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THE SECOND HYPER-GOURAVA STRESS INDEX OF GRAPHS: MATHEMATICAL PROPERTIES AND QSPR APPLICATIONS

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Abstract. The stress of a graph is the number of geodesics (shortest paths) that pass through each vertex. A topological index of a chemical structure (graph) is a number that correlates the chemical structure with its chemical reactivity or physical properties. In this paper, we introduce a new topological index for graphs called the second hyper-Gourava stress index, which is defined using the stresses of vertices. Further, we establish several inequalities, prove related results, and compute the second hyper-Gourava stress index for some standard graphs. Similarly, we establish the importance of the second hyper-Gourava stress index in predicting the physicochemical properties of lower alkanes.

1. Introduction

For standard terminology and notation in graph theory, we follow the textbook by Harary [7]. Any non-standard terminology required in this work will be introduced at the appropriate points.

Let $G = (V, E)$ be a finite, undirected graph. The distance between two vertices u and v in G, denoted by $d(u, v)$, is the number of edges in a shortest path a geodesic joining them. A geodesic P is said to pass through a vertex v if v appears as an internal vertex of P; that is, v lies on P but is not one of its endpoints. The degree of a vertex v is denoted by $d(v)$.

The notion of stress of a vertex as a centrality measure was introduced by Shimbel in 1953 [30]. This measure has since found applications in biology, sociology, psychology, and other disciplines (see [8, 29]). The stress of a vertex v in a graph G, denoted $str_G(v)$ or simply str(v), is defined as the number of geodesics that pass through v. The maximum and minimum stress among all vertices of G are denoted by Θ_G and θ_G, respectively. The concepts of the stress number and stress-regular graphs were introduced by Bhargava, Dattatreya, and Rajendra [3]. A graph G is said to be k-stress regular if $str(v) = k$, for every vertex $v \in V(G)$.

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The well-known Zagreb indices, defined in terms of vertex degrees, have been widely used to study molecular structures of chemical compounds [5, 6]. For a simple graph G, the first and second Zagreb indices are defined as:

$$M_1(G) = \sum_{v \in V(G)} d(v)^2, \tag{1.1}$$

$$M_2(G) = \sum_{uv \in E(G)} d(u)d(v). \tag{1.2}$$

Inspired by these classical indices, Rajendra et al. [24] introduced two analogous invariants based on vertex stress, called the first stress index and the second stress index. For a simple graph G, they are defined as

$$S_1(G) = \sum_{v \in V(G)} str(v)^2, \tag{1.3}$$

$$S_2(G) = \sum_{uv \in E(G)} str(u)\, str(v). \tag{1.4}$$

Motivated by these contributions, in this paper we introduce and study the second hyper-Gourava stress index of a graph.

For the discussion of stress-based indices and their QSPR analysis, the authors are encouraged to refer to the articles [1, 2, 4, 9–15, 17–28, 31, 32], as they provide valuable insights and may strengthen the scientific discussion and interpretation of the results.

2. Second Hyper-Gourava Stress Index

Definition 2.1. The second hyper-Gourava stress index $SHSI(G)$ of a graph G is defined as:

$$SHSI(G) = \sum_{uv \in E(G)} \left[(str(u) + str(v))(str(u)str(v))\right]^2. \tag{2.1}$$

Corollary 2.2. *If there is no geodesic of length ≥ 2 in a graph G, then $SHSI(G) = 0$.*

Proof. If there is no geodesic of length ≥ 2 in a graph G, then $N = 0$. Hence, by the Definition 2.1, we have $SHSI(G) = 0$.
In K_n, there is no geodesic of length ≥ 2 and so $SHSI(K_n) = 0$.

