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On Neighborhood Degree-Based Topological Analysis over Melamine-Based TriCF Structure

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Abstract: Triazine-based covalent organic frameworks (TriCFs) were synthesized using melamine, and cyanuric acid is a brand-new synthetic lubricant, which is thermo-stable and possesses a lamellar structure. This article demonstrates how topological descriptors for the TriCF structure are precisely evaluated using the degree sum of the end vertex neighbors and also some molecular descriptors with multiplicative neighborhood degree sums are evaluated. Furthermore, the neighborhood entropy measures for the outcomes are provided. The results are compared using the graph theoretical method.

Keywords: triazine-based covalent organic frameworks; neighborhood-degree sum-based topological indices; entropy measures; graph-theoretical approach

MSC: 92E10; 05C09

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1. Introduction

Chemical graph theory is the process of performing a thorough analysis to identify the key characteristics or meanings of chemical compounds graphically. It is the area of mathematics that combines graph theory and chemistry. In chemical graph theory, a compound's idiosyncrasies are mathematically described when an image of the mixture from X-ray or electron microscope diffraction is drawn into a plane and illuminated on its symmetry [1]. The chemical graph is a straightforward representation of a picture of a compound in which we suppose that the edges are bonds between atoms and the vertices are atoms. Understanding properties such as molecular structure, the kinetics of molecules, atoms, or electrons, chains or patterns of polymers, crystals and clusters, aromaticity, nuclear magnetic resonance (NMR) analysis, depicting orbitals, and electron behaviors are made possible by chemical graph theory. A few researchers who have introduced graph theory in chemistry are Ante Graovac, Alexandru Balaban, Haruo Hosoya, Iván Gutman, Nenad Trinajstic, and Milan Randić [2–4].

Graph theory connects mathematics and chemistry using a valuable tool called the topological index. A real number associated with a graph and determined by a certain rule is known as the topological index. This number is invariant for isomorphic graphs [5]. It describes the molecular structure's topology. These indices are crucial to the research of quantitative structure–property relationship/quantitative structure–activity relationship (QSPR/QSAR) since they may be used to predict various physiochemical characteristics and bioactivity, which aids in the development of new drugs. Its use in other sectors, including nanoscience and biotechnology, is equally impressive [6]. Topological indices have been used to numerically quantify various physical and chemical properties of various chemical and biological molecules, including the boiling point, anti-leishmanial action, acute toxicity, radical scavenging activity, and many more. Throughout the world, researchers are interested in this. Over the years, several vertex-degree-based topological indices have been developed [5,7].

Three nitrogen atoms replace the carbons in the triazines' six-membered planar ring, which is similar to that of benzene. The three isomers of triazine are distinguished by the positions of the nitrogen atoms [8]. The triazine structures of melamine and cyanuric chloride are two well-known examples. Melamine is a white, odorless, crystalline, nontoxic, hetero-aromatic compound utilized as a raw material in many daily products that must adhere to rigid standards for toughness and wear resistance. The synthesis of insecticides, brighteners, and reactive dyes have all benefited from the versatility and multifunctionality of cyanuric chloride (2,4,6-trichloro-1,3,5-triazine), a versatile reagent. Covalent bonding creates triazine-based covalent organic polymers (COPs), a developing subclass of porous organic framework materials. Ping Wen et al. explained the synthesis of triazine-based covalent organic frameworks (see Figure 1) utilizing melamine and cyanuric chloride [8]. The as-prepared covalent organic frameworks are referred to as TriCFs. They are exceptionally thermo-stable and possess a lamellar structure. This comprises a brand-new synthetic lubricant. The degree-based indices of this structure were studied by [9]. Currently, research on the computation of the TriCF neighborhood topological indices is needed in the literature. Future designed and produced triazine-based covalent organic frameworks could benefit from the findings of this study [8].

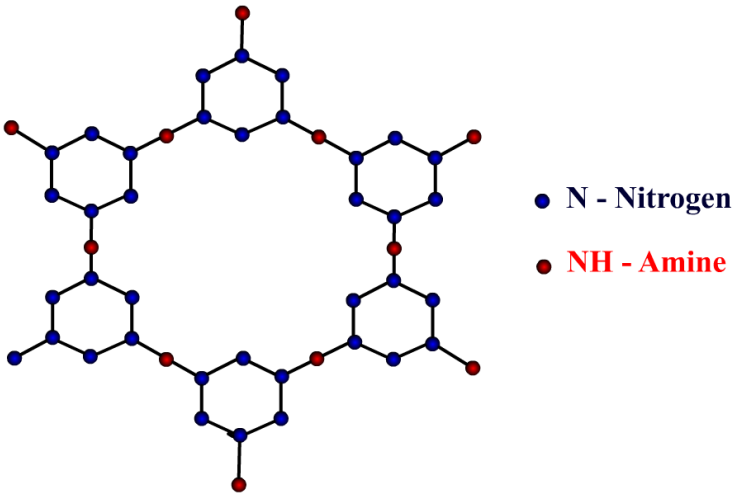


Figure 1. TriCFs' structure.

"The entropy of a probability distribution is regarded as a measure of the unpredictability of information content or a measure of the uncertainty of a system", Shannon famously wrote in his article from 1948, which established the term "entropy" [10]. Entropy later started to be applied to chemical networks and graphs. It was created for analyzing the structural data of chemical networks and graphs. There are intrinsic and extrinsic metrics for graph entropy, which correlates probability distributions with a graph's elements (vertices, edges, etc.). To estimate a network's structural information content, Shannon's entropy calculations have been applied [11]. This approach has been used to visualize live systems using graphs. Entropy measurements for graphs have also been widely used in structural chemistry, computer science, and biology [10]. Entropy network measures have a variety of uses, including quantitative structure characterization in structural chemistry and the investigation of biological or chemical aspects of molecular graphs using software [12–14].

2. Preliminaries and Mathematical Terminologies

In this study, we take γ as a connected graph. The letters $\mathscr{P}$ and $\mathscr{Q}$ stand for the vertex set (atoms) and edge set (bonds between atoms). Furthermore, $s_\gamma(u)$ stands for the total number of degrees of all vertices adjacent to u. Topological indices, which are graph-based descriptors, are often used to forecast the characteristics of chemical networks and systems. They are functions defined from a graph γ to a collection of real numbers $\mathbb{R}$. There are

primarily two kinds of topological indices. The first is a topological index based on degrees, while the second is based on distance. The motivation for using degree-based indices, also known as connectivity-based indices, comes from several research works showing that they are reliable for linking the physicochemical properties of various molecules.

Randić created the first legitimate degree-based index, which has now gained widespread acceptance as the Randić index [15]. Later, several degree-based metrics such as the Zagreb index, the atom bond connectivity index, the enhanced Zagreb index, and the geometric arithmetic index were created. Due to their excellent correlation capacity, these indices have drawn much attention [3]. Randić indices are often used to simulate molecules' physical and chemical characteristics, while Zagreb indices were developed to explore molecular complexity. A modified version of the Randić index called the "atom bond connectivity index" has shown a good correlation with the thermodynamic properties of alkanes [5]. Refer to [5] and the references there in for a thorough overview of the different degree-based topological indices.

