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Research Article

On the hyperbolic Sombor index and its applications

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Abstract

Let G be a graph with vertex V and edge set E. In this paper, we investigate the hyperbolic Sombor (HSO) index, a recently introduced degree-based topological index, defined as

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

where d_u denotes the degree of a vertex $u \in V$. We establish several bounds for this index in terms of fundamental graph parameters and classical topological indices. As a chemical application, we perform a correlation analysis to examine the relationship between the HSO index and the physicochemical properties of heptane and hexane isomers.

Keywords: hyperbolic Sombor index; topological index; physicochemical properties.

2020 Mathematics Subject Classification: 05C09, 05C90, 05C92.

1. Introduction

Throughout the development of the theory of topological molecular descriptors, numerous important degree-based topological indices have been proposed. In this paper, we present only the descriptors that are relevant to subsequent analyses.

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

$$TI(G) = \sum_{uv \in E(G)} f\big(d_u, d_v\big),$$

where $f(x, y)$ is a symmetric and non-negative real function.

We now present the mathematical formulations for several degree-based topological indices, which are characterized by distinct functional forms of $f(x, y)$. One of the oldest vertex degree-based topological indices is the first Zagreb index introduced in 1972 [7]. The first Zagreb index of a graph G can be defined as

$$M_1(G) = \sum_{uv \in E(G)} \big(d_u + d_v\big).$$

In [2], the following index was proposed, which nowadays is called the Albertson index:

$$Alb(G) = \sum_{uv \in E} |d_u - d_v|.$$

The reciprocal Randić index [1] and the sum-connectivity index [18] of a graph G are defined, respectively, as

$$RR(G) = \sum_{uv \in E} \sqrt{d_u d_v} \quad \text{and} \quad \chi(G) = \sum_{uv \in E} \frac{1}{\sqrt{d_u + d_v}}.$$

The general sum-connectivity index [19], a generalization of $\chi(G)$, is defined as

$$\chi_\alpha(G) = \sum_{uv \in E} (d_u + d_v)^\alpha,$$

where α is a real number.

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The forgotten index [4] and the sum-connectivity F-index [9] (see also [8]) are defined, respectively, as

$$F(G) = \sum_{uv \in E(G)} \left(d_u^2 + d_v^2\right) \quad \text{and} \quad SF(G) = \sum_{uv \in E} \frac{1}{\sqrt{d_u^2 + d_v^2}}.$$

The Sombor index, proposed by Gutman in [5], is defined as

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

which has attracted considerable attention for its applications in quantitative structure property/activity relationships (QSPR/QSAR) studies [5, 10, 12–14, 16, 17].

In 2024, Gutman et al. [6] proposed a topological index based on the formulation of the ellipse. This index is called the elliptic Sombor index and is defined as

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

The present paper is concerned with a recently introduced variant of the Sombor index, namely the hyperbolic Sombor (HSO) index [3], which is defined as

$$HSO(G) = \sum_{uv \in E} \frac{\sqrt{d_u^2 + d_v^2}}{\min\{d_u, d_v\}}.$$

For convenience, we write the HSO index as

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

where $d_v \geq d_u \geq 1$. In this paper, we aim to advance the study of the HSO index by exploring new bounds and its connections with the classical topological indices listed above. We also perform a correlation analysis to examine the relationship between the HSO index and the physicochemical properties of heptane and hexane isomers.

2. Bounds on the hyperbolic Sombor index of a graph

This section gives upper and lower bounds for the HSO index in terms of order, size, minimum degree, and maximum degree.

Theorem 2.1. *Let G be a simple connected graph on n vertices with maximum degree Δ and minimum degree δ. Then,*

$$\frac{n\delta^2}{\sqrt{2}\Delta} \leq HSO(G) \leq \frac{n\Delta^2}{\sqrt{2}\delta}.$$

Either of equalities holds if and only if G is a regular graph.

Proof. Let m be the size of G. By the handshake lemma, we obtain

$$n\delta \leq \sum_{v \in V(G)} d_v = 2m \leq n\Delta.$$

The left equality holds if and only if $d_v = \delta$ for any $v \in V(G)$, whereas the right equality holds if and only if $d_v = \Delta$ for any $v \in V(G)$. Hence, we obtain

$$HSO(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u^2 + d_v^2}}{d_u} \leq \sum_{uv \in E(G)} \frac{\sqrt{d_u^2 + d_v^2}}{\delta} = \frac{1}{\delta} \sum_{uv \in E(G)} \sqrt{d_u^2 + d_v^2} \leq \frac{\sqrt{2}\Delta m}{\delta} \leq \frac{n\Delta^2}{\sqrt{2}\delta}.$$

Moreover, the equality holds if and only if $d_v = d_u = \Delta$, i.e., G is regular. Similarly, we obtain the lower bound on the HSO index. □

Theorem 2.2. *Let G be a simple graph of size m and maximum degree Δ. Then,*

$$HSO(G) \leq (\sqrt{2} + \Delta - 1)m.$$

Moreover, the equality holds if and only if every component of G is K_2.