Theorem 2.3. *For a graph G, $SHSI(G) = 0$ if and only if neighbours of every vertex induce a complete subgraph of G.*

Proof. Suppose first that $SHSI(G) = 0$. By Definition 2.1, second hyper-Gourava stress index of G is:

$$SHSI(G) = \sum_{uv \in E(G)} \left[(str(u) + str(v))(str(u)str(v))\right]^2.$$

Since every summand is nonnegative and their sum is 0, each term must itself be equal to 0. Hence, for every edge $uv \in E(G)$,

$$[(str(u) + str(v))(str(u)str(v))]^2 = 0,$$

which implies

$$str(v) = 0, \qquad \text{for every } v \in V(G).$$

Let $v \in V(G)$. We show that the neighbours of v induce a complete subgraph. If v is pendant, the claim is immediate. Suppose instead that v is not pendant. Assume, for contradiction, that there exist neighbours $u, w \in N(v)$ with $uw \notin E(G)$. Then the path uvw is a geodesic of length 2 passing through v, which forces $str(v) \geq 1$, contradicting $str(v) = 0$. Thus, any two neighbours of v must be adjacent, and the subgraph induced by $N(v)$ is complete. Since v was arbitrary, this property holds for all vertices of G.

Conversely, suppose that the neighbours of every vertex of G induce a complete subgraph. Fix any $v \in V(G)$. Since every two neighbours of v are adjacent, there exists no geodesic of length at least 2 passing through v. Therefore,

$$str(v) = 0, \qquad \text{for all } v \in V(G).$$

Consequently, for each edge $uv \in E(G)$,

$$[(str(u) + str(v))(str(u)str(v))]^2 = 0.$$

Summing over all edges, we obtain

$$SHSI(G) = \sum_{uv \in E(G)} 0 = 0.$$

Proposition 2.4. *For the complete bipartite $K_{m,n}$,*

$$SHSI(K_{m,n}) = \frac{mn}{16} \left[mn(m-1)(n-1)(m^2 + n^2 - m - n)\right]^2.$$

Proof. Let $V_1 = \{v_1, \ldots, v_m\}$ and $V_2 = \{u_1, \ldots, u_n\}$ be the partite sets of $K_{m,n}$. We have:

$$str(v_i) = \frac{n(n-1)}{2} \text{ for } 1 \leq i \leq m \tag{2.2}$$

and

$$str(u_j) = \frac{m(m-1)}{2} \text{ for } 1 \leq j \leq n. \tag{2.3}$$

Using (2.2) and (2.3) in the Definition 2.1, we have

$$\begin{aligned}
SHSI(K_{m,n}) &= \sum_{uv\in E(G)} \left[(str(u)+str(v))(str(u)str(v))\right]^2 \\
&= \sum_{1\le i\le m,\ 1\le j\le m} \left[(str(v_i)+str(u_j))(str(v_i)str(u_j))\right]^2 \\
&= \sum_{1\le i\le m,\ 1\le j\le n} \left[\left(\frac{n(n-1)}{2}+\frac{m(m-1)}{2}\right)\left(\frac{mn(n-1)(m-1)}{2}\right)\right]^2 \\
&= \frac{mn}{16}\left[mn(m-1)(n-1)(m^2+n^2-m-n)\right]^2.
\end{aligned}$$

Proposition 2.5. *For the star graph $K_{1,n}$ on $n+1$ vertices ,*

$$SHSI(K_{1,n}) = 0.$$

Proof. In a star graph $K_{1,n}$, the internal vertex has stress $\frac{n(n-1)}{2}$ and the remaining n vertices have stress 0. By the Definition 2.1, we have:

$$\begin{aligned}
SHSI(K_{1,n}) &= \sum_{uv\in E(G)} \left[(str(u)+str(v))(str(u)str(v))\right]^2 \\
&= 0.
\end{aligned}$$

