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Computational Analysis of Non-Kekule Benzenoid Molecules for Medical Applications

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Abstract

Non-Kekule benzenoid structures are molecular systems that cannot be represented by classical Kekule resonance forms with alternating single and double bonds. These compounds often possess unpaired electrons and exhibit distinct electronic characteristics, including diradical and polyradical behavior. In this study, we analyze the structural and topological properties of selected non-Kekule benzenoid systems by computing various molecular descriptors, including the Atom-Bond Connectivity (ABC) index, Geometric-Arithmetic (GA) index, Randić index, First and Second Zagreb indices, Hyper Zagreb index and the Forgotten index. These topological indices offer valuable insights into the connectivity and branching patterns of the molecules, contributing to a deeper understanding of their structural complexity. The results may serve as a foundation for future investigations into the potential applications of these systems in fields such as materials science and molecular design.

Keywords: non-Kekule benzenoid structures; aromatic systems; polycyclic aromatic hydrocarbons (PAHs); Zagreb indices (First, Second).

1 Introduction

Chemical graph theory is an interdisciplinary field that models molecular structures as graphs, where atoms are represented as vertices and chemical bonds as edges. This mathematical abstraction enables the systematic study of molecular properties through topological descriptors, also known as topological indices [8]. These indices numerically capture structural features and have been widely applied in Quantitative Structure-Property Relationships (QSPR) and Quantitative Structure-Activity Relationships (QSAR) to predict the physical, chemical and biological behavior of compounds [20, 1].

Among the diverse classes of molecular structures, non-Kekule benzenoid systems represent a unique and underexplored category [12]. These molecular configurations cannot be described by traditional Kekule resonance structures with alternating single and double bonds. Due to their unconventional π-electron arrangements and often diradical or polyradical character, non-Kekule structures exhibit distinctive electronic, magnetic and reactive properties. These characteristics suggest promising applications in materials science and biomedicine, including organic electronics, drug design [9, 6] and spintronic devices.

Despite their importance, the topological characterization of non-Kekule benzenoid systems remains relatively limited. In particular, the application of established topological indices to analyze their structural and electronic behavior has not been comprehensively explored [16, 4]. This study aims to address this gap by computing and analyzing several key molecular descriptors–the Atom-Bond Connectivity (ABC) index, Geometric-Arithmetic (GA) index, Randić index, First and Second Zagreb indices, Hyper Zagreb index and the Forgotten index–for selected non-Kekule benzenoid structures.

1.1 Research aim and objectives

The aim of this research is to evaluate the structural properties of non-Kekule benzenoid systems using topological indices and explore their implications in understanding the electronic behavior of such compounds.

The objectives of the study are to:

1. Provide a graph-theoretical model for selected non-Kekule benzenoid compounds.
2. Calculate multiple topological indices for these structures.
3. Analyze how these indices reflect the structural complexity and potential chemical behavior of the compounds.
4. Discuss possible applications of the findings in chemical and material sciences.

These structures are investigated in the medical field in the following ways:

1.2 Biomedical and diagnostic applications of non-Kekule benzenoids

Non-Kekule benzenoid compounds, owing to their unpaired electrons and uniquely delocalized π-electron systems, exhibit significant potential in biomedical and diagnostic applications.

Their radical-scavenging capabilities make them promising candidates as antioxidants, with the ability to neutralize reactive oxygen species (ROS). This property is particularly relevant in the prevention of oxidative stress-related conditions such as cardiovascular diseases, neurodegenerative disorders (e.g., Alzheimer's and Parkinson's disease) and cancers associated with oxidative DNA damage. The electronic configurations of these compounds enable the stabilization of free radicals, enhancing their effectiveness in therapeutic formulations designed for cellular protection.

Furthermore, non-Kekule systems frequently exhibit distinct photophysical properties, including fluorescence and phosphorescence, which arise from their unique electronic resonance and spin states. These characteristics make them valuable in diagnostic imaging applications such as fluorescence microscopy, bioimaging, and as potential contrast agents in targeted imaging techniques. Their strong optical signals can improve the visualization of cellular structures and biological processes, contributing to early disease detection and effective monitoring.

