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RESEARCH PAPER

NM-polynomial and neighborhood degree-based indices in graph theory: a study on non-kekulean benzenoid graphs

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Abstract: In this study, we explore the neighborhood degree sum-based topological indices of Non-Kekulean Benzenoid graphs Kn using graph theory and computational tools. The novelty of this work lies in the application of the neighborhood M-polynomial (NM-polynomial) to derive various topological indices, which provide deep insights into the structural properties of Non-Kekulean Benzenoid systems. We compute several indices, including the third version of the Zagreb index, neighborhood second Zagreb index, neighborhood forgotten topological index, and others, using edge partitioning and combinatorial methods. The results are graphically represented and compared using MATLAB and Maple, revealing significant relationships between the molecular topology and the computed indices. Our findings demonstrate that the ND_3 index is the most dominant, while the F^*_N index increases more slowly compared to other indices. This study not only advances the understanding of Non-Kekulean Benzenoid graphs but also highlights the effectiveness of combining mathematical methodologies with computational tools for molecular structure analysis. The results contribute to the fields of graph theory and computational chemistry, offering a foundation for future research on diverse molecular structures.

Keywords: Graph theory, Topological indices, Benzenoid, Chemical graph theory, Degree- based indices, NM-polynomial

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INTRODUCTION

Graph theory provides essential tools for analyzing molecular structures in chemistry. Following the conventions established by Diudea et al. [1] and West [2], we define our graph theoretical framework: Every graph in this work is a simple graph Γ without any loops or multiple edges. Let the set of vertices and edges of a graph, respectively, be V (Γ) and E(Γ). The degree of the vertex $v \in V$ (Γ), indicated by d_u, is the sum of the degrees of u's neighbors in Γ, where δ_u is the number of edges incident on v. The vertices that are adjacent to a vertex are referred to as its neighbors. Chemical graph theory, a subfield of graph theory, investigates the relationship between a compound's molecular graph and its various characteristics and activities.

In drug discovery, predicting the physicochemical properties and biological activity of molecules has become increasingly important. QSPR/QSAR mathematical models relate the chemical structure of substances to their physical qualities. It characterizes molecular properties using topological indices rather than a wet lab. The first widely recognized topological index is the Wiener Index [3], introduced for alkanes, which calculates the sum of distances between all pairs of vertices in a graph. This index has proven effective in correlating molecular structure with boiling points and other physical properties of compounds. Since then, numerous topological indices have been

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proposed to capture various structural aspects of molecules.

Degree-based indices such as the Randic Index [4], which focuses on the branching of molecular structures, and the Balaban Index [5], which considers distance-based measures of atom pairs, have been extensively used in Quantitative Structure-Property Relationships (QSPR) and Quantitative Structure-Activity Relationships (QSAR) studies. These indices are particularly useful in predicting biological activity, toxicity, and molecular stability.

The aim of this work is to compute and analyze neighborhood degree sum-based topological indices for Non-Kekulean Benzenoid graphs K_n using the NM-polynomial approach, providing new insights into their structural properties and potential applications in chemical research.

The rest of the work is organized as follows. Section 2 is methodology. Section 3 is results and discussions. Section 4 concluded the work.

Table 1 displays the creation of neighborhood degree sum-based indices and how they relate to the NM-polynomial.

Here, $NM(\Gamma)$ is a function of x, y and $D_x = \frac{\partial(f(x,y))}{\partial x}$, $D_y = \frac{\partial(f(x,y))}{\partial y}$, $L_x = f(x^2, y)$, $L_y = f(x, y^2)$, $L_y = f(x, y^2)$, $S_x = \int_0^x \frac{f(t,y)}{t}\, dt$, $S_y = \int_0^y \frac{f(x,t)}{t}\, dt, J = f(x,x)$

