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Mathematical Properties of a Novel Graph-Theoretic Irregularity Index with Potential Applicability in QSPR Modeling

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Abstract: Irregularity indices are graph-theoretic parameters designed to quantify the irregularity in a graph. In this paper, we study the practical applicability of irregularity indices in QSPR modeling of the physicochemical and quantum-theoretic properties of compounds. Our comparative testing shows that the recently introduced IRA index has significant priority in applicability over other irregularity indices. In particular, we show that the correlation potential of the IRA index with certain physicochemical and quantum-theoretic properties such as the enthalpy of formation, boiling point, and π-electron energies is significant. Our QSPR modeling suggests that the regression models with the aforementioned characteristics such as strong curve fitting are, in fact, linear. Considering this the motivation, the IRA index was studied further, and we provide analytically explicit expressions of the IRA index for certain graph operations and compositions. We conclude the paper by reporting the conclusions, implications, limitations, and future scope of the current study.

Keywords: irregularity index; enthalpy of formation; boiling point; π-electronic energy; benzenoid hydrocarbon; QSPR model; transformation graph; derived graph

MSC: 05C92; 05C09; 05C76

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1. Introduction

1.1. Background

The retrieval of the biological, quantum-theoretic, and physicochemical characteristics of a compound from its structure (chemical) is a contemporary technique in reticular chemistry. Though the idea seems self-explanatory, understanding this connection, of retrieving the information of a physicochemical property from its structure, up to its full potential, is rather challenging [1]. One of the frequent challenges is the unavailability of experimental data, which are normally required in order to unveil the aforementioned connection. Thus, in order to elucidate this relationship of the structural dependence of a physicochemical feature, diverse research has been performed to estimate the missing data (e.g., normal boiling point, heat of formation); see, for instance, [2–6]. This research direction aiming at the investigation of predictive potentials frequently employs diverse methods such as machine learning [7], among others. More modern approaches such as graph signal processing (GSP) [8] are being formulated to address this old problem.

One of the contemporary tools that is frequently employed in order to predict the diverse physicochemical features of a chemical compound is provided by molecular descriptors. Their strength lies in developing QSPR/QSAR models, which are regression

models describing the so-called relationship between a chemical property and its molecular structure. These molecular descriptors have been proposed at an accelerating rate; see, for instance, [9–11]. Recently, Vladimirova et al. [12] employed QSPR modeling in correlating the sensitivity (potentiometric) of sensorial membranes. Topological descriptors are an important family of descriptors lying in the bigger class of molecular descriptors. They are numerical quantities transforming a chemical structure into a mathematical real number. Chemical graph theory, in this aspect, converts a chemical compound into a chemical graph by constructing a correspondence between non-hydrogen atoms (respectively bonds) and vertices (respectively edges). Diverse algorithms are then employed to transform such mathematical point–line objects to graph numerical invariants, also known as topological descriptors. Much of the available research [13–17] shows that these graph-based invariants, which are easily computable, efficiently encrypt a significantly higher level of the structural information of chemical compounds. Recently, Azadifar et al. [18] applied the graph-theoretic relevancy–redundancy gene selection method to cancer diagnosis.

1.2. Related Work

Based on their mathematical definitions, these graph-based topological descriptors/indices are classified into diverse groups, of which degree-based topological indices (DIs) have significantly more accuracy; see [19]. For the set of simple connected graphs $\sum$, an irregularity index $IR(\Gamma)$ is a map $IR : \sum \to \mathbb{R}^+ \cup \{0\}$ such that $IR(\Gamma) = 0 \iff \Gamma$ is regular. The motivation for defining an irregularity index was purely mathematical, and it was the quantification of the irregularity in a graph. Therefore, most of the studies conducted on irregularity indices are pure mathematical. For instance, in 2005, Gutman et al. [20] conducted a comparison between different irregularity indices for chemical trees. In the same year, Hansen and Mélot [21] found sharp upper and lower bounds on Albertson's irregularity index. Zhou and Luo [22], in 2008, further improved the extremal results on Albertson's irregularity index, which were previously published by Hansen and Mélot [21]. Luo and Zhou [23] found sharp bounds on Albertson's irregularity index of trees and unicyclic graphs with the given matching number. Mukwembi, in 2013 [24], studied maximally irregular graphs with respect to Albertson's irregularity index. Réti and Dimitrov [25] studied Albertson's irregularity index in bidegreed graphs. Dimitrov and Réti [26] studied graphs whose Albertson's irregularity indices are the same. Abdo et al. [27] studied the structural sensitivity of some well-known irregularity indices. Réti [28], in 2019, studied a relation between irregularity indices such as the σ index and the main eigenvalues of a graph. Other mathematical results on the irregularity indices can be found in [29–36]. Importantly, all of these results have primarily contributed to graph theory, but are not applicable to graph theory.

Irregularity indices for different graph operations have been studied since their conception. Abdo and Dimitrov [37] derived sharp bounds on Albertson's irregularity index of product graphs such as the strong graph, the Cartesian graph, corona graph, and join graph, among others. For the same product graphs, Abdo and Dimitrov [38] derived sharp bounds on the total irregularity index. Abdo and Dimitrov [39] derived exact expressions of the total irregularity index of certain derived graphs. De et al. [40] conducted the study of Abdo and Dimitrov [39] for Albertson's irregularity index. It is worth mentioning that all of these results on composite and product graphs have been published with no motivation from the application perspective.

Since the motivation of defining irregularity indices was purely mathematical, researcher have investigated their practical applicability to other scientific disciplines Réti et al. [41] studied the relation between various degree-based irregularity indices for isomeric octanes and showed that the correlation between irregularity indices and the physicochemical properties of alkanes is, in general, weak. Recently, in 2022, Emadi Kouchak et al. [42] presented an application of irregularity indices in computer science by employing graph irregularity indices in quantifying network structural similarities and dissimilarities. Table 1 presents an overview of current methods employing irregulaity indices.

It is noteworthy to mention that none of the literature on irregularity indices presents methods for their calculation on large-sized graphs. In Section 3, we present a two-step procedure and the MatLab code to calculate the commonly occurring irregularity indices for large-sized graphs.

Table 1. Some methods studying irregularity indices.

Method	Description
Gutman et al. [20]	Restricted to the class of chemical trees.
Hansen and Mélot [21]	Lacks applicability. Restricted to Albertson's index.
Zhou and Luo [22]	Lacks applicability. Restricted to Albertson's index.
Mukwembi in 2013 [24]	Lacks applicability. Restricted to Albertson's index.
Réti and Dimitrov [25]	Lacks applicability. Restricted to bidegreed graphs.
Dimitrov and Réti [26]	Lacks applicability. Restricted to Albertson's index.
Abdo et al. [27]	Lacks applicability.
Réti [28]	Lacks applicability
Abdo and Dimitrov [37]	Applicable to Albertson's index only.
Abdo and Dimitrov [39]	Applicable to Albertson's index only.
De et al. [40]	Applicable to Albertson's index only.
Réti et al. [41]	Chemical applicability restricted to isomeric octanes.
Emadi Kouchak et al. [42]	Applications to computer science.

1.3. Motivation

Based on related work, in this subsection, we outline the limitations of existing methods, which, in turn, motivated this study:

- Almost all of the results published on irregularity indices are purely mathematical without discussing their applicability.
- Calculating an irregularity index for graphs on a large number of vertices is rather difficult. No computational technique has been proposed so far to tackle this issue.
- The correlation ability of irregularity indices for predicting physicochemical properties of isomeric octanes, i.e., alkanes, is rather poor.
- No criteria have been published to address the proliferation of newly introduced irregularity indices.
- Mathematical results on composition and product graphs have only been studied for Albertson's irregularity and the total irregularity indices, which have no practical applicability, except the quantification of the irregularity in a graph.
- There has not been any study published that reflects on how to employ mathematical results on composition and product graphs for practical applications.

1.4. Contributions

Based on the limitations mentioned in the previous subsection, we outline the scientific contributions made in this work:

- A computational technique is proposed to compute irregularity indices, which efficiently works for large-sized graphs.
- We conduct a comparative testing of commonly occurring irregularity indices for the predicting physicochemical and quantum-theoretic properties of benzenoid hydrocarbons.
- The IRA index outperforms all the irregularity indices by correlating significantly well with the quantum-theoretic and fairly well with the physicochemical properties.

- Having potential applications in QSPR modeling, the IRA index is further studied for various transformation and derived graphs.
- We devise a method of employing mathematical results on transformation and derived graphs in correlating the physicochemical and quantum-theoretic properties of derivative hydrocarbons.

1.5. Organization of the Paper

This paper is organized as follows: Section 2 presents the definitions and preliminary results required in later sections. Section 3 conducts a comparative testing of commonly occurring irregularity indices for predicting the physicochemical and quantum-theoretic properties of benzenoid hydrocarbons. Sections 4 and 5 present the results on the IRA index of transformation graphs and derived graphs, respectively. In Section 6, we put forward a method of employing mathematical results on transformation and derived graphs in correlating the physicochemical and quantum-theoretic properties of derivative hydrocarbons. Section 7 concludes the paper by presenting the conclusions, implications, limitations, and future scope.