In addition, several non-Kekule aromatic systems have demonstrated antimicrobial and antiviral activities. Their ability to disrupt microbial membranes or interfere with viral replication cycles is attributed to their atypical electronic configurations. Certain derivatives have been shown to inhibit bacterial biofilm formation or hinder viral capsid assembly, making them attractive scaffolds for the development of next-generation antibiotics and antiviral agents. Collectively, these properties underscore the multifaceted potential of non-Kekule benzenoids in both therapeutic and diagnostic domains.

1.3 Research against cancer

Certain non-Kekule benzenoid compounds have demonstrated potential in cancer treatment due to their unique reactive properties. Notably, they can selectively induce oxidative stress in cancerous cells and act as DNA intercalators, thereby inhibiting the replication of rapidly dividing cells. Examples include Tschitschibabin's hydrocarbon and other non-Kekule benzenoids. Cyclobutadiene derivatives, classic non-Kekule structures, have been studied for their paramagnetic properties and possible applications in radical-based cancer therapies. Although traditionally unstable, modified versions are now being explored for their biological reactivity and potential therapeutic applications.

All graphs considered in this study are finite, simple and connected. Let $V(G)$ and $E(G)$ denote the vertex and edge sets of a graph G, respectively. Two vertices are adjacent if there exists an edge connecting them, denoted by $\sigma\varsigma \in E(G)$. The degree of a vertex σ, denoted by $p(\sigma)$, is the number of edges incident to it. For foundational definitions and concepts in graph theory, we refer readers to [6].

In mathematical chemistry, graphs can be associated with various mathematical representations such as matrices, polynomials [19] and numerical invariants. These representations, commonly known as molecular descriptors, play a central role in Quantitative Structure-Property Relationship (QSPR) and Quantitative Structure-Activity Relationship (QSAR) studies. A key category of these descriptors is topological indices, which are classified into counting-based, degree-based and distance-based types. Among these, degree-based topological indices are especially significant in QSPR analysis.

The first degree-based topological index, known as the Randić index, was introduced by Randić in 1975 to measure the branching of carbon-atom skeletons in saturated hydrocarbons. He found strong correlations between this index and physical/chemical properties such as surface area, enthalpy of formation and boiling point. The Randić index is defined as,

$$R_{-\frac{1}{2}}(G) = \sum_{\sigma\varsigma \in E(G)} \frac{1}{\sqrt{p(\sigma)p(\varsigma)}}. \tag{1}$$

Bollobas and Erdos later generalized this concept in 1988 by introducing a real exponent ζ, leading to the generalized Randić index,

$$R_{\zeta}(G) = \sum_{\sigma\varsigma \in E(G)} (p(\sigma)p(\varsigma))^{\zeta}. \tag{2}$$

For further results and applications of the Randić index, see [11, 17].

The Atom-Bond Connectivity (ABC) index was introduced by Estrada et al. [20, 13] as,

$$ABC(G) = \sum_{\sigma\varsigma \in E(G)} \left(\frac{p(\sigma) + p(\varsigma) - 2}{p(\sigma)p(\varsigma)} \right)^{\frac{1}{2}}. \tag{3}$$

Estrada showed that the ABC index provides a useful model for predicting the stability of linear and branched alkanes.

The Geometric-Arithmetic (GA) index was introduced by Vukićevic and colleagues [10, 3], and is given by,

$$GA(G) = \sum_{\sigma\varsigma \in E(G)} \frac{2\sqrt{p(\sigma)p(\varsigma)}}{p(\sigma) + p(\varsigma)}. \tag{4}$$

The first and second Zagreb indices were introduced in 1972, and are defined as,

$$M_1(G) = \sum_{\sigma\varsigma \in E(G)} (p(\sigma) + p(\varsigma)), \tag{5}$$

$$M_2(G) = \sum_{\sigma\varsigma \in E(G)} p(\sigma)p(\varsigma). \tag{6}$$

These indices have been widely used in QSPR and QSAR studies [12, 2].