Proof. For any edge $uv \in E(G)$ with $d_v \geq d_u \geq 1$, it follows that $\sqrt{d_u^2 + d_v^2} \leq d_v + (\sqrt{2} - 1)d_u$ with equality if and only if $d_u = d_v$. Therefore,

$$HSO(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u^2 + d_v^2}}{d_u} \leq \sum_{uv \in E(G)} \frac{d_v + (\sqrt{2}-1)d_u}{d_u} = \sum_{uv \in E(G)} \left(\frac{d_v}{d_u} + \sqrt{2} - 1 \right) \leq (\sqrt{2} + \Delta - 1)m.$$

Moreover, all equalities hold if and only if $d_u = d_v = 1$ for any $uv \in E(G)$; that is, every component of G is K_2. □

Theorem 2.3. *Let G be a connected graph with m edges and degree sequence $d_1 \geq d_2 \geq \cdots \geq d_n$. Let p be the number of vertices with minimum degree d_n, and let q be the number of edges in the subgraph induced by these p vertices. Then*

$$q\sqrt{2} + (m - pd_n + q)\sqrt{2}\frac{d_{n-p}}{d_1} + (pd_n - 2q)\sqrt{2} \leq HSO(G) \leq q\sqrt{2} + (m - pd_n + q)\sqrt{2}\frac{d_1}{d_{n-p}} + (pd_n - 2q)\frac{d_1}{d_n}\sqrt{2}.$$

Proof. Let H be the subgraph induced by the p vertices of degree d_n. For any edge $uv \in E(H)$, if $uv \in E(H)$, then

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

If $uv \in E(G) - E(H)$, then

$$\frac{d_{n-p}}{d_1}\sqrt{2} \leq \frac{\sqrt{d_u^2(G) + d_v^2(G)}}{d_u(G)} \leq \frac{d_1}{d_{n-p}}\sqrt{2}.$$

If $v \in V(H)$, $u \in V(G) - V(H)$, or $u \in V(H)$, $v \in V(G) - V(H)$, then

$$\sqrt{2} \leq \frac{\sqrt{d_n^2 + d_{n-p}^2}}{d_n} \leq \frac{\sqrt{d_u^2(G) + d_v^2(G)}}{d_u(G)} \leq \frac{\sqrt{d_n^2 + d_1^2}}{d_n} \leq \frac{d_1}{d_n}\sqrt{2}.$$

By the handshake lemma, $\sum_{v \in V(H)} d_v(H) = 2q$ as $|E(H)| = q$. Since

$$\sum_{v \in V(H)} d_v(G) = \sum_{v \in V(H)} d_v(H) + e(H, \overline{H}),$$

it follows that the number of edges between $V(H)$ and $V(G) - V(H)$ is $pd_n - 2q$, and

$$|E(G - V(H))| = m - pd_n + q.$$

Consequently,

$$HSO(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u^2(G) + d_v^2(G)}}{d_u} \leq q\sqrt{2} + (m - pd_n + q)\sqrt{2}\frac{d_1}{d_{n-p}} + (pd_n - 2q)\frac{d_1}{d_n}\sqrt{2},$$

and

$$HSO(G) = \sum_{uv \in E(G)} \frac{\sqrt{d_u^2(G) + d_v^2(G)}}{d_u(G)} \geq q\sqrt{2} + (m - pd_n + q)\sqrt{2}\frac{d_{n-p}}{d_1} + (pd_n - 2q)\sqrt{2}.$$

□

3. Relationship between the HSO index and other topological indices

This section gives upper and lower bounds for the HSO index in terms of some other degree-based topological indices.

Theorem 3.1. *Let G be a simple and connected graph of order $n \geq 2$ with the maximum degree Δ. Then*

$$\frac{\sqrt{2}}{2\Delta} Alb(G) + \frac{1}{\Delta} RR(G) \leq HSO(G) \leq \frac{1}{\delta} Alb(G) + \frac{\sqrt{2}}{\delta} RR(G).$$

Any of the equalities holds if and only if G is regular.

Proof. Since for any two real numbers $a, b \geq 0$, we have $\frac{\sqrt{2}}{2}\left(\sqrt{a} + \sqrt{b}\right) \leq \sqrt{a+b}$, and the equality holds if and only if $a = b$. Setting $a = (d_u - d_v)^2$ and $b = 2d_u d_v$, we obtain

$$\frac{\sqrt{2}}{2}\left(\sqrt{(d_u - d_v)^2} + \sqrt{2d_u d_v}\right) \leq \sqrt{d_u^2 + d_v^2}.$$

Then

$$\frac{\sqrt{2}}{2}\left(\frac{|d_u-d_v|}{d_u}+\sqrt{2}\frac{\sqrt{d_ud_v}}{d_u}\right)\leq\frac{\sqrt{d_u^2+d_v^2}}{d_u}.$$