Later, a significant number of researchers developed unique modifications to these indices that consider the neighboring degree sum for each vertex rather than the degree [16–18]. Let s_u represent the degree sum of the nearby vertices of the vertex u to define them broadly. The generic equation for bond additive and multiplicative variants of degree-sum-based indices may be written as

$$TI_s(\gamma) = \sum_{uv \in E(\gamma)} \phi(s_u, s_v) \tag{1}$$

and

$$TI_s^*(\gamma) = \prod_{uv \in E(\gamma)} \phi(s_u, s_v) \tag{2}$$

We used the edge partition approach, where the total number of edges for each structure is split into different groups according to the degrees of the end vertices of edges, to generate the degree-based indices. Similar to this, edges are divided into sections to determine degree-sum-based indices using the neighborhood degree sums of the end vertices of edges. This research employed edge partition approaches to derive multiplicative neighborhood degree sum topological indices and neighborhood degree-sum-based entropy measurements for the TriCF structure. We used Shannon's model to calculate the probabilistic entropy because it is the most widely used method [10–12]. The entropy measured using that topological index X is given by

$$E_X(\gamma) = \log(X(\gamma)) - \frac{1}{X(\gamma)}\Big(\sum_{uv \in E(\gamma)} f(e) log(f(e))\Big). \tag{3}$$

where $f(e)$ is the edge partition.

For vertices u and v, s_u and s_v denote the neighborhood degree sum of u and v. We now show various neighborhood degree-sum-based topological descriptors and neighborhood multiplicative degree-sum-based topological descriptors in Table 1 [19,20] and Table 2 [6,16–18,21–33], respectively.

Table 1. Neighborhood degree-sum-based topological indices.

Neighborhood First Zagreb Index	$NM_1(G) = \sum_{uv \in E(G)} [s_u + s_v]$
Neighborhood Second Zagreb Index	$NM_2(G) = \sum_{uv \in E(G)} [s_u \times s_v]$
Neighborhood Reduced Second Zagreb Index	$NRM_2(G) = \sum_{uv \in E(G)} [(s_u - 1)(s_v - 1)]$
Neighborhood Hyper Zagreb Index	$NHM(G) = \sum_{uv \in E(G)} [s_u + s_v]^2$
Neighborhood Augmented Zagreb Index	$NAZ(G) = \sum_{uv \in E(G)} [\frac{s_u \times s_v}{s_u + s_v - 2}]^3$

Table 1. *Cont.*

Neighborhood Randić Index	$NR(G) = \sum_{uv \in E(G)} [\frac{1}{\sqrt{s_u s_v}}]$
Neighborhood Reciprocal Randić Index	$NRR(G) = \sum_{uv \in E(G)} [\sqrt{s_u s_v}]$
Neighborhood Reduced Reciprocal Randić Index	$NRRR(G) = \sum_{uv \in E(G)} [\sqrt{(s_u - 1)(s_v - 1)}]$
Neighborhood Harmonic Index	$NH(G) = \sum_{uv \in E(G)} [\frac{2}{s_u + s_v}]$
Neighborhood Sum Connectivity Index	$NSC(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{s_u + s_v}}$
Neighborhood Geometric Arithmetic Index	$NGA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{s_u s_v}}{s_u + s_v}$
Neighborhood Inverse Sum Index	$NIS(G) = \sum_{uv \in E(G)} \frac{s_u s_v}{s_u + s_v}$
Neighborhood Forgotten index	$NF(G) = \sum_{uv \in E(G)} {s_u}^2 + {s_v}^2$
Neighborhood Symmetric Division Index	$NSDI(G) = \sum_{uv \in E(G)} \frac{{s_u}^2 + {s_v}^2}{s_u s_v}$
Neighborhood Atom Bond Connectivity Index	$NABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{s_u + s_v - 2}{s_u s_v}}$

Table 2. Multiplicative neighborhood degree-sum-based topological indices.

Multiplicative Neighborhood First Zagreb Index	$MNM_1(G) = \prod_{uv \in E(G)} [s_u + s_v]$
Multiplicative Neighborhood Second Zagreb Index	$MNM_2(G) = \prod_{uv \in E(G)} [s_u \times s_v]$
Multiplicative Neighborhood Reduced Second Zagreb Index	$MNRM_2(G) = \prod_{uv \in E(G)} [(s_u - 1)(s_v - 1)]$
Multiplicative Neighborhood Hyper Zagreb Index	$MNHM(G) = \prod_{uv \in E(G)} [s_u + s_v]^2$
Multiplicative Neighborhood Augmented Zagreb Index	$MNAZ(G) = \prod_{uv \in E(G)} [\frac{s_u \times s_v}{s_u + s_v - 2}]^3$
Multiplicative Neighborhood Randić Index	$MNR(G) = \prod_{uv \in E(G)} [\frac{1}{\sqrt{s_u s_v}}]$
Multiplicative Neighborhood Reciprocal Randić Index	$MNRR(G) = \prod_{uv \in E(G)} [\sqrt{s_u s_v}]$
Multiplicative Neighborhood Reduced Reciprocal Randić Index	$MNRRR(G) = \prod_{uv \in E(G)} [\sqrt{(s_u - 1)(s_v - 1)}]$
Multiplicative Neighborhood Harmonic Index	$MNH(G) = \prod_{uv \in E(G)} [\frac{2}{s_u + s_v}]$
Multiplicative Neighborhood Sum Connectivity Index	$MNSC(G) = \prod_{uv \in E(G)} \frac{1}{\sqrt{s_u + s_v}}$
Multiplicative Neighborhood Geometric Arithmetic Index	$MNGA(G) = \prod_{uv \in E(G)} \frac{2\sqrt{s_u s_v}}{s_u + s_v}$
Multiplicative Neighborhood Inverse Sum Index	$MNIS(G) = \prod_{uv \in E(G)} \frac{s_u s_v}{s_u + s_v}$
Multiplicative Neighborhood Forgotten index	$MNF(G) = \prod_{uv \in E(G)} {s_u}^2 + {s_v}^2$
Multiplicative Neighborhood Symmetric Division Index	$MNSDI(G) = \prod_{uv \in E(G)} \frac{{s_u}^2 + {s_v}^2}{s_u s_v}$
Multiplicative Neighborhood Atom Bond Connectivity Index	$MNABC(G) = \prod_{uv \in E(G)} \sqrt{\frac{s_u + s_v - 2}{s_u s_v}}$

3. Research Aim and Methodology

Chemical graph theory is a concept used in the mathematical chemistry field of topology. It gained popularity as its proponents presented several graph theory applications for the mathematical modeling of chemical characteristics [34,35]. Chemists have established through actual experimental data that a compound's physicochemical properties are closely related to its molecular structure. Later, additional graph-theoretical techniques were developed to describe various chemical compound properties. The idea of topological indices, specific network invariants, is an essential tool. In addition to the topological index, information entropy is a necessary tool for assessing the properties of chemical compounds. Due to its applicability, the notion, which was first applied to the communication system, has recently received respect in various scientific and technological sectors [10,12]. In chemistry, much research has been performed on the correspondence between the traditional concept of thermodynamics and the statistical mechanic's definition of entropy. The concept of information entropy may be considered a replacement for thermodynamic entropy due to its relationship to the Gibbs entropy formula employed in statistical mechanics [33,36]. They are thus primarily used in chemistry to characterize compounds' complexity, disorder, and other properties, such as phase transition energy. The relationship between information entropy and chemical properties, such as the variation in molecule stability caused by various arrangements of essential components, has been studied recently [13]. Shannon first introduced the concept of information entropy in communication networks, and the statement was purely based on terms used in that field. Later, it was changed to use it in other scientific domains [11].

