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The *IRC* Indices of Transformation and Derived Graphs

Haichang Luo [1,†], Sakander Hayat [2,*,†], Yubin Zhong [2], Zhongyuan Peng [3] and Tamás Réti [4]

[1] School of Intelligent Manufacturing, Zhanjiang University of Science and Technology, Zhanjiang 524300, China; xsk12388888@163.com
[2] School of Mathematics and Information Sciences, Guangzhou University, Guangzhou 510006, China; zhong_yb@163.com
[3] Department of Social Sciences, Maoming Polytechnic, Maoming 525000, China; tntship@126.com
[4] Donát Bánki Faculty of Mechanical and Safety Engineering, Obuda University, Népszínház str. 8, H-1081 Budapest, Hungary; reti.tamas@bgk.uni-obuda.hu
* Correspondence: sakander1566@gmail.com
† These authors contributed equally to this work.

Abstract: An irregularity index $IR(\Gamma)$ of a graph Γ is a nonnegative numeric quantity (i.e., $IR(\Gamma) \geq 0$) such that $IR(\Gamma) = 0$ iff Γ is a regular graph. In this paper, we show that IRC closely correlates with the normal boiling point T_{bp} and the standard heat of formation ΔH_f^o of lower benzenoid hydrocarbons. The correlation models that fit the data efficiently for both T_{bp} and ΔH_f^o are linear. We develop further mathematical properties of IRC by calculating its exact expressions for the recently introduced transformation graphs as well as certain derived graphs, such as the total graph, semi-total point graph, subdivision graph, semi-total line graph, double, strong double, and extended double cover graphs. Some open problems are proposed for further research on the IRC index of graphs.

Keywords: irregularity index; physicochemical property; QSAR model; benzenoid hydrocarbon; transformation graph; derived graph

MSC: 05C92; 05C09; 05C76

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1. Introduction

In modern chemistry, the dependence of the physicochemical properties of a compound on its chemical structure is a cornerstone idea. Studying this dependence up to its full potential is rather challenging [1]. Unavailability of experimental data is one of the common challenges encountered in unveiling this dependence. A lot of research [2–6] has been conducted so far to estimate the missing data. Modern tools such as machine learning [7] and graph signal processing (GSP) [8] have recently been employed to address this data retrieval. Molecular descriptors [9–11] are one of the contemporary tools to predict diverse psychochemical features of a chemical compound. Graph-theoretic descriptors are an important class of descriptors that transform a chemical compound into a graph; diverse graph-theoretic tools are then employed to retrieve the dependence. A lot of available research [12–14] shows that these graph-based invariants, which are easily computable, efficiently encrypt a significantly higher level of structural information of chemical compounds.

Diverse classes of topological indices include degree-based indices, which have significantly better efficiency. An irregularity index $IR(\Gamma)$ of a graph Γ is a nonnegative numeric quantity (i.e., $IR(\Gamma) \geq 0$), such that $IR(\Gamma) = 0$ iff Γ is a regular graph. Degree-based irregularity indices have diverse application in QSPR/QSAR modeling [15]. Thus, their mathematical properties have been studied extensively. For instance, Ascioglu and Cangul [16] studied the σ irregularity index and the forgotten index of subdivision and r-subdivision graphs. Réti [17] studied upper and lower bounds on various degree-based irregularity indices, such as the sigma index, irregularity indices based on Zagreb, forgotten

topological indices, and so on. In the same work, Réti [17] introduced the IRC index. This paper presents its potential applicability in QSPR/QSAR modeling of compounds. We also studied the IRC index for various transformation and derived graphs.

This paper is organized as follows: Section 2 presents definitions and preliminary results required in later sections. Section 3 applies the IRC index in QSAR modeling of physicochemical properties of chemical compounds. Sections 4 and 5 present results on the IRC index of transformation graphs and derived graphs, respectively. Section 6 concludes the paper and exhibits some open problems relating to the IRC index.

2. Preliminaries

A simple graph G is an ordered pair $G = (V, E)$, where V is the set of points called vertices and $E \subseteq \binom{V}{2}$ is the set of lines called edges. The cardinality $n =\mid V \mid$ (respectively, $e =\mid E \mid$) of E is called the order (respective size) of G. Two vertices, $u, v \in V(G)$, respectively, (edges $e, f \in E(G)$) are said to be adjacent if $uv \in E(G)$ (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 $u \in V(G)$ and an edge $e \in E(G)$ are called incident and written as $u \sim e$ if u is one of the end-vertex of e. The number of vertices adjacent to a vertex u is known as the degree of u and written as $d(u)$. A graph is called bipartite if it contains no cycle of added length. We refer the reader to a book on molecular topology by Diudea et al. [18].

A topological invariant $IR(G)$ of graph G is said to have an irregularity index if $IR(G) \geq 0$ and $IR(G) = 0$ iff G is regular. Based on its defining structure, an irregularity index could either be eigenvalues-based or degree-based.

The first ever proposed irregularity index is eigenvalues-based and known as the Collatz–Sinogowitz irregularity index [19], which determines the irregularity of a graph. For a n-vertex e-edge graph $G(n, e)$, it is defined as follows:

$$CS(G) = \lambda(G) - \frac{2e}{n},$$

where λ is the spectral radius of the adjacency matrix of G. Because of the lower computational complexity, irregularity indices are mostly degree-based. In 1992, Bell [20] introduced a degree-based irregularity index known as the variance of degree $Var(G)$, which has significant applications in chemistry. For a (n, e) graph G, it is defined as

$$Var(G) = \frac{1}{n}\sum_{u\in V(G)}(d(u))^2 - \frac{1}{n^2}\left(\sum_{u\in V(G)} d(u)\right)^2 = \frac{1}{n}\sum_{u\in V(G)}(d(u))^2 - \left(\frac{2e}{n}\right)^2.$$

In 1997, Albertson introduced another degree-based irregularity index, known as Albertson's irregularity index. It is defined as

$$AL(G) = \sum_{uv\in E(G)} \mid d(u) - d(v) \mid .$$

By extending Albertson's irregularity index, Gutman et al. [21] introduced the sigma index.

