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Research Article

Bounds on the neighborhood inverse sum indeg index of graphs with applications to benzenoid hydrocarbons

Deepa Balasubramaniyan[1,†], **Natarajan Chidambaram**[1,‡], **Modjtaba Ghorbani**[2,*]

[1]Department of Mathematics, Srinivasa Ramanujan Centre,
SASTRA Deemed to be University, Kumbakonam - 612 001, Tamil Nadu, India
[†]mathsdeepa2000@gmail.com
[‡]mathsnatarajan@gmail.com

[2]Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University,
Tehran 16785-163, Iran
[*]mghorbani@sru.ac.ir

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Abstract: The neighborhood inverse sum indeg index, denoted as $ISI_N(\mathcal{G})$, of a simple graph $\mathcal{G}$ is defined as the sum of the terms $(\frac{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)}{\delta_{\mathcal{G}}(r)+\delta_{\mathcal{G}}(s)}$ for all edges $rs)$ in $\mathcal{G}$. Here, $\delta_{\mathcal{G}}(r)$ represents the neighborhood degree of a vertex r, which is the sum of the degrees of the neighbours of r in $\mathcal{G}$. This article establishes bounds for the $ISI_N(\mathcal{G})$ index in relation to various graph invariants and its connection to neighborhood degree-sum-based topological indices. We also present results on the ISI_N index concerning different graph operations. Furthermore, we analyze the physico-chemical properties of 55 benzenoid hydrocarbons and validate our model with 10 more benzenoid hydrocarbons.

Keywords: inverse sum in-degree index, vertex degree, benzenoid hydrocarbons.

AMS Subject classification: 05C12, 05C50, 05C80

1. Introduction

Mathematical chemistry is a branch of theoretical chemistry that uses mathematical techniques to describe and forecast molecular structure without necessarily utilising quantum mechanics. Chemical graph theory is a branch of mathematical chemistry

* *Corresponding Author*

that uses graph theory to model chemical phenomena mathematically [14]. Topological indices study numerical characteristics of molecular structures, which are examined for the quantitative description of chemical compounds [33]. The widespread use of topological indices in QSAR(Quantitative Structure-Activity Relationship) and QSPR(Quantitative Structure-Property Relationship) studies proves they contain useful structural information. Novel graph invariants based on the vertex degree are being developed by theorists from various backgrounds. The intriguing applications of degree-based indices have drawn a lot of attention from researchers, who are now focusing on descriptors based on the neighborhood degree indices. More than 40 years ago Gutman et al. [13] defined the Zagreb indices as

$$M_1(\mathscr{G}) = \sum_{r \in \mathscr{V}(\mathscr{G})} (d_{\mathscr{G}}(r))^2,$$
$$M_2(\mathscr{G}) = \sum_{rs \in \mathscr{E}(\mathscr{G})} d_{\mathscr{G}}(r) d_{\mathscr{G}}(s).$$

Vukicevic et al.[34] studied 148 Adriatic indices according to the four benchmark sets put forward by the International Academy of Mathematical Chemistry, the inverse sum indeg index is one of the Adriatic indices with a significant predictive capability which is defined as

$$ISI(\mathscr{G}) = \sum_{rs \in \mathscr{E}(\mathscr{G})} \frac{d_{\mathscr{G}}(r) d_{\mathscr{G}}(s)}{d_{\mathscr{G}}(r) + d_{\mathscr{G}}(s)}.$$

For a comprehensive survey on ISI index, one may refer to [1].
Fajtlowicz [9] defined the harmonic index as

$$H(\mathscr{G}) = \sum_{rs \in \mathscr{E}(\mathscr{G})} \frac{2}{d_{\mathscr{G}}(r) + d_{\mathscr{G}}(s)}.$$

Shirdel et al. [31] defined the hyper-Zagreb index as

$$HM(\mathscr{G}) = \sum_{rs \in \mathscr{E}(\mathscr{G})} [d_{\mathscr{G}}(r) + d_{\mathscr{G}}(s)]^2,$$

further obtained some results on graph operations for this index. Ghorbani et al. [11, 12] were the first team of researchers to introduce the idea of neighborhood degree sum-based indices and they called them "the third version of Zagreb indices".

$$M_1'(\mathscr{G}) = \sum_{rs \in \mathscr{E}(\mathscr{G})} (\delta_{\mathscr{G}}(r) + \delta_{\mathscr{G}}(s)),$$
$$M_2'(\mathscr{G}) = \sum_{rs \in \mathscr{E}(\mathscr{G})} \delta_{\mathscr{G}}(r) \delta_{\mathscr{G}}(s),$$

where $\delta_{\mathcal{G}}(r)$ represents the sum of the degrees of the neighbours of r in $\mathcal{G}$.(i.e)$\delta_{\mathcal{G}}(r) = \sum_{s \in N_{\mathcal{G}}(r)} d_{\mathcal{G}}(s)$, $N_{\mathcal{G}}(r) = \{s \mid rs \in \mathscr{E}(\mathcal{G})\}$ and $d_{\mathcal{G}}(r)$ denotes the degree of any vertex r in $\mathcal{G}$. Also, they found the following easy relationship between the sum of the neighborhood degrees of all vertices of any graph $\mathcal{G}$ and the famous first Zagreb index $M_1(\mathcal{G})$:

$$\sum_{r \in \mathscr{V}(\mathcal{G})} \delta_{\mathcal{G}}(r) = M_1(\mathcal{G}).$$

Further, they performed some graph operations for $M_1'(\mathcal{G})$.

Basavanagoud et al. [5] introduced the first neighborhood Zagreb index tested its chemical applicability and also obtained its bounds. The index is defined as

$$NM_1(\mathcal{G}) = \sum_{r \in \mathscr{V}(\mathcal{G})} (\delta_{\mathcal{G}}(r))^2.$$

V.R.Kulli [19] introduced the neighborhood inverse sum indeg and harmonic neighborhood index of a graph $\mathcal{G}$ as

$$ISI_N(\mathcal{G}) = \sum_{rs \in \mathscr{E}(\mathcal{G})} \frac{1}{\frac{1}{\delta_{\mathcal{G}}(r)} + \frac{1}{\delta_{\mathcal{G}}(s)}} = \sum_{rs \in \mathscr{E}(\mathcal{G})} \frac{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)}{\delta_{\mathcal{G}}(r) + \delta_{\mathcal{G}}(s)},$$

$$NH(\mathcal{G}) = \sum_{rs \in \mathscr{E}(\mathcal{G})} \frac{2}{\delta_{\mathcal{G}}(r) + \delta_{\mathcal{G}}(s)},$$

In [18], Kulli defined the following new neighborhood indices namely, the general neighborhood second Zagreb index and the neighborhood hyper-Zagreb index.

$$NM_2^{\varepsilon}(\mathcal{G}) = \sum_{rs \in \mathscr{E}(\mathcal{G})} (\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s))^{\varepsilon}, \varepsilon \in \mathbb{R} - \{0\}.$$

$$NHM = \sum_{rs \in \mathscr{E}(\mathcal{G})} [\delta_{\mathcal{G}}(r) + \delta_{\mathcal{G}}(s)]^2.$$

Pattabiraman [25] explored some upper and lower bounds on inverse sum indeg (ISI) index and in addition performed composite graph operations. Balachandran et al. [4] refined some bounds obtained in [25]. Özge Çolakoglu Havare [15] studied inverse sum indeg index for graph operations. Rani et al. [28] investigated sharp bounds for inverse sum indeg index for product graphs and double graphs. Matejić et al.[20] analysed the upper bounds of inverse sum indeg index in terms of some other vertex degree-based indices. Jamal et al. [16] computed the bounds for Sombor and inverse sum indeg index of graph operations in terms of degree, size and order. Doley et al. [7] established some bounds for the ISI index of operations and also discussed some extreme cases. Falahati et al. [10] presented sharp upper and lower bounds on the ISI index of some graphs concerning radius, number of pendants and minimal non-pendant vertex degree. Nagarajan et al. [23] explored some bounds for the ISI index of some standard graphs. Khalifeh et al. [17] studied the behaviour of some graph operations for the first and second Zagreb indices. Suresh Elumalai et al. [8] established some new upper bounds on the hyper Zagreb index of a connected graph. Das et al. [6] investigated the chemical significance of the ISI_N index of molecular graphs and estimated mathematical features of this index, including the class of all trees and unicyclic graphs. Reti et al. [29] presented some sharp bounds on the neighborhood's first Zagreb index and established its relations with the first and second Zagreb indices. Mondal et al. [22] examined the chemical applicability of the neighborhood Zagreb index and computed some results of product graphs. Mondal et al. [21] derived some bounds on the neighborhood Zagreb index and also obtained some results on different graph operations. Harishchandra et al. [27] presented the vertex versions of redefined third Zagreb, reduced second Zagreb and hyper Zagreb index by using the concept of neighborhood degree sum and some results related to line graphs. Ramane et al. [26] studied the neighborhood Zagreb indices and coindices of graphs and also some new upper bounds for the neighborhood first Zagreb index. In this article, we are concerned with the neighborhood inverse sum indeg index. First, we recall some definitions used in this article and discuss the bounds related to the ISI_N index. Then, we present some results on graph operations. Recently, Arockiaraj et al. [2] conducted a comparative study of degree and neighborhood degree-based indices in predicting physico-chemical properties of skin cancer drugs. Sarkar et al. [30] investigated thermodynamic properties of benzenoid hydrocarbons using some neighborhood degree-based indices and their applications to graphene.

2. Definitions and Preliminaries

In this section, we outline some elementary inequalities and definitions used to obtain the result. Let $\mathcal{G} = (\mathscr{V}, \mathscr{E})$ denote a simple connected graph with the vertex set $\mathscr{V}$ and the edge set $\mathscr{E}$.

Definition 1. Let $\{\rho_1, \rho_2, \ldots, \rho_n\}$ be a set of positive real numbers such that the arithmetic mean (AM) and the harmonic mean (HM) are represented as follows:

$$\mathrm{AM} = \frac{\rho_1 + \rho_2 + \cdots + \rho_n}{n},$$
$$\mathrm{HM} = \frac{n}{\frac{1}{\rho_1} + \frac{1}{\rho_2} + \cdots + \frac{1}{\rho_n}}.$$

Definition 2. Let $\mathscr{G}_1$ be any connected graph. Let y be a vertex such that $y \notin \mathscr{V}(\mathscr{G}_1)$. The graph $\mathscr{G}_1 + \{y\}$ is obtained by adding the vertex y to $\mathscr{G}_1$ and connecting it to every vertex in $\mathscr{G}_1$. Formally, $\mathscr{G}_1 + \{y\} = (\mathscr{V}, \mathscr{E})$, where $\mathscr{V} = \mathscr{V}(\mathscr{G}_1) \cup \{y\}$ and
$\mathscr{E} = \mathscr{E}(\mathscr{G}_1) \cup \{ry \mid r \in \mathscr{V}(\mathscr{G}_1)\}$.

Definition 3. The join of two graphs $\mathscr{G}_1$ and $\mathscr{G}_2$, denoted by $\mathscr{G}_1 + \mathscr{G}_2$, is the graph $\mathscr{G}$ such that $\mathscr{V}(\mathscr{G}_1 + \mathscr{G}_2) = \mathscr{V}(\mathscr{G}_1) \cup \mathscr{V}(\mathscr{G}_2)$ and $\mathscr{E}(\mathscr{G}_1 + \mathscr{G}_2) = \mathscr{E}(\mathscr{G}_1) \cup \mathscr{E}(\mathscr{G}_2) \cup \mathscr{E}'$, where $\mathscr{E}' = \{rs : r \in \mathscr{V}(\mathscr{G}_1), s \in \mathscr{V}(\mathscr{G}_2)\}$.

Definition 4. For a collection of three or more disjoint graphs $\mathscr{G}_1, \mathscr{G}_2, \mathscr{G}_3, \ldots, \mathscr{G}_k$, where each graph $\mathscr{G}_p = (\mathscr{V}_p, \mathscr{E}_p)$ has vertex set $\mathscr{V}_p$ and edge set $\mathscr{E}_p$, and the graphs are pairwise disjoint (i.e., $\mathscr{V}_p \cap \mathscr{V}_q = \emptyset$ and $\mathscr{E}_p \cap \mathscr{E}_q = \emptyset$ for all $p \neq q$), the sequential join of these graphs, denoted as $\mathscr{G} = \mathscr{G}_1 + \mathscr{G}_2 + \mathscr{G}_3 + \cdots + \mathscr{G}_k = (\mathscr{V}, \mathscr{E})$, is formed by taking the union of the vertex sets $\mathscr{V} = \mathscr{V}_1 \cup \mathscr{V}_2 \cup \cdots \cup \mathscr{V}_k$ and the union of the edge sets $\mathscr{E} = \mathscr{E}_1 \cup \mathscr{E}_2 \cup \cdots \cup \mathscr{E}_k$, along with the additional edges that connect adjacent graphs in the sequence. Specifically, the sequential join is represented as $(\mathscr{G}_1 + \mathscr{G}_2) \cup (\mathscr{G}_2 + \mathscr{G}_3) \cup \cdots \cup (\mathscr{G}_{k-1} + \mathscr{G}_k)$, where edges are added between each pair of consecutive graphs $\mathscr{G}_p$ and $\mathscr{G}_{p+1}$ for $p = 1, 2, \ldots, k-1$, creating a new graph that sequentially joins the individual graphs.

Definition 5. The Cartesian product of two graphs $\mathscr{G}_1$ and $\mathscr{G}_2$, denoted by $\mathscr{G}_1 \Box \mathscr{G}_2$, is a graph with the vertex set $\mathscr{V}(\mathscr{G}_1 \Box \mathscr{G}_2) = \{(r, s) : r \in \mathscr{V}(\mathscr{G}_1), s \in \mathscr{V}(\mathscr{G}_2)\}$ and the edge set consists of (r_1, s_1) and (r_2, s_2) are adjacent if and only if $(r_1, r_2) \in \mathscr{E}(\mathscr{G}_1)$ and $s_1 = s_2$, or $r_1 = r_2$ and $(s_1, s_2) \in \mathscr{E}(\mathscr{G}_2)$.