Since $2\delta\leq d_u+d_v\leq 2\Delta$ for any $uv\in E$, we obtain

$$\begin{aligned}HSO(G)&=\sum_{uv\in E}\frac{\sqrt{d_u^2+d_v^2}}{d_u}\geq\frac{\sqrt{2}}{2}\sum_{uv\in E}\left(\frac{|d_u-d_v|}{d_u}+\sqrt{2}\frac{\sqrt{d_ud_v}}{d_u}\right)\\&\geq\frac{\sqrt{2}}{2\Delta}\sum_{uv\in E}|d_u-d_v|+\frac{1}{\Delta}\sum_{uv\in E}\sqrt{d_ud_v}=\frac{\sqrt{2}}{2\Delta}Alb(G)+\frac{1}{\Delta}RR(G).\end{aligned}$$

Equality in the above inequalities holds if and only if G is regular. For the upper bound, we use $\sqrt{a+b}\leq\sqrt{a}+\sqrt{b}$, where the equality holds if and only if $a=0$ or $b=0$. Therefore, Setting $a=(d_u-d_v)^2$ and $b=2d_ud_v$, we obtain

$$\sqrt{d_u^2+d_v^2}\leq\sqrt{(d_u-d_v)^2}+\sqrt{2d_ud_v}=|d_u-d_v|+\sqrt{2}\sqrt{d_ud_v}.$$

$$\begin{aligned}HSO(G)&=\sum_{uv\in E}\frac{\sqrt{d_u^2+d_v^2}}{d_u}\leq\sum_{uv\in E}\left(\frac{|d_u-d_v|}{d_u}+\frac{\sqrt{2}\sqrt{d_ud_v}}{d_u}\right)\\&\leq\frac{1}{\delta}\sum_{uv\in E}|d_u-d_v|+\frac{\sqrt{2}}{\delta}\sum_{uv\in E}\sqrt{d_ud_v}=\frac{1}{\delta}Alb(G)+\frac{\sqrt{2}}{\delta}RR(G).\end{aligned}$$

The equality in the above inequalities holds if and only if G is regular. □

Theorem 3.2. *Let G be a simple and connected graph of size m. Then*

$$HSO(G)\leq\frac{\sqrt{2}}{2\delta}(Alb(G)+M_1(G)).$$

The equality holds if and only if G is a regular graph.

Proof. Let a,b be two non-negative real numbers. Then, we have $\sqrt{a+b}\leq\sqrt{a}+\sqrt{b}$ with equality if and only if $a=0$ or $b=0$. Setting $a=\frac{1}{2}(d_u-d_v)^2$, $b=\frac{1}{2}(d_u+d_v)^2$, we obtain

$$\sqrt{\frac{1}{2}(d_u-d_v)^2+\frac{1}{2}(d_u+d_v)^2}\leq\frac{\sqrt{2}}{2}(\sqrt{(d_u-d_v)^2}+\sqrt{(d_u+d_v)^2}).$$

Since $\frac{1}{2}(d_u-d_v)^2+\frac{1}{2}(d_u+d_v)^2=d_u^2+d_v^2$, it follows that

$$\frac{\sqrt{d_u^2+d_v^2}}{d_u}\leq\frac{\sqrt{2}}{2}\left(\frac{|d_u-d_v|}{d_u}+\frac{d_u+d_v}{d_u}\right).$$

Therefore, we obtain

$$\begin{aligned}HSO(G)&=\sum_{uv\in E}\frac{\sqrt{d_u^2+d_v^2}}{d_u}\leq\frac{\sqrt{2}}{2}\sum_{uv\in E}\left(\frac{|d_u-d_v|}{d_u}+\frac{d_u+d_v}{d_u}\right)\\&\leq\frac{\sqrt{2}}{2\delta}\left(\sum_{uv\in E}|d_u-d_v|+\sum_{uv\in E}(d_u+d_v)\right)=\frac{\sqrt{2}}{2\delta}(Alb(G)+M_1(G)).\end{aligned}$$

The equality in the above inequalities holds if and only if G is regular. □

Lemma 3.1 (see [11]). *If $a_i,b_i\geq 0$ and $Ab_i\leq a_i\leq Bb_i$ for $1\leq i\leq n$, then*

$$\left(\sum_{i=1}^{n}a_i^2\right)\left(\sum_{i=1}^{n}b_i^2\right)\leq\frac{(A+B)^2}{4AB}\left(\sum_{i=1}^{n}a_ib_i\right)^2.$$

The equality holds if and only if $A=B$ and $a_i=Ab_i$.

Theorem 3.3. *Let G be a simple and connected graph of size m with maximum degree Δ and minimum degree δ. Then*

$$HSO(G)\geq\sqrt{\frac{m\beta}{\Delta^2}F(G)},$$

where $\beta=\frac{4\delta\sqrt{2(\delta^2+\Delta^2)}}{(\sqrt{2}\delta+\sqrt{\delta^2+\Delta^2})^2}$. The equality holds if and only if G is a regular graph.

