

Neighborhood Sum VDB Indices and Entropy for Molecular Graphs of Supertriphenylene and Superphenalene

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Abstract: The structural topology of molecular graphs can be correlated with physicochemical and biological features using topological indices (TIs), which are numerical descriptors. In this work, we calculate the neighborhood sum degree-based M-polynomial and provide closed-form analytical formulas for a wide range of topological indices based on degree and those based on the sum of neighborhood degrees of superphenalene and supertriphenylene, two polycyclic aromatic hydrocarbons (PAHs). Explicit formulas for indices like the Zagreb-type, GA, ABC, SDD, harmonic, inverse sum, and redefined Zagreb indices are produced through systematic vertex-edge partitioning and neighborhood degree-sum labeling. Additionally, structural complexity is measured using Shannon-type entropy metrics based on neighborhood information. Three-dimensional graphical representations and tabular computations are used for numerical validation and comparative studies. The findings give these PAHs—structures of growing importance in organic electronics, supramolecular chemistry, and carbon-based nanomaterials—new TI and entropy characterizations. These results support upcoming QSPR/QSAR research and add to the theoretical toolkit for benzenoid hydrocarbon analysis.

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

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1. Introduction

A key concept in theoretical and computational chemistry is the structural description of molecules using graph-theoretic models. Geometric aspects can be abstracted while maintaining the connection patterns that control chemical behavior, thanks to molecular graphs, in which vertices stand in for atoms and edges for chemical bonds [1]. Predictive modeling of physical characteristics, stability, reactivity, and biological activity is made easier by this abstraction, especially in large and complex molecular systems like polymers, nanostructures, and benzenoid hydrocarbons.

The study of several molecular characteristics, including chemical reactivity, stability, and biological activity, has been made easier by the advancement of topological approaches in chemical graph theory. Researchers can apply ideas from graph theory to a more thorough analysis of molecular structures by transforming structural formulas into mathematical graphs [2]. When studying huge, complicated materials like proteins and polymers, this method has proven to be quite helpful.

Topological indices (TIs) are numerical descriptors invariant under graph isomorphism, encoding essential structural information. Since Wiener's pioneering work correlating path distances with boiling points of alkanes, TIs have proliferated into several families—degree-based, distance-based, eigenvalue-based, and information-theoretic indices [3]. Degree-based indices, such as the Zagreb, Randić, ABC, and GA indices, have received particular attention due to their computational efficiency and their high correlation with QSPR/QSAR endpoints including boiling points, entropy, aromatic stability, and drug-likeness.

Analytical computation of numerous TIs is enabled by algebraic polynomial frameworks. Hosoya introduced distance-based generating polynomials [4], while Deutsch and Klavžar formulated the M-polynomial, from which many degree-based descriptors can be derived through differential and integral operators [5]. Recent extensions have incorporated neighborhood degree sum-based indices, which enhance sensitivity to local structural irregularity and have demonstrated applicability in statistical learning, QSPR regression models, and graph similarity analysis [6].

Inspired by Shannon's information theory, graph entropy quantifies structural complexity, heterogeneity, and information distribution within molecular networks. Entropy measures based on degree sequences, walk structures, or neighborhood sums have been applied to assess molecular stability, study molecular recognition, and examine thermochemistry and reactivity trends [3].

Graph theoretical methods are becoming the main instruments for theoretical investigations of chemical substances. In particular, QSAR/QSPR techniques are thought to be helpful strategies and computational tools for attempting to forecast the characteristics of chemical compounds [1]. Since their qualities may be estimated before synthesis, which influences the design, these technologies are essential to the development of new, more potent herbicides. Additionally, because QSPR/QSAR models require less money and time to run, they can take the place of experimental measurements. Topological indices offer a numerical depiction of molecular topology in this context [6-8].

Algebraic polynomials can be used efficiently and usefully to compute TIs. With this method, calculating many TIs is reduced to computing one polynomial [4]. For instance, Hosoya's polynomial is often used to find distance-based TIs. A similar polynomial was developed by Deutsch and Klavžar for the degree-based index computation. This method allows the computation of multiple significant degree-based benchmarks with just one polynomial, the M-polynomial. Several academic publications discuss the M-polynomial and how it is used to calculate DB indices. The DB entropy measures are computed for these structures [5].

One new advancement in the use of graph theory in chemical compound research is the neighborhood sum degree-based TIs. It's applied in QSPR and statistical regression analysis to forecast specific molecular graph chemical features. In the study of networks, the degree-based entropy metrics that are extensively researched and used in graph theory are regarded as

information functionals. The study of the chemical and biological characteristics of molecular graphs, as well as the quantitative depiction of a molecule's structure, are two applications of entropy network metrics. As of right now, there are very few examples of neighborhood sum degree-based entropy measurements and neighborhood sum degree-based M-Polynomials in academic journals [9-11].

The real motivation for choosing supertriphenylene and superphenalene is that they are large, π -conjugated polycyclic aromatic hydrocarbons (PAHs) with high symmetry as shown in Figure 1, rigid planar frameworks, and delocalized electronic structures. Supertriphenylene ($C_{18}H_{12}$) consists of three fused benzene rings and is widely studied for its semiconducting properties, π -stacking ability, and relevance to organic LEDs, OFETs, and supramolecular assemblies [12-13].

Superphenalene ($C_{96}H_{30}$) is a giant benzenoid with over half a million resonance structures and exceptional delocalization, positioning it as a potential building block for photovoltaics and molecular electronics [12-13].

Despite their significance, neighborhood sum degree-based M-polynomials and entropy measures have not been analytically derived for these PAHs, leaving a gap in the theoretical literature.

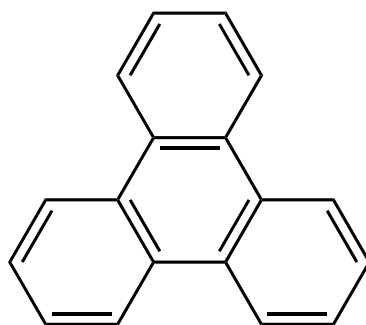


Figure 1. Triphenylene.

Superphenalene is a very large polycyclic aromatic hydrocarbon (PAH) with the chemical formula $C_{96}H_{30}$. The molecular structure of Superphenalene is shown in Figure 2, It can be formally considered to consist of three fused superbenzenes (hexa-peri-hexabenzocoronene).

This can be viewed as a three-fold symmetric overlapped structure of three hexa-peri-hexabenzocoronene (HPHBC or tribenzofluoranthene) about the center. They have also been known as building blocks of molecular electronics since 2004, being able to form self-assembled columns and nanotubes [13].

Superphenalene, on the other hand, presumably refers to a polycyclic aromatic hydrocarbon similar to phenalene but with additional features or modifications that enhance its properties or functionality. However, it's important to note that "superphenalene" isn't a widely recognized term in the scientific literature as of my last update. It's possible that it could be a hypothetical concept or a specific compound introduced after that time [12-13].

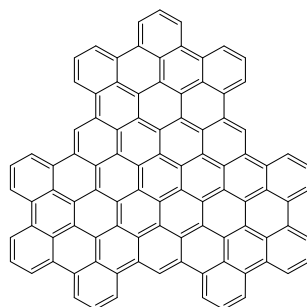


Figure 2. Superphenalene.

2. Materials and Methods

We take into account a single connected graph that has a few edges and no self-loops. The graph $\mathcal{G}$ is referred to as a connected graph when $\mathcal{V}(\mathcal{G})$ and $\mathcal{E}(\mathcal{G})$ represent the vertex set and edge set, respectively. The degree of the vertex is indicated by the symbol $\mathfrak{d}_v$.

The neighborhood sum degree-based TIs are denoted by $\mathfrak{NM}(\mathcal{G})$. The neighborhood sum degree of the molecular graph is written as $|\mathfrak{N}_{\mathcal{G}}(v)| = \sum_{v \in \mathfrak{N}_{\mathcal{G}}(v)} \mathfrak{d}_v$. The $\mathfrak{NM}(\mathcal{G})$ displays the sum of the degrees of vertices that are next to v [6-7],[14]. Let's start by building the M-polynomial of $\mathcal{G}$ based on the neighborhood sum degree:

$$\mathfrak{NM}(\mathcal{G}) = \sum_{i \leq j} (\text{Number of all edges } uv \text{ such that } \mathcal{H}_u = i, \mathcal{H}_v = j) i^i j^j \quad (1)$$

$$\mathcal{D}(\mathcal{G}) = \sum_{uv \in \mathcal{E}(\mathcal{G})} \mathcal{G}(\phi_u \phi_v) \quad \text{and} \quad \mathfrak{NM}(\mathcal{G}) = \sum_{uv \in \mathcal{E}(\mathcal{G})} g(\mathfrak{w}_u \mathfrak{w}_v) \quad (2)$$

Table 1 shows the degree-based TIs and neighborhood degree sum-based (ND) Tis.

Table 1. above lists the $\mathfrak{NM}$ -Polynomial derivatives [13,15-18].

Sl. No	Degree-based; Tis derived from $\mathfrak{NM}(\mathcal{G}; l, p)$	
1	$M_1(\mathcal{G}) = \mathbb{D}_l + \mathbb{D}_p(\mathfrak{NM}(\mathcal{G}; l, p)) _{l=p=1}$	First Zagreb Index
2	$M_2(\mathcal{G}) = \mathbb{D}_l \mathbb{D}_p(\mathfrak{NM}(\mathcal{G}; l, p)) _{l=p=1}$	Second Zagreb Index
3	$GA(\mathcal{G}) = 2[\mathbb{D}_l \mathbb{D}_p]^{-1}[\mathbb{D}_l + \mathbb{D}_p]^{-1}(\mathfrak{NM}(\mathcal{G}; l, p)) _{l=p=1}$	Geometric Arithmetic Index
4	$AG_1 = \frac{1}{2}[\mathbb{D}_l + \mathbb{D}_p][\mathbb{D}_l + \mathbb{D}_p]^{-\frac{1}{2}}(\mathfrak{NM}(\mathcal{G}; l, p)) _{l=p=1}$	Arithmetic Geometric Index
5	$RR_{\alpha}(\mathcal{G}) = \mathbb{S}_l^{\alpha} \mathbb{S}_p^{\alpha}(\mathfrak{NM}(\mathcal{G}; l, p)) _{l=p=1}$	Inverse Randic Index
6	$SDD(\mathcal{G}) = \mathbb{D}_l \mathbb{S}_p + \mathbb{D}_p \mathbb{S}_l(\mathfrak{NM}(\mathcal{G}; l, p)) _{l=p=1}$	Symmetric Division Index
7	$H(\mathcal{G}) = 2\mathbb{S}_l \mathbb{J}(\mathfrak{NM}(\mathcal{G}; l, p)) _{l=1}$	Harmonic Index
8	$I(\mathcal{G}) = \mathbb{S}_l \mathbb{J} \mathbb{D}_p(\mathfrak{NM}(\mathcal{G}; l, p)) _{l=1}$	Inverse Sum Index
9	$ABC(\mathcal{G}) = \mathbb{D}_l^{\frac{1}{2}} \mathbb{Q}_{-2} \mathbb{J} \mathbb{S}_l^{\frac{1}{2}} \mathbb{S}_p^{\frac{1}{2}}(\mathfrak{NM}(\mathcal{G}; l, p)) _{l=1}$	Atom - bond connectivity Index
10	$ABS(\mathcal{G}) = \mathbb{D}_l^{\frac{1}{2}} \mathbb{Q}_{-2} \mathbb{J}(\mathbb{S}_l^{\frac{1}{2}} + \mathbb{S}_p^{\frac{1}{2}})(\mathfrak{NM}(\mathcal{G}; l, p)) _{l=1}$	Atom – bond sum Index
11	$RR(\mathcal{G}) = \mathbb{D}_l^{\frac{1}{2}} \mathbb{D}_p^{\frac{1}{2}}(\mathfrak{NM}(\mathcal{G}; l, p)) _{l=p=1}$	Reciprocal Randic Index
12	$ReZ_2 = [\mathbb{D}_l \mathbb{D}_p][\mathbb{D}_l + \mathbb{D}_p]^{-1}(\mathfrak{NM}(\mathcal{G}; l, p)) _{l=p=1}$	Second Redefined Zagreb Index
13	$ReZ_3 = [\mathbb{D}_l \mathbb{D}_p][\mathbb{D}_l + \mathbb{D}_p](\mathfrak{NM}(\mathcal{G}; l, p)) _{l=p=1}$	Third Redefined Zagreb Index
14	$SK_2 = \frac{1}{4}[\mathbb{D}_l + \mathbb{D}_p]^2(\mathfrak{NM}(\mathcal{G}; l, p)) _{l=p=1}$	Second Shigehalli and Kanaburs Index

$\mathfrak{NM}$ -Polynomial Expressions.