Definition 6. The lexicographic product of two graphs $\mathscr{G}_1$ and $\mathscr{G}_2$, denoted $\mathscr{G}_1[\mathscr{G}_2]$, is a graph with the vertex set $\mathscr{V}(\mathscr{G}_1[\mathscr{G}_2]) = \{(r, s) : r \in \mathscr{V}(\mathscr{G}_1), s \in \mathscr{V}(\mathscr{G}_2)\}$,and the edge between vertices if only if $r_1 = r_2$ and $(s_1, s_2) \in \mathscr{E}(\mathscr{G}_2)$ or $(r_1, r_2) \in \mathscr{E}(\mathscr{G}_1)$.

Definition 7. The corona product of two graphs $\mathscr{G}_1$ and $\mathscr{G}_2$, denoted $\mathscr{G}_1 \circ \mathscr{G}_2$, is a graph $\mathscr{G}$ constructed by taking one copy of $\mathscr{G}_1$ of order n_1 and n_1 copies of $\mathscr{G}_2$, then linking the p-th vertex of $\mathscr{G}_1$ to every vertex in the p-th copy of $\mathscr{G}_2$ by an edge.

Definition 8. A function $f : \mathbb{R}^n \to \mathbb{R}$ is convex if its domain is a convex set and for every x, y in its domain and all $\lambda \in [0, 1]$, we have $f(\lambda x + (1 - \lambda) - y) \leq \lambda f(x) + (1 - \lambda) f(y)$.

Throughout our discussion δ_N denotes the minimum neighborhood degree and Δ_N denotes the maximum neighborhood degree of a graph $\mathscr{G}$.

3. Bounds for ISI_N Index

In this section, we prove some analytical inequalities that determine a lower and upper bounds for the ISI_N index.

Lemma 1. *[25] Let a_p and b_p, $1 \leq p \leq n$, be positive real numbers. Then,*

$$\left| n\sum_{p=1}^{n} a_p b_p - \sum_{p=1}^{n} a_p \sum_{p=1}^{n} b_p \right| \leq \varepsilon(n)(\mathscr{A} - a)(\mathscr{B} - b),$$

where $a, b, \mathscr{A}$, and $\mathscr{B}$ are real constants such that for each p, $1 \leq p \leq n$, $a \leq a_p \leq \mathscr{A}$ and $b \leq b_p \leq \mathscr{B}$. Further, $\varepsilon(n) = n\left\lceil \frac{n}{2} \right\rceil \left(1 - \frac{1}{n}\left\lceil \frac{n}{2} \right\rceil\right)$.

Theorem 1. *Let G be a graph on n vertices and m edges. Then*

$$ISI_N(G) \leq \varepsilon(m)\frac{(\Delta_N - \delta_N)^2(\Delta_N + \delta_N)}{m\delta_N\Delta_N} + \frac{NH(G)NM_2(G)}{2m},$$

where the equality holds if and only if G is regular.

Proof. We take $a = \frac{1}{\Delta_N}$, $\mathscr{A} = \frac{1}{\delta_N}$, $b = \delta_N^2$, and $\mathscr{B} = \Delta_N^2$ in Lemma 1. Further, $\varepsilon(m) = m\lceil \frac{m}{2} \rceil \left(1 - \frac{1}{m}\lceil \frac{m}{2} \rceil\right)$, $a_p = \frac{1}{\delta_G(r)+\delta_G(s)}$, and $b_p = \delta_G(r)\delta_G(s)$. Now, we get

$$\left| m \sum_{rs\in \mathscr{E}(G)} \frac{\delta_G(r)\delta_G(s)}{\delta_G(r)+\delta_G(s)} - \sum_{rs\in \mathscr{E}(G)} \frac{1}{\delta_G(r)+\delta_G(s)} \sum_{rs\in \mathscr{E}(G)} \delta_G(r)\delta_G(s) \right|$$
$$\leq \varepsilon(m)\left(\frac{1}{\delta_N} - \frac{1}{\Delta_N}\right)(\Delta_N^2 - \delta_N^2)$$

$$\left| mISI_N(G) - \frac{NH(G)}{2}NM_2(G) \right| \leq \varepsilon(m)\left(\frac{\Delta_N(G) - \delta_N(G)}{\delta_N(G)\Delta_N(G)}\right)(\Delta_N - \delta_N)(\Delta_N + \delta_N).$$

Therefore, we have

$$ISI_N(G) \leq \varepsilon(m)\frac{(\Delta_N - \delta_N)^2(\Delta_N + \delta_N)}{m\delta_N\Delta_N} + \frac{NH(G)NM_2(G)}{2m}.$$

The equality holds if and only if $\delta_N = \Delta_N$. Thus G is regular. □

Lemma 2. *[24](Chebyshev's Inequality) If $\varepsilon = (\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_n)$ and $\vartheta = (\vartheta_1, \vartheta_2, \ldots, \vartheta_n)$ are two real sequences such that*

(1) $\varepsilon_1 \leq \varepsilon_2 \leq \cdots \leq \varepsilon_n$ and $\vartheta_1 \leq \vartheta_2 \leq \cdots \leq \vartheta_n$, or

(2) $\varepsilon_1 \geq \varepsilon_2 \geq \cdots \geq \varepsilon_n$ and $\vartheta_1 \geq \vartheta_2 \geq \cdots \geq \vartheta_n$,

then

$$\left(\frac{1}{n}\sum_{p=1}^{n} \varepsilon_p\right)\left(\frac{1}{n}\sum_{p=1}^{n} \vartheta_p\right) \leq \frac{1}{n}\sum_{p=1}^{n} \varepsilon_p\vartheta_p.$$

Proposition 1. *Let $\mathcal{G}$ be a graph on n vertices and m edges. Then,*

$$ISI_N(\mathcal{G}) \geq \frac{1}{2m} NM_2(\mathcal{G}) NH(\mathcal{G}).$$

The equality is attained when $\mathcal{G}$ is either regular or complete bipartite.

Proof. Take $\varepsilon_p = \frac{1}{\delta_{\mathcal{G}}(r)+\delta_{\mathcal{G}}(s)}$ and $\vartheta_p = \delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)$ in the Lemma 2. Then, we have

$$\frac{1}{m}\sum_{rs\in\mathcal{E}(\mathcal{G})}\frac{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)}{\delta_{\mathcal{G}}(r)+\delta_{\mathcal{G}}(s)} \leq \left(\frac{1}{m}\sum_{rs\in\mathcal{E}(\mathcal{G})}\frac{1}{\delta_{\mathcal{G}}(r)+\delta_{\mathcal{G}}(s)}\right)\left(\frac{1}{m}\sum_{rs\in\mathcal{E}(\mathcal{G})}\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)\right)$$

This gives

$$ISI_N(\mathcal{G}) \geq \frac{1}{2m} NM_2(\mathcal{G}) NH(\mathcal{G}).$$

Equality holds in the above lower bound when $\mathcal{G}$ is regular or a complete bipartite. □

Proposition 2. *For any graph $\mathcal{G}$ with n vertices and m edges,*

$$\frac{m\delta_N^2}{2\Delta_N} \leq ISI_N(\mathcal{G}) \leq \frac{m\Delta_N^2}{2\delta_N}.$$

Proof. For any vertex $s \in \mathcal{V}(\mathcal{G})$, we have $2 \leq \delta_N \leq \delta_{\mathcal{G}}(s) \leq \Delta_N$.
So,

$$\frac{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)}{\delta_{\mathcal{G}}(r)+\delta_{\mathcal{G}}(s)} \geq \frac{\delta_N^2}{2\Delta_N}.$$

Similarly,

$$\frac{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)}{\delta_{\mathcal{G}}(r)+\delta_{\mathcal{G}}(s)} \leq \frac{\Delta_N^2}{2\delta_N}.$$

Thus, we get

$$\frac{m\delta_N^2}{2\Delta_N} \leq ISI_N(\mathcal{G}) \leq \frac{m\Delta_N^2}{2\delta_N}.$$

Equality in both bounds is attained when $\mathcal{G}$ is either regular or a complete bipartite.
□

Now, we provide another improved lower and upper bounds for $ISI_N(\mathcal{G})$ in the following result.

Lemma 3. *For any two vertices $\mathscr{r}$ and $\mathscr{s}$ in a graph $\mathscr{G}$,*

$$\delta_N \leq \frac{2\delta_{\mathscr{G}}(\mathscr{r})\delta_{\mathscr{G}}(\mathscr{s})}{\delta_{\mathscr{G}}(\mathscr{r})+\delta_{\mathscr{G}}(\mathscr{s})} \leq \Delta_N$$

Proof. We know that for any vertex $\mathscr{s}$ in $\mathscr{G}$, $\delta_N \leq \delta_{\mathscr{G}}(\mathscr{s}) \leq \Delta_N$. Also, it is noted that for any two vertices $\mathscr{r}$ and $\mathscr{s}$ in $\mathscr{G}$,

$$\delta_{\mathscr{G}}(\mathscr{r})[\delta_{\mathscr{G}}(\mathscr{s})-\delta_N]+\delta_{\mathscr{G}}(\mathscr{s})[\delta_{\mathscr{G}}(\mathscr{r})-\delta_N] \geq 0,$$

$$\delta_{\mathscr{G}}(\mathscr{r})\delta_{\mathscr{G}}(\mathscr{s})-\delta_N\delta_{\mathscr{G}}(\mathscr{r})+\delta_{\mathscr{G}}(\mathscr{r})\delta_{\mathscr{G}}(\mathscr{s})-\delta_N\delta_{\mathscr{G}}(\mathscr{s}) \geq 0.$$

This implies,

$$\delta_N \leq \frac{2\delta_{\mathscr{G}}(\mathscr{r})\delta_{\mathscr{G}}(\mathscr{s})}{\delta_{\mathscr{G}}(\mathscr{r})+\delta_{\mathscr{G}}(\mathscr{s})}.$$

Similarly,

$$\delta_{\mathscr{G}}(\mathscr{r})(\Delta_N-\delta_{\mathscr{G}}(\mathscr{s}))+\delta_{\mathscr{G}}(\mathscr{s})(\Delta_N-\delta_{\mathscr{G}}(\mathscr{r})) \geq 0,$$

$$\Delta_N\delta_{\mathscr{G}}(\mathscr{r})+\Delta_N\delta_{\mathscr{G}}(\mathscr{s})-2\delta_{\mathscr{G}}(\mathscr{r})\delta_{\mathscr{G}}(\mathscr{s}) \geq 0.$$

So,

$$\Delta_N \geq \frac{2\delta_{\mathscr{G}}(\mathscr{r})\delta_{\mathscr{G}}(\mathscr{s})}{\delta_{\mathscr{G}}(\mathscr{r})+\delta_{\mathscr{G}}(\mathscr{s})}.$$

Therefore, we have

$$\delta_N \leq \frac{2\delta_{\mathscr{G}}(\mathscr{r})\delta_{\mathscr{G}}(\mathscr{s})}{\delta_{\mathscr{G}}(\mathscr{r})+\delta_{\mathscr{G}}(\mathscr{s})} \leq \Delta_N.$$

□

Proposition 3. *For any connected graph $\mathscr{G}$ with $\mathscr{n}$ vertices and $\mathscr{m}$ edges,*

$$\frac{\mathscr{m}}{2}\delta_N \leq ISI_N(\mathscr{G}) \leq \frac{\mathscr{m}}{2}\Delta_N.$$

Proof. By Lemma 3, we get

$$\delta_N \leq \frac{2\delta_{\mathscr{G}}(\mathscr{r})\delta_{\mathscr{G}}(\mathscr{s})}{\delta_{\mathscr{G}}(\mathscr{r})+\delta_{\mathscr{G}}(\mathscr{s})} \leq \Delta_N.$$

Therefore,

$$\sum_{\mathscr{r}\mathscr{s}\in\mathscr{E}(\mathscr{G})}\delta_N \leq 2\sum_{\mathscr{r}\mathscr{s}\in\mathscr{E}(\mathscr{G})}\frac{\delta_{\mathscr{G}}(\mathscr{r})\delta_{\mathscr{G}}(\mathscr{s})}{\delta_{\mathscr{G}}(\mathscr{r})+\delta_{\mathscr{G}}(\mathscr{s})} \leq \sum_{\mathscr{r}\mathscr{s}\in\mathscr{E}(\mathscr{G})}\Delta_N.$$

Hence,

$$\frac{\mathscr{m}\delta_N}{2} \leq ISI_N(\mathscr{G}) \leq \frac{\mathscr{m}\Delta_N}{2}.$$

□

Proposition 4. *For any graph* $\mathcal{G}$, $ISI_N(\mathcal{G}) \leq \frac{\Delta_N^2}{2} NH(\mathcal{G})$.

Proof.

$$ISI_N(\mathcal{G}) = \sum_{rs \in \mathcal{E}(\mathcal{G})} \frac{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)}{\delta_{\mathcal{G}}(r) + \delta_{\mathcal{G}}(s)}$$

$$\leq \sum_{rs \in \mathcal{E}(\mathcal{G})} \frac{\Delta_N^2}{\delta_{\mathcal{G}}(r) + \delta_{\mathcal{G}}(s)}, \quad \text{since} \quad \delta_{\mathcal{G}}(r) \leq \Delta_N, \text{ for all } r \in \mathcal{V}(\mathcal{G}).$$

Now,

$$ISI_N(\mathcal{G}) \leq \frac{\Delta_N^2}{2} \sum_{rs \in \mathcal{E}(\mathcal{G})} \frac{2}{\delta_{\mathcal{G}}(r) + \delta_{\mathcal{G}}(s)}.$$

Hence,

$$ISI_N(\mathcal{G}) \leq \frac{\Delta_N^2}{2} NH(\mathcal{G}).$$

□

Corollary 1. $ISI_N(\mathcal{G}) \leq \frac{m\Delta_N^3}{2\delta_N^2}$.

