MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **95** (2026) 63–94
ISSN: 0340–6253
doi: 10.46793/match.95-1.03425

Geometric Approach to Degree-Based Topological Index: Hyperbolic Sombor Index

Jayjit Barman, Shibsankar Das*

Department of Mathematics, Institute of Science,
Banaras Hindu University, Varanasi-221005, Uttar Pradesh, India.
jayjit44@bhu.ac.in, shib.cgt@gmail.com, shibsankar@bhu.ac.in

(Received February 28, 2025)

Abstract

This article presents a new geometric approach to forming molecular structure descriptors (topological indices) based on vertex degrees. The degrees of a pair of adjacent vertices are represented by the length of the semi-major and semi-minor axes of the hyperbola that form the basis of the model. In this way, a number of previously known topological indices can now be interpreted geometrically and some new topological indices can be generated. The eccentricity of the hyperbola gives rise to a remarkably simple vertex-degree-based topological index, which we refer to as the hyperbolic Sombor index (HSO). We concentrate on some of the most important properties of this index, such as prediction power, structure sensitivity and degeneracy. We apply statistical approaches and computing methods to the octane, nonane and decane isomer data sets to compare these properties with other well-known degree-based topological indices.

1 Introduction

Graph theory is a subfield of mathematics that examines graphs, which are abstract structures that represent the relationships between objects.

*Corresponding author.

Let $G(V, E)$ be an undirected, simple and connected graph, where $V(G)$ and $E(G)$ are the collection of vertices and edges, respectively. An edge $e = uv$ in a graph is a basic element that connects two vertices u and v and represents a relationship between them.

A subfield of mathematical chemistry known as *chemical graph theory* focuses on employing graph theory to solve severe molecular difficulties. Chemical graph theory is concerned with a molecular graph in which atoms are represented as vertices and bonds between them as edges. A *topological index* of a graph is a numerical value that represents the structure of graphs and some of their topological characteristics, such as the arrangement of vertices and edges. It also contains information about the physicochemical and biological properties of molecules in $QSPR/QSAR$ analysis.

A degree-based topological index for a graph G is denoted as $TI(G)$ and stated as

$$TI(G) = \sum_{uv \in E(G)} f(d(u), d(v)), \tag{1}$$

where $f(x, y)$ is a non-negative real-valued function of x and y with the symmetric property that $f(x, y) = f(y, x)$.

We now provide formulations for several useful degree-based topological indices that have distinct theoretical forms of the function $f(x, y)$ given in Equation 1. One of the first vertex degree-based topological indices is the Zagreb index, which was first presented by I. Gutman and N. Trinajstić in 1972 [6]. The following formula defines the first Zagreb index:

$$M_1(G) = \sum_{uv \in E(G)} (d(u) + d(v)).$$

The mathematical interpretation of the modified second Zagreb index was proposed by Miličević et al. in 2004 [20], and it is represented as

$${}^{m}M_2(G) = \sum_{uv \in E(G)} \frac{1}{d(u)d(v)}.$$

The forgotten index was proposed by B. Furtula and I. Gutman in

2015 [10], which they defined as

$$F(G) = \sum_{uv \in E(G)} (d^2(u) + d^2(v)).$$

Milan Randić developed the branch connectivity metric in 1975 to measure the degree of branching in saturated hydrocarbon's carbon-atom structure. It was known as the Randić index or branching/connectivity index and presented as

$$R_{-1/2}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}.$$

Note that, it is a specific example of the well-known general Randić index [4,19] (whose mathematical formula is given by $\sum_{uv \in E(G)} (d(u)d(v))^{\alpha}$, where $\alpha \in \mathbb{R}$), with $\alpha = 1/2$. In 2009, B. Zhou and N. Trinajstić introduced the sum connectivity index (SCI), which was inspired by the development and usefulness of Randić index in a number of scientific and technological fields [32]. It is represented as

$$SCI(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u) + d(v)}}.$$

The symmetric division (deg) index (SDD) is one of the most significant bond-additive descriptors among 148 discrete adriatic indices [30]. It was started in 2010 by D. Vukičević and is described as

$$SDD(G) = \sum_{uv \in E(G)} \left(\frac{d(u)}{d(v)} + \frac{d(v)}{d(u)} \right).$$

In the article [30], the authors show that the SDD index is the most accurate predictor of the total surface area of polychlorobiphenyls. It has demonstrated a dominant nature in the $QSPR$ study compared to a number of other degree-based topological indices [9].

In 1993, Favron et al. presented the harmonic index in [8] and is de-

scribed as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}.$$

The article [8] illustrates several relationships between a graph's eigenvalues and harmonic index. The harmonic index is generalized in articles [5, 26], which also present certain related mathematical findings.

The novel topological descriptor known as the atom-bond connectivity index (ABC) was introduced by Estrada et al. in 1998 [7] and was based on the connection between atoms and bonds in a molecule. It is mathematically described as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d(u) + d(v) - 2}{d(u)d(v)}}.$$

There is a significant correlation between the enthalpy of alkane forms and the ABC index [7].

The geometric-arithmetic (GA) index based on the geometric and arithmetic means of edges' end vertex degrees has been proposed by D. Vukičević and B. Furtula in 2009 [29]. It is represented as

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}.$$

The usefulness of the GA index is evaluated in the article [29] by conducting a $QSPR$ analysis of the index with the physicochemical properties of octane isomers.

Shegehalli and Kanabur [27] introduced the arithmetic-geometric (AG) index by swapping the numerator and denominator of the GA index. It is described as

$$AG(G) = \sum_{uv \in E(G)} \frac{d(u) + d(v)}{2\sqrt{d(u)d(v)}}.$$

Sombor index (SO) was the most studied degree-based topological in-

dex proposed by Ivan Gutman [12] in 2021 and defined as

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

The distance of $(d(u), d(v))$ from the origin $(0, 0)$ in the two-dimensional plane forms a function, where u and v are two different vertices of the graph G and they correspond to an edge uv or vu. This function is used to create the Sombor index. The predictive and discriminative capabilities and mathematical relationships of the Sombor index are examined in the articles [25, 31].

In 2021, V.R. Kulli presented the modified Sombor index [17]. It is denoted as ${}^{m}SO$ and represented as

$${}^{m}SO(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d^2(u) + d^2(v)}}.$$

Inspired by effectiveness and progress of the GA index, in 2022, V.R. Kulli introduced two additional indices, the geometric-quadratic (GQ) and quadratic-geometric (QG) indices [16] derived from the geometric and quadratic means of the degrees of an edge's end vertices. Their representation is as follows:

$$GQ(G) = \sum_{uv \in E(G)} \frac{\sqrt{2d(u)d(v)}}{\sqrt{d^2(u) + d^2(v)}}$$

and

$$QG(G) = \sum_{uv \in E(G)} \frac{\sqrt{d^2(u) + d^2(v)}}{\sqrt{2d(u)d(v)}}.$$

The Nirmala index [15] was first presented by V.R. Kulli and described as

$$N(G) = \sum_{uv \in E(G)} \sqrt{d(u) + d(v)}.$$

Recently, Gutman et al. [13] proposed a novel topological descriptor based on the formulation of an ellipse. They termed it the elliptic Sombor

index and denoted it as

$$ESO(G) = \sum_{uv \in E(G)} (d(u) + d(v)) \sqrt{d^2(u) + d^2(v)}.$$

2 The hyperbolic representation of a vertex-degree pair

The standard form of an equation of a hyperbola centered at the origin O with vertices $V(a, 0)$, $V'(-a, 0)$ and co-vertices $P(0, b)$, $P'(0, -b)$ is given by

$$\frac{x^2}{a^2} - \frac{y^2}{b^2} = 1.$$

In Figure 1, we consider the hyperbola centered at the origin O to have

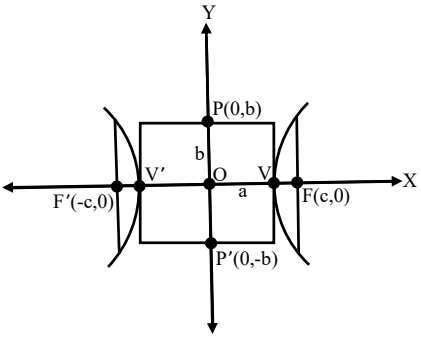

Figure 1. A hyperbola centered at the origin O with focus points F and F'.

two focus points, $F(c, 0)$ and $F'(-c, 0)$. The length of the semi-major axis OV and the semi-minor axis OP are indicated by a and b, respectively. Then we know that

$$c = \sqrt{a^2 + b^2}. \tag{2}$$

- **Eccentricity:** The eccentricity of a hyperbola is calculated by the formula

$$e = \frac{c}{a} \tag{3}$$

where c is the length of the focus point F of the hyperbola. From

Equations (2) and (3), we get the value of eccentricity of a hyperbola in terms of a and b as $e = \frac{\sqrt{a^2+b^2}}{a}$.

