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Entropy and Neighborhood Sum Degree-Based Indices for Kekulene-Type Carbon Nanostructures: A Graph-Theoretic Approach

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Abstract: A real number known as the topological index (TI), which is invariant under network isomorphism, characterizes the connection between a chemical structure and its attributes. Chemical reactivity, physical properties, and biological activity can all be predicted using TIs derived from chemical structures. A number of TIs have been identified and investigated for various molecular graphs. This article computes entropy measures and the neighborhood-sum-degree-based M-polynomial for the kekulene systems (4,4) and ZHK(3), which are polycyclic aromatic carbons composed of 12 fused benzene rings. We derive the appropriate analytical expressions for these compounds. The obtained results will facilitate a more in-depth structural investigation of these structures by theoretical chemists.

Keywords: degree-based indices; m-polynomial; entropy measures; neighborhood sum degree-based indices.

1. Introduction

Structural formulas provide a visual representation of the arrangement of atoms in a molecule, indicating the types of atoms present and how they are bonded to one another. On the other hand, topological networks represent the connectivity of atoms within a molecule without necessarily depicting the spatial arrangement. In other words, topological networks focus on the connectivity of atoms, neglecting bond angles and molecular geometry.

The development of topological methods in chemical graph theory has facilitated the exploration of various molecular properties, such as chemical reactivity, stability, and biological activity. Researchers can apply graph theory concepts to analyze molecular structures more rigorously by converting structural formulas into mathematical graphs. This approach has proven especially useful in the study of large and complex molecules, such as polymers and biomolecules.

Chemical graph theory enables scientists and mathematicians to comprehensively analyze molecular compounds by representing molecular structures as graphs. In these graphs, the vertices correspond to the atoms within individual molecules or molecular groups. The connections between these vertices, depicted as edges in the chemical graph, illustrate

interactions among chemical entities. These edges often signify reactions, reaction processes, chemical bonds, or other changes in molecular entities.

The primary techniques for theoretically investigating chemical compounds are increasingly graph theoretical tools. Specifically, QSAR/QSPR methods are considered useful quasi-strategies and computational tools for predicting chemical compound properties. These methods are crucial to the creation of new, more effective herbicides, as their properties can be estimated prior to synthesis, thereby affecting the design [1]. Furthermore, QSPR/QSAR models can replace experimental measurements because they are less expensive and time-consuming. In this context, topological indices provide a numerical representation of molecular topology.

The topological index (TI), a real number that is invariant under graph isomorphism, defines the link between a chemical structure and its properties. Physical properties, chemical reactivity, and biological activity can all be predicted by chemically determined TIs. Different kinds of transition states (TIs) have been recognized and investigated for different kinds of molecular structures. The seminal paper by chemist Wiener contains the first known example of a topological index. Using the route number, the total distance between any two atoms within the alkane was calculated, and the boiling point of the alkanes was determined [2].

After extensive research, this path number is now referred to as the Wiener index. The investigation of topological indices, whose mathematical analysis started in the 1970s, was made possible by this groundbreaking work. TIs have become increasingly significant as molecular indices in theoretical chemistry because the structures of relevant molecules strongly influence their behavior and properties.

Currently, a variety of distinct TI types are defined and studied in the literature. The degree and distance indices are the most commonly used types of TIs. Distance-based refers to a topological index computation that needs to know the distance between vertices. A degree-based topological index (TI-DBI) is a subclass of TIs that is computed using the degrees of the terminal vertices of the molecular graph.

The computation of TIs can be done effectively and practically using algebraic polynomials. With this method, estimating several TIs is reduced to computing a single polynomial. For example, to find TIs based on distance, the Hosoya polynomial [3] is widely employed. Deutsch and Klavžar created a comparable polynomial for the degree-based index calculation [4]. Using this technique, several important degree-based benchmarks are computed from a single polynomial, known as the M-polynomial. Numerous scholarly works address the M-polynomial and its application in the computation of degree-based indices [5]. Degree-based entropy measures are computed for these structures.

The neighborhood-sum degree-based TIs are a recent development in the application of graph theory to chemical compound research. They have been used in statistical regression analysis and QSPR to predict certain chemical properties of molecular graphs [6,7]. The degree-based entropy metrics widely studied and employed in graph theory are considered information functions in the study of networks. Applications of entropy network measures include the study of the chemical and biological properties of molecular graphs and the quantitative description of a molecule's structure.

There are currently only a few examples in academic articles that show how to compute neighborhood-sum degree-based M-Polynomials and neighborhood-sum degree-based entropy measurements.

A polycyclic aromatic hydrocarbon, kekulene, is composed of twelve fused benzene ring circles. Its chemical formula is $C_{48}H_{24}$, and it is thus classified as a {12}-circulene. Given the name August Kekulé in honor of his discovery of the structure of the benzene molecule, it was first synthesized in 1978. The nature of the π bonding within the molecule has been the subject of much discussion due to the variety of possible arrangements. The two most significant configurations are the "Clar" configuration, which consists of six benzene-like (aromatic 6 π electron rings) connected by bridging bonds and vinyl groups in non-aromatic rings, and the "Kekulé" configuration, which consists of two concentric aromatic rings (18 π electron inner, 30 π electron outer) linked by radial single bonds, shown in below Figure 1 and Figure 2.[26]

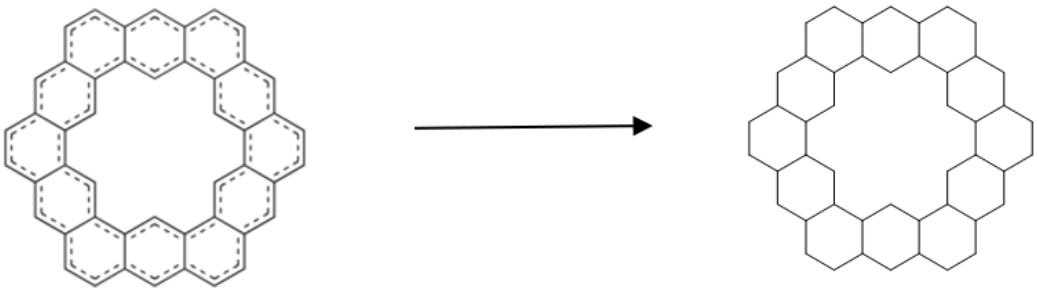


Figure 1. "Kékule" configuration: Two concentric aromatic rings.

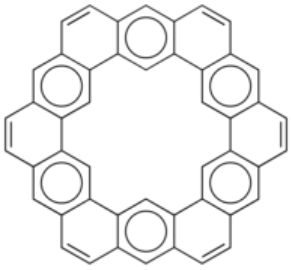


Figure 2. "Clar" configuration: Benzene rings alternating with non-aromatic linkers.

The chemical was first synthesized in 1978 and allowed the experimental determination of its electronic structure. The late 1970s saw the discovery of benzene rings using H-NMR, and X-ray analysis demonstrated the presence of alternating aromatic and non-aromatic rings in the structure, both of which were consistent with the Clar arrangement. The carbon-carbon bond lengths and bond ordering were evaluated in 2019 using single-molecule atomic force microscopy. This revealed the structure to be one of alternating non-aromatic connections and benzene-like rings. This arrangement meets Clar's requirement since it has the greatest number of disjunct aromatic π sextets. The structure is fundamentally planar, but its symmetry is only threefold, not sixfold. There is a little alternating tilt to the carbon-hydrogen bonds in the core of the ring.

The scientific community has been interested in cycloarenes, a fascinating class of polycyclic aromatic hydrocarbons (PAHs), for decades due to their unique electrical and molecular properties. These platforms are ideal for exploring fundamental questions about aromaticity, particularly those related to electron distribution in complex aromatic systems. Recently, cycloarenes have attracted renewed attention because they can serve as models for graphene pores. Kekulene has probably been studied more than any other member of its family. Its electrical structure has been known for many years; the Clar model 1a and the annulene Kekulé structure 1b are especially significant, as shown in Figure 3[26]. In fact, this molecule

was initially shown to possess traits such as hyperaromaticity, which were linked to an annulenoid that was supposedly representative.

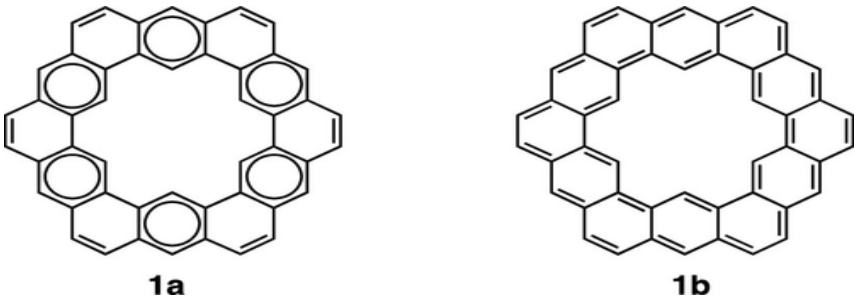


Figure 3. Clar model 1a and the annulenoid Kekule structure 1b.

We consider only one connected graph with not many edges and no self-loops. Where V(Γ) and E(Γ) are the vertex set and edge set, respectively, the graph Γ is referred to as a connected graph. The symbol d_v stands for the vertex's degree.

$N_\Gamma(v)$ represents the neighborhood sum degree-based Tis [8–10]. The NM polynomial is a mathematical tool used to characterize the structure of a chemical graph based on the distances between its vertices. The molecular graph's neighborhood sum degree can be expressed as $|N_\Gamma(v)| = d_v$. The total of the degrees of v's neighboring vertices is shown by the $N_\Gamma(v)$. First, let's construct the [24,25] M-polynomial of Γ that is based on the neighbourhood sum degree:

$$NM(\Gamma) = \sum_{i\le j}(\text{Number of all edges } uv \text{ such that } H_u = i, H_v = j)s^i p^j. \quad (1)$$

$$D(\Gamma) = \sum_{uv\in E(\Gamma)} g(\phi_u \phi_v) \quad \text{and} \quad NM(\Gamma) = \sum_{uv\in E(\Gamma)} g(\omega_u \omega_v) \quad (2)$$

For Figures 4 and 8, the degree-based Tis [11-12],[29-31] and neighborhood degree sum-based (ND) Tis are formulated in Table 1 below.

Table 1. $\mathcal{NM}$ -polynomial expressions [11-12].

