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QSPR Analysis Of Benzenoids By Linear Regression Modeling Using The Inverse Sum In-Degree Index*

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Abstract

Topological indices work as numerical molecular descriptors in quantitative structure property relationships (QSPR) models. The inverse sum in-degree index (henceforth ISI index) is a degree-based topological index, defined to design a novel descriptor in modeling molecular properties with higher accuracy than previously available descriptors. Benzenoids belong to a class of aromatic hydrocarbons containing at least one benzene ring, with several applications in household goods, electronics, healthcare, textiles, etc. From graph theoretical perspective, the formation of a chain of benzene rings can be regarded as edge fusion of cycles of length six. In this regard, a detailed study of the structure of benzenoids and their ISI index are presented. The expression and the bounds for the ISI index of benzenoids are derived in terms of the number of benzene rings present in it. Further, the predictive potential of the inverse sum in-degree index of Benzenoids is studied with the help of regression analysis. The linear regression models for the inverse sum in-degree index of benzenoids against various physicochemical and thermodynamic properties like molecular weight, complexity, density, boiling point, magnetic susceptibility, refractive index, and melting point are obtained. On the whole, the extent of the relationship between the ISI index and the physicochemical parameters of benzenoids is studied in this article.

1 Introduction

In recent years, chemical graph theory, considered an important branch of both computational chemistry and graph theory, has attracted much attention from researchers. The results obtained in this field have been applied to many chemical and pharmaceutical engineering applications. Topological indices are significant attributes in chemical graph theory to analyze the physicochemical characteristics of chemical compounds without the help of physical resources. This method of studying the properties of various pharmaceutical drugs/genetic elements is very suitable and serviceable for developing countries as it can yield and analyze information about new drugs without expensive chemical experiments.

A graph $G(V, E)$ consists of a vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and an edge set $E(G) = \{(v_i, v_j)|v_i, v_j \in V(G) \text{ and } i \neq j\}$. The degree of a vertex v_i in a graph G, denoted by $d_G(v_i)$ is the number of vertices adjacent to it. The neighborhood of v_i, denoted by $N_G(v_i)$ is the set of all vertices adjacent to v_i. The distance between any two vertices v_i and v_j is the length of the shortest path connecting v_i, v_j. We write $v_i \sim v_j$ if v_i, v_j are adjacent, and $v_i \nsim v_j$ if not. The adjacency matrix (also known as classical adjacency matrix) $A(G) = (a_{ij})$ is a square matrix of order n where $a_{ij} = 1$ if $v_i \sim v_j$ and 0 otherwise. The eigenvalues of $A(G)$ associated with their multiplicities compose the spectrum of G.

A molecular graph represents the skeleton of non-saturated hydrocarbons of molecular compounds. The vertices of this graph correspond to non-hydrogen atoms and the edges to covalent bonds between atoms. Note that hydrogen atoms are often omitted. Topological indices are numerical descriptors of a molecular graph, used to predict their physicochemical and bioactivity properties.

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The Wiener index is the first topological index, introduced by H. Wiener in 1947 to determine the physical properties of paraffins [1]. The Wiener index of a graph G is the sum of distances between every pair of vertices in G. Hundreds of topological indices are currently being researched and developed since then. These topological indices have many applications in the field of chemistry and graph theory, precisely in QSAR and QSPR studies. Topological indices are divided majorly into eccentricity-based, degree-based, distance-based and spectrum-based categories. The first topological index, the Wiener index is the distance-based one.

The ISI index is found to have a special impetus as a predictor of the total surface area of octane isomers. The inverse sum in-degree index of a graph G, is defined as

$$ISI(G) = \sum_{v_i \sim v_j} \frac{d_G(v_i)d_G(v_j)}{d_G(v_i) + d_G(v_j)}.$$

A modification of the classical adjacency matrix corresponding to the ISI index is proposed in [2] and is defined as follows: The ISI-matrix $A_{ISI}(G) = (a_{ISI})_{ij}$ of a graph G of order n is an $n \times n$ matrix where

$$(a_{ISI})_{ij} = \frac{d_G(v_i)d_G(v_j)}{d_G(v_i) + d_G(v_j)} \text{ if } v_i \sim v_j, \text{ and } 0 \text{ otherwise.}$$

