Research Article

A Comparison Study of Irregularity Descriptors of Benzene Ring Embedded in P-Type Surface Network and Its Derived Network

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Topological indices are atomic auxiliary descriptors which computationally and hypothetically portray the nature of the basic availability of nanomaterials and chemical mixes, and henceforth, they give faster techniques to look at their exercises and properties. Anomaly indices are for the most part used to describe the topological structures of unpredictable graphs. Graph anomaly examines are helpful not only for quantitative structure-activity relationship (QSAR) and also quantitative structure-property relationship (QSPR) but also for foreseeing their different physical and compound properties, including poisonousness, obstruction, softening and breaking points, the enthalpy of vanishing, and entropy. In this article, we discuss the irregularities of benzene ring and its line graph and compare them by its irregularity indices. We present graphical comparison by using Mathematica.

1. Introduction

Let $G = (V(G), E(G))$ be a simple, finite, and undirected graph, where $V(G)$ and $E(G)$ are the sets containing vertices and edges of $G$ independently. Let $du$ imply the degree of a vertex $v$ and $uv$ address an edge between the two vertices $u$ and $v$. For defined phrasings, we insinuate [1]. A graph is regular, if all its vertices have the same degree, else it is irregular. A line graph is represented by $L(G)$ and defined as edges of $G$ taken as vertices of $L(G)$, and if two edges of $G$ have a common vertex, then edge is made between vertices of $L(G)$. In history, Paul Erdos conducted the examination of irregular graphs for the first time [2]. Beginning now and into the not-so-distant future, the irregularity degree and irregular graphs have turned into the major open issue of graph theory. A graph should be perfect if all the vertices have different degrees (for instance, no two vertices have the same degree). No graph is perfect shown in [3]. The graphs lying inbetween are called semiperfect (quasiperfect) [4]. A disentangled methodology is the irregularity index for passing on the irregularity. Such irregularity index was introduced in [5]. The Albertson index, $AL(G)$, was characterized by Alberston in [6] as $AL(G) = \sum_{uv \in E(G)} |d_u - d_v|$. The irregularity index, $IRL(G)$ and $IRLU(G)$, is characterized by Vukicevic [7] as $IRL(G) = \sum_{uv \in E(G)} \ln (d_u) - \ln (d_v)$ and $IRLU(G) = \sum_{uv \in E(G)} (d_u - (d_v)/\min (d_u, d_v))$. Recently, Abdoo et al. established the new form "total irregularity measure of a graph $G$," which is described in [8–10]. The Randic index is defined as $IRA(G) = \sum_{uv \in E(G)} (d_u^{1/2} - d_v^{1/2})^2$, where irregularity indices $M_1(G), M_2(G), F(G)$, and $RR(G)$ are defined as $M_1(G) = \sum_{uv \in E(G)} (d_u + d_v), \quad M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v), \quad F(G) = \sum_{uv \in E(G)} ((d_u)^2 + (d_v)^2), \quad \text{and} \quad RR(G) = \sum_{uv \in E(G)} \sqrt{d_u d_v}$. In 1985, $C_{60}$ was discovered, and after that, study of carbon nanostructures is also the family of nanotechnology. Mackay and Terrones gave new idea by constructing solid carbon with three-dimension frames in 1991 [11]. In the same year, Lenosky et al. [12] proposed a three-dimensional structure by unit cell of 192 atoms and 216 atoms. Later on, Keeffe et al. compared six-folded and eight-folded ring structures’ energies in 1992 [13], the second one 3D benzene structure was called 6.82P (polybenzene). In 2018, Ahmad found degree-based topological indices of benzene ring
embedded in the P-type surface in the 2D network [14]. Later, in 2019, Yang determined M-polynomial and topological indices of benzene ring embedded in the P-type surface in the 2D network [15]. In the same year, Ahmad et al. computed degree-based topological indices of line graph of benzene ring embedded in the P-type surface in the 2D network [16], and recently, in 2020, Prosanta Sarkar et al. found general fifth M-Zagreb polynomials of benzene ring implanted in the P-type-surface in the 2D network [17].

2. Methodology

The graph is represented by $G = (V(G), E(G))$, where $V(G)$ denotes vertices and $E(G)$ denotes edges. In irregularity indices, we first find the order (number of vertices of graph) and size (number of edges of graph) of the graph and partition vertices by its degrees (same and different) and divide edges by its end vertices degree which is usually known as edge partition. We use edge partition as well as order and size to find irregularity indices and edge partition depending on the degree of end vertices of edges.