In this article, we explore the multiplicative neighborhood-degree sum-based indices and neighborhood-degree sum-based indices of the TriCF structure. In addition, we calculate the entropies of these structures and also determine the numerical values, which aid in the investigation of the physiochemical characteristics of the TriCF structure.

This study's computations use graph theoretical technologies, precisely the edge partition method and analytical techniques. Chem Draw Ultra describes the TriCFs' molecular structures, and Origin displays the numerical outcomes.

4. Main Results

In this section, we present the key findings of the study. In this work, based on the growth of TriCFs, the authors categorized it into three kinds. In particular, γ_1, γ_2, and γ_3 are linear chain TriCF structures, parallelogram TriCF structures, and hexagonal TriCF structures, respectively. The schematic of the triazine-based covalent organic framework synthesis can be formed into any structure such as a linear chain, parallelogram, hexagonal, etc. Figures 2–4 show the 2D structure of a linear chain, parallelogram and hexagonal TriCF structures, respectively. Figure 5 shows the unit cell of the TriCF structure. In the linear chain TriCF structure, the unit cell is repeated r-times linearly (r columns). Similarly, in the parallelogram TriCF structure, the unit cells are arranged in the shape of a parallelogram structure. In hexagonal TriCF structures, the unit cells are placed in a hexagonal structure. It is easy to understand the growth from Figures 3 and 4. From this, we can find the edge partition, which is given in Table 3.

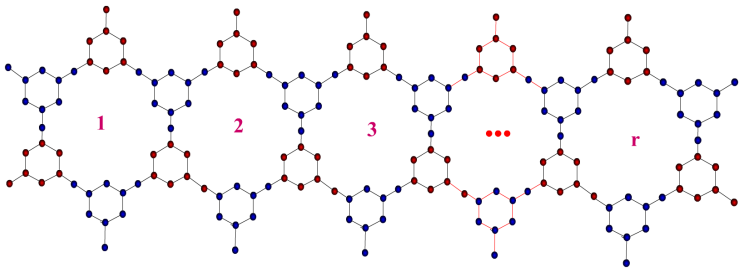


Figure 2. Linear chain TriCF structure.

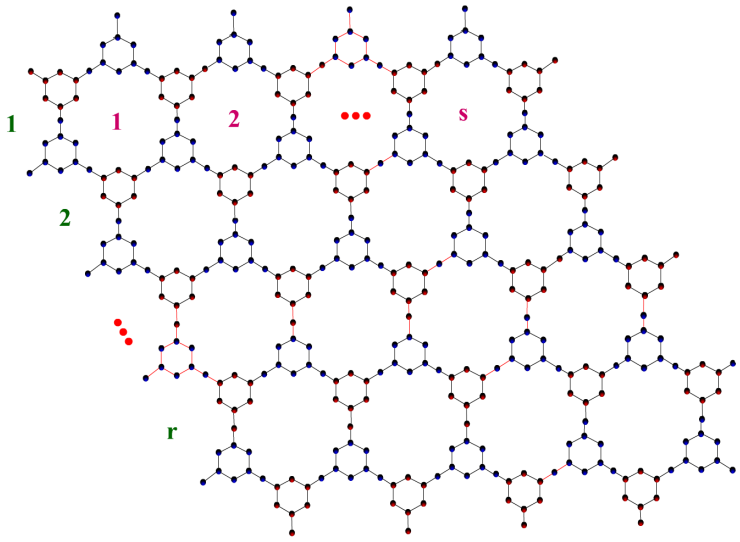


Figure 3. Parallelogram TriCF structure.

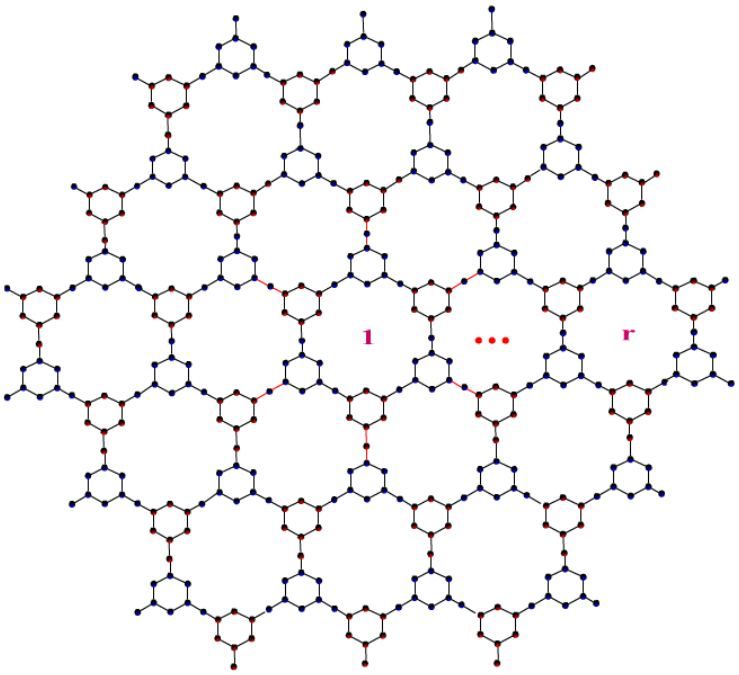


Figure 4. Hexagonal TriCF structure.

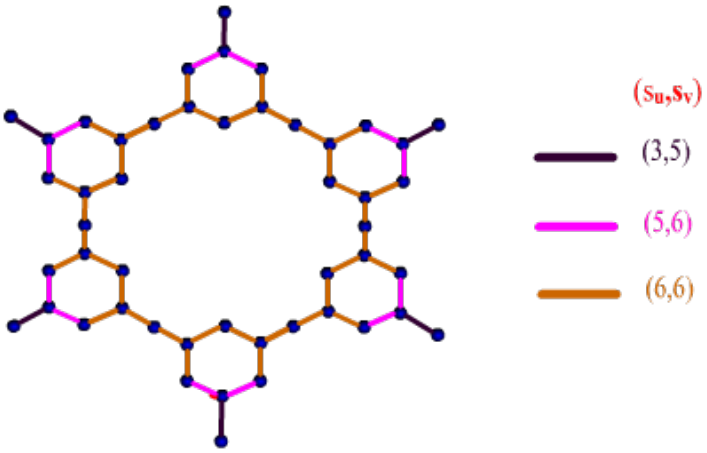


Figure 5. Neighborhood degree sum edge partition of the unit cell of the TriCF structure.

Table 3 below illustrates the total number of edges ($\mathscr{Q}$) and vertices ($\mathscr{P}$) and how the edges are partitioned in each structure.

Table 3. Edge partition of γ.

