Proceedings of the Jangjeon Mathematical Society
29 (2026), No. 3, pp. 537 - 549
www.jangjeon.or.kr
http://dx.doi.org/10.17777/pjms2026.29.3.006

A QSPR ANALYSIS AND CURVILINEAR REGRESSION MODELING OF A STRESS-BASED TOPOLOGICAL INDEX

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Abstract. We present a new topological index for graphs, termed the square root of cubic stress sum index, which is based on the stresses associated with the nodes. We have established several inequalities and proven various results related to this index. Additionally, we calculated the square root of cubic stress sum index for a selection of standard graphs. This study examines the chemical significance of the cubic stress sum index through regression analysis applied to 22 benzenoid hydrocarbons. Using logarithmic regression models, we investigate how the cubic stress sum index correlates with several physicochemical properties of these hydrocarbons.

2020 Mathematics Subject Classification. 05C09.

Keywords and Phrases: Graph, Geodesic, Topological index, Stress of a node.

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 [24]. This centrality measure has applications in biology, sociology, psychology, etc., (See [7,22]). 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 [1]. A graph G is called k-stress regular if $\mathrm{str}(v) = k$ for all $v \in V(G)$. For new stress/degree based topological indices, we suggest the reader to refer the

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papers [6, 8, 10–21, 23, 25].

In this work, a finite simple connected graph is referred to as a graph, denoted by G, and let N represent the number of geodesics of length ≥ 2 in G. Motivated by the Sombor stress index, we introduce a topological index for graphs based on the stress at nodes. This new index is termed the square root of cubic stress sum index. Furthermore, several inequalities have been established, various results have been proven, and the square root of cubic stress sum index has been computed for several standard graphs. Also examines the chemical significance of the square root of cubic stress sum index through regression analysis applied to 22 benzenoid hydrocarbons. Using logarithmic regression models, we investigate how the square root of cubic stress sum index correlates with several physicochemical properties of these hydrocarbons.

Condensed polycyclic unsaturated conjugated hydrocarbons are often referred to as benzenoid hydrocarbons. These are organic compounds composed of multiple six-membered carbon rings that are fused, with hydrogen atoms attached to maintain valency. The main characteristic of benzenoid hydrocarbons is their stable structure, where electrons are spread out over the double bonds between some carbon atoms [4]. This delocalization imparts aromatic stability to the molecule and is a fundamental aspect of their chemical behavior.

On the other hand, polycyclic aromatic hydrocarbons (PAHs) represent a broader category of compounds that include multiple fused aromatic rings but are not restricted to six-membered rings. Unlike benzenoid hydrocarbons, PAHs may contain five-membered or other ring sizes within their framework, leading to more structural variation. When rings other than six-membered are added, it often disturbs the usual way electrons are spread out in benzenoid systems, leading to different electronic and chemical properties.

A notable characteristic of most PAHs is their planar geometry. This flat shape happens because the sp^2 hybridized orbitals from neighboring carbon atoms in the same plane overlap, creating strong σ-bonds. Simultaneously, the unhybridized p orbitals overlap above and below the plane to create an extended π-electron system. The presence of these spread-out π-electrons throughout the connected structure makes the molecule more aromatic.

However, not all PAHs maintain strict planarity. In certain cases, the molecular geometry may deviate from planarity due to various factors, such as ring strain, angular distortion, or steric interactions. When non-six-membered rings are part of the molecular architecture, the resulting angles and bond lengths may lead to torsion or curvature, breaking the planar conformation. These shape limitations, affected by the arrangement and stiffness of C–C bonds, are very important in figuring out how the compound behaves physically and chemically. Understanding such deviations is important in studying the reactivity, stability, and optical properties of these aromatic systems.

2. Square root of cubic stress sum index

Definition 2.1. *The square root of cubic stress sum index $\mathcal{CSI}(G)$ of a graph G is defined as*

$$\mathcal{CSI}(G) = \sum_{uv \in E(G)} \sqrt{str(u)^3 + str(v)^3} \tag{1}$$

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

$$\sqrt{2}\, m^{\frac{3}{2}} \theta_G \leq \mathcal{CSI}(G) \leq \sqrt{2}\, m^{\frac{3}{2}} \Theta_G$$

where m is the number of edges in G.

