_G(x)^2 + 8}. \end{aligned}$$

Proof. The degree of an original vertex $x \in V(G)$ is $\deg_{R(G)}(x) = 2 \deg_G(x)$, and each new vertex w_{uv} has degree $\deg_{R(G)}(w_{uv}) = 2$. The set of connected vertex triples in $R(G)$ falls into the following three disjoint classes.

(I) Three original vertices. A triple $\{x, y, z\} \subseteq V(G)$ is connected in $R(G)$ if and only if it is connected in G . The contribution of such a triple is

$$\sqrt{\deg_{R(G)}(x)^2 + \deg_{R(G)}(y)^2 + \deg_{R(G)}(z)^2},$$

which is equal to

$$2\sqrt{\deg_G(x)^2 + \deg_G(y)^2 + \deg_G(z)^2}.$$

(II) Two original vertices and one new vertex. Let $uv \in E(G)$. For every neighbor $x \in N(u)$, the vertex w_{ux} is adjacent to u , hence the triple $\{u, v, w_{ux}\}$ is connected. Similarly, for every $y \in N(v)$ the triple $\{u, v, w_{vy}\}$ is connected. The vertex w_{uv} appears in both families; therefore, the number of distinct triples containing $\{u, v\}$ and one new vertex is $d_u + d_v - 1$. Each such triple contributes

$$\sqrt{(2d_u)^2 + (2d_v)^2 + 2^2} = \sqrt{4d_u^2 + 4d_v^2 + 4}.$$

(III) One original vertex and two new vertices. For a fixed $x \in V(G)$ and any two distinct neighbors $y, z \in N_G(x)$, the new vertices w_{xy} and w_{xz} are adjacent to x , forming a connected triple $\{x, w_{xy}, w_{xz}\}$. Its contribution is

$$\sqrt{4 \deg_G(x)^2 + 4 + 4} = \sqrt{4 \deg_G(x)^2 + 8}.$$

For each vertex x there are $\binom{\deg_G(x)}{2}$ such triples. Combining the three disjoint cases gives the desired formula. ■

Topological indices have proven invaluable in characterizing molecular structures and predicting physicochemical properties. The recent introduction of the Sombor index by Gutman has sparked considerable interest due to its geometric foundations. Now, we extend this geometric perspective to the Triplet Sombor Index, revealing its interpretation as a measure of Euclidean distances in three-dimensional space.

Recall that, for a graph $G = (V, E)$, the *Sombor index* [2] is defined as:

$$\text{SO}(G) = \sum_{uv \in E(G)} \sqrt{(\deg(u))^2 + (\deg(v))^2}.$$

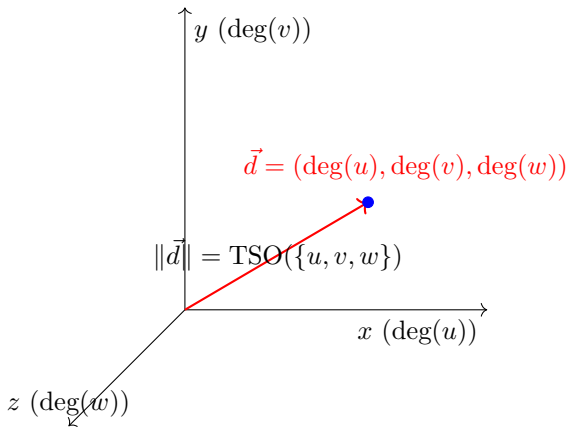
The Sombor index admits a natural geometric interpretation. For each edge uv , the term $\sqrt{(\deg(u))^2 + (\deg(v))^2}$ represents the Euclidean distance from the origin to the point $(\deg(u), \deg(v))$ in $\mathbb{R}^2$. This interpretation provides an intuitive geometric meaning: the Sombor index sums the "magnitudes" of degree vectors associated with each edge. In a similar way, the fundamental geometric interpretation of the TSO arises from the observation that for each connected triple $\{u, v, w\}$

$$\text{TSO}(\{u, v, w\}) = \sqrt{(\deg(u))^2 + (\deg(v))^2 + (\deg(w))^2}.$$

This expression is precisely the Euclidean distance from the origin to the point

$$(\deg(u), \deg(v), \deg(w))$$

in three-dimensional space.