3. Sum-based Neighborhood Degree Entropy Measures

In his foundational paper, Shannon defined entropy as a measure of the uncertainty or unpredictability of data (orbits, for example) relative to relevant information. This work laid

the groundwork for modern information theory. Entropy computations have been used to assess the structural informativeness of a wide variety of networks [19]. Because of information theory's versatility, researchers have applied it in several domains, including linguistics, electrical engineering, chemical and medical sciences, and graph theory for chemical networks [9]. Graph entropy is a way of measuring the topological information of chemical networks and graphs [20-23].

Rashevsky introduced a way to compute graph entropy using vertex orbits [24]. Building on this idea, intrinsic and extrinsic graph-entropy measures allow researchers to associate probability distributions with graph elements such as vertices and edges. Graph entropies have since found broad application across biology, ecology, chemistry, and sociology. Dehmer further advanced the field by formulating new graph-entropy measures and employing information functionals to extract structural information from graphs [20-22].

Estrada et al. explored walk-based graph entropies and developed a physically valid graph entropy metric [25]. Entropy network metrics provide a quantitative picture of molecular structure and help analyze the chemical and biological characteristics of molecular graphs. There are numerous uses for entropy measures in the study of chemical graph theory.

The node entropy is defined as:

$$\mathcal{ENT}_{\mathfrak{G}}(v_i) = - \sum_{j=1}^{d_i} p_{ij} \log(p) \quad (3)$$

If $\mathfrak{G} = (\mathcal{V}, \mathcal{E}, w)$ is an edge-weighted graph, then the entropy measure of $\mathfrak{G}$ is defined as [9],[20],[23].

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

4. Neighborhood Computation Sum Degree-Based M-polynomial for Supertriphenylene

Supertriphenylene is a polycyclic aromatic hydrocarbon (PAH) composed of three benzene rings fused in a triangular arrangement [12]. It belongs to the family of graphene fragments and exhibits interesting electronic and optical properties due to its unique structure. Researchers have studied supertriphenylene for potential applications in organic electronics, such as organic semiconductors and light-emitting diodes (LEDs). Supertriphenylene possesses several notable properties and applications. Figure 3 shows the molecular graph of supertriphenylene; its three benzene rings in a triangular configuration give the molecule a rigid, planar structure. Supertriphenylene, like other aromatic compounds, has delocalized electrons, which makes it electrically intriguing. Its uses in organic electronics depend on this feature. Because of its conjugated structure, supertriphenylene exhibits semiconductor properties. Its application in organic field-effect transistors (OFETs) and other electronic devices has been investigated. It has unique optical properties, such as fluorescence and absorption, that are useful for optoelectronic applications in solar cells and LEDs. Supertriphenylene molecules help create molecular materials and nanoscale architectures because they self-assemble into distinct configurations. They often exhibit strong thermal stability, which is crucial for processing and use in a variety of technological contexts. Supertriphenylene can undergo various chemical reactions, such as aromatic substitution and oxidative coupling, allowing for functionalization and modification to tailor its properties for

specific applications. Supertriphenylene's semiconducting characteristics make it suitable for application in organic electronic devices such as organic photovoltaic cells (OPVs), organic light-emitting diodes (OLEDs), and organic field-effect transistors (OFETs). Its light emission and efficient charge transfer are made possible by its conjugated structure. Because of its rigid, planar structure, supertriphenylene can be used in molecular electronic devices and molecular junctions, where precise control over molecular architecture and electronic properties is essential. It can be added to molecular materials to create functional surfaces, coatings, membranes, and molecular sensors, among other uses. Nanoscale designs with specific features can be produced by taking advantage of their capacity to self-assemble into organized structures. The ability of supertriphenylene to self-assemble can be used in supramolecular chemistry to create host-guest complexes, molecular recognition systems, and supramolecular structures. Because of its well-defined molecular structure and ability for bottom-up assembly, it holds promise for the creation of nanowires, nanodevices, and nanostructured materials. Supertriphenylene and its derivatives have been explored for biomedical applications such as drug delivery systems, imaging agents, and biosensors, leveraging their biocompatibility and functionalizability. Its optical properties make supertriphenylene suitable for applications in optoelectronic devices, including LEDs, organic lasers, and photonic devices. Functionalized supertriphenylene derivatives have been investigated for catalytic applications, including in organic synthesis and environmental remediation.

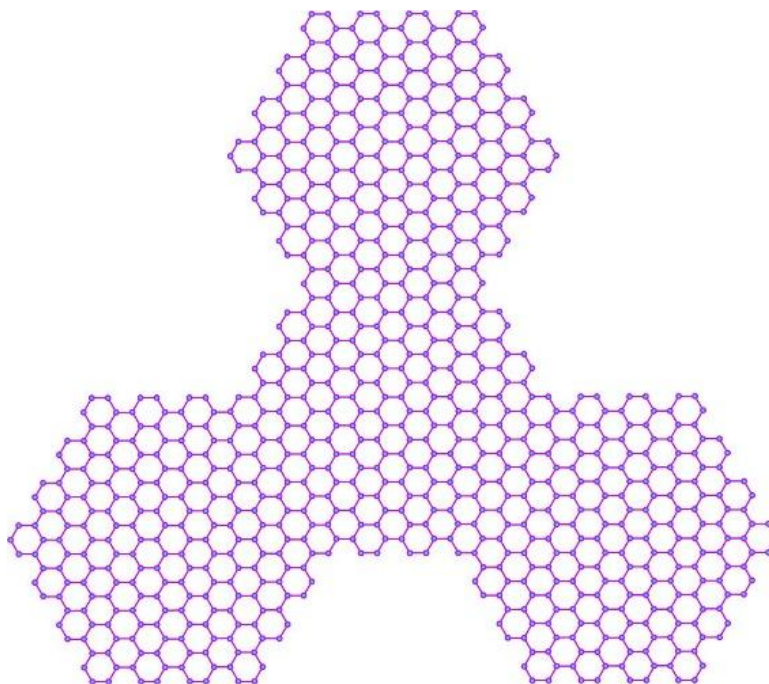


Figure 3. Molecular graph of supertriphenylene.

Table 2. Partition table for Figure 3.

(d_u, d_v)	Frequency
(4,5)	12
(5,5)	$18t - 36$
(5,8)	$36t - 48$
(6,8)	12
(8,8)	$18t - 18$
(8,9)	$36t - 36$
(9,9)	$108t^2 - 261t + 165$

Theorem 1.

Given that $\mathcal{G}$ is a Supertriphenylene, the following $\mathfrak{MM}$ -polynomial of $\mathcal{G}$.

$$\mathfrak{NM}(\mathfrak{G}; S, P) = 12l^4p^5 + (18t - 36)l^5p^5 + (36t - 48)l^5p^8 + 12l^6p^8 + (18t - 18)l^8p^8 + (36t - 36)l^8p^9 + (108t^2 - 261t + 165)l^9p^9 \quad (5)$$

Theorem 2.

If $\mathfrak{G}$ is a Supertriphenylene, then that $\mathfrak{G}$'s $\mathfrak{NM}$ -polynomial can be found.

1. $\mathfrak{NM}_{M_1}(\mathfrak{G}) = 1944t^2 - 3150t + 1362$
2. $\mathfrak{NM}_{M_2}(\mathfrak{G}) = 8748t^2 - 15507t + 16593$
3. $\mathfrak{NM}_{GA}(\mathfrak{G}) = 52.166 - 154.03t + 108.t^2$
4. $\mathfrak{NM}_{AG}(\mathfrak{G}) = 68.808 - 169.94t + 108.t^2$
5. $\mathfrak{NM}_{RR_\alpha}(\mathfrak{G}) = \frac{190421}{21600} - \frac{5911}{7200}t + \frac{4}{3}t^2$
6. $\mathfrak{NM}_{SDD}(\mathfrak{G}) = \frac{60053}{360} - \frac{3699}{10}t + 216t^2$
7. $\mathfrak{NM}_H(\mathfrak{G}) = \frac{50877}{30940} - \frac{59123}{4420}t + 12t^2$
8. $\mathfrak{NM}_I(\mathfrak{G}) = \frac{3384995}{3094} - \frac{351063}{442}t + 486t^2$
9. $\mathfrak{NM}_{ABC}(\mathfrak{G}) = 16.046 - 62.091t + 48.t^2$
10. $\mathfrak{NM}_{ABS}(\mathfrak{G}) = 50.25 - 146.20t + 101.82t^2$
11. $\mathfrak{NM}_{RR}(\mathfrak{G}) = 688.79 - 1581.8t + 972.t^2$
12. $\mathfrak{NM}_{ReZ_2}(\mathfrak{G}) = \frac{3231497}{9282} - \frac{351063}{442}t + 486t^2$
13. $\mathfrak{NM}_{ReZ_3}(\mathfrak{G}) = 157464t^2 - 294822t + 154338$
14. $\mathfrak{NM}_{SK_2}(\mathfrak{G}) = 8748t^2 - 15417t + 7515$

Proof:

Let $k(l,p)=\mathfrak{NM}(\mathfrak{G}; l, P) = 12l^4p^5 + (18t - 36)l^5p^5 + (36t - 48)l^5p^8 + 12l^6p^8 + (18t - 18)l^8p^8 + (36t - 36)l^8p^9 + (108t^2 - 261t + 165)l^9p^9$

1. $\mathbb{D}_l + \mathbb{D}_p(\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = 108l^4p^5 + 10(18t - 36)l^5p^5 + 13(36t - 48)l^5p^8 + 168l^6p^8 + 16(18t - 18)l^8p^8 + 17(36t - 36)l^8p^9 + 18(108t^2 - 261t + 165)l^9p^9$
2. $\mathbb{D}_l\mathbb{D}_p(\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = 2880l^4p^5 + 25(18t - 36)l^5p^5 + 40(36t - 48)l^5p^8 + 6912l^6p^8 + 64(18t - 18)l^8p^8 + 72(36t - 36)l^8p^9 + 81(108t^2 - 261t + 165)l^9p^9$
3. $2[\mathbb{D}_l\mathbb{D}_p]^{\frac{1}{2}}[\mathbb{D}_l + \mathbb{D}_p]^{-1}(\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = \frac{16}{3}\sqrt{5}l^4p^5 + (18t - 36)l^5p^5 + \frac{4}{3}\sqrt{10}(36t - 48)l^5p^8 + \frac{48}{7}\sqrt{3}l^6p^8 + (18t - 18)l^8p^8 + \frac{12}{17}\sqrt{2}(36t - 36)l^8p^9 + (108t^2 - 261t + 165)l^9p^9$
4. $\frac{1}{2}[\mathbb{D}_l + \mathbb{D}_p][\mathbb{D}_l + \mathbb{D}_p]^{-\frac{1}{2}}(\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = 12\left(\frac{9}{2\sqrt{20}}\right)l^4p^5 + \left(\frac{10}{2\sqrt{25}}\right)(18t - 36)l^5p^5 + \left(\frac{13}{2\sqrt{40}}\right)(36t - 48)l^5p^8 + 12\left(\frac{14}{2\sqrt{48}}\right)l^6p^8 + \left(\frac{16}{2\sqrt{64}}\right)(18t - 18)l^8p^8 + \left(\frac{17}{2\sqrt{72}}\right)(36t - 36)l^8p^9 + \left(\frac{18}{2\sqrt{81}}\right)(108t^2 - 261t + 165)l^9p^9$

