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Research Article

A Perspective Approach to Study the Valency-Based Irregular Indices for Benzenoid Planar Octahedron Structures

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The molecular topology and the chemical structures which are not regular perform a dominant character in designing the compound in connection with their physical and chemical properties. The study of topological descriptors of molecular structures is widely used in the field of cheminformatics, information technology, biomedical science, and many more. Numerous topological indices have been evolved in the theory of chemistry. Graphs which are not regular can be specified using irregular measures. In this article, we find some irregularity indices, which are useful in Quantitative structure activity relationship for benzenoid structures. Based on the exact analytic expressions, the numerical and graphical comparison for benzenoid structures is also provided.

1. Introduction

In chemical graph theory, latest innovation in graph theoretical models and simulation of molecular graphs are conducted by various researchers. They empower the researchers to develop a correlation between graph theory and chemical compounds. Also, the researches explain the physical and chemical properties like freezing point, solubility, and melting point of chemical structure of various compounds [1–3]. An irregularity index is an analytical value associated with a chemical structure that describes a structure's irregularity. Von Collatz and Ulrich defined the notion "network irregularity" in 1957 [4]. Irregularity measures are aided to denote various organizations in convoluted networks. Self-similarity, network motif, and scale-freeness are all main topological features of these organizations [5].

Let $\sigma((V(\sigma), X(\sigma))$ be an ordered pair of graphs, where $V(\sigma)$ is a nonempty vertex set and $X(\sigma)$ is an edge set. Topological descriptors can be obtained from the molecular structure. They are very helpful to explain Quantitative Structure Activity Relationship (QSAR) of medicines and chemical compounds to form their molecular characteristics by computing numerically [6].

The total number of edges incident with vertex m is called the degree of vertex l, it is denoted by $\Im(l)$. In a graph, the maximum vertex degree is denoted by $\Delta(\sigma)$. Topological study of Line graph of Remdesivir Compound used in the treatment of corona virus is discussed [7]. Degree-based topological indices and polynomials of hyaluronic acid-curcumin conjugates, locating and Multiplicative Locating Indices of Graphs with QSPR Analysis, and structural determination of Paraffin Boiling Points are well studied [3, 8–12]. Graph Irregularity Indices used as Molecular Descriptors in QSPR studies and Randic Index, Irregularity, and complex biomolecular networks are also extensively discussed [13, 14]. The expected values of arithmetic bond connectivity and geometric indices in random phenylene

chains are clearly presented [15–22]. In literature, Irregularity indices of metal organic frameworks [23], Bismuth Tri-Iodide [24], probabilistic neural network [25], and computer networks like silicate, oxide, hexagonal, and honeycomb [26] were extensively studied. Gutman studied the topological indices and irregularity measures [27]. Graphs with equal irregularity indices are well explained [28]. Irregularity indices based on Zagreb indices were studied [29]. For line graph of Dutch windmill graph, the irregularity indices were extensively studied [30]. Several irregularity indices of Dendrimers structures were clearly discussed [31].

In this article, we compute the irregularity degree based topological indices of the benzenoid planar octahedron networks and compare the results graphically.

In 1972, Gutman discussed the first and second Zagreb indices [32].

$$\begin{aligned} M_1(\sigma) &= \sum_{lm\in X(\sigma)} (\mathfrak{F}(l) + \mathfrak{F}(m)), \\ M_2(\sigma) &= \sum_{lm\in X(\sigma)} (\mathfrak{F}(l) \times \mathfrak{F}(m)). \end{aligned} \tag{1}$$

In a graph, if all the degrees are same, then the graph is called a regular graph. Otherwise, it is irregular. The selected irregularity indices for benzenoid planar octahedron networks are represented by

$$\begin{aligned} \mathrm{VAR}(\sigma) &= \frac{M_1(\sigma)}{q} - \left(\frac{2p}{q}\right)^2, \\ \mathrm{AL}(\sigma) &= \sum_{lm\in X(\sigma)} |\mathfrak{F}(l) - \mathfrak{F}(m)|, \\ \mathrm{IR1}(\sigma) &= F(\sigma) - \left(\frac{2p}{q}\right) M_1(\sigma), \\ \mathrm{IR2}(\sigma) &= \sqrt{\frac{M_2(\sigma)}{p}} - \left(\frac{2p}{q}\right), \\ \mathrm{IRF}(\sigma) &= F(\sigma) - 2M_2(\sigma), \\ \mathrm{IRFW}(\sigma) &= \frac{\mathrm{IRF}(\sigma)}{M_2(\sigma)}, \\ \mathrm{IRA}(\sigma) &= \sum_{lm\in X(\sigma)} \left((\mathfrak{F}(l))^{-1/2} - (\mathfrak{F}(m))^{-1/2}\right)^2, \\ \mathrm{IRB}(\sigma) &= \sum_{lm\in X(\sigma)} \left((\mathfrak{F}(l))^{1/2} - (\mathfrak{F}(m))^{-1/2}\right)^2, \\ \mathrm{IRC}(\sigma) &= \sum_{lm\in X(\sigma)} \frac{\sqrt{\mathfrak{F}(l)\mathfrak{F}(m)}}{p} - \frac{2p}{q}, \\ \mathrm{IRDIF}(\sigma) &= \sum_{lm\in X(\sigma)} \left|\frac{\mathfrak{F}(l)}{\mathfrak{F}(m)} - \frac{\mathfrak{F}(m)}{\mathfrak{F}(l)}\right|, \\ \mathrm{IRL}(\sigma) &= \sum_{lm\in X(\sigma)} |\ln \mathfrak{F}(l) - \ln \mathfrak{F}(m)|, \\ \mathrm{IRLU}(\sigma) &= \sum_{lm\in X(\sigma)} \frac{|\mathfrak{F}(l) - \mathfrak{F}(m)|}{\min(\mathfrak{F}(l), \mathfrak{F}(m))}, \\ \mathrm{IRLF}(\sigma) &= \sum_{lm\in X(\sigma)} \frac{|\mathfrak{F}(l) - \mathfrak{F}(m)|}{\sqrt{\mathfrak{F}(l)\mathfrak{F}(m)}}, \\ \mathrm{IRLA}(\sigma) &= 2\sum_{lm\in X(\sigma)} \frac{|\mathfrak{F}(l) - \mathfrak{F}(m)|}{\mathfrak{F}(l) + \mathfrak{F}(m)}, \\ \mathrm{IRGA}(\sigma) &= \sum_{lm\in X(\sigma)} \ln \frac{\mathfrak{F}(l) + \mathfrak{F}(m)}{2\sqrt{\mathfrak{F}(l)\mathfrak{F}(m)}}. \end{aligned} \tag{2}$$

2. Main Outcomes

The structure of Benzenoid planar octahedron is constructed and the topological properties of this structure is well discussed [33]. The 2-dimensional structure of Benzenoid planar octahedron structure is given in Figure 1. We represent the graph of Benzenoid planar octahedron by σ_n, $n \geq 2$, where n denotes the dimension of Benzenoid planar octahedron. Figure 1 depicts the 2-dimensional structure of the molecular graph of σ_2. The total number of vertices (q) and edges (p) in the structure of Benzenoid planar octahedron are $45n^2 - 3n$ and $90n^2$.

The set of edges of Benzenoid planar octahedron structure is divided into five partitions based on the degree of end vertices. The first edge partition includes of $36n^2$ edges lm, where $\mathfrak{F}(l) = 3$ and $\mathfrak{F}(m) = 3$. The second edge partition includes of $12n$ edges lm, where $\mathfrak{F}(l) = 3$ and $\mathfrak{F}(m) = 4$. The third edge partition includes of $36n^2 - 12n$ edges lm, where $\mathfrak{F}(l) = 3$ and $\mathfrak{F}(m) = 8$. The fourth edge partition includes of $12n$ edges lm, where $\mathfrak{F}(l) = 4$ and $\mathfrak{F}(m) = 8$. The fifth edge partition includes of $18n^2 - 12n$ edges lm, where $\mathfrak{F}(l) = 8$ and $\mathfrak{F}(m) = 8$. Table 1 shows the edge partition of Benzenoid planar octahedron structure.

Now the irregularity degree based topological indices is computed as.