Proposition 2.6. *If $G=(V,E)$ is a k-stress regular graph, then*

$$SHSI(G) = 2k^6|E|.$$

Proof. Suppose that G is a k-stress regular graph. Then

$$str(v)=k, \text{ for all } v\in V(G).$$

By the Definition 2.1, we have

$$\begin{aligned}
SHSI(K_{1,n}) &= \sum_{uv\in E(G)} \left[(str(u)+str(v))(str(u)str(v))\right]^2 \\
&= \sum_{uv\in E(G)} \left[(k+k)(k^2)\right]^2 \\
&= (2k^3)^2|E| \\
&= 2k^6|E|.
\end{aligned}$$

Proposition 2.7. *Let $G_1, G_2, \dots, G_m$ be the components of a disconnected graph H. Then the second hyper-Gourava stress index of H is given by*

$$SHSI(H) = SHSI(G_1)+SHSI(G_2)+\cdots+SHSI(G_m).$$

Proof. We have $H = \bigcup_{i=1}^{m} G_i$. Note that an edge $uv \in E(H)$ if and only if uv belongs to the same component. Hence,

$$SHSI(H) = SHSI\left(\bigcup_{i=1}^{m} G_i\right)$$

$$= \sum_{u_{1i}v_{1i}\in E(G_1)} [(str(u_{1i}) + str(v_{1i}))(str(u_{1i})str(v_{1i}))]^2 + \cdots$$
$$+ \sum_{u_{mi}v_{mi}\in E(G_m)} [(str(u_{mi}) + str(v_{mi}))(str(u_{mi})str(v_{mi}))]^2$$
$$=SHSI(G_1) + SHSI(G_2) + SHSI(G_3) + \cdots + SHSI(G_m).$$

Corollary 2.8. *For a cycle C_n,*

$$SHSI(C_n) = n \times \begin{cases} 2k^6, & \text{if } n \text{ is odd,} \\ 2\ell^6, & \text{if } n \text{ is even,} \end{cases}$$

where

$$k = \frac{(n-1)(n-3)}{8} \quad \text{and} \quad \ell = \frac{n(n-2)}{8}.$$

Proof. For any vertex v in C_n, we have

$$str(v) = \begin{cases} \frac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd,} \\ \frac{n(n-2)}{8}, & \text{if } n \text{ is even.} \end{cases}$$

Hence, C_n is

$$\begin{cases} \frac{(n-1)(n-3)}{8}\text{-stress regular}, & \text{if } n \text{ is odd,} \\ \frac{n(n-2)}{8}\text{-stress regular}, & \text{if } n \text{ is even.} \end{cases}$$

Since C_n has n vertices and n edges, by Proposition 2.6, we obtain

$$SHSI(C_n) = n \times \begin{cases} 2k^6, & \text{if } n \text{ is odd,} \\ 2\ell^6, & \text{if } n \text{ is even,} \end{cases}$$

where

$$k = \frac{(n-1)(n-3)}{8} \quad \text{and} \quad \ell = \frac{n(n-2)}{8}.$$

Corollary 2.9. *For the path P_n on n nodes*

$$SHSI(P_n) = \sum_{i=1}^{n-1} [((i-1)(n-i) + i(n-i-1))(i(i-1)(n-i)(n-i-1))]^2.$$

Proof. Let P_n be the path with node sequence $v_1, v_2, \ldots, v_n$. We have:

$$\mathrm{str}(v_i) = (i-1)(n-i),\ 1 \le i \le n.$$

Then

$$\begin{aligned}
SHSI(P_n) &= \sum_{uv \in E(P_n)} \left[(str(u) + str(v))(str(u)str(v))\right]^2 \\
&= \sum_{i=1}^{n-1} \left[(str(v_i) + str(v_{i+1}))(str(v_i)str(v_{i+1}))\right]^2 \\
&= \sum_{i=1}^{n-1} \left[((i-1)(n-i) + i(n-i-1))(i(i-1)(n-i)(n-i-1))\right]^2.
\end{aligned}$$

Proposition 2.10. *Let W_n denotes the wheel graph constructed on $n \ge 4$ vertices. Then*

$$SHSI(W_n) = (n-1)\left[\frac{(n-1)^2(n-4)^2}{4} + \frac{(n-1)(n-4)}{2}\right]^2 + 4(n-1).$$

