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Kepler Stress Exponential for Graphs

M. Kirankumar, K. R. Karthik, M. Pavithra* and Puttaswamy

ABSTRACT: In 1953, Alfonso Shimbel introduced the concept of vertex stress in a graph. The stress of a vertex in a graph is the number of shortest paths passing through it. This paper describes the Kepler stress exponential KS(G,x) of graphs and presents findings, including a characterization of graphs with non-zero constant vertex stress polynomials. Similarly, we established the importance of the Kepler stress exponential in predicting the physicochemical properties of butane derivatives.

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

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1. Introduction

We refer to the textbook of Harary [5] 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 [21]. This centrality measure has applications in biology, sociology, psychology, etc., (See [6,20]). The stress of a node v in a graph G, denoted by $\operatorname{str}_G(v)$ $\operatorname{str}(v)$, 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. [3] in their paper. A graph G is called k-stress regular if $\operatorname{str}(v) = k$ for all $v \in V(G)$.

Gutman introduced the concept of elliptic somber index [4]. The elliptic sombor index EI of a graph G is defined as:

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

The Kepler expression was proposed in [2,4] as: $\pi(r_1 + r_2)$, where $r_1 = \sqrt{a^2 + b^2}$, $r_2 = \frac{1}{\sqrt{2}}(a + b)$, and $a = d_u$, $b = d_v$, $a \ge b$.

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

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

The Kepler Banhatti exponential KB(G, x) of a graph G is defined as:

$$KB(G,x) = \sum_{uv \in E(G)} x^{(d(u)+d(v))+\sqrt{d(u)^2+d(v)^2}}.$$
(1.3)

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 introduces the Kepler stress exponential KS(G,x) for graphs using stress on nodes. Additionally, some results have been proven, and the Kepler stress exponential of some standard graphs has been computed. This work was motivated by the Kepler Banhatti exponential of a graph G defined by Kulli [7]. For the reader interested in new stress-based topological indices, we recommend reading the publications [1,8-19,22-24].

2. Kepler Stress Exponential of a Graph

Definition 2.1 The kepler stress exponential KS(G,x) of a graph G is defined as:

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

Example 2.1 Consider the graph G given in Figure 1:

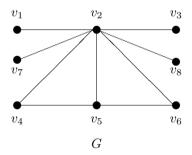


Figure 1: A graph G

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 exponential of G is:

$$\begin{split} KS(G,x) = & x^{19+\sqrt{19^2+0^2}} + x^{19+\sqrt{19^2+0^2}} + x^{19+\sqrt{19^2+0^2}} + x^{19+\sqrt{19^2+0^2}} \\ & + x^{19+\sqrt{19^2+0^2}} + x^{20+\sqrt{19^2+1^2}} + x^{19+\sqrt{19^2+0^2}} + x^{1+\sqrt{0^2+1^2}} \\ & + x^{1+\sqrt{1^2+0^2}} \\ = & 2x^2 + x^{20+\sqrt{362}} + 6x^{38}. \end{split}$$

Proposition 2.1 For the complete bipartite $K_{m,n}$,

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

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

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

and

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

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

$$KS(K_{m,n},x) = \sum_{uv \in E(G)} x^{(str(u)+str(v))+\sqrt{str(u)^2+str(v)^2}}$$

$$= \sum_{1 \le i \le m, \ 1 \le j \le m} x^{(str(v_i)+str(u_j))+\sqrt{str(v_i)^2+str(u_j)^2}}$$

$$= \sum_{1 \le i \le m, \ 1 \le j \le n} x^{\frac{n(n-1)+m(m-1)}{2}+\sqrt{\left(\frac{n(n-1)}{2}\right)^2+\left(\frac{m(m-1)}{2}\right)^2}}$$

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

Proposition 2.2 For the star graph $K_{1,n}$ on n+1 vertices,

$$KS(K_{1,n}, x) = n \cdot x^{n(n-1)}.$$

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

$$KS(K_{1,n}, x) = \sum_{uv \in E(K_{1,n})} x^{str(u) + str(v) + \sqrt{str(u)^2 + str(v)^2}}$$

$$= \sum_{uv \in E(G)} x^{\frac{n(n-1)}{2} + \sqrt{\frac{n^2(n-1)^2}{4}}}$$

$$= n \cdot x^{n(n-1)}.$$

Proposition 2.3 If G = (V, E) is a k-stress regular graph, then

$$KS(G, x) = x^{(2+\sqrt{2})k} \cdot |E|.$$

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

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

By the Definition 2.1, we have

$$KS(G, x) = \sum_{uv \in E(G)} x^{str(u) + str(v) + \sqrt{str(u)^2 + str(v)^2}}$$

$$= \sum_{uv \in E(G)} x^{2k + \sqrt{k^2 + k^2}}$$

$$= x^{(2+\sqrt{2})k} \cdot |E|.$$

Proposition 2.4 If G_1 and G_2 are any two graphs such that $G_1 \cong G_2$, then $KS(G_1, x) = KS(G_2, x)$.