2.1. Results for Benzene Ring Embedded in P-Type Surface Network

In this section, we compute some irregularity indices of benzene ring such as variance index, Albertson index, and Randic index. Benzene ring embedded in the P-type surface network having $24pq$ vertices and $32pq - 2q - 2p$ edges is depicted in Figure 1.

Theorem 1. For the benzene ring embedded in the P-type surface network $(BR[p, q])$, we have

\[
\begin{align*}
\text{VAR}(BR[p, q]) &= -\frac{(4p + 4q - 64pq)^2}{576p^2q^2} - \frac{20p + 20q - 176pq}{24pq}, \\
\text{AL}(BR[p, q]) &= 16pq, \\
\text{IR1}(BR[p, q]) &= -\frac{10(-2p^2q^2 - 2p^2q + p^2 - 2pq^2 + 2pq + q^2)}{3pq}, \\
\text{IR2}(BR[p, q]) &= \sqrt{2}\sqrt{\frac{38p + 38q - 240pq}{2(2p + 2q - 32pq)}} + \frac{4p + 4q - 64pq}{24pq}, \\
\text{IRA}(BR[p, q]) &= \frac{1213215869760357pq}{4503599627370496}, \\
\text{IRL}(BR[p, q]) &= \frac{3652105019575333pq}{562949953421312}, \\
\text{IRLU}(BR[p, q]) &= 8pq.
\end{align*}
\]

Proof. The order of graph is $n = |V(BR[p, q])| = 24pq$, and the size is $m = |E(BR[p, q])| = 32pq - 2q - 2p$. The vertex set of $BR[p, q]$ can be divided into the following classes by means of degrees:

\[
\begin{align*}
V_1(BR[p, q]) &= \{v \in V(BR[p, q]) : d_v = 2\}, \\
V_2(BR[p, q]) &= \{v \in V(BR[p, q]) : d_v = 3\}.
\end{align*}
\]

The edge set of $BR[p, q]$ can be divided into the following classes with respect to the degree of end vertices:

\[
\begin{align*}
E_1(BR[p, q]) &= \{uv \in E(BR[p, q]) : d_u = d_v = 2\}, \\
E_2(BR[p, q]) &= \{uv \in E(BR[p, q]) : d_u = d_v = 3\}, \\
E_3(BR[p, q]) &= \{uv \in E(BR[p, q]) : d_u = 2, d_v = 3\}.
\end{align*}
\]

And, the cardinality of edges are as follows:

\[
\begin{align*}
|E_1(BR[p, q])| &= 4p + 4q, \\
|E_2(BR[p, q])| &= 16pq - 6q - 6p, \\
|E_3(BR[p, q])| &= 16pq.
\end{align*}
\]

First, we find some topological indices which will be used in irregularity indices:
\[ M_1(\mathcal{B}(p, q)) = \sum_{uv \in \mathcal{E}(\mathcal{B}(p, q))} (d_u + d_v) \]
\[ = 176pq - 20q - 20p, \]

\[ M_2(\mathcal{B}(p, q)) = \sum_{uv \in \mathcal{E}(\mathcal{B}(p, q))} (d_u \times d_v) \]
\[ = 240pq - 38q - 38p, \]

\[ F(\mathcal{B}(p, q)) = \sum_{uv \in \mathcal{E}(\mathcal{B}(p, q))} \left( (d_u)^2 + (d_v)^2 \right) \]
\[ = 496pq - 76q - 76p, \]

\[ RR(\mathcal{B}(p, q)) = \sum_{uv \in \mathcal{E}(\mathcal{B}(p, q))} \sqrt{d_u d_v} \]
\[ = 48pq - 10q - 10p + 16\sqrt{6pq}, \]

\[ VAR(\mathcal{B}(p, q)) = \frac{M_1(\mathcal{B}(p, q))}{n} - \left( \frac{2m}{n} \right)^2 \]
\[ = \frac{176pq - 20q - 20p}{24pq} - \left( \frac{232pq - 2q - 2p}{24pq} \right)^2 \]
\[ = \frac{(4p + 4q - 64pq)^2}{576pq^2} - \frac{20p + 20q - 176pq}{24pq}, \]