γ	$(3,5)$	$(5,6)$	$(6,6)$	$\mathscr{Q}$	$\mathscr{P}$
γ_1	$2r+4$	$4r+8$	$30r+6$	$36r+18$	$36r+15$
γ_2	$2(r+s+1)$	$4(r+s+1)$	$(18s+12)r+12s-6$	$(18s+18)r+18s$	$(13s+20)r+18s+3$
γ_3	$6r$	$12r$	$54r^2-18r$	$54r^2$	$45r^2+3r$

4.1. Neighborhood-Degree Sum-Based Topological Indices of TriCF Structure

Theorem 1. *Let γ_1 be the Linear chain TriCF structure with dimension r. Then:*

1. $NR(\gamma_1) = \frac{2(1+\sqrt{2})(r+2)\sqrt{15}}{15} + 5r + 1.$
2. $NRR(\gamma_1) = ((4r+8)\sqrt{2} + 2r + 4)\sqrt{15} + 180r + 36.$
3. $NRRR(\gamma_1) = (4r+8)\sqrt{2} + (8r+16)\sqrt{5} + 150r + 30.$
4. $NM_1(\gamma_1) = 420r + 192.$
5. $NM_2(\gamma_1) = 1230r + 516.$
6. $NRM_2(\gamma_1) = 846r + 342.$
7. $NHM(\gamma_1) = 4932r + 2088.$
8. $NAZ(\gamma_1) = \frac{4263511r}{2700} + \frac{4311443}{6750}.$
9. $NH(\gamma_1) = \frac{137r}{22} + \frac{38}{11}.$
10. $NSC(\gamma_1) = \frac{(110r+22)\sqrt{3}}{22} + \frac{(r+2)(\sqrt{2}+\frac{8\sqrt{11}}{11})}{2}.$
11. $NGA(\gamma_1) = \frac{8(\sqrt{2}+\frac{11}{16})(r+2)\sqrt{15}}{11} + 30r + 6.$
12. $NIS(\gamma_1) = \frac{4605r}{44} + \frac{1041}{22}.$
13. $NSDI(\gamma_1) = \frac{218r}{3} + \frac{112}{3}.$
14. $NF(\gamma_1) = 2472r + 1056.$
15. $NABC(\gamma_1) = \frac{(3\sqrt{6}+6)\sqrt{5r+10}}{15} + \frac{\sqrt{75r+15}}{3}.$

Proof. Let γ_1 be a linear chain TriCF structure with $\mathscr{P}$ and $\mathscr{Q}$ (see Table 3). We performed edge partitions of γ_1 based on the neighborhood vertex degree sum. The following results were obtained by applying those edge partitions in the definitions of neighborhood degree sum-based topological indices (Table 1).

To provide the proofs, the neighborhood-degree sum-based topological indices of each TriCF linear chemical network would be too long to furnish in this paper. Hence, using the procedure mentioned below and Table 1, it is simple to construct any neighborhood-degree sum-based expression concerning each topological index.

The neighborhood-degree sum-based indices of the first Zagreb for a linear TriCF molecular graph is

$NM_1(\gamma_1) = (3+5)(2r+4) + (5+6)(4r+8) + (6+6)(30r+6)$
$= (8)(2r+4) + (11)(4r+8) + (12)(30r+6)$
$= 16r + 32 + 44r + 88 + 360r + 72$
$= 420r + 192.$ □

Theorem 2. *Let γ_2 be the parallelogram TriCF structure with dimension r and s. Then, the neighborhood-degree sum-based topological indices are:*

1. $NR(\gamma_2) = \frac{2(1+\sqrt{2})(r+s+1)\sqrt{15}}{15} + \frac{(45s+30)r}{15} + 2s - 1.$
2. $NRR(\gamma_2) = 4(r+s+1)(\sqrt{2}+\frac{1}{2})\sqrt{15} + (108s+72)r + 72s - 36.$
3. $NRRR(\gamma_2) = (4r+4s+4)\sqrt{2} + (8r+8s+8)\sqrt{5} + (90s+60)r + 60s - 30.$
4. $NM_1(\gamma_2) = (216s+204)r + 204s - 12.$
5. $NM_2(\gamma_2) = (648s+582)r + 582s - 66.$
6. $NRM_2(\gamma_2) = (450s+396)r + 396s - 54.$
7. $NHM(\gamma_2) = (2592s+2340)r + 2340s - 252.$
8. $NAZ(\gamma_2) = \frac{(11337408s+9980147)r}{13500} + \frac{9980147s}{13500} - \frac{1357261}{13500}.$
9. $NH(\gamma_2) = \frac{(66r+71)s}{22} + \frac{71r}{22} + \frac{5}{22}.$
10. $NSC(\gamma_2) = \frac{((66s+44)r+44s-22)\sqrt{3}}{22} + \frac{(r+s+1)(\sqrt{2}+\frac{8\sqrt{11}}{11})}{2}.$
11. $NGA(\gamma_2) = \frac{8(r+s+1)(\sqrt{2}+\frac{11}{16})\sqrt{15}}{11} + \frac{(396s+264)r}{22} + 12s - 6.$
12. $NIS(\gamma_2) = \frac{(2376r+2229)s}{44} + \frac{2229r}{44} - \frac{147}{44}.$
13. $NSDI(\gamma_2) = \frac{(216r+182)s}{3} + \frac{182r}{3} - \frac{34}{3}.$
14. $NF(\gamma_2) = (1296s+1176)r + 1176s - 120.$
15. $NABC(\gamma_2) = \frac{\sqrt{(45s+30)r+30s-15}}{3} + \frac{(3\sqrt{6}+6)\sqrt{5r+5s+5}}{15}.$

Proof. Let γ_2 be a parallelogram TriCF structure with $\mathscr{P}$ and $\mathscr{Q}$ be taken from Table 3. We performed edge partitions of γ_2 based on the neighborhood vertex degree sum, and the following results were obtained by applying those edge partitions in the definitions of neighborhood-degree sum-based topological indices (Table 1). To put forward the given proofs, the neighborhood-degree sum-based topological indices of each TriCF parallelogram chemical network would run into many pages. Hence, using the procedure mentioned below and Table 1, it is easy to construct any neighborhood-degree sum-based expression with regard to each topological index.

The neighborhood-degree sum-based indices of the second Zagreb for a parallelogram TriCF molecular graph is

$NM_2(\gamma_2) = (3\times 5)2(r+s+1) + (5\times 6)4(r+s+1) + (6\times 6)((18s+12)r + 12s - 6)$
$= 150r + 582s - 66 + 36(18s+12)r$
$= (648s+582)r + 582s - 66.$ □

Theorem 3. *Let γ_3 be the hexagonal TriCF structure with dimension r. Then:*

1. $NR(\gamma_3) = \frac{r(2\sqrt{15}\sqrt{2} + 2\sqrt{15} + 45r - 15)}{5}.$
2. $NRR(\gamma_3) = 6r(2\sqrt{15}\sqrt{2} + \sqrt{15} + 54r - 18).$
3. $NRRR(\gamma_3) = (4r+8)\sqrt{2} + (8r+16)\sqrt{5} + 150r + 30.$
4. $NM_1(\gamma_3) = 648r^2 - 36r.$
5. $NM_2(\gamma_3) = 1944r^2 - 198r.$
6. $NRM_2(\gamma_3) = 1350r^2 - 162r.$
7. $NHM(\gamma_3) = 7776r^2 - 756r.$
8. $NAZ(\gamma_3) = \frac{314928}{125}r^2 - \frac{1357261}{4500}r.$
9. $NH(\gamma_3) = \frac{15}{22}r + 9r^2.$
10. $NSC(\gamma_3) = \frac{3r(66\sqrt{3}r + 11\sqrt{2} + 8\sqrt{11} - 22\sqrt{3})}{22}.$

11. $NGA(\gamma_3) = \dfrac{3r(16\sqrt{15}\sqrt{2} + 11\sqrt{15} + 396r - 132)}{22}$.
12. $NIS(\gamma_3) = 162r^2 - \frac{441}{44}r$.
13. $NSDI(\gamma_3) = 108r^2 + 2r$.
14. $NF(\gamma_3) = 3888r^2 - 360r$.
15. $NABC(\gamma_3) = \left(\left(\dfrac{3\sqrt{2}}{5} + \dfrac{2\sqrt{3}}{5}\right)\sqrt{r} + \sqrt{3r^2 - r}\right)\sqrt{5}$.