Proof. In W_n with $n \ge 4$, there are $(n-1)$ peripheral vertices and one central vertex, say v. It is easy to see that

$$\mathrm{str}(v) = \frac{(n-1)(n-4)}{2}. \tag{2.4}$$

Let p be a peripheral vertex. Since v is adjacent to all the peripheral vertices in W_n, there is no geodesic passing through p and containing v. Hence contributing vertices for $\mathrm{str}(p)$ are the rest peripheral vertices. So, by denoting the cycle $W_n - p$ (on $n-1$ vertices) by C_{n-1}, we have

$$\begin{aligned}
\mathrm{str}_{W_n}(p) &= \mathrm{str}_{W_n - v}(p) \\
&= \mathrm{str}_{C_{n-1}}(p) \\
&= 1.
\end{aligned} \tag{2.5}$$

Let us denote the set of all radial edges in W_n by R, and the set of all peripheral edges by Q. Note that there are $(n-1)$ radial edges and $(n-1)$ peripheral edges in W_n. By using Definition 2.1, we have

$$\begin{aligned}
SHSI(W_n) = &\sum_{xy \in R} \left[(str(x) + str(y))(str(x)str(y))\right]^2 \\
&+ \sum_{xy \in Q} \left[(str(x) + str(y))(str(x)str(y))\right]^2 \\
=&(n-1)\left[(str(v) + str(p))(str(v)str(p))\right]^2 + (n-1)\left[(str(p)^2)(2str(p))\right]^2 \\
=&(n-1)\left[\left(\frac{(n-1)(n-4)}{2} + 1\right)\left(\frac{(n-1)(n-4)}{2}\right)\right]^2 + 4(n-1) \\
=&(n-1)\left[\frac{(n-1)^2(n-4)^2}{4} + \frac{(n-1)(n-4)}{2}\right]^2 + 4(n-1).
\end{aligned}$$

Proposition 2.11. *For the complement of a cycle C_n $(n \geq 5)$, the second hyper-Gourava stress index is given by*

$$SHSI(\overline{C_n}) = \frac{2n(n-3)\ell^6}{2}, \qquad \text{where } \ell = n-4.$$

Proof. Let $G = \overline{C_n}$ and $V(G) = \{v_1, v_2, \ldots, v_n\}$ (from [16] of Theorem 2.5)

$$st(v_i) = n-4, \quad v_i \in V(G)$$

and the total number of edges in G is

$$|E(G)| = \frac{n(n-3)}{2}$$

By the Definition 2.1, we have

$$SHSI(G) = \sum_{uv \in E(G)} \left[(str(u) + str(v))(str(u)str(v))\right]^2.$$

We have $st(u) = st(v) = n-4$, for all $u, v \in V(G)$. Then

$$SHSI(\overline{C_n}) = \sum_{uv \in E(G)} 2\ell^6$$

$$\text{SHSI}(\overline{C_n}) = \frac{2\ell^6 n(n-3)}{2}, \qquad \text{where } \ell = n-4.$$

Proposition 2.12. *For the line graph of the complete graph K_n,*

$$SHSI(L(K_n)) = 2\ell^6 n(n-1)(n-2) \qquad \text{where } \ell = (n-2)(n-3).$$

Proof. For $G = L(K_n)$, each vertex satisfies (from [16] of Theorem 2.12)

$$st(v) = (n-2)(n-3), \quad v \in V(G),$$

and the total number of edges in G is

$$|E(G)| = n(n-1)(n-2).$$

By Definition 2.1,

$$SHSI(L(K_n)) = \sum_{uv \in E(G)} \left[(str(u) + str(v))(str(u)str(v))\right]^2.$$

