M-Polynomial and Entropy Measures for Graphene Structures

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ABSTRACT

A topological index (TI) is a real number that defines the relationship between a chemical structure and its properties and remains invariant under graph isomorphism.TIs defined for chemical structures are capable of predicting physical properties, chemical reactivity and biological activity. Several kinds of TIs have been defined and studied for different molecular structures.Graphene is the thinnest material known to man and is also extremely strong while being a good conductor of heat and electricity. With such unique features, graphene and its derivatives have found commercial uses and have also fascinated theoretical chemists. In this article, the neighbourhood sum degree-based M-polynomialand entropy measures have been computed for graphenestructures. The proper analytical expressions for these indices are derived. The obtained results will enable theoretical chemists to study these exciting structures further from a structural perspective.

Keywords: Vertex degree-based TIs, M-Polynomial, neighbourhood sum degree-based indices, entropy measures

1 Introduction

Graph theoretical tools have been gaining popularity as the primary techniques for the theoretical study of chemical compounds. QSAR/QSPR techniques, in particular, are regarded as useful computational and quasi strategies for trying to predict the characteristics of chemical substances. These techniques are crucial in the development of new and more effective herbicides because their properties can be estimated prior to synthesising and thus influence the design. Furthermore, experimental measurements can be replaced by QSPR/QSAR models, which are less expensive and time-consuming [1]. In this context, TIs provide a quantitative characterisation of the molecular topology.

A topological index (TI) of a molecular graph is a specific number that describes one or more physical or chemical characteristics of the underlying molecular structure. It can also be defined as a score function which maps each component of a molecular structure to a distinct numerical value. One of the primary advantages of using TIs is that they can be used to sort a large number of molecular structures into smaller groups for more accessible analysis according to the magnitude of the indices. Therefore, the study of these indices supports the theoretical analysis of chemical compounds without involving practical experiments, thus saving time and effort involved in their research.

The first occurrence of a topological index in the literature is in the pioneering work of the eminent chemist Wiener. He described the boiling point of alkanes in terms of a path number W, which is the sum of the distances between any two atoms within the molecule. This path number later became known as the Wiener index and has been studied extensively [2].This ground-breaking work kickstarted the research on topological indices, and its mathematical investigation began in the 1970s. Since the behaviour and properties of molecules rely heavily on the corresponding molecular structures, TIs have now been established as major molecular indices in theoretical chemistry.

A considerable number of topological indices have been proven to display a strong correlation with several properties of chemical compounds. Due to their ability to characterise a large variety of physical and

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chemical properties, the study of topological indices has wide-ranging applications in various fields, including computer-assisted drug discovery, deriving multi-linear regression models [3], aromatic sextet theory [4], and thermochemistry [5]. The comparative ease of using molecular TIs to determine the physicochemical properties as opposed to the complex quantum chemical calculations has also found several applications for these TIs [6]. Thus, it becomes vital to determine the various molecular indices of molecules so that suitable indices are applied to attain the desired correlations between their properties and structures.

2 Mathematical Concepts

Throughout this research, we consider only a simple and connected graph without multiple edges and self-loops. The graph Γ is said to be a connected graph with vertex set $V(\Gamma)$ and edge set $E(\Gamma)$. The degree of the vertex is represented as d_v.

2.1 Neighbourhood Degree Sum-Based Indices

The neighbourhood sum VDB TIs are denoted by $N_\Gamma(v)$. The neighbourhood sum degree of the molecular graph is represented as $|N_\Gamma(v)| = d_v$. The $N_\Gamma(v)$ denotes the sum of the degrees of the neighbouring vertices of v. Let's define the neighbourhood sum degree-based M-polynomial of Γ,

$$NM(\Gamma) = \sum_{i \leq j} (Number\ of\ all\ edges\ pq\ \ such\ that\ H_u = i, H_v = j) r^i t^j.$$

The vertex degree and neighbourhood degree sum-based (ND) TIs are depicted as [10,11]

$$D(\Gamma) = \sum_{uv\epsilon E(\Gamma)} g(\varphi_u \varphi_v)$$

and

$$NM(\Gamma) = \sum_{uv\epsilon E(\Gamma)} g(\omega_u \omega_v).$$

The derivations of NM-Polynomial are listed below in Table 1.

