Research Article

Topological Indices of Pent-Heptagonal Nanosheets via M-Polynomials

Hafiza Bushra Mumtaz,¹ Muhammad Javaid,¹ Hafiz Muhammad Awais,¹ and Ebenezer Bonyah²

¹Department of Mathematics, School of Science, University of Management and Technology (UMT), Lahore, Pakistan
²Department of Mathematics Education, Akenten Appiah-Menka University of Skills Training and Entrepreneurial Development, Kumasi 00233, Ghana

Correspondence should be addressed to Ebenezer Bonyah; ebbonya@gmail.com

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The combination of mathematical sciences, physical chemistry, and information sciences leads to a modern field known as cheminformatics. It shows a mathematical relationship between a property and structural attributes of different types of chemicals called quantitative-structures’ activity and qualitative-structures’ property relationships that are utilized to forecast the chemical sciences and biological properties, in the field of engineering and technology. Graph theory has originated a significant usage in the field of physical chemistry and mathematics that is famous as chemical graph theory. The computing of topological indices (TIs) is a new topic of chemical graphs that associates many physiochemical characteristics of the fundamental organic compounds. In this paper, we used the M-polynomial-based TIs such as 1st Zagreb, 2nd Zagreb, modified 2nd Zagreb, symmetric division deg, general Randić, inverse sum, harmonic, and augmented indices to study the chemical structures of pent-heptagonal nanosheets of VC₅C₇ and HC₅C₇. An estimation among the computed TIs with the help of numerical results is also presented.

1. Introduction

Nanostructures [1, 2] have been studied as new materials with the size of elemental structures that has been engineered at the nanometers’ scale. Most of the materials in this size range usually show novel behavior. Therefore, intervention in the characteristics of structures at the nanoscale allows the formation of devices and nanomaterials with completely or enhanced novel functionalities and properties. Understanding the science of nanostructures is curiosity and important driven not only for the interesting nature of the topic but also for novel and overwhelming usage of nanoscale systems in various fields of science and technology. Nanotechnology can be recognized as a technology of design, application, and fabrication of nanomaterials, and nanostructures [3].

The branch of nanotechnology and nanoscience is being perused by chemists, physicists, materials scientists, engineers, biologists, computer scientists, and mathematicians [4]. So, it is also interdisciplinary. Nanostructures may be divided based on modulation and dimensionality. Most of the distinct nanotubes, zeolites, aerogel, core-shell structure, and nanoporous materials have unique properties. Numerous techniques have been utilized for the synthesis of nanomaterials with no. of degrees of success, and several direct as well as indirect methods are used for their properties [5]. The motivation to develop the nanomaterials is that the characteristics become size based in the nanometer range due to quantum confinement effect and surface effect. The chemical bonds, magnetic properties, geometric structure, electronic properties, ionization potential, mechanical strength, optical properties, and thermal properties are affected due to particle size in nanometers range. Nanostructures show characteristics mostly higher than the conventional coarse-grained material. These contain hardness/increased strength, toughness/improved ductility,
enhanced diffusivity, reduced density, higher electrical resistance, reduced elastic modulus, lower thermal conductivity, increase specific heat, higher thermal expansion coefficient, increased oscillator and strength luminescence, blue shift absorption, and superior soft magnetic characteristics in comparison to the conventional bulk material. Furthermore, these characteristics are being briefly examined to discover new tools. The interesting branch of nanotechnology has a vast range of different types of applications. The use of nanomaterials has manufactured transistors having low speed and laser having low threshold current. These are utilized in satellite receivers having low noise amplification as a source for fiber optics communications and compact disk player systems. Constructive tools of nanostructures contain UV-resistant wood coating and self-cleaning glass. On the other hand, nanoscale tools are being utilized in the field of medicine for the prevention and treatment of diseases, diagnosis, and in magnetic resonance imaging, drug delivery system, radioactive tracers, etc. [6]. The importance of nanomaterials is rising nowadays. Many other types of tools may be possible with the peculiar and novel characteristics of nanomaterials [7, 8].

Therefore, TIs are useful to define molecular nanomaterials. Nanostructures, that have a scale of less than 100 nm, contain nanosheets, nanotubes, and nanoparticles. Nanosheets (two-dimensional nanomaterials) have a sharp edge and large surface area that cause them to play a vital role in various types of tools such as catalysis, energy storage bioelectronics, and optoelectronics [9, 10]. Silicone, borophene, and graphene are specific nanosheets. Due to the rare optical, electrical, mechanical, and structural characteristics, graphene nanosheets received great recognition from industrial and academic researchers [11]. The different properties of the $C_6C_8$ nanosheet have become the most advanced field in research. A $C_6C_8$ structure is developed by alternating $C_6$ and $C_8$ [7]. In 2009, Graovac et al. studied the GA index of $TUC_4C_8$ (S) nanotubes. In 2011, Graovac et al. [12] studied the fifth geometric arithmetic index for nanostar dendrimers, and Asadpour et al. calculated, Zagreb, Randić c, and ABC indices of $TUC_4C_8$ (R) and $TUC_4C_8$ (S) $V$-Phenylenic nanotorus and nanotubes. In 2014, Al-Fozan et al. solved Szeged index of H-naphthalene nanosheets (2n, 2m) and $C_nC_q$ (S). Logman and Ashrafi studied the Padmakar–Ivan (PI) index of $TUC_4C_8$ (S) nanotubes. For further discussion, see [13–15].

