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HDR Degree Based Indices for Graphene

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ABSTRACT: Vertex degree-based HDR descriptors are numerical quantities that characterize molecular structures based on their vertex degrees. These HDR descriptors create the basis for theoretical chemists to explore and synthesize new molecular compounds. Entropic measures and multiplicative TIs are types of HDR descriptors with a wide range of applications, including quantitative structural analysis of molecular structures and certain properties of chemical structures. Poly-cyclic Aromatic Hydrocarbons (PAHs) have piqued the interest of theoretical chemists due to their distinctive electromagnetic and other properties like super aromaticity. Cycloarenes are a family of PAHs made up of sequentially (circularly) fused benzene rings that can trap metal ions in their cavities. The unique features of these kinds of compounds, as well as their ubiquitous availability, necessitate a systematic analysis to understand their nature as well as their intriguing properties. The focus of this research is to compute proper analytical expressions for different kinds of HDR indices for five major chemical compounds. The calculated numerical values of these HDR indices are also computed and compared in the form of 3D graphical representations.

Key Words: Graph-theoretical techniques, molecular descriptors, HDR index, graphene.

Contents

1. Introduction

PAHs are organic compounds that share a pair of carbon atoms and have two or more single or fused aromatic rings in their molecules. They are generally white, pale-yellow, or colourless solids. PAHs are omnipresent and are usually created by incomplete combustion of organic materials, natural disasters or leakage of coal deposits petroleum, or volcanoes. Several PAHs are carcinogenic, mutagenic, and toxic. As they are extremely fat-soluble, they are easily absorbed from the gastrointestinal tracts of mammals and are also known to be immune to suppressants [1,2,3].

PAHs, however, have commercial applications too. Thermosetting polymers, pharmaceuticals, photographic items, lubricating materials, agricultural products, and other chemical industries all use them as intermediaries. Some PAHs are also used as pigments, dyes, plastics, insecticides, and medications [4]. Thus, their ubiquity, applications, and possible toxic nature warrant significant research into the nature and properties of PAHs. This has been the motivation for the study of two prominent classes of PAHs, namely the zigzag hexagonal kekulene system (ZHK) and armchair hexagonal kekulene system (AHK). Additionally, the analytic expressions for three types of graphene structures are determined.

Cycloarenes are a type of PAH created by fusing angular and linear benzene ring annulations to form a central cavity. It was later named Kekulene, with the chemical formula $C_{48}H_{24}$, and synthesized successfully [5]. Kekulene is an aromatic compound with a $D_{6\ h}$ Clar system composed of 6 benzene rings

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sextets, according to a comparison of its geometric and magnetic properties with those of phenanthrene, 1,2:7,8-dibenzanthracene, anthracene. Kekulene has also been considered as one of the suitable anode materials for a lithium-ion battery because of its unusual properties. As a result, a theoretical analysis of its new structure can reveal more information about its properties [6,7,8].

Topological indices (TIs) are a type of molecular parameter that provide quantitative measurements based on the molecular structure's underlying connectivity. However, their applications are still being explored and verified [9,10,11]. They are numerical values derived from a molecular network in which each vertex depicts an atom and each edge indicates a chemical bond between two atoms. TIs are molecular descriptors that can be used to find a correlation between chemical compounds and their corresponding biological and other significant properties, like physico-chemical activities of chemical compounds [12, 13]. These topological descriptors are part of a set of theoretical tools for describing the structural characteristics of these molecules. There are several kinds of topological indices defined in the literature, of which the degree-based topological indices are one of the most extensively studied and applied indices.

A degree-based topological index is a sub-class of topological indices where the index is computed based on the degrees of the molecular graph. Due to their widespread applications and computational ease, degree-based indices have been studied extensively. Recently, Julietraja and Venugopal computed the degree-based indices for coronoid structures [14]. Julietraja et al. analysed the VDB indices for benzenoids [15,16]. Dehmer introduced graph entropies that capture structural information based on information functionals, and studied their properties [17].

The idea of graph entropy was first established by Rashevsky [18] in 1955, based on classifications of vertex orbits. Estrada et al. developed a physically sound graph entropy measure [19] and investigated walk-based graph entropies. In structural chemistry, computer science, and biology, entropy measures for graphs are extensively examined and studied [20,21,22]. Julietraja et al. used entropy measures to perform structural analysis on three types of PAHs [23].

Despite their unique properties and wide-ranging applications, not many studies have explored the topological characteristics of the above-described structures. In this paper, five chemical compounds are investigated by using different kinds of VDB TIs. Notably, few studies in the literature have applied degree-based to this extent to chemical structures [24,25]. Hence, this unique investigation will add significant depth to the current wealth of knowledge on these structures.

2. Graph Theoretical Concepts

Throughout this paper, Γ represents a connected graph, V and E refer to the vertex set and the edge set, respectively. The degree of a vertex $\mathfrak{v}$ in a graph Γ is the number of edges that are incident to that vertex $\mathfrak{v}$ [26] and is denoted by δ_v. The HDR entropy measures and other HDR indices are generated using the following molecular descriptors: GA index, Randić index, ABC index, SDD index, Sum-connectivity index, and Zagreb and its co-indices. The standard terminology and notations from the prior literature review are utilized in this paper. The degree-based multiplicative indices are calculated based on the end degrees of the edges.

The definitions and standard notations of the multiplicative indices have been taken from [27,28,29, 30,31].

$$MTI(\Gamma) = \Pi_{\mathfrak{u}\mathfrak{v}\in E(T)} F(\mathfrak{d}_\mathfrak{u}, \mathfrak{d}_\mathfrak{v})$$

Where Π denotes the product of the terms $F(\mathfrak{d}_u, \mathfrak{d}_v)$.

Many algebraic polynomials have been created and described in the literature as a convenient method of computing degree and distance-based TIs. The Hosoya polynomial is the most commonly used as it can be used to calculate various distance-based indices by computing a single polynomial. Deutsch and Klavžar [32] made a similar breakthrough for HDR indices in the form of M-polynomial in 2015. Like the Hosaya polynomial, the $M-$polynomial can be used to compute a variety of VDB indices.

The $M-$polynomial of Γ is defined as

$$M(\Gamma; w, k) = \sum_{\delta\leq i\leq j\leq\Delta} m_{ij}(\Gamma) w^i k^j$$

where $\delta = \min\{\mathfrak{d}_\mathfrak{v} : \mathfrak{v} \in V(\Gamma)\}$; $\Delta = \max\{\mathfrak{d}_\mathfrak{v} : \mathfrak{v} \in V(\Gamma)\}$, and $m_{ij}(\Gamma)$ is the edge $\mathfrak{uv} \in E(\Gamma)$ for which $\{\mathfrak{d}_\mathfrak{v}, \mathfrak{d}_\mathfrak{u}\} = \{i, j\}$.

3. Entropy of Weighted Graphs

Studies on information content of complex networks and graphs began in the late 1950s inspired by the pioneering work of Shannon. Several techniques for analyzing complex networks quantitatively have been documented in the literature. For example, graph entropy measures have been used extensively to characterize the structure of graph-based systems in mathematical chemistry, biology and in computer science related areas [33,34].

