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Research Article

Numerical and Scientific Investigation of Some Molecular Structures Based on the Criterion of Super Classical Average Assignments

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Numbering a graph is a very practical and effective technique in science and engineering. Numerous graph assignment techniques, including distance-based labeling, topological indices, and spectral graph theory, can be used to investigate molecule structures. Consider the graph G, with the injection Ω from the node set to $\{1, 2, \ldots, \Delta\}$, where Δ is the sum of the number of nodes and links. Assume that the induced link assignment Ω^* is the ceiling function of the average of root square, harmonic, geometric, and arithmetic means of the vertex labels of the end vertices of each edge. If the union of range of Ω of the node set and the range of Ω of the link set is the set $\{1, 2, \ldots, \Delta\}$, then Ω is called a super classical average assignment (SCAA). This is known as the SCAA criterion. In this study, the graphical structures corresponding to chemical structures based on the SCAA criterion are demonstrated. The graphical depiction of chemical substances was first defined and second, the union of any number of cycles C_n, the tadpole graph, the graph extracted by identifying a line of any two cycles C_m and C_n, and the graph extracted by joining any two cycles by a path are all examined in this work.

1. Introduction

The graph theory is also used to study molecules in chemistry [1]. The molecular graph theory is a branch of the graph theory that focuses on the study of the properties of molecules using graphs. In this context, a molecular graph is a graph where the vertices represent atoms and the edges represent chemical bonds between the atoms. The molecular graph theory uses various graph-theoretic concepts and techniques to analyze the properties of molecules. One of the main applications of the molecular graph theory is to study the topological properties of molecules, such as their connectivity, degree sequence, and distance matrix. For example, the degree sequence of a molecular graph represents the number of bonds that each atom has, which can be used to identify functional groups and other structural features of the molecule. Another application of the molecular graph theory is to study the chemical properties of molecules, such as their reactivity, stability, and biological activity. Graph-theoretic measures such as the Wiener index, the Randi index, and the Zagreb indices have been used to predict the biological activity of molecules based on their molecular graph [2, 3]. It is also used in computational chemistry, where it is used to model and simulate the behavior of molecules. For instance, molecular graphs are used in molecular dynamics simulations to depict the structure of molecules and to mimic their motion and interactions through time. It is an important tool for understanding the properties of molecules and their behavior in chemical reactions. It has applications in drug discovery, material science, and many other fields of chemistry. Graph labeling is an important tool in the molecular graph theory, which studies the properties of molecules using the graph theory. In this context, graph labeling is used to represent atoms and bonds in a molecule and to label these atoms and bonds with various attributes, such as atomic number, bond order, and hybridization. Quantitative structure-activity relationship (QSAR) studies use mathematical models to predict the biological activity of compounds based on their chemical structure. Graph labeling is used to represent the chemical structure of the compounds, and the labels can be used as input features for the QSAR model. Graph labeling is used to represent chemical reaction networks, which are networks of chemical reactions that occur in a system [4]. The labels on the nodes and edges of the graph represent the chemical species and the reactions, respectively. It can also be used to measure the similarity between two molecules. The labels on the atoms and bonds of the molecules are used to calculate a similarity score between the two molecules, which can be used to predict their biological activity or other properties.

A graph is described as a finite, undirected, and simple graph throughout this work. Considering the graph $G(V, E)$, which has p vertices and q edges, researchers are using the notations and contexts [5–8] and proposing [9–16] for a comprehensive review of the graph theory and its applications. P_n represents a path containing n vertices, while C_n represents a cycle containing n vertices. The graph $G(V, E) = G_1 \cup G_2$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 are the graphs with $V = V_1 \cup V_2$ and $E = E_1 \cup E_2$. The union of m number of cycles of equal length n is indicated by m_{C_n}.

2. Literature Survey

In [17], Barrientos examined at graceful labelings of chain and corona graphs. The mean labeling [18] of graphs was defined by Somosundaram and Ponraj, and super mean labeling [19] was discussed by Vasuki and Arockiaraj. Baskar and Arockiaraj proposed the principles of F-geometric mean labeling [20] and super geometric mean labeling [21] and highlighted them for several standard graphs. In [22], the authors introduced C-exponential mean graphs. In [23], Durai Baskar and Saratha Devi created the idea of super C-logarithmic mean labeling. The super fibonacci graceful labelings of several graphs were described by Vaidya and Prajapati [24]. Muhiuddin et al. defined classical mean graph labeling [25], whereas Alanazi et al. expanded it to specific ladder graphs [26]. Recently, the authors explained that the classical mean labeling of various graphs has been developed by duplicating operations [27]. Here, the researchers extend and investigate a super classical mean-labeling techniques based on graph operation strategies in a significant number of investigators in the area of graph labeling.

3. Methodology

Consider the graph G, with the injection Ω from the node set to $\{1, 2, \ldots, \Delta\}$, where Δ is the sum of the number of nodes and links. Assume that the induced link assignment Ω^* is the ceiling function of the average of root square, harmonic, geometric, and arithmetic means of the vertex labels of the end vertices of each edge. If the union of range of Ω of the node set and the range of Ω of the link set is the set $\{1, 2, \ldots, \Delta\}$, then Ω is called a super classical average assignment (SCAA). This is known as the SCAA criterion. Here, the researchers have demonstrated the SCAA by using the ceiling function and established the SCAA of some standard structures.