However, the combination of three fields such as mathematics, physical chemistry, and information sciences lead to a modern field known as cheminformatics [16–18]. It develops a mathematical relationship between a property and structural attributes of different types of chemicals called by quantitative-structures’ activity and qualitative-structures’ property relationships that are utilized to forecast the organic sciences and biological properties in the field of engineering and technology [19, 20]. Graph theory has originated a significant usage in the field of mathematical chemistry that is famous as chemical graph theory.

Polya gave the idea for counting polynomials in the field of chemistry [21], and Wiener introduced the concept of TI related to the paraffin’s boiling point [22]. Computing the TIs is a new field of chemical graphs that associates many physiochemical characteristics of the fundamental chemical compounds [23–27].

## 2. Preliminaries

A molecular structure $\Gamma = (V(\Gamma), E(\Gamma))$; $V(\Gamma) = \{s_1, s_2, s_3, \ldots, s_n\}$ and $E(\Gamma)$ are nodes (vertices) and edge set of $\Gamma$. $|V(\Gamma)| = v$ and $|E(\Gamma)| = e$ is the order and size of $\Gamma$. In a connected and simple molecular graph, a path is represented within two vertices and the distance between the two vertices $s$ and $t$ is mentioned as $\varphi(s,t)$, in a graph $\Gamma$, see [28–30]. In this paper, a graph is connected and simple, having no multiple edges or loops.

1st and 2nd Zagreb indices: let $\Gamma$ be a molecular structure; then, its 1st and 2nd Zagreb indices [31] are

$$M_1(\Gamma) = \sum_{v \in V(\Gamma)} [\varphi(s) + \varphi(t)],$$

$$M_2(\Gamma) = \sum_{e \in E(\Gamma)} [\varphi(s) \times \varphi(t)].$$

General Randić $c$ index: if $R$ is the real number, $\alpha \in R$, and $\Gamma$ is a molecular structure, the general Randić $c$ index [32] is

$$R_n(\Gamma) = \sum_{st \in E(\Gamma)} [\varphi(s)\varphi(t)]^n.$$  

Symmetric division deg index: for a molecular structure $\Gamma$, the symmetric division deg index [33] is

$$SDD(\Gamma) = \sum_{st \in E(\Gamma)} \left[ \frac{\min(\varphi(s), \varphi(t))}{\max(\varphi(s), \varphi(t))} + \frac{\max(\varphi(s), \varphi(t))}{\min(\varphi(s), \varphi(t))} \right].$$

Harmonic index: for a molecular structure $\Gamma$, the harmonic index [34] is

$$H(\Gamma) = \sum_{st \in E(\Gamma)} \frac{2}{\varphi(s) + \varphi(t)}.$$  

Inverse sum index: for a molecular structure $\Gamma$, the inverse sum index [35] is

$$IS(\Gamma) = \sum_{st \in E(\Gamma)} \frac{\varphi(s)\varphi(t)}{\varphi(s) + \varphi(t)}.$$  

Augmented Zagreb index: for a molecular structure $\Gamma$, the augmented Zagreb index [13] is

$$AZI(\Gamma) = \sum_{st \in E(\Gamma)} \left[ \frac{\varphi(s)\varphi(t)}{\varphi(s) + \varphi(t) - 2} \right]^3.$$

A graph polynomial is a graph invariant whose values are polynomials. So, all these invariants are discussed in algebraic graph theory [36]. Among such types of algebraic polynomials, the M-polynomial, defined in 2015, shows the same role in finding the much closed form of various degree-based TIs that correlate different types of chemical properties of the various materials under
investigation. In 2019, Yang et al. [37] find out the M-polynomial and topological indices of benzene ring embedded in P-type surface network. In 2020, Khalaf et al. [38] computed the M-polynomial and topological indices of book graph and Raza and Sakaiti [2] solved the M-polynomial and degree-based topological indices of some nanostructures. In 2021, Mondal et al. [39] find out the neighborhood M-polynomial of titanium compounds and Irfan et al. [1] computed the M-polynomials and topological indices for line graphs of chain silicate network and H-naphtalenic nanotubes. M-Polynomial: let \( \Gamma \) be a molecular structure and \( m_{ij} \), \( i, j \geq 1 \), be the number of edges \( e = st \) of \( \Gamma \) in such a way that \( \{\varphi(s)\varphi(t)\} = [i, j] \). The M-polynomial of \( \Gamma \) is

\[
M(\Gamma, \mu, \nu) = \sum_{i \leq j(\Gamma)} \left( m_{ij} \mu^i \nu^j \right).
\]

Now, we discussed the relationship between the M-polynomial and some important TIs in the form of Tables 1 and 2.

3. Pent-Heptagonal Nanosheet

Firstly, we discuss the structure of pent-heptagonal nanosheet \( V_{C_5C_7} \). For nanosheet of \( V_{C_5C_7} \), we represent the number of pentagons in the first row by \( b \), and the first four rows of nodes as well as edges are repeated. Therefore, we represent the number of repetitions as \( a \). The nanosheet \( V_{C_5C_7}(2, 4) \) has \( 16ab + 2a + 5b \) nodes or vertices and \( 24ab + 4b \) edges. Additionally, it has \( 6a + 7b \) nodes having degree 2 and \( 16ab - 4a - 2b \) nodes having degree 3. The degree-based edge partition of nanosheet \( a = 2 \) and \( b = 4 \) is shown in Table 3.