5. $S_l^\alpha S_p^\alpha(\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = \left(\frac{36}{5^\alpha}\right) l^4 p^5 + \left(\frac{1}{25^\alpha}\right) (18t - 36) l^5 p^5 + \left(\frac{1}{40^\alpha}\right) (36t - 48) l^5 p^8 + 3 l^6 p^8 + \frac{1}{64^\alpha} (18t - 18) l^8 p^8 + \frac{1}{72^\alpha} (36t - 36) l^8 p^9 + \frac{1}{81^\alpha} (108t^2 - 261t + 165) l^9 p^9$
6. $\mathbb{D}_l S_p + \mathbb{D}_p S_l(\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = \frac{123}{5} l^4 p^5 + 2(18t - 36) l^5 p^5 + \frac{89}{40} (36t - 48) l^5 p^8 + 25 l^6 p^8 + 2(18t - 18) l^8 p^8 + \frac{145}{72} (36t - 36) l^8 p^9 + 2(108t^2 - 261t + 165) l^9 p^9$
7. $2S_l J(\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=1} = \frac{24}{9} l^9 + \frac{2}{10} (18t - 36) l^{10} + \frac{2}{13} (36t - 48) l^{13} + \frac{24}{14} l^{14} + \frac{2}{16} (18t - 18) l^{16} + \frac{2}{17} (36t - 36) l^{17} + \frac{2}{18} (108t^2 - 261t + 165) l^{18}$
8. $S_l J \mathbb{D}_l \mathbb{D}_p(\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=1} = \frac{2880}{9} l^9 + \frac{25}{10} (18t - 36) l^{10} + \frac{40}{13} (36t - 48) l^{13} + \frac{6912}{14} l^{14} + \frac{64}{16} (18t - 18) l^{16} + \frac{72}{17} (36t - 36) l^{17} + \frac{81}{18} (108t^2 - 261t + 165) l^{18}$
9. $\mathbb{D}_l^{\frac{1}{2}} Q_{-2} J S_l^{\frac{1}{2}} S_p^{\frac{1}{2}}(\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=1} = 12 \sqrt{\frac{7}{20}} l^4 p^5 + \sqrt{\frac{8}{25}} (18t - 36) l^5 p^5 + \sqrt{\frac{11}{40}} (36t - 48) l^5 p^8 + 12 \sqrt{\frac{12}{48}} l^6 p^8 + \sqrt{\frac{14}{64}} (18t - 18) l^8 p^8 + \sqrt{\frac{15}{72}} (36t - 36) l^8 p^9 + \sqrt{\frac{16}{81}} (108t^2 - 261t + 165) l^9 p^9$
10. $\mathbb{D}_l^{\frac{1}{2}} Q_{-2} J \left(S_l^{\frac{1}{2}} + S_p^{\frac{1}{2}} \right) (\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=1} = 12 \sqrt{\frac{7}{9}} l^4 p^5 + \sqrt{\frac{8}{10}} (18t - 36) l^5 p^5 + \sqrt{\frac{11}{13}} (36t - 48) l^5 p^8 + 12 \sqrt{\frac{12}{14}} l^6 p^8 + \sqrt{\frac{14}{16}} (18t - 18) l^8 p^8 + \sqrt{\frac{15}{17}} (36t - 36) l^8 p^9 + \sqrt{\frac{16}{18}} (108t^2 - 261t + 165) l^9 p^9$
11. $\mathbb{D}_l^{\frac{1}{2}} \mathbb{D}_p^{\frac{1}{2}}(\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = 12\sqrt{20} l^4 p^5 + \sqrt{25} (18t - 36) l^5 p^5 + \sqrt{40} (36t - 48) l^5 p^8 + 12\sqrt{48} l^6 p^8 + \sqrt{64} (18t - 18) l^8 p^8 + \sqrt{72} (36t - 36) l^8 p^9 + \sqrt{81} (108t^2 - 261t + 165) l^9 p^9$
12. $[\mathbb{D}_l \mathbb{D}_p][\mathbb{D}_l + \mathbb{D}_p]^{-1}(\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = \frac{80}{3} l^4 p^5 + \frac{5}{2} (18t - 36) l^5 p^5 + \frac{40}{13} (36t - 48) l^5 p^8 + \frac{288}{7} l^6 p^8 + 4 (18t - 18) l^8 p^8 + \frac{72}{17} (36t - 36) l^8 p^9 + \frac{9}{2} (108t^2 - 261t + 165) l^9 p^9$
13. $[\mathbb{D}_l \mathbb{D}_p][\mathbb{D}_l + \mathbb{D}_p](\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = 2160 l^4 p^5 + 250 (18t - 36) l^5 p^5 + 520 (36t - 48) l^5 p^8 + 8064 l^6 p^8 + 1024 (18t - 18) l^8 p^8 + 1224 (36t - 36) l^8 p^9 + 1458 (108t^2 - 261t + 165) l^9 p^9$

$$^{14}. \frac{1}{4} [\mathbb{D}_l + \mathbb{D}_p]^2 (\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = 243 l^4 p^5 + 25 (18t - 36) l^5 p^5 + \frac{169}{4} (36t - 48) l^5 p^8 + 588 l^6 p^8 + 64 (18t - 18) l^8 p^8 + \frac{289}{4} (36t - 36) l^8 p^9 + 81 (108t^2 - 261t + 165) l^9 p^9$$

The aforementioned findings are obtained using Partition Table 2 and the conditions of the $\mathfrak{NM}$ -Polynomial with its derivatives [26-32].

5. Entropy Measures in Supertriphenylene by Neighborhood Degree Sum-Based

Theorem 3

If $\mathfrak{G}$ is a Supertriphenylene, then $\mathfrak{NM}$ - measures of entropy are given as follows [9,20,23,33]

1. $\mathfrak{NMEN}_{\mathcal{M}_1} = \log(1944t^2 - 3150t + 1362) - \frac{1}{1944t^2 - 3150t + 1362} (12(9) \log(9) + (18t - 36)(10) \log(10) + (36t - 48)(13) \log(13) + 12(14) \log(14) + (18t - 18)(16) \log(16) + (36t - 36)(17) \log(17) + (108t^2 - 261t + 165)(18) \log(18))$
2. $\mathfrak{NMEN}_{\mathcal{M}_2} = \log(8748t^2 - 15507t + 16593) - \frac{1}{8748t^2 - 15507t + 16593} (12(20) \log(20) + (18t - 36)(25) \log(25) + (36t - 48)(40) \log(40) + 12(48) \log(48) + (18t - 18)(64) \log(64) + (36t - 36)(72) \log(72) + (108t^2 - 261t + 165)(81) \log(81))$
3. $\mathfrak{NMEN}_{\mathcal{T}_{GA}} = \log(52.166 - 154.03t + 108.0t^2) - \frac{1}{52.166 - 154.03t + 108.0t^2} (12 \left(\frac{2\sqrt{20}}{9}\right) \log \left(\frac{2\sqrt{20}}{9}\right) + (18t - 36) \left(\frac{2\sqrt{25}}{10}\right) \log \left(\frac{2\sqrt{25}}{10}\right) + (36t - 48) \left(\frac{2\sqrt{40}}{13}\right) \log \left(\frac{2\sqrt{40}}{13}\right) + 12 \left(\frac{2\sqrt{48}}{14}\right) \log \left(\frac{2\sqrt{48}}{14}\right) + (18t - 18) \left(\frac{2\sqrt{64}}{16}\right) \log \left(\frac{2\sqrt{64}}{16}\right) + (36t - 36) \left(\frac{2\sqrt{72}}{17}\right) \log \left(\frac{2\sqrt{72}}{17}\right) + (108t^2 - 261t + 165) \left(\frac{2\sqrt{81}}{18}\right) \log \left(\frac{2\sqrt{81}}{18}\right))$
4. $\mathfrak{NMEN}_{\mathcal{T}_{AG_1}} = \log(68.808 - 169.94t + 108.0t^2) - \frac{1}{68.808 - 169.94t + 108.0t^2} (12 \left(\frac{9}{2\sqrt{20}}\right) \log \left(\frac{9}{2\sqrt{20}}\right) + (18t - 36) \left(\frac{10}{2\sqrt{25}}\right) \log \left(\frac{10}{2\sqrt{25}}\right) + (36t - 48) \left(\frac{13}{2\sqrt{40}}\right) \log \left(\frac{13}{2\sqrt{40}}\right) + 12 \left(\frac{14}{2\sqrt{48}}\right) \log \left(\frac{14}{2\sqrt{48}}\right) + (18t - 18) \left(\frac{16}{2\sqrt{64}}\right) \log \left(\frac{16}{2\sqrt{64}}\right) + (36t - 36) \left(\frac{17}{2\sqrt{72}}\right) \log \left(\frac{17}{2\sqrt{72}}\right) + (108t^2 - 261t + 165) \left(\frac{18}{2\sqrt{81}}\right) \log \left(\frac{18}{2\sqrt{81}}\right))$
5. $\mathfrak{NMEN}_{\mathcal{T}_{RR_\alpha}} = \log\left(\frac{190421}{21600} - \frac{5911}{7200}t + \frac{4}{3}t^2\right) - \frac{1}{\frac{190421}{21600} - \frac{5911}{7200}t + \frac{4}{3}t^2} (12 \left(\frac{1}{20^\alpha}\right) \log \left(\frac{1}{20^\alpha}\right) + (18t - 36) \left(\frac{1}{25^\alpha}\right) \log \left(\frac{1}{25^\alpha}\right) + (36t - 48) \left(\frac{1}{40^\alpha}\right) \log \left(\frac{1}{40^\alpha}\right) + 12 \left(\frac{1}{48^\alpha}\right) \log \left(\frac{1}{48^\alpha}\right) + (18t - 18) \left(\frac{1}{64^\alpha}\right) \log \left(\frac{1}{64^\alpha}\right) + (36t - 36) \left(\frac{1}{72^\alpha}\right) \log \left(\frac{1}{72^\alpha}\right) + (108t^2 - 261t + 165) \left(\frac{1}{81^\alpha}\right) \log \left(\frac{1}{81^\alpha}\right))$

