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A NOVEL FIRST HYPER-GOURAVA STRESS INDEX OF GRAPHS WITH 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 first hyper-Gourava stress index, which is defined using the stresses of vertices. Further, we establish several inequalities, prove related results, and compute the first hyper-Gourava stress index for some standard graphs. Similarly, we establish the importance of the first 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 [44]. This measure has since found applications in biology, sociology, psychology, and other disciplines (see [10, 42]). 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 $v \in V(G)$.

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

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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. [33] 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 first hyper-Gourava stress index of a graph.

Over the years, numerous stress-related concepts in graph theory, particularly those involving topological indices and graph energy, have been introduced, developed, and extensively investigated by several researchers, contributing significantly to the advancement of chemical graph theory and related fields (See [1–4, 8, 9, 11–23, 25–41, 43, 45–48]).

2. First Hyper-Gourava Stress Index

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

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

Corollary 2.2. *If a graph G contains no geodesic of length at least 2, then $FHSI(G) = 0$.*

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

Theorem 2.3. *Let G be a graph. The first hyper-Gourava stress index of G is zero if and only if the open neighborhood of every vertex induces a complete subgraph.*

Proof. Suppose first that $FHSI(G) = 0$. By Definition 2.1,

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

Since each summand is nonnegative, the equality $FHSI(G) = 0$ implies that every summand is zero. Hence,

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

for every edge $uv \in E(G)$. As the stress of every vertex is a nonnegative integer, the above equality is possible only when

$$str(u) = 0 \qquad \text{and} \qquad str(v) = 0.$$

Therefore,

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

We now show that the neighbourhood of every vertex induces a complete subgraph. Let $v \in V(G)$, and suppose, to the contrary, that $N(v)$ is not complete. Then there exist distinct vertices $u, w \in N(v)$ such that $uv \in E(G)$. Since u and w are both adjacent to v, the path

$$uvw$$

has length 2. As u and w are nonadjacent, no shorter path exists between them, so uvw is a geodesic. Consequently, v is an internal vertex of a geodesic, which implies

$$str(v) \geq 1,$$

contradicting $str(v) = 0$. Hence, every two neighbours of v are adjacent, and therefore $G[N(v)]$ is complete.

Conversely, suppose that the neighbourhood of every vertex induces a complete subgraph. Let $v \in V(G)$. If v were an internal vertex of some geodesic uvw, then $u, w \in N(v)$. Since $G[N(v)]$ is complete, u and w are adjacent. Thus, the edge uw is a path of length 1, contradicting the fact that uvw is a geodesic of length 2. Hence, no vertex is an internal vertex of any geodesic, and therefore

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

Substituting these values into the definition of $FHSI(G)$, we obtain

$$FHSI(G) = \sum_{uv \in E(G)} \left[str(u) + str(v) + str(u)str(v)\right]^2 = 0.$$

Therefore,

$$FHSI(G) = 0$$

if and only if the neighbourhood of every vertex induces a complete subgraph. □

Proposition 2.4. *For the complete bipartite graph $K_{m,n}$, the first hyper-Gourava stress index depends only on the sizes of its two partite sets and is expressed as*

$$FHSI(K_{m,n}) = \frac{mn}{4} \left[n(n-1) + m(m-1) + mn(n-1)(m-1)\right]^2.$$

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

$$\begin{aligned}
FHSI(K_{m,n}) &= \sum_{uv\in E(G)} [str(u)+str(v)+str(u)str(v)]^2 \\
&= \sum_{1\le i\le m,\ 1\le j\le m} [str(v_i)+str(u_j)+str(v_i)str(u_j)]^2 \\
&= \sum_{1\le i\le m,\ 1\le j\le n} \left[\frac{n(n-1)}{2}+\frac{m(m-1)}{2}+\frac{mn(n-1)(m-1)}{2}\right]^2 \\
&= \frac{mn}{4}\left[n(n-1)+m(m-1)+mn(n-1)(m-1)\right]^2.
\end{aligned}$$