From Figure 1, we note that 2 distinct types of vertices in \( V_{C_5C_7} \) are 2 and 3. So,

\[
V_1 = \{ s \in V(\Gamma_1) | \varphi(s) = 2 \}
\]

\[
V_2 = \{ s \in V(\Gamma_1) | \varphi(s) = 3 \}.
\]

We have 3 different types of edges that is based on the degree of end nodes in \( (\Gamma_1) \) that are

\[
E_{2.2} = \{ st \in (\Gamma_1) | \varphi(s) = 2, \varphi(t) = 2 \}
\]

\[
E_{2.3} = \{ st \in (\Gamma_1) | \varphi(s) = 2, \varphi(t) = 3 \}
\]

\[
E_{3.3} = \{ st \in (\Gamma_1) | \varphi(s) = 3, \varphi(t) = 3 \},
\]

where \( |E_1| = (2a + 2b + 4), \ |E_2| = (8a + 10b - 8), \ |E_3| = (24ab - 10a - 8b + 4), \) and \( a = 2 \) and \( b = 4 \). Then,

\[
|E(\Gamma_1)| = |E_1| + |E_2| + |E_3| = 16 + 48 + 144 = 208.
\]

Now, we discuss the structure of pent-heptagonal nanosheet \( H_{C_5C_7} \). For the nanosheet \( H_{C_5C_7} \), we represent the number of pentagons in the first row by \( b \), and the 1st four rows of nodes and edges are repeated. So, we represent the number of repetitions as \( a \). The nanosheets \( H_{C_5C_7}(2, 4) \) have \( 16ab + 2a + 4b \) vertices and \( 24ab + 3b \) edges. Moreover, it has \( 6a + 6b \) vertices with degree 2 and \( 16ab - 4a - 2b \) vertices with degree 3. The degree-based edge partition of nanosheets for \( a = 2 \) and \( b = 4 \) is shown in Table 4.

From Figure 2, we note that 2 distinct types of vertices in \( H_{C_5C_7} \) are 2 and 3. So,

\[
V_1 = \{ s \in V(\Gamma_2) | \varphi(u) = 2 \},
\]

\[
V_2 = \{ s \in V(\Gamma_2) | \varphi(u) = 3 \}.
\]

We have 3 different types of edges that is based on the degree of end nodes in \( (\Gamma_2) \):

\[
E_{2.2} = \{ st \in (\Gamma_2) | \varphi(s) = 2, \varphi(t) = 2 \},
\]

\[
E_{2.3} = \{ st \in (\Gamma_2) | \varphi(s) = 2, \varphi(t) = 3 \},
\]

\[
E_{3.3} = \{ st \in (\Gamma_2) | \varphi(s) = 3, \varphi(t) = 3 \}.
\]

4. Main Results

This section deals with the main results consisting of polynomials and TIs of the nanosheets.
Let $\Gamma = V C_5 C_7$ be the pent-heptagonal nanosheet. Then, the $M$-polynomial of $\Gamma$ is
\[
M(\Gamma, \mu, \nu) = (2a + 2b + 4)\mu^2 \nu^2 + (8a + 10b - 8)\mu^2 \nu^3 + (24ab - 10a - 8b + 4)\mu^3 \nu^3. 
\]  
(13)

Proof. Now, by using definition of $M$-polynomial of $(\Gamma_1)$, we obtain
\[
M(\Gamma_1, \mu, \nu) = \sum_{s \leq 1} [E_{2s}(\Gamma_1)\mu^s \nu^s]
= \sum_{2 \leq s \leq 2} [E_{2s}(\Gamma_1)\mu^s \nu^s] + \sum_{2 \leq s \leq 3} [E_{2s}(\Gamma_1)\mu^s \nu^s]
= \sum_{3 \leq s \leq 3} [E_{3s}(\Gamma_1)\mu^s \nu^s]
= [E_1(\mu^2 \nu^2) + E_2(\mu^3 \nu^3) + E_3(\mu^3 \nu^3)]
= (2a + 2b + 4)\mu^2 \nu^2 + (8a + 10b - 8)\mu^2 \nu^3 + (24ab - 10a - 8b + 4)\mu^3 \nu^3.
\]  
(14)
The $M$-polynomial of $(\Gamma_1)$ is
\[
M(\Gamma_1, \mu, \nu) = (2a + 2b + 4)\mu^2 \nu^2 + (8a + 10b - 8)\mu^2 \nu^3 + (24ab - 10a - 8b + 4)\mu^3 \nu^3.
\]  
(15)

Theorem 2. Let $\Gamma = V C_5 C_7$ be the pent-heptagonal nanosheet. Then, the $M$-polynomial of $\Gamma$ is
\[
M(\Gamma, \mu, \nu) = (2a + 2b + 4)\mu^2 \nu^2 + (8a + 10b - 8)\mu^2 \nu^3 + (24ab - 10a - 8b + 4)\mu^3 \nu^3.
\]  
(16)

So, the 1st Zagreb index ($M_1(\Gamma_1)$), 2nd Zagreb index ($M_2(\Gamma_1)$), 2nd modified Zagreb (MM$_2$($\Gamma_1$)), general Randic ($R_\alpha(\Gamma_1)$), reciprocal general Randic RR$_\alpha(\Gamma_1)$, where $\gamma \in \alpha$, and the symmetric division deg index ($SDD(\Gamma_1)$) obtained from $M$-polynomial are as follows:

(a) $M_1(\Gamma_1) = 144ab - 12a + 10b$
(b) $M_2(\Gamma_1) = 216ab - 34a - 4b + 4$
(c) $MM_2(\Gamma_1) = 8/3ab + 13/18a + 23/18b + 1/9$
(d) $R_\gamma(\Gamma_1) = (4)^\gamma(2a + 2b + 4) + (6)^\gamma(8a + 10b - 8) + (9)^\gamma(24ab - 10a - 8b + 4)$
(e) $RR_\gamma(\Gamma_1) = 2a + 2b + 4/4(4)^\gamma + 8a + 10b - 8/6\gamma(24ab - 10a - 8b + 4)^9$
(f) $SDD(\Gamma_1) = 48ab + 4/3a + 29/3b - 4/3$

Proof. Let $f(\mu, \nu) = M(\Gamma_1, \mu, \nu)$ be the $M$-polynomial of the pent-heptagonal nanosheet $VC_5 C_7$, then,
\[
f(\mu, \nu) = (2a + 2b + 4)\mu^2 \nu^2 + (8a + 10b - 8)\mu^2 \nu^3 + (24ab - 10a - 8b + 4)\mu^3 \nu^3.
\]  
(17)

Firstly, we find out the required partial derivatives and integrals as
\[
D_\mu f(\mu, \nu) = 2(2a + 2b + 4)\mu^2 \nu^2 + 2(8a + 10b - 8)\mu^2 \nu^3 + (24ab - 10a - 8b + 4)\mu^3 \nu^3
\]  
\[
D_\nu f(\mu, \nu) = 2(2a + 2b + 4)\mu^2 \nu^2 + 3(8a + 10b - 8)\mu^2 \nu^3 + 3(24ab - 10a - 8b + 4)\mu^3 \nu^3
\]  
\[
D_\mu D_\nu f(\mu, \nu) = 2(a + b + c)\mu^2 \nu^2 + (8a + 10b - 8/3)\mu^2 \nu^3 + (8ab - 10a - 8b + 4/3)\mu^3 \nu^3
\]  
\[
D_\mu T_\nu f(\mu, \nu) = D_\mu(T_\nu f(\mu, \nu)) = (a + b + c)\mu^2 \nu^2 + (8a + 10b - 8/3)\mu^2 \nu^3 + (8ab - 10a - 8b + 4/3)\mu^3 \nu^3
\]  
\[
D_\nu T_\mu f(\mu, \nu) = D_\nu(T_\mu f(\mu, \nu)) = (a + b + c)\mu^2 \nu^2 + (8a + 10b - 8/3)\mu^2 \nu^3 + (8ab - 10a - 8b + 4/3)\mu^3 \nu^3
\]  
\[
D_\mu T_\mu f(\mu, \nu) = D_\mu(T_\mu f(\mu, \nu)) = 2(a + b + c)\mu^2 \nu^2 + 3(4a + 5b - 4)\mu^2 \nu^3 + 3(8ab - 10a - 8b + 4/3)\mu^3 \nu^3
\]  
\[
D_\nu T_\nu f(\mu, \nu) = D_\nu(T_\nu f(\mu, \nu)) = 2(a + b + c)\mu^2 \nu^2 + 2/3(8a + 10b - 8)\mu^2 \nu^3 + (24ab - 10a - 8b + 4/3)\mu^3 \nu^3
\]  
\[
D_\mu D_\nu T_\nu f(\mu, \nu) = (4)^\gamma(2a + 2b + 4)\mu^2 \nu^2 + (8a + 10b - 8)\mu^2 \nu^3 + (9)^\gamma(24ab - 10a - 8b + 4)\mu^3 \nu^3
\]  
\[
T_\mu f(\mu, \nu) = (8a + 5b + 3a + 3b - 8/3)\mu^2 \nu^2 + (8a + 10b - 8)(6)\mu^2 \nu^3 + (24ab - 10a - 8b + 4)(9)\mu^3 \nu^3
\]  
\[
T_\nu f(\mu, \nu) = 8ab + 5/3a + 10/3b - 8/3
\]  
Now, we obtain $\mu = \nu = 1$:
\[
D_\mu f(\mu, \nu)|_{\mu=\nu=1} = 72ab - 10a + 4
\]  
\[
D_\nu f(\mu, \nu)|_{\mu=\nu=1} = 72ab - 2a + 10b - 4
\]  
\[
D_\mu(D_\nu f(\mu, \nu))|_{\mu=\nu=1} = 216ab - 34a - 4b + 4
\]  
\[
T_\nu f(\mu, \nu)|_{\mu=\nu=1} = 8ab + 5/3a + 10/3b - 8/3
\]  
\[
T_\nu f(\mu, \nu)|_{\mu=\nu=1} = 8ab + 1/3a + 5/3b - 4/3
\[ T_\mu (\mathcal{T}_\nu (f (\mu, \nu)))) |_{\mu = \nu = 1} = 8/3ab + 13/18a + 23/18b - 8/9 \]
\[ D_\mu (\mathcal{T}_\nu (f (\mu, \nu)))) |_{\mu = \nu = 1} = 24ab + 4a + 9b - 4 \]
\[ D_\mu (\mathcal{T}_\nu (f (\mu, \nu)))) |_{\mu = \nu = 1} = 24ab - 8/3a + 2/3b + 8/3 \]
\[ D_\mu^2 (\mathcal{T}_\nu^2 (f (\mu, \nu)))) |_{\mu = \nu = 1} = (4)T^2 (2a + 2b + 4) + (6)(8a + 10b - 8) + (9)^2 (24ab - 10a - 8b + 4) \]
\[ T_\mu^2 (\mathcal{T}_\nu^2 (f (\mu, \nu)))) |_{\mu = \nu = 1} = (2a + 2b + 4)/(4)T^2 (8a + 10b - 8)/(6)^2 + (24ab - 10a - 8b + 4)/(9)^2 \]