Table 1. Formulation of Topological Indices using NM-Polynomial for a Graph Γ

Topological Index	$f(x,y)$	Derivation from $NM(\Gamma)$	Significance
Third Version of Zagrab Index $M_1'(\Gamma)$ [11]	$x+y$	$(D_x + D_y)(M(\Gamma; x,y))\|x=y=1$	Predicting molecular stability
Neighborhood second Zagreb index $M_2^*(\Gamma)$([11])	xy	$(D_x \cdot D_y)(M(\Gamma; x,y))\|x=y=1$	Indicating branching patterns
Neighborhood forgotten topological index $F_N^*(\Gamma)$ ([11])	x^2+y^2	$(D_x^2 + D_y^2)(M(\Gamma; x,y))\|x=y=1$	Global molecular characterization
Neighborhood second modified zagreb index ${}^{nm}M_2(\Gamma)$([12])	$\frac{1}{xy}$	$(S_x S_y)(M(\Gamma; x,y))\|x=y=1$	Sensitive to local structural changes
Neighborhood general Randic index $NR\alpha(\Gamma)$([12])	$(xy)^\alpha$	$(D_x^\alpha + D_y^\alpha)(M(\Gamma; x,y))\|x=y=1$	Predicting biological activity
Third NDe Index $ND_3(\Gamma)$([12])	$xy(x+y)$	$D_x D_y (D_x + D_y)(M(\Gamma; x,y))\|x=y=1$	Predicting reactivity
Fifth NDe Index $ND_5(\Gamma)$ ([12])	$\frac{x^2+y^2}{xy}$	$(D_x S_y + D_y S_x)(M(\Gamma; x,y))\|x=y=1$	Local structural variations
Neighborhood Harmonic index $NH(\Gamma)$([11])	$\frac{2}{x+y}$	$2(S_x)J(M(\Gamma; x,y))\|x=1$	Predicting molecular stability
Neighborhood Inverse sum index $NI(\Gamma)$ ([11])	$\frac{xy}{x+y}$	$S_x J(D_x + D_y)(M(\Gamma; x,y))\|x=y=1$	Sensitive to local structural changes
Sanskruti index $S(\Gamma)$([12])	$\frac{xy}{(x+y-2)^3}$	$(S_x^3 Q_{-2} J D_x^3 D_y^3)(M(\Gamma; x,y))\|x=1$	Complex molecular structures

METHODOLOGY

Topological indexes are used in QSPR/QSAR analysis to convert graph into a real number that characterize the topology of the graph. For graphs that are isomorphic, it doesn't change. When attempting to create several indices of a certain category, it is difficult to compute topological indices using their traditional definitions. Numerous algebraic polynomials were constructed by [6–8], whose differentiation or integration—or combination of

the two—obtained at a given point gives topological indices. The M-polynomial is the most generic polynomial that could offer a significant number of degree-based topological indices [9]. To generate more indices, efforts are carried out on a daily basis.

Several academics have lately been interested in the neighborhood degree sum-based indexes [10–14]. The computation of these kinds of indices was made easier by the creation of the neighborhood M-polynomial (NM) by contemporary authors [15]. Similar to the M-polynomial for degree-based indices, it has a similar function for neighborhood degree sum-based indices. [16] Computed degree-based topological indices and M-polynomials for Vphenylenic nanotubes and nanotori.

M-polynomials were employed by [17] to produce topological indices for the praline net- work of a chosen number of beautiful structures. The use of M-polynomial-based topological descriptors of chemical crystal structures was discussed in [18]. [19] Described M-polynomials and topological indices for the linear chains of benzene, napthalene, and anthracene. Using an M-polynomial, [20] calculated the silicate network's topological indices. [21] Developed degree- based topological indices and M-polynomials for copper (I) oxide.

Using an M-polynomial, [22] created topological indices for nanotubes. [23] Included the closure formula for the topological and M-polynomial descriptors of boron triangular nanotubes. [24, 25] reported the discovery of the zigzag edge coronoid of starphene and the invention of numerous M-polynomials for nanostructures. In [26], the topological characteristics of titanium difluoride TiF_2 crystal structures were found. In [27], the M- and NM-polynomials of a few anti-COVID-19 medications were assessed. In this study, we employ edge partitioning, graph theoretical approaches, and combinatorial computation to derive the NM-polynomial and various neighborhood degree sum-based indices for Non-Kekulean Benzenoid graphs K_n. The results are computed using Maple 2020 and graphically represented using MATLAB 2017.