Proof. By using the previous Lemma 3, we get

$$ISI_N(\mathcal{G}) \leq \frac{\Delta_N^2}{2} \sum_{rs \in \mathcal{E}(\mathcal{G})} \frac{\Delta_N}{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)}$$

$$\leq \frac{\Delta_N^3}{2} \sum_{rs \in \mathcal{E}(\mathcal{G})} \frac{1}{\delta_N^2}, \quad \text{since} \quad \delta_{\mathcal{G}}(r) \geq \delta_N, \text{ for all } r \in \mathcal{V}(\mathcal{G}).$$

Therefore, $ISI_N(\mathcal{G}) \leq \dfrac{m\Delta_N^3}{2\delta_N^2}$.

□

Lemma 4. *[32] If* f *is a convex function in* $\mathbb{R}^+$ *and* $\rho_1, \rho_2, \ldots, \rho_m > 0$, *then*

$$f\left(\frac{\rho_1 + \rho_2 + \cdots + \rho_m}{m}\right) \leq \frac{1}{m}\left(f(\rho_1) + f(\rho_2) + \cdots + f(\rho_m)\right).$$

Theorem 2. *Let* $\mathcal{G}$ *be a graph on* n *vertices and* m *edges. Then,*

$$\frac{m\sqrt{m}\delta_N^2}{\sqrt{NHM(\mathcal{G})}} \leq ISI_N(\mathcal{G}) \leq \frac{\Delta_N^3}{2} NM_2^{-1}(\mathcal{G}).$$

Proof. By Lemma 3, we have

$$\frac{\delta_N}{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)} \leq \frac{2}{\delta_{\mathcal{G}}(r)+\delta_{\mathcal{G}}(s)} \leq \frac{\Delta_N}{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)}.$$

$$\begin{aligned} ISI_N(\mathcal{G}) &= \sum_{rs\in\mathcal{E}(\mathcal{G})} \frac{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)}{\delta_{\mathcal{G}}(r)+\delta_{\mathcal{G}}(s)} \\ &\leq \frac{\Delta_N^2}{2} \sum_{rs\in\mathcal{E}(\mathcal{G})} \frac{2}{\delta_{\mathcal{G}}(r)+\delta_{\mathcal{G}}(s)} \\ &\leq \frac{\Delta_N^2}{2} \sum_{rs\in\mathcal{E}(\mathcal{G})} \frac{\Delta_N}{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)}. \end{aligned}$$

So, $ISI_N(\mathcal{G}) \leq \frac{\Delta_N^3}{2} NM_2^{-1}(\mathcal{G})$, Since $f(x) = \frac{1}{x^2}$ is convex in $\mathbb{R}^+$, we get

$$f\left(\frac{1}{m}\sum_{rs\in\mathcal{E}(\mathcal{G})} \frac{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)}{\delta_{\mathcal{G}}(r)+\delta_{\mathcal{G}}(s)}\right) = \frac{1}{\frac{1}{m^2}\left[\sum_{rs\in\mathcal{E}(\mathcal{G})} \frac{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)}{\delta_{\mathcal{G}}(r)+\delta_{\mathcal{G}}(s)}\right]^2} = \frac{m^2}{(ISI_N(\mathcal{G}))^2}.$$

By Lemma 4, we have

$$\begin{aligned} f\left(\frac{1}{m}\sum_{rs\in\mathcal{E}(\mathcal{G})} \frac{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)}{\delta_{\mathcal{G}}(r)+\delta_{\mathcal{G}}(s)}\right) &\leq \frac{1}{m}\sum_{rs\in\mathcal{E}(\mathcal{G})} \frac{(\delta_{\mathcal{G}}(r)+\delta_{\mathcal{G}}(s))^2}{(\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s))^2} \\ \frac{m^2}{(ISI_N(\mathcal{G}))^2} &\leq \frac{1}{m}\sum_{rs\in\mathcal{E}(\mathcal{G})} \frac{(\delta_{\mathcal{G}}(r)+\delta_{\mathcal{G}}(s))^2}{\delta_N^4}, \end{aligned}$$

since $\delta_{\mathcal{G}}(r) \geq \delta_N$ for all $r \in \mathcal{V}(\mathcal{G})$

$$\frac{m^3}{(ISI_N(\mathcal{G}))^2} \leq \frac{1}{\delta_N^4} NHM(\mathcal{G}).$$

Therefore,

$$ISI_N(\mathcal{G}) \geq \frac{m^{\frac{3}{2}}\delta_N^2}{\sqrt{NHM(\mathcal{G})}}.$$

Thus, we have

$$\frac{m\sqrt{m}\delta_N^2}{\sqrt{NHM(\mathcal{G})}} \leq ISI_N(\mathcal{G}) \leq \frac{\Delta_N^3}{2} NM_2^{-1}(\mathcal{G}).$$

□

Lemma 5. *[15](Arithmetic-Harmonic Mean Inequality) The harmonic mean of a set of positive real numbers is always less than or equal to the arithmetic mean. The HM-AM inequality is given by*

$$\frac{n}{\frac{1}{\rho_1}+\frac{1}{\rho_2}+\cdots+\frac{1}{\rho_n}} \le \frac{\rho_1+\rho_2+\cdots+\rho_n}{n},$$

where equality holds if and only if $\rho_1=\rho_2=\cdots=\rho_n$*.*

Lemma 6. *[25](Cauchy-Schwarz Inequality) Let* $\mathscr{X}=(\rho_1,\rho_2,\ldots,\rho_n)$ *and* $\mathscr{Y}=(\phi_1,\phi_2,\ldots,\phi_n)$ *be two sequences of real numbers. Then,*

$$\left(\sum_{p=1}^{n}\rho_p\phi_p\right)^2 \le \left(\sum_{p=1}^{n}\rho_p^2\right)\left(\sum_{p=1}^{n}\phi_p^2\right),$$

with equality if and only if the sequences $\mathscr{X}$ *and* $\mathscr{Y}$ *are proportional.*

Theorem 3. *For any graph* $\mathcal{G}$*,* $ISI_N(\mathcal{G}) \le \frac{\sqrt{mNHM(\mathcal{G})}}{4}$*.*

Proof. We know that,

$$NHM(\mathcal{G}) = \sum_{rs\in\mathscr{E}(\mathcal{G})}[\delta_{\mathcal{G}}(r)+\delta_{\mathcal{G}}(s)]^2,$$

$$\frac{NHM(\mathcal{G})}{4} = \sum_{rs\in\mathscr{E}(\mathcal{G})}\left[\frac{\delta_{\mathcal{G}}(r)+\delta_{\mathcal{G}}(s)}{2}\right]^2.$$

By Lemma 5, we have

$$\frac{NHM(\mathcal{G})}{4} \ge \sum_{rs\in\mathscr{E}(\mathcal{G})}\left[\frac{2}{\frac{1}{\delta_{\mathcal{G}}(r)}+\frac{1}{\delta_{\mathcal{G}}(s)}}\right]^2.$$

Using Lemma 6, we get

$$\frac{NHM(\mathcal{G})}{4} \ge \frac{1}{m}\left[\sum_{rs\in\mathscr{E}(\mathcal{G})}\frac{2\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)}{\delta_{\mathcal{G}}(r)+\delta_{\mathcal{G}}(s)}\right]^2.$$

That is,

$$\frac{NHM(\mathcal{G})}{4} \ge \frac{4}{m}[ISI_N(\mathcal{G})]^2.$$

Therefore,

$$ISI_N(\mathcal{G}) \le \frac{\sqrt{mNHM(\mathcal{G})}}{4}.$$

□

4. ISI_N index of Graph Operations

Let $\mathcal{G}_1$ be a simple connected graph of order n_1 and size m_1, and $\mathcal{G}_2$ be a simple connected graph of order n_2 and size m_2. The following results provide insight into the ISI_N index of graph operations such as join, sequential join, cartesian product, lexicographic and corona product for connected graphs.

Lemma 7. *For the graph $\mathcal{G} = \mathcal{G}_1 + \{y\}$, we have*

(i) $\delta_{\mathcal{G}}(r) = \delta_{\mathcal{G}_1}(r) + d_{\mathcal{G}_1}(r) + n_1$

(ii) $\delta_{\mathcal{G}}(y) = 2m_1 + n_1$.

Theorem 4. *For the graph $\mathcal{G} = \mathcal{G}_1 + \{y\}$,*

$$ISI_N(\mathcal{G}) \leq \frac{1}{4}[2M_1(\mathcal{G}_1) + M_1'(\mathcal{G}_1)] + m_1 n_1 + \frac{m_1}{2} + \frac{{n_1}^2}{2}.$$

Proof. Let $\mathcal{E}'$ be the set of all edges from every vertex r of $\mathcal{G}_1$ to the new vertex y in $\mathcal{G}$.
By definition of ISI_N index, we have

$$\begin{aligned}
ISI_N(\mathcal{G}) &= \sum_{rs \in \mathcal{E}(\mathcal{G})} \frac{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)}{\delta_{\mathcal{G}}(r) + \delta_{\mathcal{G}}(s)} \\
&= \sum_{rs \in \mathcal{E}(\mathcal{G}_1)} \frac{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)}{\delta_{\mathcal{G}}(r) + \delta_{\mathcal{G}}(s)} + \sum_{ry \in \mathcal{E}'} \frac{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(y)}{\delta_{\mathcal{G}}(r) + \delta_{\mathcal{G}}(y)} \\
&= S_1 + S_2.
\end{aligned}$$

Now,by applying Lemma 5 and Lemma 7,

$$\begin{aligned}
S_1 &= \sum_{rs \in \mathcal{E}(\mathcal{G}_1)} \frac{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(s)}{\delta_{\mathcal{G}}(r) + \delta_{\mathcal{G}}(s)} \\
&\leq \frac{1}{4} \sum_{rs \in \mathcal{E}(\mathcal{G}_1)} \left(\delta_{\mathcal{G}_1}(r) + \delta_{\mathcal{G}_1}(s) + d_{\mathcal{G}_1}(r) + d_{\mathcal{G}_1}(s) + 2n_1\right) \\
&\leq \frac{1}{4} \sum_{rs \in \mathcal{E}(\mathcal{G}_1)} (\delta_{\mathcal{G}_1}(r) + \delta_{\mathcal{G}_1}(s)) + \frac{1}{4} \sum_{rs \in \mathcal{E}(\mathcal{G}_1)} (d_{\mathcal{G}_1}(r) + d_{\mathcal{G}_1}(s)) + \frac{m_1 n_1}{2} \\
&\leq \frac{1}{4} [M_1(\mathcal{G}_1) + M_1'(\mathcal{G}_1)] + \frac{m_1 n_1}{2}, \\
S_2 &= \sum_{ry \in \mathcal{E}'} \frac{\delta_{\mathcal{G}}(r)\delta_{\mathcal{G}}(y)}{\delta_{\mathcal{G}}(r) + \delta_{\mathcal{G}}(y)}
\end{aligned}$$

$$\leq \frac{1}{4}\sum_{r\in\mathscr{V}(\mathcal{G}_1)}\big(\delta_{\mathcal{G}_1}(r)+d_{\mathcal{G}_1}(r)+n_1\big)+\frac{1}{4}\sum_{ry\in\mathscr{E}'}(2m_1+n_1)$$
$$\leq \frac{M_1(\mathcal{G}_1)}{4}+\frac{m_1}{2}+\frac{m_1n_1}{2}+\frac{{n_1}^2}{2}.$$

Hence,

$$ISI_N(\mathcal{G})\leq \frac{1}{4}[2M_1(\mathcal{G}_1)+M_1'(\mathcal{G}_1)]+m_1n_1+\frac{m_1}{2}+\frac{{n_1}^2}{2}.$$

□

Lemma 8. *Let $\mathcal{G}_1$ and $\mathcal{G}_2$ be any two graphs. Then for $\mathcal{G}=\mathcal{G}_1+\mathcal{G}_2$, we have*

(i) $\delta_{\mathcal{G}}(r)=\delta_{\mathcal{G}_1}(r)+d_{\mathcal{G}_1}(r)n_2+2m_2+n_1n_2$ *, where* $r\in\mathscr{V}(\mathcal{G}_1)$

(ii) $\delta_{\mathcal{G}}(s)=\delta_{\mathcal{G}_2}(s)+d_{\mathcal{G}_2}(s)n_1+2m_1+n_1n_2$ *,where* $s\in\mathscr{V}(\mathcal{G}_2)$*.*

Theorem 5. *If $\mathcal{G}=\mathcal{G}_1+\mathcal{G}_2$, then*

$$ISI_N(\mathcal{G})\leq \frac{1}{4}\big[M_1'(\mathcal{G}_1)+M_1'(\mathcal{G}_2)\big]+\frac{1}{4}\big[(n_2+1)M_1(\mathcal{G}_1)+(n_1+1)M_1(\mathcal{G}_2)\big]$$
$$+2m_1m_2+\left[\frac{m_1n_2+m_2n_1}{2}\right]+n_1n_2\left[m_1+m_2+\frac{n_1n_2}{2}\right].$$

Proof. By definition of ISI_N index, we have

$$ISI_N(\mathcal{G})=\sum_{rs\in\mathscr{E}(\mathcal{G}_1)}\frac{\delta_{\mathcal{G}_1}(r)\delta_{\mathcal{G}_1}(s)}{\delta_{\mathcal{G}_1}(r)+\delta_{\mathcal{G}_1}(s)}+\sum_{rs\in E(\mathcal{G}_2)}\frac{\delta_{\mathcal{G}_2}(r)\delta_{\mathcal{G}_2}(s)}{\delta_{\mathcal{G}_2}(r)+\delta_{\mathcal{G}_2}(s)}$$
$$+\sum_{rs\in\mathscr{E}'}\frac{\delta_{\mathcal{G}_1}(r)\delta_{\mathcal{G}_2}(s)}{\delta_{\mathcal{G}_1}(r)+\delta_{\mathcal{G}_2}(s)}$$
$$=S_1+S_2+S_3.$$