Numerous open problems in discrete mathematics, computer science, information theory, statistics, chemistry, and biology involve investigating entropies for relational structures. Rashevsky was the first to introduce the structural information content based on partitions of vertex orbits [18]. In addition, he used the concept of graph entropy to measure the structural complexity of graphs. Mowshowitz used the same measure and theoretically proved some properties for graph operations [36].

He also introduced the entropy of a graph as an information-theoretic quantity, and he interpreted it as the structural information content of a graph. Mewshowitz also studied the mathematical properties of graph entropy measures and discussed their potential applications.

Let Γ be a graph with vertex $\mathfrak{v}_i$ and $\mathfrak{d}_i$ be the degree of $\mathfrak{v}_i$ for the given edge $\mathfrak{u}_\mathfrak{i}\mathfrak{v}_\mathfrak{j}$, then one can define

$$\mathcal{P}_{ij} = \frac{\mathfrak{w}(\mathfrak{u}_\mathfrak{i}\mathfrak{v}_\mathfrak{j})}{\sum_{j=1}^{\mathfrak{d}_\mathfrak{i}} \mathfrak{w}(\mathfrak{u}_\mathfrak{i}\mathfrak{v}_\mathfrak{j})}$$

where $\mathfrak{w}(\mathfrak{u}_\mathfrak{i}\mathfrak{v}_\mathfrak{j})$ is the weight of the edge $\mathfrak{u}_\mathfrak{i}\mathfrak{v}_\mathfrak{j}$ and $\mathfrak{w}(\mathfrak{u}_\mathfrak{i}\mathfrak{v}_\mathfrak{j}) > 0$. The node entropy is defined as

$$ENT_\Gamma(\mathfrak{v}_i) = -\sum_{j=1}^{\mathfrak{d}_\mathfrak{i}} \log(\mathcal{P}_{ij})$$

For an edge-weighted graph $\Gamma = (V, E, \mathfrak{w})$, the entropy measure of Γ is defined as Where

$$\mathcal{P}_{\mathfrak{uv}} = \frac{\mathfrak{w}(\mathfrak{uv})}{\sum_{\mathfrak{uv}\in E(\Gamma)} \mathfrak{w}(\mathfrak{uv})}, \qquad TI(\Gamma) = \chi$$

$$\begin{aligned}
\mathrm{ENT}_\chi(\Gamma) &= -\sum_{\mathfrak{uv}\in E(\Gamma)} \mathcal{P}_{\mathfrak{u},\mathfrak{v}} \log \mathcal{P}_{\mathfrak{u},\mathfrak{v}} \\
&= -\sum_{\mathfrak{uv}\in E(\Gamma)} \frac{F(\mathfrak{d}_\mathfrak{u}, \mathfrak{d}_\mathfrak{v})}{\chi(\Gamma)} \log \frac{F(\mathfrak{d}_\mathfrak{u}, \mathfrak{d}_\mathfrak{v})}{\chi(\Gamma)} \\
&= -\frac{1}{\chi} \sum_{\mathfrak{uv}\in E(\Gamma)} F(\mathfrak{d}_\mathfrak{u}, \mathfrak{d}_\mathfrak{v}) \left(F(\mathfrak{d}_\mathfrak{u}, \mathfrak{d}_\mathfrak{v})\right) - \log \chi(\Gamma)
\end{aligned}$$

4. Computing Different Kinds of HDR Indices for β - Graphene

A single-atom-thick layer of carbon atoms arranged in a hexagonal lattice is known as graphene and it forms the the core component of graphite. Graphene is a notable substance in and of itself, with many remarkable properties that have earned it the name "wonder material" on numerous occasions. With one atom thick, it is the thinnest material known to man. It is also extremely strong, about 200 times stronger than steel. Furthermore, graphene is a good conductor of electricity and heat, in addition to having intriguing physical, chemical, mechanical, thermal, and electrical properties as well as light absorption characteristics [36,37]. It is a resource that has the potential to truly change the world, with limitless applications in almost every industry [38]. The β-Graphene consists of $V(\Gamma) = 12mn+2m+10n$ and $E(\Gamma) = 18mn + m + 11n$ [25]. It is depicted in Figure 1.

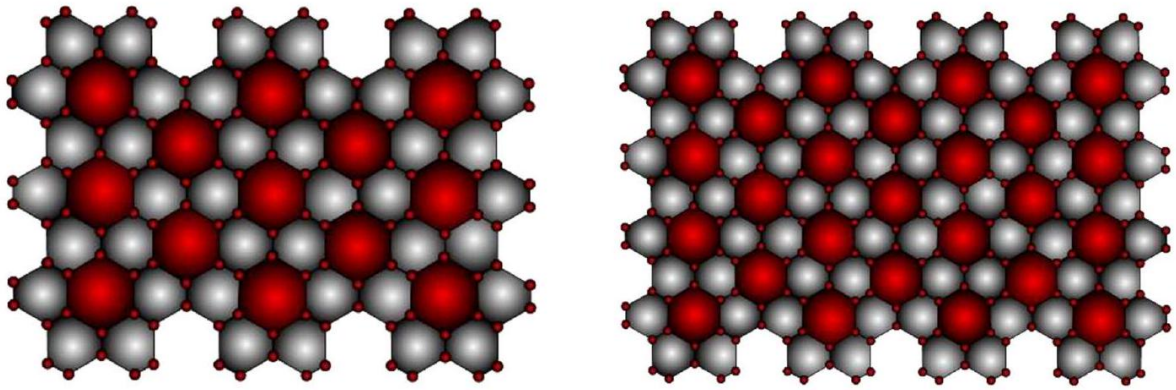

Figure 1: (a) β-Graphene (3,3), (b) β-Graphene (4,4)

Table 1: Edge Frequency for β-Graphene [26]

Edge types	Frequency
$\mathfrak{d}_{22}$	$2m+4n$
$\mathfrak{d}_{23}$	$4m+8n$
$\mathfrak{d}_{33}$	$18mn-5m-n$

Using Table 1, we compute two important types of VDB indices for β-Graphene in this section.

Theorem 4.1 *If Γ is the molecular graph of a β-Graphene, then the HDR multiplicative TIs are computed as*

1. $HDRMF_1I(\Gamma) = 39346408075296537575424^{mn} \times 1889568^{-m} \times 18^{-n} \times 1827904^{m} \times 3341233033216^{n}$.
2. $HDRMF_2I(\Gamma) = 225283995449391744118401478747726 41^{m*n} \times 3486784401^{-m} \times 81^{-n} \times 429981696^{m} \times 184884258895036416^{n}$.
3. $\mathrm{HDRMRRR}(\Gamma) = 262144^{mn} \times 2^{-3m+3n}$,
4. $\mathrm{MSDD}(\Gamma) = 262144^{mn} \times 2^{-3m+3n} \times 28561^{m} \times 815730721^{n} \times 1296^{-m} \times 1679616^{-n}$,
5. $\mathrm{HDRFMHZI}(\Gamma) = 10314424798490535546171949056^{mn} \times 60466176^{-m} \times 36^{-n} \times 100000000^{m} \times 10000000000000000^{n}$,
6. $\mathrm{HDRMHI}(\Gamma) = 4^{m} \times 16^{n} \times 625^{-m} \times 390625^{-n} \times 387420489^{-mn} \times 243^{m} \times 3^{n}$,
7. $HDRMSCI(\Gamma) = 10077696^{-mn} \times 36^{m} \times 6^{\left(\frac{1}{2}\right)m+\left(\frac{1}{2}\right)n} \times 100^{-m} \times 10000^{-n}$,
8. $\mathrm{HDRMABCI}(\Gamma) = 262144^{mn} \times 256^{-m} \times 128^{-n} \times 387420489^{-mn} \times 243^{m} \times 3^{n}$,
9. $HDRMAZI(\Gamma) = 3245185536584267267831560205762 56^{-mn} \times 281474976710656^{m} \times 4398046511104^{n} \times 338139191352272634293022147239224117019852745184856 1^{mn} \times 205891132094649^{-m} \times 729^{-n}$,
10. $HDRMReZG_1(\Gamma) = 262144^{mn} \times 387420489^{-mn} \times 1875^{m} \times 512^{-m} \times 390625^{n} \times 1119744^{-n}$,