Theorem 1. *We consider the graph σ_n, $n \geq 2$, then the irregularity indices of Benzenoid planar octahedron structure are*

$$\begin{aligned} \mathrm{VAR}(\sigma_n) &= \frac{4\left(225n^2 - 195n + 8\right)}{(1 - 15n)^2}, \\ \mathrm{AL}(\sigma_n) &= 180n^2 - 12n, \\ \mathrm{IR1}(\sigma_n) &= -3600n^6 + 384n^5 + 2700n^3 + 5292n^2 - 1152n, \\ \mathrm{IR2}(\sigma_n) &= \sqrt{\frac{2}{15}}\sqrt{n^3(195n - 44)} + \frac{60n}{1 - 15n}, \\ \mathrm{IRF}(\sigma_n) &= 900n^2 - 96n, \end{aligned}$$

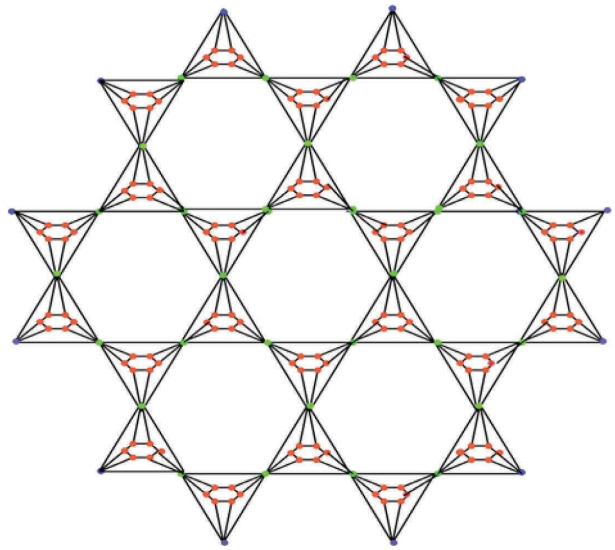

Figure 1: Benzenoid planar octahedron structure of dimension 2.

Table 1: Edge partition of benzenoid planar octahedron structure.

$(\mathfrak{F}(l), \mathfrak{F}(m))$	$(3,3)$	$(3,4)$	$(3,8)$	$(4,8)$	$(8,8)$
Number of edges	$36n^2$	$12n$	$36n^2 - 12n$	$12n$	$18n^2 - 12n$

$$
\begin{aligned}
\mathrm{IRFW}(\sigma_n) &= \frac{900n^2 - 96n}{2340n^2 - 528n},\\
\mathrm{IRA}(\sigma_n) &= 1.8030n^2 - 0.2718n,\\
\mathrm{IRB}(\sigma_n) &= 43.2734n^2 - 5.3274n,\\
\mathrm{IRC}(\sigma_n) &= \frac{428.36n - 45.345}{90n} - \frac{60n}{15n-1},\\
\mathrm{IRDIF}(\sigma_n) &= 82.5n^2 - 2.5n,\\
\mathrm{IRL}(\sigma_n) &= 35.3088n^2 - 0.0012n,\\
\mathrm{IRLU}(\sigma_n) &= 4n(15n-1),\\
\mathrm{IRLF}(\sigma_n) &= 36.74n^2 - 0.29769n,\\
\mathrm{IRLA}(\sigma_n) &= 32.7272n^2 + 0.5195n,\\
\mathrm{IRGA}(\sigma_n) &= 4.16592n^2 - 0.55824n.
\end{aligned} \tag{3}
$$

Proof. Applying the partition of edges of end vertices of each edge of the Benzenoid planar octahedron structure σ_n exploited in Table 1, we calculate the irregularity indices of the Benzenoid planar octahedron structure σ_n and the mathematical computations are given as follows:

$$
\mathrm{VAR}(\sigma_n) = \frac{M_1(\sigma_n)}{q} - \left(\frac{2p}{q}\right)^2 = \frac{900n^2 - 96n}{45n^2 - 3n} - \left(\frac{2(90n^2)}{45n^2 - 3n}\right)^2 = \frac{4\left(225n^2 - 195n + 8\right)}{(1-15n)^2},
$$

$$
\begin{aligned}
\mathrm{AL}(\sigma_n) &= \sum_{lm \in X(\sigma)} |\mathfrak{F}(l) - \mathfrak{F}(m)| = |3-3|36n^2 + |3-4|12n + |3-8|\left(36n^2 - 12n\right) + |4-8|12n + |8-8|\left(18n^2 - 12n\right)\\
&= 180n^2 - 12n,
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{IR1}(\sigma_n) &= F(\sigma_n) - \left(\frac{2p}{q}\right)M_1(\sigma_n) = \left(5580n^2 - 1152n\right) - \frac{2\left(90n^2\right)}{45n^2 - 3n}\left[900n^2 - 96n\right]\\
&= -3600n^6 + 384n^5 + 2700n^3 + 5292n^2 - 1152n,
\end{aligned}
$$

$$\mathrm{IR2}(\sigma_n) = \sqrt{\frac{M_2(\sigma_n)}{p}} - \left(\frac{2p}{q}\right) = \sqrt{\frac{2340n^2 - 528n}{90n^2}} - \left(\frac{2\left(90n^2\right)}{45n^2 - 3n}\right) = \sqrt{\frac{2}{15}}\sqrt{n^3(195n - 44)} + \frac{60n}{1 - 15n},$$

$$\mathrm{IRF}(\sigma_n) = F(\sigma_n) - 2M_2(\sigma_n) = \left(5580n^2 - 1152n\right) - 2\left(2340n^2 - 528n\right) = 900n^2 - 96n,$$

$$\mathrm{IRFW}(\sigma_n) == \frac{IRF(\sigma_n)}{M_2(\sigma_n)} = \frac{900n^2 - 96n}{2340n^2 - 528n},$$

$$IRA(\sigma_n) = \sum_{lm\in X(\sigma)} \left((\mathfrak{F}(l))^{-1/2} - (\mathfrak{F}(m))^{-1/2} \right)^2 = \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}}\right)^2 \left(36n^2\right) + \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{4}}\right)^2 (12n)$$

$$+ \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{8}}\right)^2 \left(36n^2 - 12n\right) + \left(\frac{1}{\sqrt{4}} - \frac{1}{\sqrt{8}}\right)^2 (12n) + \left(\frac{1}{\sqrt{8}} - \frac{1}{\sqrt{8}}\right)^2 \left(18n^2 - 12n\right)$$

$$= 1.8030n^2 - 0.2718n,$$

$$\mathrm{IRB}(\sigma_n) = \sum_{lm\in X(\sigma)} \left((\mathfrak{F}(l))^{1/2} - (\mathfrak{F}(m))^{1/2} \right)^2 = (\sqrt{3} - \sqrt{4})^2 (12n) + (\sqrt{3} - \sqrt{8})^2 \left(36n^2 - 12n\right) + (\sqrt{4} - \sqrt{8})^2 (12n)$$

$$= 43.2734n^2 - 5.3274n,$$

$$\mathrm{IRC}(\sigma_n) = \sum_{lm\in X(\sigma)} \frac{\sqrt{\mathfrak{F}(l)\mathfrak{F}(m)}}{p} - \frac{2p}{q}$$

$$= \frac{\sqrt{9}\left(36n^2\right) + \sqrt{12}(12n) + \sqrt{24}\left(36n^2 - 12n\right) + \sqrt{32}(12n) + \sqrt{64}\left(18n^2 - 12n\right)}{90n^2} - \left(\frac{2\left(90n^2\right)}{45n^2 - 3n}\right)$$

$$= \frac{428.36n - 45.345}{90n} - \frac{60n}{15n - 1},$$

$$\mathrm{IRDIF}(\sigma_n) = \sum_{lm\in X(\sigma)} \left| \frac{\mathfrak{F}(l)}{\mathfrak{F}(m)} - \frac{\mathfrak{F}(m)}{\mathfrak{F}(l)} \right|$$

$$= \left|\frac{3}{3} - \frac{3}{3}\right| 36n^2 + \left|\frac{3}{4} - \frac{4}{3}\right| 12n + \left|\frac{3}{8} - \frac{8}{3}\right| \left(36n^2 - 12n\right) + \left|\frac{4}{8} - \frac{8}{4}\right| 12n + \left|\frac{8}{8} - \frac{8}{8}\right| \left(18n^2 - 12n\right)$$

$$= 82.5n^2 - 2.5n,$$

$$\mathrm{IRL}(\sigma_n) = \sum_{lm\in X(\sigma)} |\ln \mathfrak{F}(l) - \ln \mathfrak{F}(m)|$$

$$= 36n^2 |\ln 3 - \ln 3| + 12n |\ln 3 - \ln 4| + \left(36n^2 - 12n\right) |\ln 3 - \ln 8| + (12n) |\ln 4 - \ln 8| + \left(18n^2 - 12n\right) |\ln 8 - \ln 8|$$

$$= 35.3088n^2 - 0.0012n,$$

$$\mathrm{IRLU}(\sigma_n) = \sum_{lm\in X(\sigma)} \frac{|\mathfrak{F}(l) - \mathfrak{F}(m)|}{\min(\mathfrak{F}(l), \mathfrak{F}(m))}$$

$$= \frac{|3 - 3|}{\min(3, 3)} \left(36n^2\right) + \frac{|3 - 4|}{\min(3, 4)} (12n) + \frac{|3 - 8|}{\min(3, 8)} \left(36n^2 - 12n\right) + \frac{|4 - 8|}{\min(4, 8)} (12n) + \frac{|8 - 8|}{\min(8, 8)} \left(18n^2 - 12n\right)$$

