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Kepler Stress Index for Graphs

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ABSTRACT: Shimbel (1953) introduced the node centrality index, which is the stress of a vertex. The number of geodesics (shortest paths) that pass through a vertex in a graph is its stress. A number that links a chemical structure to physical characteristics or chemical reactivity is called a topological index of the chemical structure (graph). In this work, we present the kepler stress index, a new topological index for graphs based on vertex stresses. Additionally, we compute the kepler stress index for a few standard graphs, prove a few results, and establish a few inequalities.Likewise, we defined the significance of the kepler stress index in predicting the physicochemical properties of butane derivatives.

Key Words: Graph, Geodesic, Topological index, Stress of a node, Kepler stress index.

Contents

1. Introduction

We refer to the textbook of Harary [4] for standard terminology and concepts in graph theory. This article will provide non-standard information when needed.

Let $G = (V, E)$ be a graph (finite, simple, connected and undirected). The degree of a node v in G is denoted by $\deg(v)$. A shortest path (graph geodesic) between two nodes u and v in G is a path between u and v with the minimum number of edges. We say that a graph geodesic P is passing through a node v in G if v is an internal node of P (i.e., v is a node in P, but not an end node of P).

The concept of stress of a node (node) in a network (graph) has been introduced by Shimbel as centrality measure in 1953 [24]. This centrality measure has applications in biology, sociology, psychology, etc., (See [6,22]). The stress of a node v in a graph G, denoted by $\mathrm{str}_G(v)$ $\mathrm{str}(v)$, is the number of geodesics passing through it. We denote the maximum stress among all the nodes of G by Θ_G and minimum stress among all the nodes of G by θ_G. Further, the concepts of stress number of a graph and stress regular graphs have been studied by Bhargava et al. in their paper [2]. A graph G is called k-stress regular if $\mathrm{str}(v) = k$ for all $v \in V(G)$.

Gutman et al. [3] introduced the concept of elliptic Somber index. The elliptic Sombor index EI of a graph G is defined as

$$EI(G) = \sum_{uv \in E(G)} (d(u) + d(v))\sqrt{d(u)^2 + d(v)^2}. \tag{1.1}$$

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The Kepler expression was proposed in [3] as: $\pi\,(r_1 + r_2)$, where $r_1 = \sqrt{a^2 + b^2}$, $r_2 = \frac{1}{\sqrt{2}}(a + b)$, and $a = d_u$, $b = d_v$, $a \geq b$.

Kulli [7] introduced the concept of Kepler Banhatti index. The Kepler Banhatti index $KB(G)$ of a graph G is defined as:

$$EI(G) = \sum_{uv \in E(G)} (d(u) + d(v)) + \sqrt{d(u)^2 + d(v)^2}. \tag{1.2}$$

In this work, a finite simple connected graph is referred to as a graph, G denotes a graph and N denotes the number of geodesics of length ≥ 2 in G. In section 2, we introduce a new topological index for graphs using stress on nodes, which we call the Kepler stress index. In section 3, we define the significance of the Kepler stress index in predicting the physicochemical properties of butane derivatives. Additionally, some inequalities have been established, some results have been proven, and the Kepler stress index of some standard graphs has been computed. This was motivated by the Kepler Banhatti index that was previously discussed. For new stress/degree based topological indices, we suggest the reader to refer the papers [1,5,8-21,23,25-28].

2. Kepler Stress Index

Definition 2.1 *The kepler stress index $KSI(G)$ of a graph G is defined as*

$$KSI(G) = \sum_{uv \in E(G)} (str(u) + str(v)) + \sqrt{str(u)^2 + str(v)^2}. \tag{2.1}$$

Observation: From the Definition 2.1, it follows that, for any graph G,

$$(2 + \sqrt{2})m\theta_G \leq KSI(G) \leq (2 + \sqrt{2})m\Theta_G,$$

where m is the number of edges in G.