Table 2: Multiplicative Vertex Degree Based Indices

Sl. No.	Name of the TIs	Mathematical Expressions
1	First Multiplicative HDR-index	$\mathrm{HDRMF_1I}(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \mathfrak{deg}_\Gamma(\mathfrak{u})^2 + \mathfrak{deg}_r(\mathfrak{v})^2$
2.	Second Multiplicative $F-$index	$\mathrm{MHDRF}_2\, I(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \mathfrak{deg}\Gamma(\mathfrak{u})^2 \times \mathfrak{deg}_r(\mathfrak{v})^2$
3.	Multiplicative reduced reciprocal HDR Randić Index	$HDR = \prod_{\mathfrak{uv}\in E(\Gamma)} \sqrt{(\mathfrak{deg}_\Gamma(\mathfrak{u})-1)\,(\mathfrak{deg}_\Gamma(\mathfrak{v})-1)}$
4.	Multiplicative HDRSDD index	$\mathrm{HDRMSDD}(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \left(\frac{\mathfrak{deg}_\Gamma(\mathfrak{u})}{\mathfrak{deg}_\Gamma(\mathfrak{v})} + \frac{\mathfrak{deg}_\Gamma(\mathfrak{v})}{\mathfrak{deg}_\Gamma(\mathfrak{u})}\right)$
5.	First Multiplicative HDR Hyper-Zagreb Index	$\mathrm{HDRFMHZI}(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} (\mathfrak{deg}_\Gamma(\mathfrak{u}) + (\mathfrak{deg}_\Gamma(\mathfrak{v}))^2$
6.	Multiplicative HDR Harmonic Index [24]	$\mathrm{HDRHGDMHI}(\Gamma) = \prod_{\mathfrak{uv}v\in E(\Gamma)} \left(\frac{2}{\mathfrak{deg}_\Gamma(\mathfrak{u})+\mathfrak{deg}_\Gamma(\mathfrak{v})}\right)$
7.	Multiplicative HDR Sum Connectivity Index	$\mathrm{HDRMSCI}(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \frac{1}{\sqrt{\mathfrak{deg}_\Gamma(\mathfrak{u})+\mathfrak{deg}_\Gamma(\mathfrak{v})}}$
8.	Multiplicative Randić Index	$\mathrm{HDRMRI}(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \frac{1}{\sqrt{\mathfrak{deg}_\Gamma(\mathfrak{u})\times\mathfrak{deg}_\Gamma(v)}}$
9.	Multiplicative HDRABC Index	$\mathrm{HDRMABCI}(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \sqrt{\frac{\mathfrak{deg}_\Gamma(\mathfrak{u})+\mathfrak{deg}_\Gamma(v)-2}{\mathfrak{deg}_\Gamma(\mathfrak{u})\times\mathfrak{deg}_\Gamma(v)}}$
10	Multiplicative HDRGA Index	$\mathrm{HDRMABCI}(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \sqrt{\frac{\mathfrak{deg}_\Gamma(\mathfrak{u})\times\mathfrak{deg}_\Gamma(v)}{\mathfrak{deg}_\Gamma(\mathfrak{u})+\mathfrak{deg}_\Gamma(v)}}$
11.	Multiplicative $HDRAG_1$ Index	$\mathrm{HDRMAG_1}(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \frac{\mathfrak{deg}_\Gamma(\mathfrak{u})+\mathfrak{deg}_\Gamma(v)}{2\sqrt{\mathfrak{deg}_\Gamma(\mathfrak{k})\times\mathfrak{deg}_\Gamma(v)-2}}$
12.	Multiplicative HDR Augmented Zagreb Index	$\mathrm{HDRMAZI}(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \left(\frac{\mathfrak{deg}_\Gamma(\mathfrak{u})\times\mathfrak{deg}_\Gamma(\mathfrak{v})}{\mathfrak{deg}_\Gamma(\mathfrak{u})+\mathfrak{deg}_\Gamma(\mathfrak{v})-2}\right)^3$
13.	First Multiplicative HDR redefined Zagreb index	$\mathrm{HDRMTeZG_1}(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \frac{\mathfrak{deg}_\Gamma(\mathfrak{u})+\mathfrak{deg}_\Gamma(\mathfrak{v})}{\mathfrak{deg}_\Gamma(\mathfrak{u})\times\mathfrak{deg}_\Gamma(\mathfrak{v})}$
14	Second Multiplicative HDR redefined Zagreb index	$\mathrm{HDRMTeZG_1}(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \left(\frac{\mathfrak{deg}_\Gamma(\mathfrak{u})\times\mathfrak{deg}_\Gamma(\mathfrak{v})}{\mathfrak{deg}_\Gamma(\mathfrak{u})+\mathfrak{deg}_\Gamma(\mathfrak{v})}\right)$
15	Third Multiplicative HDR redefined Zagreb index	$\mathrm{HDRMReZG_3}(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} (\mathfrak{deg}_\Gamma\mathfrak{u} \times \mathfrak{deg}_\Gamma\mathfrak{v})$ $(\mathfrak{deg}_\Gamma(\mathfrak{u}) + \mathfrak{deg}_\Gamma(\mathfrak{v}))$
16	Multiplicative second modified HDR Zagreb index	$\mathrm{HDRMM}_2^{\mathrm{m}}(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \left(\frac{1}{\mathfrak{deg}_\Gamma(\mathfrak{u})+\mathfrak{deg}_\Gamma(\mathfrak{v})}\right)$
17	Multiplicative reciprocal HDR Randić Index	$\mathrm{HDRMRR}(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} = \left(\sqrt{(\mathfrak{deg}_\Gamma(\mathfrak{u}) \times \mathfrak{deg}_\Gamma(\mathfrak{v}))}\right)$
18	Multiplicative $HDRSK$ Index	$\mathrm{HDRMSK}(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \left(\frac{\mathfrak{deg}_\Gamma(\mathfrak{u})+\mathfrak{deg}_\Gamma(\mathfrak{v})}{2}\right)$
19	Multiplicative $HDRSK_1$ Index	$HDRMSK_1(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \left(\frac{\mathfrak{deg}_\Gamma(\mathfrak{u})\times\mathfrak{deg}_\Gamma(\mathfrak{v})}{2}\right)$
20	Multiplicative $\mathrm{HDRSK_2}$ Index	$\mathrm{HDRMSK^2}(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)\in E(\Gamma)} \left(\frac{\mathfrak{deg}(\mathfrak{u})+\mathfrak{deg}_\Gamma(\mathfrak{v})}{2}\right)^2$