$$\sigma(G) = \sum_{uv\in E(G)} (d(u) - d(v))^2.$$

A topological index T is a map from the set of simple connected graph $\sum$ to the real set (i.e., $T : \sum \to \mathbb{R}$), and it has significant applications in chemistry. One of the earliest degree-based topological indices are the Zagreb indices. Gutman and Trinajstić [22] introduced the two Zagreb indices back in 1972 while working on the total π-electronic energy of benzenoid hydrocarbons in theoretical chemistry. They have have been employed in various chemical application since then (see for instance, Gutman and Das [23] and Gutman [24]). For a graph G, the two Zagreb indices are defined as follows:

$$M_1(G) = \sum_{uv \in E(G)} d(u) + d(v) = \sum_{u \in V(G)} d^2(u), \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

Furtula and Gutman [25] proposed a degree-based structure descriptor, which they called the forgotten topological index. It is defined as:

$$F(G) = \sum_{u \in V(G)} d^3(u).$$

In connection with the Zagreb indices, several new irregularity indices have been established. Two of those Zagreb-related irregularity indices are the following [15,26]:

$$IRM_1(G) = \sqrt{\frac{M_1(G)}{n}} - \frac{2e}{n} = Var(G)\left(\sqrt{\frac{M_1(G)}{n}} + \frac{2e}{n}\right)^{-1}.$$

$$IRM_2(G) = \sqrt{\frac{M_2(G)}{n}} - \frac{2e}{n}.$$

Moreover, based on a degree-based quantity proposed in [27], Réti [17] introduced the following irregularity index:

$$IRC(G) = \sum_{u \in V(G)} d^3(u) - \frac{2e}{n} \sum_{u \in V(G)} d^2(u) = F(G) - \frac{2e}{n} M_1(G) \geq 0.$$

This paper focuses on this new irregularity index (i.e., IRC index) and presents its potential applicability in modeling physico-chemical properties of benzenoid hydrocarbons. Then, further mathematical properties of the IRC index are studied.

For an edge $e = xy \in E(G)$, the degree of e is defined as $d(e) = d(u) + d(v) - 2$. Based on degrees of edges, Ilić and Zhou [28] proposed the reformulated Zagreb indices. For a graph G, the reformulated first Zagreb index is defined as follows:

$$EM_1(G) = \sum_{f \in E(G)} d^2(f).$$

The reformulated second Zagreb index is defined as follows:

$$EM_2(G) = \sum_{e,f \in E(G),\ e \sim f} d(e)d(f).$$

Similarly, an edge version of the forgotten index, also called the reformulated forgotten index, of G is defined as follows:

$$EF(G) = \sum_{f \in E(G)} d^3(f).$$

Recently, Ranjini et al. [29] introduced certain redefined versions of the Zagreb indices. The redefined first, second, and third Zagreb indices are defined as follows:

$$\begin{aligned} ReZG_1(G) &= \sum_{uv \in E(G)} \frac{d(u) + d(v)}{d(u)d(v)}, \quad ReZG_2(G) = \sum_{uv \in E(G)} \frac{d(u)d(v)}{d(u) + d(v)}, \\ ReZG_3(G) &= \sum_{uv \in E(G)} d(u)d(v)[d(u) + d(v)]. \end{aligned}$$

Now we introduce some derived graphs based on different graph operations. The total graph $\mathcal{T}(G)$ of a graph G was introduced by Behzad [30] in 1967, and it has the vertex

set $V(\mathcal{T}(G)) = V(G) \cup E(G)$, such that $yz, ye, ef \in E(\mathcal{T}(G))$ iff $y \sim z$, $z \sim e$ or $e \sim f$ are adjacent/incident in G.

Sampathkumar and Chikkodimath [31] extended the concept of the total graph and put forward two semi-total point and line graphs. The semi-total point graph $\mathcal{T}_1(G)$ has the vertex set $V(\mathcal{T}_1(G)) = V(G) \cup E(G)$, and any two vertices $y, z \in V(\mathcal{T}_1(G))$ are adjacent iff:

(i) $u, v \in V(G)$ such that $u \sim v$ in G, or;
(ii) $u \in V(G)$, $e \in E(G)$ or vice versa such that $u \sim e$ in G.

Similarly, the semi-total line graph $\mathcal{T}_2(G)$ has the vertex set $V(\mathcal{T}_2(G)) = V(G) \cup E(G)$, and any two vertices $u, v \in V(\mathcal{T}_2(G))$ are adjacent iff:

(i) $u, v \in E(G)$ such that $u \sim v$ in G, or;
(ii) $u \in V(G)$, $e \in E(G)$ or vice vera such that $u \sim e$ in G.

Independently, similar concepts were studied by Akiyama et al. [32], where they referred to these operations as "middled graphs".

The subdivision $S(G)$ of a graph G has the vertex set $V(S(G)) = V(G) \cup E(G)$ such that $uv \in E(S(G))$ iff $u \in V(G)$ and $v \in E(G)$ and vice versa. Informally, $S(G)$ is built by adding a degree-two vertex on each edge of G.

The line graph $L(G)$ of a graph G has the vertex set $V(L(G)) = E(G)$ such that $f, g \in V(L(G))$ are adjacent in G iff $f \sim g$ in $E(G)$.

The double graph $D(G)$ of G, having two copies G_1 and G_2, has its vertex set $V(D(G)) = V(G_1) \cup V(G_1)$, preserving $E(G_i)$ $(1 \leq i \leq 2)$, and for any $uv \in E(G)$, we add two additional edges u_1v_2 and v_1u_2 in $D(G)$. Similarly, the strong double $SD(G)$ of G is obtained from $D(G)$ by additionally adding u_iv_i for every $uv \in E(G)$.

The extended double cover G^* of G was introduced by Alon [33]. If $V(G) = \{v_1, \ldots, v_n\}$, then G^* is a bipartite graph with partition (X, Y), where $X = \{x_1 \ldots, x_n\}$ and $Y = \{y_1, \ldots, y_n\}$, in which $x_i \sim y_j$ iff either $i = j$ or $x_iy_i \in E(G)$.