Example 2.1 *Consider the graph G given in Figure 1.*

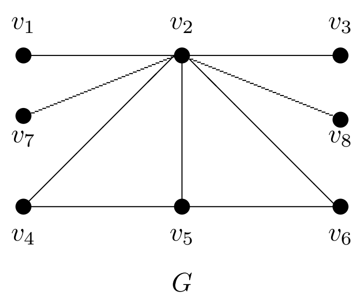

Figure 1: A graph G

The stresses of the nodes of G are as follows:
$str(v_1) = str(v_3) = str(v_7) = str(v_8) = str(v_4) = str(v_6) = 0,$
$str(v_2) = 19,\ str(v_5) = 1.$

The kepler stress index of G is:

$$\begin{aligned} KSI(G) = {} & 19 + \sqrt{19^2 + 0^2} + 19 + \sqrt{19^2 + 0^2} + 19 + \sqrt{19^2 + 0^2} + 19 + \sqrt{19^2 + 0^2} \\ & + 19 + \sqrt{19^2 + 0^2} + 20 + \sqrt{19^2 + 1^2} + 19 + \sqrt{19^2 + 0^2} + 1 + \sqrt{0^2 + 1^2} \\ & + 1 + \sqrt{1^2 + 0^2} \\ = {} & 271.026. \end{aligned}$$

Proposition 2.1 *For any graph G,*

$$0 \leq KSI(G) \leq (2+\sqrt{2})N|E|. \tag{2.2}$$

Proof: For any node v in G, we have $0 \leq \text{str}(v) \leq N$. Hence by Definition 2.1, it follows that $0 \leq KSI \leq (2+\sqrt{2})N|E|$. □

Corollary 2.1 *If there is no geodesic of length ≥ 2 in a graph G, then $KSI(G) = 0$. Moreover, for a complete graph K_n, $KSI(K_n) = 0$.*

Proof: If there is no geodesic of length ≥ 2 in a graph G, then $N = 0$. Hence, by the Proposition 2.1, we have $KSI(G) = 0$.

In K_n, there is no geodesic of length ≥ 2 and so $KSI(K_n) = 0$. □

Theorem 2.1 *For a graph G, $KSI(G) = 0$ iff G is complete.*

Proof: Suppose that $KSI(G) = 0$. Then by the Definition 2.1, $(str(u) + str(v)) + \sqrt{\text{str}(u)^2 + \text{str}(v)^2} = 0$, $\forall uv \in E(G)$. Hence $\text{str}(v) = 0$, $\forall v \in V(G)$. If $|V(G)| = 1$ or 2, then G is a complete graph as $G \cong K_1$ or K_2. Assume that $|V(G)| > 2$. Let u, v be any two distinct nodes in G. We claim that u, v are adjacent in G. For, if u, v are not adjacent in G, then there is a geodesic in G between u and v passing through at least one node, say w making $\text{str}(w) \geq 1$, which a contradiction. Hence, u, v are adjacent in G. Therefore, G is complete.

Conversely, suppose that the graph G is complete. Then by Corollary 2.1, it follows that $KSI(G) = 0$. □

Proposition 2.2 *For the complete bipartite $K_{m,n}$,*

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

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,

$$\text{str}(v_i) = \frac{n(n-1)}{2} \text{ for } 1 \leq i \leq m \tag{2.3}$$

and

$$\text{str}(u_j) = \frac{m(m-1)}{2} \text{ for } 1 \leq j \leq n. \tag{2.4}$$

Using (2.3) and (2.4) in the Definition 2.1, we have

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

□

Proposition 2.3 *For the star graph $K_{1,n}$ on $n+1$ vertices ,*

$$KSI(K_{1,n}) = n^2(n-1).$$

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

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

□

Proposition 2.4 *If $G = (V, E)$ is a k-stress regular graph, then*

$$KSI(G) = (2 + \sqrt{2})k|E|.$$

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

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

By the Definition 2.1, we have

$$\begin{aligned} KSI(G) &= \sum_{uv \in E(G)} (str(u) + str(v)) + \sqrt{\text{str}(u)^2 + \text{str}(v)^2} \\ &= \sum_{uv \in E(G)} 2k + \sqrt{k^2 + k^2} \\ &= (2 + \sqrt{2})k|E|. \end{aligned}$$

□

Proposition 2.5 *If G_1 and G_2 are any two graphs such that $G_1 \cong G_2$, then $KSI(G_1) = KSI(G_2)$.*

Proof: Obvious. □

Remark 2.1 *The converse of Proposition 2.8 is not true. There exist non-isomorphic graphs having the same kepler stress index. For instance, $KSI(K_n) = KSI(K_1) = 0$, for all $n \geq 1$, but $K_n \ncong K_1$ for $n > 1$.*

Proposition 2.6 *Let $G_1, G_2, \ldots, G_m$ be the components of a disconnected graph H. Then the kepler stress index of H is given by*