Proposition 2.5. *The first hyper-Gourava stress index of the star graph $K_{1,n}$ on $n+1$ vertices is determined by*

$$FHSI(K_{1,n}) = \frac{n^3(n-1)^2}{4}.$$

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:

$$\begin{aligned}
FHSI(K_{1,n}) &= \sum_{uv\in E(G)} [str(u)+str(v)+str(u)str(v)]^2 \\
&= \frac{n^3(n-1)^2}{4}.
\end{aligned}$$

Proposition 2.6. *For a k-stress regular graph $G=(V,E)$, the first hyper-Gourava stress index satisfies*

$$FHSI(G) = (4k^2+4k^3+k^4)|E|.$$

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:

$$\begin{aligned}
FHSI(K_{1,n}) &= \sum_{uv\in E(G)} [str(u)+str(v)+str(u)str(v)]^2 \\
&= \sum_{uv\in E(G)} (k+k+k^2)^2 \\
&= (2k+k^2)^2|E| \\
&= (4k^2+4k^3+k^4)|E|.
\end{aligned}$$

Proposition 2.7. *Let* $H = \bigcup_{i=1}^{m} G_i$ *be a disconnected graph with components* $G_1, G_2, \cdots, G_m$*. The first hyper-Gourava stress index is additive over the components of* H*, and hence*

$$FHSI(H) = \sum_{i=1}^{m} FHSI(G_i).$$

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,

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

$$\begin{aligned}
&= \sum_{u_{1i}v_{1i}\in E(G_1)} [(str(u_{1i}) + str(v_{1i}) + str(u_{1i})str(v_{1i})]^2 + \cdots \\
&\quad + \sum_{u_{mi}v_{mi}\in E(G_m)} [(str(u_{mi}) + str(v_{mi}) + str(u_{mi})str(v_{mi})]^2 \\
&= FHSI(G_1) + FHSI(G_2) + FHSI(G_3) + \cdots + FHSI(G_m) \\
&= \sum_{i=1}^{m} FHSI(G_i).
\end{aligned}$$

Corollary 2.8. *For a cycle* C_n*,*

$$FHSI(C_n) = n \times \begin{cases} 4k^2 + 4k^3 + k^4, & \text{if } n \text{ is odd,} \\ 4\ell^2 + 4\ell^3 + \ell^4, & \text{if } n \text{ is even,} \end{cases}$$

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

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

Hence, C_n is

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

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

$$FHSI(C_n) = n \times \begin{cases} 4k^2 + 4k^3 + k^4, & \text{if } n \text{ is odd,} \\ 4\ell^2 + 4\ell^3 + \ell^4, & \text{if } n \text{ is even,} \end{cases}$$

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*

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

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

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

Then

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

Proposition 2.10. *The first hyper-Gourava stress index of the wheel graph W_n with $n \geq 4$ vertices can be expressed as*

$$FHSI(W_n) = (n-1)\left[(n-1)(n-4) + 1\right]^2 + 9(n-1).$$

Proof. In W_n with $n \geq 4$, 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

$$\begin{aligned}
FHSI(W_n) = &\sum_{xy\in R} [str(x) + str(y) + str(x)str(y)]^2 \\
&+ \sum_{xy\in Q} [str(x) + str(y) + str(x)str(y)]^2 \\
=&(n-1)\left[str(v) + str(p) + str(v)str(p)\right]^2 + (n-1)\left[str(p)^2 + 2str(p)\right]^2 \\
=&(n-1)\left[\frac{(n-1)(n-4)}{2} + 1 + \frac{(n-1)(n-4)}{2}\right]^2 + 9(n-1) \\
=&(n-1)\left[(n-1)(n-4)+1\right]^2 + 9(n-1).
\end{aligned}$$

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

$$FHSI(\overline{C_n}) = \frac{n(n-3)}{2}\left(4\ell^2 + 4\ell^3 + \ell^4\right), \qquad \textit{where } \ell = n-4.$$

Proof. Let $G = \overline{C_n}$ and $V(G) = \{v_1, v_2, \ldots, v_n\}$ (from [24] 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:

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

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

$$FHSI(\overline{C_n}) = \sum_{uv\in E(G)} 4\ell^2 + 4\ell^3 + \ell^4$$

$$FHSI(\overline{C_n}) = \frac{n(n-3)}{2}\left(4\ell^2 + 4\ell^3 + \ell^4\right), \qquad \text{where } \ell = n-4.$$

Proposition 2.12. *The first hyper-Gourava stress index of the line graph $L(K_n)$ of the complete graph K_n satisfies*

$$FHSI(L(K_n)) = n(n-1)(n-2)(4\ell^2 + 4\ell^3 + \ell^4), \ \textit{where } \ell = (n-2)(n-3).$$

Proof. For $G = L(K_n)$, each vertex satisfies (from [24] 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,

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

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

$$FHSI(L(K_n)) = \sum_{uv \in E(G)} 4\ell^2 + 4\ell^3 + \ell^4$$

$$FHSI(L(K_n)) = n(n-1)(n-2)(4\ell^2 + 4\ell^3 + \ell^4) \qquad \text{where } \ell = (n-2)(n-3).$$

Proposition 2.13. *The first hyper-Gourava stress index of the line graph $L(K_{m,n})$ of the complete bipartite graph $K_{m,n}$ satisfies*

$$FHSI(L(K_{m,n}) = \frac{mn(m+n-2)}{2}(4\ell^2 + 4\ell^3 + \ell^4),$$

where $\ell = mn - m + 1$.

Proof. For $G = L(K_{m,n})$, each vertex satisfies (from [24] 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,

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

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

$$FHSI(L(K_{m,n})) = \sum_{uv \in E(G)} 4\ell^2 + 4\ell^3 + \ell^4$$

$$FHSI(L(K_{m,n})) = \frac{mn(m+n-2)}{2}(4\ell^2 + 4\ell^3 + \ell^4), \qquad \text{where } \ell = mn - m + 1.$$

Proposition 2.14. *For the Kronecker product of complete graphs K_n and K_m, denoted by $K_n \otimes K_m$, the first hyper-Gourava stress index satisfies*

$$FHSI(K_n \otimes K_m) = \frac{mn(m-1)(n-1)}{2}(4\ell^2 + 4\ell^3 + \ell^4),$$

where $\ell = \dfrac{(n-1)(m-1)(m+n-4)}{2}$.

Proof. For $G = K_n \otimes K_m$ each vertex satisfies (from [24] of Theorem 2.14)

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

Then

$$\begin{aligned} FHSI(K_n \otimes K_m) &= \sum_{uv \in E(G)} [str(u) + str(v) + str(u)str(v)]^2 \\ &= \sum_{uv \in E(G)} 4\ell^2 + 4\ell^3 + \ell^4 \\ &= \frac{mn(m-1)(n-1)}{2}(4\ell^2 + 4\ell^3 + \ell^4), \end{aligned}$$

where $\ell = \dfrac{(n-1)(m-1)(m+n-4)}{2}$.

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

Quantitative structure–property relationship (QSPR) analysis has become an essential approach in molecular modeling for predicting the physicochemical and biological properties of chemical compounds. In QSPR studies, chemometric techniques play a significant role by applying statistical and mathematical methods to extract meaningful information from molecular data sets. These methods establish quantitative relationships between molecular descriptors and the corresponding physicochemical properties of compounds.

The primary objective of QSPR modeling is to develop reliable mathematical models that correlate molecular structure descriptors with experimentally measured properties. Such models allow the prediction of properties for new compounds without requiring costly and time-consuming experimental investigations. The effectiveness of a QSPR model largely depends on the selection of suitable molecular descriptors that accurately represent the structural characteristics of molecules.

Among various molecular descriptors, topological indices have received considerable attention due to their ability to characterize molecular structures using graph-theoretical approaches. These indices, derived from molecular connectivity and structural information, are computationally efficient and have demonstrated significant applications in QSPR analysis. Their simplicity, rapid calculation, and capability to capture important structural features make them valuable tools in mathematical chemistry.