Proof. First, we prove that for any vertices $u, v \in V$

$$\sqrt{2} \leq \frac{\sqrt{d_u^2 + d_v^2}}{d_u} \leq \frac{\sqrt{\Delta^2 + \delta^2}}{\delta}.$$

Noting that $\delta \leq d_u \leq \Delta$ for any $u \in V$ and $\frac{\delta}{\Delta} \leq \frac{d_v}{d_u} \leq \frac{\Delta}{\delta}$. Therefore,

$$\frac{\sqrt{d_u^2 + d_v^2}}{d_u} = \sqrt{1 + (\frac{d_v}{d_u})^2} \leq \sqrt{1 + (\frac{\Delta}{\delta})^2} = \frac{\sqrt{\Delta^2 + \delta^2}}{\delta}.$$

On the other hand, we have $\sqrt{2} \leq \frac{\sqrt{d_u^2+d_v^2}}{d_u}$. Now apply Lemma 3.1 with $a_i = \frac{\sqrt{d_u^2+d_v^2}}{d_u}$, $b_i = 1$, $A = \sqrt{2}, B = \frac{\sqrt{\Delta^2+\delta^2}}{\delta}$. We obtain

$$\left(\sum_{uv \in E} \frac{d_u^2 + d_v^2}{d_u^2}\right)\left(\sum_{uv \in E} 1\right) \leq \frac{\left(\sqrt{2} + \frac{\sqrt{\Delta^2+\delta^2}}{\delta}\right)^2}{4\sqrt{2}\frac{\sqrt{\Delta^2+\delta^2}}{\delta}} \left(\sum_{uv \in E} \frac{\sqrt{d_u^2 + d_v^2}}{d_u}\right)^2.$$

Then

$$m \sum_{uv \in E} \frac{d_u^2 + d_v^2}{d_u^2} \leq \frac{(\sqrt{2}\delta + \sqrt{\delta^2 + \Delta^2})^2}{4\delta\sqrt{2(\delta^2 + \Delta^2)}} \left(\sum_{uv \in E} \frac{\sqrt{d_u^2 + d_v^2}}{d_u}\right)^2$$

and

$$\frac{m}{\Delta^2} \sum_{uv \in E} (d_u^2 + d_v^2) \leq \frac{(\sqrt{2}\delta + \sqrt{\delta^2 + \Delta^2})^2}{4\delta\sqrt{2(\delta^2 + \Delta^2)}} (HSO(G))^2.$$

Since $F(G) = \sum_{uv \in E}(d_u^2 + d_v^2)$, we have

$$\frac{m}{\Delta^2} F(G) \leq \frac{(\sqrt{2}\delta + \sqrt{\delta^2 + \Delta^2})^2}{4\delta\sqrt{2(\delta^2 + \Delta^2)}} (HSO(G))^2.$$

By considering $\beta = \frac{4\delta\sqrt{2(\delta^2+\Delta^2)}}{(\sqrt{2}\delta+\sqrt{\delta^2+\Delta^2})^2}$, we obtain

$$HSO(G) \geq \sqrt{\frac{m\beta}{\Delta^2} F(G)}.$$

The equality holds if and only if G is a regular graph. □

Lemma 3.2 (see [15]). *Let $x = (x_i)_{i=1}^n$ and $a = (a_i)_{i=1}^n$ be two sequences of positive real numbers. Then for any $r \geq 0$,*

$$\frac{\left(\sum_{i=1}^n x_i\right)^{r+1}}{\left(\sum_{i=1}^n a_i\right)^r} \leq \sum_{i=1}^n \frac{x_i^{r+1}}{a_i^r}.$$

The equality holds if and only if either $r = 0$ or $\frac{x_1}{a_1} = \frac{x_2}{a_2} = \cdots = \frac{x_n}{a_n}$.

Theorem 3.4. *For a simple graph G,*

$$\frac{m^2}{\Delta\, SF(G)} \leq HSO(G) \leq \frac{m}{\delta^2} F(G).$$

Any of the equalities holds if and only if G is a regular graph.

Proof. By the Cauchy-Schwarz inequality, we obtain

$$(HSO(G))^2 = \left(\sum_{uv \in E} \frac{\sqrt{d_u^2 + d_v^2}}{d_u}\right)^2 \leq \left(\sum_{uv \in E} (\sqrt{d_u^2 + d_v^2})^2\right)\left(\sum_{uv \in E} \frac{1}{d_u^2}\right) \leq \left(\sum_{uv \in E} (d_u^2 + d_v^2)\right) \frac{m}{\delta^2} = \frac{m}{\delta^2} F(G).$$

Hence

$$HSO(G) \leq \frac{m}{\delta^2} F(G).$$

For the lower bound, we use Lemma 3.2 by setting $x_i = \frac{1}{\sqrt{d_u}}, a_i = \frac{1}{\sqrt{d_u^2+d_v^2}}$, and $r = 1$. Therefore, we have

$$HSO(G) = \sum_{uv \in E} \frac{\sqrt{d_u^2 + d_v^2}}{d_u} = \sum_{uv \in E} \frac{\frac{1}{(\sqrt{d_u})^2}}{\frac{1}{\sqrt{d_u^2+d_v^2}}} \geq \frac{(\sum_{uv \in E} \frac{1}{\sqrt{d_u}})^2}{\sum_{uv \in E} \frac{1}{\sqrt{d_u^2+d_v^2}}} \geq \frac{m^2}{\Delta\, SF(G)}.$$