$$= 4n + 60n^2 - 20n + 12n$$

$$= 4n(15n - 1),$$

$$
\begin{aligned}
\mathrm{IRLF}(\sigma_n) &= \sum_{lm\in X(\sigma)} \frac{|\mathfrak{F}(l)-\mathfrak{F}(m)|}{\sqrt{\mathfrak{F}(l)\mathfrak{F}(m)}} \\
&= 36n^2\left(\frac{|3-3|}{\sqrt{9}}\right) + 12n\left(\frac{|3-4|}{\sqrt{12}}\right) + \left(36n^2-12n\right)\left(\frac{|3-8|}{\sqrt{24}}\right) + 12n\left(\frac{|4-8|}{\sqrt{32}}\right) + \left(18n^2-12n\right)\left(\frac{|8-8|}{\sqrt{64}}\right) \\
&= \sqrt{12}n + 36.74n^2 - 12.247n + 8.4852n \\
&= 36.74n^2 - 0.29769n, \\
\mathrm{IRLA}(\sigma_n) &= 2\sum_{lm\in X(\sigma)} \frac{|\mathfrak{F}(l)-\mathfrak{F}(m)|}{\mathfrak{F}(l)+\mathfrak{F}(m)} \\
&= 2\left(36n^2\right)\left(\frac{|3-3|}{3+3}\right) + 2(12n)\left(\frac{|3-4|}{3+4}\right) + 2\left(36n^2-12n\right)\left(\frac{|3-8|}{3+8}\right) + 2(12n)\left(\frac{|4-8|}{4+8}\right) + 2\left(18n^2-12n\right)\left(\frac{|8-8|}{8+8}\right) \\
&= 32.7272n^2 + 0.5195n, \\
\mathrm{IRGA}(\sigma_n) &= \sum_{lm\in X(\sigma)} \ln\frac{\mathfrak{F}(l)+\mathfrak{F}(m)}{2\sqrt{\mathfrak{F}(l)\mathfrak{F}(m)}} \\
&= 36n^2\left(\ln\frac{6}{2\sqrt{9}}\right) + 12n\left(\ln\frac{7}{2\sqrt{12}}\right) + \left(36n^2-12n\right)\left(\ln\frac{11}{2\sqrt{24}}\right) + 12n\left(\ln\frac{12}{2\sqrt{32}}\right) + \left(18n^2-12n\right)\left(\ln\frac{16}{2\sqrt{64}}\right) \\
&= 4.16592n^2 - 0.55824n.
\end{aligned} \tag{4}
$$

The structure of Benzenoid dominating planar octahedron is constructed and the topological properties of this structure is well explained [33]. The 2-dimensional structure of Benzenoid dominating planar octahedron structure is given in Figure 2. We denote the graph of Benzenoid dominating planar octahedron by ν_n, $n \geq 2$, where n denotes the dimension of Benzenoid dominating planar octahedron. Figure 2 depicts the 2-dimensional structure of the molecular graph of ν_2. The total number of vertices (t) and edges (s) in the structure of Benzenoid dominating planar octahedron are $27n^2 - 33n + 12$ and $270n^2 - 378n + 156$.

The set of edges of Benzenoid dominating planar octahedron structure is divided into five partitions based on the degree of end vertices. The first partition of edge includes of $108n^2 - 132n + 48$ edges lm, where $\mathfrak{F}(l) = 3$ and $\mathfrak{F}(m) = 3$. The second partition of edge includes of $24n - 12$ edges lm, where $\mathfrak{F}(l) = 3$ and $\mathfrak{F}(m) = 4$. The third partition of edge includes of $108n^2 - 132n + 48$ edges lm, where $\mathfrak{F}(l) = 3$ and $\mathfrak{F}(m) = 8$. The fourth partition of edge includes of $24n - 12$ edges lm, where $\mathfrak{F}(l) = 4$ and $\mathfrak{F}(m) = 8$. The fifth partition of edge includes of $54n^2 - 162n + 84$ edges lm, where $\mathfrak{F}(l) = 8$ and $\mathfrak{F}(m) = 8$. Table 2 shows the edge partition of Benzenoid dominating planar octahedron structure. □

Theorem 2. *Consider the graph ν_n, $n \geq 2$, then the irregularity indices of Benzenoid dominating planar octahedron structure are*

$$
\begin{aligned}
\mathrm{VAR}(\nu_n) &= \frac{2700n^2-4380n+1932}{27n^2-33n+12} - \left(\frac{2\left(270n^2-378n+156\right)}{27n^2-33n+12}\right)^2, \\
AL(\nu_n) &= 540n^2 - 540n + 180, \\
\mathrm{IR1}(\nu_n) &= \left(16740n^2-19044n+6732\right) - \frac{2\left(270n^2-378n+156\right)}{27n^2-33n+12}\left[2700n^2-4380n+1932\right], \\
\mathrm{IR2}(\nu_n) &= \sqrt{\frac{7020n^2-13668n+6432}{270n^2-378n+156}} - \left(\frac{2\left(270n^2-378n+156\right)}{27n^2-33n+12}\right),
\end{aligned}
$$

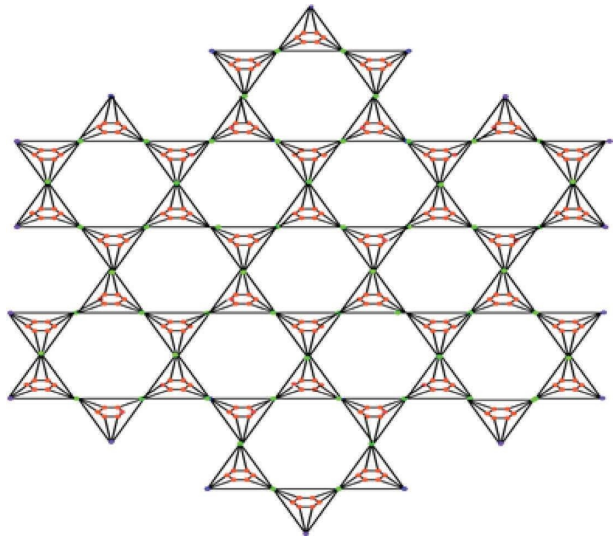

Figure 2: Benzenoid dominating planar octahedron structure of dimension 2.

Table 2: Edge partition of benzenoid dominating planar octahedron structure.

$(\mathfrak{F}(l), \mathfrak{F}(m))$	(3, 3)	(3, 4)	(3, 8)	(4, 8)	(8,8)
Number of edges	$108n^2 - 132n + 48$	$24n - 12$	$108n^2 - 132n + 48$	$24n - 12$	$54n^2 - 162n + 84$

$$
\begin{aligned}
\mathrm{IRF}(\nu_n) &= 2700n^2 + 8292n - 6132,\\
\mathrm{IRFW}(\nu_n) &= \frac{2700n^2 + 8292n - 6132}{7020n^2 - 13668n + 6432},\\
\mathrm{IRA}(\nu_n) &= 5.40692n^2 - 5.95031n + 2.074,\\
\mathrm{IRB}(\nu_n) &= 129.82n^2 - 140.4752n + 48.6009,\\
\mathrm{IRC}(\nu_n) &= \frac{1285.08n^2 - 2119.636n + 941.651}{270n^2 - 378n + 156} - \left(\frac{2\left(270n^2 - 378n + 156\right)}{27n^2 - 33n + 12}\right),\\
\mathrm{IRDIF}(\nu_n) &= -247.5n^2 + 252.5n - 85,\\
\mathrm{IRL}(\nu_n) &= -105.926n^2 - 23.53776n + 87.25368,\\
\mathrm{IRLU}(\nu_n) &= 180n^2 - 188n + 64,\\
\mathrm{IRLF}(\nu_n) &= 110.22n^2 - 110.82n + 37.0403,\\
\mathrm{IRLA}(\nu_n) &= 98.1818n^2 - 97.1429n + 32.2078,\\
\mathrm{IRGA}(\nu_n) &= 12.4977n^2 - 15.0278n + 4.72428.
\end{aligned}
\tag{5}
$$

Proof. Applying the partition of edge based on degrees of end vertices of each edge of the Benzenoid dominating planar octahedron structure ν_n depicted in Table 2, we compute the irregularity indices of the Benzenoid dominating planar octahedron structure ν_n, and the mathematical calculations are given as follows:

$$\mathrm{VAR}(\nu_n) = \frac{M_1(\nu_n)}{t} - \left(\frac{2s}{t}\right)^2 = \frac{2700n^2 - 4380n + 1932}{27n^2 - 33n + 12} - \left(\frac{2\left(270n^2 - 378n + 156\right)}{27n^2 - 33n + 12}\right)^2,$$

$$\begin{aligned}\mathrm{AL}(\nu_n) &= \sum_{lm \in X(\nu)} |\Im(l) - \Im(m)| = |3-3|\left(108n^2 - 132n + 48\right) + |3-4|(24n-12) + |3-8|\left(108n^2 - 132n + 48\right) \\ &\quad + |4-8|(24n-12) + |8-8|\left(54n^2 - 162n + 84\right) \\ &= 540n^2 - 540n + 180,\end{aligned}$$

$$\mathrm{IR1}(\nu_n) = F(\nu_n) - \left(\frac{2s}{t}\right)M_1(\nu_n) = \left(16740n^2 - 19044n + 6732\right) - \frac{2\left(270n^2 - 378n + 156\right)}{27n^2 - 33n + 12}\left[2700n^2 - 4380n + 1932\right],$$