2. Mathematical Preliminaries

A simple graph Γ is a mathematical tuple comprising a set of nodes V and a set $E \subseteq \binom{V}{2}$ of links connecting some or all nodes. The multiplicity $\varepsilon = \mid E \mid$ (respectively $v = \mid V \mid$) is known as the size (respectively order). Two vertices $y, z \in V(\Gamma)$ (respectively edges $e, f \in E(\Gamma)$) are said to be adjacent if $yz \in E(\Gamma)$ (respectively e and f share a common end-vertex). In that case, we denote adjacency with $y \sim z$ or $e \sim f$. A vertex $y \in V(\Gamma)$ and an edge $e \in E(\Gamma)$ are called incident and written as $y \sim e$ if y is one of the end-vertices of e. The degree/valency $d(y)$ of $y \in V$ is the cardinality of the neighborhood $N(y) := \{z \in V : y \sim z\}$ of y. Let μ_y be the average of the degrees of the neighbors of vertex $y \in V(\Gamma)$. A graph for which every cycle is of an even length is known as bipartite. A graph is called bipartite if it contains no cycle of an oddlength. A graph embeddable in the Euclidean space $\mathbb{R}^2$ is called planar; otherwise, it is called non-planar.

A topological invariant $IR(\Gamma)$ of graph Γ is said to be an irregularity index if $IR(\Gamma) \geq 0$ and $IR(\Gamma) = 0$ if and only if Γ is regular. Based on its defined structure, an irregularity index could either be eigenvalue-based or degree-based.

The first-ever proposed irregularity index is eigenvalue-based and known as the Collatz–Sinogowitz irregularity index [43], which determines the irregularity of a graph. For a v-vertex ε-edge graph $\Gamma(v, \varepsilon)$, it is defined as follows:

$$CS(\Gamma) = \lambda(\Gamma) - \frac{2\varepsilon}{v},$$

where λ is the spectral radius of the adjacency matrix of Γ. Because of the lesser computational complexity, irregularity indices are mostly degree-based. In 1992, Bell [44] introduced a degree-based irregularity index known as the variance of degree $Var(\Gamma)$, which has significant application in chemistry. For a (v, ε) graph Γ, it is defined as

$$Var(\Gamma) = \frac{1}{v}\sum_{y \in V(\Gamma)} (d(y))^2 - \frac{1}{v^2}\left(\sum_{y \in V(\Gamma)} d(y)\right)^2 = \frac{1}{v}\sum_{y \in V(\Gamma)} (d(y))^2 - \left(\frac{2\varepsilon}{v}\right)^2.$$

Using the variance, Réti [28] introduced the IRV irregularity index defined as $IRV(\Gamma) = v^2 Var(\Gamma)$. In 1997, Albertson introduced another degree-based irregularity index known as Albertson's irregularity index. It is defined as

$$AL(\Gamma) = \sum_{yz \in E(\Gamma)} \mid d(y) - d(z) \mid .$$

By extending Albertson's irregularity index, Gutman et al. [34] introduced the sigma index.

$$\sigma(\Gamma) = \sum_{yz \in E(\Gamma)} (d(y) - d(z))^2.$$

A topological index T is simply a map $T : \sum \to \mathbb{R}$. Topological indices have important applications in chemistry. The Randić connectivity index belongs to the oldest class of descriptors. Randić [45] introduced this topological descriptor in 1975. For a graph Γ, it is defined as

$$R(\Gamma) = \sum_{yz \in E(\Gamma)} \frac{1}{\sqrt{d(y)d(z)}}.$$

Another Randić-type invariant [46] is the reciprocal Randić index, defined as:

$$RR(\Gamma) = \sum_{yz \in E(\Gamma)} \sqrt{d(y)d(z)}.$$

Besides the Randić index, some of the other degree-based topological indices include the first and second Zagreb indices [47,48] and the forgotten topological index [49]. For a graph Γ, they are defined as follows:

$$\begin{aligned} M_1(\Gamma) &= \sum_{yz \in E(\Gamma)} (d(y) + d(z)) = \sum_{y \in V(\Gamma)} (d(y))^2, \qquad M_1(\Gamma) = \sum_{yz \in E(\Gamma)} (d(y)d(z)), \\ F(\Gamma) &= \sum_{yz \in E(\Gamma)} \left[(d(y))^2 + (d(z))^2 \right] = \sum_{y \in V(\Gamma)} (d(y))^3. \end{aligned}$$

Using the Randić index of a graph Γ i.e., $R(\Gamma)$, Li and Gutman in their book [46] introduced a novel irregularity index called the IRA index. For an v-vertex graph Γ, it is defined as

$$IRA(\Gamma) = v - 2 \sum_{yz \in E(\Gamma)} \frac{1}{\sqrt{d(y)d(z)}} = v - 2R(\Gamma).$$

Note that the definition of the IRA index suggests that any result on the Randić connectivity index gives a directed result on IRA. The Randić index has been studied so extensively that there is a whole book written on this graphical parameter. We refer the reader to the book [46] and the survey [50] on the Randić index. Estrada [51] reintroduced the IRA index from the Randić index and presented their applications to complex biomolecular networks. Later on, Estrada [52] also presented applications of the IRA index in quantifying network heterogeneity. Gutman [53] showed that, just like the transformation of the Randić index into the IRA index, other degree-based indices can also be transformed into their corresponding irregularities. Some computational results on the IRA index of chemical and neural networks are reported by Kang et al. [54] and Chu et al. [55].

Other irregularity indices for a (v, ε)-graph, which we use in the comparative testing, are listed below:

$$\begin{aligned} IR_1(\Gamma) &= F(\Gamma) - \frac{2\varepsilon}{v} M_1(\Gamma), \qquad IR_2(\Gamma) = \sqrt{\frac{M_2(\Gamma)}{\varepsilon}} - \frac{2\varepsilon}{v}, \\ IRF(\Gamma) &= F(\Gamma) - 2M_2(\Gamma), \qquad IRFW(\Gamma) = \frac{IRF(\Gamma)}{M_2(\Gamma)}, \\ IRB(\Gamma) &= M_1(\Gamma) - 2RR(\Gamma), \qquad IRC(\Gamma) = \frac{RR(\Gamma)}{\varepsilon} - \frac{2\varepsilon}{v}, \\ IRDIF(\Gamma) &= \sum_{yz \in E(\Gamma)} \left| \frac{d(y)}{d(z)} - \frac{d(z)}{d(y)} \right|, \qquad IRG(\Gamma) = \sum_{yz \in E(\Gamma)} |\ln d(y) - \ln d(z)|, \\ IRLU(\Gamma) &= \sum_{yz \in E(\Gamma)} \frac{|d(y) - d(z)|}{\min(d(y), d(z))}, \qquad IRLF(\Gamma) = \sum_{yz \in E(\Gamma)} \frac{|d(y) - d(z)|}{\sqrt{d(y), d(z)}}, \end{aligned}$$

$$IRLA(\Gamma) = \sum_{yz\in E(\Gamma)} 2\frac{|d(y)-d(z)|}{d(y)+d(z)}, \qquad IRD(\Gamma) = \sum_{yz\in E(\Gamma)} \ln[1+|d(y)-d(z)|],$$

$$IRGA(\Gamma) = \sum_{yz\in E(\Gamma)} \ln\left(\frac{d(y)+d(z)}{2\sqrt{d(y)d(z)}}\right), \qquad IRM_1(\Gamma) = \frac{1}{v}\sum_{y\in V(\Gamma)} \mu_y - \frac{2\varepsilon}{v},$$

$$IRM_2(\Gamma) = \sum_{y\in V(\Gamma)} |d(y)-\mu_y|.$$

For details on these irregularity indices, we refer to the work by Réti et al. [41].

This paper focuses on this new irregularity index, i.e., the IRA index, and presents its potential applicability in modeling the physicochemical and quantum-theoretic properties of benzenoid hydrocarbons. Then, further mathematical properties of the IRA index are investigated.

Now, we introduce some derived graphs based on different graph operations. The total graph $\mathcal{T}(\Gamma)$ of a graph Γ was introduced by Behzad [56] in 1967, and it has the vertex set $V(\mathcal{T}(\Gamma)) = V(\Gamma)\cup E(\Gamma)$ such that $yz, ye, ef \in E(\mathcal{T}(\Gamma))$ if and only if $y\sim z$, $z\sim e$, or $e\sim f$ is adjacent/incident in Γ.

Sampathkumar and Chikkodimath [57] extended the concept of the total graph and put forward two semi-total point and line graphs. The semi-total point graph $\mathcal{T}_1(\Gamma)$ has the vertex set $V(\mathcal{T}_1(\Gamma)) = V(\Gamma)\cup E(\Gamma)$, and any two vertices $y, z \in V(\mathcal{T}_1(\Gamma))$ are adjacent if and only if:

(i) $y, z \in V(\Gamma)$ such that $y\sim z$ in Γ or;
(ii) $y\in V(\Gamma)$, $z\in E(\Gamma)$, or vice versa, such that $y\sim z$ in Γ.