11. $HDRHDRMReZG(\Gamma) = 387420489^{mn} \times 262144^{-mn} \times 512^m \times 1875^{-m} \times 1119744^n \times 390625^{-n}$,

12. $HDRMReZG3(\Gamma) = 152436046569249334074776404623 36^{mn} \times 459165024^{-m} \times 54^{-n} \times 207360000^m \times 42998169600000000^n$

13. $HDRMM_{2^m}(\Gamma) = 150094635296999121^{-mn} \times 59049^m \times 9^n \times 20736^{-m} \times 429981696^{-n}$,

14. $\mathrm{MRR}(\Gamma) = 387420489^{mn} \times 243^{-m} \times 3^{-n} \times 144^m \times 20736^n$,

15. $HDRMRI(\Gamma) = 387420489^{-mn} \times 243^m \times 3^n \times 144^{-m} \times 20736^{-n}$

16. $\mathrm{MGHDRAI}(\Gamma) = 576^m \times 625^{-m} \times 331776^n \times 390625^{-n}$.

Proof: Let Γ be the molecular graph of a β-Graphene. The β-Graphene contains $V(\Gamma) = 12mn+2m+10n$ and $E(\Gamma) = 18mn + m + 11n$. Using the definitions of HDR multiplicative TIs and the edge frequency Table 1, the results are obtained as below.

1. $HDRHDRMF_1I(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \mathfrak{d}_{\mathfrak{u}}^2 + \mathfrak{deg}_\Gamma(\mathfrak{v})^2$
$= 8^{2m+4n} \times 13^{4m+8n} \times 18^{18mn-5m-n}$
$= 39346408075296537575424^{mn} \times 1889568^{-m} \times 18^{-n} \times 1827904^{m}$
$\times 3341233033216^{n}$.

2. $HDRMF_2I(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \mathfrak{deg}_\Gamma(\mathfrak{u})^2 \times \mathfrak{deg}_\Gamma(\mathfrak{v})^2$
$= 16^{2m+4n} \times 36^{4m+8n} \times 81^{18mn-5m-n}$
$= 225283995449391744118401478747726 41^{m*n} \times 3486784401^{-m} \times 81^{-n}$
$\times 429981696^{m} \times 184884258895036416^{n}$

3. $HDRMRRR(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \sqrt{(\mathfrak{deg}_\Gamma(\mathfrak{u})-1)(\mathfrak{deg}_\Gamma(\mathfrak{v})-1)}$
$= 1^{2m+4n} \times \sqrt{2}^{4m+8n} \times 2^{18mn-5m-n}$
$= 262144^{mn} \times 2^{-3m+3n}$

4. $HDRMSDD(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \left(\frac{\mathfrak{deg}_\Gamma(\mathfrak{u})}{\mathfrak{deg}_\Gamma(\mathfrak{v})} + \frac{\mathfrak{deg}_\Gamma(\mathfrak{v})}{\mathfrak{deg}_\Gamma(\mathfrak{u})}\right)$
$= 22m + 4n \times \frac{134m+8n}{6} \times 218mn - 5m - n$
$= 262144^{mn} \times 2^{-3m+3n} \times 28561^{m} \times 815730721^{n} \times 1296^{-m} \times 1679616^{-n}$

5. $HDRFMHZI = \prod_{\mathfrak{uv}\in E(\Gamma)} (\mathfrak{deg}_\Gamma(\mathfrak{u}) + (\mathfrak{deg}_\Gamma(\mathfrak{v}))^2$
$= 16^{2m+4n} \times 25^{4m+8n} \times 36^{18mn-5m-_n}$
$= 10314424798490535546171949056^{mn} \times 60466176^{-m} \times 36^{-n} \times 100000000^{m}$
$\times 10000000000000000^{n}$

6. $\mathrm{HDRHGDMHI}(\Gamma) = \prod_{\mathfrak{uv}v\in E(\Gamma)} \left(\frac{2}{\mathfrak{deg}_\Gamma(\mathfrak{u}) + \mathfrak{deg}_\Gamma(\mathrm{v})}\right)$
$= \frac{1}{2}^{2m+4n} \times \frac{2}{5}^{4m+8n} \times \frac{1^{18mn-5m-n}}{3}$
$= 4^{m} \times 16^{n} \times 625^{-m} \times 390625^{-n} \times 387420489^{-mn} \times 243^{m} \times 3^{n}$

7. $\mathrm{HDRMSCI}(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \frac{1}{\sqrt{\mathfrak{deg}_\Gamma(\mathfrak{u}) + \mathfrak{deg}_\Gamma(\mathrm{v})}}$
$= \frac{1}{2}^{2m+4n} \times \frac{1}{\sqrt{5}}^{4m+8n} \times \frac{1}{\sqrt{6}}^{18mn-5m-n}$
$= 10077696^{-mn} \times 36^{m} \times 6 \left(\frac{1}{2}\right)^{m+\left(\frac{1}{2}\right)^{n}} \times 100^{-m} \times 10000^{-n}$

$$8.\,\mathrm{HDRMABCI}(\Gamma) = \prod_{\mathfrak{u}\mathfrak{v}\in E(\Gamma)} \sqrt{\frac{\mathfrak{deg}_\Gamma(\mathfrak{u}) + \mathfrak{deg}_\Gamma(\mathfrak{v}) - 2}{\mathfrak{deg}_\Gamma(\mathfrak{u}) \times \mathfrak{deg}_\Gamma(\mathfrak{v})}}$$
$$= \sqrt{\frac{1}{2}}^{2m+4n} \times \sqrt{\frac{1}{2}}^{-m+8n} \times \frac{2}{3}^{18mn-5m-n}$$
$$= 262144^{mn} \times 256^{-m} \times 128^{-n} \times 387420489^{-mn} \times 243^{m} \times 3^{n}$$

$$9.\,\mathrm{HDRMAZI}(\Gamma) = \prod_{\mathfrak{u}\mathfrak{v}\in E(\Gamma)} \left(\frac{\mathfrak{deg}_\Gamma(\mathfrak{u}) \times \mathfrak{deg}_\Gamma(\mathfrak{v})}{\mathfrak{deg}_\Gamma(\mathfrak{u}) + \mathfrak{deg}_\Gamma(\mathfrak{v}) - 2}\right)^3$$
$$= 8^{2m+4n} \times 8^{4m+8n} \times \left(\frac{9}{4}\right)^{3^{18mn-5m-n}}$$
$$= 3245185536584267267831560205762^{-mn} \times 281474976710656^{m} \times$$
$$4398046511104^{n} \times 3381391913522726342930221472392241170198527451848561^{m+n} \times$$
$$205891132094649^{-m} \times 729^{-n}$$

$$10.\,\mathrm{HDRMABCI}(\Gamma) = \prod_{\mathfrak{u}\mathfrak{v}\in E(\Gamma)} \frac{\mathfrak{deg}_\Gamma(\mathfrak{u}) + \mathfrak{deg}_\Gamma(v)}{\mathfrak{deg}_\Gamma(\mathfrak{u}) \times \mathfrak{deg}_\Gamma(v)}$$
$$= 1^{2m+4n} \times \frac{5}{6}^{4m+8n} \times \frac{2}{3}^{18mn-5m-n}$$
$$= 262144^{mn} \times 387420489^{-mn} \times 1875^{m} \times 512^{-m} \times 390625^{n} \times 1119744^{-n}$$