SL.NO	Degree-based TIs derived from $\mathcal{NM}$ (Γ; s, p)	
1	$M_1(\Gamma) = \mathbb{D}_s + \mathbb{D}_p(\mathcal{NM}(\Gamma; s, p))\|_{s=p=1}$	First Zagreb Index
2	$M_2(\Gamma) = \mathbb{D}_s \mathbb{D}_p(\mathcal{NM}(\Gamma; s, p))\|_{s=p=1}$	Second Zagreb Index
3	$M_2^m(\Gamma) = \mathbb{S}_s \mathbb{S}_p(\mathcal{NM}(\Gamma; s, p))\|_{s=p=1}$	Second Modified Zagreb Index
4	$R_\alpha(\Gamma) = \mathbb{D}_s^\alpha \mathbb{D}_p^\alpha(\mathcal{NM}(\Gamma; s, p))\|_{s=p=1}$	General Randic Index
5	$RR_\alpha(\Gamma) = \mathbb{S}_s^\alpha \mathbb{S}_p^\alpha(\mathcal{NM}(\Gamma; s, p))\|_{s=p=1}$	Inverse Randic Index
6	$SDD(\Gamma) = \mathbb{D}_s\mathbb{S}_p + \mathbb{D}_p\mathbb{S}_s(\mathcal{NM}(\Gamma; s, p))\|_{s=p=1}$	Symmetric Division Index
7	$H(\Gamma) = 2\mathbb{S}_s J(\mathcal{NM}(\Gamma; s, p)\|_{s=1}$	Harmonic Index
8	$I(\Gamma) = \mathbb{S}_s J\mathbb{D}_s \mathbb{D}_p(\mathcal{NM}(\Gamma; s, p))\|_{s=1}$	Inverse Sum Index
9	$A(\Gamma) = \mathbb{S}_s^3 Q_{-2} J\mathbb{D}_s^3 \mathbb{D}_p^3(\mathcal{NM}(\Gamma; s, p))\|_{s=1}$	Augmented Zagreb Index
10	$ABC(\Gamma) = \mathbb{D}_s^{\frac{1}{2}} Q_{-2} J\mathbb{S}_s^{\frac{1}{2}} \mathbb{S}_p^{\frac{1}{2}}(\mathcal{NM}(\Gamma; s, p))\|_{s=1}$	Atom - bond connectivity Index
11	$ABS(\Gamma) = \mathbb{D}_s^{\frac{1}{2}} Q_{-2} J(\mathbb{S}_s^{\frac{1}{2}} + S_p^{\frac{1}{2}})(\mathcal{NM}(\Gamma; s, p))\|_{s=1}$	Atom – bond sum Index
12	$F(\Gamma) = \mathbb{D}_s^2 + \mathbb{D}_p^2(\mathcal{NM}(\Gamma; s, p))\|_{s=p=1}$	F-index
13	$RR(\Gamma) = \mathbb{D}_s^{\frac{1}{2}} \mathbb{D}_p^{\frac{1}{2}}(\mathcal{NM}(\Gamma; s, p))\|_{s=p=1}$	Reciprocal Randic Index
14	$RRR(\Gamma) = \mathbb{D}_s^{\frac{1}{2}} Q_{-1} \mathbb{D}_p^{\frac{1}{2}} Q_{-1}(\mathcal{NM}(\Gamma; s, p))\|_{s=p=1}$	Reduced Reciprocal Randic Index

The derivations of $\mathcal{NM}$-Polynomial are listed above in Table 1.

2. Neighborhood Degree Sum-Based Entropy Measures

Shannon defined entropy as a way to measure the degree of uncertainty in a system or the unexpectedness of pertinent information in his groundbreaking work. The contemporary theory of information was founded on this work. Entropy calculations have been used to quantify a network's structural information [13]. Because of its adaptability, information theory has been used extensively across a variety of fields, including the chemical and medical sciences, electrical engineering, linguistics, and graph theory for chemical networks [14]. A method for measuring the topological information of chemical networks and graphs was introduced by graph entropy.

Graph entropy was calculated by Rashevsky using vertex orbits [15]. Mathematicians can relate probability distributions to graph elements, such as edges and vertices, using intrinsic and extrinsic graph entropy measures. Numerous disciplines, including biology, ecology, chemistry, and sociology, frequently use graph entropies [16–18]. Dehmer generated graph entropies and extracted structural information from them using information functional analysis [19,20]. Walk-based graph entropies were studied [21,22], who also created a graph entropy metric that is physically sound. Applications of entropy network metrics include analyzing the chemical and biological properties of molecular graphs and providing quantitative representations of molecular structures [23,24]. Entropy metrics find wide applications in the study of chemical graph theory.

The node entropy is defined as

$$\mathcal{ENT}_{\Gamma}(v_i) = -\sum_{j=1}^{d_i} p_{ij} \log\left(p_{ij}\right) \qquad (3)$$

For an edge-weighted graph $\Gamma = (\mathcal{V}, \mathcal{E}, w)$, the entropy measure of Γ is defined as [18,25].

$$\mathcal{ENT}_{\Omega}(\Gamma) = \log_{\Omega}(\Gamma) - \frac{1}{\Omega(\Gamma)} \sum_{uv \in E(\Gamma)} \mathcal{F}(d_u, d_v) \log \mathcal{F}(d_u, d_v) \qquad (4)$$

3. Computing the Neighborhood Sum Degree-Based M-polynomial for Kekulene Systems (4,4)

This section computes the appropriate analytic formulations for entropy measures and neighborhood-degree-sum-based indices for kekulene systems (4,4) shown in Figure 4 and Table 2 [26]. Edge Partition for Kekulene System (4,4) using the M-polynomial. [10] Kekulene is a hypothesized polycyclic aromatic hydrocarbon with a unique structure, as shown in my January 2022 information update. German chemist August Kekulé, who is renowned for his contributions to the structural theory of organic chemistry, proposed it as a molecular structure.

Kekulene is composed of 60 carbon atoms arranged in five fused benzene rings and has a planar, symmetrical structure. The alternating double bonds that connect each carbon atom to two others give the molecule its aromatic character. It is important to note that kekulene has not been isolated or synthesized as a stable molecule; rather, it is a speculative idea [26,27].

Kekulene currently has no practical applications because it is a totally theoretical compound. However, speculative substances such as kekulene can inspire research and computer simulations across several areas of chemistry.

Kekulene is an intriguing topic for research in this area. Its electrical structure, stability, reactivity, and other properties can be investigated by researchers using computational methods. Despite kekulene's high instability, its structure and characteristics may serve as inspiration for the synthesis of related compounds with advantageous properties. Creating new

materials with advantageous mechanical, optical, or electrical properties can be aided by understanding the properties of polycyclic aromatic hydrocarbons, such as kekulene. The possible uses of PAHs in nanotechnology, such as in molecular electronics or as building blocks for nanomaterials, have been investigated. By studying the Kekulé, we can enhance our comprehension of aromaticity, molecular structure, and chemical bonding by developing and refining theoretical models in chemistry.

Although there may not be any practical uses for kekulene, the knowledge gained from examining its theoretical properties may have broader ramifications across a range of chemistry and materials science domains.

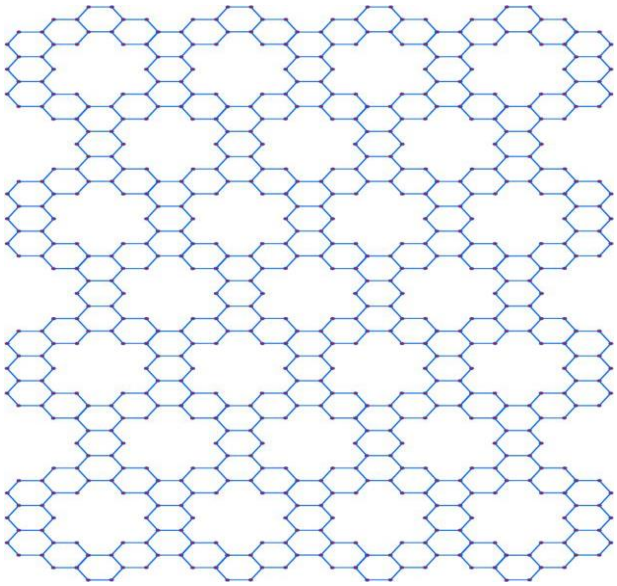


Figure 4. Kekulene System (4,4).

Let Γ be a rectangular Kekulene system RK(f, l). The number of vertices and edges of $RK(f,l)\ is\ V(\Gamma) = 36fl + 14l - 2f$ and $E(\Gamma) = 48fl + 16l - 4f$ (5)

Table 2. Edge Partition for Kekulene System (4,4) [29-31].

(d_u, d_v)	**Frequency**
(5,5)	4f + 2l
(5,7)	8f + 4l
(6,7)	8f + 4l
(6,8)	2fl − 4f − 8l
(7,8)	8f + 4l
(8,8)	24fl − 8f − 10l

Theorem 1. Assuming Γ to be a kekulene System (4,4), the $\mathcal{NM}$ -polynomial of Γ can be obtained as follows.

$$\mathcal{NM}(\Gamma; S, P) = (4f + 2l)s^5p^5 + (8f + 4l)s^5p^7 + (8f + 4l)s^6p^7 + (2fl - 4f - 8l)s^6p^8 + (8f + 4l)s^7p^8 + (24fl - 8f - 10l)s^8p^8 \quad (6)$$

Theorem 2. Assuming Γ to be a kekulene System (4,4), the $\mathcal{NM}$ -polynomial of Γ can be obtained as follows.

1. $\mathcal{NM}M_1(\Gamma) = 176f - 92l + 412fl$
2. $\mathcal{NM}M_2(\Gamma) = 1632fl + 460f - 442l$
3. $\mathcal{NM}SMZ(\Gamma) = \frac{719}{1400}f + \frac{213}{5600}l + \frac{5}{12}fl$
4. $\mathcal{NM}GRI(\Gamma) = 460f - 442l + 1632fl$

5. $\mathcal{NM}\mathrm{IRI}(\Gamma) = \frac{719}{1400} f + \frac{213}{5600} l + \frac{5}{12} fl$

6. $\mathcal{NM}\mathrm{SDD}(\Gamma) = \frac{1152}{35} f - \frac{563}{70} l + \frac{313}{6} fl$

7. $\mathcal{NM}\mathrm{H}(\Gamma) = \frac{1301}{455} f - \frac{323}{1820} l + \frac{23}{7} fl$

8. $\mathcal{NM}\mathrm{ISI}(\Gamma) = \frac{131948}{1365} f + \frac{5134}{1365} l + \frac{720}{7} fl$

.9. $\mathcal{NM}\mathrm{AZ}(\Gamma) = \frac{67990447572161}{128384384128} f - \frac{177788916841279}{256768768256} l + \frac{830336}{343} fl$

10. $\mathcal{NM}\mathrm{ABC}(\Gamma) = 8.7460 f - 1.4331 l + 12.225 fl$

11. $\mathcal{NM}\mathrm{ABS}(\Gamma) = 8.7816 f - 6.7774 l + 24.302 fl$

12. $\mathcal{NM}\mathrm{F}(\Gamma) = 3272\mathrm{fl} + 952\mathrm{f} - 892\mathrm{l}$

13. $\mathcal{NM}\mathrm{RR}(\Gamma) = 87.329 f - 45.907 l + 205.86 fl$

14. $\mathcal{NM}\mathrm{RRR}(\Gamma) = 71.192 f - 41.901 l + 179.83 fl$ (7)

Proof: let $h(s,p) = \mathcal{NM}(\Gamma; s, p) = (4f + 2l)s^5p^5 + (8f + 4l)s^5p^7 + (8f + 4l)s^6p^7 + (2fl - 4f - 8l)s^6p^8 + (8f + 4l)s^7p^8 + (24fl - 8f - 10l)s^8p^8$

$\mathbb{D}_s + \mathbb{D}_p = 10(4f + 2l)s^5p^5 + 12(8f + 4l)s^5p^7 + 13(8f + 4l)s^6p^7 + 14(2fl - 4f - 8l)s^6p^8 + 15(8f + 4l)s^7p^8 + 16(24fl - 8f - 10l)s^8p^8$