RESULTS AND DISCUSSIONS

Non-Kekulean Benzenoid graphs K_n

Non-Kekulean Benzenoid graphs are characterized by their unique arrangement of rings, result- ing in structures that cannot be represented by Kekulean forms. Since Benzenoid forms contains rings, benzene has both real and distinct Kekulean and Non-Kekulean structures. The way the structures are modified is by the unique arrangement of rings in the Benzenoid system, which results in a sequence of Benzenoid structures of the Benzenoid graph. See [28] for the series of concealed Non-Kekulean Benzenoid graph K_n, where n is the number of bridges [29] in the center of K_n, as illustrated in Figure 1. Similarly, there exist k bridges for $n \leq k$. Based on the valency of each atom, we have noticed that there are three types of atom-bonds in the Non-Kekulean Benzenoid graph K_n. In light of this understanding of atom-bonds, it can be shown that there exist two kinds of atoms, v_i and v_j, such that $d_v i \leq 2$ and $d_v j \leq 3$, where $d_v i$ and $d_v j$ denote the valency of atoms $\forall v_i, v_j \in K_n$.

From Table 2 the order and size of Non-Kekulean Benzenoid graphs K_n are

$V_K n = 2(6n + 7)$, $E_K n = 17n + 14$.

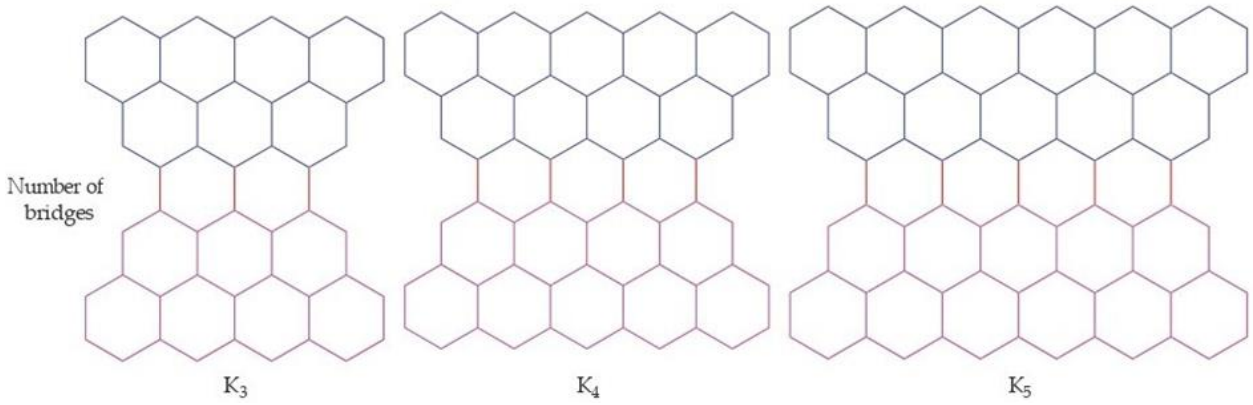

Figure 1. Benzene ring embedded in P-type surface in 2D-network

Table 2. The partitions of the edges Non-Kekulean Benzenoid K_n based on neighboring vertices

(δ_u,δ_v)	frequency
(4, 5)	8
(5, 7)	8
(6, 7)	4n
(6, 8)	4
(7, 9)	2n+4
(8, 8)	2
(8, 9)	4
(9, 9)	11n-16

NM-Polynomial of Non-Kekulean Benzenoid K_n

The neighborhood M-polynomial of a graph Γ is defined as

$$NM(\Gamma; x, y) = \sum_{i \le j} \Gamma_{i,j} x^i y^j, \quad (1)$$

where $\Gamma_{i,j} x^i y^j$ is the total count of edges $uv \in E(\Gamma)$ such that $\delta u, \delta v = i, j$.

Theorem 3.1. *Let* Γ *be the graph of chemical structures of the Non-Kekulean Benzenoid* K_n*, then*

$NM(\Gamma; x, y) = 8\,x^4y^5 + 8\,x^5y^7 + 4\,x^6y^7n + 4\,x^6y^8 + x^7y^9\,(2n + 4) + 2\,x^8y^8 + 4\,x^8y^9 + x^9y^9\,(11n - 16)$

Proof.