The eigenvalues of ISI matrix $A_{ISI}(G)$ associated with their multiplicities are called the ISI-spectrum of G. If $\xi_1, \xi_2, \ldots, \xi_n$ are the eigenvalues of the ISI matrix $A_{ISI}(G)$, then the ISI-Energy can be defined as

$$E_{ISI}(G) = \sum_{i=1}^{n} |\xi_i|.$$

Extremal values of inverse sum in-degree index across several graph classes, including connected graphs, chemical graphs, trees and chemical trees were determined in [3]. Several upper and lower bounds on the inverse sum in-degree index in terms of some molecular structural parameters and relate this index to various well-known molecular descriptors are presented in [4]. A problem posed by Sedlar, Stevanovic, and Vasilyev (2015) to characterize the structure of chemical trees with the maximal inverse sum in-degree index is resolved in [5]. The bounds related to this index for some graph operations, including the Kronecker product, join, corona product, Cartesian product, disjunction, and symmetric difference are provided in [6] and [7]. Sharp bounds for ISI index of graph operations like Cartesian product, tensor product, strong product, composition, disjunction, symmetric difference, corona product, Indu-Bala product, union of graphs, double graph, and strong double graph are determined in [8]. The ISI index of some unary graph operations and their extremal cases are studied in [9]. In [10] and [11], some properties and the bounds for the ISI eigenvalues and the energy are obtained. Authors have also constructed pairs of ISI equi-energetic graphs for each $n \geq 9$. Coming to the applications in Molecular chemistry, the inverse sum in-degree index of some nanotubes is computed in [12]. The ISI index and energy of Hyaluronic Acid-Paclitaxel conjugates used in the production of drugs used in the treatment of cancer disease are studied in [13] and hence giving information about the physicochemical properties and biological characteristics. QSPR analysis of some anti-cancer drugs like Aminopterin, Degueline, etc is carried out through ISI index/energy with the help of statistical modeling (linear, logarithmic and quadratic models) in [14]. Authors of [15] have recently introduced the generalized form of the degree-based inverse sum in-degree index which is defined as follows:

$$S_{\alpha,\beta}(G) = \sum_{v_i \sim v_j} \frac{(d_G(v_i)d_G(v_j))^{\alpha}}{(d_G(v_i) + d_G(v_j))^{\beta}}.$$

where α, β are real numbers. Many degree-based topological invariants can be derived from the generalized form of this index.

2 Motivation and Significance of the Work

Topological indices provide a pathway to determine molecular characteristics without using the long-chain process of chemical methods. Since the experiments are expensive and time-consuming, it would be practi-

cally convenient to evaluate various topological indices and conclude about the physical /biological properties of the molecule. The mathematical convergence in the study serves as a motivation for us to carry out the structure-properties analysis of benzenoids through one of the hundreds of available topological indices, named the ISI index. Further, the studies carried out in [13] and [14] also serve as a great source of motivation to choose the ISI index to analyze the physicochemical properties of a significant class of hydrocarbons.

3 ISI Index of Benzenoids

In molecular chemistry, we encounter chains of molecules joined by fusing vertices or edges. For example, two atoms/molecules joined by fusing an edge from each give rise to a new molecule. Keeping this practical convenience in mind, the graph operation of fusing the edges is considered in this section. Firstly, the linear chain of cycles joined by fusing the edges is considered in the following section.

Theorem 1 *Let $C_1, C_2, \ldots, C_k$ be cycles of length $m_1, m_2, \ldots, m_k$, respectively, where each $m_i \geq 6$. Let G be a graph of a linear chain of cycles connected by the operation of edge fusion, where every cycle C_i shares an edge with the adjacent cycle C_{i+1} for all $1 \leq i \leq (k-1)$. Then*

$$ISI(G) = \sum_{i=1}^{k} m_i + \frac{3(k-1)}{10}.$$

Proof. Clearly, the graph G has $\sum_{i=1}^{k} m_i - 2(k-1)$ vertices and $\sum_{i=1}^{k} m_i - (k-1)$ edges. Further, G has $2(k-1)$ vertices of degree 3 and the rest of degree 2. The non-zero entries of the ISI matrix $A_{ISI}(G)$ are $\frac{9}{6}$(corresponding to the pair of adjacent vertices both having degree 3), $\frac{6}{5}$ (corresponding to the pair of adjacent vertices in which one vertex is of degree 3 and the other of degree 2) and 1 (corresponding to the pair of adjacent vertices in which both vertices are of degree 2). There are $(k-1)$ pairs of adjacent vertices with each having degree 3, $4(k-1)$ pairs of adjacent vertices with one having degree 3 and the other 2. Further, since G has $\sum_{i=1}^{k} m_i - (k-1)$ edges, the number of remaining pairs of adjacent vertices are given by