$\mathbb{D}_s\,\mathbb{D}_p = 25(4f + 2l)s^5p^5 + 35(8f + 4l)s^5p^7 + 42(8f + 4l)s^6p^7 + 48(2fl - 4f - 8l)s^6p^8 + 56(8f + 4l)s^7p^8 + 64(24fl - 8f - 10l)s^8p^8$

$\mathbb{S}_s\,\mathbb{S}_p = \frac{1}{25}(4f + 2l)s^5p^5 + \frac{1}{35}(8f + 4l)s^5p^7 + \frac{1}{42}(8f + 4l)s^6p^7 + \frac{1}{48}(2fl - 4f - 8l)s^6p^8 + \frac{1}{56}(8f + 4l)s^7p^8 + + \frac{1}{64}(24fl - 8f - 10l)s^8p^8$

$\mathbb{D}_s^{\alpha}\,\mathbb{D}_p^{\alpha} = (25)^{\alpha}(4f + 2l)s^5p^5 + (35)^{\alpha}(8f + 4l)s^5p^7 + (42)^{\alpha}(8f + 4l)s^6p^7 + (48)^{\alpha}(2fl - 4f - 8l)s^6p^8 + (56)^{\alpha}(8f + 4l)s^7p^8 + (64)^{\alpha}(24fl - 8f - 10l)s^8p^8$

$\mathbb{S}_s^{\alpha}\,\mathbb{S}_p^{\alpha} = \frac{1}{25^{\alpha}}(4f + 2l)s^5p^5 + \frac{1}{35^{\alpha}}(8f + 4l)s^5p^7 + \frac{1}{42^{\alpha}}(8f + 4l)s^6p^7 + \frac{1}{48^{\alpha}}(2fl - 4f - 8l)s^6p^8 + \frac{1}{56^{\alpha}}(8f + 4l)s^7p^8 + + \frac{1}{64^{\alpha}}(24fl - 8f - 10l)s^8p^8$

$\mathbb{D}_s\mathbb{S}_p + \mathbb{D}_p\mathbb{S}_s = 2(4f + 2l)s^5p^5 + \left(\frac{74}{35}\right)(8f + 4l)s^5p^7 + \left(\frac{85}{42}\right)(8f + 4l)s^6p^7 + \left(\frac{25}{12}\right)(2fl - 4f - 8l)s^6p^8 + \left(\frac{113}{56}\right)(8f + 4l)s^7p^8 + 2(24fl - 8f - 10l)s^8p^8$

$2\mathbb{S}_s\mathrm{J} = \frac{4}{10}(4f + 2l)s^{10} + \frac{4}{12}(8f + 4l)s^{12} + \frac{4}{13}(8f + 4l)s^{13} + \frac{4}{14}(2fl - 4f - 8l)s^{14} + \frac{4}{15}(8f + 4l)s^{15} + \frac{4}{16}(24fl - 8f - 10l)s^{16}$

$\mathbb{S}_s\,\mathrm{J}\mathbb{D}_s\,\mathbb{D}_p = \frac{25}{10}(4f + 2l)s^{10} + \frac{35}{12}(8f + 4l)s^{12} + \frac{42}{13}(8f + 4l)s^{13} + \frac{48}{14}(2fl - 4f - 8l)s^{14} + \frac{156}{15}(8f + 4l)s^7p^8 + \frac{64}{16}(24fl - 8f - 10l)s^{16}$

$\mathbb{S}_s^3\mathrm{Q}_{-2}\,\mathrm{J}\mathbb{D}_s^3\,\mathbb{D}_p^3 = \left(\frac{25}{8}\right)^3(4f + 2l)s^8 + \left(\frac{7}{2}\right)^3(8f + 4l)s^{10} + \left(\frac{42}{11}\right)^3(8f + 4l)s^{11} + 64(2fl - 4f - 8l)s^{12} + \left(\frac{56}{13}\right)^3(8f + 4l)s^{13} + \left(\frac{32}{7}\right)^3(24fl - 8f - 10l)s^{14}$

$\mathbb{D}_s^{\frac{1}{2}}\mathrm{Q}_{-2}\,\mathrm{J}\mathbb{S}_s^{\frac{1}{2}}\,\mathbb{S}_P^{\frac{1}{2}} = \sqrt{\frac{8}{25}}(4f + 2l)s^5p^5 + \sqrt{\frac{10}{35}}(8f + 4l)s^5p^7 + \sqrt{\frac{11}{42}}(8f + 4l)s^6p^7 + \sqrt{\frac{12}{48}}(2fl - 4f - 8l)s^6p^8 + \sqrt{\frac{13}{56}}(8f + 4l)s^7p^8 + \sqrt{\frac{14}{64}}(24fl - 8f - 10l)s^8p^8$

$$\mathbb{D}_s^{\frac{1}{2}}Q_{-2}\,J\left(\mathbb{S}_s^{\frac{1}{2}}+\mathbb{S}_p^{\frac{1}{2}}\right)=\sqrt{\frac{8}{10}}(4f+2l)s^5p^5+\sqrt{\frac{10}{12}}(8f+4l)s^5p^7+\sqrt{\frac{11}{13}}(8f+4l)s^6p^7+\sqrt{\frac{12}{14}}(2fl-4f-8l)s^6p^8+\sqrt{\frac{13}{15}}(8f+4l)s^7p^8+\sqrt{\frac{14}{16}}(24fl-8f-10l)s^8p^8$$

$$\mathbb{D}_s^2+\mathbb{D}_p^2=50(4f+2l)s^5p^5+74(8f+4l)s^5p^7+85(8f+4l)s^6p^7+100(2fl-4f-8l)s^6p^8+113(8f+4l)s^7p^8+128(24fl-8f-10l)s^8p^8$$

$$\mathbb{D}_s^{\frac{1}{2}}\mathbb{D}_p^{\frac{1}{2}}=\sqrt{25}(4f+2l)s^5p^5+\sqrt{35}(8f+4l)s^5p^7+\sqrt{42}(8f+4l)s^6p^7+\sqrt{48}(2fl-4f-8l)s^6p^8+\sqrt{56}(8f+4l)s^7p^8+8(24fl-8f-10l)s^8p^8$$

$$\mathbb{D}_s^{\frac{1}{2}}Q_{-1}\,\mathbb{D}_p^{\frac{1}{2}}Q_{-1}=\sqrt{16}(4f+2l)s^5p^5+\sqrt{24}(8f+4l)s^5p^7+\sqrt{30}(8f+4l)s^6p^7+\sqrt{35}(2fl-4f-8l)s^6p^8+\sqrt{42}(8f+4l)s^7p^8+7(24fl-8f-10l)s^8p^8 \quad (8)$$

The partition Table 2 and the conditions of the $\mathcal{NM}$-Polynomial with its derivatives are used to derive the above results.[28–30]

4. Neighbourhood Degree Sum-Based Entropy Measures for Kekulene System (4,4)

Theorem 3. If Γ is a kekulene System (4,4), then $\mathcal{NM}$-entropy measures are given as follows

$$\mathcal{NMENT}_{NM1}=\log(176f-92l+412fl)-\frac{1}{176f-92l+412fl}((4f+2l)(10)\log10+(8f+4l)(12)\log12+(8f+4l)(13)\log13+(2fl-4l-8l)(14)\log14+(8f+4l)(15)\log15+(24fl-8f-10l)(16)\log16)$$

$$\mathcal{NMENT}_{NM2}=\log(460f-442l+1632fl)-\frac{1}{4460f-442l+1632fl}\big((4f+2l)(25)\log25+(8f+4l)(35)\log35+(8f+4l)(42)\log42+(2fl-4f-8l)(48)\log48+(8f+4l)(56)\log56+(24fl-8f-10l)(64)\log64\big)$$

$$\mathcal{NMENT}_{SMZ}=\log\left(\frac{719f}{1400}-\frac{213l}{5600}+\frac{5fl}{12}\right)-\frac{1}{\left(\frac{719f}{1400}-\frac{213l}{5600}+\frac{5fl}{12}\right)}\left((4f+2l)\left(\frac{1}{25}\right)\log\left(\frac{1}{25}\right)+(8f+4l)\left(\frac{1}{35}\right)\log\left(\frac{1}{35}\right)+(8f+4l)\left(\frac{1}{42}\right)\log\left(\frac{1}{42}\right)+(2fl-4f-8l)\left(\frac{1}{48}\right)\log\left(\frac{1}{48}\right)+(8f+4l)\left(\frac{1}{56}\right)\log\left(\frac{1}{56}\right)+(24fl-8f-10l)\left(\frac{1}{64}\right)\log\left(\frac{1}{64}\right)\right)$$

$$\mathcal{NMENT}_{GRI}=\log(GRI)-\frac{1}{GRI}\big((4f+2l)(25^\alpha)\log(25^\alpha)+(8f+4l)(35^\alpha)\log(35^\alpha)+(8f+4l)(42^\alpha)\log(42^\alpha)+(2fl-4f-8l)(48^\alpha)\log(48^\alpha)+(8f+4l)(56^\alpha)\log(56^\alpha)+(24fl-8f-10l)(64^\alpha)\log(64^\alpha)\big)$$

$$\mathcal{NMENT}_{IRI}=\log(IRI)-\frac{1}{IRI}\left((4f+2l)\left(\frac{1}{25^\alpha}\right)\log\left(\frac{1}{25^\alpha}\right)+(8f+4l)\left(\frac{1}{35^\alpha}\right)\log\left(\frac{1}{35^\alpha}\right)+(8f+4l)\left(\frac{1}{42^\alpha}\right)\log\left(\frac{1}{42^\alpha}\right)+(2fl-4f-8l)\left(\frac{1}{48^\alpha}\right)\log\left(\frac{1}{48^\alpha}\right)+(8f+4l)\left(\frac{1}{56^\alpha}\right)\log\left(\frac{1}{56^\alpha}\right)+(24fl-8f-10l)\left(\frac{1}{64^\alpha}\right)\log\left(\frac{1}{64^\alpha}\right)\right)$$

$$\mathcal{NMENT}_{\mathrm{SDD}} = \log\left(\frac{1152\mathrm{f}}{35} - \frac{563\mathrm{l}}{70} + \frac{313\mathrm{fl}}{6}\right) - \frac{1}{\frac{1152\mathrm{f}}{35} - \frac{563\mathrm{l}}{70} + \frac{313\mathrm{fl}}{6}}\left((4\mathrm{f}+2\mathrm{l})2\log(2) + (8\mathrm{f}+4\mathrm{l})\left(\frac{74}{35}\right)\log\left(\frac{74}{35}\right) + (8\mathrm{f}+4\mathrm{l})\left(\frac{85}{42}\right)\log\left(\frac{85}{42}\right) + (2\mathrm{fl}-4\mathrm{f}-8\mathrm{l})\left(\frac{25}{12}\right)\log\left(\frac{25}{12}\right) + (8\mathrm{f}+4\mathrm{l})\left(\frac{113}{56}\right)\log\left(\frac{113}{56}\right) + (24\mathrm{fl}-8\mathrm{f}-10\mathrm{l})2\log(2)\right)$$