Using Table 2 and definition of NM-polynomial, we have following computation

$$NM(\Gamma; x, y) = \sum_{i \le j} \Gamma_{i,j} x^i y^j$$

$= m(4,5)x4y5 + m(5,7)x5y7 + m(6,7)x6y7 + m(6,8)x6y8 + m(7,9)x7y9 + m(8,8)x8y8 + m(8,9)x8y9 + m(9,9)x9y9$

$= 8\,x^4y^5 + 8\,x^5y^7 + 4\,x^6y^7n + 4\,x^6y^8 + x^7y^9\,(2n + 4) + 2\,x^8y^8 + 4\,x^8y^9 + x^9y^9\,(11n - 16) + 4\,x^8y^9 + x^9y^9\,(11n - 16)$

Neighborhood Degree based Topological Indices of Non-Kekulean Benzenoid graphs K_n

Using the NM-polynomial, we compute several neighborhood degree sum-based indices, including the third version of the Zagreb index, neighborhood second Zagreb index, neighborhood forgotten topological index, and others.

Theorem 3.2. *Let* Γ *be the graph of chemical structures of the Non-Kekulean Benzenoid* K_n*, then*

$$M_1'(\Gamma, x, y) = 282n + 100$$

$$M_2^*(\Gamma, x, y) = 1185n + 4$$

$$F_N^*(\Gamma, x, y) = 282n + 100$$

$$^{nm}M_2(\Gamma, x, y) = \frac{149n}{567} + \frac{60299}{90720}$$

$$NR_\alpha(\Gamma, x, y) = (60n + 12)m + 36n)\,7^\alpha + ((60n - 12)m - 12n)8^\alpha + (16n + 8m)\,5^\alpha + (60mn + 12n)6^\alpha + 6m(n - 1)\,9^\alpha$$

$$ND_3(\Gamma, x, y) = 20238n - 4864$$

$$ND_5(\Gamma, x, y) = \frac{308n}{9} + \frac{2097}{70}$$

$$NH(\Gamma, x, y) = \frac{977n}{468} + \frac{4463}{1428}$$

$$NI(\Gamma, x, y) = 17n + 14$$

$$S(\Gamma, x, y) = \frac{9988271649n}{5451776} - \frac{3209573707}{10976000}$$

Proof. Using Table 1 and Theorem 3.1, we have following computation

$M_1'(\Gamma, x, y) = (D_x + D_y)(NM(\Gamma; x, y))|x = y = 1$

$=(D_x + D_y)(8\,x^4y^5 + 8\,x^5y^7 + 4\,x^6y^7n + 4\,x^6y^8 + x^7y^9\,(2n + 4) + 2\,x^8y^8 + 4\,x^8y^9 + x^9y^9\,(11n - 16))|x = y = 1$

$= (198\,nx^9y^9 - 288\,x^9y^9 + 32\,nx^7y^9 + 68\,x^8y^9 + 32\,x^8y^8 + 64\,x^7y^9 + 52\,x^6y^7n + 56\,x^6y^8 + 96\,x^5y^7 + 72\,x^4y^5)|x = y = 1$

$= 282n + 100$

$M_2^*(\Gamma, x, y) = (D_x \cdot D_y)(NM(\Gamma; x, y))|x = y = 1$

$= (D_x \cdot D_y)(8\,x^4y^5 + 8\,x^5y^7 + 4\,x^6y^7n + 4\,x^6y^8 + x^7y^9\,(2n + 4) + 2\,x^8y^8 + 4\,x^8y^9 + x^9y^9\,(11n - 16))|x = y = 1$

$= (891\,nx^9y^9 - 1296\,x^9y^9 + 126\,nx^7y^9 + 288\,x^8y^9 + 128\,x^8y^8 + 252\,x^7y^9 + 168\,x^6y^7n + 192\,x^6y^8 + 280\,x^5y^7 + 160\,x^4y^5)|x = y = 1$

$= 1185n + 4$

$F_N^*(\Gamma, x, y) = (D_x^2 + D_y^2)(NM(\Gamma; x, y))|x = y = 1$

$=(D_x^2 + D_y^2)(8\,x^4y^5 + 8\,x^5y^7 + 4\,x^6y^7n + 4\,x^6y^8 + x^7y^9\,(2n + 4) + 2\,x^8y^8 + 4\,x^8y^9 + x^9y^9\,(11n - 16))|x = y = 1$

$= (198\,nx^9y^9 - 288\,x^9y^9 + 32\,nx^7y^9 + 68\,x^8y^9 + 32\,x^8y^8 + 64\,x^7y^9$