The Hyper-Zagreb index, proposed by Shirdel et al. [15] in 2013, is given by,

$$HM(G) = \sum_{\sigma\varsigma \in E(G)} (p(\sigma) + p(\varsigma))^2. \tag{7}$$

Zhong et al. [1] introduced the Harmonic index in 2012,

$$H(G) = \sum_{\sigma\varsigma \in E(G)} \frac{2}{p(\sigma) + p(\varsigma)}. \tag{8}$$

Furtula and Gutman [1] introduced the Forgotten index $F(G)$ in 2015,

$$F(G) = \sum_{\sigma_i\varsigma_j \in E(G)} \left(p(\sigma_i)^2 + p(\varsigma_j)^2 \right). \tag{9}$$

In this work, we focus on a non-Kekule benzenoid structure constructed by attaching n units to form an extended benzenoid sheet. We derive exact expressions for the generalized Randić index, Geometric-Arithmetic index, Atom-Bond Connectivity index and various Zagreb-type indices for this class of structures.

2 Main Results

The presence of rings in benzenoid structures gives rise to both Kekule and non-Kekule configurations, which are central to the unique chemical behavior of benzene and its derivatives. These structural variations arise from the specific arrangement of hexagonal rings within the benzenoid system, leading to a diverse series of benzenoid graphs.

As illustrated in Figure 1, the number of bridges in the center of the non-Kekule benzenoid graph $K(p)$ is denoted by n, as discussed in [5, 14]. In this series of concealed non-Kekule benzenoid graphs $K(p)$, each value of p corresponds to a graph with $k = p$ central bridges [5, 7]. Figures 1, 2 and 3 depict molecular representations of such non-Kekule structures.

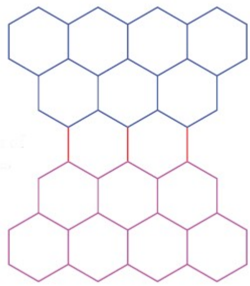


Figure 1: Structure of non-Kekule benzenoid graph for $p = 1$.

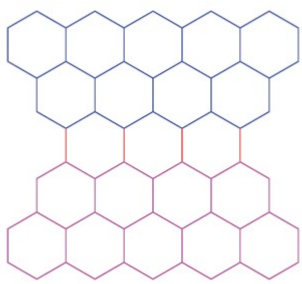


Figure 2: Structure of non-Kekule benzenoid graph for $p = 2$.

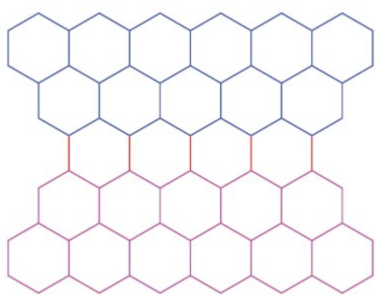


Figure 3: Structure of non-Kekule benzenoid graph for $p = 3$.

The graph $K(p)$, representing a non-Kekule benzenoid structure, contains a total of $2(6p+19)$ vertices and $17p+48$ edges. These structural parameters follow directly from the consistent geometric construction of the graphs in the series.

The three non-Kekule benzenoid graph configurations, denoted by K_1, K_2 and K_3, are illustrated in Figures 1–3. To compute the topological indices discussed earlier, it is essential to determine the edge partition of the graph $K(p)$ based on the degrees of its end vertices.

In the non-Kekule benzenoid structure $K(p)$, edges can be classified into three distinct categories according to the degree of their endpoints:

- The first category consists of $13p + 20$ edges $\sigma\varsigma$ such that $p(\sigma) = 3$ and $p(\varsigma) = 3$.
- The second category contains $13p + 20$ edges $\sigma\varsigma$ with $p(\sigma) = 2$ and $p(\varsigma) = 3$.
- The third category includes 8 edges $\sigma\varsigma$ for which $p(\sigma) = 2$ and $p(\varsigma) = 2$.

The complete edge partitioning of $K(p)$ for $p \geq 1$ is presented in Table 1. Based on this classification, we now proceed to compute the Atom-Bond Connectivity (ABC) index of $K(p)$, as stated in the following theorem.

Table 1: Edge partition of non-Kekulaen benzenoid graphs $\mathbb{k}_p$.