This means that each connected triple is associated with a point in $\mathbb{R}^3$ whose coordinates are the degrees of the constituent vertices. The TSO sums the distances of these points from the origin.

An alternative but equivalent geometric interpretation involves the centroid of points placed along the coordinate axes. For a connected triple $\{u, v, w\}$, let

- Vertex u be represented by the point $P_u = (\deg(u), 0, 0)$ on the x-axis
- Vertex v be represented by the point $P_v = (0, \deg(v), 0)$ on the y-axis
- Vertex w be represented by the point $P_w = (0, 0, \deg(w))$ on the z-axis

Then the centroid C of points P_u , P_v , and P_w is

$$C = \left(\frac{\deg(u)}{3}, \frac{\deg(v)}{3}, \frac{\deg(w)}{3} \right).$$

The distance from the origin to the centroid is

$$\|C\| = \frac{1}{3} \sqrt{(\deg(u))^2 + (\deg(v))^2 + (\deg(w))^2}.$$

Therefore

$$3 \cdot \|C\| = \sqrt{(\deg(u))^2 + (\deg(v))^2 + (\deg(w))^2} = \text{TSO}(\{u, v, w\}).$$

Then the TSO term for the triple equals three times the distance from the origin to the centroid of triangle $P_uP_vP_w$. This interpretation reveals that the TSO measures the "spread" of the degree vector of the triple from the origin, scaled by the number of vertices in the triple.

We close this section by establishing bounds for TSO in terms of some graph invariants.

Theorem 2. *For any connected graph G with n vertices, maximum degree Δ , and minimum degree δ*

$$TSO(G) \leq \frac{n\Delta^2(\Delta-1)\sqrt{3}}{2}.$$

and additionally

$$TSO(G) \geq \begin{cases} \frac{n\delta^2(\delta-1)\sqrt{3}}{6} & \text{if } \delta \geq 2, \\ (n-2)\sqrt{6} & \text{if } \delta = 1. \end{cases}$$

Proof. Let $N_c(G)$ denote the number of connected triples in G . For any connected triple $\{u, v, w\}$, we have:

$$\sqrt{3\delta^2} \leq \sqrt{(\deg(u))^2 + (\deg(v))^2 + (\deg(w))^2} \leq \sqrt{3\Delta^2}.$$

Hence, the contribution for any triple is between $\delta\sqrt{3}$ and $\Delta\sqrt{3}$, except when $\delta = 1$, where the minimum contribution per triple is $\sqrt{6}$. It is clear that

$$\frac{n}{3} \binom{\delta}{2} \leq N_c(G) \leq n \binom{\Delta}{2}.$$

For $\delta = 1$, we use $N_c(G) \geq n - 2$ (since the path minimizes connected triples). Multiplying the per-triple bounds by the bounds on $N_c(G)$ yields the result. ■

Remark. The equality in the upper bound of the above Theorem holds if and only if the graph G is Δ -regular. If no Δ -regular graph exists for the given pair (n, Δ) , then the maximum value of $TSO(G)$ is attained by graphs whose degree sequence contains the largest possible number of vertices of degree Δ .

3 Bounds for trees

Li, Wang, and Zhang [3] studied the extremal Sombor index of trees, establishing that the star maximizes the Sombor index among trees. This section establishes bounds for TSO in trees and determines the extremal trees. We prove that stars maximize TSO, while paths minimize it. We first examine the maximal possible TSO among all graphs of order n .

Theorem 3. *Among all graphs with n vertices, the complete graph K_n has the maximum TSO.*

Proof. In K_n , every vertex has degree $n - 1$, and every triple of vertices is connected. There are $\binom{n}{3}$ such triples, each contributing $(n - 1)\sqrt{3}$. Hence,

$$\text{TSO}(K_n) = \binom{n}{3} \cdot (n - 1)\sqrt{3} = \frac{n(n - 1)^2(n - 2)\sqrt{3}}{6}.$$

For any other graph G , either there are fewer connected triples, or some vertices have degree less than $n - 1$, reducing the contribution of some triples. Thus, $\text{TSO}(G) < \text{TSO}(K_n)$. ■

Before continuing, we recall important facts about the maximum of a convex function over a convex set.