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

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,

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

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

□

Corollary 2.2 *For a cycle C_n,* $KSI(C_n) = \begin{cases} \dfrac{(2+\sqrt{2})n(n-1)(n-3)}{8}, & \textit{if } n \textit{ is odd;} \\ \dfrac{(2+\sqrt{2})n^2(n-2)}{8}, & \textit{if } n \textit{ is even.} \end{cases}$

Proof: For any node v in C_n, we have, $\text{str}(v) = \begin{cases} \dfrac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd;} \\ \dfrac{n(n-2)}{8}, & \text{if } n \text{ is even.} \end{cases}$

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 nodes and n edges, by Proposition 2.4, we have

$$KSI(C_n) = (2+\sqrt{2})\, n \times \begin{cases} \dfrac{(n-1)(n-3)}{8}, & \text{if } n \text{ is odd;} \\ \dfrac{n(n-2)}{8}, & \text{if } n \text{ is even.} \end{cases}$$

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

□

Proposition 2.7 *Let T be a tree on n nodes. Then*

$$KSI(T) = \sum_{uv\in J}\left[\left(\sum_{1\le i<j\le m(u)} |C_i^u||C_j^u| + \sum_{1\le i<j\le m(v)} |C_i^v||C_j^v|\right) + \sqrt{\left(\sum_{1\le i<j\le m(u)} |C_i^u||C_j^u|\right)^2 + \left(\sum_{1\le i<j\le m(v)} |C_i^v||C_j^v|\right)^2}\;\right] + \sum_{w\in Q} 2\left(\sum_{1\le i<j\le m(w)} |C_i^w||C_j^w|\right).$$

where J is the set of internal(non-pendant) edges in T, Q denotes the set of all nodes adjacent to pendent nodes in T, and the sets $C_1^v, \dots, C_m^v$ denotes the node sets of the components of $T - v$ for an internal node v of degree $m = m(v)$.

Proof: We know that a pendant node in T has zero stress. Let v be an internal node of T of degree $m = m(v)$. Let $C_1^v, \dots, C_m^v$ be the components of $T - v$. Since there is only one path between any two nodes in a tree, it follows that,

$$\text{str}(v) = \sum_{1\le i<j\le m} |C_i^v||C_j^v| \tag{2.5}$$

Let J denotes the set of internal(non-pendant) edges, and P denotes pendant edges and Q denotes the set of all nodes adjacent to pendent nodes in T. Then using (2.5) in the Definition 2.1 ((2.1)), we have

$$KSI(T) = \sum_{uv\in J} (str(u) + str(v)) + \sqrt{\text{str}(u)^2 + \text{str}(v)^2}$$

$$+\sum_{uv\in P}(str(u)+str(v))+\sqrt{\mathrm{str}(u)^2+\mathrm{str}(v)^2}$$
$$=\sum_{uv\in J}(str(u)+str(v))+\sqrt{\mathrm{str}(u)^2+\mathrm{str}(v)^2}+\sum_{w\in Q}2\mathrm{str}(w)$$
$$=\sum_{uv\in J}\left[\left(\sum_{1\le i<j\le m(u)}|C_i^u||C_j^u|+\sum_{1\le i<j\le m(v)}|C_i^v||C_j^v|\right)+\sqrt{\left(\sum_{1\le i<j\le m(u)}|C_i^u||C_j^u|\right)^2+\left(\sum_{1\le i<j\le m(v)}|C_i^v||C_j^v|\right)^2}\;\right]$$
$$+\sum_{w\in Q}2\left(\sum_{1\le i<j\le m(w)}|C_i^w||C_j^w|\right).$$

□

Corollary 2.3 *For the path P_n on n nodes,*

$$KSI(P_n)=\sum_{i=1}^{n-1}((i-1)(n-i)+i(n-i-1))+\sqrt{(i-1)^2(n-i)^2+i^2(n-i-1)^2}.$$

Proof: The proof of this corollary follows by above Proposition 2.7. We follow the proof of the Proposition 2.7 to compute the index. Let P_n be the path with node sequence $v_1, v_2, \ldots, v_n$ (shown in Figure 2).