$$11.\,\mathrm{HDRMABCI}(\Gamma) = \prod_{\mathfrak{u}\mathfrak{v}\in E(\Gamma)} \left(\frac{\mathfrak{deg}_\Gamma(\mathfrak{u}) \times \mathfrak{deg}_\Gamma(v)}{\mathfrak{deg}_\Gamma(\mathfrak{u}) + \mathfrak{deg}_\Gamma(v)}\right)$$
$$= 1^{2m+4n} \times \frac{6}{5}^{4m+8n} \times \frac{3}{2}^{18mn-5m-n}$$
$$= 387420489^{mn} \times 262144^{-mn} \times 512^{m} \times 1875^{-m} \times 1119744^{n} \times 390625^{-n}$$

$$12.\,\mathrm{HDRMReZG_3}(\Gamma) = \prod_{\mathfrak{u}\mathfrak{v}\in E(\Gamma)} \left(\mathfrak{deg}_\Gamma\mathfrak{u} \times \mathfrak{deg}_\Gamma\mathfrak{v}\right)\left(\mathfrak{deg}_\Gamma(\mathfrak{u}) + \mathfrak{deg}_\Gamma(\mathfrak{v})\right)$$
$$= 16^{2m+4n} \times 30^{4m+8n} \times 54^{18mn-5m-n}$$
$$= 152436046569249334074776404623 36^{mn} \times 459165024^{-m} \times 54^{-n}$$
$$\times 207360000^{m} \times 42998169600000000^{n}$$

$$13.\ \mathrm{HDRMM_2^m}(\Gamma) = \prod_{\mathfrak{u}\mathfrak{v}\in E(\Gamma)} \left(\frac{1}{\mathfrak{deg}_\Gamma(\mathfrak{u}) \times \mathfrak{deg}_\Gamma(\mathfrak{v})}\right)$$
$$= \frac{1^{2m+4n}}{4} \times \frac{1^{4m+8n}}{6} \times \frac{1^{18mn-5m-n}}{}$$
$$= 150094635296999121^{-mn} \times 59049^{m} \times 9^{n} \times 20736^{-m} \times 429981696^{-n}$$

$$14.\,\mathrm{HDRMRR}(\Gamma) = \prod_{\mathfrak{u}\mathfrak{v}\in E(\Gamma)} \left(\sqrt{(\mathfrak{deg}_\Gamma(\mathfrak{u}) \times \mathfrak{deg}_\Gamma(\mathfrak{v}))}\right)$$
$$= 2^{2m+4n} \times \sqrt{6}^{4m+8n} \times 3^{18mn-5m-n}$$
$$= 387420489^{mn} \times 243^{-m} \times 3^{-n} \times 144^{m} \times 20736^{n}$$

$$15.\,\mathrm{HDRMRI}(\Gamma) = \prod_{\mathfrak{u}\mathfrak{v}\in E(\Gamma)} \frac{1}{\sqrt{\mathfrak{deg}_\Gamma(\mathfrak{u}) \times \mathfrak{deg}_\Gamma(v)}}$$
$$= \frac{1}{2}^{2m+4n} \times \frac{1}{\sqrt{6}}^{4m+8n} \times \frac{1}{3}^{18mn-5m-n}$$
$$= 387420489^{-mn} \times 243^{m} \times 3^{n} \times 144^{-m} \times 20736^{-n}.$$

$$16.\ \mathrm{HDRMAG}_1(\Gamma) = \prod_{\mathfrak{uv}\in E(\Gamma)} \frac{\mathfrak{deg}_\Gamma(\mathfrak{u}) + \mathfrak{deg}_\Gamma(v)}{2\sqrt{\mathfrak{deg}_\Gamma(\mathfrak{k}) \times \mathfrak{deg}_\Gamma(v)}}$$
$$= 1^{2m+4n} \times \frac{2\sqrt{6}}{5}^{4m+8n} \times 1^{18mn-5m-n}$$
$$= 576^m \times 625^{-m} \times 331776^n \times 390625^{-n}$$

Hence the proof.

□

Theorem 4.2 *If Γ is the molecular graph of β-Graphene, then the M-polynomial is computed as $M(\Gamma, w, k) = (2m + 4n)w^2k^2 + (4m + 8n)w^2k^3 + (18mn - 5m - n)w^3k^3$.*

Proof: Using the definition of M-polynomial and Table 1, the following result is obtained as $M(\Gamma; w, k) = (2m + 4n)w^2k^2 + (4m + 8n)w^2k^3 + (18mn - 5m - n)w^3k^3$. Hence the proof. □

Theorem 4.3 *If Γ is the molecular graph of β-Graphene, then the HDR indices are computed using M-polynomial as follows.*

1. $\mathrm{HDRABC}\,(\Gamma) = 3\sqrt{2}m + 6\sqrt{2}n + 12mn - \left(\frac{10}{3}\right) m - \left(\frac{2}{3}\right) n,$
2. $\mathrm{HDRGA}\,(\Gamma) = 18mn - 3m + 3n + \left(\frac{8}{5}\right) \sqrt{6}m + \left(\frac{16}{5}\right) \sqrt{6}n,$
3. $HDRB_1(\Gamma) = 252mn - 10m + 106n,$
4. $HDRB_2(\Gamma) = 432mn - 44m + 128n,$
5. $HDRHB_1(\Gamma) = 1764mn - 182m + 518n,$
6. $\mathrm{HDRHB}_2(\Gamma) = 5184mn - 908m + 776n,$
7. $\mathrm{HDRMB}^1(\Gamma) = \left(\frac{109}{105}\right) m + \left(\frac{488}{105}\right) n + \left(\frac{36}{7}\right)_{mn},$
8. $\mathrm{HDRMB}^2(\Gamma) = \left(\frac{23}{18}\right) m + \left(\frac{73}{18}\right) n + 3_{mn},$
9. $\mathrm{HDRH}_b(\Gamma) = \left(\frac{218}{105}\right) m + \left(\frac{976}{105}\right) n + \left(\frac{72}{7}\right)_{mn},$
10. $\mathrm{HDRReZG}_1(\Gamma) = 12mn + 2m + 10n,$
11. $\mathrm{HDRReZG}^2(\Gamma) = 27mn - \left(\frac{7}{10}\right) m + \left(\frac{121}{10}\right)_n,$
12. $\mathrm{HDRReZG}_3(\Gamma) = 972mn - 118m + 250n,$
13. $\mathrm{HDRSK}(\Gamma) = 54mn - m + 25n,$
14. $\mathrm{HDRSK}^1(\Gamma) = 81mn - \left(\frac{13}{2}\right) m + \left(\frac{55}{2}\right) n,$
15. $SK_2(\Gamma) = 162mn - 12m + 57n.$

Proof: The β-Graphene contains $V(\Gamma) = 12mn + 2m + 10n$ and $E(\Gamma) = 18mn + m + 11n$. In order to prove this theorem, the results of Theorem 2, frequency Table 1, and the differential operators of M-polynomial have been used.