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

Lemma 1. *Let G be an (n, e)-graph. Let $x \in V(G)$ and $f = uv \in E(G)$. Then, the following relations hold:*

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

Next, we introduce some transformation operations on graphs put forward by Wu and Meng [34] back in 2002. For a graph G and variables $a, b, c \in \{+, -\}$, the transformation graph G^{xyz} has the vertex set $V(G^{xyz}) = V(G) \cup E(G)$, and for any $uv \in V(G^{xyz})$, we have $u \sim v$ in G^{xyz} iff

(i) $u, v \in V(G)$, $uv \in E(G)$ if $x = +$ and $uv \notin E(G)$ if $x = -$;
(ii) $u, v \in E(G)$, $u \sim v$ in G if $y = +$ and $u \nsim v$ in G if $y = -$;
(iii) $u \in V(G)$, $e \in E(G)$, $u \sim e$ in G if $z = +$ and $u \nsim e$ in G if $z = -$.

Alternatively, the vertex set of G^{xyz} is partitioned into V_x and V_y, that is, $V(G^{xyz}) = V_x \cup V_y$, where

$$V_x = \{u \mid u \in V(G)\} \quad \text{and} \quad V_y = \{e \mid e \in E(G)\}. \tag{1}$$

Moreover, the edge set of G^{xyz} can be partitioned into E_x, E_y, and E_z, that is, $E(G^{xyz}) = E_x \cup E_y \cup E_z$, where

$$E_x = \{uv \mid u,v \in V(G)\},\ \ E_y = \{ef \mid e,f \in E(G)\},\ \ \text{and}\ \ E_z = \{ue \mid u \in V(G), e \in E(G)\}. \quad (2)$$

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

Lemma 2. *Let G be an (n,e)-graph. Let $x \in V(G)$ and $f = uv \in E(G)$. Then, the following relations hold:*

(i) $d_{G^{+++}}(x) = 2d_G(f)$ and $d_{G^{+++}}(f) = d_G(u) + d_G(v)$.
(ii) $d_{G^{++-}}(x) = e$ and $d_{G^{++-}}(f) = d_G(u) + d_G(v) + n - 4$.
(iii) $d_{G^{+-+}}(x) = 2d_G(f)$ and $d_{G^{+-+}}(f) = e - d_G(u) - d_G(v) + 3$.
(iv) $d_{G^{-++}}(x) = n - 1$ and $d_{G^{-++}}(f) = d_G(u) + d_G(v)$.
(v) $d_{G^{---}}(x) = n + e - 2d_G(x) - 1$ and $d_{G^{---}}(f) = n + e - d_G(u) - d_G(v) - 1$.
(vi) $d_{G^{--+}}(x) = n - 1$ and $d_{G^{--+}}(f) = e - d_G(u) - d_G(v) + 3$.
(vii) $d_{G^{-+-}}(x) = n + e - 1 - 2d_G(x)$ and $d_{G^{-+-}}(f) = n + d_G(u) + d_G(v) - 4$.
(viii) $d_{G^{+--}}(x) = e$ and $d_{G^{+--}}(f) = e + n - d_G(u) - d_G(v) - 1$.

Further mathematical properties of transformation graphs have been studied by Xu and Wu [35] and Yi and Wu [36].

3. Application of the *IRC* Index in QSAR Modeling

In order to investigate the potential applicability of the *IRC* irregularity index, we would have to compute it for lower benzenoid hydrocarbons. The next subsection explains the computational details, which 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 the computer saves a lot of time.

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

Our simple two-step process employs newGraph [37] and MatLab [38] to compute an irregularity index IR of a graph G.

Step 1: Draw G on 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 *IRC* index, it is easily modifiable for any arbitrary irregularity index.

Our MatLab program with a README file is publicly available on GitHub. Access the webpage https://github.com/Sakander/Irregulaity-Indices.git (accessed on 21 February 2022) in order to access the code.

3.2. QSAR Modeling of Physicochemical Properties

Following a seminal work by Gutman et al. [39], in order to assess the efficiency of a topological descriptor, we choose two basic physicochemical properties known as the standard enthalpy of formation ΔH_f^o and the normal boiling point T_{bp}. For the chemistry of the underlying chemical compounds, the enthalpy of formation exhibits the behavior of thermal properties, and the boiling point is supposed to constitute intermolecular and van der Waals interactions. The criterion to determine the performance of an irregularity index is simply the determination of the statistical correlation coefficient. The higher the value of the correlation coefficient is (i.e., closer to zero), the better the efficiency of the irregularity index.

Following the standard choice of chemical compounds, we regard lower benzenoid hydrocarbons, as they are supposed to represent both cyclic and acyclic chemical structures. For the sake of authenticity and reliability of the statistical inference, we use 22 lower benzenoid hydrocarbons. Public availability of experimental data is another considerable reason for choosing lower benzenoid hydrocarbons. Figure 1 depicts the 22 lower benzenoid hydrocarbons.

Experimental data of T_{bp} for the lower PAHs considered here have been provided by the standard NIST databases [40]. On the other hand, the experimental data for ΔH_f^o have been retrieved from Allison and Burgess [2]. For tallying the data, we confirmed it with Nikolić et al. [41].

For the molecular graphs in Figure 1, we first employ the computational method in Section 3.1 to compute their IRC indices. Then, we conduct a detailed statistical analysis of the IRC index with the experimental data of T_{bp} and ΔH_f^o for the PAHs in Figure 1. Corresponding statistical parameters, such as the correlation coefficient, the regression model with confidence interval, the standard error of fit, the determination coefficient, scatter plot, and so on, are computed to assess how closely the IRC index correlates with the experimental data. Table 1 exhibits the values of T_{bp}, ΔH_f^o and the IRC indices of the 22 lower PAH graphs in Figure 1.

