Topological Analysis of PAHs using Irregularity based Indices

Julietraja Konsalraj 1,* Venugopal Padmanabhan 2, Chellamani Perumal 3

1 Department of Mathematics, Sri Sivasubramaniam Nadar College of Engineering, Kalavakkam – 603 110, India; julietrajak@ssn.edu.in (J.K.);
2 Department of Mathematics, Shiv Nadar University Chennai, Kalavakkam – 603 110, India; venugopalp@snuchennai.edu.in (V.P.);
3 Department of Mathematics, Sacred Heart College (Autonomous), Tirupattur – 635 601, Tirupattur Dt., India; joshmani238@gmail.com (C.P.);
* Correspondence: julietrajak@ssn.edu.in (J.K.);

Abstract: Topological descriptors are non-empirical graph invariants that characterize the structures of chemical molecules. The structural descriptors are vital components of QSAR/QSPR studies which form the basis for theoretical chemists to design and investigate new chemical structures. Irregularity indices are a class of topological descriptors that have been employed to study certain chemical properties of compounds. This article aims to compute analytical expressions of irregularity indices for three important classes of polycyclic aromatic hydrocarbons. The intriguing properties of these classes of compounds have several potential applications in wide-ranging fields, which warrant a study of their properties from a structural perspective. Additionally, the 3D graphical representations of a few indices are presented, which will aid in analyzing the similarity of behavior among the indices.

Keywords: topological descriptors; benzenoid systems; graph-theoretical methods; irregularity indices.

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1. Introduction

A Polycyclic Aromatic Hydrocarbon (PAH) is an organic compound that contains at least two aromatic rings placed in linear, angular, or clustered structures. PAHs are primarily produced by anthropogenic and natural combustion processes, with palpable environmental and human health effects. They are also marked by intriguing characteristics such as spectra, specific reactivity, and photophysics [1,2]. PAHs are primarily studied for toxicity analyses as these substances are toxic and carcinogenic and are also present ubiquitously. The recent development in the field of nano-sciences, particularly in graphene-based molecules, has also rekindled the interest among researchers in the study of PAHs [3].

Hexabenzocoronene [4] (HBC) is a PAH of empirical formula C_{42}H_{18}. The molecular structure includes a coronene as its core and additional benzene placed between each pair of rings on the circumference. HBC molecules exhibit outstanding stability and self-assembly. The HBC and their derivatives are applied across wide-ranging technologies from batteries and solar cells to sensors and semiconductors [5,6].

Dodeca-benzo-circumcoronene (DBC) [7] is a PAH that consists of thirty-one benzene rings with the empirical formula C_{84}H_{24}. Twelve of these rings are placed such that they enclose...
a circumcoronene molecule at the center. The structure of DBC provides a prototype for graphene nanoflakes.

Hexa-cata-hexabenzocoronene (cHBC) is a PAH of empirical formula C_{48}H_{24}. The structure comprises a coronene molecule at its center and an additional benzene ring placed on top of each ring along the perimeter. It is also widely known as contorted hexabenzocoronene due to its twisted structure [8], which is used in several applications such as photovoltaic materials, chemoresponsive, and photoresponsive transistors, and in Li-ion batteries [9,10]. This article focuses on studying these three structures from a structural perspective using irregularity indices.

A topological index or a molecular descriptor is a distinct number that quantifies the topology of a molecular structure and its characteristics [11]. The topological descriptors provide an efficient alternative to complex quantum chemical calculations in the theoretical analysis of molecular structures and hence have been studied extensively [12]. Recently, Julietraja and Venugopal computed the degree-based indices for coronoid structures [13]. Chu et al. computed the degree- and irregularity-based molecular descriptors for benzenoid systems [14]. Julietraja et al. also computed the vertex-degree based (VDB) indices using M-polynomial for certain prominent classes of polycyclic aromatic hydrocarbons. For certain types of benzenoid systems, degree-based entropy measures were also studied [15-17]. A topological index is called an irregularity index if the index is non-zero for a non-regular molecular graph and becomes zero for a regular molecular graph [18]. Irregularity indices are particularly applied in the quantitative study of non-regular graphs based on their topology [19]. The irregularity measures of graphs are used in the quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) studies for estimating several chemical and physical characteristics, such as melting and boiling points, enthalpy of vaporization, resistance, entropy, and toxicity [20].

The scientific significance of the above structures warrants a study from a structural perspective. Prabhu et al. [21] have analyzed these molecular compounds using distance-based indices. In this article, we attempt to investigate these structures using irregularity indices. A very few articles in the literature have investigated chemical structures using irregularity indices. Hence, this article will add substantial weightage to the current understanding of PAHs.

2. Graph theoretical concepts

In this article, \( \Gamma(V, E) \) is a connected graph. \( V(\Gamma) \) represents the vertex set, and \( E(\Gamma) \) denotes the edge set of the graph. The degree of a vertex is depicted as \( \text{deg}_\Gamma(v) \) is the number of edges that contain the vertex \( v \) as an endpoint [22]. There exists a very extensive literature on degree-based topological descriptors, which show a strong correlation with several physical and chemical properties of PAHs. Some of these indices, as defined below, have been used to compute the irregularity indices.