1-ethyl-2-methylcyclobutane is an organic compound with the molecular formula C_8H_{16} [1]. Let us break down the name to apprehend its composition as follows: “1-ethyl” designates that there is an ethyl group (C_2H_5) attached to the first carbon atom of the cyclobutane ring. “2-methyl” designates that there is a methyl group (CH_3) committed to the second carbon atom of the cyclobutane ring. Now, let us visualize the molecule. It has a cyclobutane ring, which is a four-membered carbon ring, where each carbon atom is attached to two hydrogen atoms. The first carbon atom in the ring has an ethyl group (C_2H_5) attached to it, which comprises two carbon atoms and five hydrogen atoms. The second carbon atom in the ring has a methyl group (CH_3) attached to it, which consists of one carbon atom and three hydrogen atoms. The chemical formulation of 1-ethyl-2-methylcyclobutane can be written as C_8H_{16}, representing it has 8 carbon atoms and 16 hydrogen atoms in its structure. This molecule is an illustration of a cycloalkane with substituent groups, making it an attention-grabbing compound in organic chemistry. It is a cyclobutane derivative with one ethyl group and one methyl group attached to the cyclobutane ring. Figure 1 depicts 1-ethyl-2-methylcyclobutane and its corresponding SCAA in the hydrogen-depleted molecular graph. Here, the number of points and links are 7. Based on the SCAA, the vertex and edge sets are $\{1, 3, 5, 8, 10, 12, 14\}$ and $\{2, 4, 6, 7, 9, 11, 13\}$, respectively.

4. Results and Discussion

The assignment of various simple graphs and some chain graphs based on super classical averages are discussed. By implementing these super classical averages, it provides more accurate assignment values. Also, the collection of unions of node and link assignment values are $\{1, 2, \ldots, \Delta\}$, where Δ is the sum of nodes and links.

4.1. Super Classical Meanness of Some Simple Graphs

Theorem 1. *For $n \geq 5$, the union of any number of cycles C_n meets its SCAA criterion.*

Proof. Let the graph G be the union of k cycles. Let $\left\{v_j^{(i)}; 1 \leq j \leq p_i\right\}$ be the vertices of the i^{th} cycle C_{p_i} with $p_i \geq 5$ and $1 \leq i \leq k$.

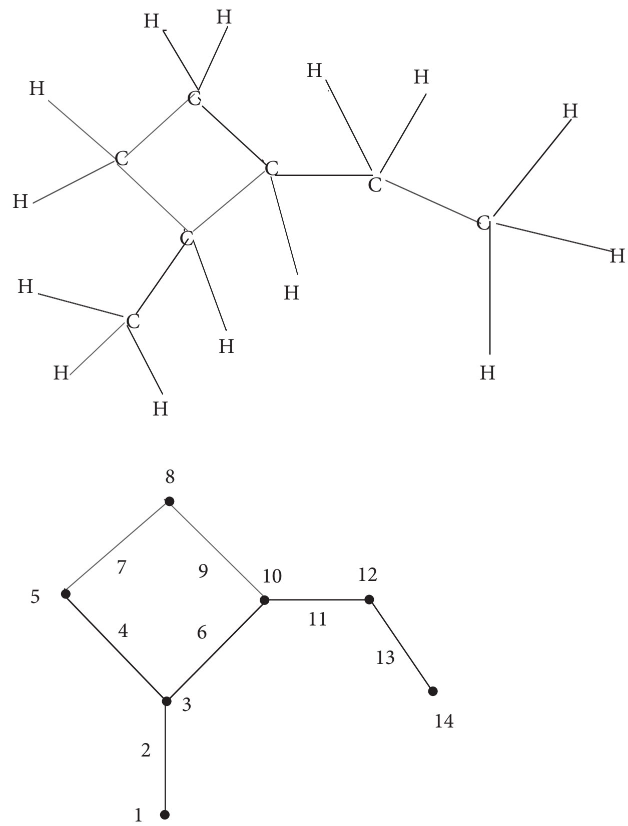

Figure 1: 1-ethyl-2-methylcyclobutane and its corresponding SCAA of the hydrogen-depleted molecular graph.

Assign the following values to $\Omega\colon V(G) \longrightarrow \{1, 2, 3, \ldots, \sum_{i=1}^{k} 2p_i\}$.