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

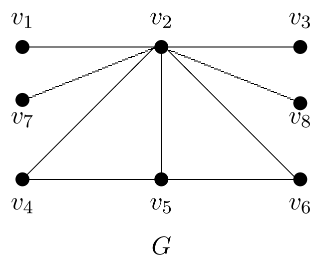


FIGURE 1. A graph G

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 square root of cubic stress sum index of G is:

$$\begin{aligned}\mathcal{CSI}(G) =& \sqrt{19^3+0^3} + \sqrt{19^3+0^3} + \sqrt{19^3+0^3} + \sqrt{19^3+0^3} + \sqrt{19^3+0^3} \\ &+ \sqrt{19^3+1^3} + \sqrt{19^3+0^3} + \sqrt{0^3+1^3} + \sqrt{1^3+0^3} \\ =& 581.0514.\end{aligned}$$

Proposition 2.2. *For any graph G,*

$$0 \leq \mathcal{CSI}(G) \leq \sqrt{2} N^{\frac{3}{2}} |E|. \tag{2}$$

Proof. For any node v in G, we have $0 \leq \mathrm{str}(v) \leq N$. Hence by Definition 2.1, it follows that $0 \leq \mathcal{CSI}(G) \leq \sqrt{2} N^{\frac{3}{2}} |E|$. ☐

Corollary 2.3. *If there is no geodesic of length ≥ 2 in a graph G, then $\mathcal{CSI}(G) = 0$. Moreover, for a complete graph K_n, $\mathcal{CSI}(K_n) = 0$.*

Proof. If there is no geodesic of length ≥ 2 in a graph G, then $N = 0$. Hence, by the Proposition 2.2, we have $\mathcal{CSI}(G) = 0$.

In K_n, there is no geodesic of length ≥ 2 and so $\mathcal{CSI}(K_n) = 0$. ☐

Theorem 2.4. *For a graph G, $\mathcal{CSI}(G) = 0$ iff G is complete.*

Proof. Suppose that $\mathcal{CSI}(G) = 0$. Then by the Definition 2.1, $\sqrt{\mathrm{str}(u)^3 + \mathrm{str}(v)^3 = 0}$, $\forall uv \in E(G)$. Hence $\mathrm{str}(v) = 0$, $\forall v \in V(G)$. 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 $\mathrm{str}(w) \geq 1$, 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 2.3, it follows that $\mathcal{CSI}(G) = 0$. □

Proposition 2.5. *For the complete bipartite $K_{m,n}$,*

$$\mathcal{CSI}(K_{m,n}) = \frac{mn}{2\sqrt{2}} \sqrt{n^3(n-1)^3 + m^3(m-1)^3}.$$

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,

$$\mathrm{str}(v_i) = \frac{n(n-1)}{2} \text{ for } 1 \leq i \leq m \tag{3}$$

and

$$\mathrm{str}(u_j) = \frac{m(m-1)}{2} \text{ for } 1 \leq j \leq n. \tag{4}$$

Using (3) and (4) in the Definition 2.1, we have

$$\begin{aligned}
\mathcal{CSI}(K_{m,n}) &= \sum_{uv \in E(G)} \sqrt{\mathrm{str}(u)^3 + \mathrm{str}(v)^3} \\
&= \sum_{1 \leq i \leq m,\ 1 \leq j \leq m} \sqrt{\mathrm{str}(v_i)^3 + \mathrm{str}(u_j)^3} \\
&= \sum_{1 \leq i \leq m,\ 1 \leq j \leq n} \sqrt{\left(\frac{n(n-1)}{2}\right)^3 + \left(\frac{m(m-1)}{2}\right)^3} \\
&= \frac{mn}{2\sqrt{2}} \sqrt{n^3(n-1)^3 + m^3(m-1)^3}.
\end{aligned}$$