**Definition 1.** The first and second Zagreb indices of a graph \( \Gamma \) are defined [23] as

\[
M_1(\Gamma) = \sum_{x_2y_2 \in E} (\text{deg}_\Gamma(x_2) + \text{deg}_\Gamma(y_2))
\]

\[
M_2(\Gamma) = \sum_{x_2y_2 \in E} (\text{deg}_\Gamma(x_2) \cdot \text{deg}_\Gamma(y_2))
\]
Definition 2. The reciprocal Randić index [24] is described as

$$RR(G) = \sum_{x_2y_2 \in E} \sqrt{(deg_F(x_2) \cdot deg_F(y_2))}$$

Definition 3. The forgotten topological index [25], which is defined as

$$F(G) = \sum_{x_2y_2 \in E} (deg_F(x_2)^2 + deg_F(y_2)^2)$$

2.1. Irregularity-based indices for QSPR/QSAR studies.

Table 1. Irregularity-based indices [20].

| S. No. | Irregularity based indices |
|--------|----------------------------|
| 1.     | $VAR(\Gamma) = \sum_{x_2y_2 \in E} \left(\frac{deg_F(x_2) - 2m}{n}\right)^2 = M_4(\Gamma) - \left(\frac{2m}{n}\right)^2$ |
| 2.     | $IR1(\Gamma) = \sum_{x_2y_2 \in E} deg_F(x_2)^3 - \frac{2m}{n} \sum_{u \in E} deg_F(x_2)^2 = F(\Gamma) - \frac{2m}{n} M_4(\Gamma)$ |
| 3.     | $IR2(\Gamma) = \sum_{x_2y_2 \in E} \frac{deg_F(x_2) \cdot deg_F(y_2)}{m} - \frac{2m}{n} = \sqrt{\frac{M_2(\Gamma)}{m} - \frac{2m}{n}}$ |
| 4.     | $IRDIF(\Gamma) = \sum_{x_2y_2 \in E} \frac{|deg_F(x_2) - deg_F(y_2)|}{deg_F(y_2)}$ |
| 5.     | $AL(\Gamma) = \sum_{x_2y_2 \in E} |deg_F(x_2) - deg_F(y_2)|$ |
| 6.     | $IRL(\Gamma) = \sum_{x_2y_2 \in E} \ln deg_F(x_2) - \ln deg_F(y_2)|$ |
| 7.     | $IRLU(\Gamma) = \sum_{x_2y_2 \in E} \min (deg_F(x_2) + deg_F(y_2))$ |
| 8.     | $IRLF(\Gamma) = \sum_{x_2y_2 \in E} \frac{|deg_F(x_2) - deg_F(y_2)|}{\sqrt{(deg_F(x_2) + deg_F(y_2))}}$ |
| 9.     | $IRF(\Gamma) = \sum_{x_2y_2 \in E} (deg_F(x_2) - deg_F(y_2))^2 = F(\Gamma) - 2M_2(\Gamma)$ |
| 10.    | $IRLA(\Gamma) = 2 \sum_{x_2y_2 \in E} \frac{|deg_F(x_2) - deg_F(y_2)|}{(deg_F(x_2) + deg_F(y_2))}$ |
| 11.    | $IRA(\Gamma) = \sum_{x_2y_2 \in E} (deg_F(x_2)^{-1/2} - deg_F(y_2)^{-1/2})^2$ |
| 12.    | $IRB(\Gamma) = \sum_{x_2y_2 \in E} (deg_F(x_2)^{1/2} - deg_F(y_2)^{1/2})^2$ |
| 13.    | $IRC(\Gamma) = \sum_{x_2y_2 \in E} \frac{deg_F(x_2) \cdot deg_F(y_2)}{m} - \frac{2m}{n} = \frac{RR(\Gamma)}{m} - \frac{2m}{n}$ |
| 14.    | $IRGA(\Gamma) = \sum_{x_2y_2 \in E} \ln \frac{(deg_F(x_2) + deg_F(y_2))}{2 \sqrt{deg_F(x_2) \cdot deg_F(y_2)}}$ |
| 15.    | $IRR_t(\Gamma) = \frac{1}{2} \sum_{x_2y_2 \in E} |deg_F(x_2) - deg_F(y_2)|$ |

3. Methods

The results presented in this article are calculated by employing the degree counting method, analytical techniques, and edge partition method. The analytical expressions of
irregularity descriptors have been computed using Maple 2016, and the 3D visualization of certain computed indices is also generated using the same tool. ChemDraw Ultra 18.1 is used in representing the molecular structures of the PAH systems visually.

4. Computing the irregularity-based indices for $HBC(r)$

Let $\Gamma$ be $HBC(r)$. The cardinality of $HBC(r)$ is $V(\Gamma) = 18r^2 - 18r + 6 = n$ and $E(\Gamma) = 27r^2 - 33r + 12 = m$, where $m$ and $n$ indicates the total number of vertices and edges of $HBC(r)$ and illustrated in Figure 1.

Table 2. Edge partition Table for $HBC(r)$.

| $(deg_r(x_2), deg_r(y_2))$ | Total number of edges $|E|$ | Set of edges |
|--------------------------|--------------------------|-------------|
| (2, 2)                  | $6r$                     | $E_{(2, 2)}^r$ |
| (2, 3)                  | $12r - 12$               | $E_{(2, 3)}^r$ |
| (3, 3)                  | $27r^2 - 51r + 24$      | $E_{(3, 3)}^r$ |

Figure 1. (i) Coronene; (ii) $HBC(2)$; (iii) $HBC(3)$; (iv) $HBC(4)$. 
Theorem 1. If \( \Gamma \) is the \( HBC(r) \), then the irregularity-based indices are computed as

1. \( VAR(\Gamma) = \frac{27r^4 - 90r^3 + 23r^2 + 28r - 16}{(3r^2 - 3r + 1)^2} \)
2. \( IR1(\Gamma) = \frac{24(9r^3 - 24r^2 + 20r - 5)}{3r^2 - 3r + 1} \)
3. \( IR2(\Gamma) = \sqrt{\frac{54r^2 - 97r + 47/9r^2 - 11r + 4}{3r^2 - 3r + 1}}(3r^2 - 3r + 1)^2 \)
4. \( IRDIF(\Gamma) = \frac{1}{3} \cdot (12r - 12) \)
5. \( AL(\Gamma) = 12r - 12 \)
6. \( IRL(\Gamma) = 0.40545 \cdot (12r - 12) \)
7. \( IRLU(\Gamma) = \frac{1}{2} \cdot (12r - 12) \)
8. \( IRLF(\Gamma) = \frac{1}{\sqrt{6}} \cdot (12r - 12) \)
9. \( IRF(\Gamma) = 12r - 12 \)
10. \( IRLA(\Gamma) = \frac{2}{5} \cdot (12r - 12) \)
11. \( IRA(\Gamma) = 0.16832 \cdot (12r - 12) \)
12. \( IRB(\Gamma) = 0.10106 \cdot (12r - 12) \)
13. \( IRC(\Gamma) = \frac{(12r^3 - 24r^2 + 16r - 4)\sqrt{5} + 27r^4 - 120r^3 + 167r^2 - 96r + 22}{27r^4 - 60r^3 + 54r^2 - 23r + 4} \)
14. \( IRGA(\Gamma) = (0.20391e - 1) \cdot (12n - 12) \)
15. \( IRR_{1}(\Gamma) = \frac{1}{2} \cdot (12r - 12) \)