When p_1 is odd,

$$\Omega\left(v_j^{(1)}\right) = \begin{cases} 2j-1, & 1 \le j \le 2, \\ 4j-6, & 3 \le j \le \left\lfloor \dfrac{p_1}{2} \right\rfloor + 2, \\ 4p_1 + 7 - 4j, & \left\lfloor \dfrac{p_1}{2} \right\rfloor + 3 \le j \le p_1. \end{cases} \tag{1}$$

The values associated with the influenced line assignment will be provided by

$$\begin{aligned} \Omega^*\left(v_j^{(1)} v_{j+1}^{(1)}\right) &= \begin{cases} 3j-1, & 1 \le j \le 2, \\ 4j-4, & 3 \le j \le \left\lfloor \dfrac{p_1}{2} \right\rfloor + 1, \\ 4p_1 + 5 - 4j, & \left\lfloor \dfrac{p_1}{2} \right\rfloor + 2 \le j \le p_1 - 1, \end{cases} \\ \Omega^*\left(v_1^{(1)} v_{p_1}^{(1)}\right) &= 4. \end{aligned} \tag{2}$$

When p_1 is even,

$$\Omega\left(v_j^{(1)}\right) = \begin{cases} 2j-1, & 1 \le j \le 2, \\ 4j-6, & 3 \le j \le \left\lfloor \dfrac{p_1}{2} \right\rfloor, \\ 4j-7, & j = \left\lfloor \dfrac{p_1}{2} \right\rfloor + 1, \\ 4j-8, & j = \left\lfloor \dfrac{p_1}{2} \right\rfloor + 2, \\ 4p_1 + 7 - 4j, & \left\lfloor \dfrac{p_1}{2} \right\rfloor + 3 \le j \le p_1. \end{cases} \tag{3}$$

The values associated with the influenced line assignment will be provided by

$$\begin{aligned} \Omega^*\left(v_j^{(1)} v_{j+1}^{(1)}\right) &= \begin{cases} 3j-1, & 1 \le j \le 2, \\ 4j-4, & 3 \le j \le \left\lfloor \dfrac{p_1}{2} \right\rfloor, \\ 4j-5, & j = \left\lfloor \dfrac{p_1}{2} \right\rfloor + 1, \\ 4j-10, & j = \left\lfloor \dfrac{p_1}{2} \right\rfloor + 2, \\ 4p_1 + 5 - 4j, & \left\lfloor \dfrac{p_1}{2} \right\rfloor + 3 \le j \le p_1 - 1, \end{cases} \\ \Omega^*\left(v_1^{(1)} v_{p_1}^{(1)}\right) &= 4. \end{aligned} \tag{4}$$

Let $P_i \doteq 0 \,(\mathrm{mod}\, 2)$ and $k \geq i \geq 2$, then

$$\Omega\left(v_j^{(i)}\right) = \begin{cases} \Omega\left(v_{\lfloor p_{i-1}/2 \rfloor + 2}^{(i-1)}\right) + 1, & j = 1, \\ \Omega\left(v_{\lfloor p_{i-1}/2 \rfloor + 2}^{(i-1)}\right) + 4j - 5, & 2 \leq j \leq \left\lfloor \dfrac{p_i}{2} \right\rfloor, \\ \Omega\left(v_{\lfloor p_{i-1}/2 \rfloor + 2}^{(i-1)}\right) + 4j - 4, & j = \left\lfloor \dfrac{p_i}{2} \right\rfloor + 1, \\ \Omega\left(v_{\lfloor p_{i-1}/2 \rfloor + 2}^{(i-1)}\right) + 4j - 11, & j = \left\lfloor \dfrac{p_i}{2} \right\rfloor + 2, \\ \Omega\left(v_{\lfloor p_{i-1}/2 \rfloor + 2}^{(i-1)}\right) + 4p_i + 6 - 4j, & \left\lfloor \dfrac{p_i}{2} \right\rfloor + 3 \leq j \leq p_i. \end{cases} \tag{5}$$

The values associated with the influenced line assignment will be provided by

$$\Omega^*\left(v_1^{(i)} v_{p_i}^{(i)}\right) = \Omega\left(v_{\lfloor p_{i-1}/2 \rfloor + 2}^{(i-1)}\right) + 4,$$

$$\Omega^*\left(v_j^{(i)} v_{j+1}^{(i)}\right) = \begin{cases} \Omega\left(v_{\lfloor p_{i-1}/2 \rfloor + 2}^{(i-1)}\right) + 2, & j = 1, \\ \Omega\left(v_{\lfloor p_{i-1}/2 \rfloor + 2}^{(i-1)}\right) + 4j - 3, & 2 \leq j \leq \left\lfloor \dfrac{p_i}{2} \right\rfloor - 1, \\ \Omega\left(v_{\lfloor p_{i-1}/2 \rfloor + 2}^{(i-1)}\right) + 4j - 2, & j = \left\lfloor \dfrac{p_i}{2} \right\rfloor, \\ \Omega\left(v_{\lfloor p_{i-1}/2 \rfloor + 2}^{(i-1)}\right) + 4j - 5, & j = \left\lfloor \dfrac{p_i}{2} \right\rfloor + 1, \\ \Omega\left(v_{\lfloor p_{i-1}/2 \rfloor + 2}^{(i-1)}\right) + 4p_i + 4 - 4j, & \left\lfloor \dfrac{p_i}{2} \right\rfloor + 2 \leq j \leq p_i - 1. \end{cases} \tag{6}$$

Hence, Ω satisfies the required numbering and also the resultant graph admits required labeling. Figure 2 depicts an SCAA of $C_6 \cup C_8 \cup C_5 \cup C_7$. □

Theorem 2. *The graphical structure $T(n,k)$ meets its SCAA criterion.*

Proof. Let $v_j \in V[P_n]$ and $u_j \in V[C_n]$. $T(n,k)$ is constructed by identifying the vertex $u_{(n+3/2)}$ and v_1 while $n \neq 0 \pmod 2$ and $u_{(n+2/2)}$ and v_1 while n is even.