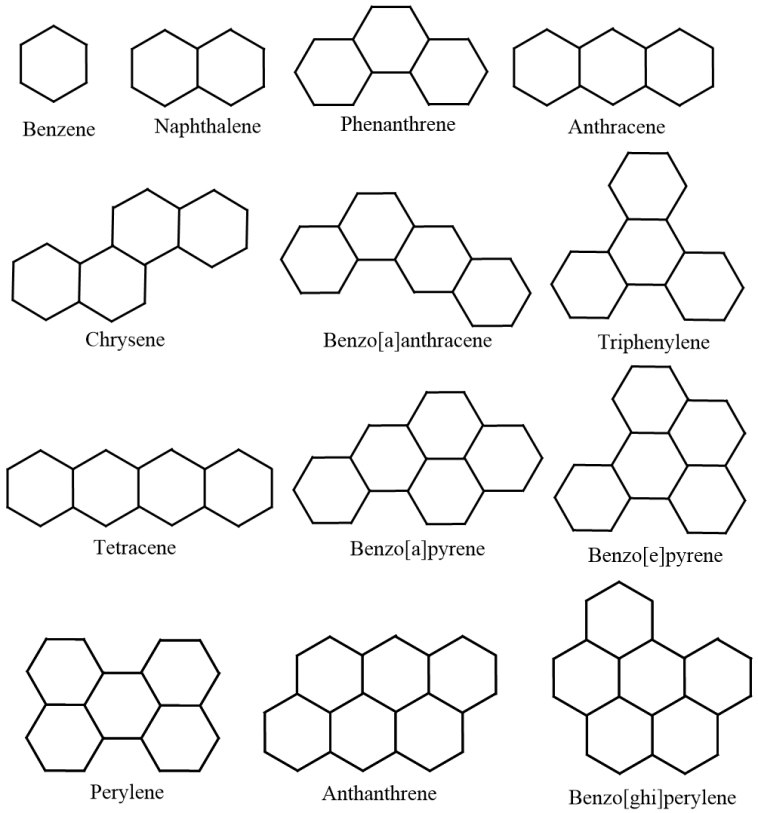


Figure 1. *Cont.*

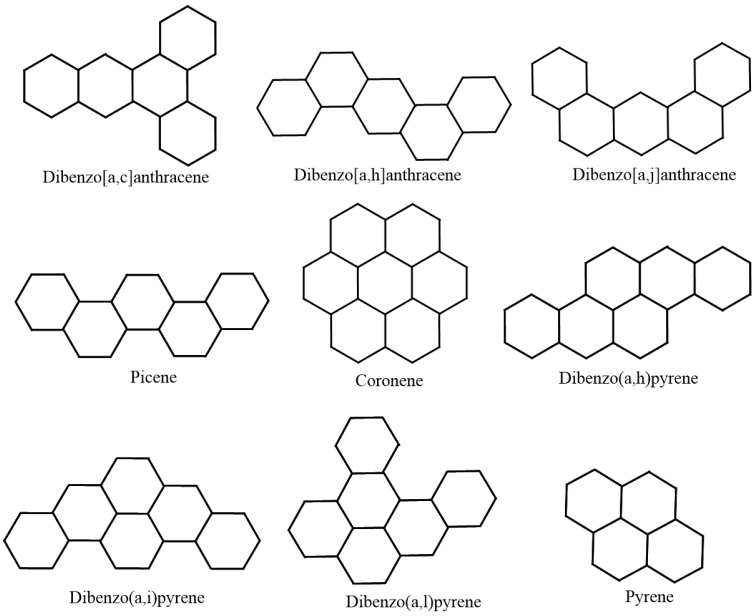


Figure 1. The 22 lower benzenoid hydrocarbon graphs.

Table 1. The experimental data of T_{bp}, ΔH_f^o, and the IRC index of the 22 lower PAHs.

Molecule	T_{bp} in °C	ΔH_f^o in kJ/mol	IRC
Benzene	80.1	75.2	0
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

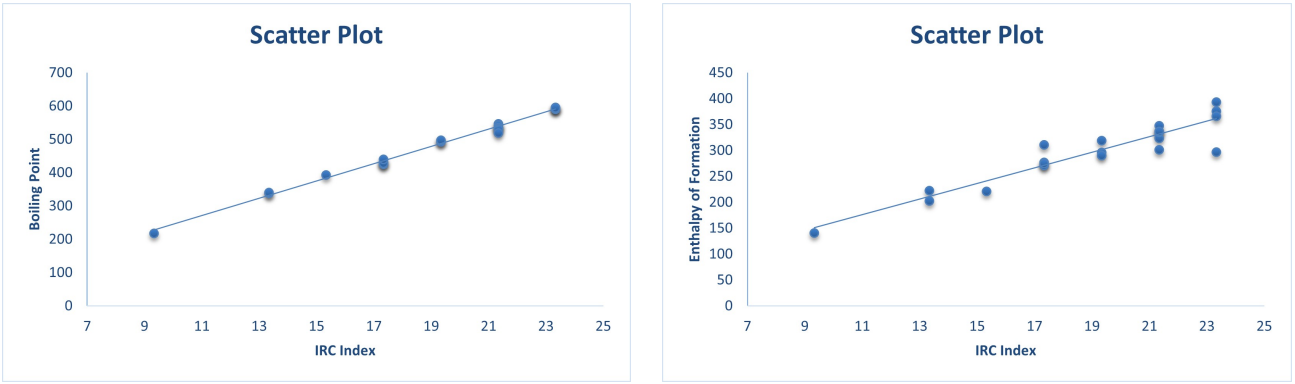
Let ρ be the correlation coefficient. Then, $\rho(\Delta H_f^o)$ and $\rho(T_{bp})$ are presented in the following expression.

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

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

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

Moreover, Figure 2 shows the scatter plot of two selected properties, that is, T_{bp} and ΔH_f^o vs. IRC index.



(**a**) (**b**)

Figure 2. Scatter plots between the IRC index and the two selected properties (i.e., T_{bp} and ΔH_f^o). (**a**) A scatter plot between IRC and T_{bp}. (**b**) A scatter plot between IRC and ΔH_f^o.

The statistical analysis shows that the IRC index correlates well with the normal boiling point and fairly well with the enthalpy of formation for lower PAHs. Thus, based on the analysis in this section, we suggest that further applications of the IRC index in quantitative structure activity/property relationship models are warranted. This also suggests a window for exploring further mathematical properties of the IRC index.

Next, we derive some mathematical properties of the IRC index. First, we compute the IRC index of various transformation graphs introduced by Wu and Meng [34].

4. The IRC Indices of Transformation Graphs

First, we define some terminologies required later in this section. For a graph G, we define

$$\xi_4(G) = \sum_{uv \in E(G)} \left(d^3(u) + d^3(v)\right), \ \chi_\alpha(G) = \sum_{uv \in E(G)} \left(d(u) + d(v)\right)^\alpha.$$

Next, we calculate the IRC indices of different transformation and total transformation graphs. The next theorem calculates the IRC index of G^{xyz}, where $x = y = z = +$.