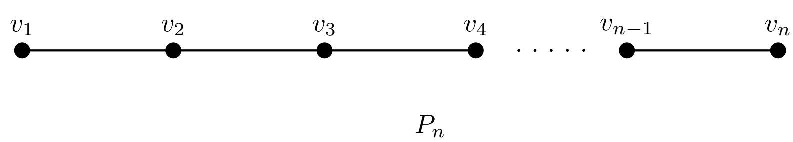

Figure 2: The path P_n on n nodes.

We have,

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

Then

$$KSI(P_n)=\sum_{uv\in E(P_n)}(str(u)+str(v))+\sqrt{\mathrm{str}(u)^2+\mathrm{str}(v)^2}$$
$$=\sum_{i=1}^{n-1}(str(v_i)+str(v_{i+1}))+\sqrt{\mathrm{str}(v_i)^2+\mathrm{str}(v_{i+1})^2}$$
$$=\sum_{i=1}^{n-1}((i-1)(n-i)+i(n-i-1))+\sqrt{(i-1)^2(n-i)^2+i^2(n-i-1)^2}.$$

□

Proposition 2.8 *Let $Wd(n,m)$ denotes the windmill graph constructed for $n\ge 2$ and $m\ge 2$ by joining m copies of the complete graph K_n at a shared universal node v. Then*

$$KSI(Wd(n,m))=m^2(m-1)(n-1)^3.$$

Hence, for the friendship graph F_k on $2k+1$ nodes,

$$KSI(F_k)=8k^2(k-1).$$

Proof: Clearly the stress of any node other than universal node is zero in $Wd(n,m)$, because neighbors of that node induces a complete subgraph of $Wd(n,m)$. Also, since there are m copies of K_n in $Wd(n,m)$ and their nodes are adjacent to v, it follows that, the only geodesics passing through v are of length 2 only. So, $\mathrm{str}(v) = \dfrac{m(m-1)(n-1)^2}{2}$. Note that there are $m(n-1)$ edges incident on v and the edges that are not incident on v have end nodes of stress zero. Hence by the Definition 2.1, we have

$$\begin{aligned} KSI(Wd(n,m)) &= m(n-1)2\,\mathrm{str}(v) \\ &= 2m(n-1)\left[\frac{m(m-1)(n-1)^2}{2}\right] \\ &= m^2(m-1)(n-1)^3. \end{aligned}$$

Since the friendship graph F_k on $2k+1$ nodes is nothing but $Wd(3,k)$, it follows that

$$KSI(F_k) = k^2(k-1)(3-1)^3 = 8k^2(k-1).$$

□

Proposition 2.9 *Let W_n denotes the wheel graph constructed on $n \geq 4$ vertices. Then*

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

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

$$\mathrm{str}(v) = \frac{(n-1)(n-4)}{2} \tag{2.6}$$

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

$$\begin{aligned} \mathrm{str}_{W_n}(p) &= \mathrm{str}_{W_n - v}(p) \\ &= \mathrm{str}_{C_{n-1}}(p) \\ &= 1 \end{aligned} \tag{2.7}$$

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

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

□

3. The significance of the Kepler Stress Index in predicting the Physicochemical Properties of Butane Derivatives

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 Kepler 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 butane derivatives, which are presented in Table 1.

Name of the Chemical Compounds	S.T.	Complexity	H.A.C	Density	Index of Refraction	Molecular Weight
1,4-Butanedithiol	31.1	17.5	6	1.03	1.51	122.3
2-Butanone	22.9	38.5	5	8.32	1.37	72.11
1,3-Butanediol	34.9	28.7	6	9.96	1.44	90.12
Butane dinitrile	40.7	92	6	1.01	1.42	82.07
Butanediamide	53	96.6	8	1.18	1.49	116.12
Butane-1-sulfonamide	41.9	133	8	1.15	1.47	137.2
1-Butanethiol	24.8	13.1	5	8.5	1.44	90.19
1,4-Diamonobutane	35.8	17.5	6	8.65	1.46	165.1
Butane-1,4-disulfonic acid	77.9	266	12	1.66	1.54	218.3
Butyraldehyde	23.1	24.8	5	8.18	1.37	72.11
2,3-Butanedione	27.3	71.5	6	9.75	1.38	86.09
1-Butanesulfonyl chloride	36.4	133	8	1.26	1.45	156.63