Consequently,

(i) First Zagreb index: \( M_1 (\Gamma, \mu, \nu) = (D_\mu + D_\nu) (f (\mu, \nu)) |_{\mu = \nu = 1} = (72ab - 10a + 4) + (72ab - 2a + 10b - 4) = 144ab - 12a + 10b \)

(ii) Second Zagreb index: \( M_2 (\Gamma, \mu, \nu) = (D_\mu D_\nu) (f (\mu, \nu)) |_{\mu = \nu = 1} = 216ab - 34a - 4b + 4 \)

(iii) Second modified Zagreb index: \( MM_2 (\Gamma, \mu, \nu) = (T_\mu T_\nu) (f (\mu, \nu)) |_{\mu = \nu = 1} = T_\mu (T_\nu (f (\mu, \nu))) |_{\mu = \nu = 1} = 8/3ab + 13/18a + 23/18b + 1/9 \)

(iv) General Randic index: \( R_\mu (\Gamma, \mu, \nu) = (D_\mu^2 D_\nu^2) (f (\mu, \nu)) |_{\mu = \nu = 1} = (4)^2 (2a + 2b + 4) + (6)^2 (8a + 10b - 8) + (9)^2 (24ab - 10a - 8b + 4) \)

(v) Reciprocal general Randic index: \( R_\mu (\Gamma, \mu, \nu) = (D_\mu D_\nu) (f (\mu, \nu)) |_{\mu = \nu = 1} = 24ab - 8/3a + 2/3b + 8/3 + (24ab + 4a + 9b - 4) = 48ab + 4/3a + 29/3b - 4/3 \)

(vi) Symmetric division deg index: \( SDD (\Gamma, \mu, \nu) = (D_\mu^3 T_\nu + D_\mu T_\nu^3) (f (\mu, \nu)) |_{\mu = \nu = 1} = (2a + 2b + 4)\mu^2 \nu^2 + (8a + 10b - 8)\mu^3 \nu^3 \]
\[ + (24ab - 10a - 8b + 4)\mu^3 \nu^3 \]

Then, harmonic index \( H (\Gamma_1) \), inverse index \( IS (\Gamma_1) \) and augmented Zagreb index \( AZI (\Gamma_1) \) obtained from \( M \)-polynomial are as follows:

(a) \( H (\Gamma_1) = 13/15a + 7/3b + 8ab + 2/15 \)

(b) \( IS (\Gamma_1) = 36ab - 17/5a + 44b + 2/5 \)

(c) \( AZI (\Gamma_1) = 273.375ab - 33.90625a + 4.875b + 13.5625 \)

Proof. Let \( f (\mu, \nu) = M (\Gamma_1, \mu, \nu) \) be the \( M \)-polynomial of the pent-heptagonal nanosheets \( VC_5C_7 \) then,

\[ f (\mu, \nu) = (2a + 2b + 4)\mu^2 \nu^2 + (8a + 10b - 8)\mu^3 \nu^3 \]
\[ + (24ab - 10a - 8b + 4)\mu^3 \nu^3 \]

Firstly, we find out the required partial derivatives and integrals are as follows:

\[ J (f (\mu, \nu)) = (2a + 2b + 4)\mu^4 + (8a + 10b - 8)\mu^5 + (24ab - 10a - 8b + 4)\mu^6 \]
\[ T_\mu^2 (J (f (\mu, \nu))) = (a/2 + b/2 + 1)\mu^4 + (8/5a + 2b - 8/5)\mu^6 + (4ab - 5/3a - 4/3b + 2/3)\mu^6 \]
\[ J (D_\mu (D_\nu (f (\mu, \nu)))) = (8a + 8b + 16)\mu^4 + (48a + 60b - 48)\mu^5 + (216ab - 90a - 72b - 36)\mu^6 \]
\[ Q_2 (J (D_\mu (D_\nu (f (\mu, \nu)))) = (8a + 8b + 16)\mu^4 + (48a + 60b - 48)\mu^5 + (216ab - 90a - 72b - 36)\mu^6 \]
\[ T_\mu^2 (J (D_\mu^2 D_\nu (f (\mu, \nu)))) = (2a + 2b + 4)\mu^4 + 1/5 (48a + 60b - 48)\mu^5 + (36ab - 15a - 12b + 6)\mu^6 \]
\[ D_\mu^3 (D_\nu (f (\mu, \nu))) = (4)^2 (2a + 2b + 4)\mu^5 + (6)^2 (8a + 10b - 8)\mu^6 + (9)^2 (24ab - 10a - 8b + 4)\mu^7 \]
\[ J (D_\mu^3 D_\nu^2 (f (\mu, \nu))) = (4)^2 (2a + 2b + 4)\mu^2 + (6)^2 (8a + 10b - 8)\mu^3 + (9)^2 (24ab - 10a - 8b + 4)\mu^4 \]