Now, by Lemma 5 and Lemma 8, we get

$$S_1=\sum_{rs\in\mathscr{E}(\mathcal{G}_1)}\left[\frac{\big(\delta_{\mathcal{G}_1}(r)+d_{\mathcal{G}_1}(r)n_2+2m_2+n_1n_2\big)\big(\delta_{\mathcal{G}_1}(s)+d_{\mathcal{G}_1}(s)n_2+2m_2+n_1n_2\big)}{\big(\delta_{\mathcal{G}_1}(r)+\delta_{\mathcal{G}_1}(s)\big)+n_2\big(d_{\mathcal{G}_1}(r)+d_{\mathcal{G}_1}(s)\big)+4m_2+2n_1n_2}\right]$$
$$\leq \frac{1}{2}\sum_{rs\in\mathscr{E}(\mathcal{G}_1)}\left[\frac{\delta_{\mathcal{G}_1}(r)+\delta_{\mathcal{G}_1}(s)}{2}+\frac{n_2}{2}\big(d_{\mathcal{G}_1}(r)+d_{\mathcal{G}_1}(s)\big)+2m_2+n_1n_2\right]$$
$$\leq \frac{1}{4}M_1'(\mathcal{G}_1)+\frac{n_2}{4}M_1(\mathcal{G}_1)+m_1m_2+\frac{n_1n_2m_1}{2},$$
$$S_2=\sum_{rs\in\mathscr{E}(\mathcal{G}_2)}\left[\frac{\big(\delta_{\mathcal{G}_2}(r)+d_{\mathcal{G}_2}(r)n_1+2m_1+n_1n_2\big)\big(\delta_{\mathcal{G}_2}(s)+d_{\mathcal{G}_2}(s)n_1+2m_1+n_1n_2\big)}{\big(\delta_{\mathcal{G}_2}(r)+\delta_{\mathcal{G}_2}(s)\big)+n_1\big(d_{\mathcal{G}_2}(r)+d_{\mathcal{G}_2}(s)\big)+4m_1+2n_1n_2}\right]$$

$$\leq \frac{1}{2}\sum_{rs\in\mathscr{E}(\mathcal{G}_2)}\left[\frac{\delta_{\mathcal{G}_2}(r)+\delta_{\mathcal{G}_2}(s)}{2}+\frac{n_1}{2}\left(d_{\mathcal{G}_2}(r)+d_{\mathcal{G}_2}(s)\right)+2m_1+n_1n_2\right]$$
$$\leq \frac{1}{4}M_1'(\mathcal{G}_2)+\frac{n_1}{4}M_1(\mathcal{G}_2)+m_1m_2+\frac{n_1n_2m_2}{2},$$

and

$$S_3=\sum_{rs\in\mathscr{E}'}\left[\frac{\left(\delta_{\mathcal{G}_1}(r)+d_{\mathcal{G}_1}(r)n_2+2m_2+n_1n_2\right)\left(\delta_{\mathcal{G}_2}(s)+d_{\mathcal{G}_2}(s)n_1+2m_1+n_1n_2\right)}{\delta_{\mathcal{G}_1}(r)+\delta_{\mathcal{G}_2}(s)+d_{\mathcal{G}_1}(r)n_2+d_{\mathcal{G}_2}(s)n_1+2(m_1+m_2)+2n_1n_2}\right]$$
$$\leq \frac{1}{4}\sum_{r\in\mathscr{V}(\mathcal{G}_1)}\delta_{\mathcal{G}_1}(r)+\frac{1}{4}\sum_{s\in\mathscr{V}(\mathcal{G}_2)}\delta_{\mathcal{G}_2}(s)+\frac{n_2}{4}\sum_{r\in\mathscr{V}(\mathcal{G}_1)}d_{\mathcal{G}_1}(r)+\frac{n_1}{4}\sum_{s\in\mathscr{V}(\mathcal{G}_2)}d_{\mathcal{G}_2}(s)$$
$$+\frac{m_1+m_2}{2}\sum_{rs\in\mathscr{E}'}1+\frac{n_1n_2}{2}\sum_{rs\in\mathscr{E}'}1$$
$$\leq \frac{1}{4}\big[M_1(\mathcal{G}_1)+M_1(\mathcal{G}_2)\big]+\frac{1}{2}\big[m_1n_2+m_2n_1+(m_1+m_2+n_1n_2)n_1n_2\big],$$

Thus, we obtain,

$$ISI_N(\mathcal{G})\leq \frac{1}{4}\left[M_1'(\mathcal{G}_1)+M_1'(\mathcal{G}_2)\right]+\frac{1}{4}\left[(n_2+1)M_1(\mathcal{G}_1)+(n_1+1)M_1(\mathcal{G}_2)\right]$$
$$+2m_1m_2+\left[\frac{m_1n_2+m_2n_1}{2}\right]+n_1n_2\left[m_1+m_2+\frac{n_1n_2}{2}\right].$$

□

Theorem 6. *Let $\mathcal{G}_1,\mathcal{G}_2,\mathcal{G}_3,\ldots,\mathcal{G}_k$ be k-disjoint graphs. Then for the sequential join of these graphs, $\mathcal{G}=\mathcal{G}_1+\mathcal{G}_2+\mathcal{G}_3+\cdots+\mathcal{G}_k$, we have*

$$ISI_N(\mathcal{G})=\frac{1}{4}\sum_{q=1}^{k}M_1'(\mathcal{G}_q)+\frac{1}{4}\sum_{q=1}^{k-2}n_{q+1}M_1(\mathcal{G}_q)+\frac{n_k}{4}M_1(\mathcal{G}_{k-1})+\frac{1}{4}\sum_{q=1}^{k-1}n_{q-1}M_1(\mathcal{G}_q)$$
$$+\frac{n_{k-1}}{2}M_1(\mathcal{G}_k)+\frac{1}{4}\sum_{q=1}^{k-2}\left[n_{q+1}M_1(\mathcal{G}_q)+n_qM_1(\mathcal{G}_{q+1})\right]$$
$$+\frac{1}{2}\sum_{q=1}^{k-2}n_qn_{q+1}\left(m_q+m_{q+1}+m_{q+2}\right)+\frac{1}{2}\sum_{q=2}^{k-1}n_qn_{q+1}m_{q-1}$$
$$+\frac{3}{2}\left[m_1m_2+m_{k-1}m_k\right]+\sum_{q=2}^{k-2}m_qm_{q+1}+\frac{1}{2}\sum_{q=2}^{k-1}m_qn_q\left(n_{q-1}+n_{q+1}\right)$$
$$+\frac{1}{2}\sum_{q=2}^{k-1}m_qn_{q+1}\left(n_{q-1}+n_{q+1}\right)+\frac{1}{2}\sum_{q=1}^{k-1}\left(n_qn_{q+1}\right)^2+\frac{1}{4}\sum_{q=2}^{k-1}n_q^2n_{q-1}n_{q+1}$$
$$+\frac{1}{4}\sum_{q=1}^{k-2}n_qn_{q+1}^2n_{q+2}+n_kn_{k-1}\left(m_k+\frac{m_{k-1}}{2}\right)+\frac{1}{2}\sum_{q=1}^{k-1}n_q^2m_{q+1}$$

$$+\frac{1}{2}\sum_{q=1}^{k-2} m_{q+1} n_q n_{q+2} + \frac{n_2 m_1}{2}(n_1+n_2).$$

Proof. We write $ISI_N(\mathcal{G}) = \sum_{p=1}^{6} S_p$, by using Lemma 8.

Now, we have

$$S_1 = \sum_{rs\in\mathcal{E}(\mathcal{G}_1)} \frac{[\delta_{\mathcal{G}_1}(r) + d_{\mathcal{G}_1}(r)n_2 + 2m_2 + n_1n_2][\delta_{\mathcal{G}_1}(s) + d_{\mathcal{G}_1}(s)n_2 + 2m_2 + n_1n_2]}{\delta_{\mathcal{G}_1}(r) + \delta_{\mathcal{G}_1}(s) + (d_{\mathcal{G}_1}(r) + d_{\mathcal{G}_1}(s))n_2 + 4m_2 + 2n_1n_2}$$

$$\leq \frac{1}{2}\sum_{rs\in\mathcal{E}(\mathcal{G}_1)} \left[\frac{\delta_{\mathcal{G}_1}(r) + \delta_{\mathcal{G}_1}(s)}{2} + \frac{n_2(d_{\mathcal{G}_1}(r) + d_{\mathcal{G}_1}(s))}{2} + 2m_2 + n_1n_2\right]$$

$$\leq \frac{M_1'(\mathcal{G}_1)}{4} + \frac{n_2}{4}M_1(\mathcal{G}_1) + m_1m_2 + \frac{n_1n_2m_1}{2},$$

$$S_2 = \sum_{rs\in\mathcal{E}(\mathcal{G}_k)} \frac{\begin{array}{c}[\delta_{\mathcal{G}_k}(r) + d_{\mathcal{G}_k}(r)n_{k-1} + 2m_{k-1} + n_k n_{k-1}]\\ [\delta_{\mathcal{G}_k}(s) + d_{\mathcal{G}_k}(s)n_{k-1} + 2m_{k-1} + n_k n_{k-1}]\end{array}}{\delta_{\mathcal{G}_k}(r) + \delta_{\mathcal{G}_k}(s) + (d_{\mathcal{G}_k}(r) + d_{\mathcal{G}_k}(s))n_{k-1} + 4m_{k-1} + 2n_k n_{k-1}}$$

$$\leq \frac{1}{2}\sum_{rs\in\mathcal{E}(\mathcal{G}_k)} \left[\frac{\delta_{\mathcal{G}_k}(r) + \delta_{\mathcal{G}_k}(s)}{2} + \frac{n_{k-1}(d_{\mathcal{G}_k}(r) + d_{\mathcal{G}_k}(s))}{2} + 2m_{k-1} + n_k n_{k-1}\right]$$

$$\leq \frac{M_1'(\mathcal{G}_k)}{4} + \frac{n_{k-1}}{4}M_1(\mathcal{G}_k) + m_k m_{k-1} + \frac{n_k n_{k-1} m_k}{2},$$

$$S_3 = \sum_{q=2}^{k-1}\sum_{rs\in\mathcal{E}(\mathcal{G}_q)} \frac{\begin{array}{c}[\delta_{\mathcal{G}_q}(r) + d_{\mathcal{G}_q}(r)(n_{q-1}+n_{q+1}) + 2(m_{q-1}+m_{q+1}) + n_q(n_{q-1}+n_{q+1})]\\ [\delta_{\mathcal{G}_q}(s) + d_{\mathcal{G}_q}(s)(n_{q-1}+n_{q+1}) + 2(m_{q-1}+m_{q+1}) + n_q(n_{q-1}+n_{q+1})]\end{array}}{\begin{array}{r}\delta_{\mathcal{G}_q}(r) + \delta_{\mathcal{G}_q}(s) + n_{q-1}n_{q+1}[d_{\mathcal{G}_q}(r) + d_{\mathcal{G}_q}(s)] + 4(m_{q-1}+m_{q+1})\\ +2n_q(n_{q-1}+n_{q+1})\end{array}}$$

$$\leq \frac{1}{2}\sum_{q=2}^{k-1}\sum_{rs\in\mathcal{E}(\mathcal{G}_q)} \left[\frac{\delta_{\mathcal{G}_q}(r) + \delta_{\mathcal{G}_q}(s)}{2} + \frac{n_{q-1}n_{q+1}}{2}[d_{\mathcal{G}_q}(r) + d_{\mathcal{G}_q}(s)] + 2(m_{q-1}+m_{q+1})\right.$$

$$\left. + n_q(n_{q-1}+n_{q+1})\right]$$

$$\leq \frac{1}{4}\sum_{q=2}^{k-1} M_1'(\mathcal{G}_q) + \frac{1}{4}\sum_{q=2}^{k-1} M_1(\mathcal{G}_q)(n_{q-1}+n_{q+1}) + \sum_{q=2}^{k-1} m_q(m_{q-1}+m_{q+1})$$

$$+ \frac{1}{2}\sum_{q=2}^{k-1} m_q n_q(n_{q-1}+n_{q+1}),$$

$$S_4 = \sum_{\substack{rs\in\mathcal{E}'\\ r\in\mathcal{V}(\mathcal{G}_1)\\ s\in\mathcal{V}(\mathcal{G}_2)}} \frac{\begin{array}{c}[\delta_{\mathcal{G}_1}(r) + d_{\mathcal{G}_1}(r)n_2 + 2m_2 + n_1n_2]\\ [\delta_{\mathcal{G}_2}(s) + d_{\mathcal{G}_2}(s)(n_1+n_3) + 2(m_1+m_3) + n_2(n_1+n_3)]\end{array}}{\begin{array}{r}\delta_{\mathcal{G}_1}(r) + \delta_{\mathcal{G}_2}(s) + d_{\mathcal{G}_1}(r)n_2 + d_{\mathcal{G}_2}(s)(n_1+n_3) + 2(m_1+m_2+m_3)\\ +2n_1n_2 + n_2n_3\end{array}}$$

$$\leq \frac{1}{2}\sum_{rs\in\mathcal{E}'} \left[\frac{\delta_{\mathcal{G}_1}(r)}{2} + \frac{\delta_{\mathcal{G}_2}(s)}{2} + \frac{d_{\mathcal{G}_1}(r)n_2}{2} + \frac{d_{\mathcal{G}_2}(s)(n_1+n_3)}{2} + (m_1+m_2+m_3)\right.$$

$$+n_1n_2+\frac{n_2n_3}{2}\Bigg]$$

$$\leq \frac{1}{4}[n_2M_1(G_1)+n_1M_1(G_2)]+\frac{m_1n_2^2}{2}+\frac{n_1m_2(n_1+n_3)}{2}+\frac{n_1n_2(m_1+m_2+m_3)}{2}$$

$$+\frac{n_1n_2^2(2n_1+n_3)}{4},$$

$$S_5=\sum_{q=2}^{k-2}\sum_{\substack{rs\in E'\\ r\in V(G_q)\\ s\in V(G_{q+1})}}\frac{\begin{array}{r}[\delta_{G_q}(r)+d_{G_q}(r)(n_{q-1}+n_{q+1})+2(m_{q-1}+m_{q+1})+n_q(n_{q-1}+n_{q+1})]\\ [\delta_{G_{q+1}}(s)+d_{G_{q+1}}(s)(n_q+n_{q+2})+2(m_q+m_{q+2})+n_{q+1}(n_q+n_{q+2})]\end{array}}{\begin{array}{c}\delta_{G_q}(r)+\delta_{G_{q+1}}(s)+d_{G_q}(r)(n_{q-1}+n_{q+1})+d_{G_{q+1}}(s)(n_q+n_{q+2})\\ +2n_qn_{q+1}+2(m_{q-1}+m_q+m_{q+1}+m_{q+2})+n_qn_{q-1}+n_{q+1}n_{q+2}\end{array}}$$