Similarly, the semi-total line graph $\mathcal{T}_2(\Gamma)$ has the vertex set $V(\mathcal{T}_2(\Gamma)) = V(\Gamma)\cup E(\Gamma)$, and any two vertices $y, z \in V(\mathcal{T}_2(\Gamma))$ are adjacent if and only if:

(i) $y, z \in E(\Gamma)$ such that $y\sim z$ in Γ or;
(ii) $y\in V(\Gamma)$, $z\in E(\Gamma)$, or vice versa, such that $y\sim z$ in Γ.

Independently, similar concepts were studied by Akiyama et al. [58], where they called these operations "middle graphs".

The subdivision $S(\Gamma)$ of a graph Γ has the vertex set $V(S(\Gamma)) = V(\Gamma)\cup E(\Gamma)$ such that $xy \in E(S(\Gamma))$ if and only if $y\in V(\Gamma)$ and $z\in E(\Gamma)$, and vice versa. Informally, $S(\Gamma)$ is built by adding a degree-two vertex on each edge of Γ.

The line graph $L(\Gamma)$ has $V(L(\Gamma)) = E(\Gamma)$ such that $g, h \in V(L(\Gamma))$ are adjacent in $L(\Gamma)$ iff $g\sim h$ in Γ.

The double-graph $D(\Gamma)$ of Γ, having two copies Γ_1 and Γ_2, has its vertex set $V(D(\Gamma)) = V(\Gamma_1)\cup V(\Gamma_1)$ preserving $E(\Gamma_i)$ $(1\le i\le 2)$ and for any $yz\in E(\Gamma)$; we add two additional edges y_1z_2 and z_1y_2 in $D(\Gamma)$. Similarly, the strong double-$SD(\Gamma)$ of Γ is obtained from $D(\Gamma)$ by additionally adding y_iz_i for every $yz\in E(\Gamma)$.

The extended double-cover Γ^* of Γ was introduced by Alon [59]. If $V(\Gamma) = \{x_1,\ldots,x_v\}$, then Γ^* is a bipartite graph with partition (Y, Z), where $Y = \{y_1\ldots, y_v\}$ and $Z = \{z_1,\ldots,z_v\}$ in which $y_i\sim z_j$ iff either $i=j$ or $y_iz_i\in E(\Gamma)$.

The definitions of some of the aforementioned derived graphs suggest the following lemma.

Lemma 1. *Let Γ be an (v,ε)-graph. Let $x\in V(\Gamma)$ and $f = yz\in E(\Gamma)$. Then, the following relations hold:*

(i) $d_{S(\Gamma)}(x) = d_\Gamma(x)$ and $d_{S(\Gamma)}(f) = 2$.
(ii) $d_{L(\Gamma)}(f) = d_\Gamma(y) + d_\Gamma(z) - 2$.
(iii) $d_{\mathcal{T}_1(\Gamma)}(x) = 2d_\Gamma(x)$ and $d_{\mathcal{T}_1(\Gamma)}(f) = 2$.
(iv) $d_{\mathcal{T}_2(\Gamma)}(x) = d_\Gamma(x)$ and $d_{\mathcal{T}_2(\Gamma)}(f) = d_{L(\Gamma)}(f)+2 = d_\Gamma(y)+d_\Gamma(z)+2$.
(v) $d_{\mathcal{T}(\Gamma)}(x) = 2d_\Gamma(x)$ and $d_{\mathcal{T}(\Gamma)}(f) = d_{L(\Gamma)}(f)+2 = d_\Gamma(y)+d_\Gamma(z)+2$.

Here, we define some auxiliary terminologies required later in this section. For an (v, ε)-graph Γ, we define

$$ERR(\Gamma) = \sum_{y \in V(\Gamma)} \sqrt{y}, \quad RA(\Gamma) = \sum_{xy, yz \in E(\Gamma)} \frac{1}{\sqrt{(d(x) + d(y) - 2) \times (d(y) + d(z) - 2)}}.$$

$$LR(\Gamma) = \sum_{xy, yz \in E(\Gamma)} \frac{1}{\sqrt{(d(x) + d(y)) \times (d(y) + d(z))}}, \quad MR(\Gamma) = \sum_{yz \in E(\Gamma)} \frac{1}{\sqrt{d(y) \times (d(y) + d(z))}}.$$

$$AR(\Gamma) = \sum_{yz \in E(\Gamma)} \frac{1}{\sqrt{(2d(y) + 1) \times (2d(z) + 1)}}, \quad BR(\Gamma) = \sum_{yz \in E(\Gamma)} \frac{1}{\sqrt{(d(y) + 1) \times (d(z) + 1)}}.$$

$$ERa(\Gamma) = \sum_{yz \in E(\Gamma)} \frac{1}{\sqrt{(\varepsilon + v - 1 - 2d(y)) \times (\varepsilon + v - 1 - 2d(z))}}.$$

$$ERRa(\Gamma) = \sum_{x \in V(\Gamma), y \in E(\Gamma), x \nsim y} \frac{1}{\sqrt{(\varepsilon + v - 1 - 2d(x)) \times (v - 2)}}.$$

Next, we introduce some transformation operations on graphs put forward by Wu and Meng [60] in 2002. For a graph Γ and variables $a, b \in \{+, -\}$, the transformation graph Γ^{ab} has the vertex set $V(\Gamma^{ab})$ partitioned into V_a and V_b, i.e., $V(\Gamma^{ab}) = V_a \cup V_b$, where

$$V_a = \{y \mid y \in V(\Gamma)\} \quad \text{and} \quad V_b = \{y \mid y \in E(\Gamma)\}. \tag{1}$$

Moreover, the edge set of Γ^{ab} can be partitioned in E_a, E_b, and E_c, i.e., $E(\Gamma^{ab}) = E_a \cup E_b \cup E_c$, where

$$E_a = \{yz \mid y, z \in V(\Gamma)\}, \quad E_b = \{ef \mid e, f \in E(\Gamma)\}, \quad \text{and} \quad E_c = \{ye \mid y \in V(\Gamma), e \in E(\Gamma)\}. \tag{2}$$

Alternatively, the vertex set of Γ^{ab} is $V(\Gamma^{ab}) = V(\Gamma) \cup E(\Gamma)$, and for any $y, z \in V(\Gamma^{ab})$, we have $y \sim z$ in Γ^{ab} iff:

(i) $y, z \in V(\Gamma)$, $yz \in E(\Gamma)$ if $a = +$ and $yz \notin E(\Gamma)$ if $a = -$.
(ii) $x \in V(\Gamma)$, $y \in E(\Gamma)$, $x \sim y$ in Γ if $b = +$ and $x \nsim y$ in Γ if $b = -$.

Figure 1 presents a graph T and its four transformation graphs.

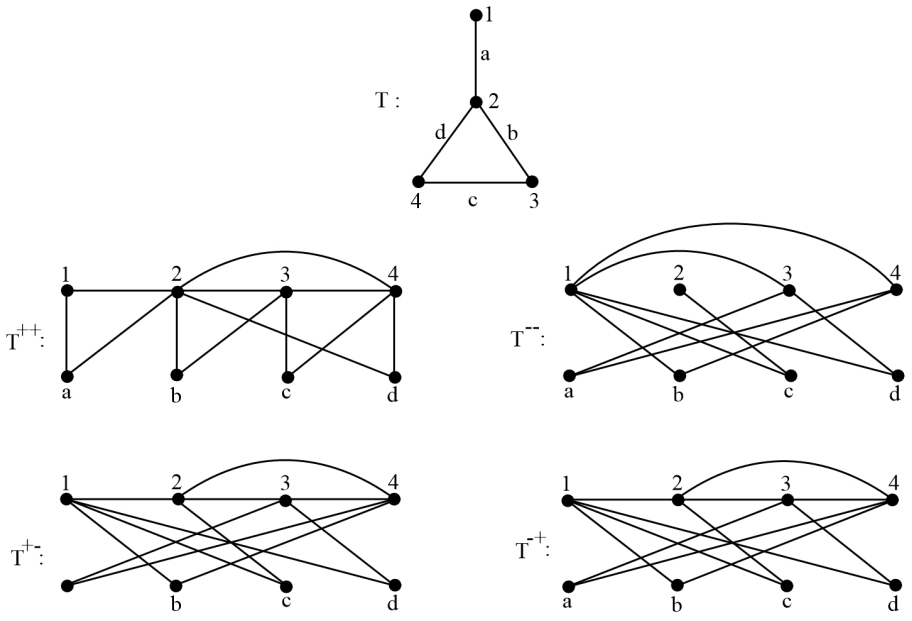


Figure 1. A graph T and its four transformation graphs.

Based on the definitions of the transformation graphs, the following properties can be deduced.