$$\sum_{i=1}^{k} m_i - (k-1) - (k-1) - 4(k-1) = \sum_{i=1}^{k} m_i - 6k + 6.$$

That is, there are $\sum_{i=1}^{k} m_i - 6k + 6$ pairs of adjacent vertices each having degree 2. Thus

$$ISI(G) = (k-1) \times \frac{9}{6} + (4k-4) \times \frac{6}{5} + \left(\sum_{i=1}^{k} m_i - 6k + 6 \right) \times 1 = \sum_{i=1}^{k} m_i + \frac{3(k-1)}{10}.$$

■

Benzene ($C6H6$) is the best-known aromatic compound and the parent to which numerous other aromatic compounds are related. Benzenoids are organic compounds that are derived from or have a benzene group in their molecular structure. Benzenoids have increased stability due to resonance in the benzene rings. It is found that the operation of edge fusion is one of the most commonly occurring operations among benzenoids. For example, the edge fusion of two benzene rings gives rise to Naphthalene, and three benzene rings to Phenantherene. In order to focus on benzenoids, where the length of the benzene cycle m_i in the above theorem is taken as 6. That is, $m_i = 6$ for $1 \leq i \leq k$ gives the ISI index of a special type of benzenoids when k benzene rings are linearly connected (Example: Naphthalene, Anthracene, Naphthacene and Pentacene in Figure 1). That is $ISI(G) = \frac{63k-3}{10}$.

Using the expression derived above, one can obtain the ISI index of Anthracene, Naphthalene, etc. Benzenoids have benzene rings connected with each other in various manners. The next theorem in this section gives the bounds for the ISI index of benzenoids containing k benzene rings. Before the theorem, a detailed note on the structural and other properties of benzenoids is given, which are required for proving the next theorem.