Now, we obtain \( \mu = \nu = 1 \):

\[ T_\mu (J (f (\mu, \nu))) |_{\mu = \nu = 1} = 13/30 a + 7/6 b + 4ab + 1/15 \]
\[ T_\mu (Q_2 (J (D_\mu (D_\nu (f (\mu, \nu)))))) |_{\mu = \nu = 1} = 36ab - 17/5 a + 2b + 2/5 \]
\[ T_\mu^3 (J (D_\mu^2 D_\nu^2 (f (\mu, \nu)))) |_{\mu = \nu = 1} = 8(2a + 2b + 4) + 8(8a + 10b - 8) \]
\[ + (729/64)(24ab - 10a - 8b + 4) \]
\[ = 273.375ab - 33.90625a + 4.875b + 13.5625 \]

Consequently,

(i) Harmonic index:
Now, by using definition of M-polynomial for $\Gamma$, we have

$$M(\Gamma_1, 2, \mu, \nu) = (2a + 3b + 2)\mu^2\nu^2 + (8a + 6b - 4)\mu^2\nu^3 + (24ab - 10a - 6b + 10)\mu^3\nu^3.$$  

Proof. For $\Gamma_2 = HC_5C_7$, we have

$$M(\Gamma_2, \mu, \nu) = (2a + 3b + 2)\mu^2\nu^2 + (8a + 6b - 4)\mu^2\nu^3 + (24ab - 10a - 6b + 10)\mu^3\nu^3.$$  

(iv) Augmented Zagreb index:

$$ AZI(\Gamma_1) = T^2_{\mu}(\chi_{\mu}(\chi_{\mu}(f(\mu, \nu)))) = \left(\frac{4}{3}ight)^3 (2a + 2b + 4) + \left(\frac{6}{3}ight)^3 (8a + 10b - 8) + \left(\frac{9}{4}ight)^3 (24ab - 10a - 8b + 4) $$

$$ = 273.375ab - 33.90625a + 4.875b + 13.5625. \tag{23}

Theorem 4. Let $\Gamma_2 = HC_5C_7$ be the second pent-heptagonal nanosheets; the M-polynomial of $(\Gamma_2)$ is

$$M(\Gamma_2, \mu, \nu) = (2a + 3b + 2)\mu^2\nu^2 + (8a + 6b - 4)\mu^2\nu^3 + (24ab - 10a - 6b + 10)\mu^3\nu^3. \tag{24}$$

Proof. Now, by using definition of M-polynomial for $(\Gamma_2)$,

$$M(\Gamma_2, \mu, \nu) = \sum_{k=1}^{\ell} \left[ E_{2,2} (\Gamma) \mu^2 \nu^2 \right] + \sum_{k=1}^{L_3} \left[ E_{3,3} (\Gamma) \mu^2 \nu^3 \right] + \sum_{k=1}^{L_3} \left[ E_{3,3} (\Gamma) \mu^2 \nu^3 \right] = E_{1,2} \mu^2 \nu^2 + E_{2,2} \mu^2 \nu^2 + E_{3,3} \mu^2 \nu^3 + E_{4,3} \mu^2 \nu^3 = (2a + 3b + 2)\mu^2\nu^2 + (8a + 6b - 4)\mu^2\nu^3 + (24ab - 10a - 6b + 10)\mu^3\nu^3. \tag{25}$$

The M-polynomial of $(\Gamma_2)$ is

$$M(\Gamma_2, \mu, \nu) = (2a + 3b + 2)\mu^2\nu^2 + (8a + 6b - 4)\mu^2\nu^3 + (24ab - 10a - 6b + 10)\mu^3\nu^3. \tag{26}$$

Theorem 5. Let $\Gamma_2 = HC_5C_7$ be the pent-heptagonal nanosheets. Then, the M-polynomial of $(\Gamma_2)$ is

$$M(\Gamma_2, \mu, \nu) = (2a + 3b + 2)\mu^2\nu^2 + (8a + 6b - 4)\mu^2\nu^3 + (24ab - 10a - 6b + 10)\mu^3\nu^3. \tag{27}$$

So, the 1st Zagreb index $(M_1(\Gamma_2))$, 2nd modified Zagreb $(MM_2(\Gamma_2))$, general Randic $(R_\gamma(\Gamma_2))$, where $\gamma \in \alpha$, reciprocal general Randic $(RR_\gamma(\Gamma_2))$, where $\gamma \in \alpha$, and the symmetric division deg index $(\text{SDD}(\Gamma_2))$ obtained from M-polynomial are as follows:

(a) $M_1(\Gamma_2) = 144ab - 12a + 6b + 48$
(b) $M_2(\Gamma_2) = 216ab - 34a - 6b + 74$
(c) $MM_2(\Gamma_2) = 8/3ab + 13/18a + 13/12b + 17/18$
(d) $R_\gamma(\Gamma_2) = (4\gamma)^2 (2a + 3b + 2) + (6\gamma)^2 (8a + 6b - 4) + (9\gamma)^2 (24ab - 10a - 6b + 10)$
(e) $RR_\gamma(\Gamma_2) = 2a + 3b + 2 (4\gamma)^2 + 8a + 6b - 4 (6\gamma)^2 + 24ab - 10a - 6b + 10$\gamma^3$
(f) $\text{SDD}(\Gamma_2) = 48ab + 4/3a + 7b + 46/3$

$$f(\mu, \nu) = (2a + 3b + 2)\mu^2\nu^2 + (8a + 6b - 4)\mu^2\nu^3 + (24ab - 10a - 6b + 10)\mu^3\nu^3. \tag{28}$$