Lemma 2. *Let* Γ *be an* (v, ε)*-graph. Let* $x \in V(\Gamma)$ *and* $f = yz \in E(\Gamma)$*. Then, the following relations hold:*

(i) $d_{\Gamma^{++}}(x) = 2d_{\Gamma}(x)$ and $d_{\Gamma^{++}}(f) = 2$.
(ii) $d_{\Gamma^{+-}}(x) = \varepsilon$ and $d_{\Gamma^{+-}}(f) = v - 2$.
(iii) $d_{\Gamma^{-+}}(x) = v - 1$ and $d_{\Gamma^{-+}}(f) = 2$.
(iv) $d_{\Gamma^{--}}(x) = v + \varepsilon - 1 - 2d_{\Gamma}(x)$ and $d_{\Gamma^{--}}(f) = v - 2$.

Further mathematical properties of transformation graphs were studied by Xu and Wu [61] and Yi and Wu [62].

3. Application of the *IRA* Index in QSPR Modeling

In order to investigate the potential applicability of irregularity indices in QSPR modeling, we would require computing them for the lower benzenoid hydrocarbons, as they represent both cyclic and acyclic chemical structures. The next subsection explains the computational details that will be carried out in subsequent subsections.

3.1. Computational Details

Although the defining structure of any degree-based irregularity index is simple enough to compute it on paper, using a computer saves much time.

Here, we devised a simple way of calculating any irregularity index for an arbitrary graph. Note that, although we used this method only for computing the *IRA* index of the lower benzenoid hydrocarbons, the method can be employed for any degree-based irregularity index and for any arbitrary graph.

Our simple two-step process employs newGraph [63] and MatLab [64] to compute a degree-based irregularity index *IR* of a graph Γ:

Step 1: Draw Γ in newGraph, and compute its adjacency matrix A.
Step 2: Input A into our program in MatLab to compute *IR*.

Although our MatLab program only computes the *IRA* index, it is easily modifiable for any arbitrary degree-based irregularity index.

Our MatLab program with a README file is publicly available on GitHub. Access the web page https://github.com/Sakander/Irregulaity-Indices.git (accessed on 18 November 2022) in order to access the code.

3.2. QSPR Modeling of Physicochemical Properties

In order to address the proliferation of molecular descriptors, Gutman et al. [65] laid down the foundation to investigate the quality of degree-based topological indices for the prediction of the physicochemical characteristics of compounds. They selected the enthalpy of formation ΔH_f^o (respectively the boiling point ΔT_{bp}) to be the monitors of thermal characteristics (respectively van der Waals-type relations) for their comparative testings. On the other hand, Gutman and Trinajstić [66] studied the dependence of degree-based descriptors on the energy of the π-electron $E_\pi = E_\pi(\beta)$ (i.e., measured in β units) for benzenoid hydrocarbons. Lučić et al. [67] and Chen [68] studied the prediction strength of the sum-connectivity and product-connectivity indices for the π-electronic energy of benzenoid hydrocarbons. Following the work in [67], we also determined the predictive potential of the *IRA* index for determining the E_π of benzenoid hydrocarbons. The criterion to determine the performance of an irregularity index is simply the determination of the statistical correlation coefficient. The higher the value (i.e., the closer to one) of the correlation coefficient is, the better the efficiency of an irregularity index.

Following the standard choice of chemical compounds, we consider the lower benzenoid hydrocarbons, as they are supposed to represent both cyclic and acyclic chemical

structures. For the sake of the authenticity and reliability of the statistical inference, we took 22 lower benzenoid hydrocarbons, claiming the number to be large enough. The public availability of experimental data is another considerable reason for choosing the lower benzenoid hydrocarbons. Note that the lower benzenoid hydrocarbons are actually polycyclic aromatic hydrocarbons (PAHs). Figures 2 and 3 depict the 22 PAHs considered with their aromaticity. For E_π, we considered 29 lower benzenoid hydrocarbons as their experimental data are easily accessible.

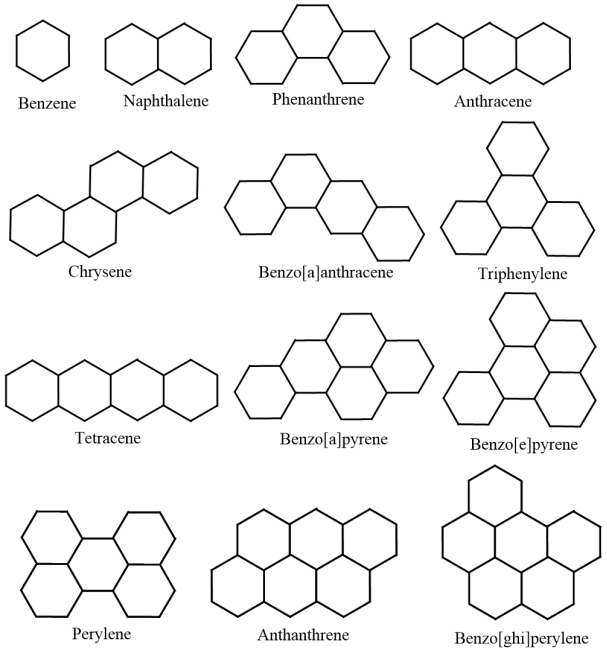


Figure 2. The 22 lower benzenoid hydrocarbons. Contd.

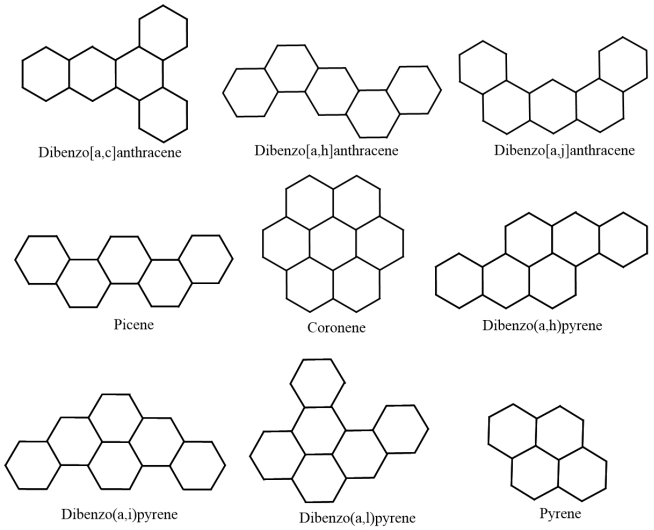


Figure 3. The 22 lower benzenoid hydrocarbons.

The experimental data of ΔT_{bp} for the lower PAHs considered here were provided by the standard NIST databases [69]. On the other hand, the experimental data for ΔH_f^o were retrieved from Allison and Burgess [2]. To tally the data, we confirmed them with Nikolić et al. [70]. The experimental data for E_π for the 29 lower benzenoid hydrocarbons was taken from Lučić et al. [67].

For the molecules in Figures 2 and 3, a degree-based irregularity index was calculated conveniently. However, to save time, one may employ the computational method

in Section 3.1 to compute all the irregularity indices in Section 2 simultaneously. After calculating the irregularity indices, we calculated the Pearson correlation coefficient ρ with E_π, ΔT_{bp}, and ΔH_f^o for the 29 lower benzenoid hydrocarbons. Table 2 presents the irregularity indices defined in Section 2 and their correlation coefficients with E_π, ΔT_{bp} and ΔH_f^o for the lower benzenoid hydrocarbons.

Table 2. The Pearson correlation coefficient ρ between irregularity indices and E_π, ΔT_{bp}, and ΔH_f^o.

Irregularity Index	E_π	ΔT_{bp}	ΔH_f^o
IRA	0.9997	0.9976	0.9343
AL	0.7393	0.8091	0.7803
σ	0.7393	0.8091	0.7803
Var	0.7835	0.9021	0.7793
IR_1	0.9951	0.9964	0.9055
IR_2	0.2924	0.6989	0.6053
IRF	0.7393	0.8091	0.7803
$IRFW$	−0.0862	−0.3355	−0.2005
IRB	0.7393	0.8091	0.7803
IRC	0.4557	0.7955	0.6886
$IRDIF$	0.7393	0.8091	0.7803
IRG	0.7393	0.8091	0.7803
$IRLU$	0.7393	0.8091	0.7803
$IRLF$	0.7393	0.8091	0.7803
$IRLA$	0.7393	0.8091	0.7803
IRD	0.7393	0.8091	0.7803
$IRGA$	0.7393	0.8092	0.7803
IRM_1	0.2186	0.1072	0.1526
IRM_2	0.7393	0.8091	0.7803

By calculating the average of all three correlation coefficients, we can easily see in Table 2 that only the IRA index warrants further usage in the QSPR modeling of the physicochemical and quantum-theoretic properties of benzenoid hydrocarbons. Based on this motivation, next, we focus on the IRA index only.