Proof. Let γ_3 be a hexagonal TriCF structure $\mathscr{P}$ and $\mathscr{Q}$ given in Table 3. We performed edge partitions of γ_3 based on the neighborhood vertex degree sum, and the following results were obtained by applying those edge partitions in the definitions of neighborhood-degree sum-based topological indices (Table 1). To provide the proof, the neighborhood-degree sum-based topological indices of each TriCF hexagonal chemical network would be too long. Using the procedure mentioned below and Table 1, it is simple to construct any neighborhood-degree sum-based expression with regard to each topological index.

The neighborhood-degree sum-based indices of the forgotten indices for a hexagonal TriCF molecular graph is $NF(\gamma_3) = (9+25)(6r) + (25+36)(12r) + (36+36)(54r^2 - 18r)$
$= (34)(6r) + (61)(12r) + (72)(54r^2 - 18r)$
$= 3888r^2 - 360r$. □

4.2. Multiplicative Neighborhood-Degree Sum-Based Topological Indices of TriCF Structure

Theorem 4. *Let γ_1 be the linear chain TriCF structure with dimension r. Then, the neighborhood-degree sum-based multiplicative indices are:*

1. $MNR(\gamma_1) = \dfrac{1}{6^{30r+6}15^{r+2}30^{2r+4}}$.
2. $MNRR(\gamma_1) = 2^{32r+10}3^{33r+12}5^{3r+6}$.
3. $MNRRR(\gamma_1) = 2^{7r+14}5^{32r+10}$.
4. $MNM_1(\gamma_1) = 8^{2r+4}11^{4r+8}12^{30r+6}$.
5. $MNM_2(\gamma_1) = 15^{2r+4}30^{4r+8}36^{30r+6}$.
6. $MNRM_2(\gamma_1) = 8^{2r+4}20^{4r+8}25^{30r+6}$.
7. $MNHM(\gamma_1) = 64^{2r+4}121^{4r+8}144^{30r+6}$.
8. $MNAZ(\gamma_1) = 2^{96r+30}3^{168r+12}5^{18-72r}$.
9. $MNH(\gamma_1) = \dfrac{1}{6^{30r+6}11^{4r+8}}$.
10. $MNSC(\gamma_1) = \dfrac{1}{1619177472\,2^{33r}3^{15r}11^{2r}}$.
11. $MNGA(\gamma_1) = \dfrac{15^{3r+6}}{2^{34r+11}11^{4r+8}}$.
12. $MNIS(\gamma_1) = \left(\dfrac{15}{8}\right)^{2r+4}\left(\dfrac{30}{11}\right)^{4r+8}3^{30r+6}$.
13. $MNSDI(\gamma_1) = \left(\dfrac{34}{15}\right)^{2r+4}\left(\dfrac{61}{30}\right)^{4r+8}2^{30r+6}$.
14. $MNF(\gamma_1) = 34^{2r+4}61^{4r+8}72^{30r+6}$.
15. $MNABC(\gamma_1) = \dfrac{5^{12r}}{36000\,2^{16r}3^{28r}}$.

Proof. Let γ_1 be a linear chain TriCF structure with vertices $\mathscr{P}$ and $\mathscr{Q}$ (see Table 3). We performed edge partitions of γ_1 based on the neighborhood vertex degree sum, and the following results were obtained by applying those edge partitions in the definitions of multiplicative neighborhood-degree sum-based topological indices (Table 2). To provide the proofs, the multiplicative neighborhood-degree sum-based topological indices of each TriCF linear chemical network would be too long. By using the below-mentioned procedure and Table 2, it is simple to construct any multiplicative neighborhood-degree sum-based expression with regard to each topological index.

The multiplicative neighborhood-degree sum-based indices of the Randić indices for a linear TriCF molecular graph is $NMR(\gamma_1) = (9+25)^{(2*r+4)}(25+36)^{(4*r+8)}(36+36)^{(30*r+6)} = 34^{2r+4}61^{4r+8}72^{30r+6}$. □

Theorem 5. *Let γ_2 be the parallelogram TriCF structure with dimension r and s. Then, the multiplicative neighborhood-degree sum-based topological indices are:*

1. $MNM_1(\gamma_2) = 8^{2r+2s+2}11^{4r+4s+4}12^{(18s+12)r+12s-6}$.
2. $MNM_2(\gamma_2) = 15^{2r+2s+2}30^{4r+4s+4}36^{(18s+12)r+12s-6}$.
3. $MNRM_2(\gamma_2) = 2^{14r+14s+14}5^{36rs+28r+28s-8}$.
4. $MNHM(\gamma_2) = 64^{2r+2s+2}121^{4r+4s+4}144^{(18s+12)r+12s-6}$.
5. $MNAZ(\gamma_2) = \left(\frac{125}{8}\right)^{2r+2s+2}\left(\frac{1000}{27}\right)^{4r+4s+4}\left(\frac{5832}{125}\right)^{(18s+12)r+12s-6}$.
6. $MNR(\gamma_2) = \left(\frac{\sqrt{15}}{15}\right)^{2r+2s+2}\left(\frac{\sqrt{30}}{30}\right)^{4r+4s+4}\left(\frac{1}{6}\right)^{(18s+12)r+12s-6}$.
7. $MNRR(\gamma_2) = \left(\sqrt{15}\right)^{2r+2s+2}\left(\sqrt{30}\right)^{4r+4s+4}6^{(18s+12)r+12s-6}$.
8. $MNRRR(\gamma_2) = 2^{7r+7s+7}5^{18rs+14r+14s-4}$.
9. $MNH(\gamma_2) = \left(\frac{1}{4}\right)^{2r+2s+2}\left(\frac{2}{11}\right)^{4r+4s+4}\left(\frac{1}{6}\right)^{(18s+12)r+12s-6}$.
10. $MNSC(\gamma_2) = \left(\frac{\sqrt{2}}{4}\right)^{2r+2s+2}\left(\frac{\sqrt{11}}{11}\right)^{4r+4s+4}\left(\frac{\sqrt{3}}{6}\right)^{(18s+12)r+12s-6}$.
11. $MNGA(\gamma_2) = 8\left(\frac{\sqrt{15}}{8}\right)^{2r+2s+2}\left(\frac{\sqrt{30}}{11}\right)^{4r+4s+4}\left(\frac{1}{2}\right)^{(18s+12)r+12s-6}$.
12. $MNIS(\gamma_2) = \left(\frac{15}{8}\right)^{2r+2s+2}\left(\frac{30}{11}\right)^{4r+4s+4}3^{(18s+12)r+12s-6}$.
13. $MNSDI(\gamma_2) = \left(\frac{34}{15}\right)^{2r+2s+2}\left(\frac{61}{30}\right)^{4r+4s+4}2^{(18s+12)r+12s-6}$.
14. $MNF(\gamma_2) = 34^{2r+2s+2}61^{4r+4s+4}72^{(18s+12)r+12s-6}$.
15. $MNABC(\gamma_2) = \left(\frac{\sqrt{10}}{5}\right)^{2r+2s+2}\left(\frac{\sqrt{30}}{10}\right)^{4r+4s+4}\left(\frac{\sqrt{10}}{6}\right)^{(18s+12)r+12s-6}$.