We have $st(u) = st(v) = (n-2)(n-3)$, for all $u, v \in V(G)$. Then

$$SHSI(L(K_n)) = \sum_{uv \in E(G)} 2\ell^6$$

$$SHSI(L(K_n)) = 2\ell^6 n(n-1)(n-2), \qquad \text{where } \ell = (n-2)(n-3).$$

Proposition 2.13. *For the line graph of $K_{m,n}$,*

$$SHSI(L(K_{m,n})) = \frac{2\ell^6 mn(m+n-2)}{2}, \qquad \text{where } \ell = mn - m + 1.$$

Proof. For $G = L(K_{m,n})$, each vertex satisfies (from [16] of Theorem 2.14)

$$st(v) = mn - m - n + 1, \quad v \in V(G),$$

and the total number of edges in G is

$$|E(G)| = \frac{mn(m+n-2)}{2}.$$

By Definition 2.1,

$$SHSI(L(K_{m,n})) = \sum_{uv\in E(G)} [(str(u) + str(v))(str(u)str(v))]^2$$

. We have $st(u) = st(v) = mn - m - n + 1$, for all $u, v \in V(G)$. Then

$$SHSI(L(K_{m,n})) = \sum_{uv\in E(G)} 2\ell^6$$

$$SHSI(L(K_{m,n})) = \frac{2\ell^6 mn(m+n-2)}{2}, \qquad \text{where } \ell = mn - m + 1.$$

Proposition 2.14. *Let K_n and K_m be complete graphs on n and m vertices, respectively. Then for the Kronecker product of K_n and K_m, denoted by $K_n \otimes K_m$,*

$$SHSI(K_n \otimes K_m) = \frac{2\ell^6 mn(m-1)(n-1)}{2}, \qquad \text{where } \ell = \frac{(n-1)(m-1)(m+n-4)}{2}.$$

Proof. For $G = K_n \otimes K_m$ each vertex satisfies (from [16] of Theorem 2.14)

$$str(v) = \frac{(n-1)(m-1)(m+n-4)}{2}. \quad v \in V(G).$$

$$\begin{aligned}
SHSI(K_n \otimes K_m) &= \sum_{uv\in E(G)} [(str(u) + str(v))(str(u)str(v))]^2 \\
&= \sum_{uv\in E(G)} 2\ell^6 \\
&= \frac{2\ell^6 mn(m-1)(n-1)}{2}, \qquad \text{where } \ell = \frac{(n-1)(m-1)(m+n-4)}{2}.
\end{aligned}$$

3. The Significance of Second Hyper-Gourava Stress Index in Predicting the Physicochemical Properties of Lower Alkanes

Quantitative structure-property relationships, also known as QSPR, continue to be the primary focus of numerous studies that are employed for the purpose of modeling and predicting the physicochemical and biological properties of molecules. In this endeavor, chemometrics is a powerful tool that can be of assistance. In order to extract the maximum amount of information possible from a data set, it employs statistical and mathematical methods. In order to describe how a particular physicochemical property varies as a function of molecular descriptors that describe the chemical structure of the molecule, quantitative spectroscopic spectroscopy (QSPR) makes use of chemometric methods. Therefore, it is possible to replace expensive biological tests or experiments of a particular physicochemical property with calculated descriptors. These descriptors can then be used to predict the responses of interest for new compounds without the need for the biological tests or experiments. To find an optimal quantitative relationship, which can be used to indicate the properties of compounds, including those that have not been measured, is the fundamental strategy behind quantitative spectrophotometry (QSPR). It should come as no surprise that the parameters that are utilized to describe the molecular structure are the primary factors that determine how well the QSPR model performs. The development of alternative molecular descriptors that can be derived solely from the information encoded in the chemical structure has been the subject of a great deal of experimentation and research. There has been a significant amount of focus placed on ”topological indices,” which are derived from the connectivity and composition of a molecule. These indices have made significant contributions to the field of QSPR research. Because of its ease of use and its rapid computation speed, the topological index has garnered the interest of researchers in the scientific community.