$$\mathcal{NMENT}_{\mathrm{H}} = \log\left(\frac{1301\mathrm{f}}{455} - \frac{323\mathrm{l}}{1820} + \frac{23\mathrm{fl}}{7}\right) - \frac{1}{\frac{1301\mathrm{f}}{455} - \frac{323\mathrm{l}}{1820} + \frac{23\mathrm{fl}}{7}}\left((4\mathrm{f}+2\mathrm{l})\left(\frac{1}{5}\right)\log\left(\frac{1}{5}\right) + (8\mathrm{f}+4\mathrm{l})\left(\frac{1}{6}\right)\log\left(\frac{1}{6}\right) + (8\mathrm{f}+4\mathrm{l})\left(\frac{2}{13}\right)\log\left(\frac{2}{13}\right) + (2\mathrm{fl}-4\mathrm{f}-8\mathrm{l})\left(\frac{1}{7}\right)\log\left(\frac{1}{7}\right) + (8\mathrm{f}+4\mathrm{l})\left(\frac{2}{15}\right)\log\left(\frac{2}{15}\right) + (24\mathrm{fl}-8\mathrm{f}-10\mathrm{l})\left(\frac{1}{8}\right)\log\left(\frac{1}{8}\right)\right)$$

$$\begin{aligned}\mathcal{NMENT}_{\mathrm{ISI}} = {} & \log\left(\frac{131948\mathrm{f}}{1365} + \frac{5134\mathrm{l}}{1365} + \frac{720\mathrm{fl}}{7}\right) \\ & - \frac{1}{\frac{131948\mathrm{f}}{1365} + \frac{5134\mathrm{l}}{1365} + \frac{720\mathrm{fl}}{7}}\left((4\mathrm{f}+2\mathrm{l})\left(\frac{5}{2}\right)\log\left(\frac{5}{2}\right)\right. \\ & + (8\mathrm{f}+4\mathrm{l})\left(\frac{35}{12}\right)\log\left(\frac{35}{12}\right) + (8\mathrm{f}+4\mathrm{l})\left(\frac{42}{13}\right)\log\left(\frac{42}{13}\right) \\ & + (2\mathrm{fl}-4\mathrm{f}-8\mathrm{l})\left(\frac{24}{7}\right)\log\left(\frac{24}{7}\right) + (8\mathrm{f}+4\mathrm{l})\left(\frac{52}{5}\right)\log\left(\frac{52}{5}\right) \\ & \left. + (24\mathrm{fl}-8\mathrm{f}-10\mathrm{l})(4)\log(4)\right)\end{aligned}$$

$$\mathcal{NMENT}_{\mathrm{az}} = \log\left(\frac{67990447572161\mathrm{f}}{128384384128} - \frac{177788916841279\mathrm{l}}{256768768256} + \frac{830336\mathrm{fl}}{343}\right) - \frac{1}{\frac{67990447572161\mathrm{f}}{128384384128} - \frac{177788916841279\mathrm{l}}{256768768256} + \frac{830336\mathrm{fl}}{343}}\left((4\mathrm{f}+2\mathrm{l})\left(\frac{15625}{512}\right)\log\left(\frac{15625}{512}\right) + (8\mathrm{f}+4\mathrm{l})\left(\frac{343}{8}\right)\log\left(\frac{343}{8}\right) + (8\mathrm{f}+4\mathrm{l})\left(\frac{74088}{1331}\right)\log\left(\frac{74088}{1331}\right) + (2\mathrm{fl}-4\mathrm{f}-8\mathrm{l})(64)\log(64) + (8\mathrm{f}+4\mathrm{l})\left(\frac{175616}{2197}\right)\log\left(\frac{175616}{2197}\right) + (224\mathrm{fl}-8\mathrm{f}-10\mathrm{l})\left(\frac{32768}{343}\right)\log\left(\frac{32768}{343}\right)\right)$$

$$\mathcal{NMENT}_{\mathrm{ABC}} = \log(\mathrm{ABC}) - \frac{1}{\mathrm{ABC}}\left\{(4\mathrm{f}+2\mathrm{l})\left(\frac{2\sqrt{2}}{5}\right)\log\left(\frac{2\sqrt{2}}{5}\right) + (8\mathrm{f}+4\mathrm{l})\left(\sqrt{\frac{10}{35}}\right)\log\left(\sqrt{\frac{10}{35}}\right) + (8\mathrm{f}+4\mathrm{l})\left(\sqrt{\frac{11}{42}}\right)\log\left(\sqrt{\frac{11}{42}}\right) + (2\mathrm{fl}-4\mathrm{f}-8\mathrm{l})\left(\sqrt{\frac{1}{4}}\right)\log\left(\sqrt{\frac{1}{4}}\right) + (8\mathrm{f}+4\mathrm{l})\left(\sqrt{\frac{13}{56}}\right)\log\left(\sqrt{\frac{13}{56}}\right) + (24\mathrm{fl}-8\mathrm{f}-10\mathrm{l})\left(\sqrt{\frac{14}{64}}\right)\log\left(\sqrt{\frac{14}{64}}\right)\right\}$$

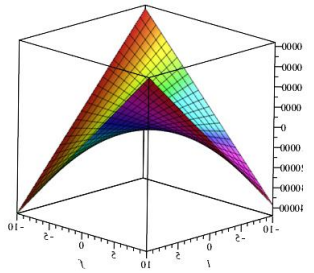
$$\mathcal{NMENT}_{\mathrm{ABS}} = \log(\mathrm{ABS}) - \frac{1}{\mathrm{ABS}}\left\{(4\mathrm{f}+2\mathrm{l})\left(\frac{2\sqrt{5}}{5}\right)\log\left(\frac{2\sqrt{5}}{5}\right) + (8\mathrm{f}+4\mathrm{l})\left(\sqrt{\frac{10}{12}}\right)\log\left(\sqrt{\frac{10}{12}}\right) + (8\mathrm{f}+4\mathrm{l})\left(\sqrt{\frac{11}{13}}\right)\log\left(\sqrt{\frac{11}{13}}\right) + (2\mathrm{fl}-4\mathrm{f}-8\mathrm{l})\left(\sqrt{\frac{12}{14}}\right)\log\left(\sqrt{\frac{12}{14}}\right) + (8\mathrm{f}+4\mathrm{l})\left(\sqrt{\frac{13}{15}}\right)\log\left(\sqrt{\frac{13}{15}}\right) + (24\mathrm{fl}-8\mathrm{f}-10\mathrm{l})\left(\sqrt{\frac{14}{16}}\right)\log\left(\sqrt{\frac{14}{16}}\right)\right\}$$

$$\begin{aligned}\mathcal{NMENT}_{\mathrm{F}} = {} & \log(952\mathrm{f}-892\mathrm{l}+3272\mathrm{fl}) \\ & - \frac{1}{952\mathrm{f}-892\mathrm{l}+3272\mathrm{fl}}\big((4\mathrm{f}+2\mathrm{l})(50)\log 50 + (8\mathrm{f}+4\mathrm{l})(74)\log 74 \\ & + (8\mathrm{f}+4\mathrm{l})(85)\log 85 + (2\mathrm{fl}-4\mathrm{f}-8\mathrm{l})(100)\log 100 \\ & + (8\mathrm{f}+4\mathrm{l})(113)\log 113 + (24\mathrm{fl}-8\mathrm{f}-10\mathrm{l})(128)\log 128\big)\mathcal{NMENT}_{\mathrm{RR}} \\ & = \log(\mathrm{RR}) - \frac{1}{\mathrm{RR}}\big((4\mathrm{f}+2\mathrm{l})(5)\log 5 + (8\mathrm{f}+4\mathrm{l})\big(\sqrt{35}\big)\log\sqrt{35} \\ & + (8\mathrm{f}+4\mathrm{l})\big(\sqrt{42}\big)\log\sqrt{42} + (2\mathrm{fl}-4\mathrm{f}-8\mathrm{l})\big(4\sqrt{3}\big)\log 4\sqrt{3} \\ & + (8\mathrm{f}+4\mathrm{l})\big(2\sqrt{14}\big)\log 2\sqrt{14} + (24\mathrm{fl}-8\mathrm{f}-10\mathrm{l})(8)\log 8\big)\end{aligned}$$

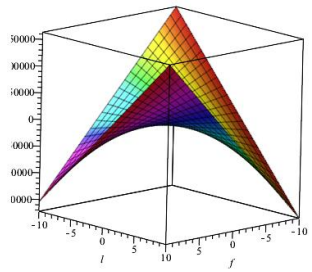
$$\mathcal{NMENT}_{\mathrm{RRR}} = \log(\mathrm{RRR}) - \frac{1}{\mathrm{RRR}}\big((4f + 2l)(4)\log 4 + (8f + 4l)\big(2\sqrt{6}\big)\log 2\sqrt{6} + (8f + 4l)\big(\sqrt{30}\big)\log\sqrt{30} + (2fl - 4f - 8l)\big(\sqrt{35}\big)\log\sqrt{35} + (8f + 4l)\big(\sqrt{42}\big)\log\sqrt{42} + (24fl - 8f - 10l)(7)\log(7)\big) \quad (9)$$

5. Comparative Analysis for Kekulene System (4,4)

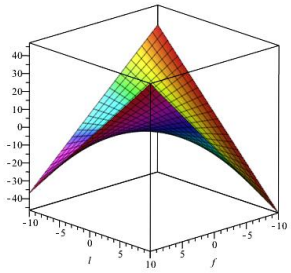
This section presents the three-dimensional graphs that represent the analytical equations for the neighborhood-degree-sum-based indices derived from Theorems 2 and 3. These graphics make it easier for the reader to understand and appreciate how the indices behave regarding the variables that define the molecular structure. Moreover, the outcomes of Theorem 2 have also been presented as comparison plots, where each neighborhood-degree-sum-based index is plotted on a single graph against a single structural variable [9,10]. The differences between the indices and the chemical structure are graphically represented in these comparison charts. Figures 2 and 3 show these charts. Tables 3–6 display the calculated numerical values for the indices [31–33]. To aid readers in understanding the numerical data, Figures 5, 6, and 7 present the data as three-dimensional graphs.