Table 1: Physiochemical properties of Butane derivatives

Name of the Chemical Compounds	Kepler stress index(KSI)
1,4-Butanedithiol	1838.685
2-Butanone	1008.835
1,3-Butanediol	1757.441
Butane dinitrile	435.852
Butanediamide	1816.841
Butane-1-sulfonamide	3103.236
1-Butanethiol	1535.015
1,4-Diamonobutane	2618.318
Butane-1,4-disulfonic acid	4931.531
Butyraldehyde	999.595
2,3-Butanedione	784.916
1-Butanesulfonyl chloride	2253.833

Table 2: Exact values of kepler stress index(KSI) of butane derivatives

Regression Models

Using Table 1 and Table 2, a study was carried out with a linear regression model

$$P = A(KSI(G)) + B,$$

where P = Physical property and $KSI(G)$ = kepler stress index.

Table 3: The correlation coefficient (r) from the linear regression model between the Kepler stress index and the physicochemical properties (surface tension(S.T.), complexity(C), hydrogen atom count(H.A.C.), density(D), index of refraction(I.R.), and molecular weight(M.W.)) of butane derivatives.

ST	C	HAC	D	IR	MW
0.782	0.718	0.856	0.370	0.780	0.925

The linear regression models for surface tension (S.T.), complexity(C), hydrogen atom count (H.A.C.), density(D), index of refraction(I.R.), and molecular weight (M.W.) of butane derivatives are given below:

$$ST = 0.0099(KSI(G)) + 18.405 \tag{3.1}$$
$$C = 0.0435(KSI(G)) - 6.0296 \tag{3.2}$$
$$HAC = 0.0014(KSI(G)) + 4.0474 \tag{3.3}$$
$$D = -0.0012(KSI(G)) + 7.4165 \tag{3.4}$$
$$IR = 0.00003(KSI(G)) + 1.3784 \tag{3.5}$$
$$MW = 0.034(KSI(G)) + 51.875 \tag{3.6}$$

From Table 3, it follows that the linear regression models (3.1)-(3.2)-(3.3)-(3.5)-(3.6) can be used as predictive tools.

4. Conclusion

Table 3, reveals that the linear regression models (3.1)-(3.2)-(3.3)-(3.5)-(3.6) are useful tools in predicting the physical properties of butane derivatives. It shows that kepler stress index can be used as predictive means in QSPR researches.

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References

1. AlFran, H. A., Somashekar, P. and Siva Kota Reddy, P., *Modified Kashvi-Tosha Stress Index for Graphs*, Glob. Stoch. Anal., 12(1), 10-20, (2025).

2. Bhargava, K., Dattatreya, N. N. and Rajendra, R., *On stress of a vertex in a graph*, Palest. J. Math., 12(3), 15–25, (2023).

3. Gutman, I., Furtula, B. and Oz, M. S. *Geometric approach to vertex-degree-based topological indices–Elliptic Sombor index, theory and application*, Int. J. Quantum Chem., 124(2), Article ID: e27346, (2024).

4. Harary, F., *Graph Theory*, Addison Wesley, Reading, Mass, (1972).

5. Hemavathi, P. S., Lokesha, V., Manjunath, M., Siva Kota Reddy, P. and Shruti, R., *Topological Aspects of Boron Triangular Nanotube And Boron-α Nanotube*, Vladikavkaz Math. J, 22(1), 66-77, (2020).

6. Indhumathy, M., Arumugam, S., Baths, Veeky and Singh, Tarkeshwar, *Graph theoretic concepts in the study of biological networks*, Applied Analysis in Biological and Physical Sciences, Springer Proceedings in Mathematics & Statistics, 186, 187-200, (2016).

7. Kulli, V. R., *Kepler Banhatti and Modified Kepler Banhatti indices*, International Journal of Mathematics and Computer Research, 12(6), 4310-4314, (2024).

8. Mahesh, K. B., Rajendra, R. and Siva Kota Reddy, P., *Square Root Stress Sum Index for Graphs*, Proyecciones, 40(4), 927-937, (2021).

9. Mangala Gowramma, H., Siva Kota Reddy, P., Kim, T. and Rajendra, R., *Taekyun Kim Stress Power α-Index*, Bol. Soc. Parana. Mat. (3), 43, Article Id: 72273, 10 Pages, (2025).

10. Mangala Gowramma, H., Siva Kota Reddy, P., Kim, T. and Rajendra, R., *Taekyun Kim α-Index of Graphs*, Bol. Soc. Parana. Mat. (3), 43, Article Id: 72275, 10 Pages, (2025).