Here, the 3D graphical representations are being generated over some of the analytical expressions from Theorem 3 to perform comparative analysis for β-Graphene system. The purpose of this comparison is to determine the similarities and differences between the various topological indices. It can be observed from these 3D plots that how the indices are varying from structural perspective.

□

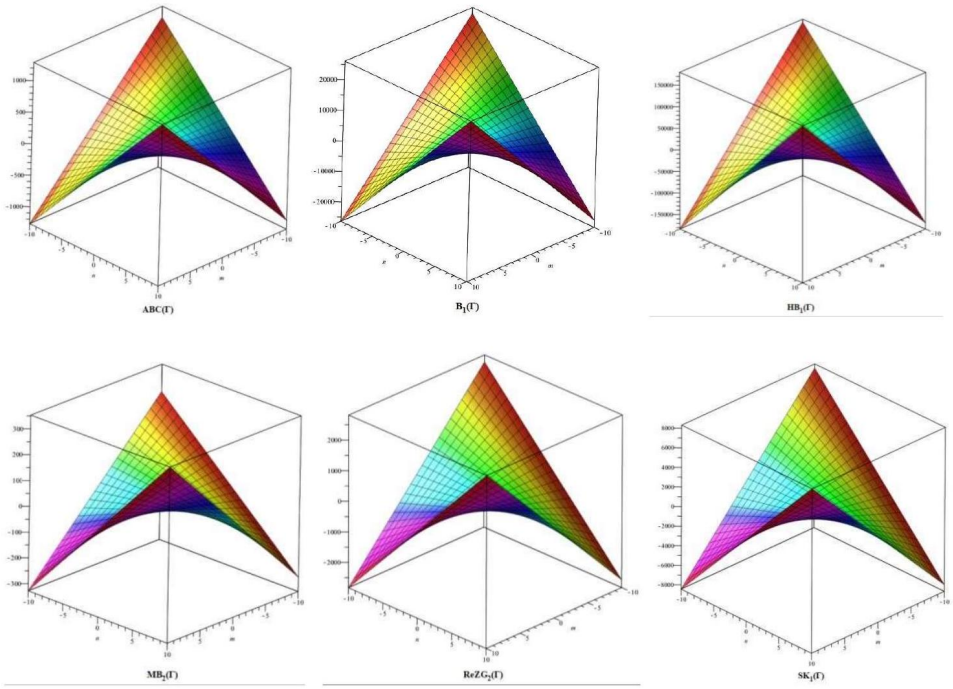

Figure 2: 3D comparison graph for Theorem 3

5. Computing HDR Indices for β-Graphyne

$\beta-$graphyne is the 2D derivative of the graphite structures. The bonds among three corresponding atoms in the graphyne layer are sequentially arranged by the chains of carbyne and thus the sp^2 atoms will be remaining as same and the desired β-graphyne layers are derived [40]. The β-Graphynes are 2D materials created by incorporating acetylenic links into a honeycomb lattice with sp-hybridisation of C atoms. Because of the presence of acetylenic groups, these structures have a diverse set of electrical, mechanical, and optoelectronic characteristics [41]. The cardinality of β-Graphynes are $V(\Gamma) = 36mn + 2m + 24n$ and $E(\Gamma) = 42mn + m + 23n$ [26] It is represented in Figure 3.

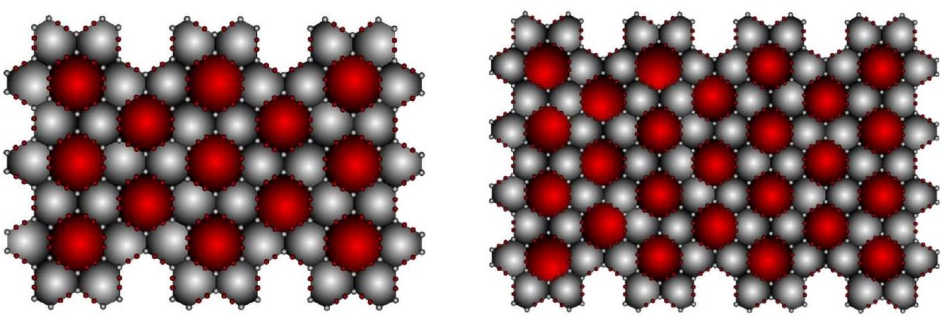

Figure 3: (a) β-Graphene (3,3), (b) β-Graphene (4,4)

Edge types	Frequency
D_{22}	$12mn + 6\ m + 18n$
D_{23}	$24mn - 4m + 4n$
D_{33}	$6mn - m + n$

Theorem 5.1 *If Γ is the molecular graph of a β - Graphyne, then the HDR multiplicative TIs are computed as*

1. $HDRMF_1I(\Gamma) = 126868945424839529040619765003881025120921190 4^{m*n} \times 131072^m \times 257049^{-m} \times 92611662449276690104 32^n$,
2. $HDRMF_2I(\Gamma) = 178488370033271965946836744880972344835984399015896537699555737 6^{mn} \times 65536^m \times 531441^{-m} \times 64247274650181814323502487961 6^n$,
3. $HDRMRRR(\Gamma) = 262144^{mn} \times 2^{-3m+3n}$,
4. $HDRMSDD(\Gamma) = 542800770374370512771595361^{mn} \times 18075490334784^{-mn} \times 41472^m \times 28561^{-m} \times 935886848^n \times 81^{-n}$,
5. $HDRFMHZI(\Gamma) = 217678233600000000000000000000000000000000000000000000000000^{mn} \times 4194304^m \times 3515625^{-m} \times 66408278665354385817600000000^n$,
6. $\mathrm{HDRMHI}(\Gamma) = 4096^{mn} \times 43451786041259765625^{-mn} \times 1875^m \times 1024^{-m} \times 30720000^{-n}$,
7. $\mathrm{HDRMSCI}(\Gamma) = 216000000000000^{-mn} \times 25^m \times 64^{-m} \times 6\,(_2)^{m-(}\Big)_2\Big) n \times 6553600^{-n}$,
8. $HDRMABCI(\Gamma) = 2985984^{-mn} \times 3^m \times 4^{-m} \times 3072^{-n}$,
9. $\mathrm{HDRMAZI}(\Gamma) = 708801874985091845381344307009569161216^{mn} \times 4096^m \times 729^{-m} \times 8404797768583914455 04^n$,
10. $HDRMReZG(\Gamma) = 59604644775390625^{mn} \times 5397312493181966745 6^{-mn} \times 1944^{m-n} \times 5 - 4m + 4n$,
11. $\mathrm{HDRMReZG_2}(\Gamma) = 5397312493181966745 6^{mn} \times 59604644775390625^{-mn} \times 5^{4m-4n} \times 1944 - m + n$,
12. $\mathrm{HDRMReZG_3}(\Gamma) = 197111727471974165070724487232199065600000000000000000000000^{mn} \times 524288^m \times 1366875^{-m} \times 2065563099607182816470630400 00^n$,
13. $\mathrm{HDRMM_{2^m}}(\Gamma) = 42247883974617233597120303333 36^{-mn} \times 729^m \times 256^{-m} \times 801543976648704^{-n}$,
14. $\mathrm{HDRMRR}(\Gamma) = 6499837226778624^{mn} \times 16^m \times 27^{-m} \times 28311552^n$,
15. $\mathrm{HDRMRI}(\Gamma) = 6499837226778624^{-mn} \times 27^m \times 16^{-m} \times 28311552^{-n}$,
16. $\mathrm{HDRMGAI}(\Gamma) = 36520347436056576^{mn} \times 59604644775390625^{-mn} \times 5^{4m-4n} \times 24^{-2m+2n}$.