$$\leq \frac{1}{2}\sum_{q=2}^{k-2}\sum_{rs\in E'}\Bigg[\frac{\delta_{G_q}(r)}{2}+\frac{\delta_{G_{q+1}}(s)}{2}+\left(\frac{n_{q-1}+n_{q+1}}{2}\right)d_{G_q}(r)+\left(\frac{n_q+n_{q+2}}{2}\right)d_{G_{q+1}}(s)$$

$$+(m_{q-1}+m_q+m_{q+1}+m_{q+2})+n_qn_{q+1}+\frac{n_qn_{q-1}}{2}+\frac{n_{q+1}n_{q+2}}{2}\Bigg]$$

$$\leq \frac{1}{4}\sum_{q=2}^{k-2}[n_{q+1}M_1(G_q)+n_qM_1(G_{q+1})]+\frac{1}{2}\sum_{q=2}^{k-2}[n_{q+1}m_q(n_{q-1}+n_{q+1})]$$

$$+n_qm_{q+1}(n_q+n_{q+2})+\frac{1}{2}\sum_{q=2}^{k-2}n_qn_{q+1}(m_{q-1}+m_q+m_{q+1}+m_{q+2}+n_qn_{q+1}$$

$$+\frac{n_qn_{q-1}}{2}+\frac{n_{q+1}n_{q+2}}{2}),$$

and

$$S_6=\sum_{\substack{rs\in E'\\ r\in V(G_{k-1})\\ s\in V(G_k)}}\frac{\begin{array}{r}[\delta_{G_{k-1}}(r)+d_{G_{k-1}}(r)(n_{k-2}+n_k)+2\,(m_{k-2}+m_k)+n_{k-1}(n_{k-2}+n_k)]\\ [\delta_{G_k}(s)+d_{G_k}(s)n_{k-1}+2m_{k-1}+n_{k-1}n_k]\end{array}}{\begin{array}{c}\delta_{G_{k-1}}(r)+\delta_{G_k}(s)+d_{G_{k-1}}(r)(n_{k-2}+n_k)+d_{G_k}(s)n_{k-1}\\ +2(m_{k-2}+m_{k-1}+m_k)+2n_{k-1}n_k+n_{k-1}n_{k-2}\end{array}}$$

$$\leq \frac{1}{2}\sum_{rs\in E'}\Bigg[\frac{\delta_{G_{k-1}}(r)}{2}+\frac{\delta_{G_k}(s)}{2}+\left(\frac{n_{k-2}+n_k}{2}\right)d_{G_{k-1}}(r)+\frac{n_{k-1}}{2}d_{G_k}(s)$$

$$+(m_{k-2}+m_k+m_{k-1})+n_{k-1}n_k+\frac{n_{k-1}n_{k-2}}{2}\Bigg]$$

$$\leq \frac{1}{4}\big[n_kM_1(G_{k-1})+n_{k-1}M_1(G_k)\big]+\frac{n_km_{k-1}(n_{k-2}+n_k)}{2}+\frac{m_kn_{k-1}^2}{2}+\frac{n_kn_{k-1}}{2}$$

$$(m_{k-2}+m_{k-1}+m_k)+\frac{(n_{k-1}n_k)^2}{2}+\frac{n_kn_{k-1}^2n_{k-2}}{4},$$

Therefore, we acquire

$$
\begin{aligned}
ISI_N(\mathcal{G}) \leq{}& \frac{1}{4}\sum_{q=1}^{k} M_1'(\mathcal{G}_q) + \frac{1}{4}\sum_{q=1}^{k-2} n_{q+1}M_1(\mathcal{G}_q) + \frac{n_k}{4}M_1(\mathcal{G}_{k-1}) + \frac{1}{4}\sum_{q=1}^{k-1} n_{q-1}M_1(\mathcal{G}_q)\\
&+ \frac{n_{k-1}}{2}M_1(\mathcal{G}_k) + \frac{1}{4}\sum_{q=1}^{k-2}\left[n_{q+1}M_1(\mathcal{G}_q) + n_qM_1(\mathcal{G}_{q+1})\right]\\
&+ \frac{1}{2}\sum_{q=1}^{k-2} n_qn_{q+1}\left(m_q + m_{q+1} + m_{q+2}\right) + \frac{1}{2}\sum_{q=2}^{k-1} n_qn_{q+1}m_{q-1}\\
&+ \frac{3}{2}\left[m_1m_2 + m_{k-1}m_k\right] + \sum_{q=2}^{k-2} m_qm_{q+1} + \frac{1}{2}\sum_{q=2}^{k-1} m_qn_q\left(n_{q-1} + n_{q+1}\right)\\
&+ \frac{1}{2}\sum_{q=2}^{k-1} m_qn_{q+1}\left(n_{q-1} + n_{q+1}\right) + \frac{1}{2}\sum_{q=1}^{k-1}\left(n_qn_{q+1}\right)^2 + \frac{1}{4}\sum_{q=2}^{k-1} n_q^2n_{q-1}n_{q+1}\\
&+ \frac{1}{4}\sum_{q=1}^{k-2} n_qn_{q+1}^2n_{q+2} + n_kn_{k-1}\left(m_k + \frac{m_{k-1}}{2}\right) + \frac{1}{2}\sum_{q=1}^{k-1} n_q^2m_{q+1}\\
&+ \frac{1}{2}\sum_{q=1}^{k-2} m_{q+1}n_qn_{q+2} + \frac{n_2m_1}{2}(n_1 + n_2).
\end{aligned}
$$

□

Lemma 9. *For the graph $\mathcal{G} = \mathcal{G}_1 \square \mathcal{G}_2$, we have*

$$\delta_{\mathcal{G}}(r, s) = \delta_{\mathcal{G}_1}(r) + \delta_{\mathcal{G}_2}(r) + 2d_{\mathcal{G}_1}(r)d_{\mathcal{G}_2}(s).$$

Theorem 7. *If $\mathcal{G} = \mathcal{G}_1 \square \mathcal{G}_2$, then*

$$
\begin{aligned}
ISI_N(\mathcal{G}) \leq{}& \frac{1}{4}\left[n_2M_1'(\mathcal{G}_1) + n_1M_1'(\mathcal{G}_2)\right] + \frac{n_1\Delta_N(\mathcal{G}_1)}{2}\left[m_2 + M_1(\mathcal{G}_2)\right]\\
&+ \frac{n_2\Delta_N(\mathcal{G}_2)}{2}\left[m_1 + M_1(\mathcal{G}_1)\right].
\end{aligned}
$$

Proof. Assume that $r_p, r_k \in \mathcal{V}(\mathcal{G}_1)$ and $s_q, s_k \in \mathcal{V}(\mathcal{G}_2)$.
By using Lemma 9, we can write the definition of ISI_N as

$$
ISI_N(\mathcal{G}) = \sum_{\substack{(r_p,s_q),(r_p,s_\ell)\in\mathcal{E}(\mathcal{G})\\ q\neq\ell}} \frac{\begin{array}{l}\left(\delta_{\mathcal{G}_1}(r_p) + \delta_{\mathcal{G}_2}(s_q) + 2d_{\mathcal{G}_1}(r_p)d_{\mathcal{G}_2}(s_q)\right)\\ \qquad\left(\delta_{\mathcal{G}_1}(r_p) + \delta_{\mathcal{G}_2}(s_l) + 2d_{\mathcal{G}_1}(r_p)d_{\mathcal{G}_2}(s_l)\right)\end{array}}{\begin{array}{l}2\delta_{\mathcal{G}_1}(r_p) + \left(\delta_{\mathcal{G}_2}(s_q) + \delta_{\mathcal{G}_2}(s_l)\right)\\ \qquad + 2d_{\mathcal{G}_1}(r_p)\left(d_{\mathcal{G}_2}(s_q) + d_{\mathcal{G}_2}(s_l)\right)\end{array}}
$$

$$
+ \sum_{\substack{(r_p,s_q),(r_k,s_q)\in\mathscr{E}(\mathcal{G})\\ p\neq k}} \frac{\big(\delta_{\mathcal{G}_1}(r_p)+\delta_{\mathcal{G}_2}(s_q)+2d_{\mathcal{G}_1}(r_p)d_{\mathcal{G}_2}(s_q)\big)\big(\delta_{\mathcal{G}_1}(r_k)+\delta_{\mathcal{G}_2}(s_q)+2d_{\mathcal{G}_1}(r_k)d_{\mathcal{G}_2}(s_q)\big)}{2\delta_{\mathcal{G}_2}(s_q)+\big(\delta_{\mathcal{G}_1}(r_p)+\delta_{\mathcal{G}_1}(r_k)\big)+2d_{\mathcal{G}_2}(s_q)\big(d_{\mathcal{G}_1}(r_p)+d_{\mathcal{G}_1}(r_k)\big)}
$$

$$
= S_1 + S_2
$$

Let $\Delta_N(\mathcal{G}_1)$and $\Delta_N(\mathcal{G}_2)$ be the maximum neighborhood degree of $\mathcal{G}_1$ and $\mathcal{G}_2$ respectively. Then, using Lemma 5 we get,

$$
\begin{aligned}
S_1 &\leq \frac{1}{2}\sum_{\substack{r_p\in\mathscr{V}(\mathcal{G}_1)\\ (s_q,s_l)\in\mathscr{E}(\mathcal{G}_2)}} \left[\delta_{\mathcal{G}_1}(r_p)+\frac{\delta_{\mathcal{G}_2}(s_q)+\delta_{\mathcal{G}_2}(s_l)}{2}+d_{\mathcal{G}_1}(r_p)\big(d_{\mathcal{G}_2}(s_q)+d_{\mathcal{G}_2}(s_l)\big)\right]\\
&\leq \frac{n_1m_2}{2}\Delta_N(\mathcal{G}_1)+\frac{n_1}{4}M_1'(\mathcal{G}_2)+\frac{n_1}{2}\Delta_N(\mathcal{G}_1)M_1(\mathcal{G}_2),
\end{aligned}
$$

and

$$
\begin{aligned}
S_2 &\leq \frac{1}{2}\sum_{\substack{s_q\in\mathscr{V}(\mathcal{G}_2)\\ (r_p,r_k)\in\mathscr{E}(\mathcal{G}_1)}} \left[\delta_{\mathcal{G}_2}(s_q)+\frac{\delta_{\mathcal{G}_1}(r_p)+\delta_{\mathcal{G}_1}(r_k)}{2}+d_{\mathcal{G}_2}(s_q)\big(d_{\mathcal{G}_1}(r_p)+d_{\mathcal{G}_1}(r_k)\big)\right]\\
&\leq \frac{n_2m_1}{2}\Delta_N(\mathcal{G}_2)+\frac{n_2}{4}M_1'(\mathcal{G}_1)+\frac{n_2}{2}\Delta_N(\mathcal{G}_2)M_1(\mathcal{G}_1)
\end{aligned}
$$

Thus, we obtain

$$
\begin{aligned}
ISI_N(\mathcal{G}) \leq{}& \frac{1}{4}\big[n_2M_1'(\mathcal{G}_1)+n_1M_1'(\mathcal{G}_2)\big]+\frac{n_1\Delta_N(\mathcal{G}_1)}{2}\big[m_2+M_1(\mathcal{G}_2)\big]\\
&+\frac{n_2\Delta_N(\mathcal{G}_2)}{2}\big[m_1+M_1(\mathcal{G}_1)\big].
\end{aligned}
$$

□

Lemma 10. *For the graph $G=\mathcal{G}_1[\mathcal{G}_2]$, we have*

$$
\delta_{\mathcal{G}}(r,s)=n_2^2\delta_{\mathcal{G}_1}(r)+\delta_{\mathcal{G}_2}(s)+2m_2d_{\mathcal{G}_1}(r)+n_2d_{\mathcal{G}_1}(r)d_{\mathcal{G}_2}(s).
$$

Theorem 8. *If $G=\mathcal{G}_1[\mathcal{G}_2]$, then*

$$
\begin{aligned}
ISI_N(\mathcal{G}) \leq{}& \frac{1}{4}\left[n_2^4M_1'(\mathcal{G}_1)+n_1M_1'(\mathcal{G}_2)\right]+\frac{n_2}{4}\left[2n_2m_2M_1(\mathcal{G}_1)+n_1\Delta_N(\mathcal{G}_1)M_1(\mathcal{G}_2)\right]\\
&+\frac{n_2^2m_1\Delta_N(\mathcal{G}_2)}{2}\left[1+n_2\Delta_N(\mathcal{G}_1)\right]+\frac{n_1m_2\Delta_N(\mathcal{G}_1)}{2}\left[n_2^2+2m_2\right].
\end{aligned}
$$