6. $\mathfrak{NMEN}\mathcal{T}_{SD} = \log\left(\frac{60053}{360} - \frac{3699}{10}t + 216t^2\right) - \frac{1}{\frac{60053}{360} - \frac{3699}{10}t + 216t^2} \left(12\left(\frac{41}{20}\right)\log\left(\frac{41}{20}\right) + (18t - 36)(2)\log(2) + (36t - 48)\left(\frac{89}{40}\right)\log\left(\frac{89}{40}\right) + 12\left(\frac{100}{48}\right)\log\left(\frac{100}{48}\right) + (18t - 18)(2)\log(2) + (36t - 36)\left(\frac{145}{72}\right)\log\left(\frac{145}{72}\right) + (108t^2 - 261t + 165)(2)\log(2)\right)$
7. $\mathfrak{NMEN}\mathcal{T}_H = \log\left(\frac{50877}{30940} - \frac{59123}{4420}t + 12t^2\right) - \frac{1}{\frac{50877}{30940} - \frac{59123}{4420}t + 12t^2} \left(12\left(\frac{2}{9}\right)\log\left(\frac{2}{9}\right) + (18t - 36)\left(\frac{2}{10}\right)\log\left(\frac{2}{10}\right) + (36t - 48)\left(\frac{2}{13}\right)\log\left(\frac{2}{13}\right) + 12\left(\frac{2}{14}\right)\log\left(\frac{2}{14}\right) + (18t - 18)\left(\frac{2}{16}\right)\log\left(\frac{2}{16}\right) + (36t - 36)\left(\frac{2}{17}\right)\log\left(\frac{2}{17}\right) + (108t^2 - 261t + 165)\left(\frac{2}{18}\right)\log\left(\frac{2}{18}\right)\right)$
8. $\mathfrak{NMEN}\mathcal{T}_I = \log\left(\frac{3384995}{3094} - \frac{3384995}{442}t + 486t^2\right) - \frac{1}{\frac{3384995}{3094} - \frac{3384995}{442}t + 486t^2} \left(12\left(\frac{240}{9}\right)\log\left(\frac{240}{9}\right) + (18t - 36)\left(\frac{25}{10}\right)\log\left(\frac{25}{10}\right) + (36t - 48)\left(\frac{40}{13}\right)\log\left(\frac{40}{13}\right) + 12\left(\frac{48}{14}\right)\log\left(\frac{48}{14}\right) + (18t - 18)\left(\frac{64}{16}\right)\log\left(\frac{64}{16}\right) + (36t - 36)\left(\frac{72}{17}\right)\log\left(\frac{72}{17}\right) + (108t^2 - 261t + 165)\left(\frac{81}{18}\right)\log\left(\frac{81}{18}\right)\right)$
9. $\mathfrak{NMEN}\mathcal{T}_{ABC} = \log(16.046 - 62.091t - 48t^2) - \frac{1}{16.046 - 62.091t - 48t^2} \left(12\left(\frac{7}{20}\right)\log\left(\frac{7}{20}\right) + (18t - 36)\left(\frac{8}{25}\right)\log\left(\frac{8}{25}\right) + (36t - 48)\left(\frac{11}{40}\right)\log\left(\frac{11}{40}\right) + 12\left(\frac{12}{48}\right)\log\left(\frac{12}{48}\right) + (18t - 18)\left(\frac{14}{64}\right)\log\left(\frac{14}{64}\right) + (36t - 36)\left(\frac{15}{72}\right)\log\left(\frac{15}{72}\right) + (108t^2 - 261t + 165)\left(\frac{16}{81}\right)\log\left(\frac{16}{81}\right)\right)$
10. $\mathfrak{NMEN}\mathcal{T}_{ABS} = \log(50.25 - 146.20t + 101.82t^2) - \frac{1}{50.25 - 146.20t + 101.82t^2} \left(12\left(\frac{7}{9}\right)\log\left(\frac{7}{9}\right) + (18t - 36)\left(\frac{8}{10}\right)\log\left(\frac{8}{10}\right) + (36t - 48)\left(\frac{11}{13}\right)\log\left(\frac{11}{13}\right) + 12\left(\frac{12}{14}\right)\log\left(\frac{12}{14}\right) + (18t - 18)\left(\frac{14}{16}\right)\log\left(\frac{14}{16}\right) + (36t - 36)\left(\frac{15}{17}\right)\log\left(\frac{15}{17}\right) + (108t^2 - 261t + 165)\left(\frac{16}{18}\right)\log\left(\frac{16}{18}\right)\right)$
11. $\mathfrak{NMEN}\mathcal{T}_{RR} = \log(688.79 - 1581.8t + 972.0t^2) - \frac{1}{688.79 - 1581.8t + 972.0t^2} \left(12(\sqrt{20})\log(\sqrt{20}) + (18t - 36)(\sqrt{25})\log(\sqrt{25}) + (36t - 48)(\sqrt{40})\log(\sqrt{40}) + 12(\sqrt{48})\log(\sqrt{48}) + (18t - 18)(\sqrt{64})\log(\sqrt{64}) + (36t - 36)(\sqrt{72})\log(\sqrt{72}) + (108t^2 - 261t + 165)(\sqrt{81})\log(\sqrt{81})\right)$
12. $\mathfrak{NMEN}\mathcal{T}_{ReZ_2} = \log\left(\frac{3231497}{9282} - \frac{351063}{442}t + 486t^2\right) - \frac{1}{\frac{3231497}{9282} - \frac{351063}{442}t + 486t^2} \left(12\left(\frac{20}{9}\right)\log\left(\frac{20}{9}\right) + (18t - 36)\left(\frac{25}{10}\right)\log\left(\frac{25}{10}\right) + (36t - 48)\left(\frac{40}{13}\right)\log\left(\frac{40}{13}\right) + 12\left(\frac{48}{14}\right)\log\left(\frac{48}{14}\right) + (18t - 18)\left(\frac{64}{16}\right)\log\left(\frac{64}{16}\right) + (36t - 36)\left(\frac{72}{17}\right)\log\left(\frac{72}{17}\right) + (108t^2 - 261t + 165)\left(\frac{81}{18}\right)\log\left(\frac{81}{18}\right)\right)$
13. $\mathfrak{NMEN}\mathcal{T}_{ReZ_3} = \log(157464t^2 - 294822t + 154338) - \frac{1}{157464t^2 - 294822t + 154338} \left(12(180)\log(180) + (18t - 36)(250)\log(250) + \right)$

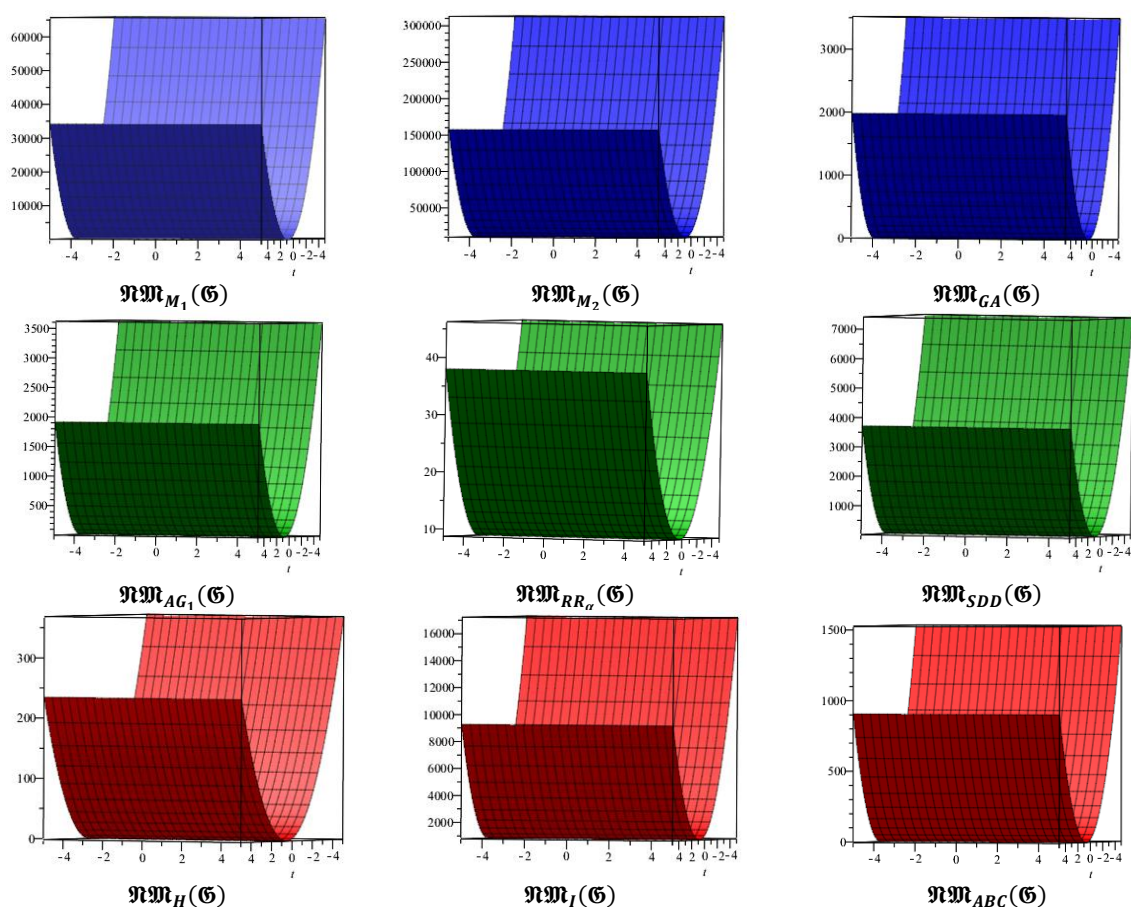
$$(36t - 48)(520) \log(520) + 12(672) \log(672) + (18t - 18)(1024) \log(1024) + (36t - 36)(1224) \log(1224) + (108t^2 - 261t + 165)(1458) \log(1458))$$

$$14. \mathfrak{NMEN}\mathcal{T}_{Sk_2} = \log(8748t^2 - 15417t + 7515) -$$

$$\frac{1}{8748t^2 - 15417t + 7515} \left(12 \left(\frac{9}{2} \right)^2 \log \left(\frac{9}{2} \right)^2 + (18t - 36) \left(\frac{10}{2} \right)^2 \log \left(\frac{10}{2} \right)^2 + \right. \\ \left. (36t - 48) \left(\frac{13}{2} \right)^2 \log \left(\frac{13}{2} \right)^2 + 12 \left(\frac{14}{2} \right)^2 \log \left(\frac{14}{2} \right)^2 + (18t - 18) \left(\frac{16}{2} \right)^2 \log \left(\frac{16}{2} \right)^2 + \right. \\ \left. (36t - 36) \left(\frac{17}{2} \right)^2 \log \left(\frac{17}{2} \right)^2 + (108t^2 - 261t + 165) \left(\frac{18}{2} \right)^2 \log \left(\frac{18}{2} \right)^2 \right)$$

6. Comparative Analysis for Supertriphenylene

This section presents three-dimensional graphs that show the analytical equations for the neighborhood degree sum-based indices, obtained from Theorems 2 and 3. These images will make it easier for the reader to understand how the indices relate to the variables that make up the molecular structure. Furthermore, we present the outcomes of Theorem 2 as comparison plots, in which each neighborhood degree sum-based index is compared to a single structural variable on a single graph. These comparison charts provide a visual representation of the differences between the indices and the chemical structure. Tables 3–6 display the calculated numerical values for the indices. To aid readers in understanding the numerical data, Figures 4, 5, and 6 present them as three-dimensional graphs.



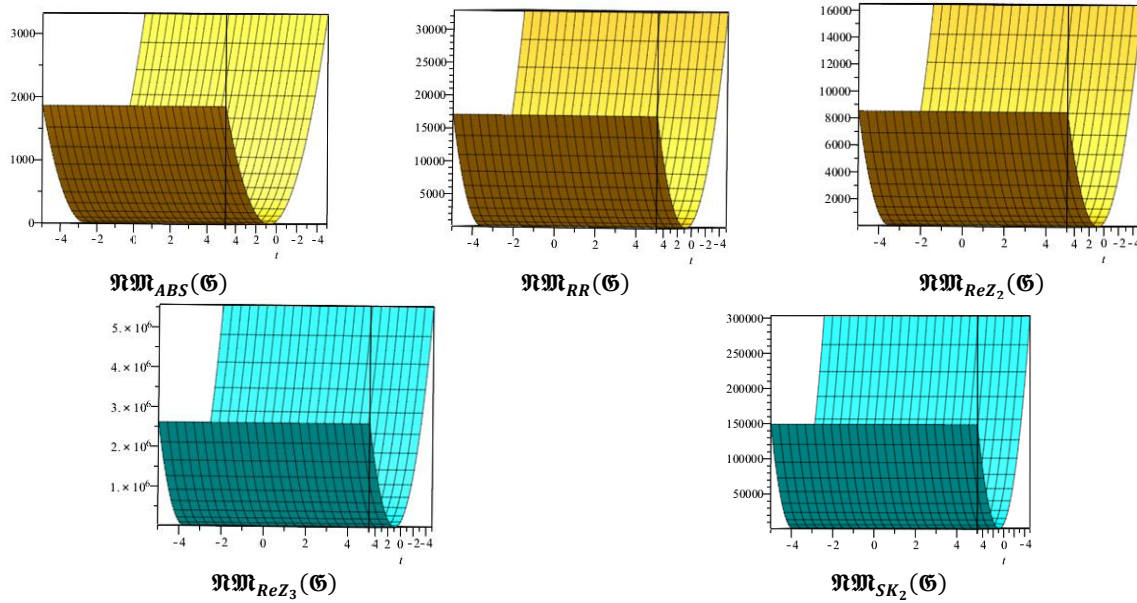


Figure 4. 3D plots for Theorem 2.