$+ 52\,x^6y^7n\ +\ 56\,x^6y^8 + 96\,x^5y^7 + 72\,x^4y^5)|x = y = 1$

$= 282\,n\ +\ 100$

$^{nm}M_2\,(\Gamma, x, y) = (S_x S_y)(\mathrm{NM}\,(\Gamma;\ x, y))|x = y = 1$

$= \ (S_x S_y)(8\,x^4y^5 + 8\,x^5y^7 + 4\,x^6y^7n\ +\ 4\,x^6y^8 + x^7y^9\,(2\,n\ +\ 4)$

$+ 2\,x^8y^8 + 4\,x^8y^9 + x^9y^9\,(11\,n - 16))|x = y = 1$

$= (\frac{11nx^9y^9}{81} - \frac{16x^9y^9}{81} + \frac{2nx^7y^9}{63} + \frac{x^8y^9}{18} + \frac{x^8y^8}{32} + \frac{4x^7y^9}{63} + \frac{2nx^6y^7}{21} + \frac{x^6y^8}{12} + \frac{8x^5y^7}{35} + \frac{2x^4y^5}{5})|x = y = 1$

$$= \frac{149n}{567} + \frac{60299}{90720}$$

$NR_\alpha\,(\Gamma, x, y) = (D_x^\alpha + D_y^\alpha)(\mathrm{NM}\,(\Gamma;\ x, y))|x = y = 1$

$= (D_x^\alpha + D_y^\alpha)\ \ (8\,x^4y^5 + 8\,x^5y^7 + 4\,x^6y^7n\ +\ 4\,x^6y^8 + x^7y^9\,(2\,n\ +\ 4)\ +\ 2\,x^8y^8$

$+ 4\,x^8y^9 + x^9y^9\,(11\,n\ -\ 16))|x = y = 1$

$= (8\cdot 4^\alpha x^4y^5\ \ + 8\cdot 5^\alpha x^5y^7 + 4\cdot 6^\alpha x^6y^7n\ +\ 4\cdot 6^\alpha x^6y^8 + 7^\alpha x^7y^9\,(2\,n\ +\ 4)$

$+ 4\cdot 8^\alpha x^8y^8 + 4\cdot 8^\alpha x^8y^9\ \ + 2\cdot 9^\alpha x^9y^9\,(11\,n\ -\ 16)\ +\ 8\cdot 5^\alpha x^4y^5 + 8\cdot 7^\alpha x^5y^7$

$+ 4\cdot 7^\alpha x^6y^7n\ +\ 4\cdot 8^\alpha x^6y^8 + 9^\alpha x^7y^9\,(2\,n\ +\ 4)\ +\ 4\cdot 9^\alpha x^8y^9)|x = y = 1$

$= (60\,n\ +\ 12)\,m\ +\ 36\,n)\,7^\alpha\ + \big((60\,n - 12)m - 12\,n\big)\,8^\alpha\ +\ (16\,n\ +\ 8\,m)5^\alpha\ +\ (60\,mn\ +\ 12\,n)6^\alpha + 6m(n - 1)\,9^\alpha$

$ND_3\,(\Gamma, x, y)\ =\ D_x D_y (D_x\ +\ D_y)(M\,(\Gamma;\ x, y))|x = y = 1$

$= D_x D_y (D_x + D_y)$

$(8\,x^4y^5 + 8\,x^5y^7 + 4\,x^6y^7n\ +\ 4\,x^6y^8 + x^7y^9\,(2\,n\ +\ 4)\ +\ 2\,x^8y^8$

$+ 4\,x^8y^9 + x^9y^9\,(11\,n\ -\ 16))|x = y = 1$

$= \ (16038\,nx^9y^9 - 23328\,x^9y^9 + 2016\,nx^7y^9 + 4896\,x^8y^9 + 2048\,x^8y^8 + 4032\,x^7y^9$

$+ 2184\,x^6y^7n\ +\ 2688\,x^6y^8 + 3360\,x^5y^7 + 1440\,x^4y^5)|x = y = 1$

$= \ 20238\,n\ -\ 4864$

$ND_5\,(\Gamma, x, y)\ =\ (D_x S_y\ +\ D_y S_x)(\mathrm{NM}\,(\Gamma;\ x, y))|x = y = 1$

$= (D_x S_y + D_y S_x)(8\,x^4y^5 + 8\,x^5y^7 + 4\,x^6y^7n\ +\ 4\,x^6y^8 + x^7y^9\,(2\,n\ +\ 4)\ +\ 2\,x^8y^8$

