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A Mathematical Analysis of Concealed Non-Kekulean Benzenoids and Subdivided Networks in Associated Line Graphs

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Abstract: In this study, an extensive examination of topological parameters derived from molecular structures is conducted, with a specific focus on the Randic index, Geometric Arithmetic (GA) index, and Atom Bond Connectivity (ABC) index. These indices are applied to concealed non-Kekulean benzenoids and subdivided networks within line graphs. The investigation reveals patterns and relationships that were previously unexplored, shedding light on the structural intricacies of chemical compounds. The utility of graph theory as an effective tool for modeling and designing interconnection devices within the realm of chemical research is underscored. Such an approach not only advances the field of mathematical chemistry but also enriches understanding of the manipulation of chemical structures for extensive scientific applications. This analysis contributes to the body of knowledge by highlighting the relevance of these indices in unveiling complex molecular topologies and their potential implications for theoretical and applied chemistry.

Keywords: Molecular; Graph theory; Chemical structure; Line graph; Indices

1 Introduction

The fields of chemistry and mathematics are combined in the field of cheminformatics. It employs graph theory to model chemical phenomena mathematically based on the topological field of chemical chemistry [1]. An atom is represented by vertices, which represent bonds. Bonds between atoms are represented by edges. Based on the degree, weight, and edge of each vertex in a molecular network, a topological index describes the topology of a graph. The topological indices of fullerenes were calculated in the study [2], and a topological index of the Dutch windmill graph was introduced in the study [3]. Additionally, Farahani [4] presented an index that computes degree-based topological properties of nanotubes and networks, Baca et al. [5] developed a GA index of nanocones, and Ali et al. [6] calculated a topological index for nanostar dendrimers. Ali [7] determined the topological indexes of polyoxide, polysilicon, DOX, and DSL networks.

Any graph of a chemical structure may be described using a descriptor, also known as a topological graph index [8]. Topological indices are based on the transformation of a graph into a value that describes the graph's topology. A descriptor, also known as a topological graph index, is a model of mathematics that may be used to characterize any graph of a chemical structure [9]. It is possible to calculate topological indices numerically by examining the invariance and topology of a graph. Indicators of topology are available in various forms; few of them are utilized in the chemistry field. Some recent graph theory literature can be seen in the studies [10, 11].

Graph theory has been used in a variety of ways. The connection indices for different graph classes were computed by different authors.

Our study investigates concealed non-Kekulean structures and subdivided networks within associated line graphs, areas that have received limited attention in previous research [12]. We believe our analysis fills a significant gap in the existing literature and offers new insights into these complex structures.

The links or lines joining different vertices of the graph are called the edges of that graph. Edges of a graph may be directional or non-directional, known as “Edges”.

A graph is a set of points that are known as vertices or nodes. Vertices are basically the corners of the graph. These corners are also called “vertices, nodes, or points [13]. Figure 1 shows a graph with three vertices.

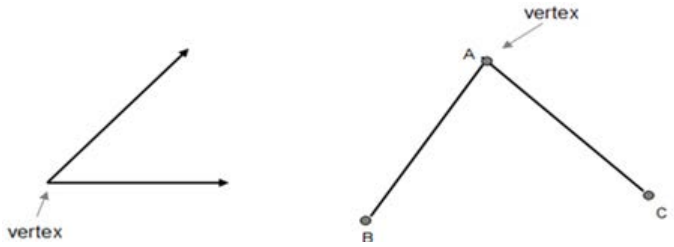

Figure 1. Graph with 3 vertices

The number of edges occurring at a vertex v of such a graph G is known as its degree. The vertex of degree one is known as the leaf vertex or end vertex. To find the degree of a vertex, count the number of edges attached to it. It is known as the “degree of vertices” [14]. In Figure 2, the degree of vertices is labeled. For example:

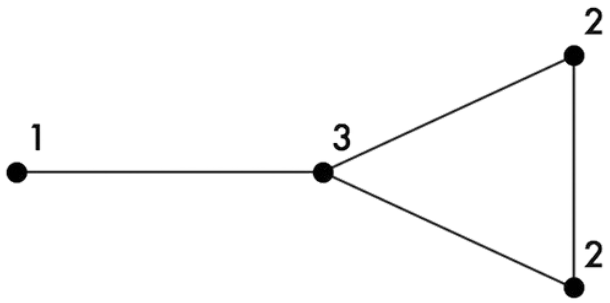

Figure 2. Degree of vertices of G

2 Subdivision

The land or buildings can be subdivided into one or more parcels, or their boundaries can be changed. The process is known as ”subdivision.” A server may be part of some computer networks. An email box, internet connection, and file storage are services that are provided by a server or a powerful computer. Clients are computers that connect to servers.