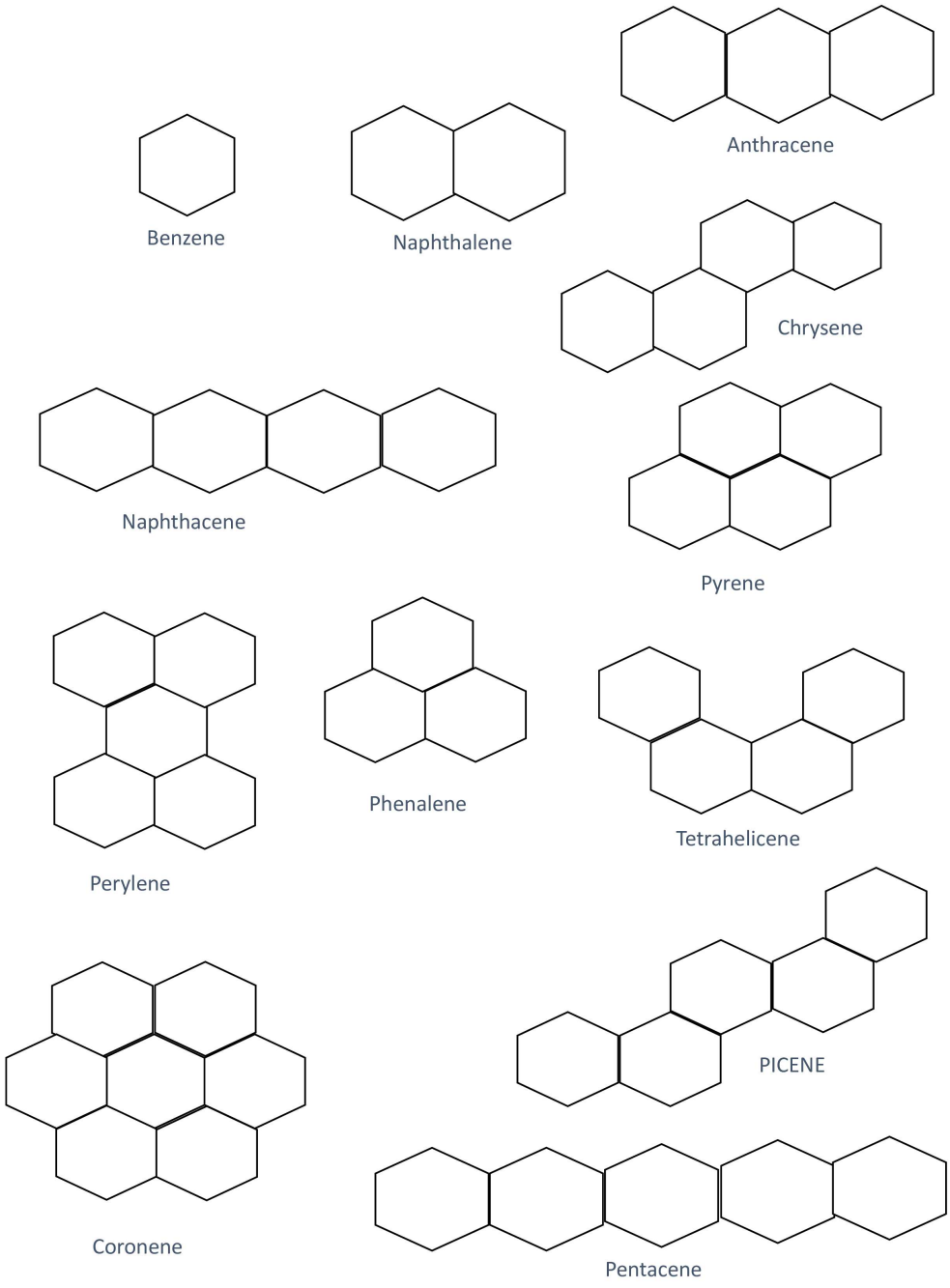

Figure 1: Some benzenoids.

One can think of formation of benzenoid structures as the addition of benzene rings one by one successively. This recurrence operation can be considered as adding the rings $R_1, R_2, \ldots, R_k$, respectively. The following are the possibilities.

- Let the first ring be R_1. The second ring R_2 added shares exactly one edge (hence 2 vertices) with R_1. Thus benzenoid with exactly 2 rings has 11 edges (10 vertices).
- The third ring R_3 added shares one edge either with R_1 or R_2 (case 1) or one edges each from both R_1 and R_2 (case 2). Thus a benzenoid with 3 rings has 16 edges (in case 1) or 15 edges (case 2).

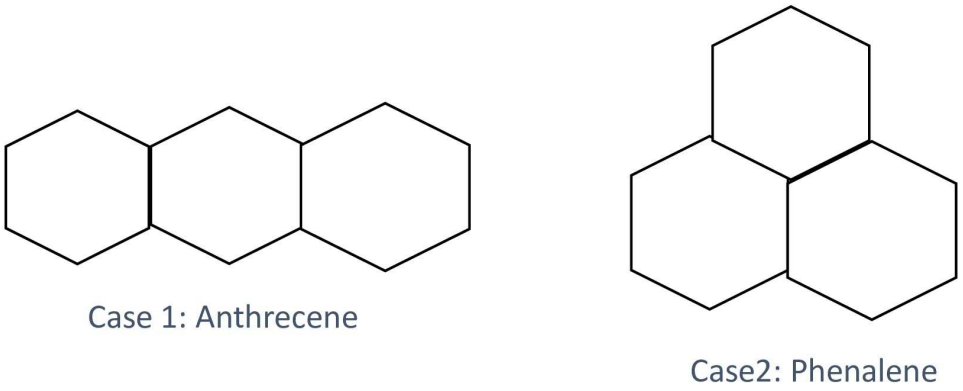

Figure 2: Benzenoids with 3 benzene rings.