Proof: Obvious.

Remark 2.1 The converse of Proposition 2.8 is not true. There exist non-isomorphic graphs having the same Kepler stress exponential. For instance, $KS(K_n, x) = KS(K_1, x) = 0$, for all $n \ge 1$, but $K_n \not\cong K_1$ for n > 1.

Proposition 2.5 Let G_1, G_2, \ldots, G_m be the components of a disconnected graph H. Then the Kepler stress exponential of H is given by

$$KS(H, x) = KS(G_1, x) + KS(G_2, x) + \dots + KS(G_m, x).$$

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,

$$KS(H,x) = KS\left(\bigcup_{i=1}^{m} G_{i}, x\right)$$

$$= \sum_{u_{1i}v_{1i} \in E(G_{1})} x^{(str(u_{1i}) + str(v_{1i})) + \sqrt{str(u_{1i})^{2} + str(v_{1i})^{2}}} + \cdots$$

$$+ \sum_{u_{mi}v_{mi} \in E(G_{m})} x^{(str(u_{mi}) + str(v_{mi})) + \sqrt{str(u_{mi})^{2} + str(v_{mi})^{2}}}$$

Corollary 2.1 For a cycle C_n ,

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

 $=KS(G_1,x)+KS(G_2,x)+KS(G_3,x)+\cdots+KS(G_m,x).$

Proof: For any node v in C_n , we have,

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

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 nodes and n edges, by Proposition 2.3, we have

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

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

Proposition 2.6 Let T be a tree on n nodes. Then

$$KS(T, x) = \sum_{uv \in J} x^{A + \sqrt{B}} + \sum_{w \in Q} x^{2(\sum_{1 \le i < j \le m(w)} |C_i^w||C_j^w|)},$$

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, \ldots, 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, \ldots, 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,

$$str(v) = \sum_{1 \le i \le j \le m} |C_i^v| |C_j^v|$$
 (2.4)

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 (2.4) in the Definition 2.1, we have:

$$\begin{split} KS(T,x) &= \sum_{uv \in J} x^{str(u) + str(v) + \sqrt{\operatorname{str}(u)^2 + \operatorname{str}(v)^2}} \\ &+ \sum_{uv \in P} x^{str(u) + str(v) + \sqrt{\operatorname{str}(u)^2 + \operatorname{str}(v)^2}} \\ &= \sum_{uv \in J} x^{str(u) + str(v) + \sqrt{\operatorname{str}(u)^2 + \operatorname{str}(v)^2}} + \sum_{w \in Q} x^{2\operatorname{str}(w)} \\ &= \sum_{uv \in J} x^{A + \sqrt{B}} + \sum_{w \in Q} x^{2\left(\sum_{1 \leq i < j \leq m(w)} |C_i^w||C_j^w|\right)}, \end{split}$$

where
$$A = \left(\sum_{1 \le i < j \le m(u)} |C_i^u| |C_j^u| + \sum_{1 \le i < j \le m(v)} |C_i^v| |C_j^v| \right)$$

and $B = \left(\sum_{1 \le i < j \le m(u)} |C_i^u| |C_j^u| \right)^2 + \left(\sum_{1 \le i < j \le m(v)} |C_i^v| |C_j^v| \right)^2$.

Corollary 2.2 For the path P_n on n nodes,

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

Proof: The proof of this corollary follows by above Proposition 2.6. We follow the proof of the Proposition 2.6 to compute the index. Let P_n be the path with node sequence v_1, v_2, \ldots, v_n (shown in Figure 2).

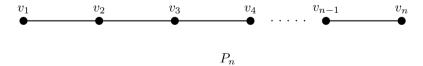


Figure 2: The path P_n on n nodes.