Motivated by the definition of eccentricity of a hyperbola, we induce a novel vertex-degree-based topological index of a graph G as

$$HSO(G) = \sum_{uv \in E(G)} \frac{\sqrt{d^2(u) + d^2(v)}}{d(u)} \tag{4}$$

where $0 < d(u) \leq d(v)$, which we named the hyperbolic Sombor index (HSO). An alternative version of the above definition can also be written as

$$HSO(G) = \sum_{uv \in E(G)} \frac{\sqrt{d^2(u) + d^2(v)}}{\min\{d(u), d(v)\}}. \tag{5}$$

Throughout this paper, we use the notion of Equation 4 of the HSO index for notational uniformity.

3 Mathematical properties of hyperbolic Sombor index

The complete graph, path graph, cycle graph and star graph with n vertices will be denoted by K_n, P_n, C_n and S_n, respectively.

We now provide a lower bound for the hyperbolic Sombor index using the size of a graph.

Theorem 1. *Let G be a simple and connected graph of size m. Then*

$$HSO(G) \geq \sqrt{2}m.$$

Moreover, the equality holds if and only if G is a complete graph.

Proof. We know that, $(x-y)^2 \geq 0$ we have

$$\begin{aligned} x^2 + y^2 \geq 2xy &\implies \sqrt{x^2+y^2} \geq \sqrt{2xy} \\ &\implies \frac{\sqrt{x^2+y^2}}{x} \geq \sqrt{\frac{2y}{x}} \end{aligned} \tag{6}$$

which holds for all positive x and y and the equality in Equation (6) is valid only if $x = y$.

Using Equation (6) and the definition of *HSO* index, we get

$$HSO(G) = \sum_{uv \in E(G)} \frac{\sqrt{d^2(u) + d^2(v)}}{d(u)} \geq \sum_{uv \in E(G)} \sqrt{\frac{2d(v)}{d(u)}} \geq \sum_{uv \in E(G)} \sqrt{2} = \sqrt{2}m.$$

Therefore, $HSO(G) \geq \sqrt{2}m$. ■

Below we present a bound for the hyperbolic Sombor index using the Sombor index and the maximum and minimum degree of a graph.

Theorem 2. *Let G be a simple connected graph. Then*

$$\frac{1}{\Delta} \cdot SO(G) \leq HSO(G) \leq \frac{1}{\delta} \cdot SO(G),$$

with equality holds on both sides if and only if G is a complete graph.

Proof. Here $\Delta = \max\{d(u) : u \in V(G)\}$ and $\delta = \min\{d(u) : u \in V(G)\}$. Also, we know that

$$\delta \leq d(u) \leq \Delta$$
$$\implies \frac{1}{\Delta} \leq \frac{1}{d(u)} \leq \frac{1}{\delta}.$$

Now

$$HSO(G) = \sum_{uv \in E(G)} \frac{\sqrt{d^2(u) + d^2(v)}}{d(u)} \leq \frac{1}{\delta} \cdot \sum_{uv \in E(G)} \sqrt{d^2(u) + d^2(v)} = \frac{1}{\delta} \cdot SO(G).$$

Similarly, $HSO(G) \geq \frac{1}{\Delta} \cdot SO(G)$.

Therefore,

$$\frac{1}{\Delta} \cdot SO(G) \leq HSO(G) \leq \frac{1}{\delta} \cdot SO(G).$$ ■

In the following theorem, we establish a bound for the hyperbolic Sombor index by utilizing the first Zagreb index along with the maximum and minimum degree of a graph.

Theorem 3. *Let G be a simple connected graph. Then*

$$\frac{1}{\sqrt{2}\Delta} \cdot M_1(G) \leq HSO(G) < \frac{1}{\delta} \cdot M_1(G),$$

with equality holds if and only if G is a complete graph.

Proof. Given elementary inequalities is

$$\frac{1}{\sqrt{2}}(x+y) \leq \sqrt{x^2+y^2} < (x+y)$$

holds for all positive value of x and y. Also, we know that

$$\frac{1}{\Delta} \leq \frac{1}{d(u)} \leq \frac{1}{\delta}. \tag{7}$$

By taking $x = d(u)$ and $y = d(v)$, we get

$$\frac{1}{\sqrt{2}}(d(u)+d(v)) \leq \sqrt{d^2(u)+d^2(v)} < (d(u)+d(v)). \tag{8}$$

Using Equations (7) and (8) and the definition of *HSO* index, we conclude that

$$\begin{aligned}\frac{1}{\sqrt{2}\Delta} \sum_{uv \in E(G)} (d(u)+d(v)) &\leq \sum_{uv \in E(G)} \frac{\sqrt{d^2(u)+d^2(v)}}{d(u)} \\ &< \sum_{uv \in E(G)} \frac{(d(u)+d(v))}{\delta} \\ \implies \frac{1}{\sqrt{2}\Delta} \cdot M_1(G) \leq HSO(G) &< \frac{1}{\delta} \cdot M_1(G).\end{aligned}$$

Therefore,

$$\frac{1}{\sqrt{2}\Delta} \cdot M_1(G) \leq HSO(G) < \frac{1}{\delta} \cdot M_1(G). \qquad \blacksquare$$

Lemma 1. *Let P_n, C_n and S_n denote the path graph, cycle graph and star graph, respectively. Then for $n \geq 2$,*

$$HSO(P_n) = 2\sqrt{5} + \sqrt{2}(n-3),\ HSO(C_n) = \sqrt{2}n \text{ and}$$
$$HSO(S_n) = (n-1)\sqrt{(n-1)^2+1}.$$

Proof. We know that $|V(P_n)| = n$ and $|E(P_n)| = (n-1)$. Based on the degree of end vertices, the edge set of P_n can be separated into two different sets:

$$E_{1,2} = \{uv \in E(P_n) | d(u) = 1, d(v) = 2\} \text{ and}$$
$$E_{2,2} = \{uv \in E(P_n) | d(u) = 2, d(v) = 2\}.$$

Therefore,

$$\begin{aligned} HSO(P_n) &= \sum_{uv \in E(G)} \frac{\sqrt{d^2(u) + d^2(v)}}{d(u)} \\ &= 2 \times \frac{\sqrt{1+4}}{1} + (n-3) \times \frac{\sqrt{4+4}}{2} \\ &= 2\sqrt{5} + \sqrt{2}(n-3). \end{aligned}$$

Now, $|V(C_n)| = n$ and $|E(C_n)| = n$. All of the vertices in C_n have degree 2. Thus,

$$\begin{aligned} HSO(C_n) &= \sum_{uv \in E(G)} \frac{\sqrt{d^2(u) + d^2(v)}}{d(u)} \\ &= n \times \frac{\sqrt{2^2+2^2}}{2} \\ &= \sqrt{2}n. \end{aligned}$$

Similarly, $|V(S_n)| = n$ and $|E(S_n)| = (n-1)$. There is only one type of edge uv based on the degree of end vertices, which satisfies $(d(u), d(v)) =$

$(1, n-1)$. Thus,

$$\begin{aligned} HSO(S_n) &= \sum_{uv \in E(G)} \frac{\sqrt{d^2(u) + d^2(v)}}{d(u)} \\ &= (n-1) \times \frac{\sqrt{1 + (n-1)^2}}{1} \\ &= (n-1)\sqrt{(n-1)^2 + 1}. \end{aligned}$$

■

Theorem 4. *Let G be a simple connected graph with $n(\geq 2)$ vertices. Let C_n and S_n be the cycle and star graph, respectively. Then,*

$$HSO(C_n) \leq HSO(G) \leq HSO(S_n).$$

The left and right inequalities hold if and only if $G \cong C_n$ and $G \cong S_n$, respectively.