- Continuing like this, at each step, a new ring added shares either one edge or 2 edges with the old rings. That is, at i^{th} step, R_i shares either one edge or two edges with any of $R_1, R_2, \ldots, R_{i-1}$. Thus if n_{i-1}, m_{i-1} are the number of vertices and the number of edges in a benzenoid containing $(i-1)$ rings, then the number of vertices n_i and the number of edges m_i in a benzenoid with i rings are given by

$$n_i = \begin{cases} n_{i-1} + 4 & \text{if } R_i \text{ shares one edge with any of } R_1, R_2, \ldots, R_{i-1}, \\ n_{i-1} + 3 & \text{if } R_i \text{ shares two edges with any of } R_1, R_2, \ldots, R_{i-1}, \end{cases}$$

and

$$m_i = \begin{cases} m_{i-1} + 5 & \text{if } R_i \text{ shares one edge with any of } R_1, R_2, \ldots, R_{i-1}, \\ m_{i-1} + 4 & \text{if } R_i \text{ shares two edges with any of } R_1, R_2, \ldots, R_{i-1}. \end{cases}$$

- Further, at each step, the vertices with degree 3 are increased during the addition of rings. If d_{i-1} is the number of vertices with degree 3 in a benzenoid containing $(i-1)$ rings, then after the addition of i^{th} ring, the number of vertices with degree 3 in a benzenoid containing i rings is $d_{i-1} + 2$. The number of vertices with degree 3 is increased by 2 irrespective of the number of edges it shares.

Next, the bounds for the ISI index of benzenoids are derived.

Theorem 2 *Let B be a benzenoid with k benzene rings with the ISI index $ISI(B)$. Then*

$$\frac{63k-3}{10} \leq ISI(B) \leq \frac{54k+15}{10}.$$

Proof. Let B be a benzenoid with k benzene rings. By definition, the ISI index is maximum when the number of vertices/edges is as maximum as possible. On constructing a benzenoid with k rings, starting with R_1 (say), the number of vertices/edges becomes the maximum if the following condition is satisfied: at each step i, the new ring added shares only one edge with any of the old rings for $2 \leq i \leq k$. Then the total number of edges is $(5k+1)$ and the total number of vertices is $(4k+2)$. Furthermore, this structure has $2(k-1)$ vertices of degree 3. The structure of such a benzenoid is a linear chain of k benzene rings connected by edge fusion. The ISI index of benzenoid with k linearly connected benzene rings is $ISI(G) = \frac{63k-3}{10}$.

Similarly, the ISI index is minimum when at each step i, the newly added ring shares the maximum number of edges with any of the old rings. But from the above notes, for every $i \geq 3$, at the i-th step, the i-th ring added shares at most 2 edges with old rings, i.e., R_1 has 6 edges, the 2^{nd} ring shares only one edge with R_1, the 3^{rd} ring shares 2 edges with old rings, and so on. Finally, even the last k-th ring shares 2 edges with old rings. Thus, the number of vertices in the 2^{nd} step is $6+4$, and from the 3^{rd} step onwards, three vertices are being added until the last. Similarly, the number of edges in the 2^{nd} step is $6+4$, and 4 edges are being added after the 3^{rd} step during every addition of a new ring. Thus, a benzenoid of this type having k benzene rings has $3k+4$ vertices and $4k+3$ edges. Further, it has $2(k-1)$ vertices of degree 3, and the remaining $(3k+4) - 2(k-1) = k+6$ vertices of degree 2.

Let G be the benzenoid with k rings obtained as mentioned above. Let S be the set of all vertices of degree 3, where $|S| = 2(k-1)$. The subgraph G_1 induced by S has only vertices of degree 3 and 1, in particular, $(k-2)$ vertices of degree 3 and k vertices of degree 1. The neighborhood of all the vertices which have degree 3 in G_1 (and G as well) contains only those vertices which have degree 3 in G. The neighborhood of all the vertices which have degree 1 in G_1 (degree 3 in G) contains one vertex of degree 3 and two vertices of degree 2 in G. Further, the neighborhood of all the other vertices of degree 2 in G has vertices of degree 2 only (which are not in G_1). The ISI matrix $A_{\mathrm{ISI}}(G)$ has $(4k+3)$ non-zero entries due to the combination of vertices with both degree 3, vertices with both degree 2, and vertices with degree $2, 3$. There are $(2k-3)$ entries given by $\frac{9}{6}$ (corresponding to vertices both of degree 3), $2k$ entries given by $\frac{6}{5}$ (corresponding to vertices of degree 3 and 2), and 6 entries given by 1 (corresponding to vertices both of degree 2). Thus,

$$\mathrm{ISI}(G) = 6 + (2k-3)\,\frac{9}{6} + 2k\frac{6}{5} = \frac{54k+15}{10}.$$