In this section, we investigate the QSPR applicability of the First Hyper-Gourava Stress Index (FHSI) for lower alkanes. The relationship between FHSI values and selected physicochemical properties is examined to evaluate the predictive potential of the proposed descriptor. The experimental data of the considered lower alkanes are presented in Table 1. The investigated physicochemical properties include boiling point ((bp) $°C$), molar volume ((mv) cm^3), molar refraction ((mr) cm^3), heat of vaporization ((hv) kJ), critical temperature ((ct) $°C$), critical pressure ((cp) atm), and surface tension ((st) $dyne\ cm^{-1}$).

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

Alkane	$FHSI(G)$	$\frac{bp}{°C}$	$\frac{mv}{cm^3}$	$\frac{mr}{cm^3}$	$\frac{hv}{kJ}$	$\frac{ct}{°C}$	$\frac{cp}{atm}$	$\frac{st}{dyne\ cm^{-1}}$
Pentane	740	36.1	115.2	25.27	26.4	196.6	33.3	16
2-Methylbutane	588	27.9	116.4	25.29	24.6	187.8	32.9	15
2,2-Dimethylpropane	144	9.5	122.1	25.72	21.8	160.6	31.6	
Hexane	3492	68.7	130.7	29.91	31.6	234.7	29.9	18.42
2-Methylpentane	4295	60.3	131.9	29.95	29.9	224.9	30	17.38
3-Methylpentane	3968	63.3	129.7	29.8	30.3	231.2	30.8	18.12
2,2-Dimethylbutane	2660	49.7	132.7	29.93	27.7	216.2	30.7	16.3
2,3-Dimethylbutane	4165	58	130.2	29.81	29.1	227.1	31	17.37
Heptane	21510	98.4	146.5	34.55	36.6	267	27	20.26
2-Methylhexane	20718	90.1	147.7	34.59	34.8	257.9	27.2	19.29
3-Methylhexane	17862	91.9	145.8	34.46	35.1	262.4	28.1	19.79
3-Ethylhexane	19470	93.5	143.5	34.28	35.2	267.6	28.6	20.44
2,2-Dimethylpentane	16722	79.2	148.7	34.62	32.4	247.7	28.4	18.02
2,3-Dimethylpentane	19510	89.8	144.2	34.32	34.2	264.6	29.2	19.96
2,4-Dimethylpentane	19926	80.5	148.9	34.62	32.9	247.1	27.4	18.15
3,3-Dimethylpentane	14166	86.1	144.5	34.33	33	263	30	19.59
2,3,3-Trimethylbutane	17235	80.9	145.2	34.37	32	258.3	29.8	18.76
Octane	80176	125.7	162.6	39.19	41.5	296.2	24.64	21.76
2-Methylheptane	78467	117.6	163.7	39.23	39.7	288	24.8	20.6
3-Methylheptane	74660	118.9	161.8	39.1	39.8	292	25.6	21.17
4-Methylheptane	73099	117.7	162.1	39.12	39.7	290	25.6	21
3-Ethylhexane	68238	118.5	160.1	38.94	39.4	292	25.74	21.51
2,2-Dimethylhexane	69500	106.8	164.3	39.25	37.3	279	25.6	19.6
2,3-Dimethylhexane	73385	115.6	160.4	38.98	38.8	293	26.6	20.99
2,4-Dimethylhexane	72951	109.4	163.1	39.13	37.8	282	25.8	20.05
2,5-Dimethylhexane	76758	109.1	164.7	39.26	37.9	279	25	19.73
3,3-Dimethylhexane	60860	112	160.9	39.01	37.9	290.8	27.2	20.63
3,4-Dimethylhexane	72272	117.7	158.8	38.85	39	298	27.4	21.62
3-Ethyl-2-methylpentane	69371	115.7	158.8	38.84	38.5	295	27.4	21.52
3-Ethyl-3-methylpentane	52704	118.3	157	38.72	38	305	28.9	21.99
2,2,3-Trimethylpentane	44202	109.8	159.5	38.92	36.9	294	28.2	20.67
2,2,4-Trimethylpentane	67791	99.2	165.1	39.26	36.1	271.2	25.5	18.77
2,3,3-Trimethylpentane	93738	114.8	157.3	38.76	37.2	303	29	21.56
2,3,4-Trimethylpentane	73671	113.5	158.9	38.87	37.6	295	27.6	21.14
Nonane	253896	150.8	178.7	43.84	46.4	322	22.74	22.92
2-Methyloctane	250456	143.3	179.8	43.88	44.7	315	23.6	21.88