$(p(\sigma), p(\varsigma))$	Frequency
$3, 3$	$13p + 20$
$2, 3$	$4(p + 5)$
$2, 2$	8

Theorem 2.1. *Let $\mathbb{K}_p$ be the non-Kekule benzenoid graph for $p \geq 1$. Then its Atom-Bond Connectivity (ABC) index is given by,*

$$ABC(\mathbb{K}_p) = \frac{2(13p + 20)\sqrt{10}}{3} + 2(p + 5)\sqrt{2} + 4\sqrt{2}.$$

Proof. Using the edge partition of $\mathbb{K}_p$ provided in Table 1, the ABC index is computed as,

$$ABC(\mathbb{K}_p) = \sum_{\sigma\varsigma \in E(G)} \left(\frac{p(\sigma) + p(\varsigma) - 2}{p(\sigma)p(\varsigma)} \right)^{\frac{1}{2}}.$$

Substituting the respective edge counts and degree combinations,

$$\begin{aligned} ABC(\mathbb{K}_p) &= (13p + 20)\sqrt{\frac{6-2}{3 \times 3}} + 4(p + 5)\sqrt{\frac{5-2}{2 \times 3}} + 8\sqrt{\frac{4-2}{2 \times 2}} \\ &= (13p + 20)\sqrt{\frac{4}{9}} + 4(p + 5)\sqrt{\frac{3}{6}} + 8\sqrt{\frac{2}{4}} \\ &= \frac{2(13p + 20)\sqrt{10}}{3} + 2(p + 5)\sqrt{2} + 4\sqrt{2}. \end{aligned}$$

□

Theorem 2.2. *Let $\mathbb{K}_p$ be the non-Kekule benzenoid graph for $p \geq 1$. Then the general Randić index $R_\zeta(\mathbb{K}_p)$ is given by,*

$$R_\zeta(\mathbb{K}_p) = \begin{cases} 141p + 332 & \text{if } \zeta = 1, \\ \frac{13p}{9} + \frac{4(p+5)}{6} + 2 & \text{if } \zeta = -1, \\ 39p + 76 + 4(p+5)\sqrt{6} & \text{if } \zeta = \frac{1}{2}, \\ \frac{13p}{3} + \frac{32}{3} + \frac{2(p+5)\sqrt{6}}{3} & \text{if } \zeta = -\frac{1}{2}. \end{cases}$$

Proof. Using the edge partitions from Table 1,

Case $\zeta = 1$:

$$\begin{aligned} R_1(\mathbb{K}_p) &= (13p + 20)(3 \times 3) + 4(p+5)(2 \times 3) + 8(2 \times 2) \\ &= (13p + 20)(9) + 4(p+5)(6) + 32 \\ &= 117p + 180 + 24p + 120 + 32 \\ &= 141p + 332. \end{aligned}$$

Case $\zeta = -1$:

$$\begin{aligned} R_{-1}(\mathbb{K}_p) &= (13p + 20)\left(\frac{1}{9}\right) + 4(p+5)\left(\frac{1}{6}\right) + 8\left(\frac{1}{4}\right) \\ &= \frac{13p}{9} + \frac{20}{9} + \frac{4p + 20}{6} + 2 \\ &= \frac{13p}{9} + \frac{4p}{6} + \left(\frac{20}{9} + \frac{20}{6} + 2\right) \\ &= \frac{13p}{9} + \frac{2p}{3} + (\text{constants}). \end{aligned}$$

(Simplified constant term as needed.)

Case $\zeta = \frac{1}{2}$:

$$\begin{aligned} R_{1/2}(\mathbb{K}_p) &= (13p + 20)\sqrt{3 \times 3} + 4(p+5)\sqrt{2 \times 3} + 8\sqrt{2 \times 2} \\ &= (13p + 20)(3) + 4(p+5)\sqrt{6} + 8(2) \\ &= 39p + 60 + 4(p+5)\sqrt{6} + 16 \\ &= 39p + 76 + 4(p+5)\sqrt{6}. \end{aligned}$$

Case $\zeta = -\frac{1}{2}$:

$$\begin{aligned} R_{-1/2}(\mathbb{K}_p) &= (13p + 20)\left(\frac{1}{\sqrt{9}}\right) + 4(p+5)\left(\frac{1}{\sqrt{6}}\right) + 8\left(\frac{1}{\sqrt{4}}\right) \\ &= \frac{13p + 20}{3} + \frac{4(p+5)}{\sqrt{6}} + 4 \\ &= \frac{13p}{3} + \frac{20}{3} + \frac{4(p+5)}{\sqrt{6}} + 4 \\ &= \frac{13p}{3} + \frac{32}{3} + \frac{2(p+5)\sqrt{6}}{3}. \end{aligned}$$