Table 3. Comparison Table for Theorem 2.

t	NM_{M_1}	NM_{M_2}	NM_{GA}	NM_{AG_1}	NM_{RR_α}	NM_{SDD}	NM_H
2	2838	20571	176.106	160.928	12.51	291.0	22.89
3	9408	48804	562.076	530.988	18.35	1001.1	69.57
4	19866	94533	1164.046	1117.048	26.865	2143.2	140.14
5	34212	157758	1982.016	1919.108	38.044	3717.3	234.76
6	52446	238479	3015.986	2937.168	51.89	5723.4	353.39
7	74568	336696	4265.956	4171.228	68.402	8161.5	496.01
8	100578	452409	5731.926	5621.288	87.581	11032	662.63
9	130476	585618	7413.896	7287.348	109.43	14334	853.26
10	164262	736323	9311.866	9169.408	133.94	18068	1067.9

Table 4. Comparison Table for Theorem 2.

t	NM_I	NM_{ABC}	NM_{ABS}	NM_{RR}	NM_{ReZ_2}	NM_{ReZ_3}	NM_{SK_2}
2	1449.50	83.864	165.13	1413.19	703.6	194550	11673
3	3085.30	261.773	528.03	4691.39	2339.4	687048	39996
4	5693.00	535.682	1094.57	9913.59	4947.1	1494474	85815
5	9272.80	905.591	1864.75	17079.79	8526.8	2616828	149130
6	13824.00	1371.5	2838.57	26189.99	13079.0	4054110	229941
7	19348.00	1933.409	4016.03	37244.19	18602.0	5806320	328248
8	25844.00	2591.318	5397.13	50242.39	25098.0	7873458	444051
9	33312.00	3345.227	6981.87	65184.59	32566.0	10255524	577350
10	41751.00	4195.136	8770.25	82070.79	41006.0	12952518	728145

Table 5. Comparison Table for Theorem 3.

t	ENT_{M_1}	ENT_{M_2}	ENT_{GA}	ENT_{AG_1}	ENT_{RR_α}	ENT_{SDD}	ENT_H
2	7.5595	9.7568	5.1763	5.0752	54.472	5.1755	2.1308
3	8.9151	10.688	6.3350	6.2791	127.97	6.4923	3.2416
4	9.6996	11.374	7.0624	7.0156	185.31	7.2785	3.9426
5	10.256	11.897	7.5939	7.5575	225.33	7.8412	4.4586
6	10.692	12.315	8.0133	7.9835	253.07	8.2797	4.8676
7	11.047	12.664	8.3598	8.3346	272.78	8.6392	5.2066
8	11.352	12.961	8.6550	8.6330	287.20	8.9437	5.4962
9	11.613	13.220	8.9122	8.8928	298.06	9.2079	5.7491
10	11.842	13.449	9.1400	9.1226	306.47	9.4412	5.9734

Table 6. Comparison Table for Theorem 3.

t	$\mathcal{ENT}_I$	$\mathcal{ENT}_{ABC}$	$\mathcal{ENT}_{ABS}$	$\mathcal{ENT}_{RR}$	$\mathcal{ENT}_{ReZ_2}$	$\mathcal{ENT}_{ReZ_3}$	$\mathcal{ENT}_{SK_2}$
2	10.028	5.810	4.1067	6.8539	7.1191	11.844	4.8633
3	10.365	5.898	5.2691	8.1577	8.0614	13.342	5.9703
4	10.591	5.996	5.9981	8.9309	8.6650	14.169	6.6763
5	10.756	6.102	6.5310	9.4847	9.1179	14.749	7.1955
6	10.880	6.212	6.9511	9.9174	9.4828	15.195	7.6097
7	10.980	6.321	7.2980	10.273	9.7894	15.558	7.9497
8	11.06	6.428	7.5936	10.574	10.053	15.866	8.2416
9	11.132	6.533	7.8512	10.836	10.286	16.132	8.4963
10	11.201	6.633	8.0791	11.066	10.495	16.367	8.7221

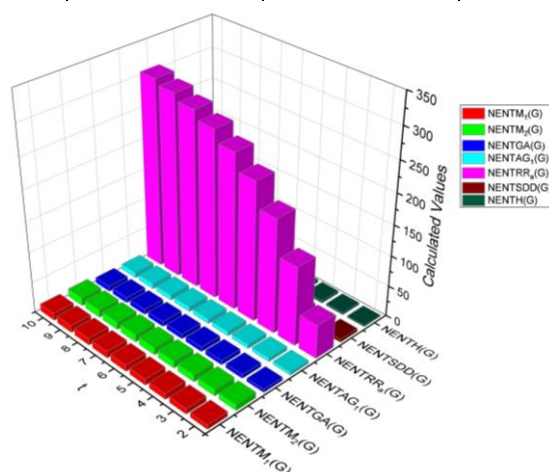


Figure 5. For comparison, Table 5.

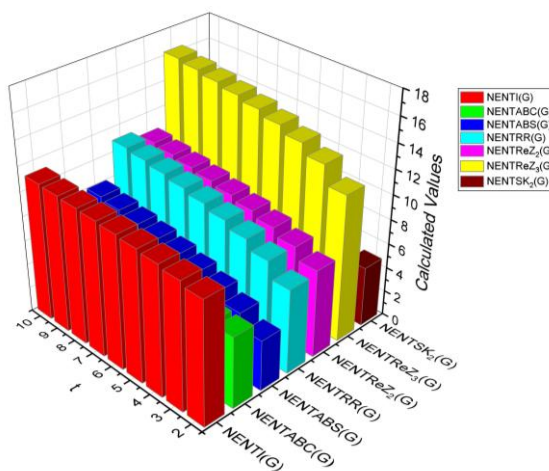


Figure 6. For comparison, Table 6.

7. Computing the Neighborhood Sum Degree-based M-polynomial for Superphenalene

With the chemical formula $C_{96}H_{30}$, superphenalene is a very big polycyclic aromatic hydrocarbon (PAH). It can be visualized as three hexa-peri-hexabenzocoronenes stacked symmetrically around a center, or as three fused super benzenes. Superphenalene's huge size and intricate structure give it several unique features, and its molecular graph is shown in Figure 7. Its planar geometry, for example, is peculiar for a molecule this size. It also has many mesomeric boundary structures, which are various representations of the molecule that show electron motion within it [12-13]. Superphenalene contains a far higher number of mesomeric boundary structures (540,000) than other big PAHs, including buckminsterfullerene (12,500), supernaphthalene (16,100), and hexabenzocoronene (250).

The goal of superphenalene research is to comprehend its special qualities and possible uses. Superphenalene may offer intriguing electrical and optical properties due to its complicated structure, which could be helpful in organic electronics or other technological applications. Nonetheless, additional investigation is required to ascertain the precise characteristics of superphenalene and to devise techniques for its mass synthesis.

This molecule is remarkably flat for its size, which may have an impact on how it interacts with other molecules [29]. Superphenalene has a high degree of electron delocalization, or spreading out, which could result in fascinating electrical properties. There are more than 540,000 ways to depict the electron distribution in this material. Photovoltaic properties: Superphenalene is a possible candidate for the construction of solar cells since theoretical studies indicate it may be helpful in capturing light energy (photovoltaics). Superphenalene's electrical characteristics make it a potential building block for this quickly emerging discipline, which focuses on carbon-based materials for devices like light-emitting diodes (LEDs) and transistors. Superphenalene's photovoltaic qualities make it a viable option for absorbing light and transforming it into electrical power for solar panels or other renewable energy uses.

Superphenalene is a relatively new area of research, and its properties are still under investigation. Large-scale synthesis methods haven't been established yet, limiting their current applications.

The cardinality of $\mathfrak{G}$ is $V(\mathfrak{G}) = 54t^2 - 72t + 24$ and $E(\mathfrak{G}) = 81t^2 - 120t + 45$

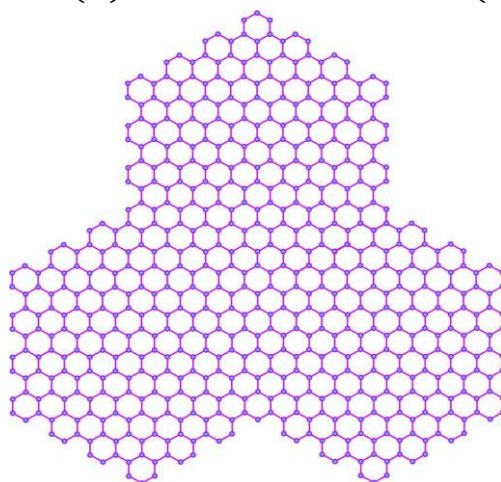


Figure 7. Molecular graph of superphenalene.

Table 7. Partition table for Figure 7 [12].

$(\mathfrak{d}_w, \mathfrak{d}_v)$	Frequency
(4,5)	18
(5,5)	$12t - 24$
(5,8)	$24t - 30$
(6,8)	6
(8,8)	$12t - 12$
(8,9)	$24t - 24$
(9,9)	$81t^2 - 192t + 111$

Theorem 4.

If $\mathfrak{G}$ is a Superphenelene, then that $\mathfrak{G}$'s $\mathfrak{NM}$ -polynomial can be found.

1. $\mathfrak{NM}_{M_1}(\mathfrak{G}) = 1458t^2 - 2424t + 1014$
2. $\mathfrak{NM}_{M_2}(\mathfrak{G}) = 6561t^2 - 11796t + 12903$

- $$\begin{aligned} \mathfrak{NM}_{GA}(\mathfrak{G}) &= 45.680 - 120.69t + 81.t^2 \\ 3. \mathfrak{NM}_{AG}(\mathfrak{G}) &= 44.301 - 119.29t + 81.t^2 \\ 4. \mathfrak{NM}_{RR\alpha}(\mathfrak{G}) &= \frac{173767}{10800} - \frac{8311}{10800}t + t^2 \\ 5. \mathfrak{NM}_{SSD}(\mathfrak{G}) &= \frac{5059}{60} - \frac{3514}{15}t + 162t^2 \\ 6. \mathfrak{NM}_H(\mathfrak{G}) &= \frac{160187}{46410} - \frac{72383}{6630}t + 9t^2 \\ 7. \mathfrak{NM}_I(\mathfrak{G}) &= \frac{3220773}{3094} - \frac{134922}{221}t + \frac{729}{2}t^2 \\ 8. \mathfrak{NM}_{ABC}(\mathfrak{G}) &= 31.250 - 56.180t + 36.t^2 \\ 9. \mathfrak{NM}_{ABS}(\mathfrak{G}) &= 65.609 - 125.18t + 76.367t^2 \\ 10. \mathfrak{NM}_{RR}(\mathfrak{G}) &= 511.68 - 1216.6t + 729.t^2 \\ 11. \mathfrak{NM}_{ReZ_2}(\mathfrak{G}) &= \frac{798613}{3094} - \frac{134922}{221}t + \frac{729}{2}t^2 \\ 12. \mathfrak{NM}_{ReZ_3}(\mathfrak{G}) &= 118098t^2 - 222792t + 105846 \\ 13. \mathfrak{NM}_{SK_2}(\mathfrak{G}) &= 6561t^2 - 11736t + 5280 \end{aligned}$$

Proof:

Let $k(l,p)=\mathfrak{NM}(\mathfrak{G}; l, P) = 18l^4p^5 + (12t - 24)l^5p^5 + (24t - 30)l^5p^8 + 6l^6p^8 + (12t - 12)l^8p^8 + (24t - 24)l^8p^9 + (81t^2 - 192t + 111)l^9p^9$