Proof. It is obvious that the value of $HSO(G)$ increases when we add edges to the graph G. A tree obtains the highest value of $HSO(G)$ of a connected graph. S_2 and S_3 demonstrate that $HSO(S_n)$ is the greatest value for trees with n vertices. Now, by the principle of mathematical induction, we shall prove for $n \geq 4$.

Let $W_{a,b}$ represent the contribution of an edge to HSO when $d(u) = a$ and $d(v) = b$ implies $W_{a,b} = \frac{\sqrt{a^2+b^2}}{a}$. Now from Lemma 1, we get for $n = 4$, $HSO(S_4) = 3\sqrt{10}$ is the greatest of all $HSO(T)$ values, where T is a four-vertex tree.

Now, assume that $HSO(S_k) = (k-1)\sqrt{(k-1)^2 + 1}$ is the greatest of all $HSO(T)$ values, where T is a k-vertex tree. If a vertex adjacent to the central vertex of S_k is provided, a star graph with $k+1$ vertices and maximal $HSO(T)$ can be created. Therefore, the highest amount of new edge that can be added is $W_{1,k} = \sqrt{k^2 + 1}$. The contribution of neighboring edges will also increase. Therefore, T must be S_{k+1} with $HSO(S_{k+1}) = k\sqrt{k^2 + 1}$. Hence, the principle of mathematical induction is valid for all n.

We know that the only graph with all of its vertices of degree 2 is C_n. Therefore, the value of $HSO(C_n)$ is minimum. So, the lower bound is obtained. ■

Theorem 5. *Let T be a tree with $n \geq 2$ vertices and let P_n be the n-vertex path graph. Then*

$$HSO(P_n) \leq HSO(T) \leq HSO(S_n).$$

The left and right inequalities hold if and only if $T \cong P_n$ and $T \cong S_n$, respectively.

Proof. To determine the upper bound, we note that $d(u) + d(v) \leq n$ for each edge uv of an n-vertex tree. The star is a tree where all of its edges have the formula $d(u) + d(v) = n$.

Through simple computation, it can be confirmed that

$$W_{1,n-1} > W_{2,n-2} > \cdots > W_{\lfloor \frac{n}{2} \rfloor, \lceil \frac{n}{2} \rceil}.$$

Thus,

$$\begin{aligned} HSO(S_n) &= (n-1)W_{1,n-1} \\ &= (n-1)\frac{\sqrt{1+(n-1)^2}}{1} \\ &= (n-1)\sqrt{(n-1)^2+1} \end{aligned}$$

is the upper bound for $HSO(T)$.

It is obvious that the value of $HSO(G)$ decreases when we remove edges from the graph G. A tree obtains the lowest value of $HSO(G)$ of a connected graph. P_2 and P_3 demonstrate that $HSO(P_n)$ is the lowest value for trees with n vertices. Now, by the principle of mathematical induction, we shall prove for $n \geq 4$.

Let $W_{a,b}$ represent the contribution of an edge to HSO when $d(u) = a$ and $d(v) = b$ implies $W_{a,b} = \frac{\sqrt{a^2+b^2}}{a}$. Now from Lemma 1, we get for $n = 4$, $HSO(P_4) = (2\sqrt{5} + \sqrt{2})$ is the lowest of all $HSO(T)$ values, where T is a four-vertex tree.

Now, assume that $HSO(P_k) = 2\sqrt{5} + \sqrt{2}(k-3)$ is the lowest of all $HSO(T)$ values, where T is a k-vertex tree. Then, if a vertex at the end is given an edge of P_k or somewhere along the path in between, a tree with $k+1$ vertices and minimal $HSO(T)$ may be created. Therefore, the

least amount of new edge that can be added is $W_{2,2} = \sqrt{2}$. Otherwise, if a vertex at the end is given an edge of the path graph or somewhere along the path in between, then the added edge will contribute $W_{1,3} = \sqrt{10}$. Likewise, the contribution of adjacent edges will rise. Therefore, T must be P_{k+1} with $HSO(P_{k+1}) = 2\sqrt{5} + \sqrt{2}(k-2)$. Hence, the principle of mathematical induction is valid for all n. ■

4 Hyperbolic Sombor index: applications

The idea of a topological index was first presented in mathematical chemistry. In the early 20^{th} century, scientists looked for techniques to mathematically describe molecular structures in order to gain a better understanding of their properties, such as stability, reactivity and boiling points. The process of determining the quality of topological indices began many years ago, but accurate processes were only recently developed [9]. A list of ideal specifications for molecular descriptors was included in the articles [9, 18, 24]. These resulted in the thirteen properties listed below:

1. It should be possible to interpret molecular descriptors structurally.
2. At least one characteristic should be positively correlated with molecular descriptors.
3. It is preferable for molecular descriptors to differentiate between isomers.
4. The local structure should be able to be described by molecular descriptors.
5. It should be feasible to generalize molecular descriptors to higher descriptors.
6. It is ideal for molecular descriptors to be independent.
7. Molecular descriptors ought to be simple.
8. It is not appropriate to base molecular descriptors on characteristics.

9. The relationship between molecular descriptors and other descriptors ought not be trivial.

10. It should be feasible to create molecular descriptors effectively.

11. Well-known structural ideas should be used in molecular descriptors.

12. The size dependency of molecular descriptors should be accurate.

13. When structures make gradual changes, then molecular descriptors should also change gradually.

Most topological indices adhere to properties 1, 4, 5, 7, 8, 10, 11 and 12, while the remaining properties must be calibrated before introducing a new topological index. The primary challenge and justification in the past was the absence of techniques for quantifying certain of the specified features. Although this issue has mostly been resolved in recent years, molecular descriptor quality assessment is still commonly disregarded. In this article, we will focus on characteristics 2, 3, 6, 9 and 13 of the renowned degree-based topological indices, which are similar to our proposed *HSO* index.

An analogous procedure will be employed here to evaluate the possible application of the hyperbolic Sombor index (HSO). The primary and most significant characteristic of a topological index is the capacity to forecast a minimum of one physicochemical property or biological activity of a group of molecules. Correlating a topological index with the physicochemical characteristics of isomeric alkanes is the most practical approach to verifying this. In order to explore the application domain of the hyperbolic Sombor index, we have chosen the boiling point (BP), enthalpy of formation ($HFORM$), entropy (S), enthalpy of vaporization ($HVAP$), acentric factor (AF) and standard enthalpy of vaporization ($DHVAP$) of octane isomers. We compare the outcomes of the above analysis with those derived from the elliptic Sombor index (ESO), the first Zagreb index (M_1), the modified second Zagreb index (${}^mM_2$), the forgotten index (F) and the atom-bond connectivity index (ABC). We selected these indices since they are closely linked to the hyperbolic Sombor index.

4.1 Correlation analysis based on *QSPR* model

In addition to the indices mentioned earlier, we used the Randić index ($R_{-1/2}$), the sum-connectivity index (SCI), the symmetric division (deg) index (SDD), the harmonic index (H), the geometric-arithmetic index (GA), the arithmetic-geometric index (AG), the Sombor index (SO), the modified Sombor index (${}^mSO$), the geometric-quadratic index (GQ), the quadratic-geometric index (QG) and the Nirmala index (N). The values of the six physicochemical properties of octane isomers are listed in Table 1, which are taken from the following papers [9, 22] and the website cited in reference [28].

As stated in article [18], we use Algorithm 1 for calculating all of the degree-based topological indices of octane isomers and listed their values in Table 2. We conduct a cross-correlation analysis among the considered degree-based topological indices. A substantial degree of correlation was found among the indices: elliptic Sombor index (ESO), first Zagreb index (M_1), modified second Zagreb index (${}^mM_2$), forgotten index (F), atom-bond connectivity index (ABC), including hyperbolic Sombor index (HSO) when we applied these indices to a collection of octane isomers and conducted a correlation analysis. These findings are displayed in Table 3. One can see that there is a strong correlation coefficient value between HSO and M_1.