Proof. By Lemma 10, we have We know that $\delta_N(\mathcal{G}) \leq \Delta_N(\mathcal{G})$ and for any $r \in \mathcal{V}(\mathcal{G}), d_{\mathcal{G}}(r) \leq \Delta_N(\mathcal{G})$. So, we obtain

$$\begin{aligned} S_1 \leq \frac{1}{2} \sum_{r_p \in \mathcal{V}(\mathcal{G}_1)} \sum_{(s_q,s_l)\in\mathcal{E}(\mathcal{G}_2)} \Bigg[& n_2^2 \delta_{\mathcal{G}_1}(r_p) + \frac{\delta_{\mathcal{G}_2}(s_q)+\delta_{\mathcal{G}_2}(s_l)}{2} + 2m_2 d_{\mathcal{G}_1}(r_p) \\ & + \frac{n_2}{2} d_{\mathcal{G}_1}(r_p)\left(d_{\mathcal{G}_2}(s_q)+d_{\mathcal{G}_2}(s_l)\right)\Bigg] \\ \leq \frac{n_1 n_2^2 m_2}{2}\Delta_N(\mathcal{G}_1) + \frac{n_1}{4} M_1'(\mathcal{G}_2) + m_2^2 n_1 \Delta_N(\mathcal{G}_1) + \frac{n_1 n_2}{4}\Delta_N(\mathcal{G}_1) M_1(\mathcal{G}_2) \end{aligned}$$

and

$$\begin{aligned} S_2 \leq \frac{1}{2} \sum_{s_q,s_l \in \mathcal{V}(\mathcal{G}_2)} \sum_{(r_p,r_k)\in\mathcal{E}(\mathcal{G}_1)} \Bigg[& \frac{n_2^2}{2}(\delta_{\mathcal{G}_1}(r_p)+\delta_{\mathcal{G}_1}(r_k)) + \frac{\delta_{\mathcal{G}_2}(s_q)+\delta_{\mathcal{G}_2}(s_l)}{2} \\ & + m_2\left(d_{\mathcal{G}_1}(r_p)+d_{\mathcal{G}_1}(r_k)\right) + \frac{n_2}{2}\left(d_{\mathcal{G}_1}(r_p)d_{\mathcal{G}_2}(s_q)+d_{\mathcal{G}_1}(r_k)d_{\mathcal{G}_2}(s_l)\right)\Bigg] \\ \leq \frac{n_2^4}{4} M_1'(\mathcal{G}_1) + \frac{n_2^2 m_1}{2}\Delta_N(\mathcal{G}_2) + \frac{m_2 n_2^2}{2} M_1(\mathcal{G}_1) + \frac{n_2^3 m_1}{2}\Delta_N(\mathcal{G}_1)\Delta_N(\mathcal{G}_2) \end{aligned}$$

Hence, we get

$$\begin{aligned} ISI_N(\mathcal{G}) \leq & \frac{1}{4}\left[n_2^4 M_1'(\mathcal{G}_1) + n_1 M_1'(\mathcal{G}_2)\right] + \frac{n_2}{4}\left[2n_2 m_2 M_1(\mathcal{G}_1) + n_1 \Delta_N(\mathcal{G}_1) M_1(\mathcal{G}_2)\right] \\ & + \frac{n_2^2 m_1 \Delta_N(\mathcal{G}_2)}{2}\left[1 + n_2 \Delta_N(\mathcal{G}_1)\right] + \frac{n_1 m_2 \Delta_N(\mathcal{G}_1)}{2}\left[n_2^2 + 2m_2\right]. \end{aligned}$$

□

Lemma 11. *For the graph $\mathcal{G} = \mathcal{G}_1 \circ \mathcal{G}_2$, we have*

(i) $\delta_{\mathcal{G}}(r) = \delta_{\mathcal{G}_1}(r) + (d_{\mathcal{G}_1}(r)+1)n_2 + 2m_2$ *, where* $r \in \mathcal{V}(\mathcal{G}_1)$

(ii) $\delta_{\mathcal{G}}(s) = \delta_{\mathcal{G}_2}(s) + d_{\mathcal{G}_2}(s) + d_{\mathcal{G}_1}(r_p) + n_2$ *, where* $s \in \mathcal{V}(\mathcal{G}_{2,p})$ *and* $\mathcal{G}_{2,p}$ *denotes the* p^{th} *copy of* $\mathcal{G}_2$.

Theorem 9. *If $\mathcal{G} = \mathcal{G}_1 \circ \mathcal{G}_2$, then*

$$\begin{aligned} ISI_N(\mathcal{G}) \leq & \frac{1}{4}\left[M_1'(\mathcal{G}_1) + n_1 M_1'(\mathcal{G}_2)\right] + \frac{(n_1+1)}{4}\left[n_2 M_1(\mathcal{G}_1) + n_1 M_1(\mathcal{G}_2)\right] \\ & + 2m_1 m_2 + \frac{n_1 n_2}{2}\left[n_1 n_2 + m_2\right] + \frac{n_1(n_2+1)}{2}\left[m_1 n_2 + n_1 m_2\right] + \frac{m_1 n_2}{2}. \end{aligned}$$

Proof. By Lemma 11, we get the definition of ISI_N as

$$\begin{aligned}
ISI_N(\mathcal{G}) &= \sum_{rs\in\mathcal{E}(\mathcal{G}_1)} \frac{\left[\delta_{\mathcal{G}_1}(r)+(d_{\mathcal{G}_1}(r)+1)n_2+2m_2\right]\left[\delta_{\mathcal{G}_1}(s)+(d_{\mathcal{G}_1}(s)+1)n_2+2m_2\right]}{\delta_{\mathcal{G}_1}(r)+\delta_{\mathcal{G}_1}(s)+n_2(d_{\mathcal{G}_1}(r)+d_{\mathcal{G}_1}(s))+2n_2+4m_2} \\
&+\sum_{p=1}^{n_1}\sum_{rs\in\mathcal{E}(\mathcal{G}_{2,p})} \frac{\left[\delta_{\mathcal{G}_2}(r)+d_{\mathcal{G}_2}(r)+d_{\mathcal{G}_1}(r_p)+n_2\right]\left[\delta_{\mathcal{G}_2}(s)+d_{\mathcal{G}_2}(s)+d_{\mathcal{G}_1}(r_p)+n_2\right]}{\delta_{\mathcal{G}_2}(r)+\delta_{\mathcal{G}_2}(s)+d_{\mathcal{G}_2}(r)+d_{\mathcal{G}_2}(s)+2d_{\mathcal{G}_1}(r_p)+2n_2} \\
&+\sum_{p=1}^{n_1}\sum_{\substack{r_ps\in\mathcal{E}' \\ r_p\in\mathcal{V}(\mathcal{G}_1),s\in\mathcal{V}(\mathcal{G}_{2,p})}} \frac{\left[\delta_{\mathcal{G}_1}(r_p)+(d_{\mathcal{G}_1}(r_p)+1)n_2+2m_2\right]\left[\delta_{\mathcal{G}_2}(s)+d_{\mathcal{G}_2}(s)+d_{\mathcal{G}_1}(r_p)+n_2\right]}{\delta_{\mathcal{G}_1}(r_p)+\delta_{\mathcal{G}_2}(s)+(n_2+1)d_{\mathcal{G}_1}(r_p)+d_{\mathcal{G}_2}(s)+2m_2+2n_2} \\
&= S_1+S_2+S_3
\end{aligned}$$

where,

$$\begin{aligned}
S_1 &\le \frac{1}{2}\sum_{rs\in\mathcal{E}(\mathcal{G}_1)}\left[\frac{\delta_{\mathcal{G}_1}(r)+\delta_{\mathcal{G}_1}(s)}{2}+\frac{n_2}{2}\left(d_{\mathcal{G}_1}(r)+d_{\mathcal{G}_1}(s)\right)+n_2+2m_2\right] \\
&\le \frac{M_1'(\mathcal{G}_1)}{4}+\frac{n_2M_1(\mathcal{G}_1)}{4}+\frac{m_1n_2}{2}+m_1m_2 \\
S_2 &\le \frac{1}{2}\sum_{p=1}^{n_1}\sum_{rs\in\mathcal{E}(\mathcal{G}_{2,p})}\left[\frac{\delta_{\mathcal{G}_2}(r)+\delta_{\mathcal{G}_2}(s)}{2}+\frac{d_{\mathcal{G}_2}(r)+d_{\mathcal{G}_2}(s)}{2}+d_{\mathcal{G}_1}(r_p)+n_2\right] \\
&\le \frac{n_1M_1'(\mathcal{G}_2)}{4}+\frac{n_1M_1(\mathcal{G}_2)}{4}+m_1m_2+\frac{n_1n_2m_2}{2}
\end{aligned}$$

and

$$\begin{aligned}
S_3 &\le \frac{1}{2}\sum_{p=1}^{n_1}\sum_{r_ps\in\mathcal{E}'}\left[\frac{\delta_{\mathcal{G}_1}(r_p)}{2}+\frac{\delta_{\mathcal{G}_2}(s)}{2}+\frac{(n_2+1)d_{\mathcal{G}_1}(r_p)}{2}+\frac{d_{\mathcal{G}_2}(s)}{2}+m_2+n_2\right] \\
&\le \frac{n_1}{4}\left[n_2M_1(\mathcal{G}_1)+n_1M_1(\mathcal{G}_2)\right]+\frac{{n_1}^2m_2}{2}(n_2+1)+\frac{n_1n_2}{2}\left[n_1n_2+m_1(n_2+1)\right].
\end{aligned}$$

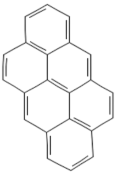
Therefore, we get

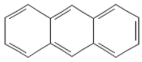
$$\begin{aligned}
ISI_N(\mathcal{G}) \le \frac{1}{4}\left[M_1'(\mathcal{G}_1)+n_1M_1'(\mathcal{G}_2)\right]&+\frac{(n_1+1)}{4}\left[n_2M_1(\mathcal{G}_1)+n_1M_1(\mathcal{G}_2)\right] \\
&+2m_1m_2+\frac{n_1n_2}{2}\left[n_1n_2+m_2\right]+\frac{n_1(n_2+1)}{2}\left[m_1n_2+n_1m_2\right] \\
&+\frac{m_1n_2}{2}.
\end{aligned}$$

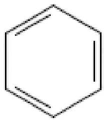
□

5. Regression Modeling of Benzenoid Hydrocarbons

In [6], the effectiveness of the ISI_N index was explored by examining the correlation between 21 benzenoid hydrocarbons ($\mathscr{BHC}$) and their boiling point (BP). In contrast, we conduct a comprehensive regression analysis using a dataset of 55 benzenoid hydrocarbons and their 11 physico-chemical properties. This dataset has been compiled from [3] and the PubChem database. Below, we present the chemical structures of the 55 $\mathscr{BHC}$:


B_1


B_2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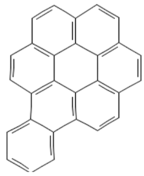
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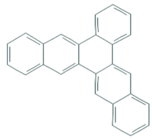
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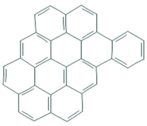
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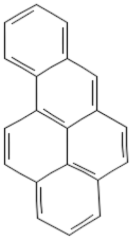
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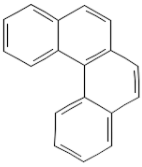
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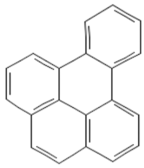
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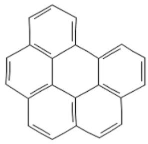
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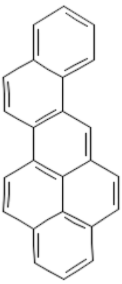
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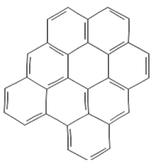
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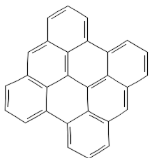
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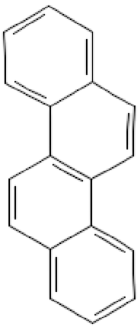
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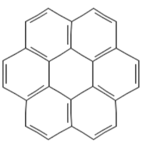
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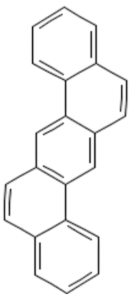
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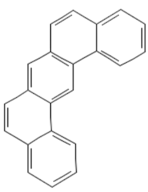
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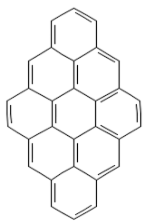
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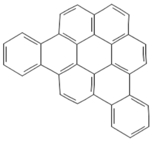
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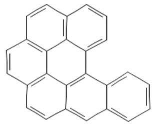
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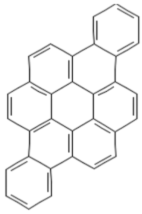
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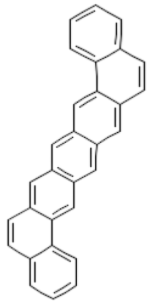
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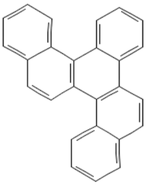
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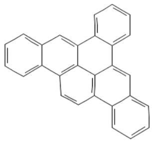
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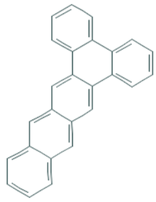
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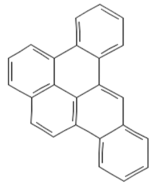
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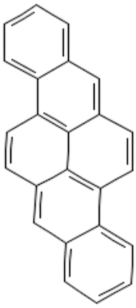
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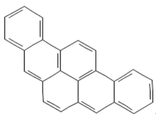
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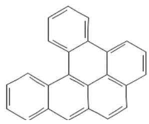
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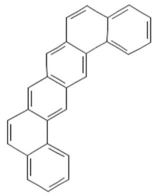
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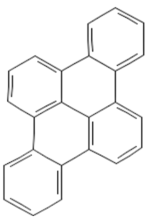
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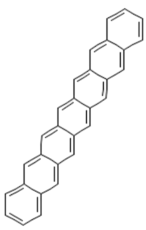
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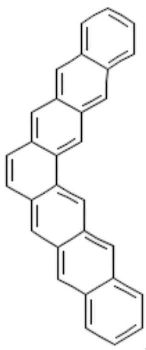
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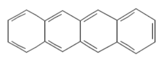
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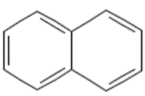
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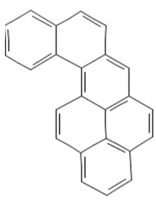
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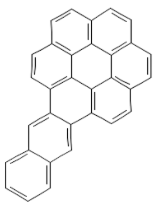
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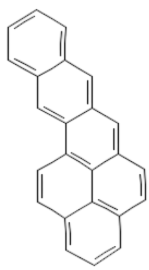
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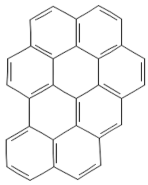
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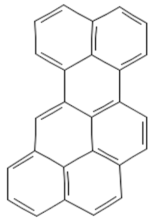
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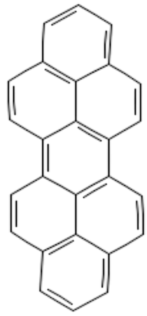
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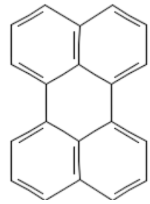
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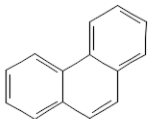
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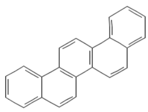
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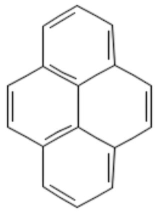
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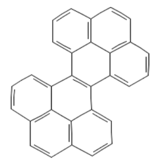
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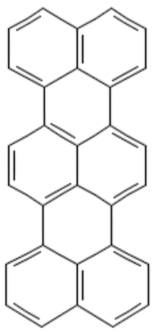
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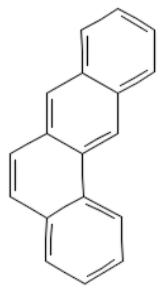
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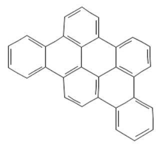
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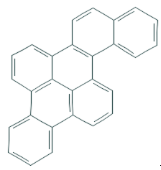
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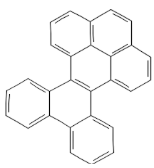
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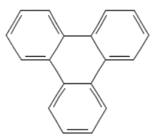
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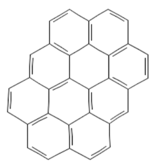
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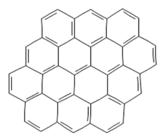
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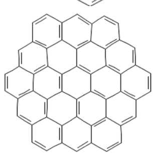