\[ AL(\mathcal{B}(p, q)) = \sum_{uv \in \mathcal{E}(\mathcal{B}(p, q))} |d_u - dv| \]
\[ = \sum_{uv \in \mathcal{E}_1(\mathcal{B}(p, q))} (0) + \sum_{uv \in \mathcal{E}_2(\mathcal{B}(p, q))} (0) \]
\[ + \sum_{uv \in \mathcal{E}_3(\mathcal{B}(p, q))} |(2) - (3)| \]
\[ = 16pb, \]

\[ IR1(\mathcal{B}(p, q)) = F(\mathcal{B}(p, q)) - \frac{2m}{n} M_1(\mathcal{B}(p, q)) \]
\[ = 496pq - 76q - 76p - \frac{2(32pq - 2q - 2p)}{24pq}176pq - 20q - 20p \]
\[ = \frac{-10\left(-8p^2q^2 - 2p^2q + p^2 - 2pq^2 + 2pq + q^2\right)}{3pq}, \]

\[ IR2(\mathcal{B}(p, q)) = \sqrt{\frac{M_2(\mathcal{B}(p, q))}{m} - \frac{2m}{n}} \]
\[ = \sqrt{\frac{240pq - 38q - 38p}{32pq - 2q - 2p} - \frac{2(32pq - 2q - 2p)}{24pq}} \]
\[ = \sqrt{\frac{\sqrt{38p + 38q - 240pq}}{2(2p + 2q - 32pq)} + \frac{4p + 4q - 64pq}{24pq},} \]
IRA(BR[p,q]) = \sum_{uv \in E(BR[p,q])} (d_u^{-1/2} - d_v^{-1/2})^2

= \sum_{uv \in E_1(BR[p,q])} (0) + \sum_{uv \in E_2(BR[p,q])} (0)
+ \sum_{uv \in E_3(BR[p,q])} (2^{-1/2} - (3)^{-1/2})^2

= \frac{1213215869760357 \ pq}{4503599627370496}

IRL(BR[p,q]) = \sum_{uv \in E(BR[p,q])} |\ln (d_u) - \ln (d_v)|

= \sum_{uv \in E_1(BR[p,q])} (0) + \sum_{uv \in E_2(BR[p,q])} (0)
+ \sum_{uv \in E_3(BR[p,q])} |\ln (2) - \ln (3)|

= \frac{365210519575333 \ pq}{562949953421312}

IRLU(BR[p,q]) = \sum_{uv \in E(BR[p,q])} \frac{|(d_u) - (dv)|}{\min (d_u, d_v)}

= \sum_{uv \in E_1(BR[p,q])} (0) + \sum_{uv \in E_2(BR[p,q])} (0)
+ \sum_{uv \in E_3(BR[p,q])} \frac{|(2) - (3)|}{\min (2, 3)}

= 8pq.

Figure 1: Benzene ring embedded in the P-type-surface network BR[p,q].
2.2. Results for Line Graph of Benzene Ring Embedded in the P-Type Surface Network. In this section, we compute some irregularity indices of the line graph of the benzene ring network such as variance index, Albertson index, and Randić irregularity indices of the line graph of the benzene ring
\[ \text{VAR}(L(BR[p,q])) = \frac{8(-8p^2q^2 - 7p^2q + 3p^2 - 7pq^2 + 6pq + 3q^2)}{(p + q - 16pq)^2}, \]
\[ \text{AL}(L(BR[p,q])) = 32pq - 8, \]
\[ \text{IR1}(L(BR[p,q])) = \frac{16(-56p^2q^2 - 37p^2q + 18p^2 - 37pq^2 + 36pq + 18q^2)}{p + q - 16pq}, \]
\[ \text{IR2}(L(BR[p,q])) = \frac{\sqrt{2}(44p + 44q - 178pq - 1/(p + q - 7pq))}{2} \cdot \frac{8p + 8q - 56pq}{p + q - 16pq}, \]
\[ \text{IRA}(L(BR[p,q])) = \frac{3(9197337752963468p + 4171150200481037q)}{144115188075855872} + \frac{3(4171150200481037p - 6470484638721904)}{144115188075855872}, \]
\[ \text{IRL}(L(BR[p,q])) = \frac{(10364838994360104p + 1060895270985307q)}{1125899906842624} + \frac{1060895270985307p - 3652105019575333}{1125899906842624}, \]
\[ \text{IRLU}(L(BR[p,q])) = \frac{4p}{3} + \frac{4q}{3} + \frac{32pq}{3} - 4. \]