The QSPR analysis of the second hyper-Gourava stress index is going to be the topic of discussion in this section. In addition, we demonstrate that the characteristics have a strong correlation with the physicochemical properties of lower alkanes, which are presented in Table 1. QSPR analysis is performed using the experimental values of the physical properties of the considered lower alkanes listed in Table 1, such as boiling points (bp) $^\circ C$, molar volumes (mv) cm^3, molar refractions (mr) cm^3, heats of vaporisation (hv) kJ, critical temperatures (ct) $^\circ C$, critical pressures (cp) atm, and surface tensions (st) $dyne\ cm^{-1}$.

TABLE 1. The experimental numerical values of the physical properties of low alkanes

Alkane	$SHSI(G)$	$\frac{bp}{^\circ C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{^\circ C}$	$\frac{cp}{atm}$	$\frac{st}{dyne\ cm^{-1}}$
Pentane	14112	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	14400	27.9	116.4	25.29	24.6	187.8	32.9	15
Hexane	244224	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	355716	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	294912	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	219024	49.7	132.7	29.93	27.7	216.2	30.7	16.3
2,3-Dimethylbutane	470596	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	3537152	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	3894340	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	3840384	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylhexane	3121200	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,2-Dimethylpentane	3956800	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	4694800	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	4251528	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	2737800	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	5143824	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	27726336	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	29052432	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	29793024	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	29968200	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	27148288	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	31510800	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	33388200	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	31119120	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	30378528	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	27493416	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	35762944	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	31502592	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	20155392	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	19662984	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	32836896	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	66215268	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	36808200	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	163040832	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	166685616	143.3	179.8	43.88	44.7	315	23.6	21.88
3-Methyloctane	170245728	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	172566756	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	164993616	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	69532960	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	177403680	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	182536132	140.5	176.7	43.63	43.8	315	23.79	22.34

2,4-Dimethylheptane	176211540	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	173890512	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	170330400	135.2	180.9	43.93	42.8	306	23.7	20.83
3,3-Dimethylheptane	171703872	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	195870960	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	177450624	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	166231584	135.2	176.9	43.6	42.7	317.8	24.18	22.01
3-Ethyl-2-methylhexane	174800052	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	168638400	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	142520616	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	194989936	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	212627556	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	184608576	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	181048464	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	183315892	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	205840336	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	186180916	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	175348656	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	209134548	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	108493056	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	215719200	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	162521496	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	189252504	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	234268020	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	109199700	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	191766528	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	200400200	141.6	169.9	43.2	41.8	334.5	26.85	23.31

TABLE 2. Statical parameters for the logarithmic QSPR model for Second hyper-Gourava stress Index $SHSI(G)$ of lower alkanes

Physiochemical properties	R	R^2	Adjusted R^2	F	Sig
boiling points (BP) $°C$	0.968	0.936	0.935	969.561	0.000
molar volumes (MV) cm^3	0.976	0.952	0.951	1300.641	0.000
molar refractions (MR) cm^3	0.988	0.977	0.976	2744.992	0.000
heats of vaporisation (HV) kJ	0.938	0.880	0.878	481.958	0.000
critical temperatures (CT) $°C$	0.954	0.910	0.909	669.444	0.000
critical pressures (cp) atm	0.860	0.740	0.736	188.044	0.000
surface tensions (ST) $dyne\ cm^{-1}$	0.874	0.765	0.761	214.409	0.000

Regression Models. By utilizing the data of Table 1 and Table 2 we have the regression model for considered physiochemical properties of compounds as in the list. The evaluation of logarithm regression model is considered as

$$P = A + B \cdot log(SHSI(G)),$$

where P = Physical property and $SHSI(G)$ = Second Hyper-Gourava Stress Index.