The equalities hold if and only if $d_u = d_v$ for any edge $uv \in E$. □

4. Chemical applications of the hyperbolic Sombor index

A topological index translates a chemical structure into a numerical quantity. It is a numerical quantity that remains unchanged under graph automorphisms and plays a crucial role in chemical graph theory. A key application of topological indices is the prediction of the physicochemical properties of molecules, such as melting and boiling points. In this section, nine structural isomers of heptane and five structural isomers of hexane are used to examine the chemical applicability of the HSO index. Subsequently, linear, quadratic, and cubic regression models are employed to investigate the fitting between the HSO index and the physicochemical properties of these isomers. The boiling points, densities, melting points, and other properties of the isomers correlate to varying degrees with the HSO index. The following regression models are examined:

$$Y = A_1X_1 + B \ (linear), \tag{1}$$

$$Y = A_2X_2^2 + A_1X_2 + B \ (quadratic), \tag{2}$$

$$Y = A_3X_3^3 + A_2X_3^2 + A_1X_3 + B \ (cubic). \tag{3}$$

In these models, Y is the dependent variable, X_i (where $i = 1, 2, 3$) is the independent variable, B is the regression constant, and A_i (where $i = 1, 2, 3$) is the regression coefficient. The graphs of nine isomers of heptane and five isomers of hexane are shown in Figure 4.1 and Figure 4.2, respectively.

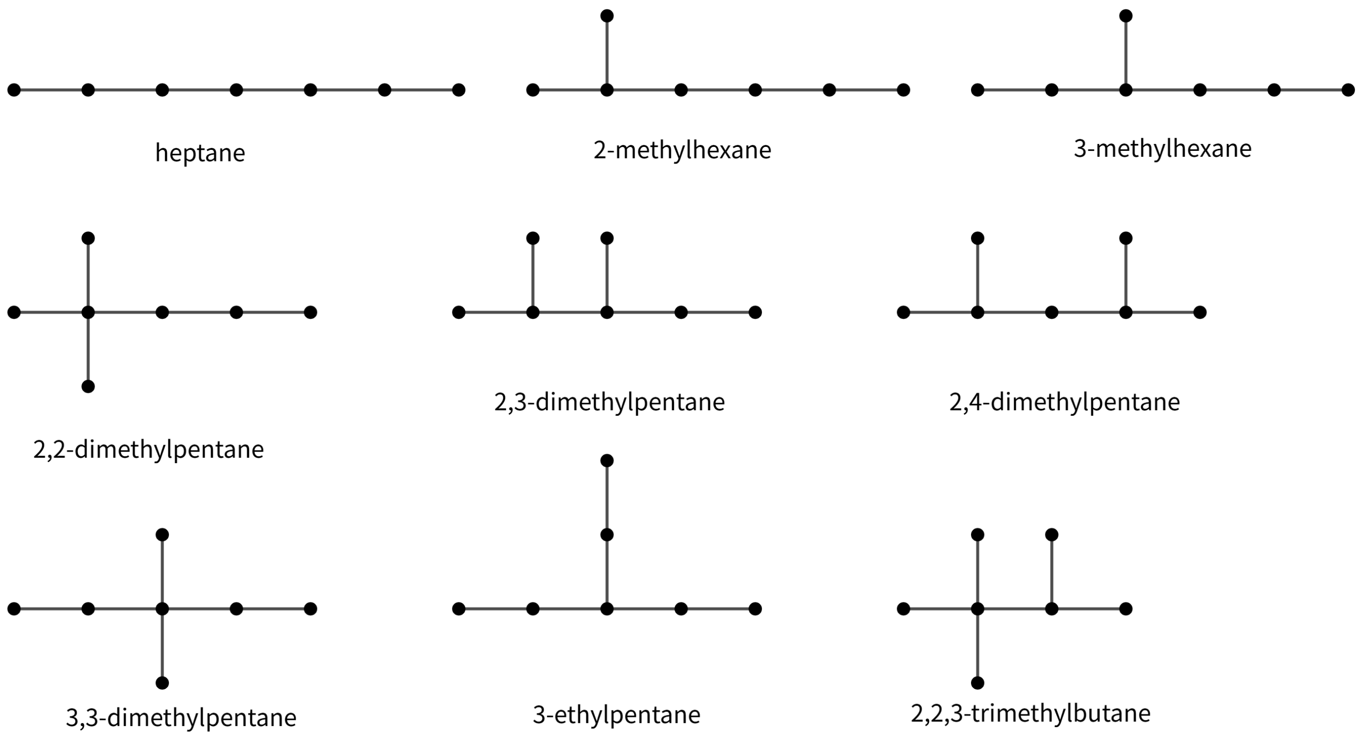

Figure 4.1: Graphs of nine isomers of heptane.