Proposition 4. ([1, Theorems 7.41, 7.42]) (i) *Let $f: C \rightarrow \mathbb{R}$ be a convex function which is not constant over the convex set C . Then f does not attain a maximum at a point in $\text{int}(C)$.*

(ii) *Let $f: C \rightarrow \mathbb{R}$ be a convex and continuous function over the nonempty convex and compact set $C \subseteq \mathbb{R}^n$. Then there exists at least one maximizer of f over C that is an extreme point of C .*

In the case of trees, the connectivity condition simplifies significantly. Suppose T is a tree with n vertices. Then the number of connected triples is $N_c(T) = \sum_{v \in V} \binom{\deg(v)}{2}$. Let $\{v_1, \dots, v_n\}$ be the vertex set of T . It is obvious that $\sum_{i=1}^n \deg(v_i) = 2(n - 1)$. Consider the real valued n -variable function f defined by

$$f(x_1, \dots, x_n) = \sum_{i=1}^n \frac{1}{2} x_i (x_i - 1)$$

As $\frac{\partial^2 f}{\partial x_i^2} = 1$ and $\frac{\partial^2 f}{\partial x_i \partial x_j} = 0$, for $i \neq j$, the Hessian matrix of f is positive definite, which implies that f is a convex function. Consider f over the compact convex simplex

$$S = \{(x_1, \dots, x_n) : 1 \leq x_1, \dots, x_n \leq n-1, x_1 + \dots + x_n = 2(n-1)\}$$

By Proposition 4, we know that the maximum of a convex function over a compact convex set occurs at an extreme point. The point $(n-1, 1, 1, \dots, 1)$ is an extreme point of S . Thus if we suppose x_i as the degree of the vertex v_i , then the extreme points of S are corresponded to the star-graphs S_n . The conclusion is that S_n has the maximum number of connected triples among all trees with n vertices. To find the minimum value of f , we can apply the Lagrange multipliers method to obtain that $x_1 = \dots = x_n = 2 - \frac{2}{n}$ the minimum of f . Hence, over the integral domain, the minimum of f is achieved by making the values as equal as possible. This gives the optimal solution, which uses only the integers 2 for $n-2$ times and 1 for two times. The corresponding graph in this case is the path graph P_n . The conclusion is that P_n has the minimum number of connected triples among all trees with n vertices.

It is clear that in a tree T , a triple $\{u, v, w\}$ is connected if and only if there exists a vertex in the triple that is adjacent to the other two vertices. This allows us to express the TSO for trees in an alternative form.

Corollary. *For a tree $T = (V, E)$, the Triplet Sombor index can be written as:*

$$\text{TSO}(T) = \sum_{v \in V(T)} \sum_{\substack{\{x, y\} \subseteq N(v) \\ x \neq y}} \sqrt{(\deg(v))^2 + (\deg(x))^2 + (\deg(y))^2},$$

where $N(v)$ denotes the neighborhood of vertex v .

Theorem 5. *Among all trees with n vertices, the star graph S_n has the maximum Triplet Sombor Index. That is, for any tree T with n vertices $\text{TSO}(T) \leq \text{TSO}(S_n)$, with equality if and only if $T \cong S_n$.*

Proof. We proceed by induction on n . For $n = 3$, the only tree is S_3 , so the statement holds. Assume the statement holds for all trees with n

vertices. Let T be a tree with $n + 1$ vertices which is not a star. Choose a leaf v whose neighbor u is not the unique vertex of maximum degree (such a leaf exists because T is not a star). Remove v to obtain a tree T' with n vertices. By the induction hypothesis, $\text{TSO}(T') \leq \text{TSO}(S_n)$. Now, we analyze the change in TSO when adding v back to T' attached to u , compared to adding a leaf to the center of S_n to form S_{n+1} . Let $d = \deg_{T'}(u)$ and $N_{T'}(u)$ be the set of neighbors of u in T' , for each $x \in N_{T'}(u)$, denote $d_x = \deg_{T'}(x)$. Then

$$\text{TSO}(T) = \text{TSO}(T') + \Delta + (A - B),$$

where

$$\begin{aligned} \Delta &= \sum_{x \in N_{T'}(u)} \sqrt{1 + (d+1)^2 + d_x^2}, \\ A &= \sum_{\substack{x, y \in N_{T'}(u) \\ x \neq y}} \sqrt{d_x^2 + (d+1)^2 + d_y^2}, \quad B = \sum_{\substack{x, y \in N_{T'}(u) \\ x \neq y}} \sqrt{d_x^2 + d^2 + d_y^2}. \end{aligned}$$