Proof: Let \( \Gamma \) be the \( HBC(r) \) network, then the number of vertices and edges of \( HBC(r) \) is

\[
V(\Gamma) = 18r^2 - 18r + 6 \quad \text{and} \quad E(\Gamma) = 27r^2 - 33r + 12.
\]

From Table 2, it is noticeable that

\[
|E^{a}_{(2,2)}| = 6r,
|E^{b}_{(2,3)}| = 12r - 12,
|E^{r}_{(3,3)}| = 27r^2 - 51r + 24.
\]

By using the definitions of \( M_1(\Gamma), M_2(\Gamma), RR(\Gamma) \) and \( F(\Gamma) \), we obtain the following result as \( M_1(\Gamma) = 216r^2 - 360r + 168 \)

\( M_2(\Gamma) = 324r^2 - 582r + 282 \)

\( RR(\Gamma) = 108r^2 + (12r - 12)\sqrt{6} - 210r + 114 \)

\( F(\Gamma) = 648r^2 - 1152r + 552 \)

\[
VAR(\Gamma) = \sum_{x_2 \in V} \left( \deg_{\Gamma}(x_2) - \frac{2m}{n} \right)^2 = \frac{M_1(\Gamma)}{n} - \left( \frac{2m}{n} \right)^2
\]

Now put the values of \( M_1(\Gamma), n \) and \( m \) in \( VAR(\Gamma) \) then the result is obtained as

\[
= \frac{(216r^2 - 360r)}{18r^2 - 18r + 6} - \left( \frac{2(27r^2 - 33r + 12)}{18r^2 - 18r + 6} \right)^2
= \frac{(27r^4 - 90r^3 + 23r^2 + 28r - 16)}{(3r^2 - 3r + 1)^2}
\]

\[
IR1(\Gamma) = \sum_{x_2 \in V} \deg_{\Gamma}(x_2)^3 - \frac{2m}{n} \sum_{x_2 \in V} \deg_{\Gamma}(x_2)^2 = F(\Gamma) - \frac{2m}{n} M_1(\Gamma)
\]
Now put the values of $F(\Gamma)$, $M_1(\Gamma)$, $n$ and $m$ in $IR1(\Gamma)$ then the result is obtained as

$$= 648r^2 - 1152r + 552 - \left(\frac{2(27r^2 - 33r + 12)}{18r^2 - 18r + 6}\right) \cdot (216r^2 - 360r + 168)$$

$$= \left(\frac{24(9r^3 - 24r^2 + 20r - 5)}{3r^2 - 3r + 1}\right)$$

$$IR2(\Gamma) = \sqrt{\sum_{x_2y_2 \in E} \frac{deg_r(x_2) \cdot deg_r(y_2)}{m} - \frac{2m}{n}} = \sqrt{\frac{M_2(\Gamma) - 2m}{m} - \frac{2m}{n}}$$

$$= \sqrt{\frac{324r^2 - 582r + 282}{27r^2 - 33r + 12} - \left(\frac{2(27r^2 - 33r + 12)}{18r^2 - 18r + 6}\right)}$$

$$= \frac{\sqrt{54r^2 - 97r + 47/9r^2 - 11r + 4 \cdot (3r^2 - 3r + 1)\sqrt{2} - 9r^2 + 11r - 4}}{3r^2 - 3r + 1}$$

$$IRDIF(\Gamma) = \sum_{x_2y_2 \in E} \left| \frac{deg_r(x_2) - deg_r(y_2)}{deg_r(y_2)} \right|$$

$$= \left| \frac{2}{2} \cdot |E^{\alpha}_{(2,2)}| + \frac{2}{3} - \frac{3}{3} \cdot |E^{\beta}_{(2,3)}| + \frac{3}{3} - \frac{3}{3} \cdot |E^{y}_{(3,3)}| \right|$$

$$= \frac{1}{3} \cdot (12r - 12)$$

$$AL(\Gamma) = \sum_{x_2y_2 \in E} |ln\deg_r(x_2) - ln\deg_r(y_2)|$$

$$= |ln2 - ln2| \cdot |E^{\alpha}_{(2,2)}| + |ln2 - ln3| \cdot |E^{\beta}_{(2,3)}| + |ln3 - ln3| \cdot |E^{y}_{(3,3)}|$$

$$= 0.40545 \cdot (12r - 12)$$

$$IRL(\Gamma) = \sum_{x_2y_2 \in E} |ln\deg_r(x_2) - ln\deg_r(y_2)|$$

$$= \left| \frac{|2 - 2|}{2} \cdot |E^{\alpha}_{(2,2)}| + \frac{|2 - 3|}{2} \cdot |E^{\beta}_{(2,3)}| + \frac{|3 - 3|}{3} \cdot |E^{y}_{(3,3)}| \right|$$

$$= \frac{1}{2} \cdot (12r - 12)$$

$$IRL(\Gamma) = \sum_{x_2y_2 \in E} |ln\deg_r(x_2) - ln\deg_r(y_2)|$$

$$= \left| \frac{|2 - 2|}{\sqrt{4}} \cdot |E^{\alpha}_{(2,2)}| + \frac{|2 - 3|}{\sqrt{6}} \cdot |E^{\beta}_{(2,3)}| + \frac{|3 - 3|}{\sqrt{6}} \cdot |E^{y}_{(3,3)}| \right|$$

$$= \frac{1}{\sqrt{6}} \cdot (12r - 12)$$

$$IRF(\Gamma) = \sum_{x_2y_2 \in E} (\deg_r(x_2) - \deg_r(y_2))^2 = F(\Gamma) - 2M_2(\Gamma)$$