**Proof.** The order of the graph is \( n = |V(L(BR[p,q]))| = 32pq - 2q - 2p \) and its size is \( m = |E(L(BR[p,q]))| = 56pq - 8q - 8p \). The vertex set of \( L(BR[p,q]) \) can be divided into the following classes by means of degrees:
\[
V_1(L(BR[p,q])) = \{v \in V(L(BR[p,q])) : d_v = 2, \}
\[
V_2(L(BR[p,q])) = \{v \in V(L(BR[p,q])) : d_v = 3, \}
\[
V_3(L(BR[p,q])) = \{v \in V(L(BR[p,q])) : d_v = 4. \}
\]

The edge set of \( L(BR[p,q]) \) can be divided into the following classes with respect to the degree of end vertices:
\[
E_1(L(BR[p,q])) = \{uv \in E(L(BR[p,q])) : d_u = d_v = 3, \}
\[
E_2(L(BR[p,q])) = \{uv \in E(L(BR[p,q])) : d_u = d_v = 4, \}
\[
E_3(L(BR[p,q])) = \{uv \in E(L(BR[p,q])) : d_u = d_v = 2, \}
\[
E_4(L(BR[p,q])) = \{uv \in E(L(BR[p,q])) : d_u = 3, d_v = 4, \}
\[
E_5(L(BR[p,q])) = \{uv \in E(L(BR[p,q])) : d_u = 3, d_v = 4. \}
\]
Figure 2: Line graph of benzene ring embedded in the P-type surface network $L(BR[p,q])$.

Figure 3: Plots for Var.
And, the cardinality of edges are as follows:

\[
\begin{align*}
|E_1(L(BR[p,q]))| &= 8pq + 4, \\
|E_2(L(BR[p,q]))| &= 16pq - 8q - 8p, \\
|E_3(L(BR[p,q]))| &= 4, \\
|E_4(L(BR[p,q]))| &= 8p + 8q - 8, \\
|E_5(L(BR[p,q]))| &= 32pq - 8q - 8p.
\end{align*}
\]

(9)

First, we find some topological indices which will be used in irregularity indices:

\[
M_1(L(BR[p,q])) = \sum_{uv \in E(L(BR[p,q]))} (d_u + d_v)
\]

\[
= 400pq - 80q - 80p,
\]

\[
M_2(L(BR[p,q])) = \sum_{uv \in E(L(BR[p,q]))} (d_u \times d_v)
\]

\[
= 712pq - 176q - 176q + 4,
\]

\[
F(L(BR[p,q])) = \sum_{uv \in E(L(BR[p,q]))} ((d_u)^2 + (d_v)^2)
\]

\[
= 1456pq - 352q - 352p,
\]

\[
RR(L(BR[p,q])) = \sum_{uv \in E(L(BR[p,q]))} \sqrt{d_u d_v}
\]

\[
= 88pq - 32q - 32p + \sqrt{6}(8p + 8q - 8) - 2\sqrt{3}(8p + 8q - 32pq) + 20.
\]

\[
VAR(L(BR[p,q])) = \frac{M_1(L(BR[p,q]))}{n} - \left(\frac{2m}{n}\right)^2
\]

\[
= \frac{400pq - 80q - 80p}{32pq - 2q - 2p} - \left(\frac{256pq - 8q - 8p}{32pq - 2q - 2p}\right)^2
\]

\[
= \frac{-8(-8p^2q^2 - 7p^2q + 3p^2 - 7pq^2 + 6pq + 3q^2)}{(p + q - 16pq)^2},
\]

\[
AL(L(BR[p,q])) = \sum_{uv \in E(L(BR[p,q]))} |d_u - dv|
\]

\[
= \sum_{uv \in E_1(L(BR[p,q]))} (0) + \sum_{uv \in E_2(L(BR[p,q]))} (0) + \sum_{uv \in E_3(L(BR[p,q]))} (0)
\]

\[
+ \sum_{uv \in E_4(L(BR[p,q]))} |(2) - (3)| + \sum_{uv \in E_5(L(BR[p,q]))} |(3) - (4)|
\]

\[
= 32pq - 8,
\]

\[
IR1(L(BR[p,q])) = F(L(BR[p,q])) - \frac{2m}{n}M_1(L(BR[p,q]))
\]