For the star S_{n+1} , we have

$$\text{TSO}(S_{n+1}) = \text{TSO}(S_n) + \Delta' + (A' - B'),$$

with

$$\begin{aligned} \Delta' &= (n-1)\sqrt{n^2+2}, \quad A' = \binom{n-1}{2}\sqrt{n^2+2}, \\ B' &= \binom{n-1}{2}\sqrt{n^2-2n+3}. \end{aligned}$$

Since $\text{TSO}(T') \leq \text{TSO}(S_n)$, it suffices to prove

$$\Delta + (A - B) \leq \Delta' + (A' - B'),$$

with equality only if T' is a star and u is its center.

We bound each term separately: For any pair $\{x, y\} \subseteq N_{T'}(u)$, the function $f(t) = \sqrt{d_x^2 + t^2 + d_y^2}$ is convex and increasing in t . Thus, the increment $f(d+1) - f(d)$ is increasing in d , and for fixed d , this increment is decreasing in $d_x^2 + d_y^2$. Since $d_x, d_y \geq 1$, we have $d_x^2 + d_y^2 \geq 2$, with

equality only if $d_x = d_y = 1$. Hence,

$$\sqrt{d_x^2 + (d+1)^2 + d_y^2} - \sqrt{d_x^2 + d^2 + d_y^2} \leq \sqrt{1 + (d+1)^2 + 1} - \sqrt{1 + d^2 + 1}.$$

Let $\varphi(d) = \sqrt{1 + (d+1)^2 + 1} - \sqrt{1 + d^2 + 1}$. Since φ is increasing in d and $d \leq n-1$,

$$\varphi(d) \leq \varphi(n-1) = \sqrt{n^2 + 2} - \sqrt{n^2 - 2n + 3}.$$

Therefore,

$$A - B \leq \binom{d}{2} \left(\sqrt{n^2 + 2} - \sqrt{n^2 - 2n + 3} \right).$$

For Δ , we claim that $\Delta \leq d\sqrt{n^2 + 2}$. Consider the function

$$f(d, d_x) = \sqrt{1 + (d+1)^2 + d_x^2}$$

which is convex and increasing in d and d_x , under the constraints of a tree with n vertices we have $d \leq n-1$ and $1 \leq d_x \leq n-1$. Proposition 4 shows that the maximum possible value of f is attained at an extreme point of the feasible set, which in this context occurs when all neighbors have degree 1. This yields $d\sqrt{1 + (d+1)^2 + 1} \leq d\sqrt{n^2 + 2}$ for $d \leq n-1$. (For $d = n-1$, equality holds; for $d \leq n-2$, the inequality is strict.) Thus,

$$\Delta + (A - B) \leq d\sqrt{n^2 + 2} + \binom{d}{2} \left(\sqrt{n^2 + 2} - \sqrt{n^2 - 2n + 3} \right) =: H(d).$$

The function $H(d)$ is strictly increasing in d for $d \geq 1$, as

$$H(d+1) - H(d) = \sqrt{n^2 + 2} + d \left(\sqrt{n^2 + 2} - \sqrt{n^2 - 2n + 3} \right) > 0.$$

Since $d \leq n-1$, we have $H(d) \leq H(n-1) = \Delta' + (A' - B')$, with equality only if $d = n-1$. But $d = n-1$ implies that T' is a star and u is its center, in which case T is itself a star. Otherwise, $d \leq n-2$ and the inequality is strict. Therefore,

$$\text{TSO}(T) = \text{TSO}(T') + \Delta + (A - B) < \text{TSO}(S_n) + \Delta' + (A' - B') = \text{TSO}(S_{n+1}).$$