Theorem 1. *Let G be an (n, e)-graph. Then, the IRC index of G^{+++} of G is*

$$IRC(G^{+++}) = 8F(G) + \xi_4(G) + 3ReZG_3(G) - \frac{M_1(G) + 4e}{e + n}\Big(4M_1(G) + F(G) + 2M_2(G)\Big).$$

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

$$IRC(G) = \sum_{u \in V(G)} d^3(u) - \frac{2e}{n} \sum_{u \in V(G)} d^2(u).$$

Following the definition of the G^{+++}, we obtain

$$IRC(G^{+++}) = \sum_{u \in V(G^{+++})} d^3(u) - \frac{2(\frac{M_1(G)}{2} + 2e)}{e + n} \sum_{u \in V(G^{+++})} d^2(u).$$

By Lemma 2 and Equation (1), we obtain

$$\begin{aligned}
IRC(G^{+++}) &= \sum_{u\in V_x(G^{+++})} d^3(u) + \sum_{u\in V_y(G^{+++})} d^3(u) - \frac{M_1(G)+4e}{e+n}\Big(\sum_{u\in V_x(G^{+++})} d^2(u) + \sum_{u\in V_y(G^{+++})} d^2(u)\Big),\\
&= \sum_{u\in V(G)} \big(2d(u)\big)^3 + \sum_{uv\in E(G)} \big(d(u)+d(v)\big)^3\\
&\quad -\frac{M_1(G)+4e}{e+n}\Big(4\sum_{u\in V(G)} \big(2d(u)\big)^2 + \sum_{uv\in E(G)} \big(d(u)+d(v)\big)^2\Big),\\
&= 8F(G) + \sum_{uv\in E(G)} \big(d^3(u)+d^3(v)\big) + 3\sum_{uv\in E(G)} d(u)d(v)\big(d(u)+d(v)\big)\\
&\quad -\frac{M_1(G)+4e}{e+n}\Big(4M_1(G) + \sum_{uv\in E(G)} \big(d^2(u)+d^2(v)\big) + 2\sum_{uv\in E(G)} \big(d(u)d(v)\big)\Big),\\
&= 8F(G) + \xi_4(G) + 3ReZG_3(G) - \frac{M_1(G)+4e}{e+n}\Big(4M_1(G)+F(G)+2M_2(G)\Big).
\end{aligned}$$

This implies that we obtain

$$IRC(G^{+++}) = 8F(G) + \xi_4(G) + 3ReZG_3(G) - \frac{M_1(G)+4e}{e+n}\Big(4M_1(G)+F(G)+2M_2(G)\Big).$$

This completes the proof. □

The next theorem computes the IRC index of G^{xyz}, where $x = y = +$, $z = -$.

Theorem 2. *Let G be an (n,e)-graph. Then, the IRC index of G^{++-} of G is*

$$\begin{aligned}
IRC(G^{++-}) &= nm^3 + EF(G) + e(n-2)^3 + 3(n-2)EM_1(G) + 3(n-2)^2(M_1(G)-2e) -\\
&\quad \frac{M_1(G)+2e(n-2)}{e+n}\Big(nm^2 + EM_1(G) + e(n-2)^2 + 2(n-2)(M_1(G)-2e)\Big).
\end{aligned}$$

Proof. Applying the definition of the IRC index, we have

$$IRC(G) = \sum_{u\in V(G)} d^3(u) - \frac{2e}{n}\sum_{u\in V(G)} d^2(u).$$

Following the definition of the G^{++-}, we obtain

$$IRC(G^{++-}) = \sum_{u\in V(G^{++-})} d^3(u) - \frac{2(\frac{M_1(G)}{2}+e(n-2))}{e+n}\sum_{u\in V(G^{++-})} d^2(u).$$

By Lemma 2 and Equation (1), we obtain

$$\begin{aligned}
IRC(G^{++-}) &= \sum_{u\in V_x(G^{++-})} d^3(u) + \sum_{u\in V_y(G^{++-})} d^3(u)\\
&\quad -\frac{M_1(G)+2e(n-2)}{e+n}\Big(\sum_{u\in V_x(G^{++-})} d^2(u) + \sum_{u\in V_y(G^{++-})} d^2(u)\Big).
\end{aligned}$$

$$\begin{aligned}
IRC(G^{++-}) &= \sum_{u\in V(G)} e^3 + \sum_{f\in E(G)} \big(d(f)+n-2\big)^3 \\
&\quad -\frac{M_1(G)+2e(n-2)}{e+n}\Big(\sum_{u\in V(G)} e^2 + \sum_{f\in E(G)} \big(d(f)+n-2\big)^2\Big), \\
&= nm^3 + \sum_{f\in E(G)} d^3(f) + \sum_{f\in E(G)} (n-2)^3 + 3(n-2)\sum_{f\in E(G)} \big(d(f)\big)^2 + 3(n-2)^2 \sum_{f\in E(G)} d(f) \\
&\quad -\frac{M_1(G)+2e(n-2)}{e+n}\Big(nm^2 + \sum_{f\in E(G)} \big(d(f)+n-2\big)^2\Big), \\
&= nm^3 + EF(G) + e(n-2)^3 + 3(n-2)EM_1(G) + 3(n-2)^2(M_1(G)-2e) \\
&\quad -\frac{M_1(G)+2e(n-2)}{e+n}\Big(nm^2 + \sum_{f\in E(G)} (d(f))^2 + \sum_{uv\in E(G)} (n-2)^2 + 2(n-2)\sum_{f\in E(G)} d(f)\Big), \\
&= nm^3 + EF(G) + e(n-2)^3 + 3(n-2)EM_1(G) + 3(n-2)^2(M_1(G)-2e) \\
&\quad -\frac{M_1(G)+2e(n-2)}{e+n}\Big(nm^2 + EM_1(G) + e(n-2)^2 + 2(n-2)(M_1(G)-2e)\Big).
\end{aligned}$$

Thus, we obtain

$$\begin{aligned}
IRC(G^{++-}) &= nm^3 + EF(G) + e(n-2)^3 + 3(n-2)EM_1(G) + 3(n-2)^2(M_1(G)-2e) - \\
&\quad \frac{M_1(G)+2e(n-2)}{e+n}\Big(nm^2 + EM_1(G) + e(n-2)^2 + 2(n-2)(M_1(G)-2e)\Big).
\end{aligned}$$

This completes the proof. □

The proofs of the remaining results in this section have structural similarities with the proofs of Theorems 1 and 2; therefore, we omit the remaining proofs. The following calculates the IRC index of G^{xyz}, where $x = +,\ y = z = -$.