□

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

$$\mathcal{CSI}(G) = \sqrt{2}k^{\frac{3}{2}}|E|.$$

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

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

By the Definition 2.1, we have

$$\begin{aligned}
\mathcal{CSI}(G) &= \sum_{uv \in E(G)} \sqrt{\mathrm{str}(u)^3 + \mathrm{str}(v)^3} \\
&= \sum_{uv \in E(G)} \sqrt{k^3 + k^3}
\end{aligned}$$

$$= \sqrt{2}k^{\frac{3}{2}}|E|. \qquad \square$$

Corollary 2.7. *For a cycle C_n,*

$$\mathcal{CSI}(C_n) = \begin{cases} \dfrac{n(n-1)^{\frac{3}{2}}(n-3)^{\frac{3}{2}}}{16}, & \text{if } n \text{ is odd;} \\ \dfrac{n^{\frac{5}{2}}(n-2)^{\frac{3}{2}}}{16}, & \text{if } n \text{ is even.} \end{cases}$$

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

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

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 2.6, we have

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

$$= \begin{cases} \dfrac{n(n-1)^{\frac{3}{2}}(n-3)^{\frac{3}{2}}}{16}, & \text{if } n \text{ is odd;} \\ \dfrac{n^{\frac{5}{2}}(n-2)^{\frac{3}{2}}}{16}, & \text{if } n \text{ is even.} \end{cases} \qquad \square$$

Proposition 2.8. *Let T be a tree on n nodes. Then*

$$\mathcal{CSI}(T) = \sum_{uv \in J} \sqrt{\left(\sum_{1 \le i < j \le m(u)} |C_i^u||C_j^u| \right)^3 + \left(\sum_{1 \le i < j \le m(v)} |C_i^v||C_j^v| \right)^3} + \sum_{w \in Q} \left(\sum_{1 \le i < j \le m(w)} |C_i^w||C_j^w| \right)^{\frac{3}{2}}.$$

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,

$$\mathrm{str}(v) = \sum_{1 \le i < j \le m} |C_i^v||C_j^v| \tag{5}$$

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 (5) in the Definition 2.1 ((1)), we have

$$\begin{aligned}
\mathcal{CSI}(T) &= \sum_{uv \in J} \sqrt{\mathrm{str}(u)^3 + \mathrm{str}(v)^3} + \sum_{uv \in P} \sqrt{\mathrm{str}(u)^3 + \mathrm{str}(v)^3} \\
&= \sum_{uv \in J} \sqrt{\mathrm{str}(u)^3 + \mathrm{str}(v)^3} + \sum_{w \in Q} \mathrm{str}(w)^{\frac{3}{2}} \\
&= \sum_{uv \in J} \sqrt{\left(\sum_{1 \le i < j \le m(u)} |C_i^u||C_j^u| \right)^3 + \left(\sum_{1 \le i < j \le m(v)} |C_i^v||C_j^v| \right)^3} \\
&\qquad + \sum_{w \in Q} \left(\sum_{1 \le i < j \le m(w)} |C_i^w||C_j^w| \right)^{\frac{3}{2}}.
\end{aligned}$$

□

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

$$\mathcal{CSI}(P_n) = \sum_{i=1}^{n-1} \sqrt{(i-1)^3(n-i)^3 + i^3(n-i-1)^3}.$$

Proof. The proof of this corollary follows by above Proposition 2.8. We follow the proof of the Proposition 2.8 to compute the index. Let P_n be the path with node sequence $v_1, v_2, \ldots, v_n$ (shown in Figure 2).

P_n

Figure 2. The path P_n on n nodes.

We have,

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

Then

$$\begin{aligned}
\mathcal{CSI}(P_n) &= \sum_{uv \in E(P_n)} \sqrt{\mathrm{str}(u)^3 + \mathrm{str}(v)^3} \\
&= \sum_{i=1}^{n-1} \sqrt{\mathrm{str}(v_i)^3 + \mathrm{str}(v_{i+1})^3} \\
&= \sum_{i=1}^{n-1} \sqrt{(i-1)^3(n-i)^3 + i^3(n-i-1)^3}.
\end{aligned}$$

□

Proposition 2.10. *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*

$$\mathcal{CSI}(Wd(n,m)) = \frac{m^{\frac{5}{2}}(m-1)^{\frac{3}{2}}(n-1)^4}{2\sqrt{2}}.$$