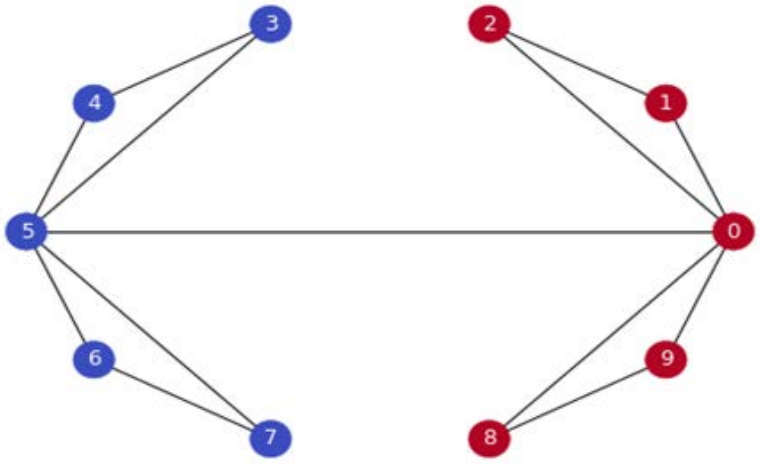

Figure 3. Subdivision graph

Subdivisions of Graph: There is no change in how land is used because of subdivision, but those who subdivide it will almost certainly change how it is used. Subdivision is an effective tool for addressing the environmental impacts of intensification and land use change. Separate consents can be inefficient if imposed later [15]. One of the subdivision graph can be seen in Figure 3.

Network: The term network refers to a group of computers that are connected, typically through a cable or a Wi-Fi connection. The process is known as "Network." See Figure 4.

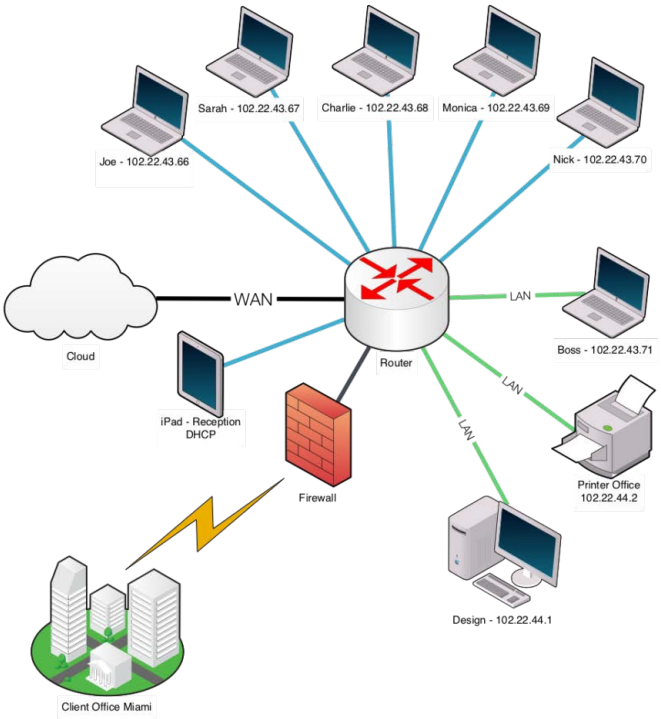

Figure 4. Network graph

An internal vertex-disjoint path is replaced with some of the edges of graph G to form a subdivision. It can be stated that the Hamiltonian graph is any graph whose degree is minimum $\frac{n}{2}$ [16]. The process is known as "subdivision of graph." See Figure 5.

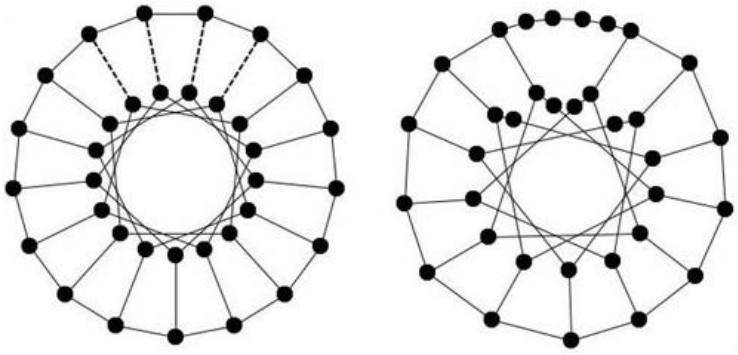

Figure 5. Examples of subdivision graphs

Definition: A Line Graph L(G) for any simple graph G is obtained by associating a vertex with each edge of the graph and connecting two vertices with an edge if the corresponding edges of G have a vertex in common. It is known as the "Line Graph".