Theorem 3. *Let G be an (n,e)-graph. Then, the IRC index of G^{+--} of G is*

$$\begin{aligned}
IRC(G^{+--}) &= nm^3 - \chi_3(G) + e(e+n-1)^3 + 3(e+n-1)\chi_2(G) - 3(e+n-1)^2 M_1(G) \\
&\quad -\frac{e^2+2mn-e-M_1(G)}{e+n}\Big(nm^2 + e(e+n-1)^2 + \chi_2(G) - 2(e+n-1)M_1(G)\Big).
\end{aligned}$$

Next we calculate the IRC index of G^{xyz}, where $x = z = +,\ y = -$.

Theorem 4. *Let G be an (n,e)-graph. Then, the IRC index of G^{+-+} of G is*

$$\begin{aligned}
IRC(G^{+-+}) &= 8F(G) - \chi_3(G) + e(e+3)^3 + 3(e+3)\chi_2(G) - 3(e+3)^2 M_1(G) \\
&\quad -\frac{e^2+7e-M_1(G)}{e+n}\Big(4M_1(G) + e(e+3)^2 + \chi_2(G) - 2(e+3)M_1(G)\Big).
\end{aligned}$$

Here, we calculate the IRC index of G^{xyz}, where $x = -,\ y = z = +$.

Theorem 5. *Let G be an (n,e)-graph. Then, the IRC index of G^{-++} of G is*

$$IRC(G^{-++}) = n(n-1)^3 + \chi_3(G) - \frac{M_1(G)+n(n-1)}{e+n}\Big(n(n-1)^2 + \chi_2(G)\Big).$$

The next theorem computes the IRC index of G^{xyz}, where $x = y = -,\ z = +$.

Theorem 6. *Let G be an (n,e)-graph. Then, the IRC index of G^{--+} of G is*

$$\begin{aligned} IRC(G^{--+}) &= n(n-1)^3 - \chi_3(G) + e(e+3)^3 + 3(e+3)\chi_2(G) - 3(e+3)^2 M_1(G) \\ &\quad - \frac{e^2 + n(n-1) + 3e - M_1(G)}{e+n}\Big(n(n-1)^2 + e(e+3)^2 + \chi_2(G) - 2(e+3)M_1(G)\Big). \end{aligned}$$

Next, we find the IRC index of G^{xyz}, where $x = y = z = -$.

Theorem 7. *Let G be an (n, e)-graph. Then, the IRC index of G^{---} of G is*

$$\begin{aligned} IRC(G^{---}) &= n(e+n-1)^3 - 8F(G) + 12(e+n-1)M_1(G) - 12(e+n-1)^2 e + e(e+n-1)^3 \\ &\quad -\chi_3(G) + 3(e+n-1)\chi_2(G) - 3(e+n-1)^2 M_1(G) - \beta(n(e+n-1)^2 \\ &\quad -\beta\Big(4M_1(G) - 8e(e+n-1) + e(e+n-1)^2 + \chi_2(G) - 2(e+n-1)M_1(G)\Big), \end{aligned}$$

where $\beta = \frac{(e+n)^2 - 5e - n - M_1(G)}{e+n}$.

Finally, we calculate the IRC index of G^{xyz}, where $x = z = -$, $y = +$.

Theorem 8. *Let G be an (n, e)-graph. Then, the IRC index of G^{-+-} of G is*

$$\begin{aligned} IRC(G^{-+-}) &= n(e+n-1)^3 - 8F(G) + 12(e+n-1)M_1(G) - 12(e+n-1)^2 e + e(n-1)^3 \\ &\quad +\chi_3(G) + 3(n-1)\chi_2(G) + 3(n-1)^2 M_1(G) - \beta(n(e+n-1)^2 \\ &\quad -\beta\Big(4M_1(G) - 8e(e+n-1) + e(n-1)^2 + \chi_2(G) + 2(n-1)M_1(G)\Big), \end{aligned}$$

where $\beta = \frac{M_1(G) + 2e(n-4) + n(n-1)}{e+n}$.

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

5. The *IRC* Indices of Derived Graphs

This section calculates the IRC indices 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 strong double graph, and the extended double cover graph.

Next, we calculate the IRC index of the subdivision graph.

Theorem 9. *Let G be an (n, e)-graph. Then, the IRC index of the subdivision graph $S(G)$ of G is*

$$IRC\big((S(G)\big) = F(G) + 8e - \frac{4mM_1(G)}{e+n} - \frac{8e^2}{e+n}.$$

Proof. By definition of the IRC index, we have

$$IRC(G) = \sum_{u \in V(G)} d^3(u) - \frac{2e}{n} \sum_{u \in V(G)} d^2(u).$$

By definition of the subdivision graph, we have

$$| V\big(L(G)\big) | = n + e, \quad | E\big(L(G)\big) | = 2e.$$

Employing this for $IRC(G)$, we obtain

$$IRC(S(G)) = \sum_{u \in V(S(G))} d^3(u) - \frac{2e}{n} \sum_{u \in V(S(G))} d^2(u).$$

By Lemma 1, we obtain

$$\begin{aligned} IRC(S(G)) &= \sum_{u\in V(G)} d^3(u) + \sum_{u\in E(G)} 2^3 - \frac{2e}{n}\Big(\sum_{u\in V(G)} d^2(u) + \sum_{u\in E(G)} 2^2\Big), \\ &= F(G) + 8e - \frac{2e}{n}\big(M_1(G) + 4e\big), \\ &= F(G) + 8e - \frac{2e}{n}M_1(G) - \frac{8e^2}{n}. \end{aligned}$$

Thus, we have

$$IRC(S(G)) = F(G) + 8e - \frac{2e}{n}M_1(G) - \frac{8e^2}{n}.$$

This completes the proof. □

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

Theorem 10. *Let G be an (n, e)-graph. Then, the IRC index of the line graph $L(G)$ of G is*

$$IRC(L(G)) = EF(G) - \frac{M_1(G) - 2e}{e}EM_1(G).$$

Proof. By definition of the IRC index, we have

$$IRC(G) = \sum_{u\in V(G)} d^3(u) - \frac{2e}{n}\sum_{u\in V(G)} d^2(u).$$

By definition of the line graph, we have

$$|\, V\big(L(G)\big) \,| = e, \quad |\, E\big(L(G)\big) \,| = \frac{M_1(G)}{2} - e.$$