Table 1. *NM-Polynomial Expressions*

S.no	VDB TIs derived from $NM(\Gamma; r, t)$
1.	$M_1(\Gamma) = D_r + D_t(NM(\Gamma; r, t))\|_{r=t=1}$
2.	$M_2(\Gamma) = D_r D_t(NM(\Gamma; r, t))\|_{r=t=1}$
3.	$M_2^m(\Gamma) = S_r S_t(NM(\Gamma; r, t))\|_{r=t=1}$
4.	$R_\alpha(\Gamma) = D_r^\alpha D_t^\alpha(NM(\Gamma; r, t))\|_{r=t=1}$
5.	$RR_\alpha(\Gamma) = S_r^\alpha S_t^\alpha(NM(\Gamma; r, t))\|_{r=t=1}$
6.	$SDD(\Gamma) = (D_r S_t + D_t S_r)(NM(\Gamma; r, t))\|_{r=t=1}$

7.	$H(\Gamma) = 2S_r J(NM(\Gamma;r,t))\|_{r=1}$
8.	$I(\Gamma) = S_r J D_r D_t (NM(\Gamma;r,t))\|_{r=1}$
9.	$A(\Gamma) = S_r^3 Q_{-2} J D_r^3 D_t^3 (NM(\Gamma;r,t))\|_{r=1}$
10.	$ABC(\Gamma) = D_r^{\frac{1}{2}} Q_{-2} J S_r^{\frac{1}{2}} S_t^{\frac{1}{2}} (NM(\Gamma;r,t))\|_{r=1}$
11.	$GA(\Gamma) = 2S_r J D_r^{\frac{1}{2}} D_t^{\frac{1}{2}} (NM(\Gamma;r,t))\|_{r=1}$
12.	$B_1(\Gamma) = (D_r + D_t + 2D_r Q_{-2} J)(NM(\Gamma;r,t))\|_{r=t=1}$
13.	$B_2(\Gamma) = D_r Q_{-2} J (D_r + D_t)(NM(\Gamma;r,t))\|_{r=1}$
14.	$HB_1(\Gamma) = D_r^2 + D_t^2 + 2D_r^2 Q_{-2} J + 2D_r Q_{-2} J (D_r + D_t)(NM(\Gamma;r,t))\|_{r=t=1}$

2.2 Neighbourhood Degree Sum-Based Entropy Measures

In his seminal work, Shannon defined entropy as a measure of the unpredictable nature of relevant information or a way of measuring a system's uncertainty. This paper laid the foundation for modern information theory. The entropy formulae have been used to quantify a network's structural informativeness [12]. Though information theory was initially used exclusively in electrical engineering and linguistics, its versatile nature found applications in life sciences like chemistry and biology [13] and in graph theory for chemical networks. The notion of graph entropy was proposed to quantify the topological information of chemical networks and graphs.

Rashevsky [14] developed the concept of graph entropy depending on the vertex orbits. The graph entropy measures enable mathematicians to relate graph components such as edges and vertices with probability distributions, categorised as intrinsic and extrinsic measures. Graph entropies have wide-ranging applications in many fields, including chemistry, ecology, sociology, and biology [15,16].Dehmer introduced graph entropies that captured the structural information based on information functionals and studied their properties [17,18]. Estrada et al. [19] introduced a physically-sound graph entropy measure and analysed the walk-based graph entropies [20]. The applications of entropy network measures range from quantitatively describing a molecular structure to exploring biological and chemical features of molecular graphs. The entropy measures have several applications in the fields of chemical graph theory. It is used to analyse complex networks and their chemical properties.

For the connected graphΓ Shannon's entropy is depicted as

Let Γ be a graph with vertex v_i and d_i be the degree of v_i for the given edge u_iv_j , then one can define

$$P_{ij} = \frac{w(u_iv_j)}{\sum_{j=1}^{d_i} w(u_iv_j)};$$

Where $w(u_iv_j)$ be the weight of the edge u_iv_j and $w(u_iv_j) > 0$. The node entropy is defined as

$$ENT_{\Gamma}(v_i) = -\sum_{j=1}^{d_i} P_{ij} log\ (P_{ij})$$

For an edge weighted graph $\Gamma = (V, E, w)$, the entropy measure of Γ is defined as [21]

$$ENT_{\Gamma}(\Gamma, w) = -\sum_{uv \in E(\Gamma)} P_{uv}\ log\ log\ P_{uv}\ ,$$