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

$$\mathcal{CSI}(F_k) = 4\sqrt{2}k^{\frac{5}{2}}(k-1)^{\frac{3}{2}}.$$

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

$$\begin{aligned}\mathcal{CSI}(Wd(n,m)) &= m(n-1)\,\mathrm{str}(v)^{\frac{3}{2}}\\ &= m(n-1)\left[\frac{m(m-1)(n-1)^2}{2}\right]^{\frac{3}{2}}\\ &= \frac{m^{\frac{5}{2}}(m-1)^{\frac{3}{2}}(n-1)^4}{2\sqrt{2}}.\end{aligned}$$

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

$$\mathcal{CSI}(F_k) = \frac{k^{\frac{5}{2}}(k-1)^{\frac{3}{2}}(3-1)^4}{2\sqrt{2}} = 4\sqrt{2}k^{\frac{5}{2}}(k-1)^{\frac{3}{2}}.$$

□

3. Logarithmic Regression Model

Regression analysis is a statistical technique that models a dependent variable and one or more independent variables and examines the relationship between them. In a variety of fields, including economics, finance, the social sciences, and engineering, it is widely used to understand how independent factors affect the dependent variable and to produce forecasts or estimates.

Finding the line or curve that most accurately depicts the relationship between the variables is the basic tenet of regression analysis. The dependent variable (also known as the response variable) is the one we are trying to predict or explain. Independent variables, also called predictor variables or explanatory variables, are the variables that are projected to have an effect on the dependent variable.

We used the SPSS program for these analyses. While there are many different types of regression analysis, the most popular kind is basic linear regression, which requires only one independent variable. Basic linear regression assumes that there is a linear relationship between the variables. The line's equation is displayed as:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \cdots + \beta_z X_z + \varepsilon$$

where Y is the dependent variable, β_0 is the Y-intercept, β_i is the coefficient of the independent variable for $i = 1, \ldots, z$, X is the independent variable, and ε is the error term.

By estimating the values of β_0 and β_1, regression analysis seeks to minimize the sum of squared differences between the observed values of Y and the expected values from the model. This estimation procedure frequently employs the least squares method. Additionally, regression analysis provides a number of statistical metrics to assess the quality of the model, including the coefficient of determination (R^2), which indicates the proportion of the variance of the dependent variable that can be explained by the independent variables.

Regression analysis is a powerful tool for determining the relationships between variables, creating predictions, and examining cause-and-effect relationships. It is extensively utilized in numerous fields for research, data analysis, and decision-making.

A statistical technique called logarithmic regression analysis, logarithmic transformation, or log-linear regression is used to model the relationship between a dependent variable and one or more independent variables when a logarithmic scale may more accurately symbolize the relationship. The logarithmic model is expressed as:

$$Y = \beta_0 + \beta_1 \log X_1 + \beta_2 \log X_2 + \beta_3 \log X_3 + \cdots + \beta_z \log X_z + \varepsilon$$

where Y is the dependent variable, β_0 is the Y-intercept, β_i is the coefficient of the independent variable, log is the logarithmic function, and ε is the error term.

Relationships in which the independent variables have multiplicative rather than additive effects on the dependent variable can be modeled using the logarithmic transformation. It is commonly used in situations where there is a curvilinear relationship between the variables, meaning that rates of change or declining returns are both present.

Economic, financial, biological, and environmental sciences are just a few of the fields in which logarithmic regression can be used to analyze data. Researchers can use the logarithmic scale to make predictions or derive insights, as well as to document and assess non-linear correlations between variables.

We perform a QSPR analysis on the physical properties of 22 benzenoid hydrocarbons using the square root of the cubic stress sum index of their molecular graphs. Table 1 gives the square root of the cubic stress sum index $\mathcal{CSI}(G)$ of molecular graphs and the experimental values for the physical properties—boiling point (BP), π-electron energy (π-ele), molecular weight (MW), polarizability (PO), molar volume (MV), and molar refractivity (MR)—of benzenoid hydrocarbons.