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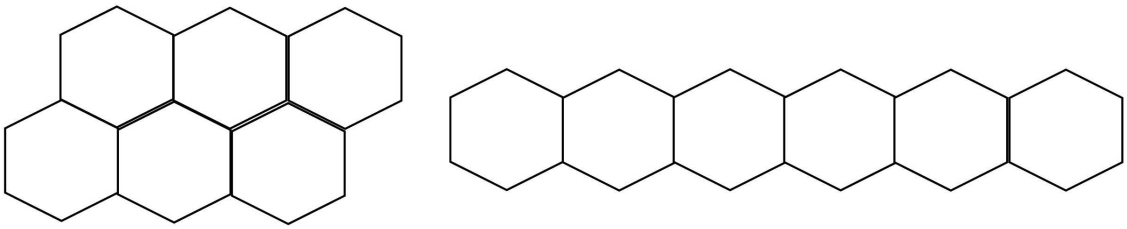

Figure 3: Benzenoids with 6 benzene rings attaining the minimum (right) and maximum (left) ISI index.

4 Correlation Analysis

Correlation analysis is a statistical method that is used to discover if there is a relationship between two variables/datasets, and how strong that relationship may be. In terms of market research, this means that the correlation analysis is used to analyze quantitative data gathered from research methods such as surveys and polls, to identify whether there are any significant connections, patterns, or trends between the two. Correlation coefficients provide a numerical summary of the direction and strength of the linear relationship between two variables. The correlation between two variables is contemplated either graphically through a scatter plot or quantified as a coefficient R^2 (known as the coefficient of determination) and its value

ranges from 0 to 1. The coefficient R^2 measures the strength of the relationship between the model and the dependent variable on a convenient $0-100\%$ scale. That is, the value of R^2 evaluates the scatter of the data points around the fitted regression line. Usually, the larger the R^2, the better the regression model fits your observations. In practice, we never see a regression model with an R^2 of 100%. In that case, the fitted values equal the data values and, consequently, all the observations fall exactly on the regression line. In this article, we first fit a linear regression model for the ISI index of benzenoids and some of their physicochemical parameters and determine how well the data fits the regression model (the goodness of fit) using R^2.

The graphs below present the relationship between the ISI index and some of the physicochemical properties of benzenoids namely, Molar mass m (g/mol), Complexity C, Boiling point BP(^oC), density ρ (g/mL), Refractive Index RI, Melting Point MP (^oC), $Log(P)$, where P is the partition coefficient) and Magnetic susceptibility χ (in cm^3/mol). The empircial data used for the analysis is given in the table below (Source: PubChem database).

Compound G	$ISI(G)$	m	C	BP	ρ	RI	MP	$LogP$	χ
Benzene	6	78.11	15.5	80.1	0.8765	1.5011	5.537	2.13	-54.8×10^{-6}
Naphthalene	12.3	128.17	80.6	217.9	1.0253	1.5898	78.2	3.34	-91.9×10^{-6}
Phenantherene	18.6	178.23	335	338	1.18	1.59427	101	4.68	-127.9×10^{-6}
Chrysene	25.1	228.29	264	448	1.274	1.771	448	5.73	-166.7×10^{-6}
Tetraphene	25	228.29	294	438	1.19	1.771	158	5.8	
Triphenylene	25.2	228.294	217	438	1.308	1.5500	198	5.146	-156.6×10^{-6}
Tetrahelicene	25.1	228.29	266	436	1.19	1.771	68	4.46	
Naphathcene	24.9	228.29	304	440	1.21	1.771	357	5.91	
Pyrene	24.9	202.25	236	404	1.2721	1.85	150.62	4.88	
Perylene	29.6	252.31	217	467	1.35	1.62	276	6.3	-168×10^{-6}
Benzo[a]pyrene	36	253.30	372	495	1.24	1.853	179	6.13	-137.5×10^{-6}
Benzo[e]pyrene	36	252.31	372	492.2	1.286	1.853	177.7	6.44	
Anthracene	18.6	178.23	154	341.3	1.28	1.595	216	4.56	-129.8×10^{-6}
Picene	32.7	278.33	361	693	1.2	1.812	366	7.14	
Coronene	38.4	300.35	376	525	1.371	1.48	437	6.05	-243.3×10^{-6}
Heptacene	43.8	378.45		677.2	1.3	1.867			
Triangulene	33.9	276.33		410			171		
Benzopyrene	36	252.31	372	496	1.24	1.887	178		
Ovalene	53.7	398.45	696	456.6	1.496	1.469	472	0.853	-353.8×10^{-6}
Phenalene	17.7	166.22	216	70	1.139	1.692	159		-205.5×10^{-6}
Pentacene	31.2	278.36	42	1.3	1.812		301	7.14	-205.5×10^{-6}