We conducted a detailed statistical analysis of the IRA index with the experimental data of ΔT_{bp} and ΔH_f^o for the benzenoid hydrocarbons in Figures 2 and 3. The corresponding statistical parameters such as the correlation coefficient, the regression model with the confidence interval, the standard error of the fit, the determination coefficient, the scatter plot, etc., were computed to assess how closely the IRA index correlated with the experimental data. A similar treatment was given for the π-electronic energy E_π and the IRA index for the lower 29 benzenoid hydrocarbons. Table 3 (respectively Table 4) exhibits the values of ΔT_{bp} and ΔH_f^o (respectively E_π) and the IRA index of the 22 (respectively 29) lower benzenoid hydrocarbons.

For E_π, the linear regression model with the 95% confidence intervals for the slope and intercepts of the model and the corresponding statistical parameters are given as follows:

$$E_\pi = 1.2808_{\pm 0.0820} IRA + 3.5939_{\pm 1.6409}, \quad \rho = 0.999, \ r^2 = 0.9734, \ s = 0.3128.$$

Between E_π and the IRA index, Figure 4 depicts the scatter plot.

Table 3. The experimental data of ΔT_{bp} and ΔH_f^0 and the IRA index of the 22 lower PAHs.

Molecule	ΔT_{bp} in °C	ΔH_f^o in kJ/mol	IRA
Naphthalene	218	141	9.3333
Phenanthrene	338	202.7	13.3333
Anthracene	340	222.6	13.3333
Chrysene	431	271.1	17.3333
Benzo[a]anthracene	425	277.1	17.3333
Triphenylene	429	275.1	17.3333
Tetracene	440	310.5	17.3333
Benzo[a]pyrene	496	296	19.3333
Benzo[e]pyrene	493	289.9	19.3333
Perylene	497	319.2	19.3333
Anthanthrene	547	323	21.3333
Benzo[ghi]perylene	542	301.2	21.3333
Dibenzo[a,c]anthracene	535	348	21.3333
Dibenzo[a,h]anthracene	535	335	21.3333
Dibenzo[a,j]anthracene	531	336.3	21.3333
Picene	519	336.9	21.3333
Coronene	590	296.7	23.3333
Dibenzo(a,h)pyrene	596	375.6	23.3333
Dibenzo(a,i)pyrene	594	366	23.3333
Dibenzo(a,l)pyrene	595	393.3	23.3333
Pyrene	393	221.3	15.3333

Table 4. The experimental data of E_π and the IRA index of the 29 lower PAHs.

Molecule	E_π (in β Units)	IRA
Naphthalene	13.6832	9.3333
Anthracene	19.3137	13.3333
Phenanthrene	19.4483	13.3333
Tetracene	24.9308	17.3333
Benzo[c]phenanthrene	25.1875	17.3333
Benzo[a]anthracene	25.1012	17.3333
Chrysene	25.1922	17.3333
Triphenylene	25.2745	17.3333
Pyrene	22.5055	15.3333
Pentacene	30.544	21.3333
Benzo[a]tetracene	30.7255	21.3333
Dibenzo[a,h]anthracene	30.8805	21.3333
Dibenzo[a,j]anthracene	30.8795	21.3333

Table 4. *Cont.*

Molecule	E_π (in β Units)	IRA
Pentaphene	30.7627	21.3333
Benzo[g]chrysene	30.999	21.3333
Pentahelicene	30.9362	21.3333
Benzo[c]chrysene	30.9386	21.3333
Picene	30.9432	21.3333
Benzo[b]chrysene	30.839	21.3333
Dibenzo[a,c]anthracene	30.9418	21.3333
Dibenzo[b,g]phenanthrene	30.8336	21.3333
Perylene	28.2453	19.3333
Benzo[e]pyrene	28.3361	19.3333
Benzo[a]pyrene	28.222	19.3333
Hexahelicene	36.6814	25.3333
Benzo[ghi]perylene	31.4251	21.3333
Hexacene	36.1557	25.3333
Coronene	34.5718	23.3333
Ovalene	46.4974	31.3333

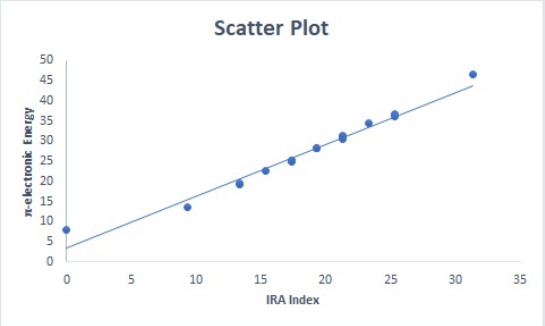


Figure 4. Scatter plot between the IRA index and the π-electronic energy.

Let ρ be the correlation coefficient. Then, $\rho(\Delta H_f^o)$ and $\rho(\Delta T_{bp})$ are presented in the following expression.

$$\rho(\Delta T_{bp}) = 0.9967, \quad \rho(\Delta H_f^o) = 0.9343.$$

The corresponding linear regression models with the 95% confidence intervals for the slope and intercepts of the models, the determination coefficients, and the standard error of the estimates are given as follows:

$$\begin{aligned} \Delta T_{bp} &= 25.937_{\pm 19.8399} IRA - 13.847_{\pm 1.0223}, \quad r^2 = 0.9933, \; s = 8.3218. \\ \Delta H_f^o &= 15.003_{\pm 53.3614} IRA + 11.309_{\pm 2.7496}, \quad r^2 = 0.8728, s = 22.3824. \end{aligned}$$

Moreover, Table 5 gives the scatter plots between the IRA index and the two selected properties, i.e., ΔT_{bp} and ΔH_f^o.

Table 5. Scatter plots between the IRA index and the two selected properties, i.e., ΔT_{bp} and ΔH_f^o.

	
Between IRA and ΔT_{bp}	Between IRA and ΔH_f^o

The statistical analysis shows that the IRA index correlates very well with E_π, well with ΔT_{bp}, and fairly well with ΔH_f^o for the lower PAHs. Thus, based on the analysis in this section, further applications of the IRA index in the quantitative structure activity/property relationship models are warranted. This also suggests a window for exploring further mathematical properties of the IRA index.

Next, we derived some mathematical properties of the IRA index. First, we computed the IRA index of various transformation graphs introduced by Wu and Meng [60].

4. The IRA Index of Transformation Graphs

Next, we calculated the IRA index of different transformation and total transformation graphs. The next theorem calculates the IRA index of Γ^{ab}, where $a = b = +$.

Theorem 1. *Let Γ be an (v, ε)-graph. Then, the IRA index of Γ^{++} of Γ is*

$$IRA(\Gamma^{++}) = (v + \varepsilon) - R(\Gamma) - ERR(\Gamma).$$

Proof. By the definition of the IRA index, we have

$$IRA(\Gamma) = v - 2 \sum_{yz \in E(\Gamma)} \frac{1}{\sqrt{d(y) \times d(z)}}.$$

Employing the definition of Γ^{++}, we have

$$\begin{aligned}
IRA(\Gamma^{++}) &= (v+\varepsilon) - 2 \sum_{yz \in E(\Gamma^{++})} \frac{1}{\sqrt{d(y) \times d(z)}}, \\
&= (v+\varepsilon) - 2 \sum_{yz \in E_a(\Gamma^{++})} \frac{1}{\sqrt{d(y) \times d(z)}} - 2 \sum_{yz \in E_c(\Gamma^{++})} \frac{1}{\sqrt{d(y) \times d(z)}}, \\
&= (v+\varepsilon) - 2 \sum_{yz \in E(\Gamma)} \frac{1}{\sqrt{2d(y) \times 2d(z)}} - 2 \sum_{y \in V(\Gamma), f \in E(\Gamma), f \sim y} \frac{1}{\sqrt{2d(y) \times 2}}, \\
&= (v+\varepsilon) - \sum_{yz \in E(\Gamma)} \frac{1}{\sqrt{d(y) \times d(z)}} - 2 \sum_{y \in V(\Gamma), f \in E(\Gamma), f \sim y} \frac{1}{\sqrt{4d(y)}}, \\
&= (v+\varepsilon) - R(\Gamma) - \sum_{y \in V(\Gamma)} d(y) \frac{1}{\sqrt{d(y)}}, \\
&= (v+\varepsilon) - R(\Gamma) - \sum_{y \in V(\Gamma)} \sqrt{d(y)}, \\
&= (v+\varepsilon) - R(\Gamma) - ERR(\Gamma).
\end{aligned}$$

This completes the proof. □

The next theorem computes the IRA index of Γ^{ab}, where $a = +,\ b = -$.