According to a chemical point of view, benzenoid hydrocarbon systems can be categorized into two types:

(1) Kekulean structure

Benzenoid hydrocarbons that possess the Kekulean Structure are said to be the Kekulean structure of benzenoid hydrocarbons.

(2) Non-Kekulean structure

Benzenoid hydrocarbons that do not possess Kekulean structures are said to be non-Kekulean structures of benzenoid hydrocarbons.

According to a class of chemists, Kekulean structures are only useful within resonance theory, which is another simplified version of valence bond theory. Whereas modern research shows that Kekulean structures are more important than is usually assumed. Furthermore, we can divide Kekulean benzenoid systems into two types:

(1) Strongly Disconnected Benzenoid Systems

Kekulean benzenoid systems, which have fixed double bonds, single bonds, or both double and single bonds, are called strongly disconnected benzenoid systems [17].

(2) Normal Benzenoid Systems

Kekulean benzenoid systems, which do not have fixed bonds, are called normal benzenoid systems. Similarly, non-Kekulean benzenoid systems are divided into two types:

(3) Obvious non-Kekulean benzenoid system

If the color excess of benzenoid systems is not zero, then benzenoid systems are called obvious non-Kekulean benzenoid systems.

(4) Concealed non-Kekulean benzenoid system

If the color excess of benzenoid systems is zero, then benzenoid systems are called concealed non-Kekulean benzenoid systems.

Topological indices are based on the transformation of a graph into a value that describes the graph's topology. A descriptor, also known as a topological graph index, is a model of mathematics that may be used to characterize.

Any graph of a chemical structure. It is possible to calculate topological indices numerically by examining the invariance and topology of a graph. The Randic index R, the ABC index, and the Geometric Arithmetic (GA) Index are among some of the topological indices [18, 19]. Researchers investigated several topological indices, including the Randic index, the ABC Index, and the Geometric Index, to obtain precise information about geometrically molecular structures [20]. Consider a simple connected, undirected graph with n vertices. Then the Randic index is defined as follows:

$$X(G) = \frac{1}{\sqrt{d_u d_v}} \tag{1}$$

where, d_u is the degree of vertex u.

Take the example of a simple connected undirected graph G(V, E) that has n nodes. Then the ABC index is defined as follows:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \tag{2}$$

where, d_u is the degree of vertex u.

In addition, the GA index is defined by considering the degrees of vertices in a graph.

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{(d_u + d_v)} \tag{3}$$

3 Main Results

Let L(G) be the line graph of concealed non-Kekulean benzenoid hydrocarbons. We calculate topological indices for molecules of the line graph and subdivisions of the line graph of Concealed Non-kekulean Benzenoid Hydrocarbons (CNBH) for different cases depending upon the values of n.

Theorem 1

Consider L (CNBH), for $n \geq 2$. The Randic index, the GA index, and the ABC index for the molecule of L (CNBH) are as follows, respectively.

i) $X(G) = 9 + \frac{1}{\sqrt{8}}n + \frac{1}{\sqrt{6}}n$

ii) $GA(G) = 28 + \frac{1}{\sqrt{28}}n + \frac{1}{\sqrt{7}}n^2$

iii) $ABC(G) = 2\sqrt{2} + 4\sqrt{2} + \frac{28}{3}n + 4\sqrt{15}n + 7\sqrt{6}n^2$

Proof: Consider the Table 1 of labeling for molecule L (CNBH) for $n \geq 2$ in Figure 6.