B_{55}

Table 1: Physico-chemical properties of 55 $\mathscr{BHC}$

Compounds	$logP$	RI	BP	ω	C	EV	FP	MR	P	ST	IR
$\mathscr{B}_1$: Anthanthrene	7.04	3215	497.1	-	411	73.6	247.2	100.8	40	74.2	2.009
$\mathscr{B}_2$: Anthracene	4.45	1804	337.4	0.477	154	55.8	146.6	61.9	24.6	48	1.715
$\mathscr{B}_3$: Benzene	2.04	979	80	0.21	15.5	30.7	-11.1	26.3	10.4	28.9	1.499
$\mathscr{B}_4$: Benzo[a]coronene	8.61	-	604.8	-	594	86.6	315.2	129.2	51.2	85.8	2.13
$\mathscr{B}_5$: Benzo[h]pentaphene	8.37	-	604.1	-	462	86.5	314.6	115.5	45.8	60.9	1.843
$\mathscr{B}_6$: Benzo[a]ovalene	10.83	-	-	-	950	-	-	168.1	66.6	104.4	2.333
$\mathscr{B}_7$: Benzo[a]pyrene	6.13	2763	495	-	372	73.4	228.6	90.3	35.8	63.5	1.887
$\mathscr{B}_8$: Benzo[c]phenanthrene	5.7	2427	436.7	-	266	66.7	209.1	79.8	31.6	53.5	1.771
$\mathscr{B}_9$: Benzo[e]pyrene	6.44	2753	467.5	-	336	70.2	228.6	90.3	35.8	63.5	1.887
$\mathscr{B}_{10}$: Benzo[ghi]perylene	6.63	3150	501	-	721	89.6	278.2	73.1	29	53.1	1.762

$\mathcal{B}_{11}$: Benzo[pqr]picene	7.63	-	552.3	-	480	80.2	282	108.1	42.9	66.5	1.913
$\mathcal{B}_{12}$: Benzobisanthene	9.11	-	-	-	676	-	-	139.7	55.4	96.2	2.248
$\mathcal{B}_{13}$: Bisanthene	8.61	-	604.8	-	542	86.6	315.2	129.2	51.2	85.8	2.13
$\mathcal{B}_{14}$: Chrysene	5.81	2429	448	0.46	264	67.9	209.1	79.8	31.6	53.5	1.771
$\mathcal{B}_{15}$: Coronene	7.64	3498	525.6	0.751	376	77	265.2	111.4	44.1	85.8	2.14
$\mathcal{B}_{16}$: Dibenz[a,h]anthracene	6.75	3137	524.7	-	361	76.9	264.5	97.6	38.7	57.7	1.812
$\mathcal{B}_{17}$: Dibenz[a,j]anthracene	6.54	3063	524.7	-	363	76.9	264.5	97.6	38.7	57.7	1.812
$\mathcal{B}_{18}$: Dibenz[Bc,kl]coronene	9.11	-	-	-	620	-	-	139.7	55.4	96.2	2.248
$\mathcal{B}_{19}$: Dibenzo[a,g]coronene	9.85	-	-	-	704	-	-	147	58.3	85.8	2.122
$\mathcal{B}_{20}$: Dibenzo[a,ghi]perylene	8.12	-	579	-	564	83.4	298.8	118.7	47	75.8	2.018
$\mathcal{B}_{21}$: Dibenzo[a,j]coronene	9.85	-	-	-	644	-	-	147	58.3	85.8	2.122
$\mathcal{B}_{22}$: Dibenzo[a,l]pentacene	9.6	-	677	-	568	95.8	360.6	133.3	52.8	63.5	1.867
$\mathcal{B}_{23}$: Dibenzo[c,p]chrysene	8.37	-	604.1	-	508	86.5	314.6	115.5	45.8	60.9	1.843
$\mathcal{B}_{24}$: Dibenzo[h,rst]pentaphene	8.86	-	629.3	-	541	89.7	330.5	126	49.9	68.8	1.932
$\mathcal{B}_{25}$: Dibenzo[a,c]tetracene	8.37	-	604.1	-	462	86.5	314.6	115.5	45.8	60.9	1.843
$\mathcal{B}_{26}$: Dibenzo[a,e]pyrene	7.28	3507	552.3	-	480	80.2	282	108.1	42.9	66.5	1.913
$\mathcal{B}_{27}$: Dibenzo[a,h]pyrene	7.28	3537	552.3	-	436	80.2	282	108.1	42.9	66.5	1.913
$\mathcal{B}_{28}$: Dibenzo[a,i]pyrene	7.28	3526	552.3	-	436	80.2	282	108.1	42.9	66.5	1.913
$\mathcal{B}_{29}$: Dibenzo[a,l]pyrene	7.71	3423	552.3	-	480	80.2	282	108.1	42.9	66.5	1.913
$\mathcal{B}_{30}$: Dibenzo[a,l]tetracene	8.37	-	604.1	-	464	86.5	314.6	115.5	45.8	60.9	1.843
$\mathcal{B}_{31}$: Dibenzo[e,l]pyrene	7.63	3508	552.3	-	396	80.2	282	108.1	42.9	66.5	1.913
$\mathcal{B}_{32}$: Heptacene	9.6	-	677	-	516	95.8	360.6	133.3	52.8	63.5	1.867
$\mathcal{B}_{33}$: Heptaphene	9.6	-	677	-	568	95.8	360.6	133.3	52.8	63.5	1.867
$\mathcal{B}_{34}$: Naphthacene	5.76	-	436.7	0.583	236	66.7	209.1	79.8	31.6	53.5	1.771
$\mathcal{B}_{35}$: Naphthalene	3.3	1194	218	0.308	80.6	43.9	78.9	44.1	17.5	40.2	1.632
$\mathcal{B}_{36}$: Naptho[1,2-a]pyrene	7.63	-	552.3	-	480	80.2	282	108.1	42.9	66.5	1.913
$\mathcal{B}_{37}$: Naptho[2,3-a]coronene	9.85	-	-	-	704	-	-	147	58.3	85.8	2.122
$\mathcal{B}_{38}$: Naptho[2,3-a]pyrene	7.63	-	552.3	-	480	80.2	282	108.1	42.9	66.5	1.913
$\mathcal{B}_{39}$: Naptho[5,4,3-abc]coronene	9.11	-	-	-	738	-	-	139.7	55.4	96.2	2.248
$\mathcal{B}_{40}$: Naphtho[8,1,2-bcd]perylene	8.12	-	579	-	564	83.4	298.8	118.7	47	75.8	2.018
$\mathcal{B}_{41}$: Peropyrene	8.12	-	579	-	470	83.4	298.8	118.7	47	75.8	2.018
$\mathcal{B}_{42}$: Perylene	6.25	2846	467.5	0.49	304	70.2	228.6	90.3	35.8	63.5	1.887
$\mathcal{B}_{43}$: Phenanthrene	4.46	1730	337.4	0.394	174	55.8	146.6	61.9	24.6	48	1.715
$\mathcal{B}_{44}$: Picene	7.11	3159	519	0.54	361	76.2	264.5	97.6	38.7	57.7	1.812
$\mathcal{B}_{45}$: Pyrene	4.88	2119	404	0.547	217	63	168.8	72.5	28.7	59.4	1.852
$\mathcal{B}_{46}$: Pyreno[4,5-e]pyrene	9.35	-	653.8	-	566	92.8	346	136.5	54.1	77.1	2.025
$\mathcal{B}_{47}$: Terylene	9.35	-	653.8	-	570	92.8	346	136.5	54.1	77.1	2.025
$\mathcal{B}_{48}$: Tetraphene	5.76	-	436.7	0.46	294	66.7	209.1	79.8	31.6	53.5	1.771
$\mathcal{B}_{49}$: Tribenzo[b,n,pqr]perylene	9.35	-	653.8	-	622	92.8	346	136.5	54.1	77.1	2.025
$\mathcal{B}_{50}$: Tribenzo[a,fg,op]tetracene	8.86	-	629.3	-	593	89.7	330.5	126	49.9	68.8	1.932
$\mathcal{B}_{51}$: Tribenzo[f,ij,no]tetraphene	8.86	-	629.3	-	541	89.7	330.5	126	49.9	68.8	1.932
$\mathcal{B}_{52}$: Triphenylene	5.49	-	425	0.46	217	65.3	209.1	79.8	31.6	53.5	1.771
$\mathcal{B}_{53}$: Ovalene	9.6	-	-	-	696	-	-	150.3	59.6	107.2	2.374
$\mathcal{B}_{54}$: Circumpyrene	12.3	-	-	-	1050	-	-	199.7	79.2	135.3	2.705
$\mathcal{B}_{55}$: Circumcoronene	15.5	-	-	-	1320	-	-	259.6	102.9	169.1	3.167

Note: "–" indicates that the specific physico-chemical property values for the compound are not available in PubChem and ChemSpider database.

Table 1 gives experimental values of physico-chemical properties such as $logP$, Kovats chromatographic retention index (RI), Boiling point (BP), Pitzer's acentric factor (ω), Complexity (C), Enthalpy of vaporization (EV), Flash Point (FP), Molar refractivity (MR), Polarizability (P), Surface tension (ST) and Index of refractivity (IR) for 55 $\mathcal{BHC}$. The data concerning the first four properties were taken from [3]. The predictive ability of the ISI_N index is evaluated using the following regression models

$$PC = \alpha_1(ISI_N) + \alpha_2 \; (Linear)$$
$$PC = \beta_1(ISI_N)^2 + \beta_2(ISI_N) + \beta_3 \; (Quadratic)$$
$$PC = \gamma_1(ISI_N)^3 + \gamma_2(ISI_N)^2 + \gamma_3(ISI_N) + \gamma_4 \; (Cubic)$$

where PC-properties, α_i , β_i and γ_i $(1 \leq i \leq 4)$ are fitting parameters.
Table 2 represents the computed values of ISI_N for 65 $\mathscr{BHC}$.

Table 2. **Computed values of 65** $\mathscr{BHC}$

$\mathscr{BHC}$	ISI_N	$\mathscr{BHC}$	ISI_N	$\mathscr{BHC}$	ISI_N	$\mathscr{BHC}$	ISI_N	$\mathscr{BHC}$	ISI_N
$\mathscr{B}_1$	87.270299	$\mathscr{B}_{14}$	61.329915	$\mathscr{B}_{27}$	91.09858	$\mathscr{B}_{40}$	104.331286	$\mathscr{B}_{53}$	143.923077
$\mathscr{B}_2$	44.478632	$\mathscr{B}_{15}$	100.625	$\mathscr{B}_{28}$	91.09858	$\mathscr{B}_{41}$	104.221091	$\mathscr{B}_{54}$	200.721154
$\mathscr{B}_3$	12	$\mathscr{B}_{16}$	77.79475	$\mathscr{B}_{29}$	91.583446	$\mathscr{B}_{42}$	74.568313	$\mathscr{B}_{55}$	271.019231
$\mathscr{B}_4$	114.889392	$\mathscr{B}_{17}$	77.79475	$\mathscr{B}_{30}$	94.217827	$\mathscr{B}_{43}$	44.676068	$\mathscr{B}_{56}$	40.701389
$\mathscr{B}_5$	94.791209	$\mathscr{B}_{18}$	130.568376	$\mathscr{B}_{31}$	91.834339	$\mathscr{B}_{44}$	77.983761	$\mathscr{B}_{57}$	28.055556
$\mathscr{B}_6$	161.141681	$\mathscr{B}_{19}$	132.840787	$\mathscr{B}_{32}$	110.17094	$\mathscr{B}_{45}$	57.472222	$\mathscr{B}_{58}$	70.825823
$\mathscr{B}_7$	74.285401	$\mathscr{B}_{20}$	94.648946	$\mathscr{B}_{33}$	103.281563	$\mathscr{B}_{46}$	121.551156	$\mathscr{B}_{59}$	74.877218
$\mathscr{B}_8$	61.41749	$\mathscr{B}_{21}$	134.987117	$\mathscr{B}_{34}$	60.901709	$\mathscr{B}_{47}$	121.317182	$\mathscr{B}_{60}$	78.071336
$\mathscr{B}_9$	74.653281	$\mathscr{B}_{22}$	110.640904	$\mathscr{B}_{35}$	28.055556	$\mathscr{B}_{48}$	61.136691	$\mathscr{B}_{61}$	74.893428
$\mathscr{B}_{10}$	87.596657	$\mathscr{B}_{23}$	95.33997	$\mathscr{B}_{36}$	91.026823	$\mathscr{B}_{49}$	121.958773	$\mathscr{B}_{62}$	74.380616
$\mathscr{B}_{11}$	90.976793	$\mathscr{B}_{24}$	99.884141	$\mathscr{B}_{37}$	134.304227	$\mathscr{B}_{50}$	108.606888	$\mathscr{B}_{63}$	57.882447
$\mathscr{B}_{12}$	130.894734	$\mathscr{B}_{25}$	95.807509	$\mathscr{B}_{38}$	90.548221	$\mathscr{B}_{51}$	108.692748	$\mathscr{B}_{64}$	42.804274
$\mathscr{B}_{13}$	117.86639	$\mathscr{B}_{26}$	91.504005	$\mathscr{B}_{39}$	130.822084	$\mathscr{B}_{52}$	61.794872	$\mathscr{B}_{65}$	107.360637

The regression equations with high correlation are identified using statistical parameters such as the squared correlation coefficient (R^2), standard error (SE), and the F-statistic (confidence statistic value). Among the three regression models we analyzed, only the cubic regression model yielded superior results concerning the relevant statistical parameters. The best-fitting regression equations are provided below.