TABLE 1. square root of cubic stress sum index ($\mathcal{CSI}$), boiling point (BP), π-electron energy (π-ele), molecular weight (MW), polarizability (PO), molar volume (MV), and molar refractivity (MR) of benzenoid hydrocarbons

Derivatives of benzene	$\mathcal{CSI}$	**BP**	**π-ele**	**MW**	**PO**	**MV**	**MR**
Benzene	44.09	78.8	8	78.11	10.4	89.4	26.3
Naphthalene	642.211	221.5	13.683	128.17	17.5	123.5	44.1
Phenanthrene	3351.643	337.4	19.448	178.23	24.6	157.7	61.9
Anthracene	3411.226	337.4	19.314	178.23	24.6	157.7	61.9
Chrysene	12320.849	448	25.192	228.3	31.6	191.8	79.8
Benzo[a]anthracene	12072.079	436.7	25.101	228.3	31.6	191.8	79.8
Triphenylene	9564.445	425	25.275	228.3	31.6	191.8	79.8
Tetracene	11880.064	436.7	25.188	228.3	31.6	191.8	79.8
Benzo[a]pyrene	19069.428	495	28.222	252.3	35.8	196.1	90.3
Benzo[e]pyrene	15097.167	467.5	28.336	252.3	35.8	196.1	90.3
Perylene	14442.27	467.5	28.245	252.3	35.8	196.1	90.3
Anthanthrene	27665.205	497.1	31.253	276.3	40	200.4	100.8
Benzo[ghi]perylene	22738.229	501	31.425	276.3	40	200.4	100.8
Dibenz[a,c]anthracene	25923.675	518	30.942	278.3	38.7	225.9	97.6
Dibenz[a,h]anthracene	39913.048	524.7	30.881	278.3	38.7	225.9	97.6
Dibenz[a,j]anthracene	27785.664	524.7	30.88	278.3	38.7	225.9	97.6
Picene	41955.082	519	30.943	278.3	38.7	225.9	97.6
Coronene	34823.75	525.6	34.572	300.4	44.1	204.7	111.4
Dibenzo[a,h]pyrene	51664.187	552.3	33.928	302.4	42.9	230.2	108.1
Dibenzo[a,i]pyrene	54779.025	552.3	33.954	302.4	42.9	230.2	108.1
Dibenzo[a,l]pyrene	34271.787	552.3	34.031	302.4	42.9	230.2	108.1
Pyrene	5676.499	404	22.506	202.25	28.7	162	72.5

Regression Models. Using Table 1, a study was carried out with a logarithmic regression model

$$P = A \cdot ln(\mathcal{CSI}(G)) + B,$$

where P is the Physical property , $\mathcal{CSI}(G)$ is the square root of cubic stress sum index , B is the intercept of the model and A is the coefficient that represents the change in P for a unit change in the logarithm of $\mathcal{CSI}(G)$.

TABLE 2. The correlation coefficient r from logarithmic regression model between square root of cubic stress sum index and physicochemical properties (BP, π-ele, MW, PO, MV, MR) of benzenoid hydrocarbons.

BP	$\pi - ele$	MW	PO	MV	MR
0.991	0.964	0.969	0.960	0.965	0.960

Figure 1: Graphical representation of the scattered points and its logarithmic fit using $\mathcal{CSI}$ for boiling point

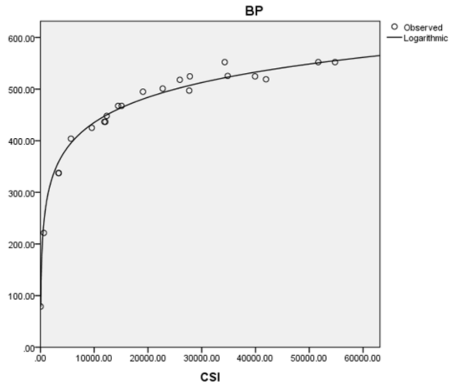
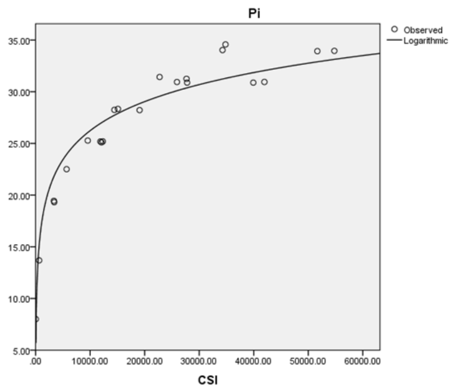


Figure 2: Graphical representation of the scattered points and its logarithmic fit using $\mathcal{CSI}$ for $\pi - ele$