Case (i). $m \geq 5$.

Sub case (i). m is odd.

Assign the following values to Ω: $V(G) \longrightarrow \{1, 2, 3, \ldots, 2n+2k-2\}$.

$$\Omega(u_i) = \begin{cases} 2i-1, & 1 \leq i \leq 2, \\ 4i-6, & 3 \leq i \leq \left\lfloor \dfrac{n}{2} \right\rfloor + 2, \\ 4n+7-4i, & \left\lfloor \dfrac{n}{2} \right\rfloor + 3 \leq i \leq n, \end{cases} \tag{7}$$

$$\Omega(v_i) = 2n+2i-2, \quad \text{for } 2 \leq i \leq k.$$

The values associated with the influenced line assignment will be provided by

$$\Omega^*(u_i u_{i+1}) = \begin{cases} 3i-1, & 1 \leq i \leq 2, \\ 4i-4, & 3 \leq i \leq \left\lfloor \dfrac{n}{2} \right\rfloor + 1, \\ 4n+5-4i, & \left\lfloor \dfrac{n}{2} \right\rfloor + 3 \leq i \leq n-1, \end{cases} \tag{8}$$

$$\Omega^*(u_1 u_n) = 4,$$

$$\Omega^*(v_i v_{i+1}) = 2n+2i-1, \quad \text{for } 1 \leq i \leq k-1.$$

Sub case (ii). m is even.

Assign the following values to Ω: $V(G) \longrightarrow \{1, 2, 3, \ldots, 2n+2k-2\}$.

$$\Omega(u_i) = \begin{cases} 3, & i = 1, \\ 4i-2, & 2 \leq i \leq \left\lfloor \dfrac{n}{2} \right\rfloor - 1, \\ 4i-3, & i = \left\lfloor \dfrac{n}{2} \right\rfloor, \\ 4i-4, & i = \left\lfloor \dfrac{n}{2} \right\rfloor + 1, \\ 4n+3-4i, & \left\lfloor \dfrac{n}{2} \right\rfloor + 2 \leq i \leq n-1, \end{cases} \tag{9}$$

$$\Omega(u_n) = 1,$$

$$\Omega(v_i) = 2n+2i-2, \quad \text{for } 2 \leq i \leq k.$$

The values associated with the influenced line assignment will be provided by

$$\Omega^*(u_i u_{i+1}) = \begin{cases} 5, & i = 1, \\ 4i, & 2 \leq i \leq \left\lfloor \dfrac{n}{2} \right\rfloor - 1, \\ 4i-1, & i = \left\lfloor \dfrac{n}{2} \right\rfloor, \\ 4i-6, & i = \left\lfloor \dfrac{n}{2} \right\rfloor + 1, \\ 4n-4i, & \left\lfloor \dfrac{n}{2} \right\rfloor + 2 \leq i \leq n-1, \end{cases} \tag{10}$$

$$\Omega^*(u_1 u_n) = 2,$$

$$\Omega^*(v_i v_{i+1}) = 2n+2i-1, \quad \text{for } 1 \leq i \leq k-1.$$

Case (ii). $n = 4$.

Assign the following values to Ω: $V(G) \longrightarrow \{1, 2, 3, \ldots, 2k+6\}$.

$$\begin{aligned} \Omega(u_1) &= 3, \\ \Omega(u_2) &= 1, \\ \Omega(u_3) &= 8, \\ \Omega(u_4) &= 6, \\ \Omega(v_i) &= 6+2i, \quad \text{for } 1 \leq i \leq k. \end{aligned} \tag{11}$$

The values associated with the influenced line assignment will be provided by

$$\begin{aligned} \Omega^*(u_1 u_2) &= 2, \\ \Omega^*(u_2 u_3) &= 4, \\ \Omega^*(v_i v_{i+1}) &= 2i+7, \quad \text{for } 1 \leq i \leq k-1, \\ \Omega^*(u_1 u_4) &= 5, \\ \Omega^*(u_3 u_4) &= 7. \end{aligned} \tag{12}$$

Hence, Ω satisfies the required numbering and also the resultant graph admits required labeling. Figure 3 depicts an SCAA of $T(7, 5)$. □

Theorem 3. *For any m and $n \geq 5$, the graphical structure obtained by identifying an edge of any two cycles C_m and C_n meets its SCAA criterion.*

Proof. Let $u_m \in V[C_m]$ and $v_n \in V[C_n]$. Let G be the resultant graph obtained by identifying the edge $u_{(m+1/2)} u_{(m+3/2)}$ of the cycle C_m with the edge $v_n v_1$ of the cycle C_n when m is odd and $u_{(m/2)} u_{(m+2/2)}$ of C_m with the edge $v_n v_1$ of C_n when m is even.