\[
= 1456pq - 352q - 352p - \frac{2(56pq - 8q - 8p)}{32pq - 2q - 2p} \cdot 400pq - 80q - 80p
\]
\[
\begin{align*}
\text{IR2} (L[B(p, q)]) &= \sqrt{M_2 (L[B(p, q)]) - \frac{2m}{n}} \\
&= \sqrt{\frac{712pq - 176q - 176p + 4}{56pq - 8q - 8p} - \frac{2(56pq - 8q - 8p)}{32pq - 2q - 2p}} \\
&= \frac{\sqrt{2} \sqrt{(44p + 44q - 178pq - 1/7(p + q - 7pq))}}{2} - \frac{8p + 8q - 56pq}{p + q - 16pq} \\
\text{IRA} (L[B(p, q)]) &= \sum_{uv \in E(L[B(p, q)])} \left( d_u^{-1/2} - dv^{-1/2} \right)^2 \\
&= \sum_{uv \in E_1 (L[B(p, q)])} (0) + \sum_{uv \in E_2 (L[B(p, q)])} (0) + \sum_{uv \in E_3 (L[B(p, q)])} (0) \\
&+ \sum_{uv \in E_4 (L[B(p, q)])} \left( \left( 2 \right)^{-1/2} - \left( 3 \right)^{-1/2} \right)^2 + \sum_{uv \in E_5 (L[B(p, q)])} \left( \left( 3 \right)^{-1/2} - \left( 4 \right)^{-1/2} \right)^2 \\
&= \frac{3(9197337752963468p + 4171150200481037q)}{144115188075855872} + \frac{3(4171150200481037p - 6470484638721904)}{144115188075855872} \\
\text{IRL} (L[B(p, q)]) &= \sum_{uv \in E(L[B(p, q)])} \left| \ln (d_u) - \ln (dv) \right| \\
&= \sum_{uv \in E_1 (L[B(p, q)])} (0) + \sum_{uv \in E_2 (L[B(p, q)])} (0) + \sum_{uv \in E_3 (L[B(p, q)])} (0) \\
&+ \sum_{uv \in E_4 (L[B(p, q)])} \left| \ln (2) - \ln (3) \right| + \sum_{uv \in E_5 (L[B(p, q)])} \left| \ln (3) - \ln (4) \right| \\
&= \frac{(1036438994360104p + 1060895270985307q)}{112589906842624} + \frac{1060895270985307p - 3652105019575333}{112589906842624} \\
\text{IRLU} (L[B(p, q)]) &= \sum_{uv \in E(L[B(p, q)])} \frac{\left| (d_u) - (dv) \right|}{\min (d_u, dv)} \\
&= \sum_{uv \in E_1 (L[B(p, q)])} (0) + \sum_{uv \in E_2 (L[B(p, q)])} (0) + \sum_{uv \in E_3 (L[B(p, q)])} (0) \\
&+ \sum_{uv \in E_4 (L[B(p, q)])} \left| \ln (2) - \ln (3) \right| + \sum_{uv \in E_5 (L[B(p, q)])} \left| \ln (3) - \ln (4) \right| \\
&= \frac{4p}{3} + \frac{4q}{3} + \frac{32pq}{3} - 4.
\end{align*}
\]
Figure 4: Plots for AL.

Figure 5: Plots for IR1.
Figure 6: Plots for the IRLU.

Figure 7: Plots for the IR2.
3. Graphical Comparison and Conclusion

In this section, we compare irregularity indices of benzene ring and line of benzene ring. Here, we plot characteristics that decide the properties of $BR[p,q]$ with parameters $p$ and $q$. Thus, we can conclude the properties of benzene and line of benzene ring on the basis of parameters $p$ and $q$. Figure 3 shows the variances of both plots which are increasing and parallel. Figures 4–6 depict the same behavior of AL, IR1, and IRL, as $BR[p,q]$ is more rapid than $L(BR[p,q])$, but one can see Figure 5 is more sharp than remaining. Figure 7 incorporates the plotting of IR1 which is overlapped by increasing the values of $p$ and $q$. The behavior of IRA and IRL of $BR[p,q]$ are the same in Figures 8 and 9, but the
behavior of $L(\text{BR}[p,q])$ is much slower than all other irregularity indices. In this paper, we have registered a few degree-based irregularity indices. It is demonstrated that topological indices help to foresee numerous properties without heading off to the wet lab.

**Data Availability**

The data used to support the findings of this study are available from the corresponding author upon request.

**Conflicts of Interest**

The authors declare that they have no conflicts of interest.

**Authors’ Contributions**

All authors contributed equally to this work.

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