Now put the values of $F(\Gamma)$ and $M_2(\Gamma)$ in $IRF(\Gamma)$ then the result is obtained as

$$= 648r^2 - 1152r + 552 - 2(324r^2 - 582r + 282)$$

$$= 12r - 12$$

$$IRLA(\Gamma) = 2 \sum_{x_2y_2 \in E} \left| \frac{deg_r(x_2) - deg_r(y_2)}{deg_r(x_2) + deg_r(y_2)} \right|$$

$$= 2 \left( \frac{|2 - 2|}{4} \cdot |E^{\alpha}_{(2,2)}| + \frac{|2 - 3|}{5} \cdot |E^{\beta}_{(2,3)}| + \frac{|3 - 3|}{6} \cdot |E^{y}_{(3,3)}| \right)$$
$$= \frac{2}{5} \cdot (12r - 12)$$

$$IRA(\Gamma) = \sum_{x_2y_2 \in E} \left( \text{deg}_t(x_2)^{-\frac{1}{2}} - \text{deg}_t(y_2)^{-\frac{1}{2}} \right)^2$$

$$= \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \right)^2 \cdot |E^\alpha_{(2,2)}| + \left( \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}} \right)^2 \cdot |E^\beta_{(2,3)}| + \left( \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}} \right)^2 \cdot |E^\gamma_{(3,3)}|$$

$$= 0.16832 \cdot (12r - 12)$$

$$IRB(\Gamma) = \sum_{x_2y_2 \in E} \left( \text{deg}_t(x_2)^{\frac{1}{2}} - \text{deg}_t(y_2)^{\frac{1}{2}} \right)^2$$

$$= (\sqrt{2} - \sqrt{2})^2 \cdot |E^\alpha_{(2,2)}| + (\sqrt{2} - \sqrt{3})^2 \cdot |E^\beta_{(2,3)}| + (\sqrt{3} - \sqrt{3})^2 \cdot |E^\gamma_{(3,3)}|$$

$$= 0.10106 \cdot (12r - 12)$$

$$IRC(\Gamma) = \sum_{x_2y_2 \in E} \sqrt{\left( \text{deg}_t(x_2) \cdot \text{deg}_t(y_2) \right)} - \frac{2m}{n} = RR(\Gamma) - \frac{2m}{n}$$

Now put the values of $RR(\Gamma), n$ and $m$ in $IRC(\Gamma)$ then the result is obtained as

$$= \left( \frac{108r^2 + (12r - 12)\sqrt{6} - 210r + 114}{27r^2 - 33r + 12} \right) - \left( \frac{2(27r^2 - 33r + 12)}{18r^2 - 18r + 6} \right)$$

$$= \left( \frac{12r^3 - 24r^2 + 16r - 4\sqrt{6} + 27r^4 - 120r^3 + 167r^2 - 96r + 22}{27r^4 - 60r^3 + 54r^2 - 23r + 4} \right)$$

$$IRGA(\Gamma) = \sum_{x_2y_2 \in E} \ln \left( \frac{\text{deg}_t(x_2) + \text{deg}_t(y_2)}{2\sqrt{(\text{deg}_t(x_2) \cdot \text{deg}_t(y_2))}} \right)$$

$$= \ln \left( \frac{4}{5} \right) \cdot |E^\alpha_{(2,2)}| + \ln \left( \frac{5}{2\sqrt{6}} \right) \cdot |E^\beta_{(2,3)}| + \ln \left( \frac{6}{\sqrt{3}} \right) \cdot |E^\gamma_{(3,3)}|$$

$$= 0.20391 e - 1 \cdot (12n - 12)$$

$$IRR_t(\Gamma) = \frac{1}{2} \sum_{x_2y_2 \in E} |\text{deg}_t(x_2) - \text{deg}_t(y_2)|$$

$$= \frac{1}{2} \cdot (|2 - 2| \cdot |E^\alpha_{(2,2)}| + |2 - 3| \cdot |E^\beta_{(2,3)}| + |3 - 3| \cdot |E^\gamma_{(3,3)}|)$$

$$= \frac{1}{2} \cdot (12r - 12)$$

5. Computing the irregularity-based indices for $DBC(r)$

Let $\Gamma$ be $DBC(r)$. The vertex set and edge set of $DBC(r)$ is $V(\Gamma) = 18r^2 + 6r = n$ and $E(\Gamma) = 27r^2 + 3r = m$, where $m$ and $n$ represent the total number of vertices and edges of $HBC(r)$ and they are picturized in Figure 2.
Figure 2. (i) $DBC(2)$; (ii) $DBC(3)$; (iii) $DBC(4)$.

Table 3. Edge partition Table for $DBC(r)$.

| $(deg_r(x_2), deg_r(y_2))$ | Total number of edges | Set of edges |
|---------------------------|-----------------------|--------------|
| (2,2)                     | $6r$                  | $E_{[2,2]}^A$ |
| (2,3)                     | $12r$                 | $E_{[2,3]}^B$ |
| (3,3)                     | $27r^2 - 15r$         | $E_{[3,3]}^C$ |

Theorem 2: If $\Gamma$ is $DBC(r)$, then the irregularity-based indices are computed as

1. $VAR(\Gamma) = \left( \frac{6r - 2}{(3r + 1)^2} \right)$
2. \( IR1(\Gamma) = \left( \frac{180r^2 - 60r}{3r+1} \right) \)

3. \( IR2(\Gamma) = \frac{\sqrt{(81r-13)/(9r+1)(3r+1-9r-1)}}{3r+1} \)

4. \( IRDIF(\Gamma) = \frac{1}{3} \cdot (12r) \)

5. \( AL(\Gamma) = 12r \)