Case (i). m and n are odd.

Assign the following values to Ω: $V(G) \longrightarrow \{1, 2, 3, \ldots, 2m+2n-3\}$.

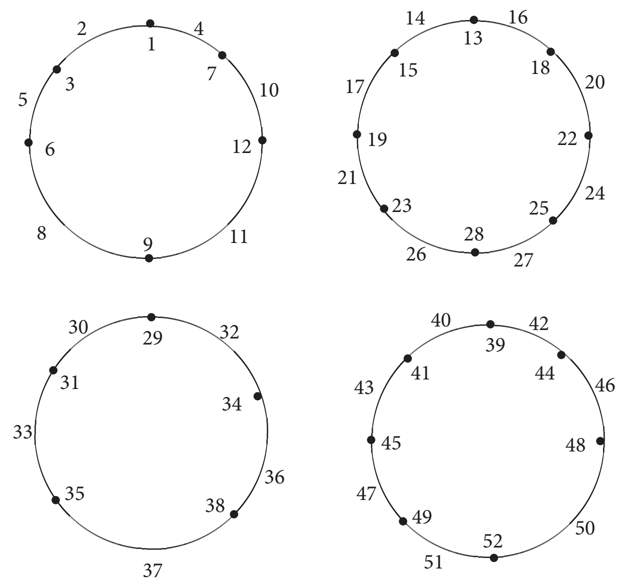

Figure 2: An SCAA of $C_6 \cup C_8 \cup C_5 \cup C_7$.

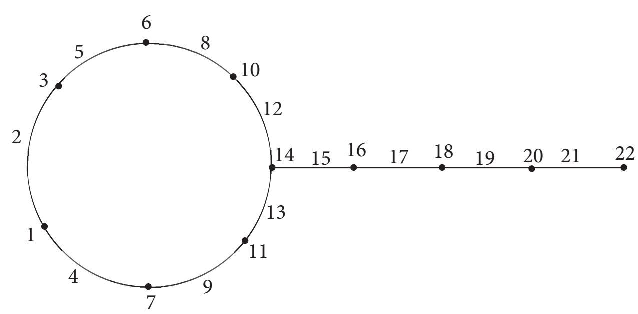

Figure 3: An SCAA of $T(7,5)$.

$$\Omega(u_i) = \begin{cases} 3, & i = 1, \\ 4i - 2, & 2 \le i \le \left\lfloor \dfrac{m}{2} \right\rfloor + 1, \\ 4m + 3 - 4i, & \left\lfloor \dfrac{m}{2} \right\rfloor + 2 \le i \le m - 1, \end{cases}$$

$$\Omega(u_m) = 1,$$

$$\Omega(v_i) = \begin{cases} 2m + 4i - 5, & 2 \le i \le \left\lfloor \dfrac{n}{2} \right\rfloor + 1, \\ 2m + 4n - 4i, & \left\lfloor \dfrac{n}{2} \right\rfloor + 2 \le i \le n - 1. \end{cases} \tag{13}$$

The values associated with the influenced line assignment will be provided by

$$\Omega^*(u_i u_{i+1}) = \begin{cases} 5, & i = 1, \\ 4i, & 2 \le i \le \left\lfloor \dfrac{m}{2} \right\rfloor, \\ 4m + 1 - 4i, & \left\lfloor \dfrac{m}{2} \right\rfloor + 1 \le i \le m - 2, \end{cases}$$

$$\Omega^*(u_{m-1} u_m) = 4,$$

$$\Omega^*(u_m u_1) = 2,$$

$$\Omega^*(v_i v_{i+1}) = \begin{cases} 2m + 2, & i = 1, \\ 2m + 4i - 3, & 2 \le i \le \left\lfloor \dfrac{n}{2} \right\rfloor, \\ 2m + 4n - 4i - 2, & \left\lfloor \dfrac{n}{2} \right\rfloor + 1 \le i \le n - 2, \end{cases}$$

$$\Omega^*(v_{n-1} v_n) = 2m + 1. \tag{14}$$

Case (ii). m is odd and $n \doteq 0 \pmod 2$

Assign the following values to Ω: $V(G) \longrightarrow \{1, 2, 3, \ldots, 2m+2n-3\}$.

$$\Omega(u_i) = \begin{cases} 3, & i = 1, \\ 4i-2, & 2 \le i \le \left\lfloor \frac{m}{2} \right\rfloor + 1, \\ 4m+3-4i, & \left\lfloor \frac{m}{2} \right\rfloor + 2 \le i \le m-1, \end{cases}$$

$$\Omega(u_m) = 1,$$

$$\Omega(v_i) = \begin{cases} 2m+4i-5, & 2 \le i \le \left\lfloor \frac{n}{2} \right\rfloor - 1, \\ 2m+4i-6, & i = \left\lfloor \frac{n}{2} \right\rfloor, \\ 2m+4i-7, & i = \left\lfloor \frac{n}{2} \right\rfloor + 1, \\ 2m+4n-4i, & \left\lfloor \frac{n}{2} \right\rfloor + 2 \le i \le n-1. \end{cases} \quad (15)$$