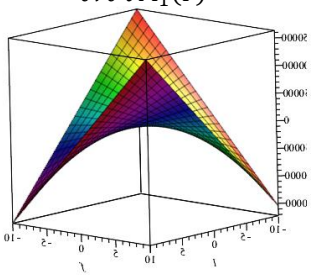
$\mathcal{NM}\mathrm{M}_1(\Gamma)$



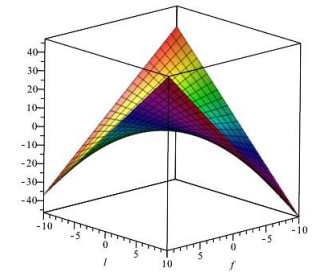
$\mathcal{NM}\mathrm{M}_2(\Gamma)$



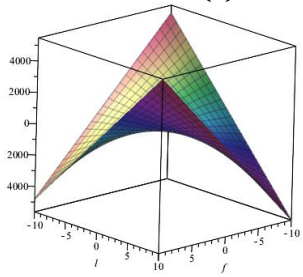
$\mathcal{NM}\mathrm{SMZ}(\Gamma)$



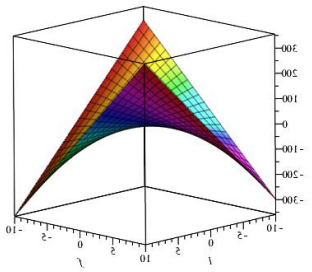
$\mathcal{NM}\mathrm{GRI}(\Gamma)$



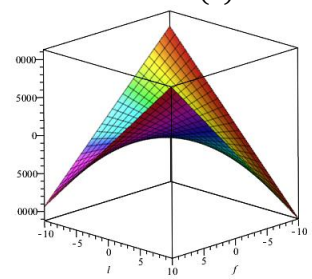
$\mathcal{NM}\mathrm{IRI}(\Gamma)$



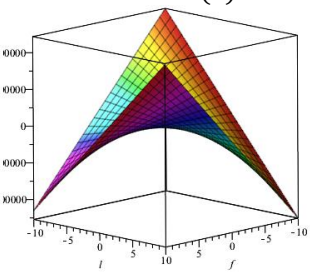
$\mathcal{NM}\mathrm{SDD}(\Gamma)$



$\mathcal{NM}\mathrm{H}(\Gamma)$



$\mathcal{NM}\mathrm{ISI}(\Gamma)$



$\mathcal{NM}\mathrm{AZ}(\Gamma)$

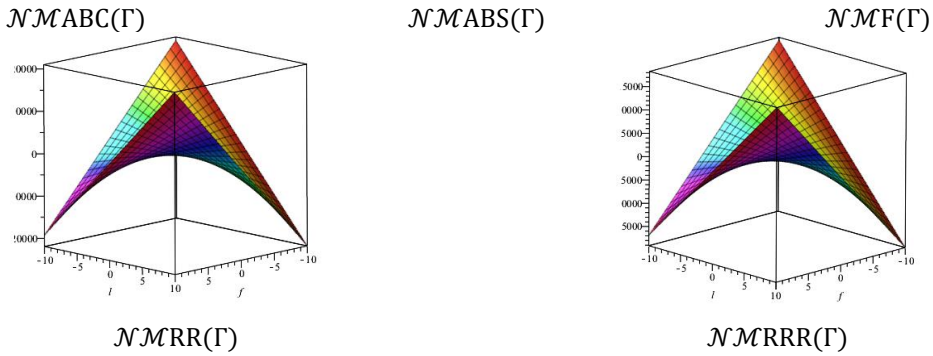


Figure 5. 3D plots for Theorem 2.

Table 3. Comparison Table for Theorem 2.

(f,l)	$\mathcal{NM}\mathbf{M_1}(\Gamma)$	$\mathcal{NM}\mathbf{M_2}(\Gamma)$	$\mathcal{NM}$SMZ(Γ)	$\mathcal{NM}$GRI(Γ)	$\mathcal{NM}$IRI(Γ)	$\mathcal{NM}$SDD(Γ)	$\mathcal{NM}$H(Γ)
(1,1)	496	1650	0.96827	1650	0.96827	77.038	5.9676
(2,2)	1816	6564	2.7699	6564	2.7699	258.41	18.507
(3,3)	3960	14742	5.4048	14742	5.4048	544.11	37.617
(4,4)	6928	26184	8.8731	26184	8.8731	934.15	63.299
(5,5)	10720	40890	13.175	40890	13.175	1428.5	95.552
(6,6)	15336	58860	18.31	58860	18.31	2027.2	134.38
(7,7)	20776	80094	24.278	80094	24.278	2730.3	179.77
(8,8)	27040	104592	31.08	104592	31.08	3537.6	231.74
(9,9)	34128	132354	38.714	132354	38.714	4449.3	290.28

Table 4. Comparison Table for Theorem 2.

(f,l)	$\mathcal{NM}$ISI(Γ)	$\mathcal{NM}$AZ(Γ)	$\mathcal{NM}$ABC(Γ)	$\mathcal{NM}$ABS(Γ)	$\mathcal{NM}$F(Γ)	$\mathcal{NM}$RR(Γ)	$\mathcal{NM}$RRR(Γ)
(1,1)	203.28	2258	19.538	34.885	3332	247.28	209.13
(2,2)	612.28	9357.6	63.527	118.37	13208	906.28	777.91
(3,3)	1227	21299	131.96	250.47	29628	1977	1706.4
(4,4)	2047.4	38082	224.85	431.16	52592	3459.4	2994.5
(5,5)	3073.6	59706	342.19	660.47	82100	5353.5	4642.1
(6,6)	4305.4	86172	483.99	938.37	118152	7659.4	6649.7
(7,7)	5743	1.1748*10^5	650.22	1264.9	160748	10377	9016.8
(8,8)	7386.3	1.5363*10^5	840.88	1640	209888	13506	11743
(9,9)	9235.3	1.9462*10^5	1056	2063.7	265572	17047	14830

Table 5. Comparison Table for Theorem 3.

(f,l)	$\mathcal{NMENT}_{\mathbf{NM1}}$	$\mathcal{NMENT}_{\mathbf{NM2}}$	$\mathcal{NMENT}_{\mathbf{SMZ}}$	$\mathcal{NMENT}_{\mathbf{GRI}}$	$\mathcal{NMENT}_{\mathbf{IRI}}$	$\mathcal{NMENT}_{\mathbf{SDD}}$	$\mathcal{NMENT}_{\mathbf{H}}$
(2,2)	7.5038	8.7135	1.0189	8.7135	0.65177	5.1744	16.385
(3,3)	8.2837	9.526	1.9901	9.526	1.5023	5.9288	17.856
(4,4)	8.8432	10.101	2.6221	10.101	2.0703	6.4743	18.822
(5,5)	9.2798	10.55	3.095	10.55	2.5024	6.9024	19.526
(6,6)	9.6379	10.914	3.4743	10.914	2.8528	7.2548	20.074
(7,7)	9.9416	11.221	3.7915	11.221	3.1484	7.5542	20.518
(8,8)	10.205	11.491	4.0645	11.491	3.4044	7.8145	20.891
(9,9)	10.438	11.725	4.3043	11.725	3.6304	8.0449	21.211
(10,10)	10.646	11.935	4.518	11.935	3.8328	8.2514	21.49

Table 6. Comparison Table for Theorem 3.

(f,l)	$\mathcal{NMENT}_{\mathbf{ISI}}$	$\mathcal{NMENT}_{\mathbf{AZ}}$	$\mathcal{NMENT}_{\mathbf{ABC}}$	$\mathcal{NMENT}_{\mathbf{ABS}}$	$\mathcal{NMENT}_{\mathbf{F}}$	$\mathcal{NMENT}_{\mathbf{RR}}$	$\mathcal{NMENT}_{\mathbf{RRR}}$
(2,2)	6.4156	9.1438	4.8496	4.8746	9.4441	4.8402	4.8355
(3,3)	7.1115	9.9664	5.5963	5.6144	10.254	5.5887	5.5857
(4,4)	7.6238	10.547	6.1381	6.1523	10.828	6.1319	6.1289
(5,5)	8.0303	10.997	6.5638	6.5753	11.277	6.5583	6.5558
(6,6)	8.3674	11.364	6.9143	6.9242	11.639	6.9097	6.9075
(7,7)	8.6555	11.674	7.2127	7.221	11.949	7.2085	7.2064
(8,8)	8.9073	11.942	7.472	7.4795	12.214	7.4681	7.4664
(9,9)	9.1307	12.179	7.7016	7.7084	12.449	7.6981	7.6964
(10,10)	9.3316	12.39	7.9075	7.9137	12.659	7.9042	7.9027

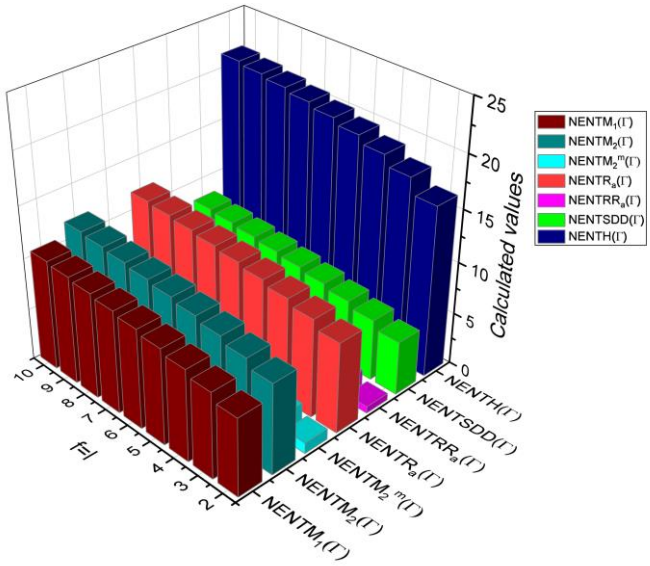


Figure 6. For the comparison, Table 5.

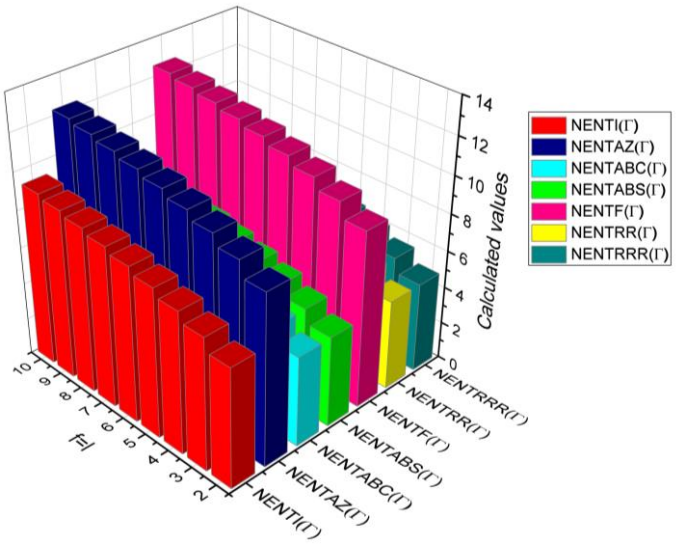


Figure 7. For the comparison, Table 6.

6. Computing the Neighborhood Sum Degree-Based M-polynomial for Kekulene Systems ZHK(3)

Kekulene systems are a class of artificial or fictitious compounds inspired by the concept of kekulene, as shown in Figure 8 and in the Edge Partition for kekulene systems ZHK(3) in Table 7. Kekulene is a potential compound that joins benzene rings in a zigzag manner, increasing the aromaticity of benzene within a larger system.

Researchers study Kekulene systems to understand the properties and potential applications of compounds with extended conjugation and aromaticity. These systems may impact several fields, including organic electronics, materials research, and drug design [26,27].

Organic synthesis is often used to develop kekulene systems, and spectroscopic methods are employed to characterize them, with the goal of predicting their properties. Despite the lack of synthesis of kekulene, efforts are underway to generate molecules with similar structures or properties.