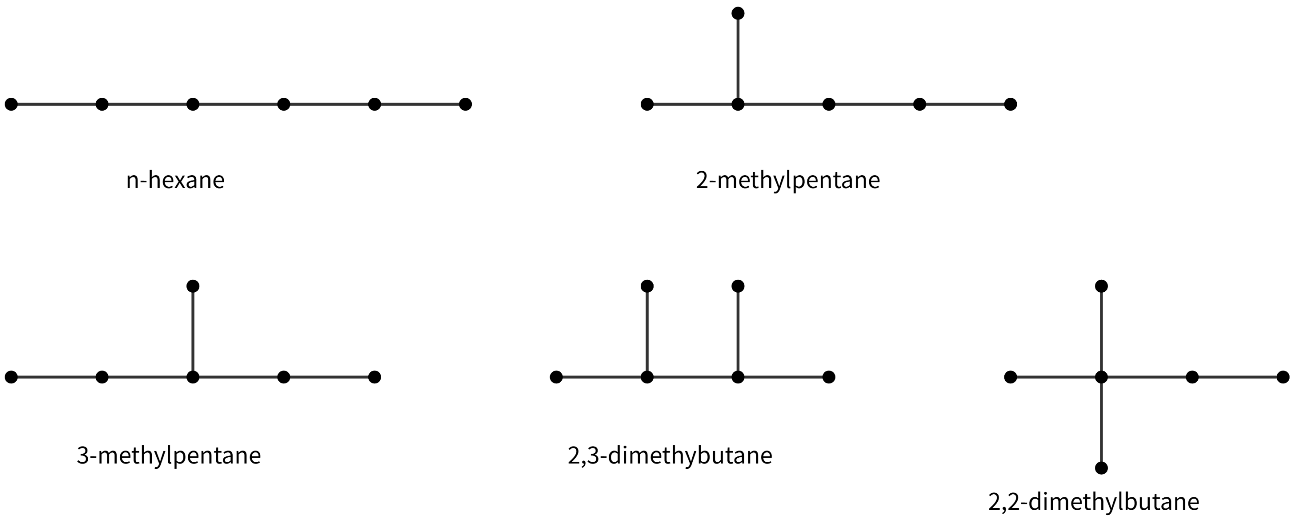

Figure 4.2: Graphs of five isomers of hexane.

Isomers	HSO	BP	DHVAP	S	HVAP	AcenFac
n-heptane	10.1290	98.4	36.00	328.57	36.6	0.3460
2-methylhexane	13.1918	90.0	34.98	323.34	34.8	0.3298
3-methylhexane	12.6542	92.0	35.16	309.60	35.0	0.3240
2,2-diethylpentane	18.2557	79.2	32.56	300.29	31.0	0.2886
3,3-diethylpentane	17.1905	86.1	33.15	305.60	33.2	0.2697
2,3-diethylpentane	14.9399	89.8	34.30	297.10	34.5	0.2986
2,4-diethylpentane	16.2547	80.5	33.02	303.17	32.7	0.3059
3-ethylpentane	12.1165	93.5	35.32	314.56	34.1	0.3101
2,2,3-trimethylbutane	20.3605	80.9	32.04	292.25	32.4	0.2510

Table 4.1: HSO-values of heptane isomers and experimental values of their five physicochemical properties.

Isomers	HSO	BP	MP
n-hexane	8.7148	155.7	-136.9
3-methypentane	11.2400	145.9	-180.4
2-methypentane	11.7776	140.5	-244.6
2,3-dimethybutane	14.0633	136.4	-199.4
2,2-dimethybutane	16.8415	121.5	-147.8

Table 4.2: HSO-values of hexane isomers and experimental values of their two physicochemical properties.

Table 4.1 presents the physicochemical properties of heptane isomers, namely the boiling point (BP), standard enthalpy of vaporization (DHVAP), entropy (S), enthalpy of vaporization (HVAP), acentric factor (AcenFac), and their corresponding HSO-values. Also, Table 4.2 displays the boiling points (BP), melting points (MP), and HSO-values of hexane isomers.

Linear regression models of heptane isomers with respect to the HSO index are given as follows:

$$BP = -1.848(HSO) + 115.56,$$
$$DHVAP = -0.420(HSO) + 40.37,$$
$$S = -3.130(HSO) + 355.26,$$
$$HVAP = -0.445(HSO) + 40.49,$$
$$AcenFac = -0.008(HSO) + 0.43.$$

Quadratic regression models of heptane isomers with respect to the HSO index are given below

$$BP = 0.122(HSO)^2 - 5.554(HSO) + 142.63,$$
$$DHVAP = 0.004(HSO)^2 - 0.547(HSO) + 41.29,$$
$$S = 0.198(HSO)^2 - 9.152(HSO) + 399.24,$$
$$HVAP = 0.028(HSO)^2 - 1.296(HSO) + 46.70,$$
$$AcenFac = -0.00(HSO)^2 - 0.003(HSO) + 0.39.$$