$+ 4\,x^8y^9 + x^9y^9\,(11\,n\ -\ 16))|x = y = 1$

$= \frac{308n}{9} + \frac{2097}{70}$

$H\,(\Gamma, x, y)\ = 2(S_x)J(\mathrm{NM}\,(\Gamma;\ x, y))|x = 1$

$= 2(S_x)J\ \ \ (8\,x^4y^5 + 8\,x^5y^7 + 4\,x^6y^7n\ +\ 4\,x^6y^8 + x^7y^9\,(2\,n\ +\ 4)\ +\ 2\,x^8y^8$

$+ 4\,x^8y^9 + x^9y^9\,(11\,n\ -\ 16))|x = 1$

$(\frac{11nx^{18}}{9} - \frac{16x^{18}}{9} + \frac{8x^{17}}{17} + \frac{nx^{16}}{4} + \frac{3x^{16}}{4} + \frac{4x^{14}}{7} + \frac{8nx^{13}}{13} + \frac{4x^{12}}{3} + \frac{16x^9}{9})|x = 1$

$$= \frac{977n}{468} + \frac{4463}{1428}$$

$NI(\Gamma, x, y)\ = S_x J(D_x + D_y)(\mathrm{NM}\,(\Gamma;\ x, y))|x = y = 1$

$= S_x J(D_x + D_y)\ \ \ (x^5y^5\ \ \ \ (4\,n\ +\ 2\,m)\ +\ x^5y^7\,(8\,n\ +\ 4\,m)\ +\ x^6y^7\,(40\,mn\ +\ 4\,m\ +\ 16\,n)$

$+ x^6y^8\,(20\,mn\ -\ 4\,m\ -\ 4\,n)\ +\ x^7y^7\,(10\,mn\ +\ 2\,n)\ +\ x^7y^8\,(8\,n\ +\ 4\,m)$

$+ x^8y^8\,(18\,mn\ -\ 4\,m\ -\ 8\,n)\ +\ x^8y^9\ \ (4\,mn\ -\ 4\,m)\ +\ x^9y^9\,(mn\ -\ m))|x = 1$

$= \ (11n\,x^{18} - 16\,x^{18}$

$+ 2n\,x^{16} + 4\,x^{17} + 6\,x^{16} + 4\,nx^{13} + 4\,x^{14} + 8\,x^{12}$

$+ 8\,x^9)|x = 1$

$= \ 17\,n\ +\ 14$

$S(\Gamma, x, y)\ = (S_x^3 Q_{-2} J D_x^3 D_y^3)(\mathrm{NM}\,(\Gamma;\ x, y))|x = 1$

$= (S_x^3 Q_{-2} J D_x^3 D_y^3)\ \ \ (8\,x^4y^5 + 8\,x^5y^7 + 4\,x^6y^7n\ +\ 4\,x^6y^8 + x^7y^9\,(2\,n\ +\ 4)\ +\ 2\,x^8y^8$

$+ 4\,x^8y^9 + x^9y^9\,(11\,n\ -\ 16))|x = 1$

$= (\frac{5845851nx^{16}}{4096} - \frac{531441x^{16}}{256} + \frac{55296x^{15}}{125} + \frac{729nx^{14}}{4} + \frac{381119x^{14}}{686} + 256x^{12} + \frac{296352nx^{11}}{1331} + 343x^{10} + \frac{64000x^7}{343})|x = 1$

$$= \frac{9988271649n}{5451776} - \frac{3209573707}{10976000}$$

Graphical representation and Comparison with Existing Studies

The NM-polynomials of the structures are graphically represented in Figure 2. Figure 3 pro- vides a 3D graphical representation of the neighborhood degree sum-based topological indices, while Figure 4 compares these indices across different structures.

From Figure 2, it is evident that the NM-polynomials vary significantly with the structure of K_n, reflecting the complexity of the molecular topology. Figure 3 shows that the ND_3 index is the most dominant, while the F_N^*

index increases more slowly compared to other indices. This suggests that ND_3 is more sensitive to changes in the molecular structure, making it a valuable tool for analyzing Non-Kekulean Benzenoid graphs.

Figure 4 provides a comparative analysis of the indices, highlighting the differences in their behavior across various structures. The results indicate that the graph parameters increase in tandem with the indices, demonstrating the effectiveness of the NM-polynomial approach in capturing the structural properties of K_n.