Using this information for $IRC(G)$, we obtain

$$IRC(L(G)) = \sum_{u\in V(L(G))} d^3(u) - \frac{2(\frac{M_1(G)}{2} - e)}{e}\sum_{u\in V(L(G))} d^2(u).$$

By Lemma 1, we obtain

$$\begin{aligned} IRC(L(G)) &= \sum_{f\in E(G)} d^3(f) - \frac{M_1(G) - 2e}{e}\sum_{f\in E(G)} d^2(f), \\ &= EF(G) - \frac{M_1(G) - 2e}{e}EM_1(G). \end{aligned}$$

Therefore, we obtain

$$IRC(S(G)) = EF(G) - \frac{M_1(G) - 2e}{e}EM_1(G).$$

This completes the proof. □

Next, we calculate the exact expression of the the IRC index of the semi-total point graph.

Theorem 11. *Let G be an (n, e)-graph. Then, the IRC index of the semi-total point graph $\mathcal{T}_1(G)$ of G is*

$$IRC\big(\mathcal{T}_1(G)\big) = 8F(G) + 8e - \frac{24e}{n+e}\big(M_1(G) - e\big).$$

Proof. By definition of the IRC index, we have

$$IRC(G) = \sum_{u \in V(G)} d^3(u) - \frac{2e}{n} \sum_{u \in V(G)} d^2(u).$$

By definition of the semi-total point graph, we have

$$| V\big(\mathcal{T}_1(G)\big) | = n + e, \quad | E\big(\mathcal{T}_1(G)\big) | = 3e.$$

Using this information for $IRC(G)$, we obtain

$$IRC\big(\mathcal{T}_1(G)\big) = \sum_{u \in V(S(G))} d^3(u) - \frac{2 \cdot 3e}{n+e} \sum_{u \in V(S(G))} d^2(u).$$

By Lemma 1, we obtain

$$\begin{aligned} IRC\big(\mathcal{T}_1(G)\big) &= \sum_{u \in V(G)} (2d(u))^3 + \sum_{u \in E(G)} 2^3 - \frac{6e}{n+e}\Big(\sum_{u \in V(G)} (2d(u))^2 + \sum_{u \in E(G)} 2^2\Big), \\ &= 8F(G) + 8e - \frac{6e}{n+e}(4M_1(G) + 4e), \\ &= 8F(G) + 8e - \frac{24e}{n+e}M_1(G) - \frac{24e^2}{n+e}. \end{aligned}$$

This shows that

$$IRC(G_1(G)) = 8F(G) + 8e - \frac{24e}{n+e}\big(M_1(G) - e\big).$$

This completes the proof. □

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

Theorem 12. *Let G be an (n, e)-graph. Then, the IRC index of the semi-total line graph $\mathcal{T}_2(G)$ of G is*

$$IRC\big(\mathcal{T}_2(G)\big) = F(G) + \chi_3(G) - \frac{2e + M_1(G)}{n+e}\Big(M_1(G) + F(G) + 2M_2(G)\Big).$$

Proof. By definition of the IRC index, we have

$$IRC(G) = \sum_{u \in V(G)} d^3(u) - \frac{2e}{n} \sum_{u \in V(G)} d^2(u).$$

By definition of the semi-total line graph, we have

$$| V\big(\mathcal{T}_2(G)\big) | = n + e, \quad | E\big(\mathcal{T}_2(G)\big) | = e + \frac{M_1(G)}{2}.$$

Using this information for $IRC(G)$, we obtain

$$IRC\big(\mathcal{T}_2(G)\big) = \sum_{u \in V\left(\mathcal{T}_2(G)\right)} d^3(u) - \frac{2(e + \frac{M_1(G)}{2})}{n+e} \sum_{u \in V\left(\mathcal{T}_2(G)\right)} d^2(u).$$

By Lemma 1, we obtain

$$\begin{aligned} IRC(\mathcal{T}_2(G)) &= \sum_{u\in V(G)}(d^3(u)) + \sum_{v=v_1v_2\in E(G)}\big(d(v_1)+d(v_2)\big)^3 - \frac{2e+M_1(G)}{n+e}\sum_{u\in V(\mathcal{T}_2(G))}d^2(u), \\ &= F(G)+\chi_3(G) - \frac{2e+M_1(G)}{n+e}\Big(\sum_{u\in V(G)}(d^2(u)) + \sum_{v=v_1v_2\in E(G)}\big(d(v_1)+d(v_2)\big)^2\Big), \\ &= F(G)+\chi_3(G) - \frac{2e+M_1(G)}{n+e}\Big(M_1(G)+F(G)+2M_2(G)\Big). \end{aligned}$$

Thus, we have

$$IRC(G_2(G)) = 3F(G)+3M_1(G)M_2(G) - \frac{2e+M_1(G)}{n+e}(M_1(G)+F(G)+2M_2(G)).$$

This completes the proof. □

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

Theorem 13. *Let G be an (n,e)-graph. Then, the IRC index of the total graph $\mathcal{T}(G)$ of G is*

$$IRC\big(\mathcal{T}(G)\big) = 8F(G)+\chi_3(G) - \frac{4e+M_1(G)}{n+e}\big(4M_1(G)+F(G)+2M_2(G)\big).$$

Proof. By definition of the IRC index, we have

$$IRC(G) = \sum_{u\in V(G)}d^3(u) - \frac{2e}{n}\sum_{u\in V(G)}d^2(u).$$

By definition of the total graph, we have

$$|\,V\big(\mathcal{T}(G)\big)\,| = n+e, \quad |\,E\big(\mathcal{T}(G)\big)\,| = 2e+\frac{M_1(G)}{2}.$$

Using this information for $IRC(G)$, we obtain

$$IRC\big(\mathcal{T}(G)\big) = \sum_{u\in V\left(\mathcal{T}(G)\right)}d^3(u) - \frac{2\big(2e+\frac{M_1(G)}{2}\big)}{n+e}\sum_{u\in V\left(\mathcal{T}(G)\right)}d^2(u).$$