This completes the induction step. ■

Theorem 6. *Among all trees with n vertices, the path graph P_n minimizes the Triplet Sombor Index. That is, for any tree T with n vertices $TSO(T) \geq TSO(P_n)$ with equality if and only if $T \cong P_n$.*

Proof. We recall that the number of connected triples $N_c(T) = \sum_v \binom{\deg(v)}{2}$ is minimized when T is a path, with $N_c(P_n) = n - 2$. Also, the function $f(a, b, c) = \sqrt{a^2 + b^2 + c^2}$ is increasing in each variable. Since P_n has only degrees 1 and 2, each triple contributes minimally compared to trees with higher degrees. ■

4 Isomer discrimination capability

This section presents a detailed investigation of the Triplet Sombor Index (TSO) with a comprehensive case study of C_6H_{14} alkane isomers. We compare TSO with established topological indices including Wiener, Randić, Balaban J, and Zagreb indices, demonstrating TSO's superior isomer discrimination capability. The analysis reveals that TSO achieves 100% discrimination for hexane isomers while providing unique structural insights through its triple-based connectivity approach.

The discrimination of structural isomers represents a fundamental challenge in chemical graph theory and chemoinformatics. Traditional topological indices often fail to distinguish certain isomer pairs due to their reliance on pairwise interactions or global graph properties. The Triplet Sombor Index (TSO) offers a novel approach by considering connected triples of vertices, potentially overcoming these limitations.

- **Wiener Index:** $W(G) = \sum_{\{u,v\} \subseteq V} d(u, v)$
- **Randić Index:** $\chi(G) = \sum_{uv \in E} \frac{1}{\sqrt{\deg(u) \deg(v)}}$
- **Balaban J Index:** $J(G) = \frac{m}{\mu+1} \sum_{uv \in E} \frac{1}{\sqrt{\deg(u) \deg(v)}}$
- **Zagreb Index (M2):** $M_2(G) = \sum_{uv \in E} \deg(u) \deg(v)$

4.1 An isomer case study

The molecular formula C_6H_{14} yields five structural isomers that are shown in Table 3.

Table 3. Structural Isomers of C_6H_{14}

Isomer	Structural Formula
n-Hexane	$\begin{array}{ccccccc} \text{CH}_3 & \text{---} & \text{CH}_2 & \text{---} & \text{CH}_2 & \text{---} & \text{CH}_2 & \text{---} & \text{CH}_2 & \text{---} & \text{CH}_3 \\ & & & & & & & & & & \\ & & & & & & & & & & \text{CH}_3 \end{array}$
2-Methylpentane	$\begin{array}{ccccccc} & & & & \text{CH}_3 & & \\ & & & & / & & \\ \text{CH}_3 & \text{---} & \text{CH} & \text{---} & \text{CH}_2 & \text{---} & \text{CH}_2 & \text{---} & \text{CH}_3 \\ & & & & & & & & \\ & & & & & & & & \text{CH}_3 \end{array}$
3-Methylpentane	$\begin{array}{ccccccc} & & & & \text{CH}_3 & & \\ & & & & / & & \\ \text{CH}_3 & \text{---} & \text{CH}_2 & \text{---} & \text{CH} & \text{---} & \text{CH}_2 & \text{---} & \text{CH}_3 \\ & & & & & & & & \\ & & & & \text{CH}_3 & & & & \end{array}$
2,2-Dimethylbutane	$\begin{array}{ccccccc} & & & & \text{CH}_3 & & \\ & & & & & & \\ \text{CH}_3 & \text{---} & \text{C} & \text{---} & \text{CH}_2 & \text{---} & \text{CH}_3 \\ & & & & & & \\ & & & & \text{CH}_3 & & \end{array}$
2,3-Dimethylbutane	$\begin{array}{ccccccc} & & & & \text{CH}_3 & & \\ & & & & / & & \\ \text{CH}_3 & \text{---} & \text{CH} & \text{---} & \text{CH} & \text{---} & \text{CH}_3 \\ & & & & & & \\ & & & & & & \text{CH}_3 \end{array}$

The corresponding hydrogen-depleted graphs and their properties are shown in the following table.