Our findings align with previous studies on topological indices and their applications in molecular structure analysis. For instance, the dominance of the ND_3 index is consistent with the results reported by 11, who also observed similar trends in other molecular networks. How- ever, our study extends these findings by providing a comprehensive analysis of Non-Kekulean Benzenoid graphs, which have not been extensively studied in the context of neighborhood degree sum-based indices. In summary, this study leverages graph theory and computational tools to explore neighborhood degree-based topological indices for Non-Kekulean Benzenoid graphs K_n. The computed indices offer precise insights into the structural characteristics of K_n, revealing nuanced relationships between molecular topology and topological features. The integration of MATLAB for graph plotting enhances the interpretability of the findings, providing a comprehensive understanding of the molecular variations within Non-Kekulean Benzenoid graphs. This study not only advances our knowledge of molecular structures but also underscores the effectiveness of combining mathematical methodologies and computational tools for rigorous analysis. The results contribute significantly to graph theory and computational chemistry, guiding future investigations into diverse molecular structures and their unique properties.

Limitations of the Study

While this study provides valuable insights into the topological indices of Non-Kekulean Benzenoid graphs, it is not without limitations. First, the analysis is limited to a specific class of molecular structures, and the results may not generalize to other types of graphs. Second, the computational complexity of deriving the NM-polynomial and associated indices increases with the size of the graph, which could limit the applicability of this approach to very large molecular systems. Finally, the study relies on theoretical computations, and further experimental validation is needed to confirm the practical utility of these indices in real-world chemical applications.

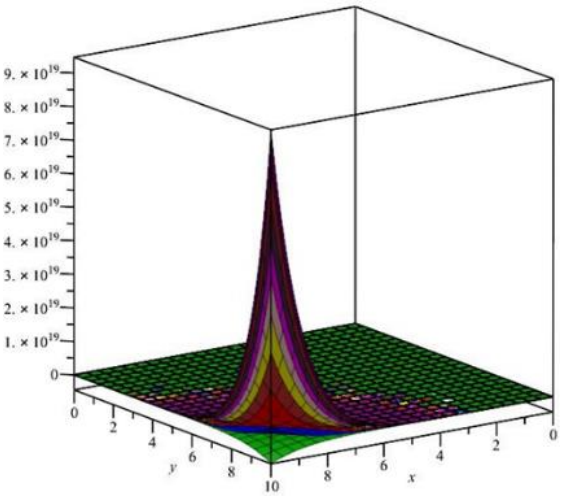

Figure 2. Graphical representation of the NM-polynomial for Non- Kekulean Benzenoid, illustrating the frequency distribution of different degree-based interactions in the molecular structure.

[4,5] [5,7] [6,7] [6,8]
[7,9] [8,8] [8,9] [9,9]

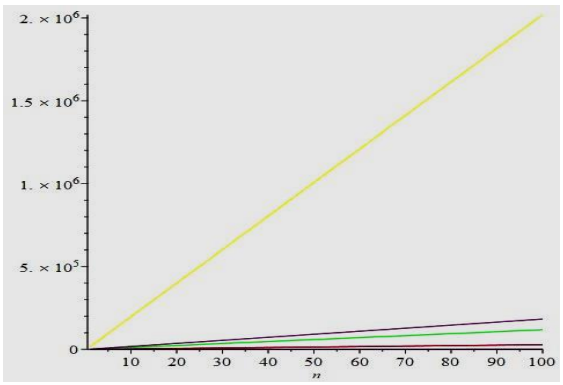

Figure 4: Comparison of Indices of Non-Kekulean Benzenoid K_n

M_1
M_2^*
F_N^*
$^{nm}M_2$
ND_3
ND_5
NH
NI
S

CONCLUSION

This research provides a detailed analysis of neighborhood degree sum-based topological indices for Non-Kekulean Benzenoid graphs

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K_n using the NM-polynomial approach. The computed in- dices, including the third version of the Zagreb index, neighborhood second Zagreb index, and neighborhood forgotten topological index, offer valuable insights into the structural properties of K_n. The graphical representation and comparative analysis highlight the dominance of the ND_3 index and the slower increase of the F_N^* index, providing a foundation for future research in this area. The integration of computational tools with mathematical methodologies enhances the interpretability of the results, contributing to the fields of graph theory and computational chemistry.