$D_{\mu}(f(\mu, \nu)) = 2(2a + 3b + 2)\mu^2\nu^2 + 2(8a + 6b - 4)\mu^2\nu^3 + 3(24ab - 10a - 6b + 10)\mu^3\nu^3$
$D_{\mu}(f(\mu, \nu)) = 2(2a + 3b + 2)\mu^2\nu^2 + 3(8a + 6b - 4)\mu^2\nu^3 + 3(24ab - 10a - 6b + 10)\mu^3\nu^3$
$D_{\mu}(f(\mu, \nu)) = 4(2a + 3b + 2)\mu^2\nu^2 + 6(8a + 6b - 4)\mu^2\nu^3 + 9(24ab - 10a - 6b + 10)\mu^3\nu^3$
$T_{\mu}(f(\mu, \nu)) = (a + (3/2)b + 1)\mu^2\nu^2 + (4a + 3b + 2)\mu^2\nu^3 + (8ab - (10/3)a - 2b + (10/3)\mu^3\nu^3)$
$T_{\mu}(f(\mu, \nu)) = (a + (3/2)b + 1)\mu^2\nu^2 + ((8/3)a + 2b - (4/3))\mu^2\nu^3 + (8ab - (10/3)a - 2b + (10/3)\mu^3\nu^3)$
$T_{\mu}(f(\mu, \nu)) = 1/4(2a + 3b + 2)\mu^2\nu^2 + 1/6(8a + 6b - 4)\mu^2\nu^3 + 1/9(24ab - 10a - 6b + 10)\mu^3\nu^3$
$D_{\mu}T_{\mu}(f(\mu, \nu)) = D_{\mu}(T_{\mu}(f(\mu, \nu))) = (2a + 3b + 2)\mu^2\nu^2 + 3(4a + 3b + 2)\mu^2\nu^3 + 3(8ab - 10/3a - 2b + (10/3)\mu^3\nu^3)$
$D_{\mu}T_{\mu}(f(\mu, \nu)) = D_{\mu}(T_{\mu}(f(\mu, \nu))) = (2a + 3b + 2)\mu^2\nu^2 + 2(8/3a + 2b - 4/3)\mu^2\nu^3 + (24ab - 10a - 6b + 10)\mu^3\nu^3$
Consequently, 

(i) First Zagreb index: \( M_1(\Gamma_2) = (D_\mu + D_\nu) (f (\mu, \nu)) \bigg|_{\mu = \nu = 1} = 72ab - 10a + 26 \)

(ii) Second Zagreb index: \( M_2(\Gamma_2) = (D_\mu D_\nu) (f (\mu, \nu)) \bigg|_{\mu = \nu = 1} = 216ab - 34a - 6b + 74 \)

(iii) Second modified Zagreb index: \( MM_2(\Gamma_2) = (T_\mu T_\nu) (f (\mu, \nu)) \bigg|_{\mu = \nu = 1} = 8/3ab + 13/18a + 13/12b + 17/18 \)

(iv) General Randic index: \( R_\nu(\Gamma_2) = (D_\mu D_\nu^\nu) (f (\mu, \nu)) \bigg|_{\mu = \nu = 1} = (4)^y (2a + 3b + 2) + (6)^y (8a + 6b - 4) \)

(v) Reciprocal general Randic index: \( RR_\nu(\Gamma_2) = (T_\mu T_\nu^\nu) (f (\mu, \nu)) \bigg|_{\mu = \nu = 1} = (2a + 3b + 2) (4)^y (8a + 6b - 4) \)

(vi) Symmetric division deg index: \( SDD(\Gamma_2) = (D_\mu T_\nu + D_\nu T_\nu) (f (\mu, \nu)) \bigg|_{\mu = \nu = 1} = (24ab - 8/3a + b + 28/3) + (24ab + 4a + 6b + 6) \)

\( T_\mu (f (\mu, \nu)) \bigg|_{\mu = \nu = 1} = 1/4 (2a + 3b + 2) + 1/5 (8a + 6b - 4) + 1/6 (24ab - 10a - 6b + 10) \)

\[ = \frac{13}{30} a + \frac{19}{20} + 4ab + \frac{41}{30}, \]

\[ = \frac{1}{5} (180ab - 17a - 6b + 36), \]

\[ T_\mu (Q_2 (f (\mu, \nu))) \bigg|_{\mu = \nu = 1} = \frac{1}{4} (8a + 12b + 8) + \frac{1}{5} (48a + 36b - 24) + \frac{1}{6} (216ab - 90a - 54b + 90) \]

\[ = \frac{1}{5} (180ab - 17a - 6b + 36), \]
\begin{equation}
T^{3}_{\mu}(f(D^{3}_{\mu}D^{3}_{\nu}(f(\mu, \nu)))) = 8(2a + 3b + 2) + 8(8a + 6b - 4) + \left(\frac{9}{4}\right)^3(24ab - 10a - 6b + 10)
\end{equation}

\begin{align*}
&= 8(2a + 3b + 2) + 8(8a + 6b - 4) + (11.3906)(24ab - 10a - 6b + 10) \\
&= 273.3744ab - 33.90625a + 3.6564b + 97.906.
\end{align*}

Consequently, (i) Harmonic index:
\[ H(\Gamma_2) = 2T_\mu (J(\mu, \nu)) \big|_{\mu=\nu=1} \]
\[ = 2 \left[ \frac{1}{4} (2a + 3b + 2) + \frac{1}{5} (8a + 6b - 4) + \frac{1}{6} (24ab - 10a - 6b + 10) \right] \]
\[ = 8ab + \frac{13}{15} a + \frac{19}{10} b - \frac{11}{3} \]

(ii) Inverse index:

**Figure 4:** Graphical comparison between \( M_1(\Gamma_2), M_2(\Gamma_2), MM_1(\Gamma_2), \) and SDD(\( \Gamma_2 \)) of \( HC_5C_7 \) and comparison between \( H(\Gamma_1), IS(\Gamma_1), \) and AZI(\( \Gamma_1 \)) of \( VC_5C_7 \).