The logarithm Regression Model for second hyper-Gourava stress Index of Graph G:

The logarithmic regression models for boiling points (BP) $°C$, molar volumes (MV) cm^3, molar refractions (MR) cm^3, heats of vaporisation (HV) kJ, critical temperatures (CT) $°C$, critical pressures (cp) atm and surface tensions (ST) $dyne\ cm^{-1}$ of lower alkanes are as follows:

$$BP = -88.162 + 11.820 \cdot log(SHSI(G)) \tag{3.1}$$

$$MV = 43.728 + 6.914 \cdot log(SHSI(G)) \tag{3.2}$$

$$MR = 3.261 + 2.107 \cdot log(SHSI(G)) \tag{3.3}$$

$$HV = 4.714 + 1.986 \cdot log(SHSI(G)) \tag{3.4}$$

$$CT = 49.467 + 14.099 \cdot log(SHSI(G)) \tag{3.5}$$

$$CP = 42.389 - 0.935 \cdot log(SHSI(G)) \tag{3.6}$$

$$ST = 8.530 + 0.718 \cdot log(SHSI(G)). \tag{3.7}$$

Figure 1: Graphical representation of the scattered points and its logarithm fit using $SHSI(G)$ for boiling point

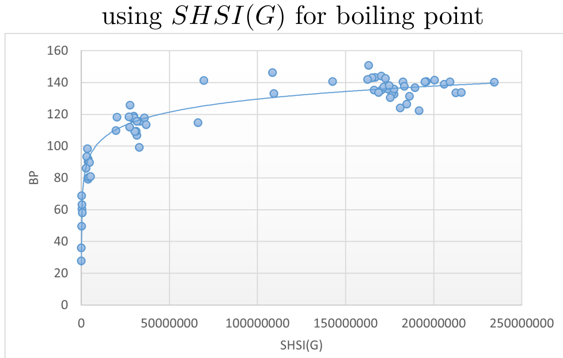


Figure 2: Graphical representation of the scattered points and its logarithm fit using $SHSI(G)$ for molar volumes

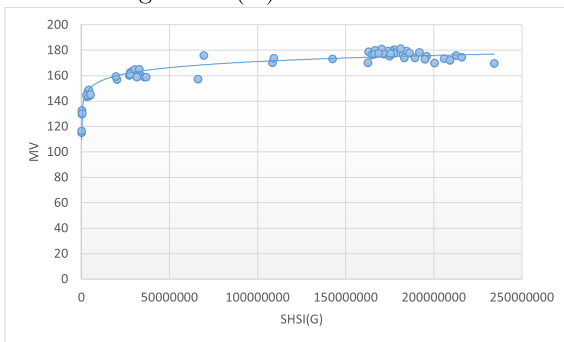


Figure 3: Graphical representation of the scattered points and its logarithm fit using $SHSI(G)$ for molar refractions

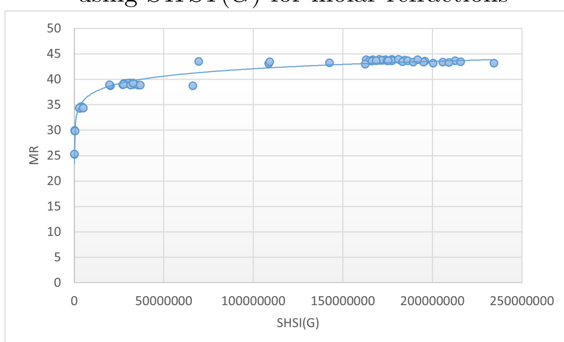


Figure 4: Graphical representation of the scattered points and its logarithm fit using $SHSI(G)$ for heats of vaporisation

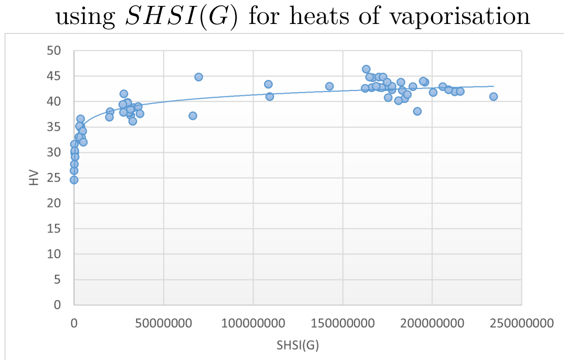


Figure 5: Graphical representation of the scattered points and its logarithm fit using $SHSI(G)$ for critical temperatures