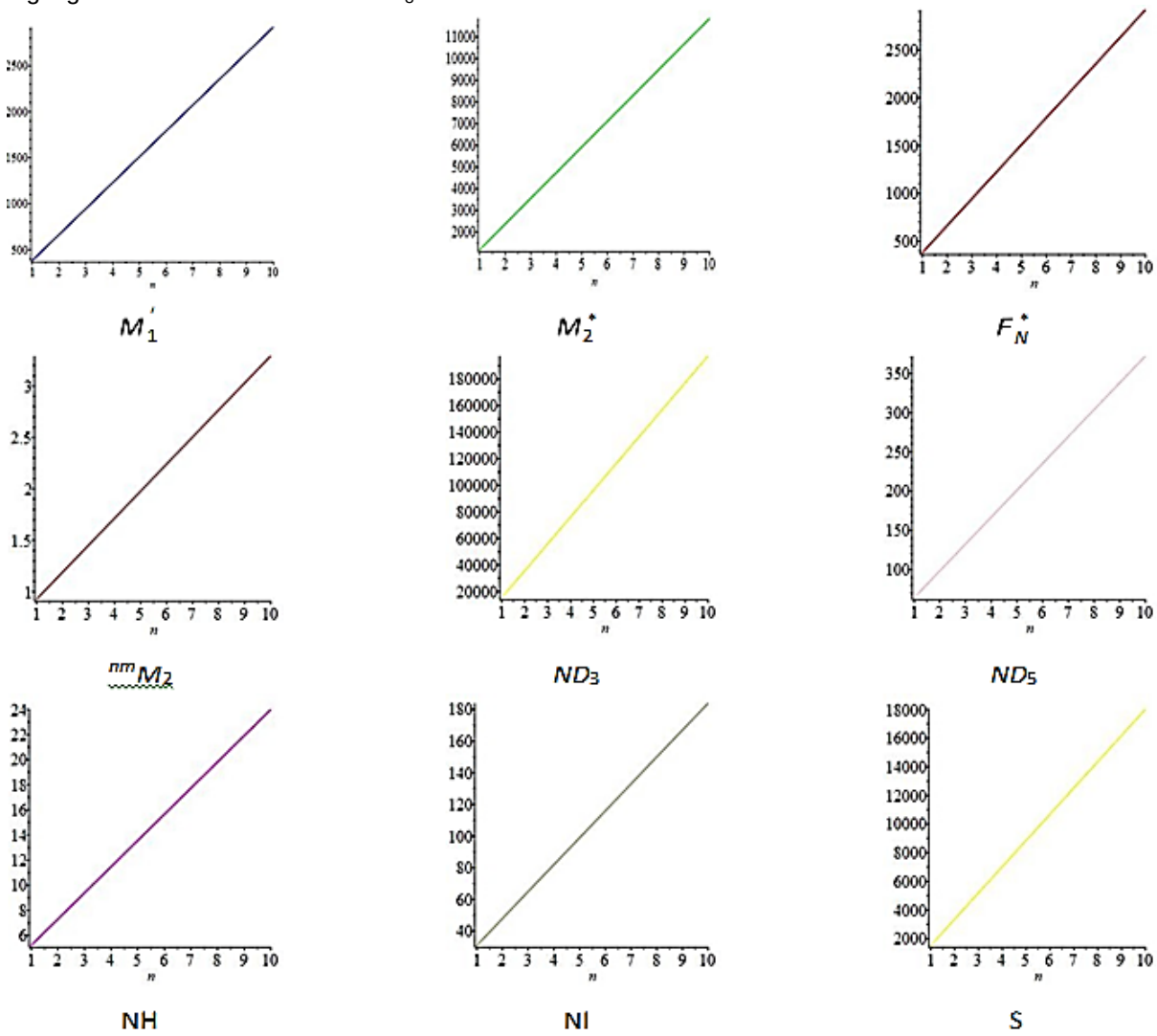

Figure 3. 3D visualization of neighborhood degree sum-based topological indices of Non- Kekulean Benzenoid, highlighting the relative magnitudes of various indices.

Author Contributions

Adnan Asghar: concept, design, analysis, writing, or revision of the manuscript.

Data Availability

No data were used to support this study.

Disclosure of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Ethical Approval

This article does not contain any studies with human participants or animals performed by any of the authors.

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