The values associated with the influenced line assignment will be provided by

$$\Omega^*(u_{m-1}u_m) = 4,$$

$$\Omega^*(u_m u_1) = 2,$$

$$\Omega^*(v_{n-1}v_n) = 2m+1,$$

$$\Omega^*(v_i v_{i+1}) = \begin{cases} 2m+2, & i = 1, \\ 2m+4i-3, & 2 \le i \le \left\lfloor \frac{n}{2} \right\rfloor - 1, \\ 2m+4i-4, & i = \left\lfloor \frac{n}{2} \right\rfloor, \\ 2m+4n-4i-1, & i = \left\lfloor \frac{n}{2} \right\rfloor + 1, \\ 2m+4n-4i-2, & \left\lfloor \frac{n}{2} \right\rfloor + 2 \le i \le n-2. \end{cases} \quad (16)$$

Case (iii). m is even and $n \ne 0 \pmod 2$.

Assign the following values to Ω: $V(G) \longrightarrow \{1, 2, 3, \ldots, 2m+2n-3\}$.

$$\Omega(u_i) = \begin{cases} 3, & i = 1, \\ 4i-2, & 2 \le i \le \left\lfloor \frac{m}{2} \right\rfloor - 1, \\ 4i-3, & \left\lfloor \frac{m}{2} \right\rfloor \le i \le \left\lfloor \frac{m}{2} \right\rfloor + 1, \\ 4m+3-4i, & \left\lfloor \frac{m}{2} \right\rfloor + 2 \le i \le m-1, \end{cases}$$

$$\Omega(u_m) = 1,$$

$$\Omega(v_i) = \begin{cases} 2m+4i-6, & 2 \le i \le \left\lfloor \frac{n}{2} \right\rfloor, \\ 2m+4i-5, & i = \left\lfloor \frac{n}{2} \right\rfloor + 1, \\ 2m+4n-4i, & i = \left\lfloor \frac{n}{2} \right\rfloor + 2, \\ 2m+4n+1-4i, & \left\lfloor \frac{n}{2} \right\rfloor + 3 \le i \le n-1. \end{cases} \quad (17)$$

The values associated with the influenced line assignment will be provided by

$$\Omega^*(u_{m-1}u_m) = 4,$$

$$\Omega^*(u_m u_1) = 2,$$

$$\Omega^*(v_i v_{i+1}) = \begin{cases} 2m+4i-4, & 1 \le i \le \left\lfloor \frac{n}{2} \right\rfloor - 1, \\ 2m+4i-3, & i = \left\lfloor \frac{n}{2} \right\rfloor, \\ 2m+4i-6, & i = \left\lfloor \frac{m}{2} \right\rfloor + 1, \\ 2m+4n-4i-1, & \left\lfloor \frac{n}{2} \right\rfloor + 1 \le i \le n-1, \end{cases} \quad (18)$$

Case (iv). m and n are even.

Assign the following values to Ω: $V(G) \longrightarrow \{1, 2, 3, \ldots, 2m+2n-3\}$.

$$\Omega(u_m) = 1,$$

$$\Omega(v_i) = \begin{cases} 2m+4i-6, & 2 \le i \le \left\lfloor \frac{n}{2} \right\rfloor, \\ 2m+4n-4i+1, & \left\lfloor \frac{n}{2} \right\rfloor + 1 \le i \le n-1, \end{cases}$$

$$\Omega(u_i) = \begin{cases} 3, & i = 1, \\ 4i-2, & 2 \le i \le \left\lfloor \frac{m}{2} \right\rfloor - 1, \\ 2m-3, & i = \left\lfloor \frac{m}{2} \right\rfloor, \\ 2m+1, & i = \left\lfloor \frac{m}{2} \right\rfloor + 1, \\ 4m-4i+3, & \left\lfloor \frac{m}{2} \right\rfloor + 2 \le i \le m-1. \end{cases} \quad (19)$$

The values associated with the influenced line assignment will be provided by

$$\Omega^*\left(u_{m-1}u_m\right) = 4,$$

$$\Omega^*\left(v_i v_{i+1}\right) = \begin{cases} 2m + 4i - 4, & 1 \leq i \leq \left\lfloor \dfrac{n}{2} \right\rfloor, \\ 2m + 4n - 4i - 1, & \left\lfloor \dfrac{n}{2} \right\rfloor + 1 \leq i \leq n - 1, \end{cases}$$

$$\Omega^*\left(u_m u_1\right) = 2,$$

$$\Omega^*\left(u_i u_{i+1}\right) = \begin{cases} 5, & i = 1, \\ 4i, & 2 \leq i \leq \left\lfloor \dfrac{m}{2} \right\rfloor - 1, \\ 2m - 1, & i = \left\lfloor \dfrac{m}{2} \right\rfloor, \\ 2m - 2, & i = \left\lfloor \dfrac{m}{2} \right\rfloor + 1, \\ 4m - 4i + 1, & \left\lfloor \dfrac{m}{2} \right\rfloor + 2 \leq i \leq m - 2. \end{cases} \tag{20}$$