6. \( IRL(\Gamma) = 0.40545 \cdot (12r) \)

7. \( IRLU(\Gamma) = \frac{1}{2} \cdot (12r) \)

8. \( IRLF(\Gamma) = \frac{1}{\sqrt{6}} \cdot (12r) \)

9. \( IRF(\Gamma) = 12r \)

10. \( IRLA(\Gamma) = \frac{2}{5} \cdot (12r) \)

11. \( IRA(\Gamma) = 0.16832 \cdot (12r) \)

12. \( IRB(\Gamma) = 0.10106 \cdot (12r) \)

13. \( IRC(\Gamma) = \frac{(12r+4)\sqrt{5-24r-12}}{27r^2+12r+1} \)

14. \( IRGA(\Gamma) = (0.20391e - 1) \cdot (12r) \)

15. \( IRR_e(\Gamma) = \frac{1}{2} \cdot (12r) \)

**Proof:** Consider \( \Gamma \) is the \( DBC(r) \). The total number of vertices and edges of \( DBC(r) \) are \( V(\Gamma) = 18r^2 + 6r \) and \( E(\Gamma) = 27r^2 + 3r \).

From Table 3, it can be observed that
\[
\begin{align*}
|E_{(2,2)}^A| &= 6r \\
|E_{(2,3)}^B| &= 12r \\
|E_{(3,3)}^C| &= 27r^2 - 15r. \\
\end{align*}
\]

By using the definitions of \( M_1(\Gamma), M_2(\Gamma), RR(\Gamma) \) and \( F(\Gamma) \), we get the following result as
\[
\begin{align*}
M_1(\Gamma) &= 162r^2 - 6r \\
M_2(\Gamma) &= 243r^2 - 39r \\
RR(\Gamma) &= 81r^2 + 12r\sqrt{6} - 33r \\
F(\Gamma) &= 486r^2 - 66rs \\
\end{align*}
\]

\[
VAR(\Gamma) = \sum_{x_2 \in V} \left( deg_r(x_2) - \frac{2m}{n} \right)^2 = \frac{M_1(\Gamma)}{n} - \left( \frac{2m}{n} \right)^2
\]

Now put the values of \( M_1(\Gamma), n \) and \( m \) in \( VAR(\Gamma) \) then the result is obtained as
\[
= \left( \frac{162r^2 - 6r}{18r^2 + 6r} \right) - \left( \frac{2(27r^2 + 3r)}{18r^2 + 6r} \right)^2
\]
\[
= \left( \frac{6r - 2}{3r + 1} \right)^2
\]

\[
IR1(\Gamma) = \sum_{x_2 \in V} deg_r(x_2)^3 - \frac{2m}{n} \sum_{x_2 \in V} deg_r(x_2)^2 = F(\Gamma) - \frac{2m}{n} M_1(\Gamma)
\]

Now put the values of \( F(\Gamma), M_1(\Gamma), n \) and \( m \) in \( VAR(\Gamma) \) then the result is obtained as

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\[(486r^2 - 66r) - \left(\frac{2(27r^2 + 3r)}{18r^2 + 6r}\right) \cdot (162r^2 - 6r)
\]
\[= \left(180r^2 - 60r\right)\]
\[= \frac{\sum_{x,y \in E} (\text{deg}_r(x) \cdot \text{deg}_r(y))}{m} \cdot \frac{2m}{n} = \frac{M_2(\Gamma)}{m} - \frac{2m}{n}\]

Now put the values of \(M_2(\Gamma), n\) and \(m\) in \(IR2(\Gamma)\) then the result is obtained as
\[
\sqrt{\frac{243r^2 - 39r}{27r^2 + 3r}} - \frac{2(27r^2 + 3r)}{18r^2 + 6r}
\]
\[
= \sqrt{(81r - 13)/(9r + 1)} (3r + 1 - 9r - 1)
\]
\[
IRDIF(\Gamma) = \sum_{x,y \in E} \left| \frac{\text{deg}_r(x)}{\text{deg}_r(y)} - \frac{\text{deg}_r(y)}{\text{deg}_r(y)} \right|
\]
\[
= \frac{2}{1} - \frac{2}{1} \cdot |E^\lambda_{(2,2)}| + \frac{2}{3} - \frac{3}{3} \cdot |E^\mu_{(2,2)}| + \frac{3}{3} - \frac{3}{3} \cdot |E^\nu_{(3,3)}|
\]
\[
= \frac{1}{3} \cdot (12r)
\]
\[
AL(\Gamma) = \sum_{x,y \in E} |\text{deg}_r(x) - \text{deg}_r(y)|
\]
\[
= |2 - 2| \cdot |E^\lambda_{(2,2)}| + |2 - 3| \cdot |E^\mu_{(2,3)}| + |3 - 3| \cdot |E^\nu_{(3,3)}|
\]
\[
= 12r
\]
\[
IRL(\Gamma) = \sum_{x,y \in E} \ln |\text{deg}_r(x) - \text{deg}_r(y)|
\]
\[
= |\ln 2 - \ln 2| \cdot |E^\lambda_{(2,2)}| + |\ln 2 - \ln 3| \cdot |E^\mu_{(2,3)}| + |\ln 3 - \ln 3| \cdot |E^\nu_{(3,3)}|
\]
\[
= 0.40545 \cdot (12r)
\]
\[
IRLU(\Gamma) = \sum_{x,y \in E} \frac{|\text{deg}_r(x) - \text{deg}_r(y)|}{\min(\text{deg}_r(x), \text{deg}_r(y))}
\]
\[
= \frac{|2 - 2|}{2} \cdot |E^\lambda_{(2,2)}| + \frac{|2 - 3|}{2} \cdot |E^\mu_{(2,2)}| + \frac{|3 - 3|}{2} \cdot |E^\nu_{(3,3)}|
\]
\[
= \frac{1}{2} \cdot (12r)
\]
\[
IRLF(\Gamma) = \sum_{x,y \in E} \frac{|\text{deg}_r(x) - \text{deg}_r(y)|}{\sqrt{|\text{deg}_r(x) - \text{deg}_r(y)|}}
\]
\[
= \frac{|2 - 2|}{\sqrt{4}} \cdot |E^\lambda_{(2,2)}| + \frac{|2 - 3|}{\sqrt{6}} \cdot |E^\mu_{(2,2)}| + \frac{|3 - 3|}{\sqrt{6}} \cdot |E^\nu_{(3,3)}|
\]
\[
= \frac{1}{\sqrt{6}} \cdot (12r)
\]
\[
IRF(\Gamma) = \sum_{x,y \in E} (\text{deg}_r(x) - \text{deg}_r(y))^2 = F(\Gamma) - 2M_2(\Gamma)
\]