**Table 7:** Comparison between \( H(\Gamma_1), IS(\Gamma_1), \) and AZI(\( \Gamma_1 \)) of \( VC_5C_7 \).

| \( a, b \) | \( H(\Gamma_1) \) | \( IS(\Gamma_1) \) | \( AZI(\Gamma_1) \) |
|---|---|---|---|
| \( a = 2, b = 4 \) | 75.208 | 105.6 | 2152.25 |
| \( a = 4, b = 6 \) | 209.68 | 586 | 6468.18 |
| \( a = 6, b = 8 \) | 408 | 1354 | 12971.12 |
| \( a = 8, b = 10 \) | 670.454 | 2413.2 | 21661.1125 |
| \( a = 10, b = 12 \) | 996.864 | 3758.4 | 32538.0625 |
| \( a = 12, b = 14 \) | 1387.274 | 5391.6 | 45602.0125 |
| \( a = 14, b = 16 \) | 1841.684 | 7312.8 | 60852.9625 |
| \( a = 16, b = 18 \) | 2360.094 | 9522 | 78290.9125 |
| \( a = 18, b = 20 \) | 2942.504 | 12019.2 | 97915.8625 |
| \( a = 20, b = 22 \) | 3588.914 | 14804.4 | 119727.8125 |

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\[ H(\Gamma_1) = IS(\Gamma_1) = AZI(\Gamma_1) \]

\[
\begin{align*}
\text{IS}(\Gamma_2) &= T_\mu(Q_2(J(D_\mu(D_\gamma(f(\mu, v))))))_{\mu=1} \\
&= \frac{1}{4} (8a + 12b + 8) + \frac{1}{5} (48a + 36b - 24) + \frac{1}{6} (216ab - 90a - 54b + 90) \\
&= 36ab - \frac{17}{5}a - \frac{9}{5}b + \frac{61}{5}.
\end{align*}
\]

(iii) Augmented Zagreb index:
5. Conclusion

In this section, we used the various degree-based TIs and show the comparison in the form of tables and figures. Comparison between $M_1(\Gamma_1)$, $M_2(\Gamma_1)$, $MM_1(\Gamma_1)$, and $SDD(\Gamma_1)$ of VC$_5$C$_7$.

The comparison of 1st Zagreb, 2nd Zagreb, 2nd modified Zagreb, and symmetric division deg indices of pent-heptagonal nanosheets ($\Gamma_1$) is computationally computed by using these M-polynomials. We calculated these indices for different values of $a$ and $b$ in Table 5, and we noted that when we increase the values of $a$ and $b$, then all of the TIs of VC$_5$C$_7$ are increasing with the same order, as shown in Figure 3.

The comparison of the harmonic index, the inverse sum index, and the augmented Zagreb index of pent-heptagonal nanosheets ($\Gamma_1$) is computationally computed by using these M-polynomials. We calculated these indices for different values of $a$ and $b$ in Table 6, and we noted that when we increase the values of $a$ and $b$, then all of the TIs of HC$_5$C$_7$ are increasing with the same order, as shown in Figure 4.

The comparison of the harmonic index, the inverse sum index, and the augmented Zagreb index of pent-heptagonal nanosheets ($\Gamma_2$) is computationally computed by using these M-polynomials. We calculated these indices for different values of $a$ and $b$ in Table 7, and we noted that when we increase the values of $a$ and $b$, then all of the TIs of VC$_5$C$_7$ are increasing with the same order, as shown in Figure 5.

In this paper, the calculated M-polynomials and enumerated TIs assist us to recognize the physical characteristic, chemical sensitivity, and biological animation of the pent-heptagonal nanosheets ($\Gamma_1$) and ($\Gamma_2$). These consequences give us remarkable ascertainment in the field of pharmaceutical production.

However, the problem is still open to compute the different TIs (degree and distance based) for various nanosheets:

(i) To compute the nanosheet for other topological indices
(ii) To compute the various nanosheets for different topological indices

\[ AZI(\Gamma_2) = T^3_\mu\left(f\left(D^1_\mu D^1_\nu f(\mu, \nu)\right)\right)_{\mu \nu = 1} \]

\[ = (2a + 3b + 2) + 8(8a + 6b - 4) + \left(\frac{9}{4}\right)(24ab - 10a - 6b + 10) \]

\[ = 8(2a + 3b + 2) + 8(8a + 6b - 4) + (11.3906)(24ab - 10a - 6b + 10) \]

\[ = 273.3744ab - 33.90625a + 3.6564b + 97.906 \]
Data Availability
No data were used to support this study.

Conflicts of Interest
The authors declare that there are no conflicts of interest regarding this publication.

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