1. $logP = 6.3e^{-7}(ISI_N)^3 - 0.00036(ISI_N)^2 + 0.106549(ISI_N) + 0.42965$
   $R^2 = 0.9618,\ SE = 0.434842,\ F - Stat = 427.7008$

2. $RI = -0.00547(ISI_N)^3 + 0.980774(ISI_N)^2 - 18.1734(ISI_N) + 1069.39$
   $R^2 = 0.9846,\ SE = 105.369,\ F - Stat = 363.0339$

3. $BP = -0.02754(ISI_N)^2 + 8.782568(ISI_N) - 8.37465$
   $R^2 = 0.9472,\ SE = 28.13256,\ F - Stat = 376.6304$

4. $\omega = 1.71e^{-6}(ISI_N)^3 - 0.00029(ISI_N)^2 + 0.019579(ISI_N) - 0.00368$
   $R^2 = 0.8790,\ SE = 0.055389,\ F - Stat = 19.36746$

5. $C = -2.6e^{-5}(ISI_N)^3 + 0.00598(ISI_N)^2 + 5.413723(ISI_N) - 74.2593$
   $R^2 = 0.9345,\ SE = 59.32763,\ F - Stat = 242.3583$

6. $EV = -4.4e^{-5}(ISI_N)^3 + 0.006144(ISI_N)^2 + 0.416828(ISI_N) + 27.07018$
   $R^2 = 0.9191,\ SE = 4.008208,\ F - Stat = 155.2616$

7. $FP = -0.00018(ISI_N)^3 + 0.019124(ISI_N)^2 + 3.438339(ISI_N) - 40.1403$
   $R^2 = 0.9360,\ SE = 19.70052,\ F - Stat = 199.9505$

8. $MR = 4.39e^{-6}(ISI_N)^3 - 0.0025(ISI_N)^2 + 1.275828(ISI_N) + 9.56984$
   $R^2 = 0.9764,\ SE = 5.763331,\ F - Stat = 703.9474$

9. $P = 1.74e^{-6}(ISI_N)^3 - 0.00099(ISI_N)^2 + 0.505513(ISI_N) + 3.80346$
$R^2 = 0.9766,\ SE = 2.275845,\ F - Stat = 709.3646$

10. $ST = -4.9e^{-6}(ISI_N)^3 + 0.002661(ISI_N)^2 + 0.144358(ISI_N) + 34.46332$
$R^2 = 0.9230,\ SE = 6.360153,\ F - Stat = 203.8213$

11. $IR = -3.9e^{-8}(ISI_N)^3 + 2.68r^{-5}(ISI_N)^2 + 0.001601(ISI_N) + 1.567664$
$R^2 = 0.9182,\ SE = 0.076098,\ F - Stat = 190.8128$

Figures 1 to 5 exhibit the scatter plot of the best-fitting cubic regression models.

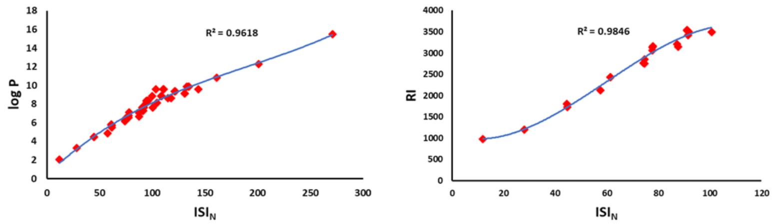


Figure 1. **Scatter plot of** *log P* **and** *RI*

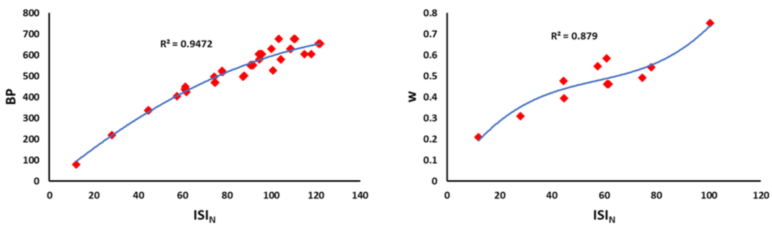


Figure 2. **Scatter plot of** BP **and** ω

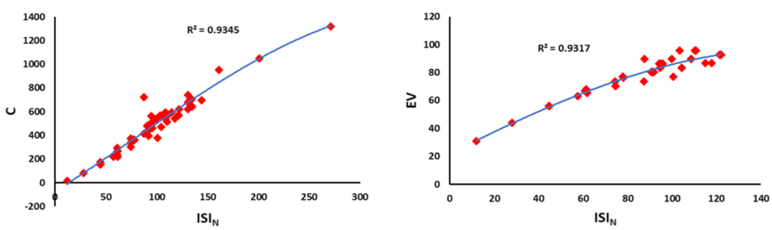


Figure 3. **Scatter plot of** C **and** EV

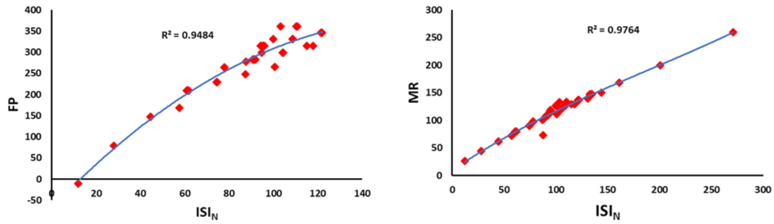


Figure 4. **Scatter plot of FP and MR**

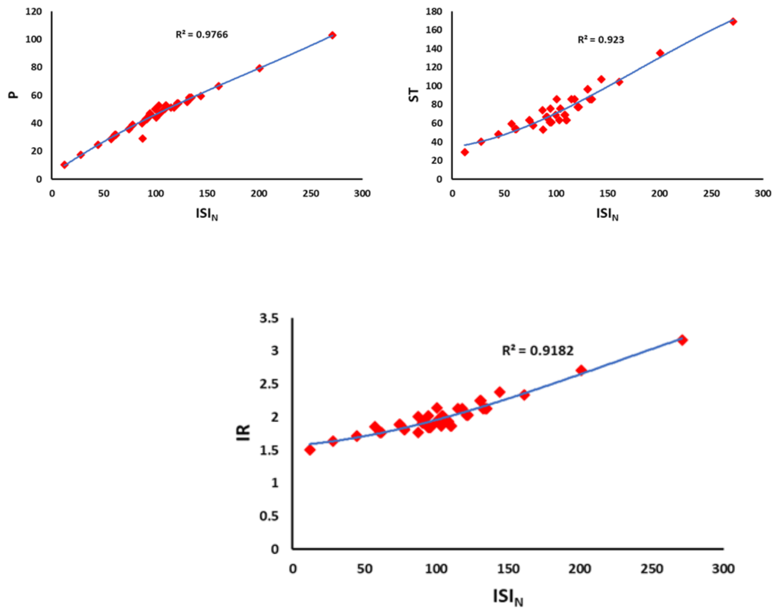
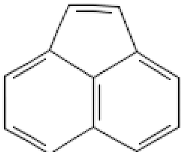
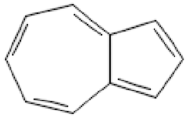
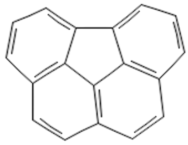


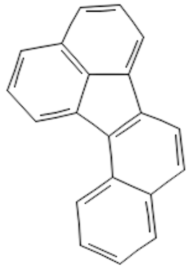
Figure 5. **Scatter plot of P, ST and IR**

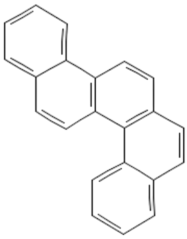
To validate the efficiency of the regression models obtained for physico-chemical properties, we considered ten $\mathcal{BHC}$ compounds for regression analysis that are not included in the dataset of 55 $\mathcal{BHC}$. The chemical structures of the ten $\mathcal{BHC}$ are given below:

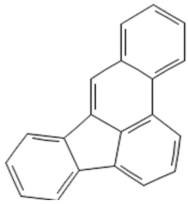

B_{56}

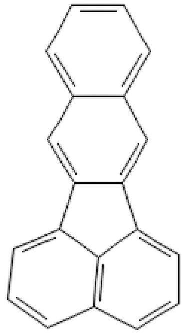

B_{57}

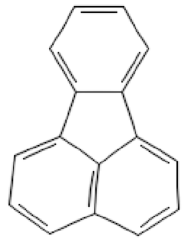

B_{58}

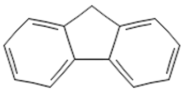

B_{59}

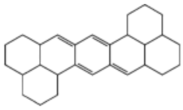

B_{60}


B_{61}


B_{62}


B_{63}


B_{64}


B_{65}

The predicted physico-chemical properties are compared with the available experimental data which are shown in Table 3. Here, P represents the predicted value of the physico-chemical property obtained from the respective regression model equation, while E stands for the experimental value of the corresponding physico-chemical property.

6. Conclusion

The neighborhood degree-sum-based topological indices have garnered considerable attention in chemical graph theory, demonstrating strong correlations with the physico-chemical properties of drugs compared to traditional degree-based indices. This necessitates further mathematical exploration of these indices to uncover valuable insights.

This study focused on the neighborhood inverse sum indeg index (ISI_N), establishing new bounds and examining its relationships with other neighborhood degree-based indices in connected graphs. Furthermore, the research investigated graph operations such as join, sequential join, composition, cartesian product, and corona product, deriving results for the ISI_N index of the resulting graphs. These operations and their subsequent analysis via the ISI_N index contribute to the broader understanding of complex molecular structures and their properties.

Topological indices, beyond their mathematical significance, hold practical applica-

Table 3. **Experimental and predictive values for 10 $\mathscr{BHC}$**

Compounds	$logP$		RI		BP		w		C		EV		FP		MR		P		ST		IR	
	E	P	E	P	E	P	E	P	E	P	E	P	E	P	E	P	E	P	E	P	E	P
B_{56}: Acenaphthylene	4.26	4.21	1425	1585.64	270	303.47	-	0.4281	184	154.24	51.7	51.25	137.2	119.35	51.3	57.65	20.3	22.86	54.7	44.42	1.732	1.675
B_{57}: Azulene	3.45	3.15	1326	1210.71	245	216.35	-	0.3551	94.6	81.76	43.9	42.63	76.7	67.40	44.1	43.49	17.5	17.25	40.2	40.50	1.632	1.633
B_{58}: Benzo[ghi]fluoranthene	5.66	6.39	2438	2758.70	432	475.51	-	0.5358	314	329.93	63.2	71.78	189.9	235.36	83	88.95	32.9	35.26	72	56.30	1.997	1.802
B_{59}: Benzo[j]fluoranthene	-	6.65	2756	2911.08	480	494.83	-	0.5543	372	353.72	70.2	74.26	228.6	248.97	90.3	92.93	35.8	36.83	63.5	58.13	1.887	1.821
B_{60}: Benzo[c]chrysene	7.14	6.85	-	3025.59	-	509.43	-	0.5710	399	372.47	76.9	76.12	264.5	259.20	97.6	96.03	38.7	38.06	57.7	59.62	1.812	1.837
B_{61}: Benzo[b]fluoranthene	-	6.65	-	2911.68	481	494.91	-	0.5544	372	353.80	70.2	74.27	228.6	249.02	90.3	92.94	35.8	36.84	63.5	58.14	1.881	1.822
B_{62}: Benzo[k]fluoranthene	-	6.62	2761	2892.80	481	492.51	-	0.5519	338	350.80	71.6	73.96	228.6	247.34	90.3	92.44	35.8	36.64	63.5	57.91	1.887	1.819
B_{63}: Fluoranthene	5.17	5.51	2057	2242.65	383	407.71	-	0.4896	243	254.09	59.8	63.25	168.4	188.04	72.5	75.89	28.7	30.08	59.4	50.78	1.887	1.743
B_{64}: Fluorene	4.16	4.38	1557	1659.48	294	317.10	-	0.4372	164	166.39	51.2	52.72	133.1	127.96	53.8	59.94	21.3	23.76	46.2	45.13	1.852	1.682
B_{65}: Heptazethrene	-	8.5	-	3654.01	-	617.09	-	0.8718	-	543.71	-	88.19	-	326.69	-	123.16	-	48.82	-	74.57	1.645	2.000

tions in drug design and cheminformatics for analyzing the physico-chemical and thermodynamic properties of chemical compounds. To this end, a regression model was developed to identify the best predictive fit for 11 physico-chemical properties of 55 benzenoid hydrocarbons, using the ISI_N index as a molecular descriptor, and validated the model's efficiency with an external set of 10 benzenoid hydrocarbons. The models developed, which show high correlation coefficients and statistical significance, highlight the ISI_N index's potential in predicting molecular properties, aligning with up-to-date research in QSAR/QSPR studies .

The findings of this study not only offer new avenues for further investigation of the ISI_N index but also provide valuable insights for researchers in mathematical chemistry and related fields. By bridging theoretical results with practical applications, this work contributes to the ongoing efforts to leverage topological indices in the rational design and analysis of chemical compounds, potentially accelerating the discovery and development of novel drugs and materials.

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Conflict of Interest: The authors declare that they have no conflict of interest.

Data Availability: Data sharing is not applicable to this article as no datasets were generated or analyzed during the current study.

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