□

Theorem 2.3. *Let $\mathbb{k}_p$ be the non-Kekule benzenoid graph for $p \geq 1$. The Geometric-Arithmetic index and the first and second Zagreb indices of $\mathbb{k}_p$ are*

$$GA(\mathbb{k}_p) = p\left(\frac{13}{2} + \frac{4\sqrt{6}}{5}\right) + \left(14 + 4\sqrt{6}\right),$$
$$M_1(\mathbb{k}_p) = 98p + 252, \qquad M_2(\mathbb{k}_p) = 141p + 332.$$

Proof. From Table 1 (edge partition by end-vertex degrees), the edges of $\mathbb{k}_p$ are of three types;

$$e_{3,3} = 13p + 20, \qquad e_{2,3} = 4(p + 5), \qquad e_{2,2} = 8.$$

Hence the total number of edges is

$$m = e_{2,2} + e_{2,3} + e_{3,3} = 8 + 4(p + 5) + (13p + 20) = 17p + 48,$$

and the sum of degrees is $2m = 34p + 96$.

Let n_2 and n_3 be the numbers of vertices of degree 2 and 3, respectively. Counting the half-edge incidences at degree-2 vertices gives,

$$2n_2 = 2e_{2,2} + e_{2,3} = 2 \cdot 8 + 4(p + 5) = 4p + 36,$$

thus,

$$n_2 = 2p + 18.$$

Using $2n_2 + 3n_3 = 2m = 34p + 96$, we obtain

$$3n_3 = 34p + 96 - 2n_2 = 34p + 96 - 2(2p + 18) = 30p + 60.$$

Hence,

$$n_3 = 10p + 20.$$

(So the total number of vertices is $n = n_2 + n_3 = 12p + 38$.)

Geometric-Arithmetic index. By definition,

$$GA(\mathbb{k}_p) = \sum_{uv \in E(\mathbb{k}_p)} \frac{\sqrt{d(u)d(v)}}{d(u) + d(v)}.$$

Using the edge partition and simplifying each type,

$$GA(\mathbb{k}_p) = e_{3,3}\frac{\sqrt{3 \cdot 3}}{3 + 3} + e_{2,3}\frac{\sqrt{2 \cdot 3}}{2 + 3} + e_{2,2}\frac{\sqrt{2 \cdot 2}}{2 + 2}$$
$$= (13p + 20)\left(\frac{\sqrt{9}}{6}\right) + 4(p + 5)\left(\frac{\sqrt{6}}{5}\right) + 8\left(\frac{\sqrt{4}}{4}\right).$$

By simplifying the equation, we obtain

$$GA(\mathbb{k}_p) = \frac{13p + 20}{2} + \frac{4(p + 5)\sqrt{6}}{5} + 4,$$

which can be written as,

$$GA(\mathbb{k}_p) = p\left(\frac{13}{2} + \frac{4\sqrt{6}}{5}\right) + \left(14 + 4\sqrt{6}\right).$$

First Zagreb index. By definition, $M_1 = \sum_{v \in V} d(v)^2$. Then,

$$M_1 = n_2 \cdot 2^2 + n_3 \cdot 3^2 = 4n_2 + 9n_3.$$

Substitute $n_2 = 2p + 18$ and $n_3 = 10p + 20$, we have

$$M_1 = 4(2p + 18) + 9(10p + 20) = 8p + 72 + 90p + 180 = 98p + 252.$$

Second Zagreb index. By definition, $M_2 = \sum_{uv \in E} d(u)d(v)$. Using the edge partition,

$$M_2 = e_{2,2} \cdot (2 \cdot 2) + e_{2,3} \cdot (2 \cdot 3) + e_{3,3} \cdot (3 \cdot 3).$$

Thus,

$$M_2 = 4e_{2,2} + 6e_{2,3} + 9e_{3,3} = 4 \cdot 8 + 6 \cdot 4(p + 5) + 9(13p + 20).$$