3-Methyloctane	240760	144.2	178	43.73	44.8	318	23.7	22.34
4-Methyloctane	233368	142.5	178.2	43.77	44.8	318.3	23.06	22.34
3-Ethylheptane	221608	143	176.4	43.64	44.8	318	23.98	22.81
4-Ethylheptane	136390	141.2	175.7	43.49	44.8	318.3	23.98	22.81
2,2-Dimethylheptane	231604	132.7	180.5	43.91	42.3	302	22.8	20.8
2,3-Dimethylheptane	233808	140.5	176.7	43.63	43.8	315	23.79	22.34
2,4-Dimethylheptane	229928	133.5	179.1	43.74	42.9	306	22.7	21.3
2,5-Dimethylheptane	237320	136	179.4	43.85	42.9	307.8	22.7	21.3
2,6-Dimethylheptane	247016	135.2	180.9	43.93	42.8	306	23.7	20.83
3,3-Dimethylheptane	208264	137.3	176.9	43.69	42.7	314	24.19	22.01
3,4-Dimethylheptane	227768	140.6	175.3	43.55	43.8	322.7	24.77	22.8
3,5-Dimethylheptane	227624	136	177.4	43.64	43	312.3	23.59	21.77
4,4-Dimethylheptane	199892	135.2	176.9	43.6	42.7	317.8	24.18	22.01
3-Ethyl-2-methylhexane	217144	138	175.4	43.66	43.8	322.7	24.77	22.8
4-Ethyl-2-methylhexane	2181792	133.8	177.4	43.65	43	330.3	25.56	21.77
3-Ethyl-3-methylhexane	180968	140.6	173.1	43.27	43	327.2	25.66	23.22
3-Ethyl-4-methylhexane	218792	140.46	172.8	43.37	44	312.3	23.59	23.27
2,2,3-Trimethylhexane	222718	133.6	175.9	43.62	41.9	318.1	25.07	21.86
2,2,4-Trimethylhexane	218468	126.5	179.2	43.76	40.6	301	23.39	20.51
2,2,5-Trimethylhexane	228164	124.1	181.3	43.94	40.2	296.6	22.41	20.04
2,3,3-Trimethylhexane	203809	137.7	173.8	43.43	42.2	326.1	25.56	22.41
2,3,4-Trimethylhexane	228208	139	173.5	43.39	42.9	324.2	25.46	22.8
2,3,5-Trimethylpentane	230368	131.3	177.7	43.65	41.4	309.4	23.49	21.27
2,4,4-Trimethylhexane	204824	130.6	177.2	43.66	40.8	309.1	23.79	21.17
3,3,4-Trimethylhexane	208368	140.5	172.1	43.34	42.3	330.6	26.45	23.27
3,3-Diethylpentane	158600	146.2	170.2	43.11	43.4	342.8	26.94	23.75
2,2-Dimethyl-3-ethylpentane	215252	133.8	174.5	43.46	42	338.6	25.96	22.38
2,3-Dimethyl-3-ethylpentane	186152	142	170.1	42.95	42.6	322.6	26.94	23.87
2,4-Dimethyl-3-ethylpentane	219848	136.7	173.8	43.4	42.9	324.2	25.46	22.8
2,2,3,3-Tetramethylpentane	206417	140.3	169.5	43.21	41	334.5	27.04	23.38
2,2,3,4-Tetramethylpentane	143073	133	173.6	43.44	41	319.6	25.66	21.98
2,2,4,4-Tetramethylpentane	209312	122.3	178.3	43.87	38.1	301.6	24.58	20.37
2,3,3,4-Tetramethylpentane	207726	141.6	169.9	43.2	41.8	334.5	26.85	23.31