The cardinality of ZHK(t) is

$$V(\Gamma) = 54t^2 - 6t \text{ and } E(\Gamma) = 72t^2 - 12t \qquad (10)$$

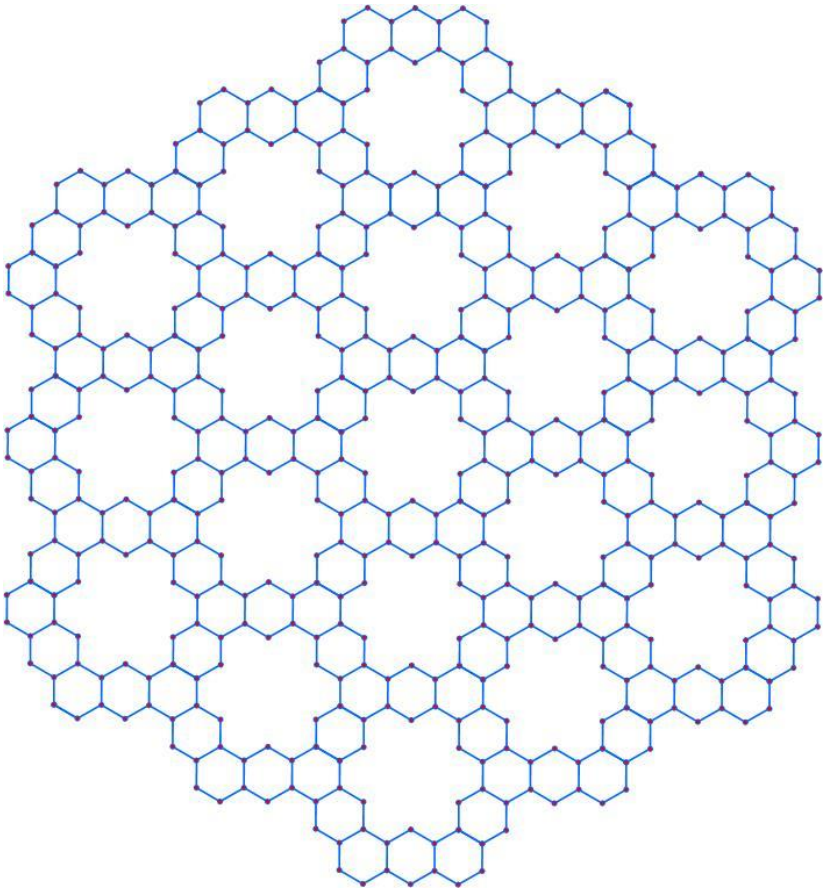


Figure 8. Kekulene systems ZHK(3).

Table 7. Edge Partition for kekulene systems ZHK(3).[29-31]

(d_u, d_v)	**Frequency**
(5,5)	6l
(5,7)	12l
(6,7)	12l
(6,8)	$36l^2 - 24l$
(7,8)	12l
(8,8)	$36l^2 - 30l$

Theorem 4. Assuming Γ to be a kekulene systems ZHK(3), the $\mathcal{NM}$ -polynomial of Γ can be obtained as follows.

$$\mathcal{NM}(\Gamma; S, P) = 6l\, s^5p^5 + 12l\, s^5p^7 + 12l\, s^6p^7 + (36l^2 - 24l)\, s^6p^8 + 12l\, s^7p^8 + (36l^2 - 30l)s^8p^8 \qquad (11)$$

Theorem 5. Assuming Γ to be a kekulene systems ZHK(3), the $\mathcal{NM}$ -polynomial of Γ can be obtained as follows.

1. $\mathcal{NM}M_1(\Gamma) = 1080\, l^2 - 276\, l$
2. $\mathcal{NM}M_2(\Gamma) = 4032\, l^2 - 1326\, l$
3. $\mathcal{NM}SMZ(\Gamma) = \frac{639}{5600}\, l + \frac{21}{16}\, l^2$
4. $\mathcal{NM}GRI(\Gamma) = 4032\, l^2 - 1326\, l$
5. $\mathcal{NM}IRI(\Gamma) = \frac{639}{5600}\, l + \frac{21}{16}\, l^2$

6. $\mathcal{NM}\mathrm{SDD}(\Gamma) = -\frac{1689}{70}\,l + 147\,l^2$

7. $\mathcal{NM}\mathrm{H}(\Gamma) = -\frac{969}{1820}\,l + \frac{135}{14}\,l^2$

8. $\mathcal{NM}\mathrm{ISI}(\Gamma) = -\frac{31266}{455}\,l + \frac{1872}{7}\,l^2$

9. $\mathcal{NM}\mathrm{AZ}(\Gamma) = -\frac{533366750523837}{256768768256}\,l + \frac{1969920}{343}\,l^2$

10. $\mathcal{NM}\mathrm{ABC}(\Gamma) = -4.2996\,l + 34.838\,l^2$

11. $\mathcal{NM}\mathrm{ABS}(\Gamma) = -11.752\,l + 67.006\,l^2$

12. $\mathcal{NM}\mathrm{F}(\Gamma) = 8208\,l^2 - 2676\,l$

13. $\mathcal{NM}\mathrm{RR}(\Gamma) = -137.72\,l + 537.42\,l^2$

14. $\mathcal{NM}\mathrm{RRR}(\Gamma) = -125.70\,l + 464.98\,l^2$ (12)

Proof:

$\mathbb{D}_s + \mathbb{D}_p = 60ls^5p^5 + 144ls^5p^7 + 156ls^6p^7 + 14(36l^2 - 24l)s^6p^8 + 180ls^7p^8 + 16(36l^2 - 30l)s^8p^8$

$\mathbb{D}_s\,\mathbb{D}_p = 6(25)ls^5p^5 + 12(35)ls^5p^7 + 12(42)ls^6p^7 + 48(36l^2 - 24l)s^6p^8 + 12(56)ls^7p^8 + 64(36l^2 - 30l)s^8p^8$

$\mathbb{S}_s^{\alpha}\,\mathbb{S}_p^{\alpha} = \frac{6}{25}ls^5p^5 + \frac{12}{35}ls^5p^7 + \frac{12}{42}ls^6p^7 + \frac{1}{48}(36l^2 - 24l)s^6p^8 + \frac{12}{56}ls^7p^8 + \frac{1}{64}(36l^2 - 30l)s^8p^8$

$\mathbb{D}_s^{\alpha}\,\mathbb{D}_p^{\alpha} = 6(25)^{\alpha}ls^5p^5 + 12(35)^{\alpha}ls^5p^7 + 12(42)^{\alpha}ls^6p^7 + (48)^{\alpha}(36l^2 - 24l)s^6p^8 + 12\,(56)^{\alpha}ls^7p^8 + (64)^{\alpha}(36l^2 - 30l)s^8p^8$

$\mathbb{S}_s^{\alpha}\,\mathbb{S}_p^{\alpha} = \frac{6}{25^{\alpha}}ls^5p^5 + \frac{12}{35^{\alpha}}ls^5p^7 + \frac{12}{42^{\alpha}}ls^6p^7 + \frac{1}{48^{\alpha}}(36l^2 - 24l)s^6p^8 + \frac{12}{56^{\alpha}}ls^7p^8 + \frac{1}{64^{\alpha}}(36l^2 - 30l)s^8p^8$

$\mathbb{D}_s\mathbb{S}_p + \mathbb{D}_p\mathbb{S}_s = 12\,ls^5p^5 + \left(\frac{60}{7} + \frac{84}{5}\right)ls^5p^7 + \left(\frac{72}{7} + 14\right)ls^6p^7 + \left(\frac{3}{4} + \frac{4}{3}\right)(36l^2 - 24l)s^6p^8 + \left(\frac{21}{2} + \frac{96}{7}\right)ls^7p^8 + 2\,(36l^2 - 30l)s^8p^8$

$2\mathbb{S}_s J = \frac{6}{5}\,l\,s^{10} + 2\,l\,s^{12} + \frac{24}{13}\,l\,s^{13} + \frac{2}{14}\,(36l^2 - 24l)\,s^{14} + \frac{24}{15}\,l\,s^{15} + \frac{2}{16}\,(36l^2 - 30l)\,s^{16}$

$\mathbb{S}_s\,J\mathbb{D}_s\,\mathbb{D}_p = 6\left(\frac{25}{10}\right)l\,s^{10} + 12\left(\frac{35}{12}\right)l\,s^{12} + 12\left(\frac{42}{13}\right)l\,s^{13} + \left(\frac{48}{14}\right)(36l^2 - 24l)\,s^{14} + 12\left(\frac{56}{15}\right)l\,s^{15} + \left(\frac{64}{16}\right)(36l^2 - 30l)\,s^{16}$

$\mathbb{S}_s^3Q_{-2}\,J\mathbb{D}_s^3\,\mathbb{D}_p^3 = 6\left(\frac{25}{8}\right)^3 l\,s^8 + 12\left(\frac{35}{10}\right)^3 l\,s^{10} + 12\left(\frac{42}{11}\right)^3 l\,s^{11} + \left(\frac{48}{12}\right)^3(36l^2 - 24l)\,s^{12} + 12\left(\frac{56}{13}\right)^3 l\,s^{13} + \left(\frac{64}{14}\right)^3(36l^2 - 30l)s^{14}$

$\mathbb{D}_s^{\frac{1}{2}}Q_{-2}\,J\mathbb{S}_s^{\frac{1}{2}}\,\mathbb{S}_p^{\frac{1}{2}} = 6\sqrt{\frac{8}{25}}ls^5p^5 + 12\sqrt{\frac{10}{35}}ls^5p^7 + 12\sqrt{\frac{11}{42}}ls^6p^7 + \sqrt{\frac{12}{48}}(36l^2 - 24n)s^6p^8 + 12\sqrt{\frac{13}{56}}ls^7p^8 + \sqrt{\frac{14}{64}}(36l^2 - 30l)s^8p^8$

$\mathbb{D}_s^{\frac{1}{2}}Q_{-2}\,J(\mathbb{S}_s^{\frac{1}{2}} + S_p^{\frac{1}{2}}) = 6\sqrt{\frac{8}{10}}\,l\,s^5p^5 + 12\sqrt{\frac{10}{12}}\,l\,s^5p^7 + 12\sqrt{\frac{11}{13}}l\,s^6p^7 + \sqrt{\frac{12}{14}}(36l^2 - 24l)\,s^6p^8 + 12\sqrt{\frac{13}{15}}l\,s^7p^8 + \sqrt{\frac{14}{16}}(36l^2 - 30l)\,s^8p^8$

$$\mathbb{D}_s^2 + \mathbb{D}_p^2 = 6\,(50)ls^5p^5 + 12(25+49)\,l\,s^5p^7 + 12(36+49)l\,s^6p^7 + (36+64)(36l^2-24l)\,s^6p^8 + 12\,(49+64)\,l\,s^7p^8 + (64+64)(36l^2-30l)\,s^8p^8$$

$$\mathbb{D}_s^{\frac{1}{2}}\mathbb{D}_p^{\frac{1}{2}} = 6\sqrt{25}\,ls^5p^5 + 12\sqrt{35}\,l\,s^5p^7 + 12\sqrt{42}\,l\,s^6p^7 + \sqrt{48}\,(36l^2-24l)\,s^6p^8 + 12\sqrt{56}\,l\,s^7p^8 + \sqrt{64}\,(36l^2-30l)\,s^8p^8$$

$$\mathbb{D}_s^{\frac{1}{2}}Q_{-1}\,\mathbb{D}_p^{\frac{1}{2}}Q_{-1} = 6\sqrt{16}\,l\,s^5p^5 + 12\sqrt{24}\,l\,s^5p^7 + 12\sqrt{30}\,l\,s^6p^7 + \sqrt{35}\,(36l^2-24l)\,s^6p^8 + 12\sqrt{42}\,l\,s^7p^8 + \sqrt{49}\,(36l^2-30l)\,s^8p^8$$

The partition Table 5 and the conditions of the $\mathcal{NM}$-Polynomial with its derivatives are used to derive the above results [28–30].