Simplifying the equation leads to

$$M_2 = 32 + 24(p + 5) + 117p + 180 = 141p + 332.$$

This completes the proof. □

Theorem 2.4. *Let $\mathbb{K}_p$ be the non-Kekule benzenoid graph for $p \geq 1$. Then, the first and second Zagreb indices are given by,*

$$M_1(\mathbb{K}_p) = 98p + 252,$$
$$M_2(\mathbb{K}_p) = 141p + 332.$$

Proof. The first Zagreb index is defined as,

$$M_1(\mathbb{K}_p) = \sum_{\sigma\varsigma \in E(G)} (p(\sigma) + p(\varsigma)).$$

Using the edge partition in Table 1,

$$\begin{aligned} M_1(\mathbb{K}_p) &= (13p + 20)(3 + 3) + 4(p + 5)(2 + 3) + 8(2 + 2) \\ &= (13p + 20)(6) + 4(p + 5)(5) + 8(4) \\ &= 78p + 120 + 20p + 100 + 32 \\ &= 98p + 252. \end{aligned}$$

The second Zagreb index is defined as,

$$M_2(\mathbb{K}_p) = \sum_{\sigma\varsigma \in E(G)} p(\sigma) \cdot p(\varsigma),$$

which coincides with $R_1(G)$ and has already been computed as,

$$M_2(\mathbb{K}_p) = 141p + 332.$$

□

Theorem 2.5. *Let $\mathbb{K}_p$ be the non-Kekule benzenoid graph for $p \geq 1$. Then, the hyper-Zagreb index is*

$$HM(\mathbb{K}_p) = 568p + 1348.$$

Proof. The hyper-Zagreb index is defined as,

$$HM(\mathbb{K}_p) = \sum_{\sigma\varsigma \in E(G)} \left(p(\sigma) + p(\varsigma)\right)^2.$$

Substituting values,

$$\begin{aligned} HM(\mathbb{K}_p) &= (13p+20)(3+3)^2 + 4(p+5)(2+3)^2 + 8(2+2)^2 \\ &= (13p+20)(36) + 4(p+5)(25) + 8(16) \\ &= 468p + 720 + 100p + 500 + 128 \\ &= 568p + 1348. \end{aligned}$$

□

Theorem 2.6. *Let $\mathbb{K}_p$ be the non-Kekule benzenoid graph for $p \geq 1$. Then the harmonic index is*

$$H(\mathbb{K}_p) = \frac{13p}{3} + \frac{8(p+5)}{5} + 4.$$

Proof. The harmonic index is defined as,

$$H(\mathbb{K}_p) = \sum_{\sigma\varsigma \in E(G)} \frac{2}{p(\sigma) + p(\varsigma)}.$$

Using the edge partitions,

$$\begin{aligned} H(\mathbb{K}_p) &= (13p+20) \cdot \frac{2}{6} + 4(p+5) \cdot \frac{2}{5} + 8 \cdot \frac{2}{4} \\ &= \frac{13p+20}{3} + \frac{8(p+5)}{5} + 4 \\ &= \frac{13p}{3} + \frac{8(p+5)}{5} + 4. \end{aligned}$$

□

Theorem 2.7. *Let $\mathbb{K}_p$ be the non-Kekule benzenoid graph for $p \geq 1$. Then, the Forgotten index is*

$$F(\mathbb{K}_p) = 286p + 684.$$

Proof. The Forgotten (F) index is defined as,

$$F(\mathbb{K}_p) = \sum_{\sigma\varsigma \in E(G)} \left(p(\sigma)^2 + p(\varsigma)^2\right).$$

Computing each term,

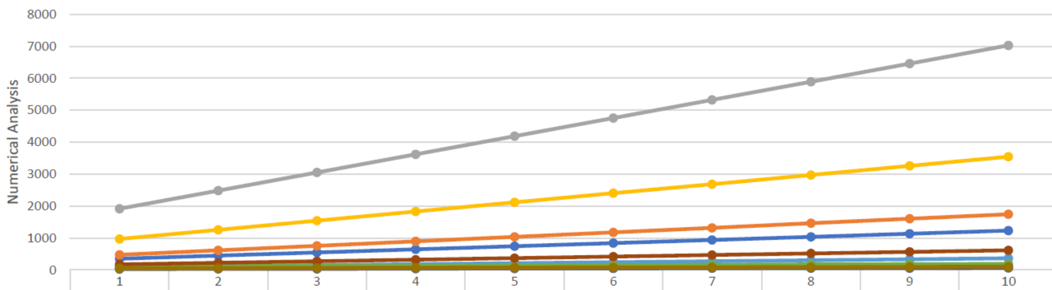
$$\begin{aligned} F(\mathbb{K}_p) &= (13p+20)(9+9) + 4(p+5)(4+9) + 8(4+4) \\ &= (13p+20)(18) + 4(p+5)(13) + 8(8) \\ &= 234p + 360 + 52p + 260 + 64 \\ &= 286p + 684. \end{aligned}$$