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

Physiochemical properties	R	R^2	Adjusted R^2	F	Sig
boiling points (BP) $°C$	0.975	0.951	0.951	1293.58	0.000
molar volumes (MV) cm^3	0.983	0.967	0.966	1918.36	0.000
molar refractions (MR) cm^3	0.991	0.983	0.983	3825.959	0.000
heats of vaporisation (HV) kJ	0.955	0.911	0.910	678.047	0.000
critical temperatures (CT) $°C$	0.952	0.906	0.904	632.851	0.000
critical pressures (cp) atm	0.886	0.785	0.781	240.476	0.000
surface tensions (ST) $dyne\ cm^{-1}$	0.875	0.765	0.762	215.355	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 logarithmic regression model is considered as

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

where P = Physical property and $FHSI(G)$ = First hyper-Gourava stress Index.

The logarithm Regression Model for first 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:

$$BP = -95.079 + 18.866 \cdot log(FHSI(G)) \tag{3.1}$$
$$MV = 39.708 + 11.033 \cdot log(FHSI(G)) \tag{3.2}$$
$$MR = 2.205 + 3.348 \cdot log(FHSI(G)) \tag{3.3}$$
$$HV = 3.207 + 3.201 \cdot log(FHSI(G)) \tag{3.4}$$
$$CT = 43.882 + 22.266 \cdot log(FHSI(G)) \tag{3.5}$$
$$CP = 43.293 - 1.525 \cdot log(FHSI(G)) \tag{3.6}$$
$$ST = 18.922 + 1.54 \times 10^{-5} \cdot log(FHSI(G)). \tag{3.7}$$

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

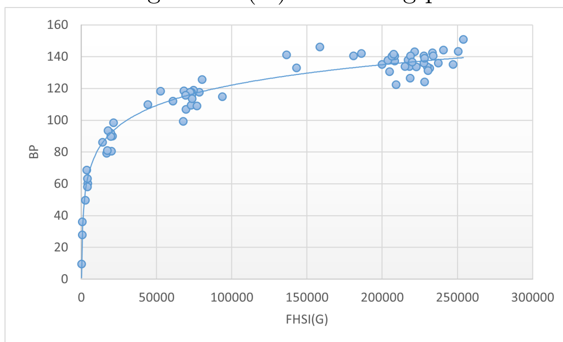


Figure 2: Graphical representation of the scattered points and its logarithm fit using $FHSI(G)$ for molar volumes

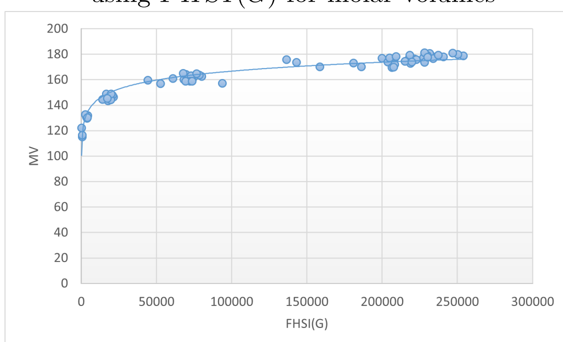


Figure 3: Graphical representation of the scattered points and its logarithm fit using $FHSI(G)$ for molar refractions

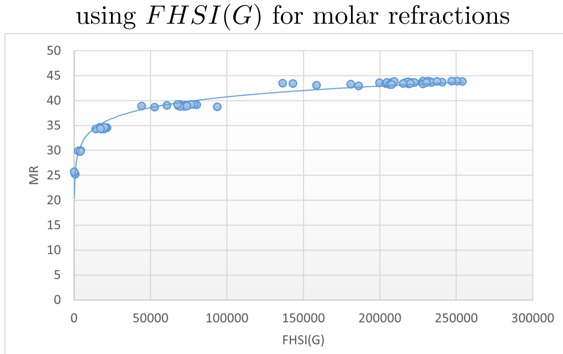


Figure 4: Graphical representation of the scattered points and its logarithm fit using $FHSI(G)$ for heats of vaporisation