Theorem 2. *Let Γ be an (v, ε)-graph. Then, the IRA index of Γ^{+-} of Γ is*

$$IRA(\Gamma^{+-}) = (v+\varepsilon) - 2 - \frac{2}{\sqrt{\varepsilon(v-2)}}\Big[\frac{v!}{(v-2)!} - 2\varepsilon\Big].$$

Proof. By the definition of the IRA index, we have

$$IRA(\Gamma) = v - 2\sum_{yz\in E(\Gamma)} \frac{1}{\sqrt{d(y)\times d(z)}}$$

Employing the definition of Γ^{+-}, we have

$$\begin{aligned}
IRA(\Gamma^{+-}) &= (v+\varepsilon) - 2\sum_{yz\in E(\Gamma^{+-})} \frac{1}{\sqrt{d(y)\times d(z)}},\\
&= (v+\varepsilon) - 2\sum_{yz\in E_a(\Gamma^{+-})} \frac{1}{\sqrt{d(y)\times d(z)}} - 2\sum_{yz\in E_c(\Gamma^{+-})} \frac{1}{\sqrt{d(y)\times d(z)}},\\
&= (v+\varepsilon) - 2\sum_{yz\in E(\Gamma)} \frac{1}{\sqrt{\varepsilon\times\varepsilon}} - 2\sum_{y\in V(\Gamma), f\in E(\Gamma), f\sim y} \frac{1}{\sqrt{\varepsilon\times(v-2)}},\\
&= (v+\varepsilon) - 2\sum_{yz\in E(\Gamma)} \frac{1}{\sqrt{\varepsilon^2}} - 2\sum_{y\in V(\Gamma), f\in E(\Gamma), f\sim y} \frac{1}{\sqrt{\varepsilon(v-2)}},\\
&= (v+\varepsilon) - 2\sum_{yz\in E(\Gamma)} \frac{1}{\varepsilon} - 2\sum_{y\in V(\bar{\Gamma})} d(y)\frac{1}{\sqrt{\varepsilon(v-2)}},\\
&= (v+\varepsilon) - 2 - \frac{2}{\sqrt{\varepsilon(v-2)}}\Big[\frac{v!}{(v-2)!} - 2\varepsilon\Big],\\
&= (v+\varepsilon) - 2 - \frac{2}{\sqrt{\varepsilon(v-2)}}\Big[\frac{v!}{(v-2)!} - 2\varepsilon\Big].
\end{aligned}$$

This completes the proof. □

The next result calculates the IRA index of Γ^{ab}, where $a = -,\ b = +$.

Theorem 3. *Let Γ be an (v, ε)-graph. Then, the IRA index of Γ^{-+} of Γ is*

$$IRA(\Gamma^{-+}) = (v+\varepsilon) - \frac{2}{v-1}\Big[\frac{v!}{2!(v-2)!} - \varepsilon\Big] - \frac{4\varepsilon}{\sqrt{2(v-1)}}.$$

Proof. By the definition of the IRA index, we have

$$IRA(\Gamma) = v - 2\sum_{yz\in E(\Gamma)} \frac{1}{\sqrt{d(y)\times d(z)}}$$

Employing the definition of Γ^{-+}, we have

$$\begin{aligned}
IRA(\Gamma^{-+}) &= (v+\varepsilon) - 2\sum_{yz\in E(\Gamma^{-+})} \frac{1}{\sqrt{d(y)\times d(z)}},\\
&= (v+\varepsilon) - 2\sum_{yz\in E_a(\Gamma^{-+})} \frac{1}{\sqrt{d(y)\times d(z)}} - 2\sum_{yz\in E_c(\Gamma^{-+})} \frac{1}{\sqrt{d(y)\times d(z)}},\\
&= (v+\varepsilon) - 2\sum_{yz\in E(\bar{\Gamma})} \frac{1}{\sqrt{(v-1)\times(v-1)}} - 2\sum_{y\in V(\Gamma), f\in E(\Gamma), f\sim y} \frac{1}{\sqrt{(v-1)\times 2}},
\end{aligned}$$

$$\begin{aligned}
&= (v+\varepsilon) - 2\sum_{yz\in E(\overline{\Gamma})} \frac{1}{\sqrt{(v-1)^2}} - 2\sum_{y\in V(\Gamma), f\in E(\Gamma), f\sim y} \frac{1}{\sqrt{2(v-1)}},\\
&= (v+\varepsilon) - 2\sum_{yz\in E(\overline{\Gamma})} \frac{1}{v-1} - 2\sum_{y\in V(\Gamma)} d(y)\frac{1}{\sqrt{2(v-1)}},\\
&= (v+\varepsilon) - \frac{2}{v-1}\Big[\frac{v!}{2!(v-2)!} - \varepsilon\Big] - 2\frac{2\varepsilon}{\sqrt{2(v-1)}},\\
&= (v+\varepsilon) - \frac{2}{v-1}\Big[\frac{v!}{2!(v-2)!} - \varepsilon\Big] - \frac{4\varepsilon}{\sqrt{2(v-1)}}.
\end{aligned}$$

This completes the proof. □

Next, we calculated the IRA index of Γ^{ab}, where $a = b = -$.

Theorem 4. *Let Γ be an (v,ε)-graph. Then, the IRA index of Γ^{--} of Γ is*

$$IRA(\Gamma^{--}) = (v+\varepsilon) - 2ERa(\overline{\Gamma}) - 2ERRa(\Gamma).$$

Proof. By the definition of the IRA index, we have

$$IRA(\Gamma) = v - 2\sum_{yz\in E(\Gamma)} \frac{1}{\sqrt{d(y)\times d(z)}}$$

Employing the definition of Γ^{--}, we have

$$\begin{aligned}
IRA(\Gamma^{--}) &= (v+\varepsilon) - 2\sum_{yz\in E(\Gamma^{--})} \frac{1}{\sqrt{d(y)\times d(z)}},\\
&= (v+\varepsilon) - 2\sum_{yz\in E_a(\Gamma^{--})} \frac{1}{\sqrt{d(y)\times d(z)}} - 2\sum_{yz\in E_c(\Gamma^{--})} \frac{1}{\sqrt{d(y)\times d(z)}},\\
&= (v+\varepsilon) - 2\sum_{yz\in E(\overline{\Gamma})} \frac{1}{\sqrt{(\varepsilon+v-1-2d(y))\times(\varepsilon+v-1-2d(z))}}\\
&\quad -2\sum_{y\in V(\Gamma), f\in E(\Gamma), f\sim y} \frac{1}{\sqrt{(\varepsilon+v-1-2d(y))\times(v-2)}},\\
&= (v+\varepsilon) - 2ERa(\overline{\Gamma}) - 2ERRa(\Gamma).
\end{aligned}$$

This completes the proof. □

The next section calculates the analytically closed formulas of the IRA for various derived graphs introduced in Section 2.

5. The IRA Index of Derived Graphs

This section calculates the IRA index of various derived graphs including the subdivision graph, the line graph, the semi-total point graph, the semi-total line graph, the total graph, the double-graph, the double-graph, the strong double-graph, and the extended double-cover graph.

Next, we calculated the IRA index of the subdivision graph.

Theorem 5. *Let Γ be an (v,ε)-graph. Then, the IRA index of the subdivision graph $S(\Gamma)$ of Γ is*

$$IRA(S(\Gamma)) = (v+\varepsilon) - \sqrt{2}ERR(\Gamma).$$

Proof. By the definition of the IRA index, we have

$$IRA(\Gamma) = v - 2\sum_{yz\in E(\Gamma)} \frac{1}{\sqrt{d(y)\times d(z)}}$$

By using the structure of the subdivision graph, we have

$$\begin{aligned}
IRA(S(\Gamma)) &= (v+\varepsilon) - 2\sum_{yz\in E\left(S(\Gamma)\right)} \frac{1}{\sqrt{d(y)\times d(z)}},\\
&= (v+\varepsilon) - 2\sum_{yz\in E_c\left(S(\Gamma)\right)} \frac{1}{\sqrt{d(y)\times d(z)}},\\
&= (v+\varepsilon) - 2\sum_{y\in V(\Gamma), f\in E(\Gamma), y\sim f} \frac{1}{\sqrt{d(y)\times d(f)}},\\
&= (v+\varepsilon) - 2\sum_{y\in V(\Gamma), f\in E(\Gamma), y\sim f} \frac{1}{\sqrt{d(y)\times 2}},\\
&= (v+\varepsilon) - \sqrt{2}\sum_{y\in V(\Gamma)} d(y)\frac{1}{\sqrt{d(y)}},\\
&= (v+\varepsilon) - \sqrt{2}\sum_{y\in V(\Gamma)} \sqrt{d(y)},\\
&= (v+\varepsilon) - \sqrt{2}ERR(\Gamma).
\end{aligned}$$

This completes the proof. □

The following theorem computes the IRA index of the line graph.

Theorem 6. *Let Γ be an (v,ε)-graph. Then, the IRA index of the line graph $L(\Gamma)$ of Γ is*

$$IRA(L(\Gamma)) = \varepsilon - 2RA(\Gamma).$$

Proof. By the definition of the IRA index, we have

$$IRA(\Gamma) = v - 2\sum_{yz\in E(\Gamma)} \frac{1}{\sqrt{d(y)\times d(z)}}$$

By using the structure of the line graph, we have

$$\begin{aligned}
IRA(L(\Gamma)) &= \varepsilon - 2\sum_{yz\in E(\Gamma)} \frac{1}{\sqrt{d(y)\times d(z)}},\\
&= \varepsilon - 2\sum_{yz\in E_b(\Gamma)} \frac{1}{\sqrt{d(y)\times d(z)}},\\
&= \varepsilon - 2\sum_{xy,yz\in E(\Gamma)} \frac{1}{\sqrt{(d(x)+d(y)-2)\times(d(y)+d(z)-2)}},\\
&= \varepsilon - 2RA(\Gamma).
\end{aligned}$$

This completes the proof. □

Next, we calculated the exact expression of the IRA index of the semi-total point graph.