The scatter plots for the above collection of data are given below. For each of the parameter, a linear regression model is derived and the coefficient R^2, which describes the strength of the model is given. The linear relationship of the ISI index with the molar mass is found to be the strongest. Also, the relationship between the ISI index and the complexity is relatively stronger and that with the magnetic susceptibility and density are fairly good. The details of the regression models along with the coefficient of determination are listed separately for all the parameters in the next table. The variable x in the above table represents the ISI index of benzenoids.

5 Concluding Remarks and Future Directions

The article highlights the detailed study of the structure of a special class of polycyclic aromatic hydrocarbons, named benzenoids, where the bond formation between benzene rings is considered as the graphical operation of edge fusion. This may be very useful in further research to investigate many other topological indices efficiently.

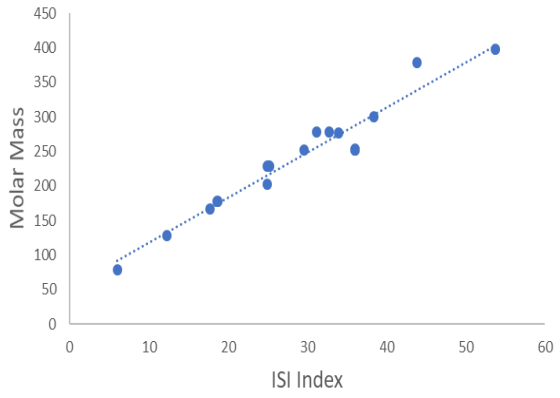

Figure 4: ISI index versus Molar Mass with $R^2 = 0.9333$.

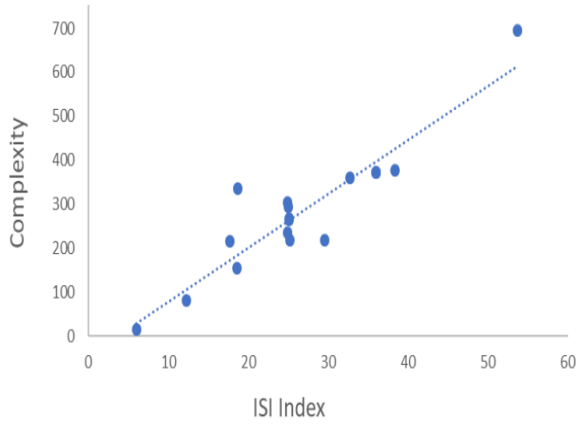

Figure 5: ISI index versus Complexity with $R^2 = 0.8507$.

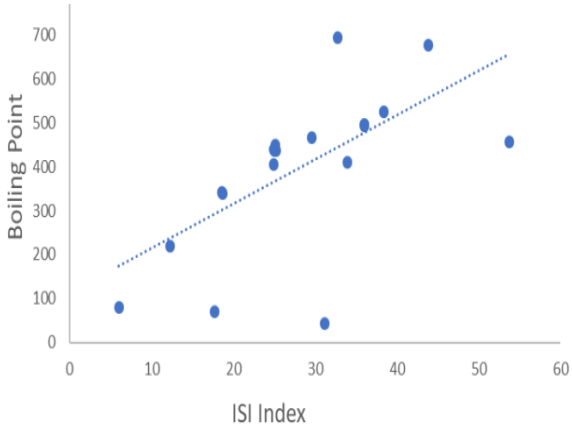

Figure 6: ISI index versus Boiling point with $R^2 = 0.3969$.