7. Neighbourhood Degree Sum-Based Entropy Measures for Kekulene Systems ZHK(3)

Theorem 6. If Γ is a kekulene systems ZHK(3), then $\mathcal{NM}$-entropy measures are given as follows:

$$\mathcal{NMENT}_{M_1} = \log(1080l^2-276l) - \frac{1}{(1080l^2-276l)}(6l\,(10)\log 10 + 12l\,(12)\log 12 + 12l\,(13)\log 13 + (36l^2-24l)(14)\log 14 + 12l(15)\log 15 + (36l^2-30l)(15)\log 15)$$

$$\mathcal{NMENT}_{M_2} = \log(4032l^2-1326l) - \frac{1}{(4032l^2-1326l)}(6l\,(25)\log 25 + 12l\,(35)\log 35 + 12l\,(42)\log 42 + (36l^2-24l)(48)\log 48 + 12l(56)\log 56 + (36l^2-30l)(64)\log 64)$$

$$\mathcal{NMENT}_{SMZ} = \log\left(\frac{639}{5600}l + \frac{21}{16}l^2\right) - \frac{1}{\left(\frac{639}{5600}l + \frac{21}{16}l^2\right)}\left(6l\left(\frac{1}{25}\right)\log\frac{1}{25} + 12l\left(\frac{1}{35}\right)\log\frac{1}{35} + 12l\left(\frac{1}{42}\right)\log\frac{1}{42} + (36l^2-24l)\left(\frac{1}{48}\right)\log\frac{1}{48} + 12l\left(\frac{1}{56}\right)\log\frac{1}{56} + (36l^2-30l)\left(\frac{1}{64}\right)\log\frac{1}{64}\right)$$

$$\mathcal{NMENT}_{GRI} = \log(GRI) - \frac{1}{(GRI)}(6l\,(25)^{\alpha}\log(25)^{\alpha} + 12n\,(35)^{\alpha}\log(35)^{\alpha} + 12n\,(42)^{\alpha}\log(42)^{\alpha} + (36n^2-24n)(48)^{\alpha}\log(48)^{\alpha} + 12n(56)^{\alpha}\log(56)^{\alpha} + (36n^2-30n)(64)^{\alpha}\log(64)^{\alpha})$$

$$\mathcal{NMENT}_{IRI} = \log\left(\frac{639}{5600}n + \frac{21}{16}n^2\right) - \frac{1}{\left(\frac{639}{5600}n+\frac{21}{16}n^2\right)}\left(6n\left(\frac{1}{(25)^{\alpha}}\right)\log\left(\frac{1}{(25)^{\alpha}}\right) + 12n\left(\frac{1}{35^{\alpha}}\right)\log\left(\frac{1}{(35)^{\alpha}}\right) + 12n\left(\frac{1}{(42)^{\alpha}}\right)\log\left(\frac{1}{(422)^{\alpha}}\right) + (36n^2-24n)\left(\frac{1}{(48)^{\alpha}}\right)\log\left(\frac{1}{(48)^{\alpha}}\right) + 12n\left(\frac{1}{(56)^{\alpha}}\right)\log\left(\frac{1}{(56)^{\alpha}}\right) + (36n^2-30n)\left(\frac{1}{(64)^{\alpha}}\right)\log\left(\frac{1}{(64)^{\alpha}}\right)\right)$$

$$\mathcal{NMENT}_{SDD} = \log\left(-\frac{1689}{70}n + 147n^2\right) - \frac{1}{\left(-\frac{1689}{70}n+147n^2\right)}\left(6n\,(2)\log 2 + 12n\left(\frac{74}{35}\right)\log\left(\frac{74}{35}\right) + 12n\left(\frac{85}{42}\right)\log\left(\frac{85}{42}\right) + (36n^2-24n)\left(\frac{25}{12}\right)\log\left(\frac{25}{12}\right) + 12n\left(\frac{113}{56}\right)\log\left(\frac{113}{56}\right) + (36n^2-30n)(2)\log 2\right)$$

$$\mathcal{NMENT}_{\mathrm{H}} = \log\left(\frac{135}{14}n^2 - \frac{969}{1820}n\right) - \frac{1}{\left(\frac{135}{14}n^2 - \frac{969}{1820}n\right)}(6n\left(\frac{1}{5}\right)\log\left(\frac{1}{5}\right) + 12n\left(\frac{1}{6}\right)\log\left(\frac{1}{6}\right) + 12n\left(\frac{2}{13}\right)\log\left(\frac{2}{13}\right) + (36n^2 - 24n)\left(\frac{1}{7}\right)\log\left(\frac{1}{7}\right) + 12n\left(\frac{2}{15}\right)\log\left(\frac{2}{15}\right) + (36n^2 - 30n)\left(\frac{1}{8}\right)\log\left(\frac{1}{8}\right))$$

$$\mathcal{NMENT}_{\mathrm{ISI}} = \log\left(\frac{1872}{7}n^2 - \frac{31266}{455}n\right) - \frac{1}{\left(\frac{1872}{7}n^2 - \frac{31266}{455}n\right)}(6n\left(\frac{25}{10}\right)\log\left(\frac{25}{10}\right) + 12n\left(\frac{35}{12}\right)\log\left(\frac{35}{12}\right) + 12n\left(\frac{42}{13}\right)\log\left(\frac{42}{13}\right) + (36n^2 - 24n)\left(\frac{48}{14}\right)\log\left(\frac{48}{14}\right) + 12n\left(\frac{56}{15}\right)\log\left(\frac{56}{15}\right) + (36n^2 - 30n)\left(\frac{64}{16}\right)\log\left(\frac{64}{16}\right))$$

$$\mathcal{NMENT}_{\mathrm{AZ}} = \log\left(\frac{1969920}{343}n^2 - \frac{533366750523837}{256768768256}n\right) - \frac{1}{\left(\frac{1969920}{343}n^2 - \frac{533366750523837}{256768768256}n\right)}(6n\left(\frac{25}{8}\right)^3\log\left(\frac{25}{8}\right)^3 + 12n\left(\frac{35}{10}\right)^3\log\left(\frac{35}{10}\right)^3 + 12n\left(\frac{42}{11}\right)^3\log\left(\frac{42}{11}\right)^3 + (36n^2 - 24n)\left(\frac{48}{12}\right)^3\log\left(\frac{48}{12}\right)^3 + 12n\left(\frac{56}{13}\right)^3\log\left(\frac{56}{13}\right)^3 + (36n^2 - 30n)\left(\frac{64}{14}\right)^3\log\left(\frac{64}{14}\right)^3)$$

$$\mathcal{NMENT}_{\mathrm{ABC}} = \log(34.838n^2 - 4.2996n) - \frac{1}{(34.838n^2 - 4.2996n)}(6n\sqrt{\left(\frac{8}{25}\right)}\log\sqrt{\left(\frac{8}{25}\right)} + 12n\sqrt{\left(\frac{10}{35}\right)}\log\sqrt{\left(\frac{10}{35}\right)} + 12n\sqrt{\left(\frac{11}{42}\right)}\log\sqrt{\left(\frac{11}{42}\right)} + (36n^2 - 24n)\sqrt{\left(\frac{12}{48}\right)}\log\sqrt{\left(\frac{12}{48}\right)} + 12n\sqrt{\left(\frac{13}{56}\right)}\log\sqrt{\left(\frac{13}{56}\right)} + (36n^2 - 30n)\sqrt{\left(\frac{14}{64}\right)}\log\sqrt{\left(\frac{14}{64}\right)})$$

$$\mathcal{NMENT}_{\mathrm{ABS}} = \log(67.006n^2 - 11.752n) - \frac{1}{(67.006n^2 - 11.752n)}(6n\sqrt{\left(\frac{8}{10}\right)}\log\sqrt{\left(\frac{8}{10}\right)} + 12n\sqrt{\left(\frac{10}{12}\right)}\log\sqrt{\left(\frac{10}{12}\right)} + 12n\sqrt{\left(\frac{11}{13}\right)}\log\sqrt{\left(\frac{11}{13}\right)} + (36n^2 - 24n)\sqrt{\left(\frac{12}{14}\right)}\log\sqrt{\left(\frac{12}{14}\right)} + 12n\sqrt{\left(\frac{13}{15}\right)}\log\sqrt{\left(\frac{13}{15}\right)} + (36n^2 - 30n)\sqrt{\left(\frac{14}{16}\right)}\log\sqrt{\left(\frac{14}{16}\right)})$$

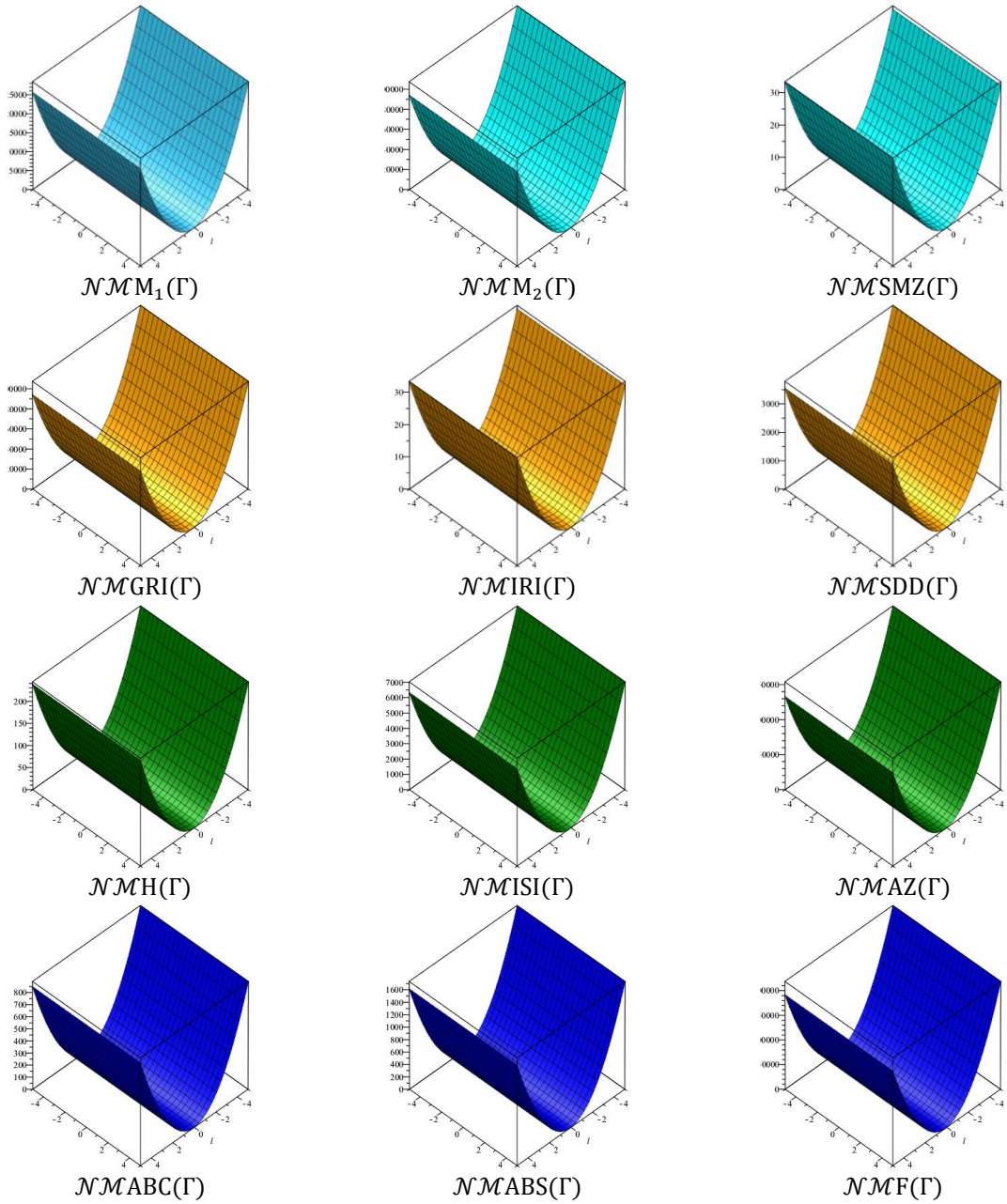
$$\mathcal{NMENT}_{\mathrm{F}} = \log(8208n^2 - 2676n) - \frac{1}{(\log(8208n^2 - 2676n)}(6n\ (50)\log(50) + 12n\ (74)\log(74) + 12n\ (85)\log(85) + (36n^2 - 24n)\ (100)\log(100) + 12n\ (113)\log(113) + (36n^2 - 30n)\ (128)\log(128))$$