Cubic regression models of heptane isomers with respect to the HSO index are presented as follows:

$$BP = 0.017(HSO)^3 - 0.650(HSO)^2 + 5.908(HSO) + 87.50,$$
$$DHVAP = 0.005(HSO)^3 - 0.216(HSO)^2 + 2.726(HSO) + 25.55,$$
$$S = -0.051(HSO)^3 - 2.532(HSO)^2 + -43.815(HSO) + 565.95,$$
$$HVAP = 0.005(HSO)^3 - 0.198(HSO)^2 + 5.2.058(HSO) + 30.57,$$
$$AcenFac = -0.000(HSO)^3 - 0.004(HSO)^2 - 0.060(HSO) + 0.66.$$

Linear regression models of hexane isomers with respect to the HSO index are given as follows:

$$BP = -4.060(HSO) + 190.86,$$
$$MP = -0.166(HSO) - 179.44.$$

Quadratic regression models of hexane isomers with respect to the HSO index are presented below

$$BP = -0.035(HSO)^2 - 3.160(HSO) + 185.34,$$
$$MP = 4.609(HSO)^2 - 118.816(HSO) + 548.52.$$

Cubic regression models of hexane isomers with respect to the HSO index are given as follows:

$$BP = -0.092(HSO)^3 + 3.441(HSO)^2 - 45.834(HSO) + 354.44,$$
$$MP = -0.239(HSO)^3 + 13.674(HSO)^2 - 230.093(HSO) + 989.47.$$

Figure 4.3 and Figure 4.4 show the variations in linear, quadratic, and cubic models for each physicochemical property. Table 4.3 and Table 4.4 give the correlation coefficients (R^2) between d if and only iferent physicochemical properties and the HSO index, which indicate the predictive power of the HSO index.

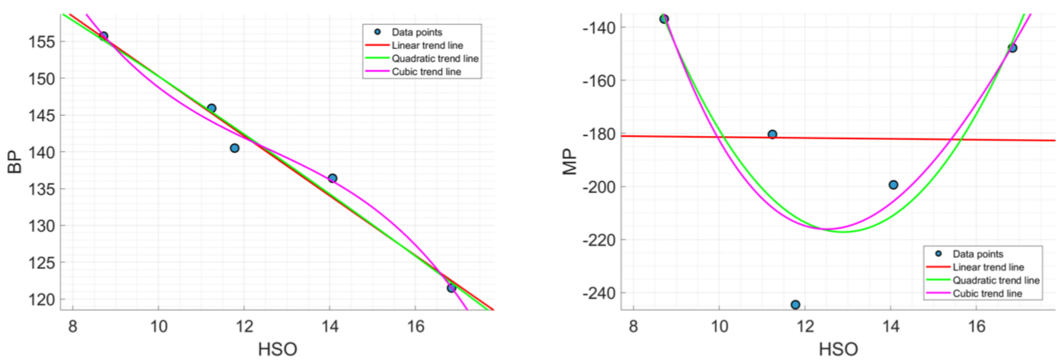

Figure 4.3: Regression models between the HSO index of hexane isomers and their two properties.