1. $\mathbb{D}_l + \mathbb{D}_p(\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = 162l^4p^5 + 10(12t - 24)l^5p^5 + 13(24t - 30)l^5p^8 + 84l^6p^8 + 16(12t - 12)l^8p^8 + 17(24t - 24)l^8p^9 + 18(81t^2 - 192t + 111)l^9p^9$
2. $\mathbb{D}_l \mathbb{D}_p(\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = 18(360)l^4p^5 + 25(12t - 24)l^5p^5 + 40(24t - 30)l^5p^8 + 6(288)l^6p^8 + 64(12t - 12)l^8p^8 + 72(24t - 24)l^8p^9 + 81(81t^2 - 192t + 111)l^9p^9$
3. $2[\mathbb{D}_l \mathbb{D}_p]^{\frac{1}{2}}[\mathbb{D}_l + \mathbb{D}_p]^{-1}(\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = 18\left(\frac{2\sqrt{20}}{9}\right)l^4p^5 + \left(\frac{2\sqrt{25}}{10}\right)(12t - 24)l^5p^5 + \left(\frac{2\sqrt{40}}{13}\right)(24t - 30)l^5p^8 + 6\left(\frac{2\sqrt{48}}{14}\right)l^6p^8 + \left(\frac{2\sqrt{64}}{16}\right)(12t - 12)l^8p^8 + \left(\frac{2\sqrt{72}}{17}\right)(24t - 24)l^8p^9 + \left(\frac{2\sqrt{81}}{18}\right)(81t^2 - 192t + 111)l^9p^9$
4. $\frac{1}{2}[\mathbb{D}_l + \mathbb{D}_p][\mathbb{D}_l + \mathbb{D}_p]^{-\frac{1}{2}}(\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = 18\left(\frac{9}{2\sqrt{20}}\right)l^4p^5 + \left(\frac{10}{2\sqrt{25}}\right)(12t - 24)l^5p^5 + \left(\frac{13}{2\sqrt{40}}\right)(24t - 30)l^5p^8 + 6\left(\frac{14}{2\sqrt{48}}\right)l^6p^8 + \left(\frac{16}{2\sqrt{64}}\right)(12t - 12)l^8p^8 + \left(\frac{17}{2\sqrt{72}}\right)(24t - 24)l^8p^9 + \left(\frac{18}{2\sqrt{81}}\right)(81t^2 - 192t + 111)l^9p^9$
5. $\mathbb{S}_l^\alpha \mathbb{S}_p^\alpha(\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = \frac{324}{20^\alpha}l^4p^5 + \frac{1}{25^\alpha}(12t - 24)l^5p^5 + \frac{1}{40^\alpha}(24t - 30)l^5p^8 + \frac{36}{48^\alpha}l^6p^8 + \frac{1}{64^\alpha}(12t - 12)l^8p^8 + \frac{1}{72^\alpha}(24t - 24)l^8p^9 + \frac{1}{81^\alpha}(81t^2 - 192t + 111)l^9p^9$

6. $\mathbb{D}_l \mathbb{S}_p + \mathbb{D}_p \mathbb{S}_l (\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = 18 \left(\frac{41}{20} \right) l^4 p^5 + 2(12t - 24) l^5 p^5 +$
 $\left(\frac{5}{8} + \frac{8}{5} \right) (24t - 30) l^5 p^8 + 6 \left(\frac{6}{8} + \frac{8}{6} \right) l^6 p^8 + 2(12t - 12) l^8 p^8 + \left(\frac{8}{9} + \frac{9}{8} \right) (24t -$
 $24) l^8 p^9 + 2(81t^2 - 192t + 111) l^9 p^9$
7. $2\mathbb{S}_l \mathbb{J}(\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=1} = 18 \left(\frac{2}{9} \right) l^9 + \frac{2}{10} (12t - 24) l^{10} + \frac{2}{13} (24t - 30) l^{13} +$
 $6 \left(\frac{2}{14} \right) l^{14} + \frac{2}{16} (12t - 12) l^{16} + \frac{2}{17} (24t - 24) l^{17} + \frac{2}{18} (81t^2 - 192t + 111) l^{18}$
8. $\mathbb{S}_l \mathbb{J} \mathbb{D}_l \mathbb{D}_p (\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=1} = 18 \left(\frac{360}{9} \right) l^9 + \frac{25}{10} (12t - 24) l^{10} + \frac{40}{13} (24t - 30) l^{13} +$
 $6 \left(\frac{288}{14} \right) l^{14} + \frac{64}{16} (12t - 12) l^{16} + \frac{72}{17} (24t - 24) l^{17} + \frac{81}{18} (81t^2 - 192t + 111) l^{18}$
9. $\mathbb{D}_l^{\frac{1}{2}} \mathbb{Q}_{-2} \mathbb{J} \mathbb{S}_l^{\frac{1}{2}} \mathbb{S}_p^{\frac{1}{2}} (\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=1} = 18 \left(\sqrt{\frac{7}{20}} \right) l^5 p^5 + \sqrt{\frac{8}{25}} (12t - 24) l^5 p^8 +$
 $\sqrt{\frac{11}{40}} (24t - 30) l^5 p^8 + 6 \sqrt{\frac{12}{48}} l^6 p^8 + \sqrt{\frac{14}{64}} (12t - 12) l^8 p^8 + \sqrt{\frac{15}{72}} (24t - 24) l^8 p^9 +$
 $\sqrt{\frac{16}{81}} (81t^2 - 192t + 111) l^9 p^9$
10. $\mathbb{D}_l^{\frac{1}{2}} \mathbb{Q}_{-2} \mathbb{J} (\mathbb{S}_l^{\frac{1}{2}} + \mathbb{S}_p^{\frac{1}{2}}) (\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=1} = 18 \left(\sqrt{\frac{7}{9}} \right) l^5 p^5 + \sqrt{\frac{8}{10}} (12t - 24) l^5 p^8 +$
 $\sqrt{\frac{11}{13}} (24t - 30) l^5 p^8 + 6 \sqrt{\frac{12}{14}} l^6 p^8 + \sqrt{\frac{14}{16}} (12t - 12) l^8 p^8 + \sqrt{\frac{15}{17}} (24t - 24) l^8 p^9 +$
 $\sqrt{\frac{16}{18}} (81t^2 - 192t + 111) l^9 p^9$
11. $\mathbb{D}_l^{\frac{1}{2}} \mathbb{D}_p^{\frac{1}{2}} (\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = 18\sqrt{20} l^4 p^5 + \sqrt{25} (12t - 24) l^5 p^5 +$
 $\sqrt{40} (24t - 30) l^5 p^8 + 6\sqrt{48} l^6 p^8 + \sqrt{64} (12t - 12) l^8 p^8 + \sqrt{72} (24t - 24) l^8 p^9 +$
 $\sqrt{81} (81t^2 - 192t + 111) l^9 p^9$
12. $[\mathbb{D}_l \mathbb{D}_p] [\mathbb{D}_l + \mathbb{D}_p]^{-1} (\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = 18 \left(\frac{20}{9} \right) l^4 p^5 + \left(\frac{25}{10} \right) (12t - 24) l^5 p^5 +$
 $\left(\frac{40}{13} \right) (24t - 30) l^5 p^8 + 6 \left(\frac{48}{14} \right) l^6 p^8 + \left(\frac{64}{16} \right) (12t - 12) l^8 p^8 + \left(\frac{72}{17} \right) (24t - 24) l^8 p^9 +$
 $\left(\frac{81}{18} \right) (81t^2 - 192t + 111) l^9 p^9$
13. $[\mathbb{D}_l \mathbb{D}_p] [\mathbb{D}_l + \mathbb{D}_p] (\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = 18(180) l^4 p^5 + (250) (12t - 24) l^5 p^5 +$
 $(520) (24t - 30) l^5 p^8 + 6(672) l^6 p^8 + (1024) (12t - 12) l^8 p^8 + (1224) (24t -$
 $24) l^8 p^9 + (1458) (81t^2 - 192t + 111) l^9 p^9$
14. $\frac{1}{4} [\mathbb{D}_l + \mathbb{D}_p]^2 (\mathfrak{NM}(\mathfrak{G}; l, p))|_{l=p=1} = 18 \left(\frac{81}{4} \right) l^4 p^5 + 25 (12t - 24) l^5 p^5 +$
 $\left(\frac{169}{4} \right) (24t - 30) l^5 p^8 + 6(49) l^6 p^8 + (64) (12t - 12) l^8 p^8 + \left(\frac{289}{4} \right) (24t -$
 $24) l^8 p^9 + (81) (81t^2 - 192t + 111) l^9 p^9$

The aforementioned findings are obtained using partition table 7 and the conditions of the $\mathfrak{NM}$ -Polynomial with its derivatives [26-32].

8. Entropy Measures in Superphenalene by Neighborhood Degree Sum-based

Theorem 5.

If $\mathfrak{G}$ is a Superphenalene, then $\mathfrak{NM}$ -entropy measures are given as follows[9,20,23,33].