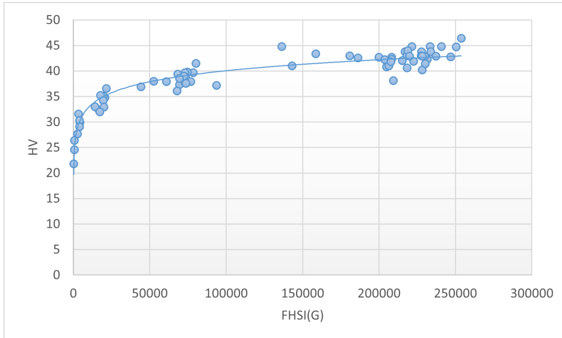


Figure 5: Graphical representation of the scattered points and its logarithm fit using $FHSI(G)$ for critical temperatures

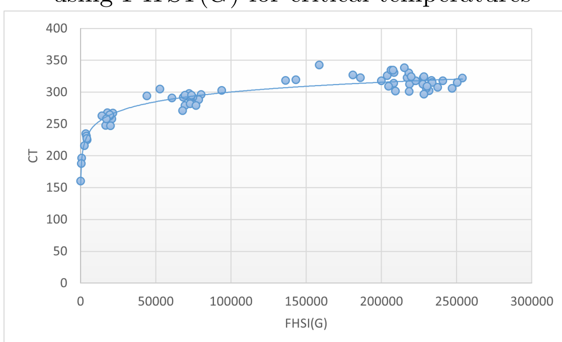


Figure 6: Graphical representation of the scattered points and its logarithm fit using $FHSI(G)$ for critical pressures

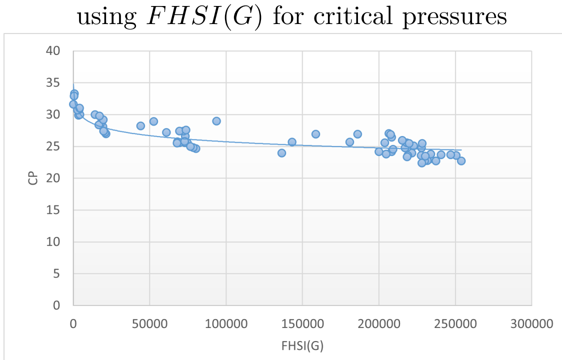
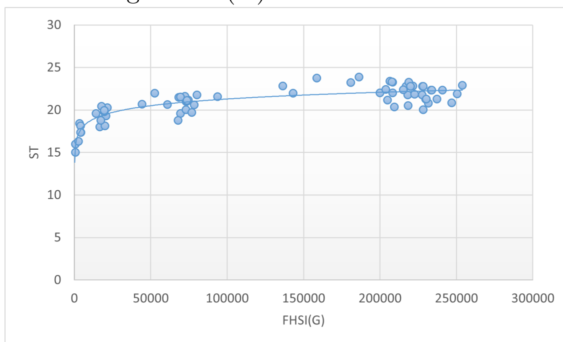


Figure 7: Graphical representation of the scattered points and its logarithm fit using $FHSI(G)$ for surface tensions.



Conclusion

In this study, we introduced a novel graph invariant, namely the first hyper-Gourava stress index, which combines the concepts of vertex stress and Gourava-type topological descriptors. The proposed index provides a new approach for characterizing the structural properties of graphs by incorporating the contribution of shortest paths through vertices. We established several mathematical properties, derived useful inequalities, and obtained exact expressions for the first hyper-Gourava stress index of various standard graph families. These results demonstrate the applicability and effectiveness of the proposed invariant in graph-theoretical analysis.

Furthermore, the QSPR investigation highlights the potential of the first hyper-Gourava stress index as a valuable molecular descriptor for predicting physicochemical properties of lower alkanes. The observed correlations indicate that this index can serve as an effective tool in chemical graph theory and molecular property modeling. The proposed invariant opens new avenues for exploring stress-based topological indices and their applications in mathematical chemistry. Future research may focus on extending this concept to other classes of graphs, developing additional stress-based descriptors, and investigating their predictive performance for a wider range of chemical compounds.

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