We have,

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

Then

$$KS(P_n, x) = \sum_{uv \in E(P_n)} x^{str(u) + str(v) + \sqrt{\operatorname{str}(u)^2 + \operatorname{str}(v)^2}}$$

$$= \sum_{i=1}^{n-1} x^{str(v_i) + str(v_{i+1}) + \sqrt{str(v_i)^2 + str(v_{i+1})^2}}$$

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

Proposition 2.7 Let Wd(n,m) denotes the windmill graph constructed for $n \geq 2$ and $m \geq 2$ by joining m copies of the complete graph K_n at a shared universal node v. Then

$$KS(Wd(n,m),x) = m(n-1)x^{m(m-1)(n-1)^2}$$

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

$$KS(F_k, x) = 2k \cdot x^{4k(k-1)}.$$

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, $str(v) = \frac{m(m-1)(n-1)^2}{2}$. 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

$$KS(Wd(n,m),x) = m(n-1)x^{2\operatorname{str}(v)}$$
$$= m(n-1)x^{m(m-1)(n-1)^2}$$

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

$$KS(F_k, x) = 2k \cdot x^{4k(k-1)}.$$

Proposition 2.8 Let W_n denotes the wheel graph constructed on $n \geq 4$ vertices. Then

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

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

$$str(v) = \frac{(n-1)(n-4)}{2}.$$
 (2.5)

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 $\operatorname{str}(p)$ are the rest peripheral vertices. So, by denoting the cycle $W_n - p$ (on n-1 vertices) by C_{n-1} , we have

$$str_{W_n}(p) = str_{W_n - v}(p)
= str_{C_{n-1}}(p)
= 1.$$
(2.6)

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

$$KS(W_n, x) = \sum_{xy \in R} x^{(\text{str}(x) + \text{str}(y)) + \sqrt{\text{str}(x)^2 + \text{str}(y)^2}}$$

$$+ \sum_{xy \in Q} x^{\text{str}(x) + \text{str}(y) + \sqrt{\text{str}(x)^2 + \text{str}(y)^2}}$$

$$= (n-1) \left[x^{(\text{str}(v) + \text{str}(p)) + \sqrt{\text{str}(v)^2 + \text{str}(p)^2}} \right] + (n-1) \cdot x^{(2+\sqrt{2}) \text{str}(p)}$$

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

3. The Significance of the Kepler Stress Exponential 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 Exponential 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 exponential $(KS(G,2))$
1,4-Butanedithiol	7.27×10^{68}
2-Butanone	1.63×10^{43}
1,3-Butanediol	2.57×10^{70}
Butane dinitrile	4.95×10^{25}
Butanediamide	7.27×10^{68}
Butane-1-sulfonamide	1.35×10^{97}
1-Butanethiol	1.36×10^{60}
1,4-Diamonobutane	2.30×10^{87}
Butane-1,4-disulfonic acid	5.31×10^{121}
Butyraldehyde	5.24×10^{44}
2,3-Butanedione	8.81×10^{34}
1-Butanesulfonyl chloride	7.97×10^{75}

Table 2: Exact values of Kepler stress exponential (KS(G,2)) of butane derivatives

Regression Model

Using Table ${1\over 2}$, a study was carried out with a linear regression model Linear Model:

$$P = A \cdot KS(G, 2) + B,$$

where P = Physical property and <math>KS(G, 2) = Kepler stress exponential.

Table 3: Statical parameters for the linear QSPR model for Kepler stress exponential (KS(G,2)) of butane derivatives

Physiochemical properties	R	R^2	Adjusted \mathbb{R}^2	F	Sig
S.T.	0.822	0.675	0.643	20.777	0.001
Complexity	0.801	0.641	0.605	17.875	0.002
H.A.C	0.824	0.680	0.647	21.202	0.001
Density	0.264	0.070	-0.023	0.75	0.407
Index of Refraction	0.552	0.305	0.235	4.385.	0.063
Molecular Weight	0.707	0.5	0.45	10.001	0.010