Table 1. Number of edges in each partition of L (CNBH) for $n \geq 2$ based on the degree of end vertices of each edge

Edges Point	Number of Pair
(2,2)	4
(2,3)	8
(3,3)	7n
(3,4)	24
(4,4)	4n+4

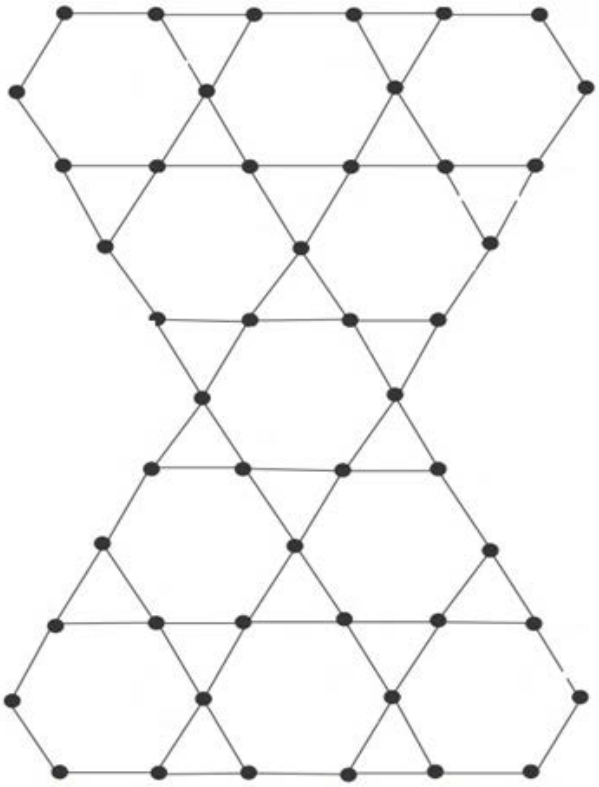

Figure 6. Molecule L(CNBH) for $n = 2$

According to Figure 1:
Case 1: By Eq. (1)

$$X(G) = \frac{1}{\sqrt{d_u d_v}}$$

$$X(G) = 2 + 7 + \frac{1}{\sqrt{8}}n + \frac{1}{\sqrt{6}}n$$

$$X(G) = 9 + \frac{1}{\sqrt{8}}n + \frac{1}{\sqrt{6}}n$$

Case 2: By Eq. (2)

$$GA(G) = \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

$$GA(G) = 4 + 14 + \frac{1}{\sqrt{28}}n + \frac{1}{\sqrt{7}}n^2$$

$$GA(G) = 28 + \frac{1}{\sqrt{28}}n + \frac{1}{\sqrt{7}}n^2$$

Case 3: By Eq. (3)

$$ABC(G) = \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

$$ABC(G) = 2\sqrt{2} + 4\sqrt{2} + \frac{28}{3}n + 4\sqrt{15}n + 7\sqrt{6}n^2$$

Theorem 2

Consider L(CNBH), for $n \geq 1$. The Randic index, the GA index, and the ABC index for the molecule of L(CNBH) are as follows, respectively.

i) $X(G) = 6n + \frac{2}{3}n + \sqrt{15}n$

ii) $GA(G) = 26 + \frac{2\sqrt{5}}{6}n + \frac{2\sqrt{5}}{13}n^2$

iii) $ABC(G) = 2\sqrt{2}n + 4\sqrt{2}n^2 + \sqrt{\frac{4}{9}}n$

Proof: Consider the Table 2 of labeling for the molecule of L(CNBH) for $n \geq 1$ in Figure 7.

Table 2. Number of edges in each partition of L (CNBH) for $n \geq 1$ based on the degree of end vertices of each edge

Edges Point	Number of Pair
(2,2)	4
(2,3)	2n
(3,3)	3n
(3,4)	4n
(4,4)	6

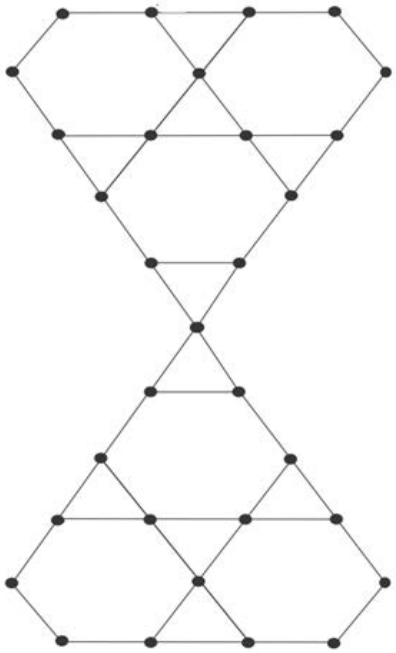

Figure 7. Molecule structure of L(CNBH) for $n = 2$

According to Figure 2:

Case 1: By Eq. (1)

$$X(G) = \frac{1}{\sqrt{d_u d_v}}$$

$$X(G) = 6n + \frac{2}{3}n + \sqrt{15}n$$

Case 2: By Eq. (2)

$$GA(G) = \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$

$$GA(G) = 22 + 4 + \frac{2\sqrt{5}}{6}n + \frac{2\sqrt{5}}{13}n^2$$

$$GA(G) = 26 + \frac{2\sqrt{5}}{6}n + \frac{2\sqrt{5}}{13}n^2$$

Case 3: By Eq. (3)

$$ABC(G) = \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$

$$ABC(G) = \sqrt{\frac{2}{4}}n + \sqrt{\frac{3}{6}}n^2 + \sqrt{\frac{4}{9}}n$$

$$ABC(G) = 2\sqrt{2}n + 4\sqrt{2}n^2 + \sqrt{\frac{4}{9}n}$$

Theorem 3

Consider the subdivision line graph L(SCNBH), for $n \geq 1$. The Randic index, the GA index, and the ABC index for the molecule of L(CNBH) are as follows, respectively.

i) $X(G) = \frac{1}{\sqrt{4}}n + \frac{1}{\sqrt{6}}n^2 + \frac{1}{\sqrt{9}}$

ii) $GA(G) = \frac{2\sqrt{4}}{4}n + \frac{2\sqrt{6}}{5}n^2 + \frac{\sqrt{9}}{3}$

iii) $ABC(G) = \sqrt{2}n + n^2\sqrt{2} + \sqrt{\frac{4}{9}}$

Proof: Consider the Table 3 of labeling for the molecule of L(CNBH) for $n \geq 1$ in Figure 8.

Table 3. Number of edges in each partition of L (CNBH) for $n \geq 2$ based on the degree of end vertices of each edge

Edges Point	Number of Pair
(2,2)	8n
(2,3)	2n
(3,3)	37

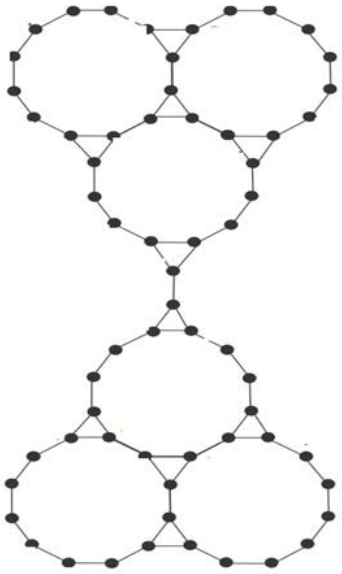

Figure 8. Molecule L(SCNBH) for $n = 1$

According to Figure 3:

Case 1: By Eq. (1)

$$X(G) = \frac{1}{\sqrt{d_u d_v}}$$
$$X(G) = \frac{1}{\sqrt{4}}n + \frac{1}{\sqrt{6}}n^2 + \frac{1}{\sqrt{9}}$$
$$X(G) = \frac{1}{\sqrt{4}}n + \frac{1}{\sqrt{6}}n^2 + \frac{1}{\sqrt{9}}$$

Case 2: By Eq. (2)

$$GA(G) = \frac{2\sqrt{d_u d_v}}{d_u + d_v}$$
$$GA(G) = \frac{2\sqrt{4}}{4}n + \frac{2\sqrt{6}}{5}n^2 + \frac{2\sqrt{9}}{6}$$
$$GA(G) = \frac{2\sqrt{4}}{4}n + \frac{2\sqrt{6}}{5}n^2 + \frac{\sqrt{9}}{3}$$

Case 2: By Eq. (2)

$$ABC(G) = \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$$
$$ABC(G) = \sqrt{\frac{2}{4}}n + \sqrt{\frac{3}{6}}n^2 + \sqrt{\frac{4}{9}}$$
$$ABC(G) = \sqrt{2}n + n^2\sqrt{2} + \sqrt{\frac{4}{9}}$$

4 Conclusions

In this study, we computed various topological descriptors, including the Randic index, GA Index, and ABC index. These descriptors will be organized based on order and distance to generate comprehensive topological indexes in subsequent analyses. These numerical parameters play crucial roles in elucidating the physical properties, chemical reactivity, and biological activities of chemical structures. Their intriguing structure and invariance hold promise for diverse applications. Specifically, in the chemical and pharmaceutical industries, our findings can contribute to identifying the significance of concealed non-Kekulean benzenoid hydrocarbons, offering valuable insights for further research and development efforts.

Data Availability

The data used to support the research findings are available from the corresponding author upon request.

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Conflicts of Interest

The authors declare no conflict of interest.

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