We use the linear regression model

$$P = c \cdot TI + d$$

to examine the relationship between the topological indices and the physicochemical characteristics, where TI stands for the topological index, P for the physicochemical property, and constants c and d for the fitting coefficients. In a linear regression model, the following statistical metrics are present:

$$R^2 = 1 - \frac{\sum_{i=1}^{N}(P_i - \widehat{P}_i)^2}{\sum_{i=1}^{N}(P_i - \overline{P})^2},\ \text{Adjusted-}R^2 = 1 - \frac{(1-R^2)(N-1)}{N-p-1},$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}(P_i - \widehat{P}_i)^2}{N}} \text{ and } SSE = \sum_{i=1}^{N}(P_i - \widehat{P}_i)^2,$$

Table 1. Physicochemical properties of octane isomers.

Properties → / **Octane isomers ↓**	***BP***	***HFORM***	***S***	***HVAP***	***AF***	***DHVAP***
n-octane	125.6650	−49.8200	111.6700	73.1900	0.3979	9.9150
2-methylheptane	117.6470	−51.5000	109.8400	70.3000	0.3779	9.4840
3-methylheptane	118.9250	−50.8200	111.2600	71.3000	0.3710	9.5210
4-methylheptane	117.7090	−50.6900	109.3200	70.9100	0.3715	9.4830
3-ethylhexane	118.5340	−50.4000	109.4300	71.7000	0.3625	9.4760
2,2-dimethylhexane	106.8400	−53.7100	103.4200	67.7000	0.3394	8.9150
2,3-dimethylhexane	115.6070	−51.1300	108.0200	70.2000	0.3482	9.2720
2,4-dimethylhexane	109.4290	−52.4400	106.9800	68.5000	0.3442	9.0290
2,5-dimethylhexane	109.1030	−53.2100	105.7200	68.6000	0.3568	9.0510
3,3-dimethylhexane	111.9690	−52.6100	104.7400	68.5000	0.3226	8.9730
3,4-dimethylhexane	117.7250	−50.9100	106.5900	70.2000	0.3403	9.3160
3-ethyl-2-methylpentane	115.4500	−50.4800	106.0600	69.7000	0.3324	9.2090
3-ethyl-3-methylpentane	118.2590	−51.3800	101.4800	69.3000	0.3069	9.0810
2,2,3-trimethylpentane	109.8410	−52.6100	101.3100	67.3000	0.3008	8.8260
2,2,4-trimethylpentane	99.2380	−53.5700	104.0900	64.8700	0.3054	8.4020
2,3,3-trimethylpentane	114.7600	−51.7300	102.0600	68.1000	0.2932	8.8970
2,3,4-trimethylpentane	113.4670	−51.9700	102.3900	68.3700	0.3174	9.0140
2,2,3,3-tetramethylbutane	106.4700	−53.9900	93.0600	66.2000	0.2553	8.4100

where P_i, $\widehat{P}_i$ and $\overline{P}$ stand for the physicochemical property's experimental value, predicted value and mean, respectively. Additionally, p is the

Table 2. Calculated values of the various degree-based topological indices of octane isomers.

Topological indices → / Octane isomers ↓	HSO	ESO	M_1	$^mM_2$	F	$R_{-1/2}$	SCI	SDD	H	ABC	GA	AG	SO	^mSO	GQ	QG	N
n-octane	10.4252	69.9850	26.0000	2.2500	50.0000	3.9142	3.6547	15.0000	3.8333	4.9497	6.8856	7.1213	18.6143	2.6622	6.7889	7.2361	13.4641
2-methylheptane	10.7789	83.9753	28.0000	2.0833	62.0000	3.7701	3.5246	17.3333	3.5667	5.1685	6.6547	7.3907	20.6515	2.4177	6.4044	7.7409	13.9681
3-methylheptane	10.2412	84.7484	28.0000	2.1667	62.0000	3.8081	3.5491	16.6667	3.6333	5.0591	6.7112	7.3173	20.5024	2.4725	6.4850	7.6087	13.9362
4-methylheptane	10.2412	84.7484	28.0000	2.1667	62.0000	3.8081	3.5491	16.6667	3.6333	5.0591	6.7112	7.3173	20.5024	2.4725	6.4850	7.6087	13.9362
3-ethylhexane	10.0928	85.5216	28.0000	2.2500	62.0000	3.8461	3.5737	16.0000	3.7000	4.9497	6.7678	7.2438	20.3533	2.5272	6.5656	7.4766	13.9044
2,2-dimethylhexane	14.3415	118.0150	32.0000	1.8750	92.0000	3.5607	3.3272	21.7500	3.2000	5.4265	6.2856	7.8713	24.7344	2.1055	5.8468	8.6093	14.8897
2,3-dimethylhexane	12.1377	99.4528	30.0000	2.0278	74.0000	3.6807	3.4328	18.6667	3.4000	5.2375	6.5207	7.5454	22.3995	2.2625	6.1790	8.0319	14.4176
2,4-dimethylhexane	10.2057	98.7388	30.0000	2.0000	74.0000	3.6639	3.4190	19.0000	3.3667	5.2779	6.4803	7.5866	22.5396	2.2279	6.1005	8.1135	14.4403
2,5-dimethylhexane	12.8516	97.9657	30.0000	1.9167	74.0000	3.6259	3.3944	19.6667	3.3000	5.3873	6.4237	7.6600	22.6886	2.1732	6.0199	8.2456	14.4721
3,3-dimethylhexane	13.2763	119.6268	32.0000	2.0000	92.0000	3.6213	3.3656	20.5000	3.3000	5.2676	6.3712	7.7426	24.4910	2.1803	5.9497	8.3876	14.8352
3,4-dimethylhexane	11.9893	100.2260	30.0000	2.1111	74.0000	3.7187	3.4574	18.0000	3.4667	5.1281	6.5773	7.4720	22.2504	2.3173	6.2596	7.8997	14.3857
3-ethyl-2-methylpentane	11.9893	100.2260	30.0000	2.1111	74.0000	3.7187	3.4574	18.0000	3.4667	5.1281	6.5773	7.4720	22.2504	2.3173	6.2596	7.8997	14.3857
3-ethyl-3-methylpentane	12.2111	121.2386	32.0000	2.1250	92.0000	3.6820	3.4040	19.2500	3.4000	5.1087	6.4569	7.6140	24.2477	2.2550	6.0526	8.1659	14.7807
2,2,3-trimethylpentane	16.0091	134.2317	34.0000	1.8333	104.0000	3.4814	3.2442	22.8333	3.0524	5.4743	6.1784	7.9963	26.3732	1.9684	5.6676	8.8437	15.3221
2,2,4-trimethylpentane	16.4142	132.0054	34.0000	1.7083	104.0000	3.4165	3.1971	24.0833	2.9333	5.6453	6.0547	8.1407	26.7716	1.8610	5.4624	9.1141	15.3938
2,3,3-trimethylpentane	15.0924	135.0703	34.0000	1.8750	104.0000	3.5040	3.2580	22.2500	3.0857	5.4248	6.2074	7.9411	26.2790	1.9883	5.6898	8.7542	15.2994
2,3,4-trimethylpentane	14.4234	114.1572	32.0000	1.8889	86.0000	3.5534	3.3165	20.6667	3.1667	5.4158	6.3301	7.7735	24.2967	2.0525	5.8730	8.4550	14.8990
2,2,3,3-tetramethylbutane	16.8759	168.9480	38.0000	1.5625	134.0000	3.2500	3.0368	27.5000	2.6500	5.8085	5.8000	8.5000	30.3955	1.6320	5.1160	9.7464	16.2448

Table 3. Cross-correlation matrix of the hyperbolic Sombor, the elliptic Sombor, the first Zagreb, the modified second Zagreb, the forgotten and the atom-bond connectivity indices.

	HSO	ESO	M_1	${}^{m}M_2$	F	ABC
HSO	1.0000					
ESO	0.9083	1.0000				
M_1	0.9204	0.9970	1.0000			
${}^{m}M_2$	−0.9143	−0.8799	−0.9051	1.0000		
F	0.9146	0.9991	0.9964	−0.8925	1.0000	
ABC	0.9097	0.8711	0.8978	−0.9997	0.8839	1.0000

number of predictors utilized in the regression model and N is the sample size. When the value of R^2 and adjusted-R^2 approaches 1, and the value of $RMSE$ (root mean squared error) and SSE (sum of squared error) approaches 0, then the regression model is considered good. See the articles [2, 18] for further information.