Now put the values of \(M_2(\Gamma)\) and \(F(\Gamma)\) in \(IRF(\Gamma)\) then the result is obtained as
\[
= 486r^2 - 66r - 2(243r^2 - 39r)
\]
\[
= 12r
\]
\[
IRLA(\Gamma) = 2 \sum_{x,y \in E} \frac{|\text{deg}_r(x) - \text{deg}_r(y)|}{|\text{deg}_r(x) + \text{deg}_r(y)|}
\]
\[
= 2 \left(\frac{1}{4} \cdot |E^\lambda_{(2,2)}| + \frac{1}{5} \cdot |E^\mu_{(2,2)}| + \frac{1}{6} \cdot |E^\nu_{(3,3)}|\right)
\]
\[
= \frac{2}{5} \cdot (12r)
\]
\[
IRA(\Gamma) = \sum_{x_2y_2 \in E} \left( \text{deg}_r(x_2)^{-1/2} - \text{deg}_r(y_2)^{-1/2} \right)^2
\]

\[
= \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \right)^2 \cdot |E^\lambda_{(2,2)}| + \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right)^2 \cdot |E^\mu_{(2,3)}| + \left( \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}} \right)^2 \cdot |E^\nu_{(3,3)}|
\]

\[
= 0.16832 \cdot (12r)
\]

\[
IRB(\Gamma) = \sum_{x_2y_2 \in E} \left( \text{deg}_r(x_2)^{1/2} - \text{deg}_r(y_2)^{1/2} \right)^2
\]

\[
= (\sqrt{2} - \sqrt{2})^2 \cdot |E^\lambda_{(2,2)}| + (\sqrt{2} - \sqrt{3})^2 \cdot |E^\mu_{(2,3)}| + (\sqrt{3} - \sqrt{3})^2 \cdot |E^\nu_{(3,3)}|
\]

\[
= 0.10106 \cdot (12r)
\]

\[
IRC(\Gamma) = \frac{\Sigma_{x_2y_2 \in E} \sqrt{\text{deg}_r(x_2) \cdot \text{deg}_r(y_2)}}{m} - \frac{2m}{n} = \frac{RR(\Gamma)}{m} - \frac{2m}{n}
\]

Now put the values of \(RR(\Gamma), m\) and \(n\) in \(IRC(\Gamma)\) then the result is obtained as

\[
= \left( \frac{81r^2 + 12r\sqrt{6} - 33r}{27r^2 + 3r} \right) - \left( \frac{2(27r^2 + 3r)}{18r^2 + 6r} \right)
\]

\[
= \left( \frac{12r + 4\sqrt{6} - 24r - 12}{27r^2 + 12r + 1} \right)
\]

\[
IRGA(\Gamma) = \sum_{x_2y_2 \in E} \ln \left( \frac{\text{deg}_r(x_2) + \text{deg}_r(y_2)}{2 \sqrt{\text{deg}_r(x_2) \cdot \text{deg}_r(y_2)}} \right)
\]

\[
= \ln \left( \frac{4}{4} \cdot |E^\lambda_{(2,2)}| + \ln \left( \frac{5}{2\sqrt{6}} \right) \cdot |E^\mu_{(2,3)}| + \ln \left( \frac{6}{6} \right) \cdot |E^\nu_{(3,3)}| \right)
\]

\[
= (0.20391e - 1) \cdot (12r)
\]

\[
IRR_t(\Gamma) = \frac{1}{2} \sum_{x_2y_2 \in E} |\text{deg}_r(x_2) - \text{deg}_r(y_2)|
\]

\[
= \frac{1}{2} \cdot \left( |2 - 2| \cdot |E^\lambda_{(2,2)}| + |2 - 3| \cdot |E^\mu_{(2,3)}| + |3 - 3| \cdot |E^\nu_{(3,3)}| \right)
\]

\[
= \frac{1}{2} \cdot (12r)
\]

6. Computing irregularity-based indices for \(cHBC(r)\)

Let \(\Gamma\) be \(cHBC(r)\). The vertex set and edge set of \(cHBC(r)\) is \(V(\Gamma) = 24r^2 - 30r + 12 = n\) and \(E(\Gamma) = 36r^2 - 54r + 24 = m\), where \(m\) and \(n\) represent the total number of vertices and edges of \(HBC(r)\) and they are picturized in Figure 3.
Figure 3. (i) Coronene; (ii) cHBC(2); (iii) cHBC(3); (iv) cHBC(4).