$$IR2(\nu_n) = \sqrt{\frac{M_2(\nu_n)}{s}} - \left(\frac{2s}{t}\right) = \sqrt{\frac{7020n^2 - 13668n + 6432}{270n^2 - 378n + 156}} - \left(\frac{2\left(270n^2 - 378n + 156\right)}{27n^2 - 33n + 12}\right),$$

$$\begin{aligned}\mathrm{IRF}(\nu_n) &= F(\nu_n) - 2M_2(\nu_n) = \left(16740n^2 - 19044n + 6732\right) - 2\left(7020n^2 - 13668n + 6432\right) \\ &= 2700n^2 + 8292n - 6132,\end{aligned}$$

$$\mathrm{IRFW}(\nu_n) == \frac{IRF(\nu_n)}{M_2(\nu_n)} = \frac{2700n^2 + 8292n - 6132}{7020n^2 - 13668n + 6432},$$

$$\begin{aligned}IRA(\nu_n) &= \sum_{lm \in X(\nu)} \left((\Im(l))^{-1/2} - (\Im(m))^{-1/2}\right)^2 = \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}}\right)^2\left(108n^2 - 132n + 48\right) + \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{4}}\right)^2(24n-12) \\ &\quad + \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{8}}\right)^2\left(108n^2 - 132n + 48\right) + \left(\frac{1}{\sqrt{4}} - \frac{1}{\sqrt{8}}\right)^2(24n-12) + \left(\frac{1}{\sqrt{8}} - \frac{1}{\sqrt{8}}\right)^2\left(54n^2 - 162n + 84\right) \\ &= 5.40692n^2 - 5.95031n + 2.074,\end{aligned}$$

$$\begin{aligned}\mathrm{IRB}(\nu_n) &= \sum_{lm \in X(\nu)} \left((\Im(l))^{1/2} - (\Im(m))^{1/2}\right)^2 = (\sqrt{3} - \sqrt{4})^2(24n-12) \\ &\quad + (\sqrt{3} - \sqrt{8})^2\left(108n^2 - 132n + 48\right) + (\sqrt{4} - \sqrt{8})^2(24n-12) \\ &= 129.82n^2 - 140.4752n + 48.6009,\end{aligned}$$

$$\begin{aligned}\mathrm{IRC}(\nu_n) &= \sum_{lm \in X(\nu)} \frac{\sqrt{\Im(l)\Im(m)}}{s} - \frac{2s}{t} \\ &= \frac{\sqrt{9}\left(108n^2 - 132n + 48\right) + \sqrt{12}(24n-12) + \sqrt{24}\left(108n^2 - 132n + 48\right) + \sqrt{32}(24n-12) + \sqrt{64}\left(54n^2 - 162n + 84\right)}{270n^2 - 378n + 156} - \\ &\quad \left(\frac{2\left(270n^2 - 378n + 156\right)}{27n^2 - 33n + 12}\right) \\ &= \frac{1285.08n^2 - 2119.636n + 941.651}{270n^2 - 378n + 156} - \left(\frac{2\left(270n^2 - 378n + 156\right)}{27n^2 - 33n + 12}\right),\end{aligned}$$

$$\mathrm{IRDIF}(\nu_n) = \sum_{lm \in X(\nu)} \left|\frac{\Im(l)}{\Im(m)} - \frac{\Im(m)}{\Im(l)}\right|,$$

$$= \left|\frac{3}{3}-\frac{3}{3}\right|\left(108n^2-132n+48\right)+\left|\frac{3}{4}-\frac{4}{3}\right|(24n-12)+\left|\frac{3}{8}-\frac{8}{3}\right|\left(108n^2-132n+48\right)+\left|\frac{4}{8}-\frac{8}{4}\right|(24n-12)$$

$$+\left|\frac{8}{8}-\frac{8}{8}\right|\left(54n^2-162n+84\right)$$

$$= -247.5n^2+252.5n-85,$$

$$\mathrm{IRL}\left(\nu_n\right) = \sum_{lm\in X(\nu)} \left|\ln \mathfrak{F}(l)-\ln \mathfrak{F}(m)\right|$$

$$= \left(108n^2-132n+48\right)|\ln 3-\ln 3|+(24n-12)|\ln 3-\ln 4|+\left(108n^2-132n+48\right)|\ln 3-\ln 8|$$

$$+(24n-12)|\ln 4-\ln 8|+\left(54n^2-162n+84\right)|\ln 8-\ln 8|$$

$$= -105.926n^2-23.53776n+87.25368,$$

$$\mathrm{IRLU}\left(\nu_n\right) = \sum_{lm\in X(\nu)} \frac{|\mathfrak{F}(l)-\mathfrak{F}(m)|}{\min\left(\mathfrak{F}(l),\mathfrak{F}(m)\right)}$$

$$= \frac{|3-3|}{\min(3,3)}\left(108n^2-132n+48\right)+\frac{|3-4|}{\min(3,4)}(24n-12)+\frac{|3-8|}{\min(3,8)}\left(108n^2-132n+48\right)$$

$$+\frac{|4-8|}{\min(4,8)}(24n-12)+\frac{|8-8|}{\min(8,8)}\left(54n^2-162n+84\right)$$

$$= 180n^2-188n+64,$$

$$\mathrm{IRLF}\left(\nu_n\right) = \sum_{lm\in X(\nu)} \frac{|\mathfrak{F}(l)-\mathfrak{F}(m)|}{\sqrt{\mathfrak{F}(l)\mathfrak{F}(m)}}$$

$$= \left(108n^2-132n+48\right)\left(\frac{|3-3|}{\sqrt{9}}\right)+(24n-12)\left(\frac{|3-4|}{\sqrt{12}}\right)+\left(108n^2-132n+48\right)\left(\frac{|3-8|}{\sqrt{24}}\right)$$

$$+(24n-12)\left(\frac{|4-8|}{\sqrt{32}}\right)+\left(54n^2-162n+84\right)\left(\frac{|8-8|}{\sqrt{64}}\right)$$

$$= 110.22n^2-110.82n+37.0403,$$

$$\mathrm{IRLA}\left(\nu_n\right) = 2\sum_{lm\in X(\nu)} \frac{|\mathfrak{F}(l)-\mathfrak{F}(m)|}{\mathfrak{F}(l)+\mathfrak{F}(m)}$$

$$= 2\left(108n^2-132n+48\right)\left(\frac{|3-3|}{3+3}\right)+2(24n-12)\left(\frac{|3-4|}{3+4}\right)+2\left(108n^2-132n+48\right)\left(\frac{|3-8|}{3+8}\right)$$

$$+2(24n-12)\left(\frac{|4-8|}{4+8}\right)+2\left(54n^2-162n+84\right)\left(\frac{|8-8|}{8+8}\right)$$

$$= 98.1818n^2-97.1429n+32.2078,$$

$$\begin{aligned}\mathrm{IRGA}(\nu_n) &= \sum_{lm\in X(\nu)} \ln\frac{\mathfrak{I}(l)+\mathfrak{I}(m)}{2\sqrt{\mathfrak{I}(l)\mathfrak{I}(m)}}\\ &= \left(108n^2-132n+48\right)\left(\ln\frac{6}{2\sqrt{9}}\right)+(24n-12)\left(\ln\frac{7}{2\sqrt{12}}\right)+\left(108n^2-132n+48\right)\left(\ln\frac{11}{2\sqrt{24}}\right)\\ &\quad+(24n-12)\left(\ln\frac{12}{2\sqrt{32}}\right)+\left(54n^2-162n+84\right)\left(\ln\frac{16}{2\sqrt{64}}\right)\\ &= 12.4977n^2-15.0278n+4.72428.\end{aligned} \tag{6}$$

The structure of Benzenoid hex planar octahedron is constructed and the topological properties of this structure are well discussed [33]. The 2-dimensional structure of Benzenoid hex planar octahedron structure is given in Figure 3. We represent the graph of Benzenoid hex planar octahedron by μ_n, $n\geq 2$, where n denotes the dimension of Benzenoid hex planar octahedron. Figure 3 depicts the 2-dimensional structure of the molecular graph of μ_2. The total number of vertices (u) and edges (v) in the structure of Benzenoid hex planar octahedron are $45n^2+51n+6$ and $90n^2+24n+6$.