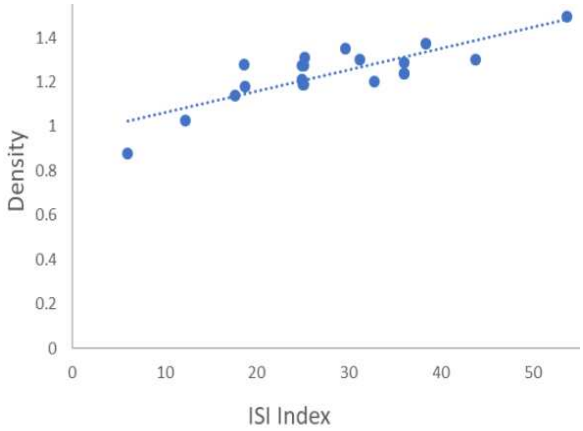

Figure 7: ISI index versus density with $R^2 = 0.6738$.

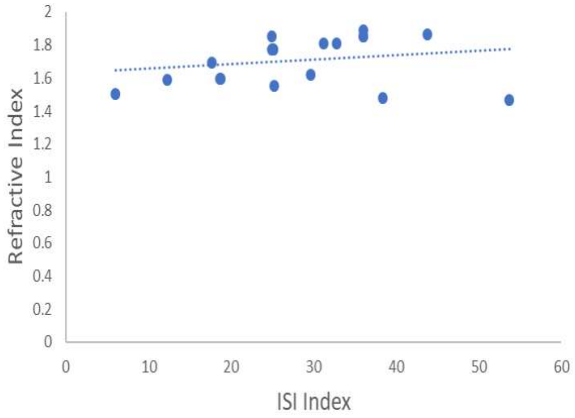

Figure 8: ISI index versus Refractive Index with $R^2 = 0.0462$.

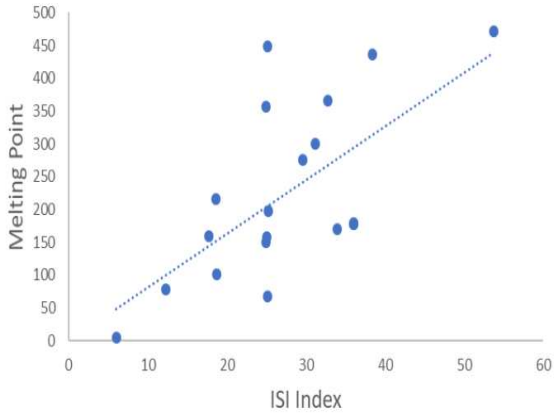

Figure 9: ISI index versus Melting point with $R^2 = 0.4146$.

Figure 10: ISI index versus Log P with $R^2 = 0.0168$.

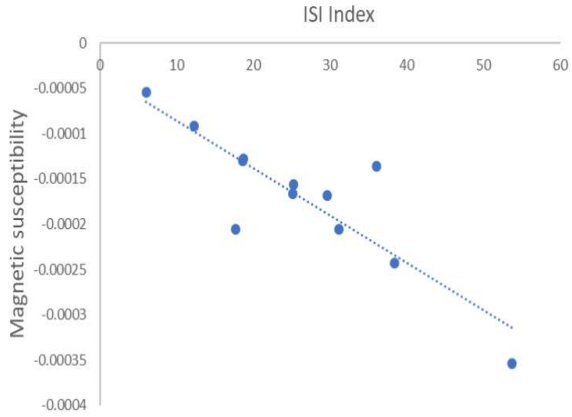

Figure 11: ISI index versus Magnetic susceptibility with $R^2 = 0.756$.

Parameter P	Linear equation modelled	R^2
Molar mass	$P = 6.519x + 53.171$	0.9333
Complexity	$P = 12.232x + 44.222$	0.8507
Boiling Point	$P = 10.089x + 114.47$	0.3969
Density	$P = 0.0095x + 0.9689$	0.6738
Refractive Index	$P = 0.0028x + 1.6279$	0.0462
Meling Point	$P = 8.1593x + 0.0424$	0.4146
Log P	$P = 0.0201x + 4.4964$	0.0168
Magnetic susceptibility	$P = \left(5 \times 10^{-6}\right) x - \left(3 \times 10^{-6}\right)$	0.7560

Analysis of the correlation between physicochemical entities of benzenoids with the ISI index with the help of linear regression models is made in this article. One can construct other statistical models like logarithmic and quadratic modeling for the same, which may lead to better conclusions.

In recent years a plethora of various graph energies appeared in the literature. Hundreds of graph energies related to molecular graphs are proven to be well-known descriptors. In this context, one can think of a similar analysis with the ISI energy, instead of the ISI index, and correlate the physical properties of benzenoids with the ISI Energy.

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