Where,

$$P_{uv} = \frac{w(uv)}{\sum_{uv \in E(\Gamma)} w(uv)}$$

$$ENT_X(\Gamma) = -\sum_{uv \in E(\Gamma)} P_{u,v}\ log\ log\ P_{u,v}$$

$$= -\sum_{uv \in E(\Gamma)} \frac{F(d_u,d_v)}{X(\Gamma)} log\ log\ \frac{F(d_u,d_v)}{X(\Gamma)}$$

$$= -\frac{1}{X(\Gamma)} \sum_{uv \in E(\Gamma)} F(d_u, d_v)\ log\ log\ \frac{F(d_u, d_v)}{X(\Gamma)}$$

$$= -\frac{1}{X(\Gamma)} \sum_{uv \in E(\Gamma)} F(d_u, d_v)(log\ log\ F(d_u, d_v)\ ) - (log\ log\ X(\Gamma)\ )$$

$$=log\ log\ X(\Gamma)\ - \frac{1}{X(\Gamma)} \sum_{uv \in E(\Gamma)} F(d_u, d_v)\ log\ log\ F(d_u, d_v)\ .$$

Where $TI(\Gamma) = X$.

2.3 Computing the Neighbourhood Sum Degree-Based M-polynomial for β-Graphene

In this section, the proper analytical expressions of neighbourhood degree sum-based indices and entropy measures are computed using the M-polynomial for β-Graphene. Graphene is a carbon allotrope, a two-dimensional hexagonal network in which the carbon atoms form vertices with sp_2hybridisation. Graphene has many exceptional properties, including mechanical strength, optical transparency, and electric and thermal conductivity. Furthermore, the one-atomic layer structure of graphene makes it ultralight and super thin. Graphene has a thickness of about 0.35 nm, which is approximately 1/200,000th of the thickness of human hair. However, the closely arranged carbon atoms and the sp_2 orbital hybridisation provide exceptional stability to the graphene structure. Thus, graphene shows extraordinary transparency of 97.7 percent, which means that it only absorbs 2.3 percent of visible light [22].

Due to its high conductivity, graphene can provide a possible alternative to many common substances used as membranes, including indium tin oxide (ITO) and fluorine-doped tin oxide (FTO). The use of graphene for these applications could address the issues of limited indium resources, pollution, and fragility. A membrane with graphene as the primary component could be used as a window barrier in dye-sensitised LEDs and solar cells. It is also possible for graphene to also exist as a nanoribbon in which a lateral charge movement causes an energy barrier to form close to the central point. A reduction in the thickness of the nanoribbon raises this energy barrier. [23]. Hence, by carefully adjusting the width of the graphene nanoribbon, the energy barrier can be accurately regulated, which is a promising advantage for graphene-based electronic devices. Graphene can also be used in the partial detection of external magnetic fields, electric fields, and deformations due to it being a low-noise electrical substance [24].

In terms of its structure, graphene can be considered the basic unit of graphite, fullerene [25], carbon nanotube [26], graphyne [27], and other related materials such as amorphous carbon, carbon fiber, charcoal [28], as well as aromatic molecules such as polycyclic aromatic hydrocarbons. As they all have the same structure, they all have some properties in common, even though their different sizes and shapes make them very different. Thus, the structural study of graphene helps understand the above listed materials. The β-Graphene consists $V(\Gamma) = 12mn + 2m + 10n$ and $E(\Gamma) = 18mn + m + 11n$. It is depicted in Figure 1.