The set of edges of Benzenoid hex planar octahedron structure is divided into five partitions based on the degree of end vertices. The first partition of edge includes of 12 edges lm, where $\mathfrak{I}(l)=2$ and $\mathfrak{I}(m)=5$. The second partition of edge includes of $36n^2-36n$ edges lm, where $\mathfrak{I}(l)=3$ and $\mathfrak{I}(m)=3$. The third partition of edge includes of $24n$ edges lm, where $\mathfrak{I}(l)=3$ and $\mathfrak{I}(m)=5$. The fourth partition of edge includes of $36n^2+12n$ edges lm, where $\mathfrak{I}(l)=3$ and $\mathfrak{I}(m)=8$. The fifth partition of edge includes of $12n-6$ edges lm, where $\mathfrak{I}(l)=5$ and $\mathfrak{I}(m)=5$. The sixth partition of edge includes of $12n$ edges lm, where $\mathfrak{I}(l)=5$ and $\mathfrak{I}(m)=8$. The seventh partition of edge includes of $18n^2$ edges lm, where $\mathfrak{I}(l)=8$ and $\mathfrak{I}(m)=8$. Table 3 shows the edge partition of Benzenoid hex planar octahedron structure. □

Theorem 3. *Consider the graph μ_n, $n\geq 2$, then the irregularity indices of Benzenoid hex planar octahedron structure are*

$$\mathrm{VAR}(\mu_n) = \frac{900n^2-384n+24}{45n^2+51n+6}-\left(\frac{180n^2+48n+12}{45n^2+51n+6}\right)^2,$$

$$AL(\mu_n) = 180n^2+144n+36,$$

$$\mathrm{IR1}(\mu_n) = \frac{413100n^4+490860n^3+243360n^2+29952n}{45n^2+51n+6},$$

$$\mathrm{IR2}(\mu_n) = \sqrt{\frac{2340n^2+1104n-30}{90n^2+24n+6}}-\left(\frac{180n^2+48n+12}{45n^2+51n+6}\right),$$

$$\mathrm{IRF}(\mu_n) = 900n^2+1800n+108,$$

$$\mathrm{IRFW}(\mu_n) = \frac{900n^2+1800n+108}{2340n^2+1104n-30},$$

$$\mathrm{IRA}(\mu_n) == 1.80311184n^2+1.11276567n+0.810495,$$

$$\mathrm{IRB}(\mu_n) == 43.2734n^2+24.7318n+8.10533616,$$

$$\mathrm{IRC}(\mu_n) = \frac{428.3632n^2-179.63401n+7.94733}{90n^2+24n+6}-\left(\frac{180n^2+48n+12}{45n^2+51n+6}\right),$$

$$\mathrm{IRDIF}(\mu_n) = 82.49976n^2+64.783n+25.2,$$

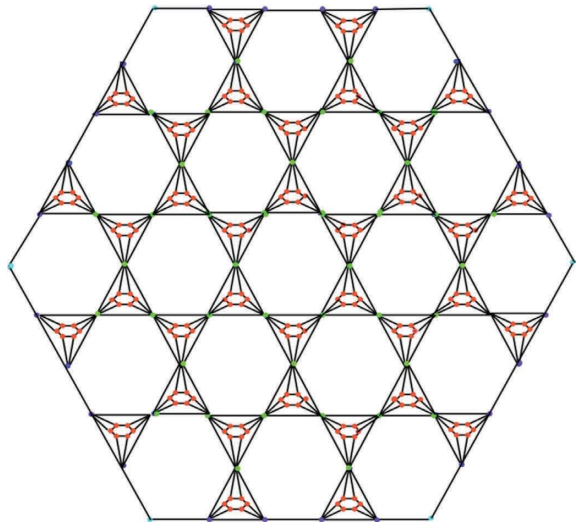

Figure 3: Benzenoid hex planar octahedron structure of dimension 2.

Table 3: Edge partition of benzenoid hex planar octahedron structure.

$(\mathfrak{F}(l), \mathfrak{F}(m))$	$(2, 5)$	$(3, 3)$	$(3, 5)$	$(3, 8)$	$(5, 5)$	$(5, 8)$	$(8, 8)$
Number of edges	12	$36n^2 - 36n$	$24n$	$36n^2 + 12n$	$12n - 6$	$12n$	$18n^2$

$$\begin{aligned}
\mathrm{IRL}(\mu_n) &= 73.7612n^2 + 84.72643n + 18.62010,\\
IRLU(\mu_n) &= 60n^2 + 43.2n + 18,\\
\mathrm{IRLF}(\mu_n) &= 36.74234n^2 + 30.3329867n + 11.3841996,\\
\mathrm{IRLA}(\mu_n) &= 32.7272n^2 + 28.44746n + 10.2857,\\
\mathrm{IRGA}(\mu_n) &= 118.5759n^2 + 84.894662n + 28.8486661.
\end{aligned} \tag{7}$$

Proof. Applying the partition of edge based on degrees of end vertices of each edge of the Benzenoid hex planar octahedron structure μ_n depicted in Table 3, we compute the irregularity indices of the Benzenoid hex planar octahedron structure μ_n and the mathematical calculations are given as follows:

$$\mathrm{VAR}(\mu_n) = \frac{M_1(\mu_n)}{u} - \left(\frac{2v}{u}\right)^2 = \frac{900n^2 - 384n + 24}{45n^2 + 51n + 6} - \left(\frac{180n^2 + 48n + 12}{45n^2 + 51n + 6}\right)^2,$$

$$\begin{aligned}
\mathrm{AL}(\mu_n) &= \sum_{lm \in X(\mu)} |\mathfrak{F}(l) - \mathfrak{F}(m)| = |2-5|(12) + |3-3|\left(36n^2 - 36n\right) + |3-5|(24n) + |3-8|\left(36n^2 + 12n\right)\\
&\quad + |5-5|(12n-6) + |5-8|(12n) + |8-8|\left(18n^2\right)\\
&= 180n^2 + 144n + 36,
\end{aligned}$$

$$\mathrm{IR1}(\mu_n) = F(\mu_n) - \left(\frac{2v}{u}\right)M_1(\mu_n) = \left(5580n^2 + 4008n + 48\right) - \left(\frac{180n^2 + 48n + 12}{45n^2 + 51n + 6}\right)\left[900n^2 - 384n + 24\right]$$

$$= \frac{413100n^4 + 490860n^3 + 243360n^2 + 29952n}{45n^2 + 51n + 6},$$

$$\mathrm{IR2}(\mu_n) = \sqrt{\frac{M_2(\mu_n)}{v}} - \left(\frac{2v}{u}\right) = \sqrt{\frac{2340n^2 + 1104n - 30}{90n^2 + 24n + 6}} - \left(\frac{180n^2 + 48n + 12}{45n^2 + 51n + 6}\right),$$

$$\mathrm{IRF}(\mu_n) = F(\mu_n) - 2M_2(\mu_n) = \left(5580n^2 + 4008n + 48\right) - 2\left(2340n^2 + 1104n - 30\right)$$

$$= 900n^2 + 1800n + 108,$$

$$\mathrm{IRFW}(\mu_n) = \frac{IRF(\mu_n)}{M_2(\mu_n)}$$

$$= \frac{900n^2 + 1800n + 108}{2340n^2 + 1104n - 30},$$

$$\mathrm{IRA}(\mu_n) = \sum_{lm\epsilon X(\mu)} \left((\mathfrak{I}(l))^{-1/2} - (\mathfrak{I}(m))^{-1/2} \right)^2 = \left(\frac{1}{\sqrt{2}} - \frac{1}{\sqrt{5}}\right)^2 (12) + \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{3}}\right)^2 \left(36n^2 - 36n\right) + \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{5}}\right)^2 (24n)$$

$$+ \left(\frac{1}{\sqrt{3}} - \frac{1}{\sqrt{8}}\right)^2 \left(36n^2 + 12n\right) + \left(\frac{1}{\sqrt{5}} - \frac{1}{\sqrt{5}}\right)^2 (12n - 6) + \left(\frac{1}{\sqrt{5}} - \frac{1}{\sqrt{8}}\right)^2 (12n) + \left(\frac{1}{\sqrt{8}} - \frac{1}{\sqrt{8}}\right)^2 \left(18n^2\right)$$

$$= 1.80311184n^2 + 1.11276567n + 0.810495,$$

$$\mathrm{IRB}(\mu_n) = \sum_{lm\epsilon X(\mu)} \left((\mathfrak{I}(l))^{1/2} - (\mathfrak{I}(m))^{1/2} \right)^2 = (\sqrt{2} - \sqrt{5})^2 (12) + (\sqrt{3} - \sqrt{3})^2 \left(36n^2 - 36n\right) + (\sqrt{3} - \sqrt{5})^2 (24n)$$

$$+ (\sqrt{3} - \sqrt{8})^2 \left(36n^2 + 12n\right) + (\sqrt{5} - \sqrt{5})^2 (12n - 6) + (\sqrt{5} - \sqrt{8})^2 (12n) + (\sqrt{8} - \sqrt{8})^2 \left(18n^2\right)$$

$$= 43.2734n^2 + 24.7318n + 8.10533616,$$

$$\mathrm{IRC}(\mu_n) = \sum_{lm\epsilon X(\mu)} \frac{\sqrt{\mathfrak{I}(l)\mathfrak{I}(m)}}{v} - \frac{2v}{u}$$

$$= \frac{\sqrt{10}(12) + \sqrt{9}\left(36n^2 - 36n\right) + \sqrt{15}(24n) + \sqrt{24}\left(36n^2 + 12n\right) + \sqrt{25}(12n - 6) + \sqrt{40}(12n) + \sqrt{64}\left(18n^2\right)}{90n^2 + 24n + 6}$$