Recently, $QSPR$ research among some physicochemical characteristics and several degree-based topological indices was examined to the data set of octane isomers. For example, article [9] presents a $QSPR$ study for physicochemical characteristics (BP, AF, S, $HFORM$ and $HVAP$) with some significant degree-based topological indices M_1, M_2, SDD, GA, ABC and ISI; article [25] shows the Sombor index's chemical application with the attributes S and $HVAP$; article [21] shows how to estimate features like S, AF, $HVAP$ and $DHVAP$ using linear regression models for the first hyper-Zagreb index; article [3] provides the linear regression models of the GA index are shown with all of our physicochemical features taken into consideration.

We perform statistical analysis between the datasets in Table 1 and the values of our considered topological indices for correlation analysis in Table 2. We extended the number of degree-based topological indices and calculated correlation coefficients between them in the context of octanes to investigate the relationship between the hyperbolic Sombor index and other indices more deeply. The physicochemical features of octane isomers with the hyperbolic Sombor index are represented graphically by linear regression models in Figures 2–4. Next, the outcomes of the comparative analysis of the considered degree-based topological indices from the linear

regression models are displayed in Tables 4–9.

Table 4. Linear regression models with statistical measures for boiling point.

Linear Models	R	R^2	$Adjusted - R^2$	$RMSE$	SSE
$BP = -1.95 \times HSO + 138.6$	-0.7311	0.5345	0.5054	4.302	296.1
$BP = -0.1713 \times ESO + 132.3$	-0.6844	0.4684	0.4352	4.597	338.2
$BP = -1.505 \times M_1 + 160.2$	-0.7203	0.5188	0.4887	4.374	306.1
$BP = 28.27 \times {}^{m}M_2 + 57.23$	0.8562	0.7330	0.7163	3.258	169.8
$BP = -0.2064 \times F + 130.6$	-0.7048	0.4967	0.4652	4.473	320.2
$BP = -22.6 \times ABC + 232.9$	-0.8631	0.7450	0.7291	3.184	162.2

Table 5. Linear regression models with statistical measures for enthalpy of formation.

Linear Models	R	R^2	$Adjusted - R^2$	$RMSE$	SSE
$HFORM = -0.4109 \times HSO - 46.59$	-0.7529	0.5669	0.5398	0.849	11.530
$HFORM = -0.03789 \times ESO - 47.73$	-0.7398	0.5473	0.5191	0.8679	12.050
$HFORM = -0.3258 \times M_1 - 41.77$	-0.7623	0.5811	0.5550	0.8349	11.150
$HFORM = 6.017 \times {}^{m}M_2 - 63.85$	0.8905	0.7930	0.7801	0.5869	5.512
$HFORM = -0.04566 \times F - 48.09$	-0.7618	0.5806	0.5544	0.8354	11.170
$HFORM = -4.792 \times ABC - 26.56$	-0.8945	0.8001	0.7876	0.5767	5.322

Table 6. Linear regression models with statistical measures for entropy.

Linear Models	R	R^2	$Adjusted - R^2$	$RMSE$	SSE
$S = -1.665 \times HSO + 126.6$	-0.8452	0.7144	0.6965	2.489	99.10
$S = -0.1771 \times ESO + 124.6$	-0.9576	0.9170	0.9118	1.341	28.79
$S = -1.472 \times M_1 + 150.9$	-0.9543	0.9107	0.9051	1.392	30.99
$S = 20.23 \times {}^{m}M_2 + 65.01$	0.8295	0.6880	0.6685	2.601	108.20
$S = -0.2061 \times F + 122.3$	-0.9527	0.9077	0.9019	1.415	32.03
$S = -15.86 \times ABC + 189.1$	-0.8202	0.6727	0.6522	2.664	113.6

Table 7. Linear regression models with statistical measures for enthalpy of vaporization.

Linear Models	R	R^2	$Adjusted - R^2$	$RMSE$	SSE
$HVAP = -0.7704 \times HSO + 78.99$	-0.8720	0.7604	0.7454	1.0220	16.730
$HVAP = -0.07132 \times ESO + 76.89$	-0.8599	0.7395	0.7233	1.0660	18.180
$HVAP = -0.6131 \times M_1 + 88.1$	-0.8860	0.7850	0.7716	0.9684	15.000
$HVAP = 10.14 \times {}^{m}M_2 + 48.91$	-0.9268	0.8590	0.8502	0.7842	9.839
$HVAP = -0.08456 \times F + 76.1$	-0.8716	0.7596	0.7446	1.0240	16.780
$HVAP = -8.065 \times ABC + 111.7$	-0.9298	0.8646	0.8561	0.7687	9.454

According to the R-value for every physicochemical property, the topological indices maintain the following ordering relationship:

Table 8. Linear regression models with statistical measures for acentric factor.

Linear Models	R	R^2	$Adjusted - R^2$	$RMSE$	SSE
$AF = -0.01317 \times HSO + 0.5038$	-0.8522	0.7263	0.7091	0.019120	0.005848
$AF = -0.001414 \times ESO + 0.4888$	-0.9744	0.9494	0.9462	0.008222	0.001082
$AF = -0.01178 \times M_1 + 0.6996$	-0.9731	0.9469	0.9435	0.008424	0.001135
$AF = 0.1534 \times {}^{m}M_2 + 0.02937$	0.8016	0.6425	0.6201	0.021850	0.007638
$AF = -0.001638 \times F + 0.4701$	-0.9650	0.9313	0.9270	0.009577	0.001467
$AF = -0.1203 \times ABC + 0.9703$	-0.7929	0.6287	0.6055	0.022260	0.007932

Table 9. Linear regression models with statistical measures for standard enthalpy of vaporization.

Linear Models	R	R^2	$Adjusted - R^2$	$RMSE$	SSE
$DHVAP = -0.1467 \times HSO + 11$	-0.8776	0.7702	0.7558	0.1894	0.5740
$DHVAP = -0.01438 \times ESO + 10.68$	-0.9166	0.8401	0.8302	0.1580	0.3993
$DHVAP = -0.1225 \times M_1 + 12.91$	-0.9362	0.8764	0.8686	0.1389	0.3088
$DHVAP = 1.915 \times {}^{m}M_2 + 5.302$	0.9253	0.8562	0.8472	0.1499	0.3593
$DHVAP = -0.01696 \times F + 10.52$	-0.9240	0.8538	0.8447	0.1511	0.3651
$DHVAP = -1.518 \times ABC + 17.13$	-0.9253	0.8562	0.8472	0.1498	0.3592

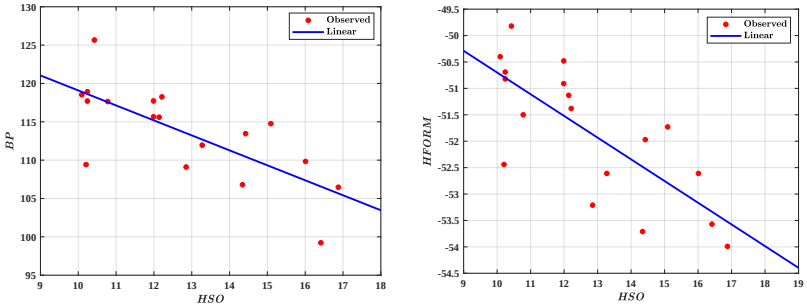

Figure 2. Pictorial representation of linear regression models for boiling point (BP) and enthalpy of formation ($HFORM$) of octane isomers with HSO index.

1. Boiling point (BP):

$$ESO < F < M_1 < HSO < {}^{m}M_2 < ABC,$$

2. Enthalpy of formation ($HFORM$):

$$ESO < HSO < F < M_1 < {}^{m}M_2 < ABC,$$

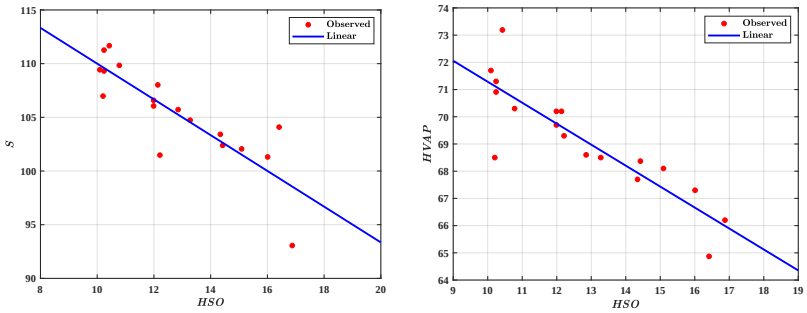

Figure 3. Pictorial representation of linear regression models for entropy (S) and enthalpy of vaporization ($HVAP$) of octane isomers with HSO index.