Proof: Let Γ be the molecular graph of a β - Graphyne. The β-Graphyne, consists of $V(\Gamma) = 36mn + 2m + 24n$ and $E(\Gamma) = 42mn + m + 23n$. To compute the analytical expressions for Theorem 4, the definitions of HDR multiplicative TIs and the partition Table 3 have been used. The proof of this Theorem is similar to that of Theorem 1. □

Theorem 5.2 *If Γ is the molecular graph of β-Graphyne, then the M-polynomial is computed as* $M(\Gamma; w, k) = (12mn + 6\ m + 18n)w^2k^2 + (24mn - 4m + 4n)w^2k^3 + (6mn - m + n)w^3k^3$.

Proof: Using the definition of M-polynomial and the partition Table 3, the result is obtained as $M(\Gamma; w, k) = (12mn + 6m + 18n)w^2k^2 + (24mn - 4m + 4n)w^2k^3 + (6mn - m + n)w^3k^3$. Hence the proof. □

Theorem 5.3 *If Γ is the molecular graph of β-Graphyne, then the HDR indices are computed using M-polynomial as follows.*

1. $HDRABC(\Gamma) = 18\sqrt{2}mn + \sqrt{2}m + 11\sqrt{2}n + 4mn - \left(\frac{2}{3}\right)m + \left(\frac{2}{3}\right)n$,
2. $GA(\Gamma) = \left(\frac{576}{5}\right)\sqrt{6}m^2n^2 + \left(\frac{192}{5}\right)\sqrt{6}m^2n + 192\sqrt{6}mn^2 - \left(\frac{48}{5}\right)\sqrt{6}m^2 - \left(\frac{96}{5}\right)\sqrt{6}mn + \left(\frac{144}{5}\right)\sqrt{6}n^2 + 6mn - m + n$
3. $HDRB_1(\Gamma) = 444mn - 10m + 202n$,
4. $\mathrm{HDRB}_2(\Gamma) = 600\mathrm{mn} - 36m + 228n$,
5. $\mathrm{HDRHB}_1(\Gamma) = 2436mn - 150m + 918n$,
6. $\mathrm{HDRHB}_2(\Gamma) = 4920mn - 564m + 1332n$,
7. $HDRMB_1(\Gamma) = \left(\frac{578}{35}\right)mn + \left(\frac{131}{105}\right)m + \left(\frac{1129}{105}\right)n$,
8. $\mathrm{HDRMB}_2(\Gamma) = \left(\frac{41}{3}\right)mn + \left(\frac{31}{18}\right)m + \left(\frac{185}{18}\right)n$,
9. $\mathrm{HDRH}_b(\Gamma) = \left(\frac{1156}{35}\right)mn + \left(\frac{262}{105}\right)m + \left(\frac{2258}{105}\right)n$,
10. $\mathrm{HDRReZG}_1(\Gamma) = 36mn + 2m + 22n$,
11. $HD\,\mathrm{ReZ}\,G_2(\Gamma) = \left(\frac{249}{5}\right)mn - \left(\frac{3}{10}\right)m + \left(\frac{243}{10}\right)n$,
12. $HD\,\mathrm{ReZG}\,G_3(\Gamma) = 1236mn - 78m + 462n$,
13. $HDRSK = 102mn - m + 49n$, 14. $H^1_{DRSK} = 123mn - \left(\frac{9}{2}\right)m + \left(\frac{105}{2}\right)n$,
14. $\mathrm{HDRSK}_2 = 252mn - 10m + 106n$.
15. $HDRSK_2 = 252mn - 10m + 106n$

Proof: The β - Graphyne contains $V(\Gamma) = 36mn + 2m + 24n$ and $E(\Gamma) = 42mn + m + 23n$. In order to prove this theorem, we use the result of Theorem 5, frequency Table 3, and differential operators of M-Polynomial. The derived results are represented as above in Theorem 6. □

The computed expressions have been plotted against the variables m and n to better understand the behaviour of the degree-based indices in relation to the molecular structure. The graphical representation of the indices will assist the reader in recognising similarities in the behaviour of the computed indices. It is represented in Figure 4.

In this section, the numerical values of HDR TIs are calculated using the analytical expressions of two chemical compounds, by changing the values of the variable t from 1 to 9 . These values are presented in Table 7, Table 8 , Table 9, and Table 10. This comparative analysis is done to find out the similarities and differences between the individual topological indices, and they can be observed based on their numerical values. The results of the computations indicate that HDR TIs are highly dependent on the value of t, or the molecular structure. As a result, the magnitude of the indices increases as the value of t goes from 1 to 9 . The 3 D graphical representation for these numerical values is depicted in Figure 11, Figure 12, Figure 13, and Figure 14.

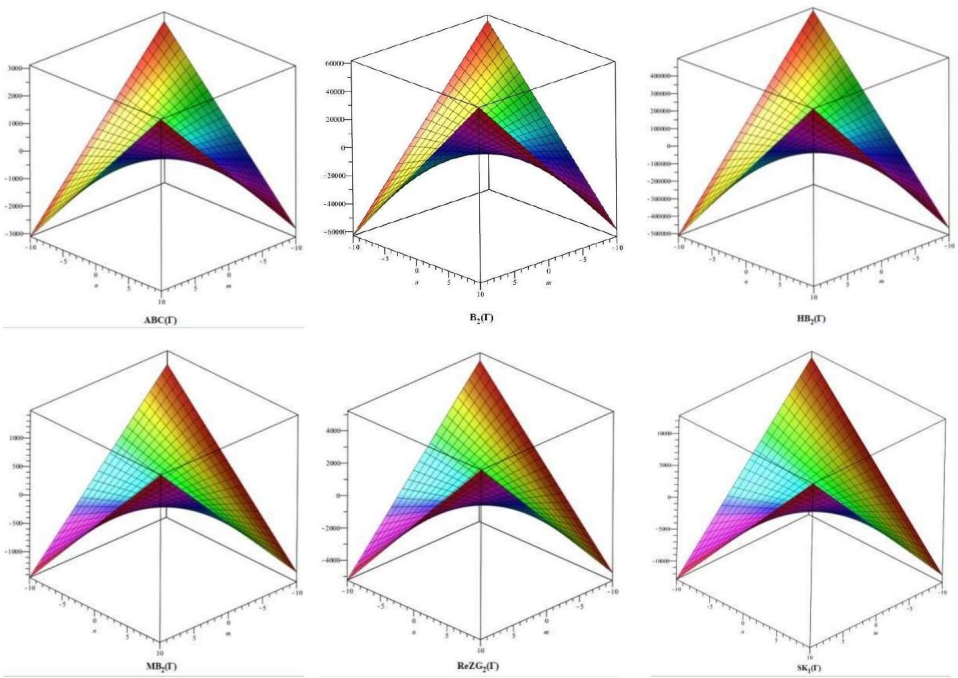

Figure 4: 3D comparison graph for Theorem 6

Table 3: Comparison Table for $ZHK(t)$

	ENT $_{M2m}$ (Γ)	ENT$_{Rm2}$ (Γ)	ENTHm ((	$ENT_A(\Gamma)$		
1	4.09	4.07	4.05	4.01	4.07	4.08
2	5.57	5.55	5.54	5.50	5.55	5.56
3	6.41	6.39	6.38	6.35	6.40	6.40
4	7.00	6.98	6.97	6.94	6.99	6.99
5	7.46	7.44	7.43	7.40	7.44	7.45