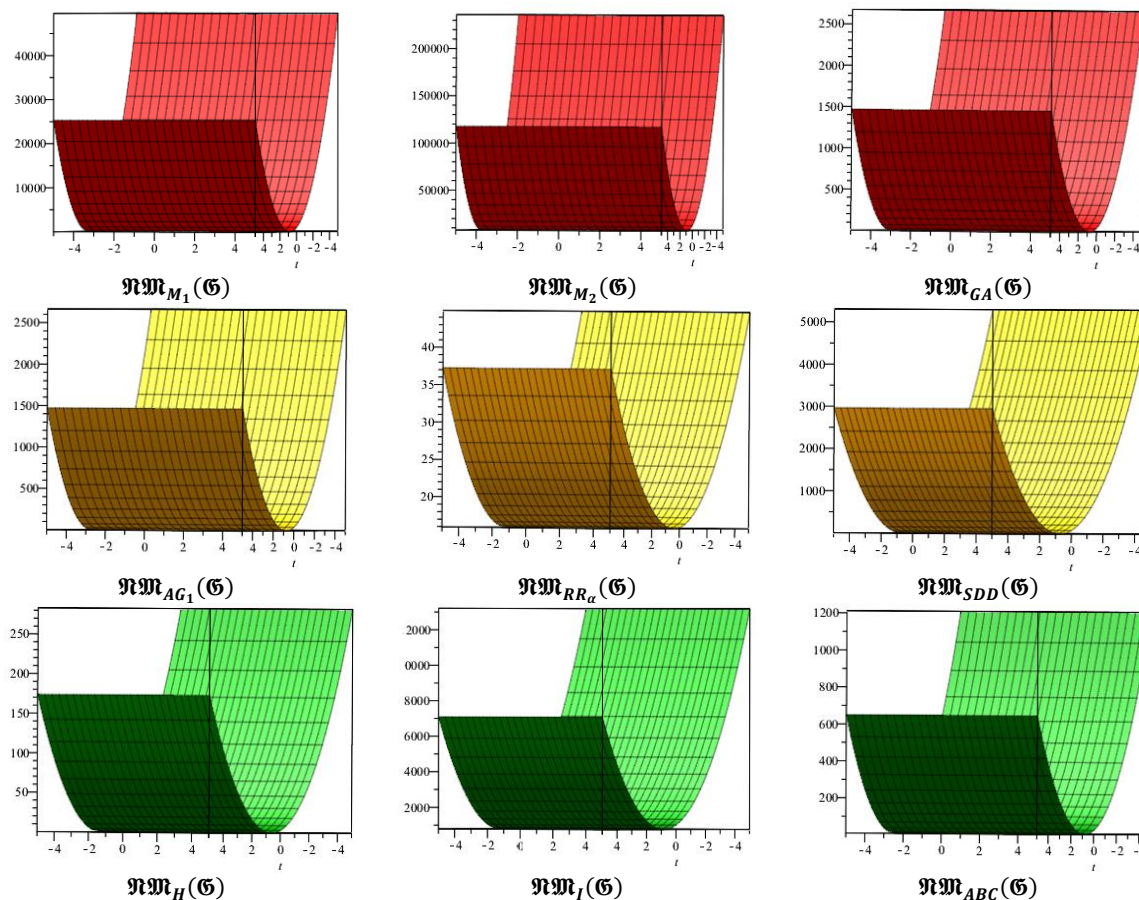
1. $\mathfrak{NMEN}\mathcal{T}_{M_1} = \log(1458t^2 - 2424t + 1014) - \frac{1}{(1458t^2 - 2424t + 1014)} (18(9)\log(9) + (12t - 24)(10)\log(10) + (24t - 30)(13)\log(13) + 6(14)\log(14) + (12t - 12)(16)\log(16) + (24t - 24)(17)\log(17) + (81t^2 - 192t + 111)(18)\log(18))$
2. $\mathfrak{NMEN}\mathcal{T}_{M_2} = \log(6561t^2 - 11796t + 12903) - \frac{1}{(6561t^2 - 11796t + 12903)} (18(20)\log(20) + (12t - 24)(25)\log(25) + (24t - 30)(40)\log(40) + 6(48)\log(48) + (12t - 12)(64)\log(64) + (24t - 24)(72)\log(72) + (81t^2 - 192t + 111)(81)\log(81))$
3. $\mathfrak{NMEN}\mathcal{T}_{GA} = \log(45.680 - 120.69t + 81.0t^2) - \frac{1}{(45.680 - 120.69t + 81.0t^2)} (18\left(\frac{2\sqrt{20}}{9}\right)\log\left(\frac{2\sqrt{20}}{9}\right) + (12t - 24)\left(\frac{2\sqrt{25}}{10}\right)\log\left(\frac{2\sqrt{25}}{10}\right) + (24t - 30)\left(\frac{2\sqrt{40}}{13}\right)\log\left(\frac{2\sqrt{40}}{13}\right) + 6\left(\frac{2\sqrt{48}}{14}\right)\log\left(\frac{2\sqrt{48}}{14}\right) + (12t - 12)\left(\frac{2\sqrt{64}}{16}\right)\log\left(\frac{2\sqrt{64}}{16}\right) + (24t - 24)\left(\frac{2\sqrt{72}}{17}\right)\log\left(\frac{2\sqrt{72}}{17}\right) + (81t^2 - 192t + 111)\left(\frac{2\sqrt{81}}{18}\right)\log\left(\frac{2\sqrt{81}}{18}\right))$
4. $\mathfrak{NMEN}\mathcal{T}_{AG_1} = \log(44.301 - 119.29t + 81.0 - t^2) - \frac{1}{(44.301 - 119.29t + 81.0 - t^2)} (18\left(\frac{9}{2\sqrt{20}}\right)\log\left(\frac{9}{2\sqrt{20}}\right) + (12t - 24)\left(\frac{10}{2\sqrt{25}}\right)\log\left(\frac{10}{2\sqrt{25}}\right) + (24t - 30)\left(\frac{13}{2\sqrt{40}}\right)\log\left(\frac{13}{2\sqrt{40}}\right) + 6\left(\frac{14}{2\sqrt{48}}\right)\log\left(\frac{14}{2\sqrt{48}}\right) + (12t - 12)\left(\frac{16}{2\sqrt{64}}\right)\log\left(\frac{16}{2\sqrt{64}}\right) + (24t - 24)\left(\frac{17}{2\sqrt{72}}\right)\log\left(\frac{17}{2\sqrt{72}}\right) + (81t^2 - 192t + 111)\left(\frac{18}{2\sqrt{81}}\right)\log\left(\frac{18}{2\sqrt{81}}\right))$
5. $\mathfrak{NMEN}\mathcal{T}_{RR_\alpha} = \log\left(\frac{173767}{10800} - \frac{8311}{10800}t + t^2\right) - \frac{1}{\left(\frac{173767}{10800} - \frac{8311}{10800}t + t^2\right)} (18\left(\frac{1}{20^\alpha}\right)\log\left(\frac{1}{20^\alpha}\right) + (12t - 24)\left(\frac{1}{25^\alpha}\right)\log\left(\frac{1}{25^\alpha}\right) + (24t - 30)\left(\frac{1}{40^\alpha}\right)\log\left(\frac{1}{40^\alpha}\right) + 6\left(\frac{1}{48^\alpha}\right)\log\left(\frac{1}{48^\alpha}\right) + (12t - 12)\left(\frac{1}{64^\alpha}\right)\log\left(\frac{1}{64^\alpha}\right) + (24t - 24)\left(\frac{1}{72^\alpha}\right)\log\left(\frac{1}{72^\alpha}\right) + (81t^2 - 192t + 111)\left(\frac{1}{81^\alpha}\right)\log\left(\frac{1}{81^\alpha}\right))$
6. $\mathfrak{NMEN}\mathcal{T}_{SDD} = \log\left(\frac{5059}{60} - \frac{3514}{15}t + 162t^2\right) - \frac{1}{\left(\frac{5059}{60} - \frac{3514}{15}t + 162t^2\right)} (18\left(\frac{41}{20}\right)\log\left(\frac{41}{20}\right) + (12t - 24)(2)\log(2) + (24t - 30)\left(\frac{89}{40}\right)\log\left(\frac{89}{40}\right) + 6\left(\frac{100}{48}\right)\log\left(\frac{100}{48}\right) + (12t - 12)(2)\log(2) + (24t - 24)\left(\frac{145}{72}\right)\log\left(\frac{145}{72}\right) + (81t^2 - 192t + 111)(2)\log(2))$

7. $\mathfrak{NMEN}\mathcal{T}_H = \log\left(\frac{160187}{46410} - \frac{72383}{6630}t + 9t^2\right) - \frac{1}{\left(\frac{160187}{46410} - \frac{72383}{6630}t + 9t^2\right)} \left(18 \left(\frac{2}{9}\right) \log\left(\frac{2}{9}\right) + (12t - 24) \left(\frac{2}{10}\right) \log\left(\frac{2}{10}\right) + (24t - 30) \left(\frac{2}{13}\right) \log\left(\frac{2}{13}\right) + 6 \left(\frac{2}{14}\right) \log\left(\frac{2}{14}\right) + (12t - 12) \left(\frac{2}{16}\right) \log\left(\frac{2}{16}\right) + (24t - 24) \left(\frac{2}{17}\right) \log\left(\frac{2}{17}\right) + (81t^2 - 192t + 111) \left(\frac{2}{18}\right) \log\left(\frac{2}{18}\right)\right)$
8. $\mathfrak{NMEN}\mathcal{T}_I = \log\left(\frac{3220773}{3094} - \frac{134922}{221}t + \frac{729}{2}t^2\right) - \frac{1}{\left(\frac{3220773}{3094} - \frac{134922}{221}t + \frac{729}{2}t^2\right)} \left(18 \left(\frac{360}{9}\right) \log\left(\frac{360}{9}\right) + (12t - 24) \left(\frac{25}{10}\right) \log\left(\frac{25}{10}\right) + (24t - 30) \left(\frac{40}{13}\right) \log\left(\frac{40}{13}\right) + 6 \left(\frac{288}{14}\right) \log\left(\frac{288}{14}\right) + (12t - 12) \left(\frac{64}{16}\right) \log\left(\frac{64}{16}\right) + (24t - 24) \left(\frac{72}{17}\right) \log\left(\frac{72}{17}\right) + (81t^2 - 192t + 111) \left(\frac{81}{18}\right) \log\left(\frac{81}{18}\right)\right)$
9. $\mathfrak{NMEN}\mathcal{T}_{ABC} = \log(31.250 - 56.180t + 36.0t^2) - \frac{1}{(31.250 - 56.180t + 36.0t^2)} \left(18 \left(\sqrt{\frac{7}{20}}\right) \log\left(\sqrt{\frac{7}{20}}\right) + (12t - 24) \left(\sqrt{\frac{8}{25}}\right) \log\left(\sqrt{\frac{8}{25}}\right) + (24t - 30) \left(\sqrt{\frac{11}{40}}\right) \log\left(\sqrt{\frac{11}{40}}\right) + 6 \left(\sqrt{\frac{12}{48}}\right) \log\left(\sqrt{\frac{12}{48}}\right) + (12t - 12) \left(\sqrt{\frac{14}{64}}\right) \log\left(\sqrt{\frac{14}{64}}\right) + (24t - 24) \left(\sqrt{\frac{15}{72}}\right) \log\left(\sqrt{\frac{15}{72}}\right) + (81t^2 - 192t + 111) \left(\sqrt{\frac{16}{81}}\right) \log\left(\sqrt{\frac{16}{81}}\right)\right)$
10. $\mathfrak{NMEN}\mathcal{T}_{ABS} = \log(65.609 - 125.18t + 76.367t^2) - \frac{1}{(65.609 - 125.18t + 76.367t^2)} \left(18 \left(\sqrt{\frac{7}{9}}\right) \log\left(\sqrt{\frac{7}{9}}\right) + (12t - 24) \left(\sqrt{\frac{8}{10}}\right) \log\left(\sqrt{\frac{8}{10}}\right) + (24t - 30) \left(\sqrt{\frac{11}{13}}\right) \log\left(\sqrt{\frac{11}{13}}\right) + 6 \left(\sqrt{\frac{12}{14}}\right) \log\left(\sqrt{\frac{12}{14}}\right) + (12t - 12) \left(\sqrt{\frac{14}{16}}\right) \log\left(\sqrt{\frac{14}{16}}\right) + (24t - 24) \left(\sqrt{\frac{15}{17}}\right) \log\left(\sqrt{\frac{15}{17}}\right) + (81t^2 - 192t + 111) \left(\sqrt{\frac{16}{18}}\right) \log\left(\sqrt{\frac{16}{18}}\right)\right)$
11. $\mathfrak{NMEN}\mathcal{T}_{RR} = \log(511.68 - 1216.6t + 729.0t^2) - \frac{1}{(511.68 - 1216.6t + 729.0t^2)} \left(18 (\sqrt{20}) \log(\sqrt{20}) + (12t - 24) (\sqrt{25}) \log(\sqrt{25}) + (24t - 30) (\sqrt{40}) \log(\sqrt{40}) + 6 (\sqrt{48}) \log(\sqrt{48}) + (12t - 12) (\sqrt{64}) \log(\sqrt{64}) + (24t - 24) (\sqrt{72}) \log(\sqrt{72}) + (81t^2 - 192t + 111) (\sqrt{81}) \log(\sqrt{81})\right)$
12. $\mathfrak{NMEN}\mathcal{T}_{ReZ_2} = \log\left(\frac{798613}{3094} - \frac{134922}{221}t + \frac{729}{2}t^2\right) - \frac{1}{\left(\frac{798613}{3094} - \frac{134922}{221}t + \frac{729}{2}t^2\right)} \left(18 \left(\frac{20}{9}\right) \log\left(\frac{20}{9}\right) + (12t - 24) \left(\frac{25}{10}\right) \log\left(\frac{25}{10}\right) + (24t - 30) \left(\frac{40}{13}\right) \log\left(\frac{40}{13}\right) + 6 \left(\frac{48}{14}\right) \log\left(\frac{48}{14}\right) + (12t - 12) \left(\frac{64}{16}\right) \log\left(\frac{64}{16}\right) + (24t - 24) \left(\frac{72}{17}\right) \log\left(\frac{72}{17}\right) + (81t^2 - 192t + 111) \left(\frac{81}{18}\right) \log\left(\frac{81}{18}\right)\right)$

$$\begin{aligned}
 13. \mathfrak{NNEN}\mathcal{T}_{ReZ_3} &= \log(118098t^2 - 222792t + 105846) - \\
 &\quad \frac{1}{(118098t^2 - 222792t + 105846)} (18(180)\log(180) + (12t - 24)(250)\log(250) + \\
 &\quad (24t - 30)(520)\log(520) + 6(672)\log(672) + (12t - 12)(1024)\log(1024) + \\
 &\quad (24t - 24)(1224)\log(1224) + (81t^2 - 192t + 111)(1458)\log(1458)) \\
 14. \mathfrak{NNEN}\mathcal{T}_{SK_2} &= \log(6561t^2 - 11736t + 5380) - \\
 &\quad \frac{1}{(6561t^2 - 11736t + 5380)} (18\left(\frac{81}{4}\right)\log\left(\frac{81}{4}\right) + (12t - 24)(25)\log(25) + \\
 &\quad (24t - 30)\left(\frac{169}{4}\right)\log\left(\frac{169}{4}\right) + 6(49)\log(49) + (12t - 12)(64)\log(64) + \\
 &\quad (24t - 24)\left(\frac{289}{4}\right)\log\left(\frac{289}{4}\right) + (81t^2 - 192t + 111)(81)\log(81))
 \end{aligned}$$

9. Comparative Analysis for Superphenalene

This section displays the three-dimensional graphs that reveal the analytical equations for the neighborhood degree sum-based indices and are derived from Theorems 4 and 5. These images will make it easier for the reader to understand how the indices relate to the variables that make up the molecular structure. We also present the outcomes of Theorem 5 as comparison plots, where each neighborhood degree sum-based index is compared against a single structural variable in a single graph. These comparison charts provide a visual representation of the differences between the indices and the chemical structure. The computed numerical values for the indices are shown in Tables 8–11. Figures 8, 9, and 10 display the numerical data to help readers comprehend it.