Proof. Let γ_2 be a parallelogram TriCF structure with vertex and edge set $\mathscr{P}$ and $\mathscr{Q}$, respectively (Table 3). We performed edge partitions of γ_2 based on the neighborhood vertex degree sum (Table 3), and the following results were obtained by applying those edge partitions in the definitions of multiplicative neighborhood-degree sum-based topological indices (Table 2).

To provide the proofs, the multiplicative neighborhood-degree sum-based topological indices of each TriCF parallelogram chemical network would be too long. By using the below-mentioned procedure and Table 2, it is simple to construct any multiplicative neighborhood-degree sum-based expression with regard to each topological index.

Multiplicative neighborhood-degree-based indices of the first Zagreb for a parallelogram TriCF molecular graph is $MNM1(\gamma_2) = (3+5)^{(2r+2s+2)}(5+6)^{(4r+4s+4)}(6+6)^{((18*s+12)r+12s-6)} = 8^{(2r+2s+2)}11^{(4r+4s+4)}12^{((18s+12)r+12s-6)}$. □

Theorem 6. *Let γ_3 be the hexagonal TriCF structure with dimension r. Then, the multiplicative neighborhood-degree sum-based topological indices are:*

1. $MNM_1(\gamma_3) = 8^{6r}11^{12r}12^{54r^2-18r}$.
2. $MNM_2(\gamma_3) = 15^{6r}30^{12r}36^{54r^2-18r}$.
3. $MNRM_2(\gamma_3) = 8^{6r}20^{12r}25^{54r^2-18r}$.
4. $MNHM(\gamma_3) = 64^{6r}121^{12r}144^{54r^2-18r}$.

5. $MNAZ(\gamma_3) = \left(\frac{125}{8}\right)^{6r}\left(\frac{1000}{27}\right)^{12r}\left(\frac{5832}{125}\right)^{54r^2-18r}$.
6. $MNR(\gamma_3) = \left(\frac{\sqrt{15}}{15}\right)^{6r}\left(\frac{\sqrt{30}}{30}\right)^{12r}\left(\frac{1}{6}\right)^{54r^2-18r}$.
7. $MNRR(\gamma_3) = \left(\sqrt{15}\right)^{6r}\left(\sqrt{30}\right)^{12r}6^{54r^2-18r}$.
8. $MNRRR(\gamma_3) = \left(2\sqrt{2}\right)^{6r}\left(2\sqrt{5}\right)^{12r}5^{54r^2-18r}$.
9. $MNH(\gamma_3) = \left(\frac{1}{4}\right)^{6r}\left(\frac{2}{11}\right)^{12r}\left(\frac{1}{6}\right)^{54r^2-18r}$.
10. $MNSC(\gamma_3) = \left(\frac{\sqrt{2}}{4}\right)^{6r}\left(\frac{\sqrt{11}}{11}\right)^{12r}\left(\frac{\sqrt{3}}{6}\right)^{54r^2-18r}$.
11. $MNGA(\gamma_3) = 8\left(\frac{\sqrt{15}}{8}\right)^{6r}\left(\frac{\sqrt{30}}{11}\right)^{12r}\left(\frac{1}{2}\right)^{54r^2-18r}$.
12. $MNIS(\gamma_3) = \left(\frac{15}{8}\right)^{6r}\left(\frac{30}{11}\right)^{12r}3^{54r^2-18r}$.
13. $MNSDI(\gamma_3) = \left(\frac{34}{15}\right)^{6r}\left(\frac{61}{30}\right)^{12r}2^{54r^2-18r}$.
14. $MNF(\gamma_3) = 34^{6r}61^{12r}72^{30r+6}$.
15. $MNABC(\gamma_3) = \left(\frac{\sqrt{10}}{5}\right)^{6r}\left(\frac{\sqrt{30}}{10}\right)^{12r}\left(\frac{\sqrt{10}}{6}\right)^{54r^2-18r}$.

Proof. Let γ_3 be a hexagonal TriCF structure. The cardinality of vertices $\mathscr{P}$ and edges $\mathscr{Q}$ is given in Table 3. We performed edge partitions of γ_3 based on the neighborhood vertex degree sum, and the following results were obtained by applying those edge partitions in the definitions of multiplicative neighborhood-degree sum-based topological indices (Table 2). To provide the proofs, the multiplicative neighborhood-degree sum-based topological indices of each TriCF hexagonal chemical network would be too long. By using the below-mentioned procedure and Table 2, it is simple to construct any multiplicative neighborhood-degree sum-based expression with regard to each topological index.

The multiplicative neighborhood-degree sum-based indices of the first Zagreb for a hexagonal TriCF molecular graph is $MNM_1(\gamma_3) = (3+5)^{(6r)}(5+6)^{(12r)}(6+6)^{(54r^{(2)}-18r)} = 8^{6r}11^{12r}12^{54r^2-18r}$.

□

4.3. Neighborhood-Degree Sum-Based Entropy Measures

This section discusses constructing the probability function using neighborhood-degree sum-based topological indices to compute the entropy values using Shannon's approach. The calculation procedure is illustrated below by using Equation (3) to calculate the entropy value of the first Zagreb index for the TriCF structure. Furthermore, Figure 6 is the 3D plot of the entropy of the first Zagreb index.

The first Zagreb entropy for the linear chain TriCF molecular graph is

$$ENM_1(\gamma_1) = \log(420r+192) - \frac{(2r+4)(3+5)\log(3+5) + (4r+8)(5+6)\log(5+6) + (30r+6)(6+6)\log(6+6)}{420r+192}$$
$$= \log(420r+192) - \frac{24(2r+4)\log(2) + 11(4r+8)\log(11) + 12(30r+6)\log(12)}{420r+192}.$$

After simplifying this, we obtain

$$ENM_1(\gamma_1) = \frac{(105r+48)\log(35r+16) + 18(r+2)(\log(2) + \frac{5\log(3)}{6} - \frac{11\log(11)}{18})}{105r+48}.$$

Figure 6 illustrates the entropy of the first Zagreb index of the TriCF linear chain structure using Maple 2020. Using the parameters r and s, we established a horizontal grid and, then, constructed a surface on top of that grid. This graph illustrates how the entropy values exhibit unique patterns corresponding to various causes. These graphs show various entropy features based on the parameters. We can regulate various variables and actions by varying the topological indices and entropy via these elements. Each TriCF chemical network's general entropy formulation is too lengthy to be given as a theorem. As mentioned above, the method makes it easy to generate any neighborhood-degree sum-based entropy expression for each topological index.