Table 4. Edge partition Table for cHBC(r).

| (degR(x_1), degR(y_2)) | Total number of edges | Set of edges |
|-------------------------|-----------------------|-------------|
| (2,2)                   | 12r - 6               | \(E_{(2,2)}^r\) |
| (2,3)                   | 12r - 12              | \(E_{(2,3)}^r\) |
| (3,3)                   | 36r^2 - 78r + 42      | \(E_{(3,3)}^r\) |

Theorem 3. If \( \Gamma \) is the cHBC(r) network, then the irregularity-based indices are computed as

1. \( VAR(\Gamma) = \frac{24r^2 - 42r + 20}{4r^2 - 5r + 2} \)
2. \( IR1(\Gamma) = \frac{120(r-1)^2(3r-2)}{4r^2 - 5r + 2} \)
3. \( IR2(\Gamma) = \frac{\sqrt{54r^2 - 97r + 47} + 4(4r^2 - 5r + 2) - 12r^2 + 18r - 8}{4r^2 - 5r + 2} \)
4. \( IRDIF(\Gamma) = \frac{1}{3} \cdot (12r - 12) \)
5. \( AL(\Gamma) = 12r - 12 \)
6. \( IRL(\Gamma) = 0.40545 \cdot (12r - 12) \)
7. \( IRLU(\Gamma) = \frac{1}{2} \cdot (12r - 12) \)
8. \( IRLF(\Gamma) = \frac{1}{\sqrt{6}} \cdot (12r - 12) \)
9. \( IRF(\Gamma) = 12r - 12 \)
10. \( IRA(\Gamma) = \frac{2}{5} \cdot (12r - 12) \)
11. \( IRB(\Gamma) = 0.16832 \cdot (12r - 12) \)
12. \( IRA(\Gamma) = 0.10106 \cdot (12r - 12) \)
13. \( IRC(\Gamma) = \frac{(r^2 - 1)(6\sqrt{5}r^2 + 10\sqrt{3}r - 14r^2 + 4\sqrt{15} - 15r - 6)}{24r^3 - 66r^2 + 73r^2 - 38r + 8} \)
14. \( IRGA(\Gamma) = (0.20391e - 1) \cdot (12r - 12) \)
15. \( IRR_t(\Gamma) = \frac{1}{2} \cdot (12r - 12) \)

**Proof:** Consider \( \Gamma \) is the cHBC \( (r) \). The total number of vertices and edges of \( cHBC(r) \) are \( V(\Gamma) = 24r^2 - 30r + 12 \) and \( E(\Gamma) = 36r^2 - 54r + 24 \).

From Table 4, it can be observed that
\[
|E^c_{(2,2)}| = 12r - 6 \\
|E^r_{(2,3)}| = 12r - 12 \\
|E^v_{(3,3)}| = 36r^2 - 78r + 42.
\]

By using the definitions of \( M_1(\Gamma), M_2(\Gamma), RR(\Gamma) \) and \( F(\Gamma) \), we get the following result as
\[
M_1(\Gamma) = 216r^2 - 360r + 168 \\
M_2(\Gamma) = 324r^2 - 582r + 282 \\
RR(\Gamma) = 108r^2 + (12r - 12)\sqrt{6} - 210r + 114 \\
F(\Gamma) = 648r^2 - 1152r + 552
\]

\[
VAR(\Gamma) = \sum_{u \in V} \left( deg_G(x_2) - \frac{2m}{n} \right)^2 = \frac{M_1(\Gamma)}{n} - \left( \frac{2m}{n} \right)^2
\]

Now put the values of \( M_1(\Gamma), n \) and \( m \) in \( VAR(\Gamma) \) then the result is obtained as
\[
= \left( \frac{216r^2 - 360r + 168}{24r^2 - 30r + 12} \right) - \left( \frac{2(36r^2 - 54r + 24)}{24r^2 - 30r + 12} \right)^2 \\
= \left( \frac{24r^2 - 42r + 20}{4r^2 - 5r + 2} \right)
\]

\[
IR1(\Gamma) = \sum_{x_2 \in V} deg_G(x_2)^3 - \frac{2m}{n} \sum_{x_2 \in V} deg_G(x_2)^2 = F(\Gamma) - \frac{2m}{n} M_1(\Gamma)
\]

Now put the values of \( F(\Gamma), M_1(\Gamma), n \) and \( m \) in \( IR1(\Gamma) \) then the result is obtained as
\[
= 648r^2 - 1152r + 552 - \left( \frac{2(36r^2 - 54r + 24)}{24r^2 - 30r + 12} \right)(216r^2 - 360r + 168) \\
= \left( \frac{120(r - 1)^2(3r - 2)}{4r^2 - 5r + 2} \right)
\]

\[
IR2(\Gamma) = \sqrt{\frac{\sum_{x_2y_2 \in E} \left( deg_G(x_2) \cdot deg_G(y_2) \right)}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(\Gamma)}{m} - \frac{2m}{n}}
\]

Now put the values of \( M_2(\Gamma), n \) and \( m \) in \( IR2(\Gamma) \) then the result is obtained as
\[
= \left( \frac{\sqrt{324r^2 - 582r + 282}}{36r^2 - 54r + 24} \right) - \left( \frac{2(36r^2 - 54r + 24)}{24r^2 - 30r + 12} \right) \\
= \left( \frac{\sqrt{54r^2 - 97r + 47/6r^2 - 9r + 4 \cdot (4r^2 - 5r + 2) - 12r^2 + 18r - 8}}{4r^2 - 5r + 2} \right)
\]

\[
IRDIF(\Gamma) = \sum_{x_2y_2 \in E} \left| \frac{deg_G(x_2)}{deg_G(y_2)} \cdot \frac{deg_G(y_2)}{deg_G(x_2)} \right| \\
= \frac{1}{2} - \frac{2}{2} \cdot |E_{(2,2)}| + \frac{2}{3} - \frac{3}{3} \cdot |E_{(2,3)}| + \frac{3}{3} - \frac{3}{3} \cdot |E_{(3,3)}| \\
= \frac{1}{3} \cdot (12r - 12)
\]
\[ AL(\Gamma) = \sum_{x_2y_2 \in E} |\text{deg}_G(x_2) - \text{deg}_G(y_2)| \]
\[ = |2 - 2| \cdot |E_{[2,2]}| + |2 - 3| \cdot |E_{[2,3]}| + |3 - 3| \cdot |E_{[3,3]}| \]
\[ = 12r - 12 \]

\[ IRL(\Gamma) = \sum_{x_2y_2 \in E} |\ln \text{deg}_G(x_2) - \ln \text{deg}_G(y_2)| \]
\[ = |\ln 2 - \ln 2| \cdot |E_{[2,2]}| + |\ln 2 - \ln 3| \cdot |E_{[2,3]}| + |\ln 3 - \ln 3| \cdot |E_{[3,3]}| \]
\[ = 0.40545 \cdot (12r - 12) \]