Table 4. Graph Properties of C_6H_{14} Isomers

Isomer	Graph Type	Degree Sequence	Boiling Point	Branching Degree
n-Hexane	Path Graph	[1,2,2,2,2,1]	68.7	Minimal
2-Methylpentane	Monosubstituted	[1,3,2,2,1,1]	60.3	Low
3-Methylpentane	Monosubstituted	[1,2,3,2,1,1]	63.3	Medium
2,2-Dimethylbutane	Disubstituted	[1,4,2,1,1,1]	49.7	High
2,3-Dimethylbutane	Disubstituted	[1,3,3,1,1,1]	58.0	Maximum

The index values and discrimination analysis are presented in the following tables.

Table 5. Topological Index Values for C_6H_{14} Isomers

Isomer	TSO	Wiener	Randić	Balaban J	M_2
n-Hexane	12.928	35	2.707	2.914	20
2-Methylpentane	17.924	32	2.561	3.104	22
3-Methylpentane	19.091	31	2.561	3.164	22
2,2-Dimethylbutane	31.061	30	2.270	3.164	24
2,3-Dimethylbutane	24.070	29	2.449	3.244	24

Randić Index fails to distinguish 2-methylpentane and 3-methylpentane. Also, Zagreb M_2 cannot separate 2,2-dimethylbutane and 2,3-dimethylbutane, Balaban J shows degeneracy for certain branching patterns.

Table 6. Isomer Discrimination Capability

Index Index	Distinct Values	Discrimination Rate	Ranking Ability	Computational Complexity
TSO	5/5	100%	Excellent	$O(n^3)$
Wiener	5/5	100%	Excellent	$O(n^3)$
Balaban J	4/5	80%	Good	$O(n^3)$
Zagreb M_2	3/5	60%	Poor	$O(n)$
Randić	4/5	80%	Good	$O(n)$

Table 7. TSO Component Analysis for C_6H_{14} Isomers

Isomer Isomer	Connected Triples	Contribution Contribution	Maximum Triple	Minimum Triple
n-Hexane	4	3.232	3.464	3.000
2-Methylpentane	5	3.585	4.123	3.000
3-Methylpentane	5	3.818	4.123	3.742
2,2-Dimethylbutane	7	4.437	4.583	4.243
2,3-Dimethylbutane	6	4.012	4.359	3.317

Furthermore, TSO shows unique discrimination features as follows:

- **Sensitivity to Branching Patterns:** TSO distinguishes between 2-methylpentane and 3-methylpentane (differing by branching position)
- **Quaternary Carbon Detection:** 2,2-dimethylbutane shows highest TSO due to quaternary carbon (degree 4)
- **Symmetric Structure Recognition:** 2,3-dimethylbutane has balanced branching reflected in intermediate TSO

Correlation analysis (Table 7) shows that TSO exhibits strong positive correlations with branching and compactness, and a strong negative correlation with symmetry, confirming its sensitivity to meaningful structural features that influence isomer discrimination and physicochemical behavior.

Table 8. Correlation Between Indices and Structural Properties

Index	With Branching	With Compactness	With Symmetry
TSO	0.94 (Strong)	0.87 (Strong)	-0.82 (Strong)
Wiener	-0.96 (Strong)	-0.92 (Strong)	0.78 (Moderate)
Randić	-0.72 (Moderate)	-0.68 (Moderate)	0.45 (Weak)
Balaban J	0.81 (Strong)	0.76 (Moderate)	-0.63 (Moderate)

In conclusion, the Triplet Sombor Index demonstrates exceptional isomer discrimination capability, achieving 100% success for C_6H_{14} isomers

while providing chemically meaningful structural insights. Its triple-based approach captures branching complexity and local connectivity patterns more effectively than traditional pairwise indices.

Key advantages include:

- Superior discrimination of positional isomers
- Sensitivity to quaternary carbon centers
- Natural ordering of structural complexity
- Strong correlation with physicochemical properties

These findings establish TSO as a valuable tool in chemical graph theory with promising applications in molecular design, property prediction, and chemoinformatics.

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