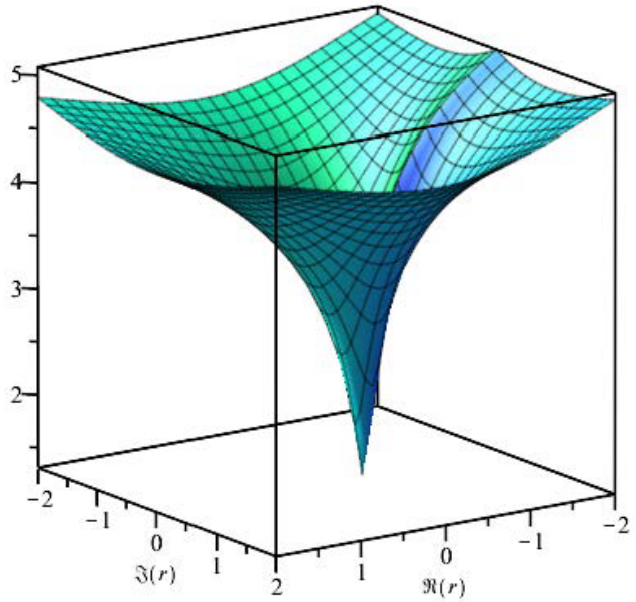


Figure 6. Three-dimensional plot of $ENM_1(\gamma_1)$.

5. Numerical Computation

This section displays the numerical outcomes of neighborhood-degree sum-based topological descriptors created for three distinct TriCF structures using entropy measurements. The values of the variables r and s range from 1 to 10. The generated topological descriptors were plotted using the Origin 2020 b application for a graphical comparison. The outcomes are summarized in Tables 4–6. Figure 5 depicts this tendency in three dimensions. These 3D charts illustrate the variation of each topological index for a particular structure. The behavior of a specific index for each of the three alternative structures that are the subject of this article can also be compared using 3D graphs. The following tables and figures analyze various entropies for all the possible structures of the TriCF molecular graph in numerical and graphical form.

Table 4. Numerical values for neighborhood-degree sum-based entropies of a linear chain TriCF structure.

$r \rightarrow$	1	2	3	4	5	6	7	8	9	10
$ER(\gamma_1)$	3.9779	4.4903	4.8276	5.0793	5.2803	5.4476	5.5908	5.7161	5.8274	5.9276
$ERR(\gamma_1)$	3.9814	4.4935	4.8306	5.0823	5.2831	5.4503	5.5936	5.7188	5.8301	5.9302
$ERRR(\gamma_1)$	3.977	4.4899	4.8274	5.0792	5.2802	5.4475	5.5908	5.7161	5.8274	5.9276
$EM_1(\gamma_1)$	3.9824	4.4943	4.8313	5.0829	5.2838	5.451	5.5942	5.7194	5.8307	5.9308
$EM_2(\gamma_1)$	3.9643	4.4795	4.818	5.0704	5.2718	5.4394	5.5828	5.7083	5.8197	5.92
$ERM_2(\gamma_1)$	3.9523	4.4698	4.8093	5.0623	5.2641	5.4319	5.5755	5.7011	5.8127	5.9131
$EHM(\gamma_1)$	3.9671	4.4818	4.82	5.0723	5.2736	5.4411	5.5845	5.71	5.8214	5.9216
$EAZ(\gamma_1)$	3.954	4.4712	4.8105	5.0634	5.2651	5.4329	5.5765	5.7021	5.8136	5.914
$EH(\gamma_1)$	9.1795	11.7376	14.0571	16.2695	18.4211	20.5336	22.6189	24.684	26.7338	28.7714
$ESC(\gamma_1)$	3.9868	4.498	4.8346	5.086	5.2867	5.4538	5.597	5.7222	5.8334	5.9335
$EGA(\gamma_1)$	3.9889	4.4998	4.8362	5.0876	5.2882	5.4553	5.5984	5.7236	5.8348	5.9349
$EIS(\gamma_1)$	3.9804	4.4927	4.8299	5.0816	5.2825	5.4497	5.5929	5.7182	5.8295	5.9296
$EAZI(\gamma_1)$	3.9882	4.4991	4.8357	5.087	5.2877	5.4548	5.5979	5.7231	5.8343	5.9344
$EF(\gamma_1)$	3.9696	4.4838	4.8218	5.074	5.2753	5.4427	5.5861	5.7115	5.8229	5.9231
$EABC(\gamma_1)$	4.5889	5.7275	6.6214	7.376	8.0385	8.6346	9.1802	9.6858	10.1586	10.6041

Table 5. Numerical values for the neighborhood-degree sum-based entropies of a parallelogram TriCF structure.

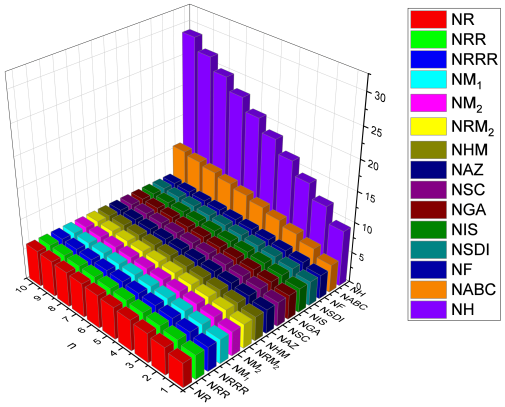
$(r,s) \rightarrow$	1	2	3	4	5	6	7	8	9	10
$ER(\gamma_2)$	−150.6809	−158.9867	−162.4445	−164.3874	−165.6278	−166.4793	−167.0923	−167.5486	−167.8965	−168.1668
$ERR(\gamma_2)$	−14.3228	−13.8865	−13.4802	−13.1369	−12.8428	−12.5861	−12.3585	−12.1542	−11.9688	−11.7991
$ERRR(\gamma_2)$	−9.3014	−8.7902	−8.3518	−7.9898	−7.6833	−7.4176	−7.1833	−6.9737	−6.7841	−6.6109
$EM_1(\gamma_2)$	3.9824	4.9654	5.595	6.0657	6.4434	6.7595	7.0317	7.2708	7.484	7.676
$EM_2(\gamma_2)$	3.9643	4.9536	5.5861	6.0584	6.4373	6.7543	7.0271	7.2667	7.4803	7.6731
$ERM_2(\gamma_2)$	3.9523	4.946	5.5804	6.0539	6.4335	6.751	7.0242	7.2641	7.4779	7.671
$EHM(\gamma_2)$	3.9671	4.9554	5.5875	6.0595	6.4382	6.7551	7.0278	7.2673	7.4808	7.6736
$EAZ(\gamma_2)$	4.3707	5.1949	5.7625	6.1985	6.5538	6.8541	7.1144	7.3444	7.5503	7.7368
$EH(\gamma_2)$	3.9796	4.9632	5.5932	6.0641	6.442	6.7584	7.0306	7.2698	7.4832	7.6757
$ESC(\gamma_2)$	3.9868	4.9683	5.5973	6.0675	6.4449	6.7609	7.0329	7.2718	7.485	7.6774
$EGA(\gamma_2)$	3.9889	4.9698	5.5984	6.0684	6.4457	6.7616	7.0335	7.2724	7.4855	7.6779
$EIS(\gamma_2)$	3.9804	4.9641	5.5941	6.0649	6.4427	6.759	7.0312	7.2703	7.4836	7.6762
$EAZI(\gamma_2)$	3.9509	4.944	5.5786	6.0523	6.4321	6.7497	7.0231	7.263	7.477	7.6701
$EF(\gamma_2)$	3.9696	4.957	5.5887	6.0605	6.439	6.7558	7.0284	7.2678	7.4814	7.6741
$EABC(\gamma_2)$	4.5889	7.071	9.4073	11.7079	14.002	16.3001	18.6062	20.2467	23.2467	25.5816

Table 6. Numerical values for the neighborhood-degree sum-based entropies of a hexagonal TriCF structure.