$$\mathcal{NMENT}_{\mathrm{RR}} = \log(537.42n^2 - 137.72n) - \frac{1}{(537.42n^2 - 137.72n)}(6n\left(\sqrt{25}\right)\log\left(\sqrt{25}\right) + 12n\ \left(\sqrt{35}\right)\log\left(\sqrt{35}\right) + 12n\ \left(\sqrt{42}\right)\log\left(\sqrt{42}\right) + (36n^2 - 24n)\left(\sqrt{48}\right)\log\left(\sqrt{48}\right) + 12n\left(\sqrt{56}\right)\log\left(\sqrt{56}\right) + (36n^2 - 30n)\left(\sqrt{64}\right)\log\left(\sqrt{64}\right)$$

$$\mathcal{NMENT}_{\mathrm{RRR}} = \log(464.98n^2 - 196.99n) - \frac{1}{(464.98n^2 - 196.99n)}(6n\left(\sqrt{16}\right)\log\left(\sqrt{16}\right) + 12n\ \left(\sqrt{24}\right)\log\left(\sqrt{24}\right) + 12n\ \left(\sqrt{30}\right)\log\left(\sqrt{30}\right) + (36n^2 - 24n)\left(\sqrt{35}\right)\log\left(\sqrt{35}\right) + 12n\left(\sqrt{42}\right)\log\left(\sqrt{42}\right) + (36n^2 - 30n)\left(\sqrt{49}\right)\log\left(\sqrt{49}\right) \quad (13)$$

8. Comparative Analysis for- Kekulene Systems ZHK(3)

The analytical equations for the neighborhood-degree-sum-based indices, derived from Theorems 5 and 6, are shown as three-dimensional graphs in this section. Thanks to these charts, the reader can more easily appreciate and understand the behavior of the indices relative to the variables that define the molecular structure. Furthermore, the results of Theorem 5 have also been presented as comparison plots, in which each neighborhood-degree-sum-based index is displayed against a single structural variable on a single graph [9,10]. These comparison charts provide a graphical representation of the discrepancies between the indices and the chemical structure. These charts are displayed in Figures 2 and 3. The indices' computed numerical values are shown in Tables 8–11. In Figures 9, 10, and 11, the numerical data are presented as three-dimensional plots to help readers visualize them [33,34].



$\mathcal{NM}$RR(Γ) $\mathcal{NM}$RRR(Γ)

Figure 9. 3D plots for Theorem 5.

Table 8. Comparison Table for Theorem 5.

l	$\mathcal{NM}M_1(\Gamma)$	$\mathcal{NM}M_2(\Gamma)$	$\mathcal{NM}$SMZ(Γ)	$\mathcal{NM}$GRI(Γ)	$\mathcal{NM}$IRI(Γ)	$\mathcal{NM}$SDD(Γ)	$\mathcal{NM}$H(Γ)
1	804	2706	1.4266	2706	1.4266	122.87	9.1104
2	3768	13476	5.4782	13476	5.4782	539.74	37.507
3	8892	32310	12.155	32310	12.155	1250.6	85.188
4	16176	59208	21.456	59208	21.456	2255.5	152.16
5	25620	94170	33.383	94170	33.383	3554.4	238.41
6	37224	137196	47.935	137196	47.935	5147.2	343.95
7	50988	188286	65.111	188286	65.111	7034.1	468.77
8	66912	247440	84.913	247440	84.913	9215	612.88
9	84996	314658	107.34	314658	107.34	11690	776.28

Table 9. Comparison Table for Theorem 5.

l	$\mathcal{NM}$ISI(Γ)	$\mathcal{NN}$AZ(Γ)	$\mathcal{NM}$ABC(Γ)	$\mathcal{NM}$ABS(Γ)	$\mathcal{NM}$F(Γ)	$\mathcal{NM}$RR(Γ)	$\mathcal{NM}$RRR(Γ)
1	198.71	3666	30.538	55.253	5532	399.7	267.99
2	932.28	18818	130.75	244.52	27480	1874.2	1466
3	2200.7	45457	300.64	567.79	65844	4423.7	3593.9
4	4004	83582	540.21	1025.1	120624	8047.9	6651.7
5	6342.1	1.3319*10^5	849.44	1616.4	191820	12747	10639
6	9215.1	1.9429*10^5	1228.4	2341.6	279432	18521	15557
7	12623	2.6688*10^5	1677	3201	383460	25370	21405
8	16566	3.5095*10^5	2195.3	4194.3	503904	33293	28183
9	21043	4.4650*10^5	2783.1	5321.5	640764	42292	35890

Table 10. Comparison Table for Theorem 6.

l	$\mathcal{NMENT}_{NM1}$	$\mathcal{NMENT}_{NM2}$	$\mathcal{NMENT}_{SMZ}$	$\mathcal{NMENT}_{GRI}$	$\mathcal{NMENT}_{IRI}$	$\mathcal{NMENT}_{SDD}$	$\mathcal{NMENT}_{H}$
1	4.1142	5.4507	86.415	5.8575	86.877	4.2056	7.4806
2	5.6531	8.4808	152.06	7.2419	152.3	5.8251	13.912
3	6.51	9.7125	175.5	8.0616	175.67	6.7064	16.343
4	7.1076	10.482	1187.63	8.6441	187.75	7.3158	17.716
5	7.5667	11.039	195.09	9.0931	195.19	7.7821	18.639
6	7.9412	11.476	200.17	9.4609	200.25	8.16	19.317
7	8.2545	11.834	203.85	9.7702	203.92	8.4778	19.85
8	8.5255	12.139	206.66	10.039	206.72	8.7517	20.286
9	8.7648	12.403	208.88	10.276	208.93	8.9928	20.657

Table 11. Comparison Table for Theorem 6.

l	$\mathcal{NMENT}_{ISI}$	$\mathcal{NMENT}_{ABC}$	$\mathcal{NMENT}_{ABS}$	$\mathcal{NMENT}_{F}$	$\mathcal{NMENT}_{RR}$	$\mathcal{NMENT}_{RRR}$
1	4.6093	4.0928	4.0943	4.0861	4.0861	4.5104
2	6.3445	5.5747	5.5759	5.5541	5.5694	5.9772
3	7.2547	6.4155	6.4168	6.4002	6.4112	6.8147
4	7.8771	7.0057	7.0066	6.9911	7.002	7.4034
5	8.351	7.4606	7.4618	7.4466	7.4573	7.8575
6	8.7335	7.8315	7.832	7.8196	7.828	8.2272
7	9.0544	8.1436	8.1443	8.1327	8.1405	8.5389
8	9.331	8.4136	8.4144	8.4021	8.4105	8.8095
9	9.5738	8.6518	8.6526	8.6413	8.6485	9.0465

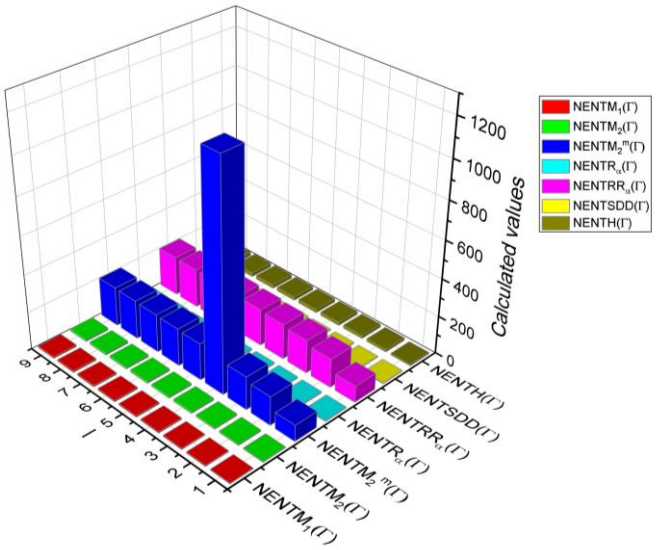


Figure 10. For comparison, Table 9.

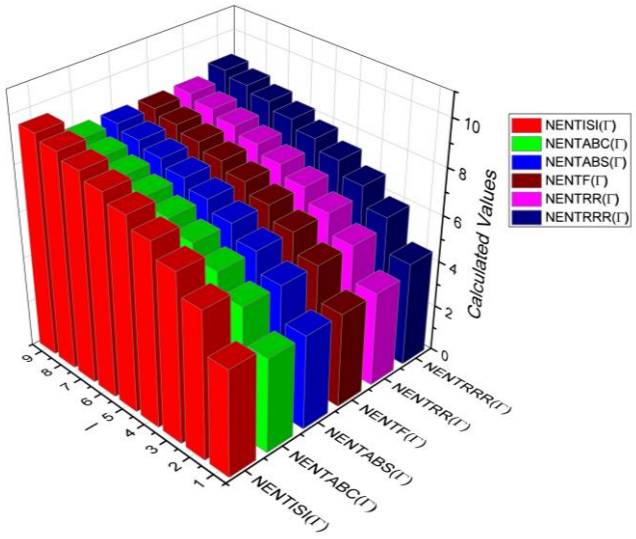


Figure 11. Comparison Table for Table 11.

9. Conclusions

This article uses the M-Polynomial to obtain closed-form analytical formulas for the neighborhood-sum degree-based indices of two types of Kekulene systems. The resulting indices are shown as separate three-dimensional plots and comparison plots to aid in the comprehension of the mathematical expressions. For all three kinds of graphene structures, entropy estimates based on the neighborhood sum degree have also been computed. Moreover, they are displayed as three-dimensional graphs to support the idea that these indices depend on the underlying molecular structure. This work is unique because these markers have never been examined for these structures before. This finding will provide fresh perspectives for future research on topological indices for these intriguing structures.

Author Contributions

Conceptualization, V.K., M.S., and K.J.; methodology, V.K., M.S., and K.J.; formal analysis, V.K., M.S., and K.J.; investigation, V.K., M.S., and K.J.; writing—original draft preparation,

V.K., M.S., and K.J.; writing—review and editing, V.K., M.S., and K.J. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest

The authors declare that none of the work reported in this study could have been influenced by any known competing financial interests or personal relationships.

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