$$\left(\frac{180n^2 + 48n + 12}{45n^2 + 51n + 6}\right)$$

$$= \frac{428.3632n^2 - 179.63401n + 7.94733}{90n^2 + 24n + 6} - \left(\frac{180n^2 + 48n + 12}{45n^2 + 51n + 6}\right),$$

$$\mathrm{IRDIF}(\mu_n) = \sum_{lm\epsilon X(\mu)} \left| \frac{\mathfrak{I}(l)}{\mathfrak{I}(m)} - \frac{\mathfrak{I}(m)}{\mathfrak{I}(l)} \right|$$

$$= \left|\frac{2}{5}-\frac{5}{2}\right|(12)+\left|\frac{3}{3}-\frac{3}{3}\right|\left(36n^2-36n\right)+\left|\frac{3}{5}-\frac{5}{3}\right|(24n)+\left|\frac{3}{8}-\frac{8}{3}\right|\left(36n^2+12n\right)+\left|\frac{5}{5}-\frac{5}{5}\right|(12n-6)$$

$$+\left|\frac{5}{8}-\frac{8}{5}\right|(12n)+\left|\frac{8}{8}-\frac{8}{8}\right|\left(18n^2\right)$$

$$= 82.49976n^2 + 64.783n + 25.2,$$

$$\mathrm{IRL}(\mu_n) = \sum_{lm\in X(\mu)} |\ln \mathfrak{I}(l) - \ln \mathfrak{I}(m)|,$$

$$= (12)|\ln 2 - \ln 5| + \left(36n^2-36n\right)|\ln 3 - \ln 3| + (24n)|\ln 3 - \ln 5| + \left(36n^2+12n\right)|\ln 3 - \ln 8|$$

$$+(12n-6)|\ln 5 - \ln 5| + (12n)|\ln 5 - \ln 8| + \left(18n^2\right)|\ln 8 - \ln 8|$$

$$= 73.7612n^2 + 84.72643n + 18.62010,$$

$$\mathrm{IRLU}(\mu_n) = \sum_{lm\in X(\mu)} \frac{|\mathfrak{I}(l) - \mathfrak{I}(m)|}{\min(\mathfrak{I}(l), \mathfrak{I}(m))}$$

$$= \frac{|2-5|}{\min(2,5)}(12) + \frac{|3-3|}{\min(3,3)}\left(36n^2-36n\right) + \frac{|3-5|}{\min(3,5)}(24n) + \frac{|3-8|}{\min(3,8)}\left(36n^2+12n\right) + \frac{|5-5|}{\min(5,5)}(12n-6)$$

$$+\frac{|5-8|}{\min(5,8)}(12n) + \frac{|8-8|}{\min(8,8)}\left(18n^2\right)$$

$$= 60n^2 + 43.2n + 18,$$

$$\mathrm{IRLF}(\mu_n) = \sum_{lm\in X(\mu)} \frac{|\mathfrak{I}(l) - \mathfrak{I}(m)|}{\sqrt{\mathfrak{I}(l)\mathfrak{I}(m)}}$$

$$= (12)\left(\frac{|2-5|}{\sqrt{10}}\right) + \left(36n^2-36n\right)\left(\frac{|3-3|}{\sqrt{9}}\right) + (24n)\left(\frac{|3-5|}{\sqrt{15}}\right) + \left(36n^2+12n\right)\left(\frac{|3-8|}{\sqrt{24}}\right) + (12n-6)\left(\frac{|5-5|}{\sqrt{25}}\right)$$

$$+(12n)\left(\frac{|5-8|}{\sqrt{40}}\right) + \left(18n^2\right)\left(\frac{|8-8|}{\sqrt{64}}\right)$$

$$= 36.74234n^2 + 30.3329867n + 11.3841996,$$

$$\mathrm{IRLA}(\mu_n) = 2\sum_{lm\in X(\mu)} \frac{|\mathfrak{I}(l) - \mathfrak{I}(m)|}{\mathfrak{I}(l) + \mathfrak{I}(m)}$$

$$= 2(12)\left(\frac{|2-5)|}{2+5}\right) + 2\left(36n^2-36n\right)\left(\frac{|3-3|}{3+3}\right) + 2(24n)\left(\frac{|3-5)|}{3+5}\right) + 2\left(36n^2+12n\right)\left(\frac{|3-8|}{3+8}\right) + 2(12n-6)\left(\frac{|5-5|}{5+5}\right)$$

$$+2(12n)\left(\frac{|5-8|}{5+8}\right) + 2\left(18n^2\right)\left(\frac{|8-8|}{8+8}\right)$$

$$= 32.7272n^2 + 28.44746n + 10.2857,$$

Table 4: Numerical values of irregularity indices for σ_n.

Irregularity indices	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
VAR (σ_n)	0.7755	2.4637	2.9917	3.2496	3.4024
AL (σ_n)	168	696	1584	2832	4440
IR1 (σ_n)	3624	−17764	−2414016	−14099520	−54585960
IR2 (σ_n)	0.2013	15.073	40.0407	75.1820	120.5118
IRF (σ_n)	804	3408	7812	14016	22020
IRFW (σ_n)	0.44370	0.41040	0.40110	0.39673	0.39419
IRA (σ_n)	1.5312	6.6684	15.4116	27.7608	43.716
IRB (σ_n)	37.946	162.4388	373.4784	671.0648	1055.198
IRC (σ_n)	−0.29992	0.36970	0.50070	0.56580	0.6047
IRDIF (σ_n)	80	325	735	1310	2050
IRL (σ_n)	35.3076	141.2328	317.7756	564.93	882.714
IRLU (σ_n)	56	232	528	944	1480
IRLF (σ_n)	36.44231	146.364	329.766	586.6492	917.01155
IRLA (σ_n)	33.2467	131.9478	296.1033	525.7132	820.7775
IRGA (σ_n)	3.60768	15.5472	35.81856	64.4217	101.3568

Table 5: Numerical values of irregularity indices for ν_n.

Irregularity indices	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
VAR (ν_n)	−214	−242.49	−262.60	−272.5	−278.28
AL (ν_n)	180	1260	3420	6660	10980
IR1 (ν_n)	396	−35009.3	−143453	−326232	−583477
IR2 (ν_n)	−16 + 2.12	−13.9112	−14.1766	−14.35032	−14.4596
IRF (ν_n)	4860	21252	43044	70236	102828
IRFW (ν_n)	−22.5	2.9615	1.5046	1.0960	0.9052
IRA (ν_n)	1.53061	11.80106	32.885	64.783	107.495
IRB (ν_n)	37.9457	286.9305	795.5553	1563.8201	2591.7249
IRC (ν_n)	−13.76885	−13.9388	−14.38090	−14.6058	−14.7386
IRDIF (ν_n)	−80	−570	−1555	−3035	−5010
IRL (ν_n)	−42.21002	−383.525	−936.693	−1701.713	−2678.58
IRLU (ν_n)	56	408	1120	2192	3624
IRLF (ν_n)	36.4403	256.2803	696.5603	1357.2803	2238.4403
IRLA (ν_n)	33.246	230.6492	624.41	1214.545	2001.0383
IRGA (ν_n)	2.19418	24.6594	72.12018	144.576	242.027

Table 6: Numerical values of irregularity indices for μ_n.

Irregularity indices	$n = 1$	$n = 2$	$n = 3$	$n = 4$	$n = 5$
VAR (μ_n)	−0.24221	1.65104	2.445903	2.86135	3.11069
AL (μ_n)	360	1044	2088	3492	5256
IR1 (μ_n)	8365.41176	22173	40337.6170	62621.72903	88945.7142
IR2 (μ_n)	2.98091	2.40416	2.0867263	1.89199	1.761016
IRF (μ_n)	2808	7308	13608	21708	31608
IRFW (μ_n)	0.8224956	0.63338	0.559033	0.51900	0.49395
IRA (μ_n)	3.726372	10.2484	20.376798	34.11134	51.45211
IRB (μ_n)	76.11053	230.6625	471.76133	799.406	1213.599
IRC (μ_n)	−0.2139701	0.415174	0.594660	0.6678025	0.703944
IRDIF (μ_n)	172.48	484.765	962.04684	1604.328	2411.609
IRL (μ_n)	177.1077	483.11776	936.65019	1537.70	2286.28
IRLU (μ_n)	121.2	344.4	687.6	1150.8	17346
IRLF (μ_n)	78.4595263	219.019533	433.06421	720.5935	1081.6076
IRLA (μ_n)	71.46036	198.089	390.172	647.7107	970.703
IRGA (μ_n)	232.31922	672.94	1350.715	2265.64	3417.71