Theorem 7. *Let Γ be an (v,ε)-graph. Then, the IRA index of the semi-total point graph $\mathcal{T}_1(\Gamma)$ of Γ is*

$$IRA\big(\mathcal{T}_1(\Gamma)\big) = (\varepsilon + v) - Ra(\Gamma) - ERR(\Gamma).$$

Proof. By the definition of the IRA index, we have

$$IRA(\Gamma) = v - 2\sum_{yz\in E(\Gamma)} \frac{1}{\sqrt{d(y)\times d(z)}}$$

By using the structure of the semi-total point graph, we have:

$$\begin{aligned}
IRA\big(\mathcal{T}_1(\Gamma)\big) &= (\varepsilon + v) - 2\sum_{yz\in E\left(\mathcal{T}_1(\Gamma)\right)} \frac{1}{\sqrt{d(y)\times d(z)}},\\
&= (\varepsilon + v) - 2\sum_{yz\in E_a\left(\mathcal{T}_1(\Gamma)\right)} \frac{1}{\sqrt{d(y)\times d(z)}} - 2\sum_{yz\in E_c\left(\mathcal{T}_1(\Gamma)\right)} \frac{1}{\sqrt{d(y)\times d(z)}}\\
&= (\varepsilon + v) - 2\sum_{yz\in E(\Gamma)} \frac{1}{\sqrt{2d(y)\times 2d(z)}} - 2\sum_{y\in V(\Gamma), f\in E(\Gamma), y\sim f} \frac{1}{\sqrt{2d(y)\times 2}},\\
&= (\varepsilon + v) - \sum_{yz\in E(\Gamma)} \frac{1}{\sqrt{d(y)\times d(z)}} - \sum_{y\in V(\Gamma)} d(y)\frac{1}{\sqrt{d(y)}},\\
&= (\varepsilon + v) - Ra(\Gamma) - \sum_{y\in V(\Gamma)} \sqrt{d(y)},\\
&= (\varepsilon + v) - Ra(\Gamma) - ERR(\Gamma).
\end{aligned}$$

This completes the proof. □

The next theorem calculates the IRA index of the semi-total line graph.

Theorem 8. *Let Γ be an (v,ε)-graph. Then, the IRA index of the semi-total line graph $\mathcal{T}_2(\Gamma)$ of Γ is*

$$IRA\big(\mathcal{T}_2(\Gamma)\big) = (\varepsilon + v) - 2LRa(\Gamma) - 2MRa(\Gamma).$$

Proof. By the definition of the IRA index, we have

$$IRA(\Gamma) = v - 2\sum_{yz\in E(\Gamma)} \frac{1}{\sqrt{d(y)\times d(z)}}$$

By using the structure of the semi-total line graph, we have

$$\begin{aligned}
IRA\big(\mathcal{T}_2(\Gamma)\big) &= (\varepsilon + v) - 2\sum_{yz\in E\left(\mathcal{T}_2(\Gamma)\right)} \frac{1}{\sqrt{d(y)\times d(z)}}\\
&= (\varepsilon + v) - 2\sum_{yz\in E_b\left(\mathcal{T}_2(\Gamma)\right)} \frac{1}{\sqrt{d(y)\times d(z)}} - 2\sum_{yz\in E_c\left(\mathcal{T}_2(\Gamma)\right)} \frac{1}{\sqrt{d(y)\times d(z)}},\\
&= (\varepsilon + v) - 2\sum_{xy,yz\in E(\Gamma)} \frac{1}{\sqrt{(d(x)+d(y))\times(d(y)+d(z))}} - 2\sum_{y\in V(\Gamma), f\in E(\Gamma), y\sim f} \frac{1}{\sqrt{d(y)\times d(f)}},\\
&= (\varepsilon + v) - 2LRa(\Gamma) - 2\sum_{yz\in E(\Gamma)} \frac{1}{\sqrt{d(y)\times(d(y)+d(z))}},\\
&= (\varepsilon + v) - 2LRa(\Gamma) - 2MRa(\Gamma).
\end{aligned}$$

This completes the proof. □

The following theorem calculates the IRA index of the total graph.

Theorem 9. *Let Γ be an (v,ε)-graph. Then, the IRA index of the total graph $\mathcal{T}(\Gamma)$ of Γ is*

$$IRA\big(\mathcal{T}(\Gamma)\big) = (\varepsilon + v) - Ra(\Gamma) - 2LRa(\Gamma) - 2MRa(\Gamma).$$

Proof. By the definition of the IRA index, we have

$$IRA(\Gamma) = v - 2\sum_{yz\in E(\Gamma)} \frac{1}{\sqrt{d(y)\times d(z)}}$$

By using the structure of the total graph, we have

$$\begin{aligned}
IRA\big(\mathcal{T}(\Gamma)\big) &= (\varepsilon+v) - 2\sum_{yz\in E\left(\mathcal{T}(\Gamma)\right)} \frac{1}{\sqrt{d(y)\times d(z)}} \\
&= (\varepsilon+v) - 2\sum_{yz\in E_a\left(\mathcal{T}(\Gamma)\right)} \frac{1}{\sqrt{d(y)\times d(z)}} - 2\sum_{yz\in E_b\left(\mathcal{T}(\Gamma)\right)} \frac{1}{\sqrt{d(y)\times d(z)}} \\
&\quad -2\sum_{yz\in E_c\left(\mathcal{T}(\Gamma)\right)} \frac{1}{\sqrt{d(y)\times d(z)}}, \\
&= (\varepsilon+v) - 2\sum_{yz\in E(\Gamma)} \frac{1}{\sqrt{2d(y)\times 2d(z)}} - 2\sum_{xy,yz\in E(\Gamma)} \frac{1}{\sqrt{(d(x)+d(y))\times(d(y)+d(z))}} \\
&\quad -2\sum_{y\in V(\Gamma), f\in E(\Gamma), y\sim f} \frac{1}{\sqrt{2d(y)\times d(f)}}, \\
&= (\varepsilon+v) - Ra(\Gamma) - 2LRa(\Gamma) - 2\sum_{yz\in E(\Gamma)} \frac{1}{\sqrt{d(y)\times(d(y)+d(z))}}, \\
&= (\varepsilon+v) - Ra(\Gamma) - 2LRa(\Gamma) - 2MRa(\Gamma).
\end{aligned}$$

This completes the proof. □

Next, we calculated the exact expression of the IRA index of the double-graph.

Theorem 10. *Let Γ be an (v,ε)-graph. Then, the IRA index of the double-graph $D(\Gamma)$ of Γ is*

$$IRA\big(D(\Gamma)\big) = (\varepsilon + v) - 4Ra(\Gamma).$$

Proof. By the definition of the IRA index, we have

$$IRA(\Gamma) = v - 2\sum_{yz\in E(\Gamma)} \frac{1}{\sqrt{d(y)\times d(z)}}$$

By using the structure of the double-graph, we have

$$\begin{aligned}
IRA\big(D(\Gamma)\big) &= (\varepsilon+v) - 2\sum_{yz\in E\left(D(\Gamma)\right)} \frac{1}{\sqrt{d(y)\times d(z)}} \\
&= (\varepsilon+v) - 2\times 2\sum_{yz\in E\left(D(\Gamma)\right)} \frac{1}{\sqrt{2d(y)\times 2d(z)}} - 2\times 2\sum_{yz\in E\left(D(\Gamma)\right)} \frac{1}{\sqrt{2d(y)\times 2d(z)}}, \\
&= (\varepsilon+v) - 2Ra(\Gamma) - 2Ra(\Gamma), \\
&= (\varepsilon+v) - 4Ra(\Gamma).
\end{aligned}$$

This completes the proof. □

For the strong double-graph, the following theorem computes the IRA index.