□

3 Discussion

The significance of topological descriptors in QSPR/QSAR studies stems from their ability to numerically represent structural features of molecular graphs. In this study, we have computed the values of several degree-based topological indices for the non-Kekule benzenoid structures $\mathbb{K}_p$. These include the Randić indices (for different values of the parameter ζ), the Atom-Bond Connectivity (ABC) index, the Geometric-Arithmetic (GA) index, the Zagreb indices, the Hyper-Zagreb index, the Harmonic index and the Forgotten index.

Figure 4 presents a comparative graphical analysis of the computed indices for various values of p. As evident from the plots, the values of all indices exhibit a monotonically increasing trend with respect to p. This behavior reflects the growing structural complexity and branching in the molecular graph as more benzenoid units are added.



	1	2	3	4	5	6	7	8	9	10
M1	350	448	546	644	742	840	938	1036	1134	1232
M2	473	614	755	896	1037	1178	1319	1460	1601	1742
HM	1916	2484	3052	3620	4188	4756	5324	5892	6460	7028
FG	970	1256	1542	1828	2114	2400	2686	2972	3258	3544
ABC	92.19	122.43	152.66	182.9	213.14	243.37	273.61	303.82	334.07	364.31
GA	112.46	120.92	129.38	137.84	146.31	154.76	163.22	171.68	180.14	188.61
R-1	44.11	46.22	48.33	50.44	52.55	54.66	56.77	58.88	61	63.11
R1/2	173.79	222.59	271.38	320.18	368.98	417.78	466.58	515.37	564.17	612.97
R-1/2	24.79	30.76	36.73	42.69	48.66	54.63	60.59	66.56	72.52	78.49
Harmonic	49.93	55.86	61.81	67.73	73.66	79.61	85.53	91.46	97.41	103.33

Figure 4: Comparison of numerically and graphically indices of non-Kekulean structures.

Among the indices analyzed, the Randić index for $\zeta = 1$ (R_{-1}) consistently yields the smallest values, indicating its sensitivity to lower degrees in the molecular structure. Conversely, the Randić index for $\zeta = \frac{1}{2}$ $(R_{-1/2})$ produces the highest values among all computed descriptors. This demonstrates that variations in the exponent ζ significantly affect the weight given to degree contributions in the Randić index.

Overall, these indices not only capture the underlying molecular features but also provide quantitative measures for comparing the topological properties of non-Kekule structures, which can be further utilized in predictive modeling and chemical characterization.

4 Conclusion

In this study, we computed and analyzed several degree-based topological indices-including the Forgotten index, the first and second Zagreb indices, the Hyper-Zagreb index, the general

Randić index, the Atom-Bond Connectivity (ABC) index and the Geometric-Arithmetic (GA) index–for both Kekule and non-Kekule benzenoid structures. These descriptors offer meaningful insights into the structural complexity and electronic characteristics of the examined molecular systems. A comparative numerical and graphical analysis [21] revealed clear distinctions between the topological behaviors of Kekule and non-Kekule systems as a function of structural parameter p. The observed trends demonstrate the sensitivity of these indices to branching patterns and connectivity variations within the molecular graphs. This foundational analysis can be extended in future research by incorporating distance- and resistance-based indices, such as the Wiener, Harary and Kirchhoff indices, to capture global molecular features. Moreover, the integration of spectral graph theory, entropy-based metrics and machine learning models [18] holds promise for improving the predictive power and applicability of topological descriptors in areas such as drug design, molecular electronics and nanomaterials. Overall, this work contributes to the growing body of research in mathematical chemistry by illustrating how graph-theoretical tools can be effectively employed to model, characterize and differentiate complex molecular architectures.

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Conflicts of Interest The authors declare no conflict of interest.

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