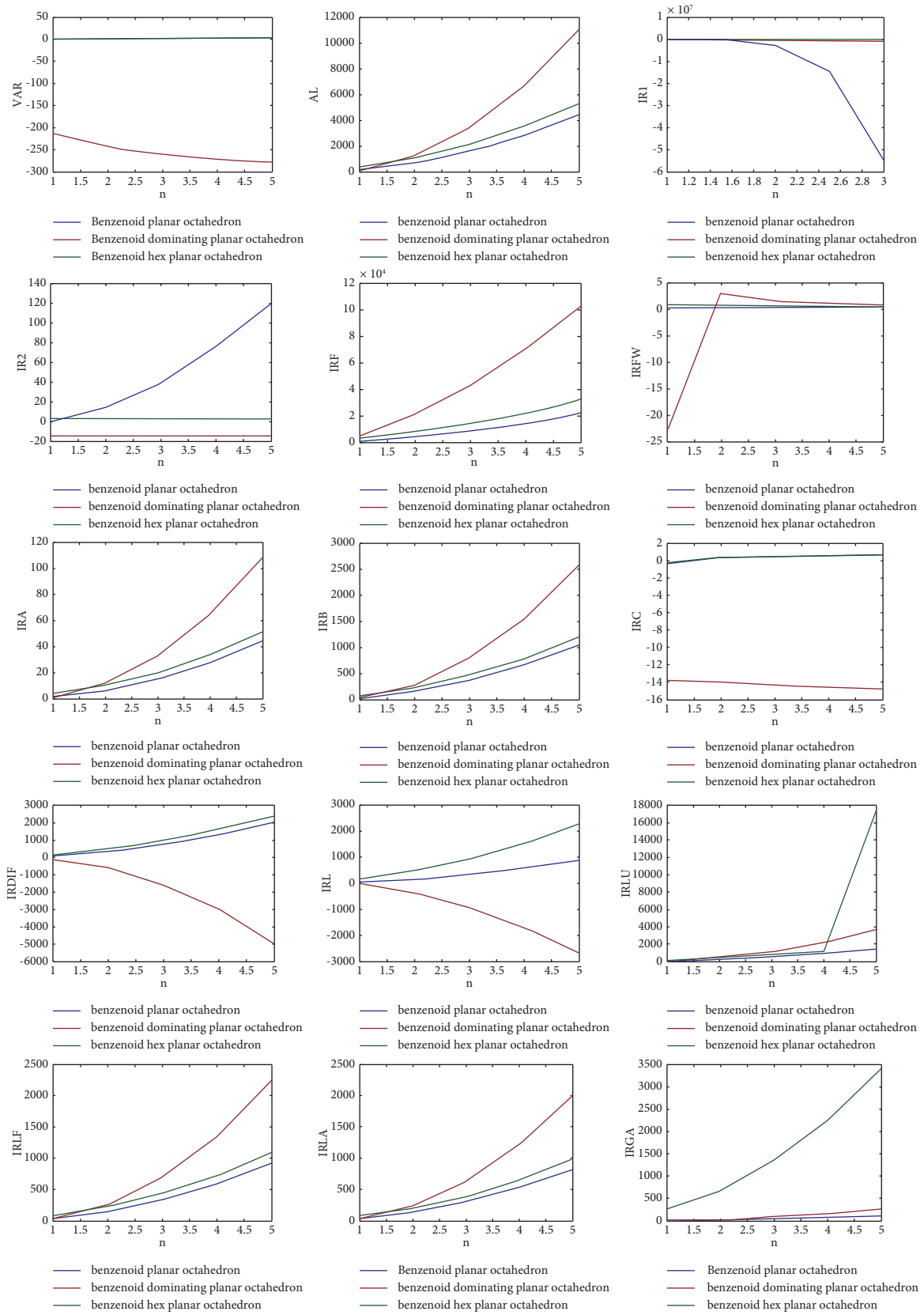

Figure 4: 2D plot for irregularity indices of benzenoid planar octahedron structure, benzenoid dominating planar octahedron structure, and benzenoid hex planar octahedron structure.

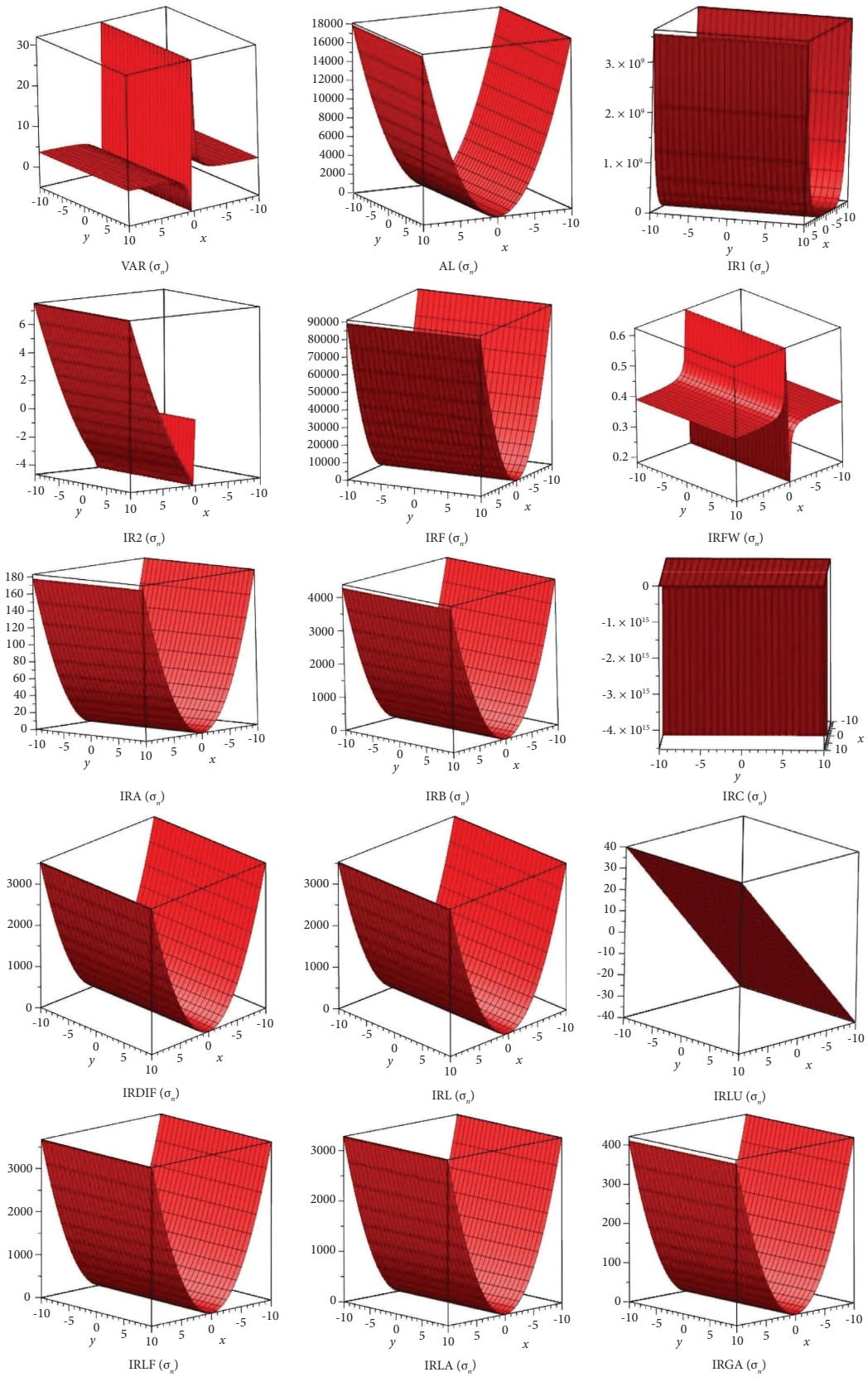

Figure 5: 3D plot for irregularity indices for σ_n.