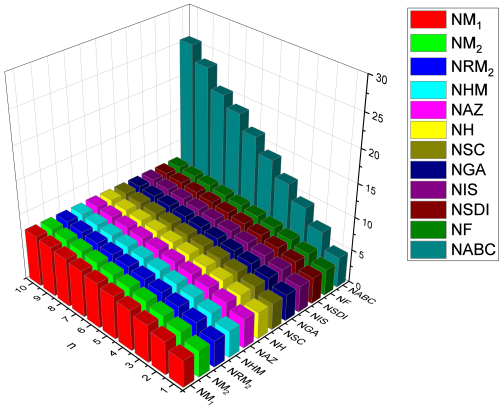
$r \rightarrow$	1	2	3	4	5	6	7	8	9	10
$ER(\gamma_3)$	3.9779	5.3687	6.1816	6.758	7.205	7.5701	7.8787	8.146	8.3818	8.5927
$ERR(\gamma_3)$	3.9814	5.37127	6.1834	6.7594	7.2061	7.5711	7.8796	8.1468	8.3825	8.5933
$ERRR(\gamma_3)$	3.977	5.3688	6.1818	6.7582	7.2052	7.5703	7.8789	8.1462	8.3819	8.5928
$EM_1(\gamma_3)$	3.9824	5.3717	6.1837	6.7597	7.2063	7.5712	7.8797	8.1469	8.3826	8.5934
$EM_2(\gamma_3)$	3.9643	5.3622	6.1773	6.7548	7.2024	7.568	7.8769	8.1445	8.3804	8.5914
$ERM_2(\gamma_3)$	3.9523	5.3561	6.1732	6.7518	7.2	7.5659	7.8752	8.1429	8.379	8.5902
$EHM(\gamma_3)$	3.9671	5.3636	6.1783	6.7556	7.203	7.5685	7.8773	8.1448	8.3807	8.5917
$EAZ(\gamma_3)$	3.954	5.3569	6.1738	6.7522	7.2003	7.5662	7.8754	8.1431	8.3792	8.5904
$EH(\gamma_3)$	9.1795	16.6571	23.3695	29.7961	36.0729	42.2578	48.3802	54.4577	60.5011	66.5179
$ESC(\gamma_3)$	3.9868	5.374	6.1853	6.7609	7.2073	7.5721	7.8804	8.1475	8.3831	8.5939
$EGA(\gamma_3)$	3.9889	5.3753	6.1862	6.7616	7.2078	7.5725	7.8808	8.1479	8.3834	8.5941
$EIS(\gamma_3)$	3.9804	5.3706	6.183	6.7592	7.2059	7.5709	7.8794	8.1466	8.3823	8.5932
$EAZI(\gamma_3)$	3.9882	5.3748	6.1859	6.7613	7.2077	7.5723	7.8807	8.1477	8.3833	8.5941
$EF(\gamma_3)$	3.9696	5.3649	6.1791	6.7562	7.2036	7.5689	7.8777	8.1452	8.381	8.592
$EABC(\gamma_3)$	4.5889	8.5204	12.4547	16.4326	20.4534	24.5118	28.6026	32.7216	36.8652	41.0305

Results and Discussion

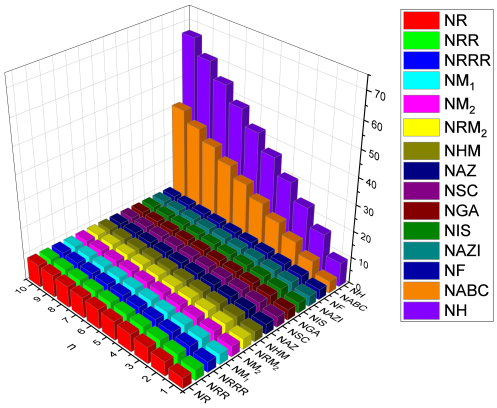
If we examine the entropy measures in Figure 7a,c, we can see that the neighborhood harmonic (NH) significantly impacts the initial structure more than the other indices. At the same time, Figure 7b shows that the NABC outperforms the other entropy measures. The stability study of the generalized TriCF structure using numerical information entropy values and the derived entropy formulae are new findings that can connect Shannon's entropy with traditional thermodynamic entropy.



(**a**) Entropy of γ_1



(**b**) Entropy of γ_2



(**c**) Entropy of γ_3

Figure 7. Comparison of entropy measures for TriCF structures.

In this study, we determined the neighborhood degree sum indices, multiplicative neighborhood degree sum indices, and entropy of TriCF structure using the neighborhood degree sum edge partition. From the computation and analysis, we obtained that the neighborhood harmonic indices and neighborhood ABC indices both have more impact than other indices and are highly correlated to the thermodynamic properties of the TriCF structures [16–18,22,23,37]. In the previous study [9], we determined degree-based indices, multiplicative degree-based indices, and the entropy values of the TriCF structure by the edge partition method based on the degrees of the end vertices and reciprocal Randić indices showed a higher impact. This will simulate molecules' physical and chemical characteristics [3,5,15] regarding the structure. Therefore, by employing degree-based and neighborhood degree-sum-based approaches, future researchers can easily compute the topological indices of upcoming TriCF structures, and also, these studies will help them produce different types of TriCF structures for different applications.

6. Conclusions

In this study, neighborhood-degree-based topological indices were computed using multiplicative and entropy measures. Using these indices, scientists can predict a range of molecular compound properties without requiring expensive or time-consuming studies. The computed findings are, therefore, crucial in predicting TriCF system properties. This is a newly synthesized lubricant whose physical, chemical, and experimental properties have yet to be investigated. As a result, the researchers will be able to advance their work with the support of this current study. For further use, we also generated the multiplicative neighborhood topological indices for the TriCF structure. Both theoretical chemists and industry experts will find this paper's graphical representation and numerical comparison of the computed findings beneficial. With the aid of the observations produced regarding the effectiveness of various indices, other researchers will be able to choose the indices more efficiently. The same classes, distance-based indices, QSAR, and QSPR, are being developed because they are also crucial for research.

Author Contributions: Conceptualization, T.A.; formal analysis, T.A.; methodology, T.A.; software, T.A.; supervision, R.S.; validation, T.A. and R.S.; visualization, T.A.; writing—original draft, T.A.; writing—review and editing, R.S. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: The authors declare no conflict of interest.

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