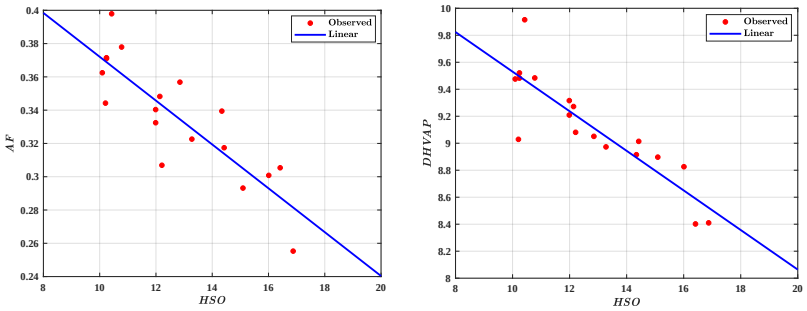

Figure 4. Pictorial representation of linear regression models for acentric factor (AF) and standard enthalpy of vaporization ($DHVAP$) of octane isomers with HSO index.

3. Entropy (S):

$$ABC < {}^{m}M_2 < HSO < F < M_1 < ESO,$$

4. Enthalpy of vaporization ($HVAP$):

$$ESO < F < HSO < M_1 < {}^{m}M_2 < ABC,$$

5. Acentric factor (AF):

$$ABC < {}^{m}M_2 < HSO < F < M_1 < ESO,$$

6. Standard enthalpy of vaporization ($DHVAP$):

$$HSO < ESO < F < {}^{m}M_2 < ABC < M_1.$$

4.2 Smoothness of hyperbolic Sombor index

A molecular descriptor's smoothness indicates that mild changes in the molecular structure cause the topological index value to fluctuate gradually. Two metrics, structural sensitivity (SS) and abruptness (Abr), were established by B. Furtula, I. Gutman and M. Dehmer in 2013 [11] to assess the smoothness of molecular descriptors and compare them to other topological indices. In order to determine the SS and Abr of a topological index of a certain class of connected graphs, we now outline an exiting algorithm [11]. The steps are:

- **Step (1):** Determine the topological index $TI(G)$ of a graph G that belongs to the class of connected graphs Ψ.
- **Step (2):** Create the set $S(G) = \{\Phi \in \Psi | GED(\Phi, G) = 2\}$, where GED is the graph edit distance between two graphs. (To know more about GED and the creation of $S(G)$, follow the articles [9, 11, 23])
- **Step (3):** Determine the topological index $TI(\Omega)$ for each $\Omega \in S(G)$. The following mathematical formulas are used to calculate the structure sensitivity and abruptness of the topological index (TI) for graph G:

$$SS(TI, G) = \frac{1}{|S(G)|} \sum_{\Omega \in S(G)} \left| \frac{TI(\Omega) - TI(G)}{TI(G)} \right|$$

and

$$Abr(TI, G) = \max_{\Omega \in S(G)} \left| \frac{TI(\Omega) - TI(G)}{TI(G)} \right|$$

where $|S(G)|$ is the total number of graphs in the set $S(G)$.

- **Step (4):** In a class of connected graphs Ψ, the overall structure sensitivity and abruptness of a topological index (TI) are determined

by averaging the SS and Abr values of a topological index generated for all G in Ψ. They are given by

$$SS(TI) = \frac{1}{|\Psi|} \sum_{G \in \Psi} SS(TI, G)$$

and

$$Abr(TI) = \frac{1}{|\Psi|} \sum_{G \in \Psi} Abr(TI, G)$$

where $|\Psi|$ is the total number of graphs in the set Ψ.

The SS value needs to be as high as feasible, while the Abr value should be as minimal as possible for a topological index to be considered acceptable. As stated in article [18], we use Algorithm 2 to compute the abruptness (Abr) and structure sensitivity (SS) of the degree-based topological indices of decane, nonane and octane isomers. For additional information on abruptness, graph edit distance and structure sensitivity, readers may refer to [1, 9, 11, 23]. The HSO index is proposed here to evaluate and compare these features with other topological indices. Two programming applications are utilized to implement the aforementioned Algorithm 2 [18] on the datasets of decane, nonane and octane isomers. Initially, the topological indices of a given molecular tree are calculated using Python's NetworkX module to identify which molecular trees have graph edit distance two. Following the completion of steps (1) and (2) in Python, we utilize Algorithm 2 (mentioned in [18]) in MATLAB R2019a software to determine the mathematical equations given in steps (3) and (4). The determined values of abruptness and structural sensitivity of the topological indices of the decane, nonane and octane isomers are listed in Table 10. The contrast of Abr and SS for the decane, nonane and octane isomers of each of our topological indices is displayed in Figures 5–7, respectively.

Observe that the structural sensitivity (SS) of several topological indices of each of the decane, nonane and octane isomers preserves the order connections listed below:

$$SS(ABC) < SS(GA) < SS(AG) < SS(R_{-1/2}) \approx SS(SCI) < SS(N)$$

Table 10. The obtained values of SS and Abr of several topological indices of the octane, nonane and decane isomers.

Sl. No.	Topological Indices		Octane	Nonane	Decane
1	HSO	SS	0.1539	0.1392	0.1061
		Abr	0.3336	0.3244	0.2671
2	ESO	SS	0.1936	0.1616	0.1387
		Abr	0.4008	0.3649	0.3419
3	M_1	SS	0.0793	0.0659	0.0566
		Abr	0.1583	0.1428	0.1336
4	${}^{m}M_2$	SS	0.0753	0.0612	0.0516
		Abr	0.1404	0.1286	0.1177
5	F	SS	0.2157	0.1794	0.1527
		Abr	0.4465	0.4015	0.3735
6	$R_{-1/2}$	SS	0.0379	0.0311	0.0263
		Abr	0.0720	0.0645	0.0588
7	SCI	SS	0.0379	0.0311	0.0264
		Abr	0.0723	0.0642	0.0591
8	SDD	SS	0.1303	0.1078	0.0907
		Abr	0.2576	0.2322	0.2099
9	H	SS	0.0749	0.0610	0.0515
		Abr	0.1409	0.1255	0.1143
10	ABC	SS	0.0346	0.0279	0.0233
		Abr	0.0656	0.0596	0.0537
11	GA	SS	0.0357	0.0290	0.0241
		Abr	0.0680	0.0595	0.0535
12	AG	SS	0.0372	0.0305	0.0255
		Abr	0.0722	0.0643	0.0579
13	SO	SS	0.1042	0.0864	0.0735
		Abr	0.2078	0.1866	0.1720
14	${}^{m}SO$	SS	0.0993	0.0807	0.0681
		Abr	0.1854	0.1648	0.1509
15	GQ	SS	0.0590	0.0479	0.0398
		Abr	0.1117	0.0974	0.0875
16	QG	SS	0.0631	0.0519	0.0436
		Abr	0.1223	0.1090	0.0984
17	N	SS	0.0390	0.0323	0.0276
		Abr	0.0767	0.0688	0.0641

$$< SS(GQ) < SS(QG) < SS(H) < SS({}^{m}M_2) < SS(M_1) < SS({}^{m}SO)$$
$$< SS(SO) < SS(SDD) < SS(HSO) < SS(ESO) < SS(F).$$

On the other hand, the following order links are maintained by the abruptness (Abr) of a number of topological indices of octane, nonane and decane isomers:

$$Abr(ABC) < Abr(GA) < Abr(R_{-1/2}) < Abr(AG) < Abr(SCI) < Abr(N)$$

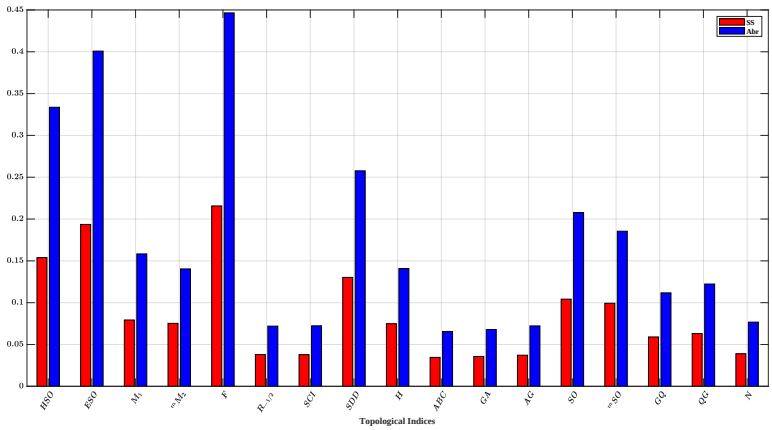

Figure 5. Structure sensitivity and abruptness of topological indices for octane isomers.