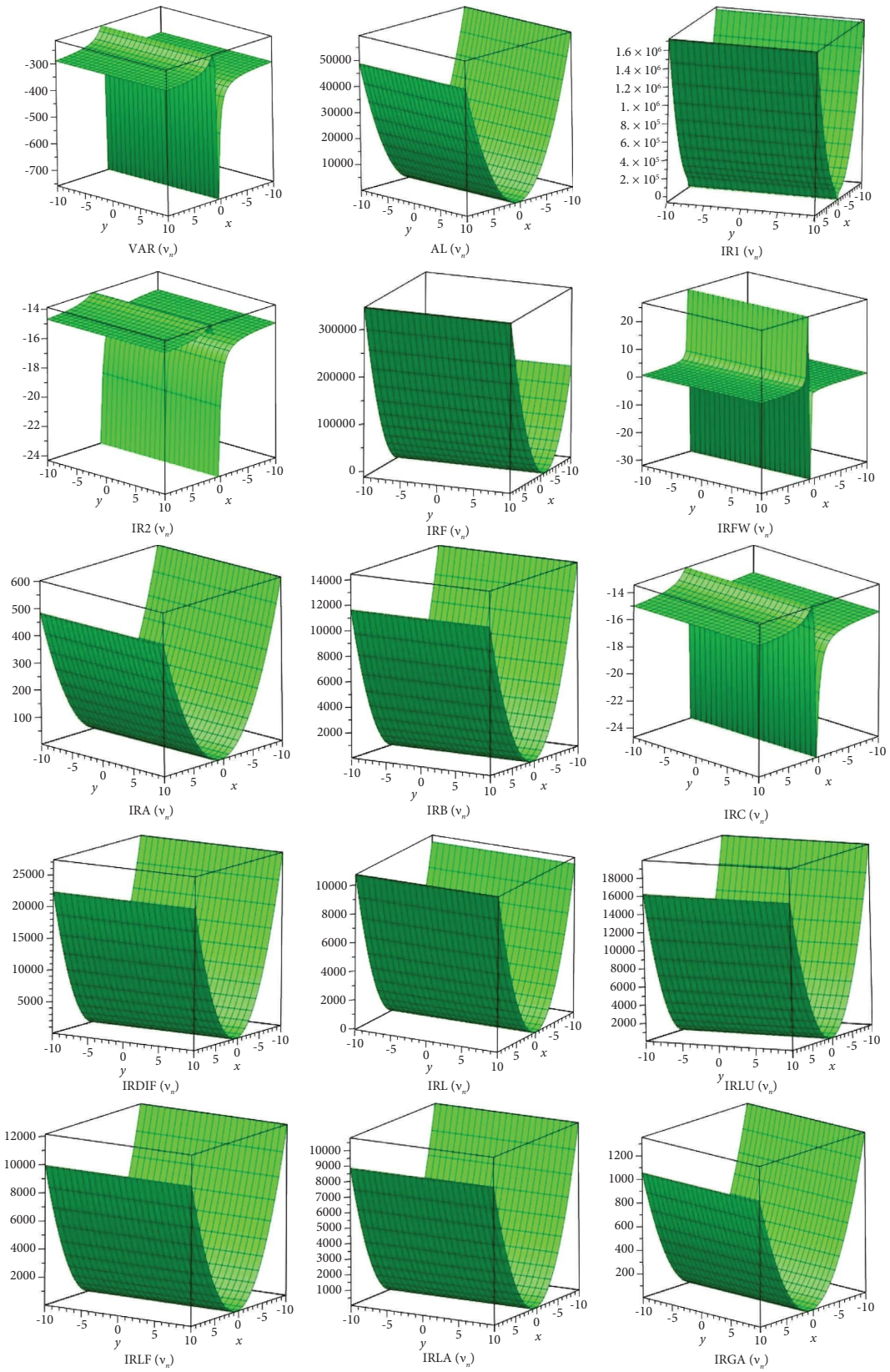

Figure 6: 3D plot for irregularity indices for v_n.

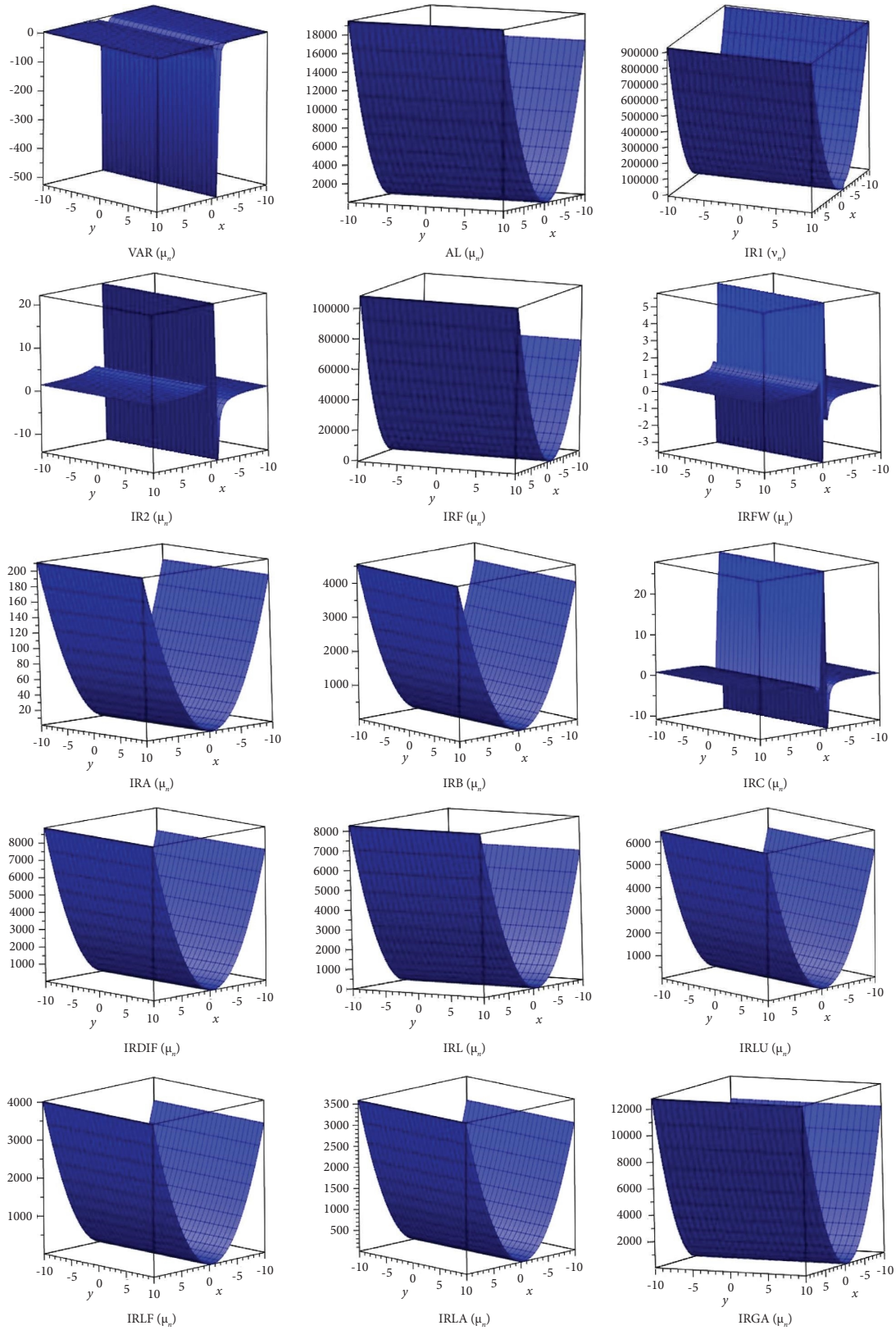

Figure 7: 3D plot for irregularity indices for μ_n.

$$\begin{aligned}\mathrm{IRGA}(\mu_n) &= \sum_{lm\in X(\mu)} \ln\frac{\mathfrak{I}(l)+\mathfrak{I}(m)}{2\sqrt{\mathfrak{I}(l)\mathfrak{I}(m)}}\\ &= (12)\left(\ln\frac{7}{2\sqrt{10}}\right)+\left(36n^2-36n\right)\left(\ln\frac{6}{2\sqrt{9}}\right)+(24n)\left(\ln\frac{8}{2\sqrt{15}}\right)+\left(36n^2+12n\right)\left(\ln\frac{11}{2\sqrt{24}}\right)\\ &\quad+(12n-6)\left(\ln\frac{10}{2\sqrt{25}}\right)+(12n)\left(\ln\frac{13}{2\sqrt{40}}\right)+\left(18n^2\right)\left(\ln\frac{16}{2\sqrt{64}}\right),\\ &= 118.5759n^2+84.894662n+28.8486661.\end{aligned} \tag{8}$$

3. Graphical Representation of the Chemical Structures

Here, we differentiate the outcomes of irregularity indices of chemical structures graphically. Three different colours have been exploited to show the graphical behaviour of irregularity indices for chemical structures. These graphs have been existed by substituting the numerical values of n through the X-axis with respect to the outcomes of irregularity indices through the Y-axis. Tables 4–6 depict such numerical values of outcomes, which can be existed after substituting the numerical values of n, and these numerical values exhibited in the tables can aid us to make graphical outcomes. Graphical lines with three distinct colours have been employed from Figure 4. Blue colour denotes the behaviour of irregular indices in the Benzenoid planar octahedron structure, red colour denotes the behaviour of irregular indices in the Benzenoid dominating planar octahedron structure, and green colour denotes the behaviour of irregular indices in the Benzenoid hex planar octahedron structure. Numerical values of n are plotted through the X-axis and two dimensional graphical behaviour of the irregularity indices through the Y-axis are shown in Figure 4. The three dimensional graphical behaviour of the irregularity indices of benzenoid structures are shown in Figures 5–7.

4. Conclusion

In the analysis of the quantitative structure property relationships (QSPRs) and (QSARs), chemical indices are important tools to approximate the characteristics of the bioactivity, physical, biomedicine, and chemical compounds. In this paper, we have provided the results on irregularity chemical indices as depicted in Figures 4–7 for Benzenoid planar octahedron structure, Benzenoid dominating planar octahedron structure, and Benzenoid hex planar octahedron structure, besides indices showed increased values for Benzenoid planar octahedron structure, Benzenoid dominating planar octahedron structure, and Benzenoid hex planar octahedron structure. The computational results which we get will aid the investigators to recognise the preferred structure more easily and would inspire the others to concentrate on the Benzenoid planar octahedron structure, Benzenoid dominating planar octahedron structure, and Benzenoid hex planar octahedron structure.

Data Availability

All the data and material used in this research is included in the paper.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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