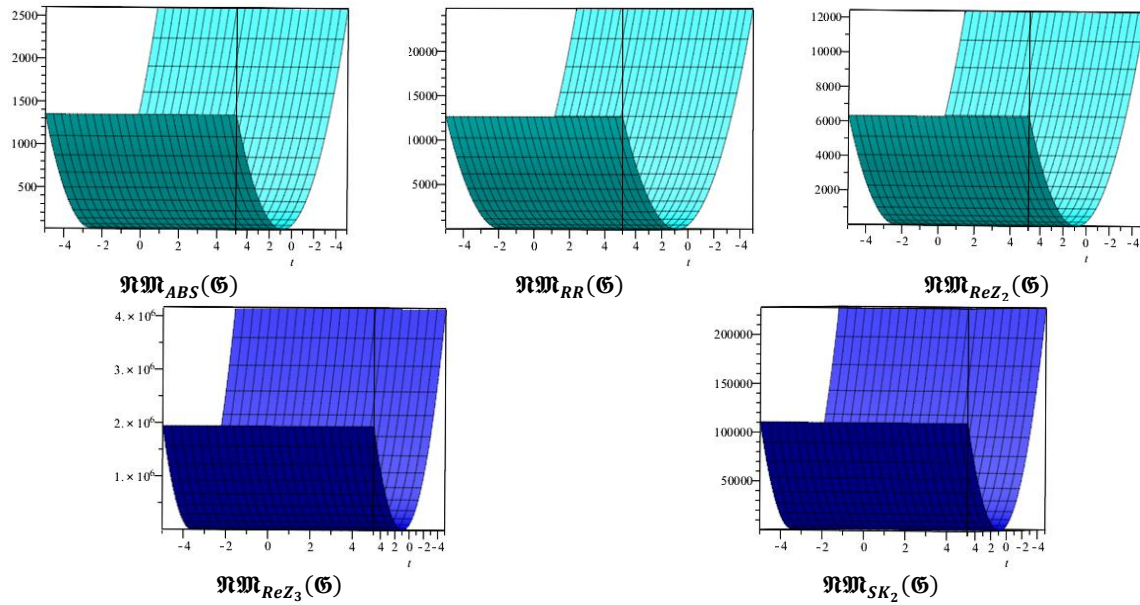


Figure 8. 3D plots for Theorem 4.

Table 8. Comparison Table for Theorem 4.

t	$\mathfrak{NM}_{M_1}$	$\mathfrak{NM}_{M_2}$	$\mathfrak{NM}_{GA}$	$\mathfrak{NM}_{AG_1}$	$\mathfrak{NM}_{RR_\alpha}$	$\mathfrak{NM}_{SDD}$	$\mathfrak{NM}_H$
2	1998	15555	128.3	129.721	18.55	263.78	17.617
3	6864	36564	412.61	415.431	22.781	839.52	51.699
4	14646	70695	858.92	863.141	29.011	1739.2	103.78
5	25344	117948	1467.23	1472.851	37.242	2963	173.86
6	38958	178323	2237.54	2244.561	47.472	4510.7	261.95
7	55488	251820	3169.85	3178.271	59.703	6382.4	368.03
8	74934	338439	4264.16	4273.981	73.933	8578.2	492.11
9	97296	438180	5520.47	5531.691	90.164	11098	634.19
10	122574	551043	6938.78	6951.401	108.39	13942	794.28

Table 9. Comparison Table for Theorem 4.

t	$\mathfrak{NM}_I$	$\mathfrak{NM}_{ABC}$	$\mathfrak{NM}_{ABS}$	$\mathfrak{NM}_{RR}$	$\mathfrak{NM}_{ReZ_2}$	$\mathfrak{NM}_{ReZ_3}$	$\mathfrak{NM}_{SK_2}$
2	1278	62.89	120.717	994.48	495.1	132654	8052
3	2490	186.71	377.372	3422.88	1707.1	500352	29121
4	4430.9	382.53	786.761	7309.28	3648.1	1104246	63312
5	7100.9	650.35	1348.884	12653.68	6318.1	1944336	110625
6	10500	990.17	2063.741	19456.08	9717.1	3020622	171060
7	14628	1401.99	2931.332	27716.48	13845	4333104	244617
8	19485	1885.81	3951.657	37434.88	18702	5881782	331296
9	25071	2441.63	5124.716	48611.28	24288	7666656	431097
10	31386	3069.45	6450.509	61245.68	30603	9687726	544020

Table 10. Comparison Table for Theorem 5.

t	$\mathcal{ENT}_{M_1}$	$\mathcal{ENT}_{M_2}$	$\mathcal{ENT}_{GA}$	$\mathcal{ENT}_{AG_1}$	$\mathcal{ENT}_{RR_\alpha}$	$\mathcal{ENT}_{SDD}$	$\mathcal{ENT}_H$
2	7.5595	9.7568	5.1763	5.0752	54.472	5.1755	2.1308
3	8.9151	10.688	6.3350	6.2791	127.97	6.4923	3.2416
4	9.6996	11.374	7.0624	7.0156	185.31	7.2785	3.9426
5	10.256	11.897	7.5939	7.5575	225.33	7.8412	4.4586
6	10.692	12.315	8.0133	7.9835	253.07	8.2797	4.8676
7	11.047	12.664	8.3598	8.3346	272.78	8.6392	5.2066
8	11.352	12.961	8.6550	8.6330	287.20	8.9437	5.4962
9	11.613	13.220	8.9122	8.8928	298.06	9.2079	5.7491
10	11.842	13.449	9.1400	9.1226	306.47	9.4412	5.9734

Table 11. Comparison Table for Theorem 5.

T	$\mathcal{ENT}_I$	$\mathcal{ENT}_{ABC}$	$\mathcal{ENT}_{ABS}$	$\mathcal{ENT}_{RR}$	$\mathcal{ENT}_{ReZ_2}$	$\mathcal{ENT}_{ReZ_3}$	$\mathcal{ENT}_{SK_2}$
2	4.6669	5.5501	4.8699	6.4773	5.7897	11.464	8.6766
3	6.3793	6.8984	6.0058	7.8372	7.0823	13.031	10.150
4	7.4394	7.6877	6.7379	8.6240	7.8543	13.872	10.966
5	8.1446	8.2483	7.2757	9.1838	8.4085	14.454	11.538
6	8.6612	8.6842	7.6997	9.6194	8.8414	14.901	11.982
7	9.0669	9.0412	8.0499	9.9781	9.1970	15.267	12.343
8	9.4006	9.3436	8.3480	10.278	9.4986	15.575	12.649
9	9.6841	9.6061	8.6075	10.543	9.7618	15.842	12.912
10	9.9295	9.8376	8.8373	10.773	9.9918	16.076	13.147

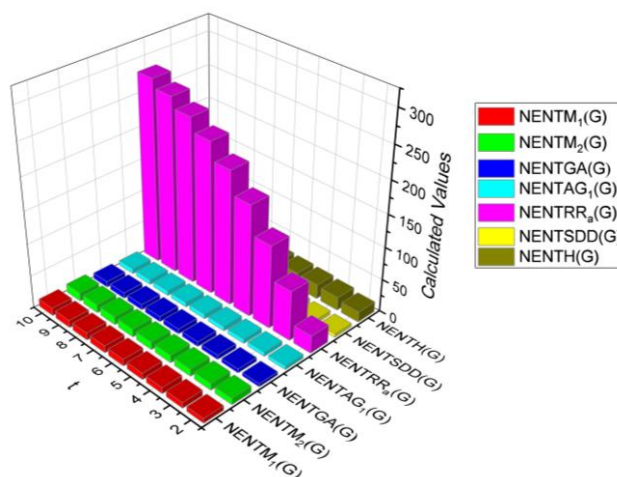


Figure 9. For comparison, Table 10.

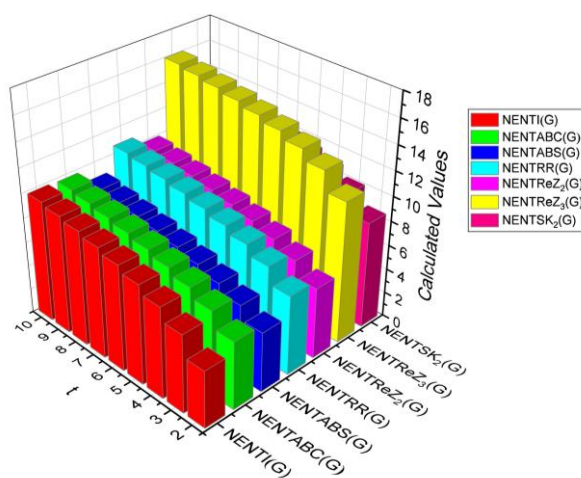


Figure 10. For comparison, Table 11.

10. Conclusion

For the polycyclic aromatic hydrocarbons supertriphenylene and superphenalene, this work provides the first analytical derivation of neighborhood-sum degree-based M-polynomials, related topological indices, and entropy measures. For a wide range of classical and neighborhood-based degree indices, closed-form formulas were found through systematic structural decomposition and vertex–edge partitioning. The accuracy of the obtained equations is confirmed by numerical tables and graphical representations, which also show how the indices rely on molecular size and connectivity. Beyond providing a basis for future QSPR/QSAR modeling, stability estimates, and electronic-property prediction for carbon-

based nanostructures, these findings improve the mathematical characterization of large PAHs. This process can be applied to benzenoid lattices, nanoribbons, and other graphene fragments.

Author Contributions

Conceptualization, V.K. and K.J.; methodology, V.K.; software, K.J.; validation, M.S. and S.K.K.; formal analysis, V.K. and K.J.; investigation, M.S.; resources, S.K.K.; data curation, V.K.; writing—original draft preparation, V.K.; writing—review and editing, M.S. and K.J.; visualization, V.K.; supervision, M.S. and K.J.; project administration, M.S. and K.J. All authors have read and agreed to the published version of the manuscript.

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Not applicable.

Data Availability Statement

The data supporting the findings of this study are available within the article.

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Conflict of Interest

The authors declare that no known competing financial interests or personal relationships influenced the work reported in this study.

Abbreviations

The following abbreviations are used in this manuscript:

Abbreviation	Definition
$\mathcal{V}(\mathcal{G})$ and	Vertex Set of Graph $\mathcal{G}$
$\mathcal{E}(\mathcal{G})$	Edge Set of Graph $\mathcal{G}$
d_v	Degree of Vertex v
$\mathfrak{N}_{\mathcal{G}}(v)$	Neighborhood Degree Sum
$\mathfrak{NM}(\mathcal{G})$	M-polynomial of $\mathcal{G}$
$\mathfrak{NM}_{TI}(\mathcal{G})$	Neighborhood Sum Degree-based Topological Index

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