\[ IRLU(\Gamma) = \sum_{x_2y_2 \in E} \frac{|\text{deg}_G(x_2) - \text{deg}_G(y_2)|}{\min(\text{deg}_G(x_2), \text{deg}_G(y_2))} \]
\[ = \frac{|2 - 2|}{\sqrt{2}} \cdot |E_{[2,2]}| + \frac{|2 - 3|}{\sqrt{5}} \cdot |E_{[2,3]}| + \frac{|3 - 3|}{\sqrt{3}} \cdot |E_{[3,3]}| \]
\[ = \frac{1}{\sqrt{6}} \cdot (12r - 12) \]

\[ IRLF(\Gamma) = \sum_{x_2y_2 \in E} \frac{(\text{deg}_G(x_2) - \text{deg}_G(y_2))^2}{\text{deg}_G(x_2) + \text{deg}_G(y_2)} \]
\[ = 12r - 12 \]

\[ IRLA(\Gamma) = 2 \sum_{x_2y_2 \in E} \frac{|\text{deg}_G(x_2) - \text{deg}_G(y_2)|}{(\text{deg}_G(x_2) + \text{deg}_G(y_2))} \]
\[ = 2 \left( \frac{|2 - 2|}{4} \cdot |E_{[2,2]}| + \frac{|2 - 3|}{5} \cdot |E_{[2,3]}| + \frac{|3 - 3|}{6} \cdot |E_{[3,3]}| \right) \]
\[ = \frac{2}{5} \cdot (12r - 12) \]

\[ IRA(\Gamma) = \sum_{x_2y_2 \in E} \left( \text{deg}_G(x_2) \cdot \text{deg}_G(y_2) \right)^{1/2} \]
\[ = \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{2}} \right)^2 \cdot |E_{[2,2]}| + \left( \frac{1}{\sqrt{2}} - \frac{1}{\sqrt{3}} \right)^2 \cdot |E_{[2,3]}| + \left( \frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}} \right)^2 \cdot |E_{[3,3]}| \]
\[ = 0.16832 \cdot (12r - 12) \]

\[ IRB(\Gamma) = \sum_{x_2y_2 \in E} \left( \text{deg}_G(x_2) \cdot \text{deg}_G(y_2) \right)^{1/2} \]
\[ = (\sqrt{2} - \sqrt{2})^2 \cdot |E_{[2,2]}| + (\sqrt{2} - \sqrt{3})^2 \cdot |E_{[2,3]}| + (\sqrt{3} - \sqrt{3})^2 \cdot |E_{[3,3]}| \]
\[ = 0.10106 \cdot (12r - 12) \]

\[ IRC(\Gamma) = \sum_{x_2y_2 \in E} \sqrt{\text{deg}_G(x_2) \cdot \text{deg}_G(y_2)} \]
\[ = \frac{2m}{n} - \frac{RR(\Gamma)}{n} \]

Now put the values of \( RR(\Gamma) \), \( n \) and \( m \) in \( IRC(\Gamma) \) then the result is obtained as
\[ = \left( \frac{108r^2 + (12r - 12)\sqrt{6} - 210r + 114}{36r^2 - 54r + 24} \right) - \left( \frac{2(36r^2 - 54r + 24)}{24r^2 - 30r + 12} \right) \]
\[ = \left( \frac{(r - 1)(8\sqrt{6}r^2 - 10\sqrt{6}r - 14r^2 + 4\sqrt{6} + 15r - 6)}{24r^4 - 66r^3 + 73r^2 - 38r + 8} \right) \]
**IRGA(Γ)** = \[ \sum_{x_2y_2 \in E} \ln \left( \frac{(deg_r(x_2) + deg_r(y_2))}{2\sqrt{\text{deg}_r(x_2) \cdot \text{deg}_r(y_2)}} \right) \]

\[ = \ln \left( \frac{4}{4} \cdot |E_{(2,2)}| \right) + \ln \left( \frac{5}{2\sqrt{6}} \right) \cdot |E_{(2,3)}| + \ln \left( \frac{6}{6} \right) \cdot |E_{(3,3)}| \]

\[ = (0.20391e - 1) \cdot (12r - 12) \]

**IRR_r(Γ)** = \[ \frac{1}{2} \sum_{x_2y_2 \in E} |\text{deg}_r(x_2) - \text{deg}_r(y_2)| \]

\[ = \frac{1}{2} \left( (2 - 2) \cdot |E_{(2,2)}| + (2 - 3) \cdot |E_{(2,3)}| + (3 - 3) \cdot |E_{(3,3)}| \right) \]

\[ = \frac{1}{2} \cdot (12r - 12) \]

7. Graphical Representations of the Obtained Results

The chemical structures are visualized as molecular graphs by employing the graph-theoretical methods. Based on the molecular graphs, the irregularity descriptors are computed as functions of \( r \), the parameter which defines the underlying molecular topology. To understand the relationship and behavioral pattern of the calculated indices, the analytical expressions of a few selected indices are represented as 3D plots against variable \( r \). The 3D plots of Theorems 1, 2, and 3 are provided in Figures 4, 5, and 6, respectively. It is obvious from the graphs that the indices vary depending upon the molecular structure.

![3D Plots](image_url)

**Figure 4.** 3D Plots for the results obtained in Theorem 1
8. Conclusions

In this article, the analytical expressions of irregularity indices have been computed for three types of PAH structures, namely, hexaperi-hexabenzocoronene (HBC), dodeca-benzocircumcoronene (DBC), and hexa-cata-hexabenzocoronene (cHBC). The 3D graphical...
representations of the analytical expressions provide a visual conceptualization of the relationship between the irregularity indices and the corresponding molecular structures. The computation of eccentricity-based indices for these structures can also contribute to further studies on these structures, as they have not been explored before. This remains an open problem for future researchers.

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**Conflict of interest**

The authors declare that there is no conflict of interest regarding the publication of this article.

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