By Lemma 1, we obtain

$$\begin{aligned} IRC\big(\mathcal{T}(G)\big) &= \sum_{u\in V(G)}\big(2d(u)\big)^3 + \sum_{v=v_1v_2\in E(G)}\big(d(v_1)+d(v_2)\big)^3 - \frac{4e+M_1(G)}{n+e}\sum_{u\in V\left(\mathcal{T}(G)\right)}d^2(u), \\ &= 8F(G)+\chi_3(G) - \frac{4e+M_1(G)}{n+e}\Big(\sum_{u\in V(G)}\big(2d(u)\big)^2 + \sum_{v=v_1v_2\in E(G)}\big(d(v_1)+d(v_2)\big)^2\Big), \\ &= 8F(G)+\chi_3(G) - \frac{4e+M_1(G)}{n+e}\Big(\sum_{u\in V(G)}\big(2d(u)\big)^2 + \sum_{v=v_1v_2\in E(G)}\big(d(v_1)+d(v_2)\big)^2\Big), \\ &= 8F(G)+\chi_3(G) - \frac{4e+M_1(G)}{n+e}\big(4M_1(G)+F(G)+2M_2(G)\big). \end{aligned}$$

Thus, we obtain

$$IRC(\mathcal{T}(G)) = 10F(G)+3M_1(G)M_2(G) - \frac{4e+M_1(G)}{n+e}(4M_1(G)+F(G)+2M_2(G)).$$

This completes the proof. □

Next, we calculate the exact expression of the the IRC index of the double graph.

Theorem 14. *Let G be an (n, e)-graph. Then, the IRC index of the double graph $D(G)$ of G is*

$$IRC\big(D(G)\big) = 16F(G) - \frac{32mM_1(G)}{n}.$$

Proof. By definition of the IRC index, we have

$$IRC(G) = \sum_{u\in V(G)} d^3(u) - \frac{2e}{n}\sum_{u\in V(G)} d^2(u).$$

By definition of the double graph, we have

$$\begin{aligned} IRC\big(D(G)\big) &= \sum_{u\in V\left(D(G)\right)} d^3(u) - \frac{2\times 4e}{2n}\sum_{u\in V\left(D(G)\right)} d^2(u) \\ &= 2\sum_{u\in V(G)} \big(2d(u)\big)^3 - \frac{4e}{n}\Big(2\sum_{u\in V(G)} \big(2d(u)\big)^2\Big), \\ &= 16F(G) - \frac{4e}{n}\big(8M_1(G)\big), \\ &= 16F(G) - \frac{32e}{n}\big(M_1(G)\big). \end{aligned}$$

Thus, we obtain

$$IRC(D(G)) = 16F(G) - \frac{32e}{n}M_1(G).$$

This completes the proof. □

The following theorem computes the IRC index of the strong double graph.

Theorem 15. *Let G be an (n, e)-graph. Then, the IRC index of the strong double graph $SD(G)$ of G is*

$$IRC\big(SD(G)\big) = 16F(G) + 2n + 24M_1(G)M_2(G) + 24e - \frac{5e}{n}\big(8M_1(G) + 2n + 16e\big).$$

Proof. By definition of the IRC index, we have

$$IRC(G) = \sum_{u\in V(G)} d^3(u) - \frac{2e}{n}\sum_{u\in V(G)} d^2(u).$$

By definition of the strong double graph, we have

$$\begin{aligned} IRC(SD(G)) &= \sum_{u\in V\left(SD(G)\right)} d^3(u) - \frac{2\times 5e}{2n}\sum_{u\in V\left(SD(G)\right)} d^2(u) \\ &= 2\sum_{u\in V(G)} \big(2d(u)+1\big)^3 - \frac{5e}{n}\big(2\sum_{u\in V(G)} \big(2d(u)+1\big)^2 \\ &= 2\big(8F(G) + n + 12M_1(G) + 12e\big) - \frac{5e}{n}\Big(2\big(4M_1(G) + n + 8e\big)\Big) \\ &= 16F(G) + 2n + 24M_1(G) + 24e - \frac{5e}{n}\big(8M_1(G) + 2n + 16e\big). \end{aligned}$$

Thus, we have

$$IRC\big(SD(G)\big) = 16F(G) + 2n + 24M_1(G) + 24e - \frac{5e}{n}(8M_1(G) + 2n + 16e).$$

This completes the proof. □

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

Theorem 16. *Let G be an (n, e)-graph. Then, the IRC index of the extended double cover graph G^* of G is*

$$IRC(G^*) = 2F(G) + 2n + 6M_1(G)M_2(G) + 12e - \frac{3e}{n}(2M_1(G) + 2n + 8e).$$

Proof. By definition of the IRC index, we have

$$IRC(G) = \sum_{u \in V(G)} d^3(u) - \frac{2e}{n} \sum_{u \in V(G)} d^2(u)$$

By definition of the extended double cover graph, we have

$$\begin{aligned} IRC(G^*) &= \sum_{u \in V(G^*)} d^3(u) - \frac{2 \cdot 3e}{2n} \sum_{u \in V(G^*)} d^2(u) \\ &= 2 \sum_{u \in V(G)} (d(u)+1)^3 - \frac{3e}{n}(2 \sum_{u \in V(G)} (d(u)+1)^2 \\ &= 2\big(F(G) + n + 3M_1(G) + 6e\big) - \frac{3e}{n}\Big(2\big(M_1(G) + n + 4e\big)\Big) \\ &= 2F(G) + 2n + 6M_1(G) + 12e - \frac{3e}{n}\Big(2M_1(G) + 2n + 8e\Big). \end{aligned}$$

Thus, we have

$$IRC(G^\star) = 2F(G) + 2n + 6M_1(G) + 12e - \frac{3e}{n}(2M_1(G) + 2n + 8e).$$

This completes the proof. □

6. Conclusions

This paper employs a recently introduced irregularity index (i.e., the IRC index) in QSAR modeling of physicochemical properties of chemical compounds. The results show that the IRC index correlates closely with certain physicochemical properties of benzenoid hydrocarbons. A detailed statistical analysis has been conducted to propose appropriate regression models, which in our case are linear. Considering this as a motivation to study the IRC index further, we calculate the IRC indices for various transformation and derived graphs. Moreover, further mathematical investigation of this IRC index is proposed herein.

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