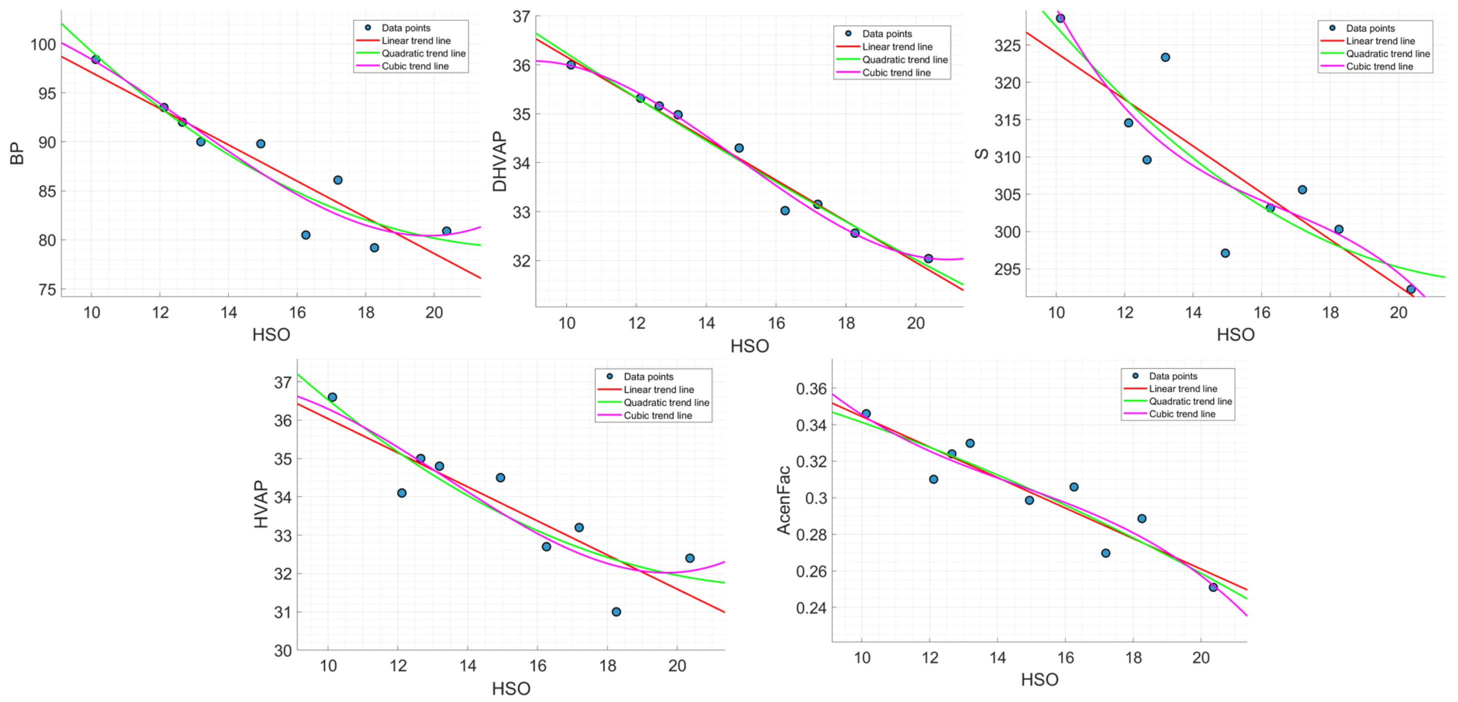

Figure 4.4: Regression models between the HSO index of heptane isomers and their five properties.

Model	BP	DHVAP	S	HVAP	AcenFac
Linear	0.8464	0.9724	0.7315	0.7701	0.8486
Quadratic	0.8797	0.9733	0.7580	0.7976	0.8520
Cubic	0.8858	0.9844	0.7749	0.8058	0.8596

Table 4.3: Correlation coefficients between the HSO index of heptane isomers and their physicochemical properties.

Model	BP	MP
Linear	0.9766	0.0001
Quadratic	0.9771	0.7547
Cubic	0.9884	0.7613

Table 4.4: Correlation coefficients between the HSO index of hexane isomers and their physicochemical properties.

5. Conclusions

In this paper, we established several bounds for the HSO index and investigated its connections with other degree-based topological indices. We also employed linear and curvilinear regression models to assess the effectiveness of the HSO index in predicting five properties of heptane isomers and two properties of hexane isomers. Among the properties considered, the HSO index demonstrated strong predictive capability for the standard enthalpy of vaporization of heptane isomers and the boiling points of hexane isomers.

We define the monotonicity of the HSO index as the monotonic increase or decrease of its value under the addition or removal of edges in a graph G. We note that the monotonicity of the HSO index is uncertain. Let $e = uv$. For $e \notin E$, let $G + e$ denote the graph obtained from G by adding the edge e. In general, we cannot determine the magnitude relationship between $HSO(G)$ and $HSO(G + e)$, as illustrated in Figure 5.1.

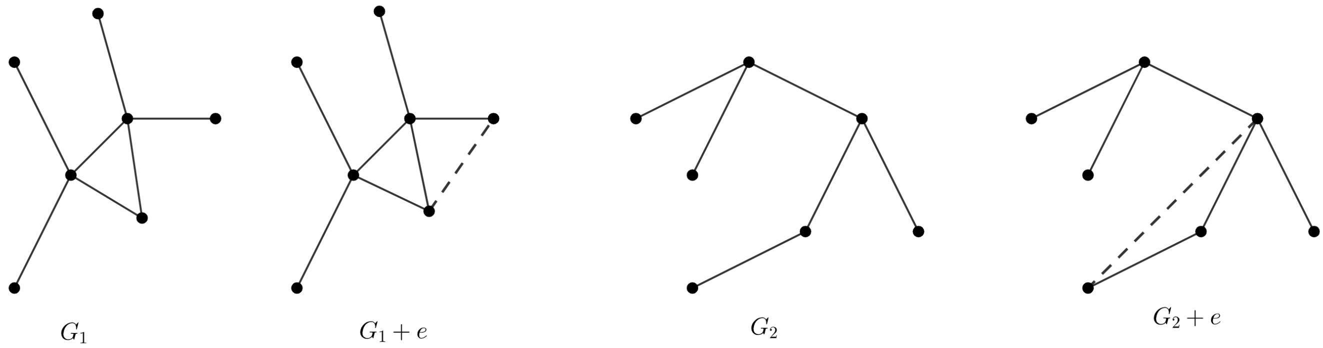

Figure 5.1: The graphs G_1 and G_2 satisfying $HSO(G_1) > HSO(G_1 + e)$ and $HSO(G_2) < HSO(G_2 + e)$.

Therefore, it is natural to consider the following problem.

Problem 5.1. *Characterize the graphs for which the HSO index is monotonic with respect to edge addition or deletion.*

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