The logarithmic regression models for boiling point, π-electron energy, molecular weight, polarizability, molar volume, and molar refractivity of benzenoid hydrocarbons are as follows:

$$BP = 70.414 \cdot ln(\mathcal{CSI}(G)) - 213.26 \tag{6}$$

$$\pi - ele = 4.056 \cdot ln(\mathcal{CSI}(G)) - 11.124 \tag{7}$$

$$MW = 34.846 \cdot ln(\mathcal{CSI}(G)) - 85.189 \tag{8}$$

$$PO = 5.0709 \cdot ln(\mathcal{CSI}(G)) - 13.548 \tag{9}$$

$$MV = 21.472 \cdot ln(\mathcal{CSI}(G)) - 8.199 \tag{10}$$

$$MR = 12.783 \cdot ln(\mathcal{CSI}(G)) - 34.107 \tag{11}$$

From Table 2, it follows that the logarithmic regression models (6)-(7)-(8)-(9)-(10)-(11) can be used as predictive tools.

Figure 3: Graphical representation of the scattered points and its logarithmic fit using $\mathcal{CSI}$ for molecular weight

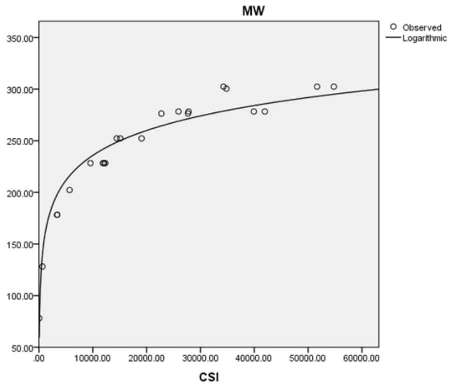


Figure 4: Graphical representation of the scattered points and its logarithmic fit using $\mathcal{CSI}$ for polarizability

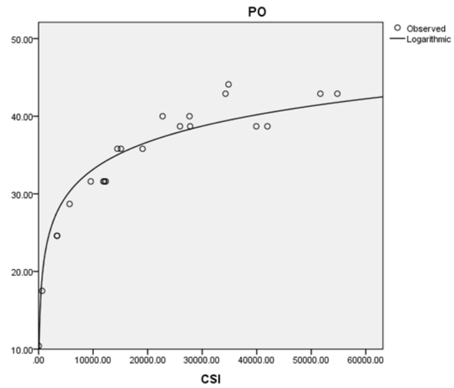


Figure 5: Graphical representation of the scattered points and its logarithmic fit using $\mathcal{CSI}$ for molar volume

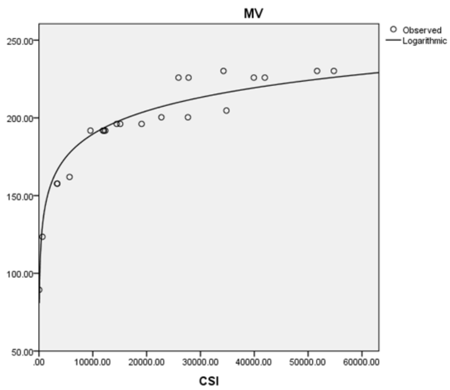
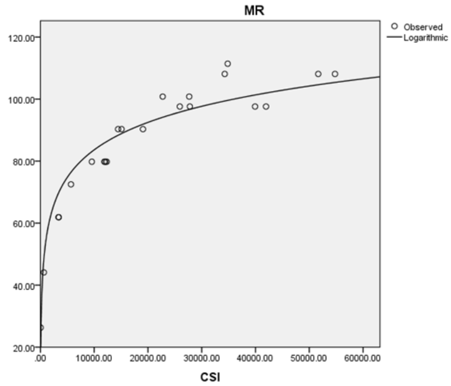


Figure 6: Graphical representation of the scattered points and its logarithmic fit using $\mathcal{CSI}$ for molar refractivity



4. Conclusion

Table 2, reveals that the logarithmic regression models (6)-(7)-(8)-(9)-(10)-(11) are useful tools in predicting the physical properties of benzenoid hydrocarbons. It shows that square root of cubic stress sum index can be used as predictive means in QSPR researches.

Acknowledgments

The authors would like to thank the referees for their invaluable comments and suggestions which led to the improvement of the manuscript.

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