Hence, Ω satisfies the required numbering and also the resultant graph admits required labeling. □

Theorem 4. *For any m and $n \geq 5$, the graphical structure obtained by joining any two cycles C_m and C_n by a path P_k meets its SCAA criterion.*

Proof. Let $u_m \in V[C_m]$ and $v_n \in V[C_n]$. Let $w_1, w_2, \ldots, w_k$ be the vertices of the path P_k with $u_{(m+3/2)} = w_1$ when m is odd, $u_{(m+2/2)} = w_1$ when m is even, and $w_k = v_n$.

Case (i). m is odd.

Assign the following values to Ω: $V(G) \longrightarrow \{1, 2, 3, \ldots, 2m + 2k + 2n - 3\}$.

$$\Omega\left(u_i\right) = \begin{cases} 2i - 1, & 1 \leq i \leq 2, \\ 4i - 6, & 3 \leq i \leq \left\lfloor \dfrac{m}{2} \right\rfloor + 2, \\ 4m - 4i + 7, & \left\lfloor \dfrac{m}{2} \right\rfloor + 3 \leq i \leq m, \end{cases}$$

$$\Omega\left(w_i\right) = 2m + 2i - 2, \quad \text{for } 2 \leq i \leq k,$$

$$\Omega\left(v_i\right) = \begin{cases} 2m + 2k + 4i - 8, & 2 \leq i \leq \left\lfloor \dfrac{n}{2} \right\rfloor, \\ 2m + 2k + 4i - 8, & i = \left\lfloor \dfrac{n}{2} \right\rfloor + 1 \text{ and } n \neq 0 \,(\operatorname{mod} 2), \\ 2m + 2k + 4i - 7, & i = \left\lfloor \dfrac{n}{2} \right\rfloor + 1 \text{ and } n \doteq 0 \,(\operatorname{mod} 2), \\ 2m + 2k + 4i - 9, & i = \left\lfloor \dfrac{n}{2} \right\rfloor + 2 \text{ and } n \neq 0 \,(\operatorname{mod} 2), \\ 2m + 2k + 4i - 14, & i = \left\lfloor \dfrac{n}{2} \right\rfloor + 2 \text{ and } n \doteq 0 \,(\operatorname{mod} 2), \\ 2m + 2k + 4n - 4i + 3, & \left\lfloor \dfrac{n}{2} \right\rfloor + 3 \leq i \leq n. \end{cases} \tag{21}$$

The values associated with the influenced line assignment will be provided by

$$\Omega^*(u_iu_{i+1}) = \begin{cases} 3i-1, & 1 \le i \le 2, \\ 4i-4, & 3 \le i \le \left\lfloor \frac{m}{2} \right\rfloor + 1, \\ 4m-4i+5, & \left\lfloor \frac{m}{2} \right\rfloor + 2 \le i \le m-1, \end{cases}$$

$$\Omega^*(u_1u_m) = 4,$$

$$\Omega^*(w_iw_{i+1}) = 2m+2i-1, \quad \text{for } 2 \le i \le k-1,$$

$$\Omega^*(v_iv_{i+1}) = \begin{cases} 2m+2k-1, & i=1, \\ 2m+2k+4i-6, & 2 \le i \le \left\lfloor \frac{n}{2} \right\rfloor - 1, \\ 2m+2k+4i-6, & i = \left\lfloor \frac{n}{2} \right\rfloor \text{ and } n \neq 0 \, (\mathrm{mod}\, 2), \\ 2m+2k+4i-5, & i = \left\lfloor \frac{n}{2} \right\rfloor \text{ and } n \doteq 0 \, (\mathrm{mod}\, 2), \\ 2m+2k+4i-6, & i = \left\lfloor \frac{n}{2} \right\rfloor + 1 \text{ and } n \neq 0 \, (\mathrm{mod}\, 2), \\ 2m+2k+4i-8, & i = \left\lfloor \frac{n}{2} \right\rfloor + 1 \text{ and } n \doteq 0 \, (\mathrm{mod}\, 2), \\ 2m+2k+4n-4i+1, & \left\lfloor \frac{n}{2} \right\rfloor + 2 \le i \le n-1 \text{ and}, \end{cases} \tag{22}$$

$$\Omega^*(v_1v_n) = 2m+2k+1.$$

Case (ii). m is even.