Theorem 11. *Let* Γ *be an* (v, ε)*-graph. Then, the* IRA *index of the strong double-graph* $SD(\Gamma)$ *of* Γ *is*

$$IRA\big(SD(\Gamma)\big) = (\varepsilon + v) - 8ARa(\Gamma).$$

Proof. By the definition of the IRA index, we have

$$IRA(\Gamma) = v - 2 \sum_{yz \in E(\Gamma)} \frac{1}{\sqrt{d(y) \times d(z)}}$$

By using the structure of the strong double-graph, we have

$$\begin{aligned} IRA(SD(\Gamma)) &= (\varepsilon + v) - 2 \sum_{yz \in E\left(SD(\Gamma)\right)} \frac{1}{\sqrt{d(y) \times d(z)}} \\ &= (\varepsilon + v) - 2 \times 2 \sum_{yz \in E\left(D(\Gamma)\right)} \frac{1}{\sqrt{(2d(y)+1) \times (2d(z)+1)}} \\ &\quad -2 \times 2 \sum_{yz \in E\left(D(\Gamma)\right)} \frac{1}{\sqrt{(2d(y)+1) \times (2d(z)+1)}}, \\ &= (\varepsilon + v) - 8 \sum_{yz \in E\left(D(\Gamma)\right)} \frac{1}{\sqrt{(2d(y)+1) \times (2d(z)+1)}}, \\ &= (\varepsilon + v) - 8ARa(\Gamma). \end{aligned}$$

This completes the proof. □

The next theorem calculates the IRA index of the extended double-cover graph.

Theorem 12. *Let* Γ *be an* (v, ε)*-graph. Then, the* IRA *index of the extended double-cover graph* Γ^* *of* Γ *is*

$$IRA(\Gamma^*) = (\varepsilon + v) - 6BRa(\Gamma).$$

Proof. By the definition of the IRA index, we have

$$IRA(\Gamma) = v - 2 \sum_{yz \in E(\Gamma)} \frac{1}{\sqrt{d(y) \times d(z)}}$$

By using the structure of the extended double-cover graph, we have

$$\begin{aligned} IRA(\Gamma^*) &= (\varepsilon + v) - 2 \sum_{yz \in E(\Gamma)} \frac{1}{\sqrt{d(y) \times d(z)}} \\ &= (\varepsilon + v) - 2 \times 3 \sum_{yz \in E\left(D(\Gamma)\right)} \frac{1}{\sqrt{(d(y)+1) \times (d(z)+1)}} \\ &= (\varepsilon + v) - 6 \sum_{yz \in E\left(D(\Gamma)\right)} \frac{1}{\sqrt{(d(y)+1) \times (d(z)+1)}}, \\ &= (\varepsilon + v) - 6BRa(\Gamma). \end{aligned}$$

This completes the proof. □

6. Applications of Mathematical Results

In this section, we describe how to use the mathematical results in this paper to find the IRA index derivative organic compounds.

Note that all the graph operations employed in the derived and transformation graphs are applicable in both planar and non-planar graphs. However, from the application perspective, all chemical structures are planar, either embeddable in $\mathbb{R}^2$ or $\mathbb{R}^3$. Thus, first, we redefine some related operations for planar graphs and devise a way to use the results.

Let $\Omega = (V, E, F)$ be a planar graph with the set of vertices (respectively edges) V (respectively E) and the set of faces F. Let $v := |V|$, $\varepsilon := |E|$, and $\xi := |F|$ be the number of vertices, edges, and faces of Ω, respectively. The *stellation/capping/triangulation* $St(\Omega)$ of Ω is obtained by assigning a new node to each face and adjoining it to all the vertices of the respective face. The *Poincaré dual* $Du(\Omega)$ of a graph Ω is obtained by locating a point in the center of each face and joining two such points if their corresponding faces share a common edge. The *medial* $Me(\Omega)$ of Ω is constructed by putting the new vertices as the midpoints of the original edges. Join two such vertices if and only if the original edges span an angle. The *leapfrog* $Le(\Gamma)$ is a composite operation defined as $Le(\Gamma) = Du(St(\Omega))$.

Table 6 presents some carbon nanotubes on a finite number of vertices, edges, and faces. Note that

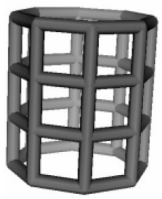
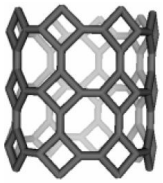
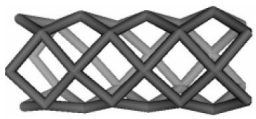
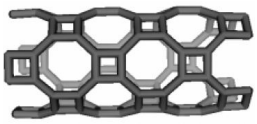
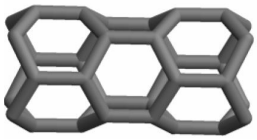
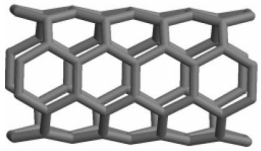
$$Me(TUC_4[8,4]) = TUHRC_4[8,4] \tag{3}$$

$$Le(TUHRC_4[8,4]) = TUVSC_4C_8[8,12] \tag{4}$$

$$Le(TUZ[8,4]) = TUA[8,9]. \tag{5}$$

Equations (3)–(5) imply that, if we know the IRA index of $TUC_4[8,4]$ and $TUZ[8,4]$, we could calculate the IRA index of all the other nanotubes. The results in this paper could also be applied to different inorganic structures in a similar fashion.

Table 6. Some finite-dimensional carbon nanotubes.

		
$TUC_4[8,4]$	$TURC_4C_8[8,4]$	$TUHRC_4[8,4]$
		
$TUVSC_4C_8[8,12]$	$TUZ[8,4]$	$TUA[8,9]$

7. Concluding Remarks

7.1. Conclusions

In this paper, we conducted a quality testing for irregularity indices to correlate with the physicochemical and quantum-theoretic properties of benzenoid hydrocarbons. The normal boiling point ΔT_{bp} and the enthalpy of formation ΔH_f^o were chosen as representatives of the physicochemical properties, and the π-electronic energy E_π was chosen as a representative of the quantum-theoretic properties. A computer-based computational technique was proposed to calculate commonly occurring irregularity indices of any given graph. The computational method was used to calculate irregularity indices for lower benzenoid hydrocarbons. A detailed statistical analysis of the irregularity indices and the experimental values of ΔT_{bp}, ΔH_f^o, and E_π of the lower benzenoid hydrocarbons revealed that the IRA index has the best performance among all commonly occurring irregularity indices.

The IRA index was further studied in context with the derived and transformation graphs. In particular, the IRA index was calculated for the four transformation graphs

and various derived graphs such as the semi-total point/line, total, and subdivision graph, among others. Finally, planar versions of those operations for Γ were introduced to propose a way of using those mathematical results to calculate the IRA index of those operated graphs from $IRA(\Gamma)$.

7.2. Implications

The implications of the research conducted in this paper include:

- The strong predictive potential of the IRA index warrants its further usage in the quantitative structure activity/property relationship models.
- The IRA index of all the derived and transformation graphs of a graph Γ can be calculated simply from the information of Γ and $IRA(\Gamma)$.
- The planar version of those operations can be employed to study the physicochemical and quantum-theoretic properties of the derivatives of organic compounds.

7.3. Limitations

The construction of a chemical graph does not distinguish between the nature of atoms and bonds in a chemical structure and the corresponding vertices and edges of the graph. This leads to the degeneracy of a topological descriptor. For instance, the IRA indices of chlorobenzene and bromobenzene would be the same, as they lead to the same chemical graph. Similarly, the IRA indices of ethane, ethylene, and acetylene would be the same as they also correspond to the same chemical graph. See Figure 5 for a depiction of this phenomenon.

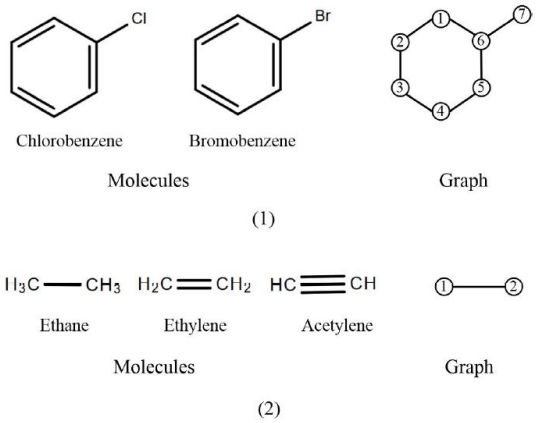


Figure 5. Cases where the degeneracy of the IRA index would occur.

Thus, the current study has a limitation where the degeneracy of topological descriptors occurs.

7.4. Future Scope

The degeneracy of a topological descriptor mentioned in the Limitations Section motivates us to focus on the following problem:

Problem 1. *Employ graph signal processing (GSP) in addressing the degeneracy of irregularity indices or, in general, topological descriptors.*

Further mathematical investigation of this IRA index is proposed herewith. Some particular problems that can be studied are as follows:

Problem 2. *Find sharp upper and lower bounds on the IRA index of v-vertex graphs with a given number of cut-vertices. Moreover, characterize the corresponding extremal cases.*

Problem 3. *Find sharp upper/lower bounds on the IRA index of v-vertex bipartite graphs with a given diameter. Furthermore, characterize the corresponding extremal cases.*

Problem 4. *Find sharp upper/lower bounds on the IRA index of v-vertex trees with a given domination number. Moreover, characterize the corresponding extremal cases.*

Problem 5. *Find sharp upper/lower bounds on the IRA index of v-vertex graphs with a given vertex/edge connectivity.*

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