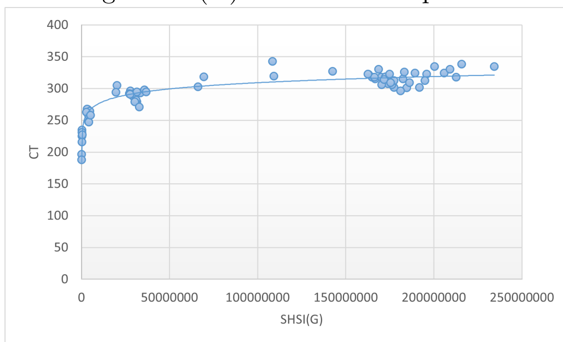


Figure 6: Graphical representation of the scattered points and its logarithm fit using $SHSI(G)$ for critical pressures

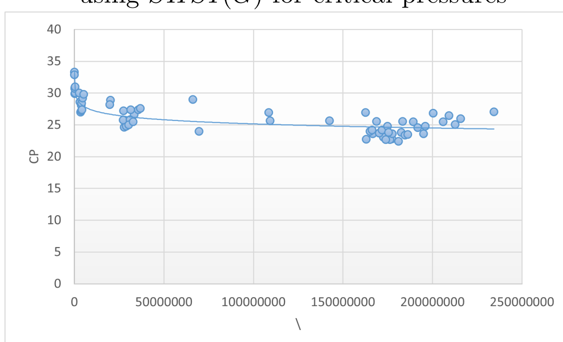
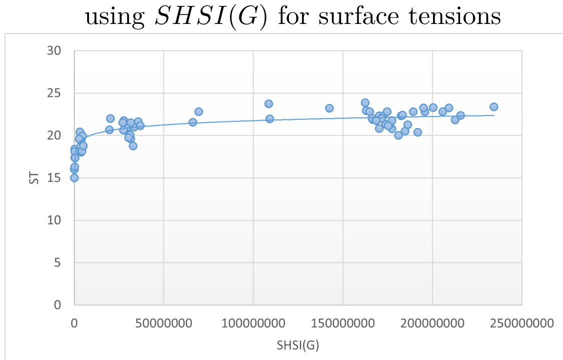


Figure 7: Graphical representation of the scattered points and its logarithm fit using $SHSI(G)$ for surface tensions



Conclusion

In this work, we introduced a new vertex stress-based topological descriptor, namely the second hyper-Gourava stress index, and investigated its mathematical and chemical significance. We established several fundamental properties and inequalities associated with this index and derived exact expressions for various standard classes of graphs, thereby providing a theoretical foundation for its study.

To assess its practical applicability, we employed the second hyper-Gourava stress index in quantitative structure–property relationship (QSPR) analysis of lower alkanes. The obtained results demonstrate that this index serves as an effective molecular descriptor for predicting selected physicochemical properties, indicating its potential usefulness in mathematical chemistry and cheminformatics. The combination of rigorous mathematical analysis and successful QSPR modeling highlights the relevance of the proposed index as both a graph invariant and a predictive tool.

The present work opens several directions for future research. Exact formulas for broader families of graphs may be derived, and extremal problems involving the second hyper-Gourava stress index can be investigated. Moreover, its relationships with other stress-based and Gourava-type topological indices deserve further exploration. From an application perspective, the predictive capability of the proposed index may be examined for larger and more diverse classes of chemical compounds, as well as in quantitative structure–activity relationship (QSAR) studies, to further establish its effectiveness in chemical graph theory and molecular property prediction.

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