Assign the following values to $\Omega: V(G) \longrightarrow \{1, 2, 3, \ldots, 2m+2k+2n-3\}$.

$$\Omega(u_i) = \begin{cases} 3, & i=1, \\ 4i-2, & 2 \le i \le \left\lfloor \frac{m}{2} \right\rfloor - 1, \\ 4i-3, & i = \left\lfloor \frac{m}{2} \right\rfloor, \\ 4i-4, & i = \left\lfloor \frac{m}{2} \right\rfloor + 1, \\ 4m-4i+3, & \left\lfloor \frac{m}{2} \right\rfloor + 2 \le i \le m-1, \end{cases}$$

$$\Omega(u_m) = 1,$$

$$\Omega(w_i) = 2m+2i-2, \quad \text{for } 2 \le i \le k,$$

$$\Omega(v_i) = \begin{cases} 2m + 2k + 4i - 8, & 2 \le i \le \left\lfloor \frac{n}{2} \right\rfloor, \\ 2m + 2k + 4i - 8, & i = \left\lfloor \frac{n}{2} \right\rfloor + 1 \text{ and } n \neq 0 \, (\text{mod } 2), \\ 2m + 2k + 4i - 7, & i = \left\lfloor \frac{n}{2} \right\rfloor + 1 \text{ and } n \doteq 0 \, (\text{mod } 2), \\ 2m + 2k + 4i - 9, & i = \left\lfloor \frac{n}{2} \right\rfloor + 2 \text{ and } n \neq 0 \, (\text{mod } 2), \\ 2m + 2k + 4i - 14, & i = \left\lfloor \frac{n}{2} \right\rfloor + 2 \text{ and } n \doteq 0 \, (\text{mod } 2), \\ 2m + 2k + 4n - 4i + 3, & \left\lfloor \frac{n}{2} \right\rfloor + 3 \le i \le n. \end{cases} \tag{23}$$

The values associated with the influenced line assignment will be provided by

$$\begin{aligned} \Omega^*(u_i u_{i+1}) &= \begin{cases} 5, & i = 1, \\ 4i, & 2 \le i \le \left\lfloor \frac{m}{2} \right\rfloor - 1, \\ 4i - 1, & i = \left\lfloor \frac{m}{2} \right\rfloor, \\ 4i - 6, & i = \left\lfloor \frac{m}{2} \right\rfloor + 1, \\ 4m - 4i, & \left\lfloor \frac{m}{2} \right\rfloor + 2 \le i \le m - 1, \end{cases} \\ \Omega^*(u_1 u_m) &= 2, \\ \Omega^*(w_i w_{i+1}) &= 2m + 2i - 1, \quad \text{for } 1 \le i \le k - 1, \\ \Omega^*(v_i v_{i+1}) &= \begin{cases} 2m + 2k - 1, & i = 1, \\ 2m + 2k + 4i - 6, & 2 \le i \le \left\lfloor \frac{n}{2} \right\rfloor - 1, \\ 2m + 2k + 4i - 6, & i = \left\lfloor \frac{n}{2} \right\rfloor \text{ and } n \neq 0 \, (\text{mod } 2), \\ 2m + 2k + 4i - 5, & i = \left\lfloor \frac{n}{2} \right\rfloor \text{ and } n \doteq 0 \, (\text{mod } 2), \\ 2m + 2k + 4i - 6, & i = \left\lfloor \frac{n}{2} \right\rfloor + 1 \text{ and } n \neq 0 \, (\text{mod } 2), \\ 2m + 2k + 4i - 8, & i = \left\lfloor \frac{n}{2} \right\rfloor + 1 \text{ and } n \doteq 0 \, (\text{mod } 2), \\ 2m + 2k + 4n - 4i + 1, & \left\lfloor \frac{n}{2} \right\rfloor + 2 \le i \le n - 1, \end{cases} \\ \Omega^*(v_1 v_n) &= 2m + 2k + 1. \end{aligned} \tag{24}$$

Hence, Ω satisfies the required numbering and also the resultant graph admits required labeling. □

5. Conclusion

The assignment of various simple graphs and some chain graphs based on super classical averages were discussed. By the implementation of the SCAA criterion on the various chain-related graphs, namely, the union of any number of cycles C_n, the tadpole graph, the graph extracted by identifying a line of any two cycles C_m and C_n, and the graph extracted by joining any two cycles by a path were discussed in detail. Also, the collection of unions of vertex and edge assignment values are $\{1, 2, \ldots, \Delta\}$, where Δ is the sum of nodes and links. The following are the primary benefits of the suggested method: For getting the assignment values of chemical compounds, they will be constructed as a corresponding graph. So, this interpretation provides a simple graph structure. This method can be applied in the chemical sciences, and so many complicated chemical structures are easily analyzed by its characterization. The following are some restrictions on this work: This work mainly focuses on some standard graphs. This method is tedious when the number of vertices and edges is huge. To find out whether the graph admits that the assignment itself is a difficult problem, it is better to study for the class of graphs. For example, a complete graph has no such assignment. The future potential studies determined on the SCAA of the lines and linkages in the structures involve (i) preservation of line graph operation, (ii) Cartesian product operation of two graphs, (iii) tensor products of two graphs, etc. Using alternative graph operations, similar results can be found for a variety of other graphs. Furthermore, the results can be used to develop and investigate unknown electrochemical systems using graph-labeling techniques.

Data Availability

The data used to support the findings of this study are available from the corresponding author without undue reservation.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors' Contributions

All authors contributed equally to this work. All the authors have read and approved the final version manuscript.

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