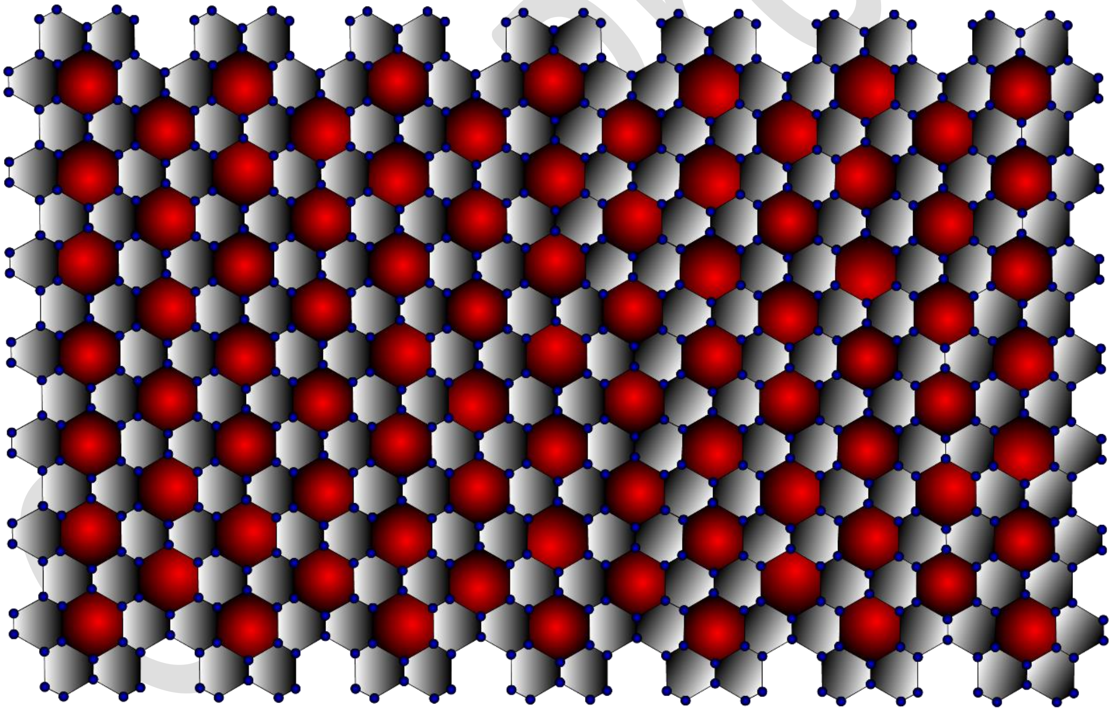

Figure 1:β*-Graphene (7,7)*

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Table 2: *Partition table for β-Graphene*

Edge types	Frequency
d_{55}	$4m + 2n$
d_{57}	$4m + 8$
d_{58}	$4m + 4n - 8$
d_{79}	$2m + 4$
d_{88}	$2n - 2$
d_{89}	$8m + 4n - 12$
d_{99}	$18mn - 21m - n + 10$

Theorem 1. If Γ is a β-Graphene system, then NM-polynomial of Γ is given as follows

$NM(\Gamma; r, t) = (4m + 2n)r^5t^5 + (4m + 8)r^5t^7 + (4m + 4n - 8)r^5t^8 + (2m + 4)r^7t^9 + (2n - 2)r^8t^8 + (8m + 4n - 12)r^8t^9 + (18mn - 21m - n + 10)r^9t^9$.

Theorem 2. If Γ is a β-Graphene system, then NM-polynomial of Γ is given as follows

1. $NMM_1(\Gamma) = 324mn - 70m + 154n$,

2. $NMM_2(\Gamma) = 1458mn - 599m + 545n + 30$,

3. $NMM_2^m(\Gamma) = \left(\frac{2437}{9450}\right)m + \left(\frac{16489}{64800}\right)n + \left(\frac{2}{9}\right)mn + \frac{1597}{90720}$,

4. $NMR_\alpha(\Gamma) = 25^\varphi(4m + 2n) + 35^\varphi(4m + 8) + 40^\varphi(4m + 4n - 8) + 63^\varphi(2m + 4) + 64^\varphi(2n - 2) + 72^\varphi(8m + 4n - 12) + 81^\varphi(18mn - 21m - n + 10)$,

5. $NMRR_\alpha(\Gamma) = 1/25^\varphi\ (4m + 2n) + 1/35^\varphi(4m + 8) + 1/40^\varphi(4m + 4n - 8) + 1/63^\varphi(2m + 4) + 1/64^\varphi(2n - 2) + 1/72^\varphi(8m + 4n - 12) + 1/81^\varphi(18mn - 21m - n + 10)$,

6. $NMSDD(\Gamma) = \left(\frac{151}{42}\right)m + \left(\frac{1033}{45}\right)n + 36mn - \frac{503}{630}$,

7. $NMH(\Gamma) = \left(\frac{12463}{13260}\right)m + \left(\frac{64637}{39780}\right)n + \frac{413}{7956} + 2mn$,

8. $NMI(\Gamma) = \left(\frac{16685}{442}\right)n + 81mn - \left(\frac{99547}{5304}\right)m + \frac{1709}{2652}$,

9. $NMA(\Gamma) = \left(\frac{176959019139103}{233744896000}\right)n + \left(\frac{4782969}{2048}\right)mn - \left(\frac{798535392483}{681472000}\right)m + \frac{11934914516533}{116872448000}$,