Table 4: Comparison Table for $ZHK(t)$

$ZHK(t)$	$ENT_{ABC}(\Gamma)$	$ENT_{GA}(\Gamma)$	$ENT_{SDD}(\Gamma)$	$ENT_R(\Gamma)$	$ENT_F(\Gamma)$	$ENT_\chi(\Gamma)$
1	4.10	4.10	4.32	4.13	4.07	4.10
2	5.58	5.58	5.69	5.65	5.56	5.58
3	6.42	6.42	6.49	6.51	6.40	6.42
4	7.01	7.01	7.06	7.10	6.99	7.01
5	7.47	7.47	7.51	7.56	7.45	7.46

Table 5: Comparison Table for $AHK(t)$

$AHK(t)$	$ENT_{M_1(\Gamma)}$	$ENT_{M2}(\Gamma)$	$ENT_{M2m}(\Gamma)$	$ENT_{RM_2(\Gamma)}$	$ENT_{HM}(\Gamma)$	$ENT_A(\Gamma)$
1	4.09	4.07	4.04	4.01	4.07	4.08
2	6.14	6.12	6.10	6.08	6.13	6.13
3	7.17	7.15	7.13	7.11	7.16	7.16
4	7.85	7.83	7.81	7.79	7.84	7.84
5	8.36	8.34	8.32	8.30	8.34	8.35

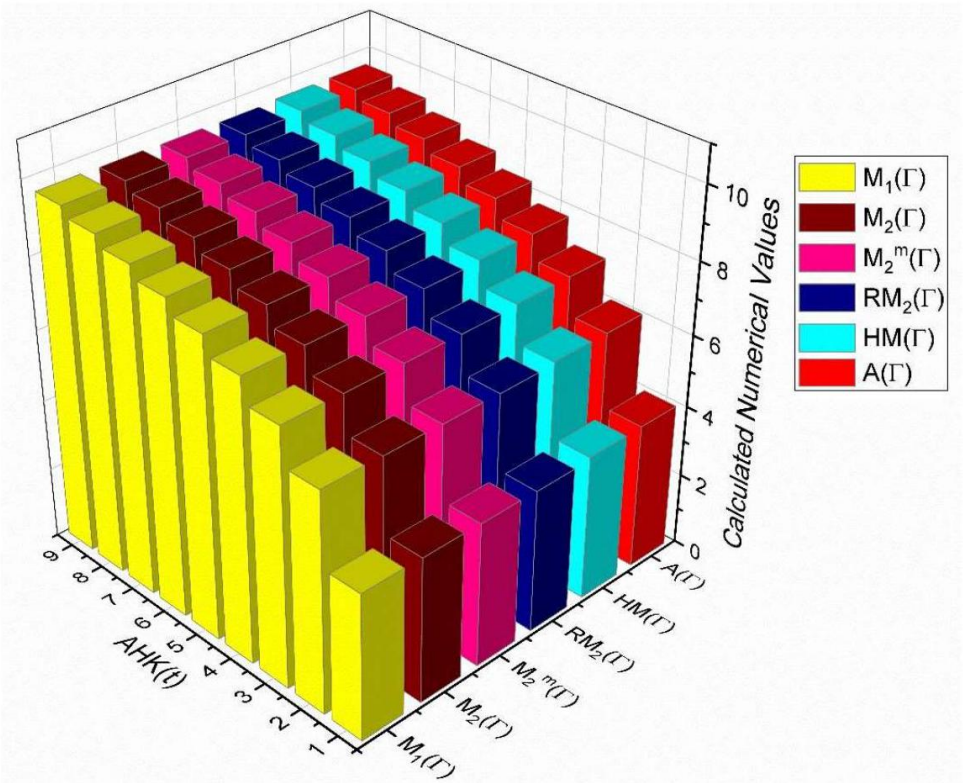

Figure 5: 3D plots for Table 9

Table 6: Comparison Table for $AHK(t)$

$ZHK(t)$	$ENT_{ABC}(\Gamma)$	$ENT_{GA}(\Gamma)$	$ENT_{SDD}(\Gamma)$	$E_T(\Gamma)$	$ENT_F(\Gamma)$	$ENT_\chi(\Gamma)$
1	4.10	4.10	4.10	4.09	4.07	4.10
2	6.15	6.15	6.15	6.14	6.13	6.15
3	7.18	7.18	7.18	7.17	7.16	7.18
4	7.86	7.86	7.86	7.85	7.84	7.86
5	8.37	8.37	8.36	8.36	8.35	8.36

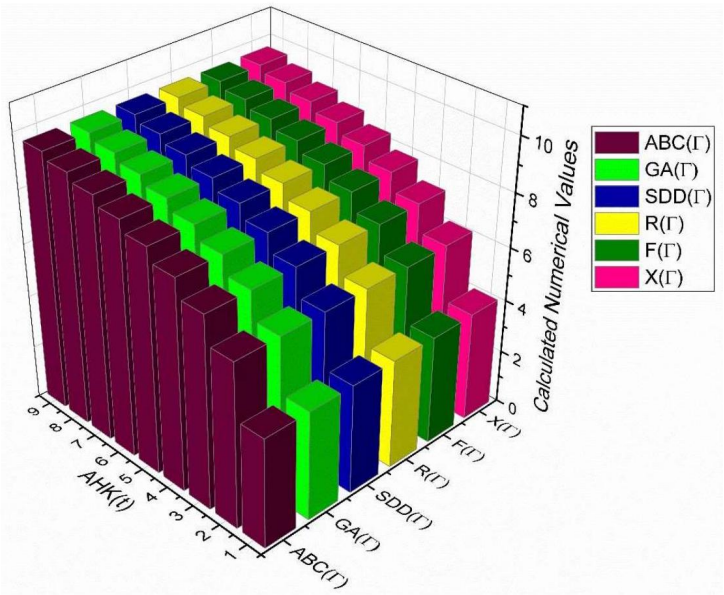

Figure 6: 3D plots for Table 10

6. Conclusion

In this research, the exact analytical expressions of different VDB TIs have been calculated for five significant classes of chemical compounds. Moreover, the analytical expressions obtained have been used to determine the numerical values for these expressions of different kinds of VDB TIs for five chemical compounds. The graphical representations of these numerical values create a visual representation of the relationship between the analytical expressions of VDB indices as well as the molecular graphs. These structures can also be studied using Wiener polarity-based indices, eccentricity-based TIs and the recent development of VDB indices, which have never been done before. It is still an area where more research could be done in the future.

Conflict of Interests

The authors declare that there is no conflict of interest regarding the publication of this paper.

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