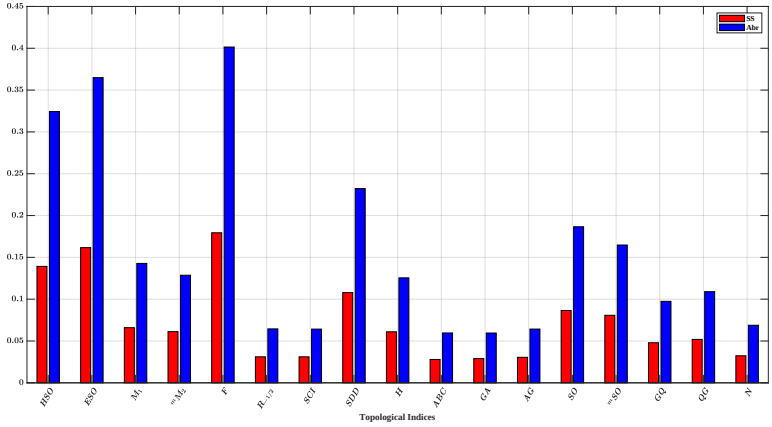

Figure 6. Structure sensitivity and abruptness of topological indices for nonane isomers.

$$< Abr(GQ) < Abr(QG) < Abr({}^{m}M_2) < Abr(H) < Abr(M_1)$$
$$< Abr({}^{m}SO) < Abr(SO) < Abr(SDD) < Abr(HSO) < Abr(ESO)$$
$$< Abr(F)$$

(for octane isomers),

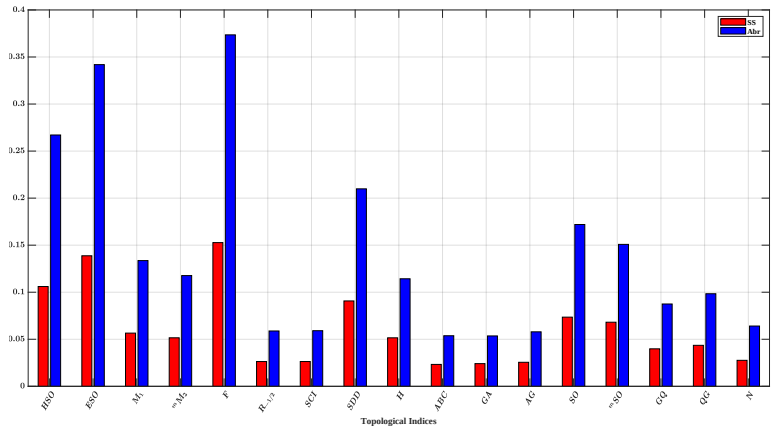

Figure 7. Structure sensitivity and abruptness of topological indices for decane isomers.

$$Abr(GA) < Abr(ABC) < Abr(SCI) < Abr(AG) < Abr(R_{-1/2}) < Abr(N) < Abr(GQ) < Abr(QG) < Abr(H) < Abr({}^{m}M_2) < Abr(M_1) < Abr({}^{m}SO) < Abr(SO) < Abr(SDD) < Abr(HSO) < Abr(ESO) < Abr(F)$$

(for nonane isomers)

and

$$Abr(GA) < Abr(ABC) < Abr(AG) < Abr(R_{-1/2}) < Abr(SCI) < Abr(N) < Abr(GQ) < Abr(QG) < Abr(H) < Abr({}^{m}M_2) < Abr(M_1) < Abr({}^{m}SO) < Abr(SO) < Abr(SDD) < Abr(HSO) < Abr(ESO) < Abr(F)$$

(for decane isomers).

The SS-values of HSO index is greater than ABC, GA, AG, $R_{-1/2}$, SCI, N, GQ, QG, H, ${}^{m}M_2$, M_1, ${}^{m}SO$, SO and SDD indices. Compared to the ABC, GA, AG, $R_{-1/2}$, SCI, N, GQ, QG, H, ${}^{m}M_2$, M_1, ${}^{m}SO$, SO and SDD indices, it is hence smoother and exhibits finer changes in structure. The abruptness of the HSO index is less than that of the ESO and F

indices. Here, we observe that when the number of alkane isomers rises from octane to decane, the values of SS of the topological indices fall. But when it comes to Abr, it is different.

4.3 Degeneracy of hyperbolic Sombor index

Topological indices make an effort to understand a molecular compound's structural properties in a meaningful way. It must be possible for a perfect topological index to discriminate between two distinct molecular configurations. The primary drawback of the majority of topological indices is degeneracy, which is the state in which two or more isomers have the same topological index values. The discriminative power of a molecular descriptor reflects its ability to capture structural statistics, with higher or lower values indicating greater sensitivity to structural characteristics. In the article [14], Konstantinova suggested a way to evaluate a topological index's degeneracy. The degeneracy measure formula is provided as

$$S_{TI} = \frac{N - N_{TI}}{N},$$

where N_{TI} is the number of isomers that the topological index (TI) is unable to distinguish, and N is the total number of isomers considered for computational testing.

In this study, we examined the discriminative power of the HSO index and contrasted it with other degree-based topological indices as mentioned in Section 1. The molecular data set of octane, nonane and decane isomers is used to test the discriminative capability. Figure 8 displays the contrast as a bar graph, while Table 11 lists the obtained outcomes.

According to Figure 8 and Table 11, the first Zagreb index (M_1) and the forgotten index (F) exhibit significantly less degeneracy for octane, nonane and decane isomers than other topological indices. Additionally, the hyperbolic Sombor index (HSO) has demonstrated dominance over other topological indices for both nonane and decane isomers.

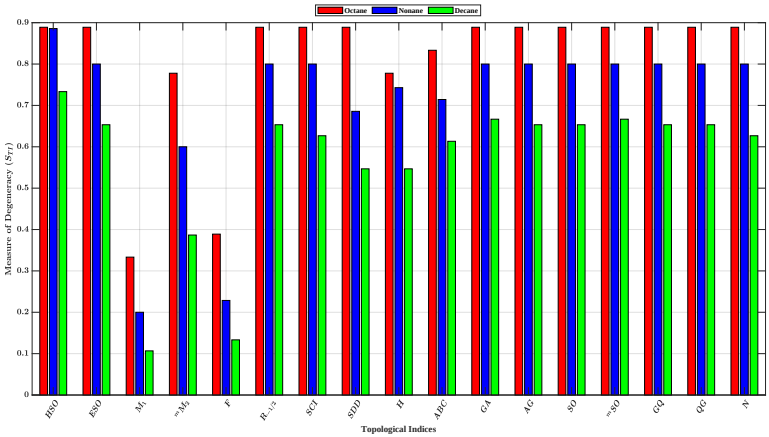

Figure 8. A bar graph representation to show contrasts of the discriminative power of topological indices between the octane, nonane and decane isomers.

Table 11. Sensitivity values $S_{TI}s$' of the several topological indices of octane, nonane and decane isomers.