The linear regression models for S.T, Complexity, H.A.C, Density(D), Index of Refraction (IR) and Molecular Weight (MW) of butane derivatives are as follows:

$$S.T = 8 \times 10^{-121} \cdot KS(G, 2) + 33.809 \tag{3.1}$$

$$C = 4 \times 10^{-120} \cdot KS(G, 2) + 60.564 \tag{3.2}$$

$$H.A.C = 1 \times 10^{-121} \cdot KS(G, 2) + 6.273$$
 (3.3)

$$D = -7 \times 10^{-122} \cdot KS(G, 2) + 5.363 \tag{3.4}$$

$$RF = 2 \times 10^{-123} \cdot KS(G, 2) + 1.436$$
 (3.5)

$$MW = 2 \times 10^{-120} \cdot KS(G, 2) + 108.185. \tag{3.6}$$

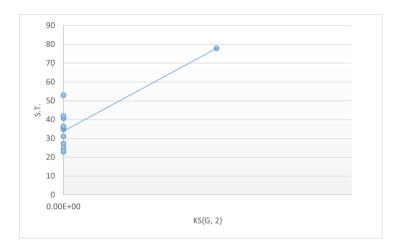


Figure 3: Graphical representation of the scattered points and its linear fit using KS(G,2) for S.T

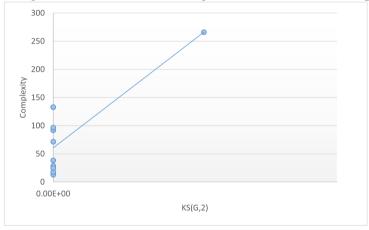


Figure 4: Graphical representation of the scattered points and its linear fit using KS(G,2) for complexity

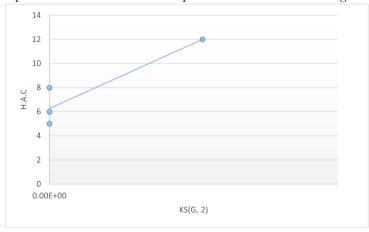


Figure 5: Graphical representation of the scattered points and its linear fit using KS(G,2) for H.A.C

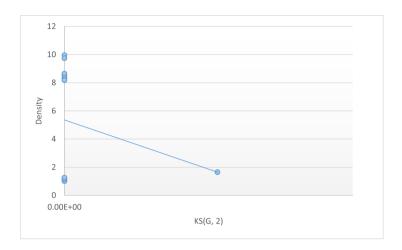


Figure 6: Graphical representation of the scattered points and its linear fit using KS(G,2) for density

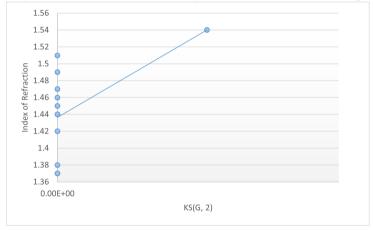


Figure 7: Graphical representation of the scattered points and its linear fit using KS(G,2) for index of refraction

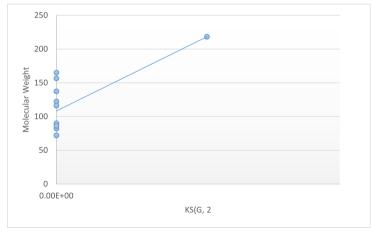


Figure 8: Graphical representation of the scattered points and its linear fit using KS(G,2) for molecular weight

4. Conclusion

In this exploration we proposed explicit formulae for KS(G,e) of some standard graphs. And table 3 shows that the linear regression models (3.1)-(3.2)-(3.3)-(3.4)-(3.5)-(3.6) are effective in predicting the physical properties of butane derivatives. It demonstrates that the Kepler stress exponential index may be utilized as a forecasting tool in QSPR research.

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M. Kirankumar

Department of Mathematics

Vidyavardhaka College of Engineering

Mysuru-570 002, India.

(Affiliated to Visvesvaraya Technological University, Belagavi-590 018, INDIA)

E-mail address: kiran.maths@vvce.ac.in

and

K. R. Karthik

 $Department\ of\ Mathematics$

 $PET\ Research\ Foundation$

(Affiliated to University of Mysore)

P.E.S College of Engineering

 $Mandya-571\ 401,\ INDIA$

E-mail address: karthikgowdru777@gmail.com

and

M. Pavithra (Corresponding author)

 $Department\ of\ Studies\ in\ Mathematics$

Karnataka State Open University

 $Mysuru-570\ 006,\ INDIA$

E-mail address: sampavi08@gmail.com

and

Puttaswamy

Department of Mathematics

PET Research Foundation

(Affiliated to University of Mysore)

P.E.S College of Engineering

 $Mandya-571\ 401,\ INDIA$

 $E\text{-}mail\ address: \verb"prof.puttaswamy@gmail.com""}$