11. Mangala Gowramma, H., Siva Kota Reddy, P., Hemavathi, P. S., Pavithra, M. and Rajendra, R., *Total Stress as a Topological Index*, Proc. Jangjeon Math. Soc., 28(2), 181-188, (2025).

12. Pinto, R. M., Rajendra, R., Siva Kota Reddy, P. and Cangul, I. N., *A QSPR Analysis for Physical Properties of Lower Alkanes Involving Peripheral Wiener Index*, *Montes Taurus J. Pure Appl. Math.*, 4(2), 81–85, (2022).

13. Rai, P. S., Rajendra, R. and Siva Kota Reddy, P., *Vertex Stress Polynomial of a Graph*, Bol. Soc. Parana. Mat. (3), 43, Article Id: 68311, 6 Pages, (2025).

14. Rajendra, R., Mahesh, K. B. and Siva Kota Reddy, P., *Mahesh Inverse Tension Index for Graphs*, Adv. Math., Sci. J., 9(12), 10163-10170, (2020).

15. Rajendra, R., Siva Kota Reddy, P. and Cangul, I. N., *Stress indices of graphs*, Adv. Stud. Contemp. Math. (Kyungshang), 31(2), 163-173, (2021).

16. Rajendra, R., Siva Kota Reddy, P. and Harshavardhana, C. N., *Tosha Index for Graphs*, Proc. Jangjeon Math. Soc., 24(1), 141-147, (2021).

17. Rajendra, R., Siva Kota Reddy, P. and Harshavardhana, C. N., *Rest of a vertex in a graph*, Adv. Math., Sci. J., 10(2), 697-704, (2021).

18. Rajendra, R., Siva Kota Reddy, P., Mahesh, K.B. and Harshavardhana, C. N., *Richness of a Vertex in a Graph*, South East Asian J. Math. Math. Sci., 18(2), 149-160, (2022).

19. Rajendra, R., Siva Kota Reddy, P. and Prabhavathi, M., *Computation of Wiener Index, Reciprocal Wiener index and Peripheral Wiener Index Using Adjacency Matrix*, South East Asian J. Math. Math. Sci., 18(3) (2022), 275-282.

20. Rajendra, R., Siva Kota Reddy, P., Harshavardhana, C. N., and Alloush, Khaled A. A., *Squares Stress Sum Index for Graphs*, Proc. Jangjeon Math. Soc., 26(4), 483-493, (2023).

21. Rajendra, R., Siva Kota Reddy, P. and Harshavardhana, C. N., *Stress-Difference Index for Graphs*, Bol. Soc. Parana. Mat. (3), 42, 1-10, (2024).

22. Shannon, P., Markiel, A., Ozier, O., Baliga, N. S., Wang, J. T., Ramage, D., Amin, N., Schwikowski, B., and Idekar, T., *Cytoscape: a software environment for integrated models of biomolecular interaction networks*, Genome Res., 13(11), 2498–2504, (2003).

23. Shanthakumari, Y., Siva Kota Reddy, P., Lokesha, V. and Hemavathi, P. S., *Topological Aspects of Boron Triangular Nanotube and Boron-Nanotube-II*, South East Asian J. Math. Math. Sci., 16(3), 145-156, (2020).

24. Shimbel, A., *Structural Parameters of Communication Networks*, Bulletin of Mathematical Biophysics, 15, 501-507, (1953).

25. Siva Kota Reddy, P., Prakasha, K. N. and Cangul, I. N., *Randić Type Hadi Index of Graphs*, Trans. Natl. Acad. Sci. Azerb. Ser. Phys.-Tech. Math. Sci., 40(4), 175-181, (2020).

26. Siva Kota Reddy, P., Somashekar, P. and Pavithra, M., *Sombor Stress Index for Graphs*, Proc. Jangjeon Math. Soc., 28(2), 217-227, (2025).

27. Somashekar, P., Siva Kota Reddy, P., Harshavardhana, C. N. and Pavithra, M., *Cangul Stress Index for Graphs*, J. Appl. Math. Inform., 42(6), 1379-1388, (2024).

28. Somashekar, P. and Siva Kota Reddy, P., *Kashvi-Tosha Stress Index for Graphs*, Dyn. Contin. Discrete Impuls. Syst., Ser. B, Appl. Algorithms, 32, 137-148, (2025).

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