Sl. No.	Topological Indices	Octane	Nonane	Decane
1	HSO	0.8889	0.8857	0.7333
2	ESO	0.8889	0.8000	0.6533
3	M_1	0.3333	0.2000	0.1067
4	$^mM_2$	0.7778	0.6000	0.3867
5	F	0.3889	0.2286	0.1333
6	$R_{-1/2}$	0.8889	0.8000	0.6533
7	SCI	0.8889	0.8000	0.6267
8	SDD	0.8889	0.6857	0.5467
9	H	0.7778	0.7429	0.5467
10	ABC	0.8333	0.7143	0.6133
11	GA	0.8889	0.8000	0.6667
12	AG	0.8889	0.8000	0.6533
13	SO	0.8889	0.8000	0.6533
14	^mSO	0.8889	0.8000	0.6667
15	GQ	0.8889	0.8000	0.6533
16	QG	0.8889	0.8000	0.6533
17	N	0.8889	0.8000	0.6267

5 Conclusion

In this article, we introduced the hyperbolic Sombor index (HSO), whose formation is inspired by the eccentricity of a hyperbola. Our discussion

focused on the octane, nonane and decane isomers by examining their uses as well as the data that is available for testing their molecular and usable characteristics. According to the outcomes of the *QSPR* analysis, *HSO* is a better predictor of boiling point than *ESO*, *F* and M_1; *HSO* predicts enthalpy of formation better than *ESO*; *HSO* predicts entropy more accurately than *ABC* and ${}^mM_2$; *HSO* is a more accurate predictor of enthalpy of vaporization than *ESO* and *F*; *HSO* outperforms *ABC* and ${}^mM_2$ in predicting acentric factor. The results of the *HSO* index for *SS* are superior to those of various well-known topological indices in terms of smoothness. To be more precise, it outperforms the outcomes of the *SDD*, *SO*, ${}^mSO$, *GQ* and *QG* indices. According to this, the *HSO* index exhibits slight structural variations in contrast to these indices. The *HSO* index has a lower *Abr*-value than the *ESO* and *F* indices, suggesting that it is a more acceptable topological indicator. The measurements of the discriminative power of the *HSO* index are similar to all of the topological indices except M_1, ${}^mM_2$, *F*, *H* and *ABC* indices for octane isomers. In the case of nonane and decane isomers, the *HSO* index responds better to isomer discrimination than other topological indices. The *HSO* index could emerge as an attractive alternative for *QSPR* analysis and for predicting the physicochemical characteristics in diverse molecular structures and graphical representations.

***Acknowledgment*:** The first author (Jayjit Barman) is grateful to the UNIVERSITY GRANTS COMMISSION, Ministry of Social Justice and Empowerment, New Delhi, India for awarding the National Fellowship for Scheduled Caste Students (NFSC) with reference to UGC-Ref. No.: 211610011412/(CSIR-UGC NET JUNE 2021) dated 11-May-2022. The second author (Dr. Shibsankar Das) is obliged to the Development Cell, Banaras Hindu University for financially supporting this work through the Faculty "Incentive Grant" under the Institute of Eminence (IoE) Scheme for the year 2024-25 (Project sanction order number: R/Dev/D/IoE/ Incentive (Phase-IV)/2024-25/82483, dated 7 January 2025).

References

[1] S. Brezovnik, M. Dehmer, N. Tratnik, P. Žigert Pleteršek, Szeged and Mostar root-indices of graphs, *Appl. Math. Comput.* **442** (2023) #127736.

[2] V. Consonni, D. Ballabio, R. Todeschini, Comments on the definition of the Q 2 parameter for QSAR validation, *J. Chem. Inf. Model.* **49**

(2009) 1669–1678.

[3] K. C. Das, I. Gutman, B. Furtula, Survey on geometric-arithmetic indices of graphs, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 595–644.

[4] S. Das, V. Kumar, On M-polynomial of the two-dimensional silicon-carbons, *Palest. J. Math.* **11** (2022) 136–157.

[5] S. Das, S. Rai, M-polynomial and related degree-based topological indices of the third type of Hex-derived network, *Nanosyst. Phys. Chem. Math.* **11** (2020) 267–274.

[6] S. Das, S. Rai, M. Mandal, M-polynomial and correlated topological indices of antiviral drug Molnupiravir used as a therapy for COVID-19, *Polycyc. Arom. Comp.* **43** (2023) 7027–7041.

[7] E. Estrada, L. Torres, L. Rodriguez, I. Gutman, An atom-bond connectivity index: modelling the enthalpy of formation of alkanes, *Indian J. Chem.* **37A** (1998) 849–855.

[8] O. Favaron, M. Mahéo, J.-F. Saclé, Some eigenvalue properties in graphs (conjectures of Graffiti-II), *Discr. Math.* **111** (1993) 197–220.

[9] B. Furtula, K. Ch. Das, I. Gutman, Comparative analysis of symmetric division deg index as potentially useful molecular descriptor, *Int. J. Quantum Chem.* **118** (2018) #e25659.

[10] B. Furtula, I. Gutman, A forgotten topological index, *J. Math. Chem.* **53** (2015) 1184–1190.

[11] B. Furtula, I. Gutman, M. Dehmer, On structure-sensitivity of degree-based topological indices, *Appl. Math. Comput.* **219** (2013) 8973–8978.

[12] I. Gutman, Geometric approach to degree-based topological indices: Sombor indices, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 11–16.

[13] I. Gutman, B. Furtula, M. S. Oz, Geometric approach to vertex-degree-based topological indices–Elliptic Sombor index, theory and application, *Int. J. Quantum Chem.* **124** (2024) #e27346.

[14] E. V. Konstantinova, The discrimination ability of some topological and information distance indices for graphs of unbranched hexagonal systems, *J. Chem. Inf. Comput. Sci.* **36** (1996) 54–57.

[15] V. Kulli, Nirmala index, *Int. J. Math. Trends Technol.* **67** (2021) #IJMTT-V67I3P502.

[16] V. Kulli, Geometric-quadratic and quadratic-geometric indices, *Ann. Pure Appl. Math.* **25** (2022) 1–5.

[17] V. Kulli, I. Gutman, Computation of Sombor indices of certain networks, *SSRG Int. J. Appl. Chem.* **8** (2021) 1–5.

[18] V. Kumar, S. Das, Comparative study of GQ and QG indices as potentially favorable molecular descriptors, *Int. J. Quantum Chem.* **124** (2024) #e27334.

[19] B. Liu, I. Gutman, On general Randić indices, *MATCH Commun. Math. Comput. Chem.* **58** (2007) 147–154.

[20] A. Miličević, S. Nikolić, N. Trinajstić, On reformulated Zagreb indices, *Mol. Divers.* **8** (2004) 393–399.

[21] K. G. Mirajkar, B. R. Doddamani, H. Huchesh, The hyper Zagreb index for some molecular structures, *South East Asian J. Math. Sci.* **17** (2021) 331–346.

[22] S. Mondal, A. Dey, N. De, A. Pal, QSPR analysis of some novel neighbourhood degree-based topological descriptors, *Complex Intell. Syst.* **7** (2021) 977–996.

[23] M. Rakić, B. Furtula, A novel method for measuring the structure sensitivity of molecular descriptors, *J. Chemom.* **33** (2019) #e3138.

[24] M. Randić, Molecular bonding profiles, *J. Math. Chem.* **19** (1996) 375–392.

[25] I. Redžepović, Chemical applicability of Sombor indices, *J. Serb. Chem. Soc.* **86** (2021) 445–457.

[26] J. Rodrıguez, J. Sigarreta, New results on the harmonic index and its generalizations, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 387–404.

[27] V. Shegehalli, R. Kanabur, Arithmetic-geometric indices of path graph, *J. Math. Comput. Sci.* **16** (2015) 19–24.

[28] Molecular Descriptors - the free online resource, `https://web.archive.org/web/20180912171255if_/http://www.moleculardescriptors.eu/index.htm` (Accessed on February, 2025).

[29] D. Vukičević, B. Furtula, Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges, *J. Math. Chem.* **46** (2009) 1369–1376.

[30] D. Vukičević, M. Gašperov, Bond additive modeling 1. Adriatic indices, *Croat. Chem. Acta* **83** (2010) 243–260.

[31] Z. Wang, Y. Mao, Y. Li, B. Furtula, On relations between Sombor and other degree-based indices, *J. Appl. Math. Comput.* **68** (2022) 1–17.

[32] B. Zhou, N. Trinajstić, On a novel connectivity index, *J. Math. Chem.* **46** (2009) 1252–1270.