10. $NMABC(\Gamma) = \left(\frac{34}{15}\right)\sqrt{2}m + \left(\frac{4}{5}\right)\sqrt{2}n + \left(\frac{4}{7}\right)\sqrt{2}\sqrt{7}m + \left(\frac{25}{28}\right)\sqrt{2}\sqrt{7} + \left(\frac{1}{5}\right)\sqrt{11}\sqrt{2}\sqrt{5}m + \left(\frac{1}{5}\right)\sqrt{11}\sqrt{2}\sqrt{5}n - \left(\frac{2}{5}\right)\sqrt{11}\sqrt{2}\sqrt{5} + \left(\frac{4}{3}\right)\sqrt{2} + \left(\frac{1}{4}\right)\sqrt{2}\sqrt{7}n + \left(\frac{2}{3}\right)\sqrt{5}\sqrt{3}\sqrt{2}m + (1/3)\sqrt{5}\sqrt{3}\sqrt{2}n - \sqrt{5}\sqrt{3}\sqrt{2} + 8mn - \left(\frac{28}{3}\right)m - \left(\frac{4}{9}\right)n + \frac{40}{9}$,

11. $NMGA(\Gamma) = 3n + \left(\frac{2}{3}\right)\sqrt{7}\sqrt{5}m + \left(\frac{4}{3}\right)\sqrt{7}\sqrt{5} + \left(\frac{16}{13}\right)\sqrt{2}\sqrt{5}m + \left(\frac{16}{13}\right)\sqrt{2}\sqrt{5}n - \left(\frac{32}{13}\right)\sqrt{2}\sqrt{5} + \left(\frac{3}{4}\right)\sqrt{7}m + \left(\frac{3}{2}\right)\sqrt{7} + 8 + \left(\frac{96}{17}\right)\sqrt{2}m + \left(\frac{48}{17}\right)\sqrt{2}n - \left(\frac{144}{17}\right)\sqrt{2} + 18mn - 17m$,

12. $NMB_1(\Gamma) = 900mn - 214m + 418n$,

13. $NMB_2(\Gamma) = 5184mn - 2188m + 1912n + 84,$

14. $NMHB_1(\Gamma) = 746496mn - 473476m + 188680n + 4801.$

Proof. Let $f(r,t) = NM(\Gamma; r,t) = (4m+2n)r^5t^5 + (4m+8)r^5t^7 + (4m+4n-8)r^5t^8 + (2m+4)r^7t^9 + (2n-2)r^8t^8 + (8m+4n-12)r^8t^9 + (18mn-21m-n+10)r^9t^9$

$D_r\big(f(r,t)\big) = 5(4m+2n)r^5t^5 + 5(4m+8)r^5t^7 + 5(4m+4n-8)r^5t^8 + 7(2m+4)r^7t^9 + 8(2n-2)r^8t^8 + 8(8m+4n-12)r^8t^9 + 9(18mn-21m-n+10)r^9t^9,$

$D_t\big(f(r,t)\big) = 5(4m+2n)r^5t^5 + 7(4m+8)r^5t^7 + 8(4m+4n-8)r^5t^8 + 9(2m+4)r^7t^9 + 8(2n-2)r^8t^8 + 8(8m+4n-12)r^8t^9 + 9(18mn-21m-n+10)r^9t^9,$

$D_r + D_t\big(f(r,t)\big) = 10(4m+2n)r^5t^5 + 12(4m+8)r^5t^7 + 13(4m+4n-8)r^5t^8 + 16(2m+4)r^7t^9 + 16(2n-2)r^8t^8 + 17(8m+4n-12)r^8t^9 + 18(18mn-21m-n+10)r^9t^9,$

$D_rD_t\big(f(r,t)\big) = 25(4m+2n)r^5t^5 + 35(4m+8)r^5t^7 + 40(4m+4n-8)r^5t^8 + 63(2m+4)r^7t^9 + 64(2n-2)r^8t^8 + 72(8m+4n-12)r^8t^9 + 81(18mn-21m-n+10)r^9t^9,$

$S_r\big(f(r,t)\big) = \frac{1}{5}(4m+2n)r^5t^5 + \frac{1}{5}(4m+8)r^5t^7 + \frac{1}{5}(4m+4n-8)r^5t^8 + \frac{1}{7}(2m+4)r^7t^9 + \frac{1}{8}(2n-2)r^8t^8 + \frac{1}{8}(8m+4n-12)r^8t^9 + \frac{1}{9}(18mn-21m-n+10)r^9t^9,$

$S_t\big(f(r,t)\big) = \frac{1}{5}(4m+2n)r^5t^5 + \frac{1}{7}(4m+8)r^5t^7 + \frac{1}{8}(4m+4n-8)r^5t^8 + \frac{1}{9}(2m+4)r^7t^9 + \frac{1}{8}(2n-2)r^8t^8 + \frac{1}{9}(8m+4n-12)r^8t^9 + \frac{1}{9}(18mn-21m-n+10)r^9t^9,$

$S_tS_r\big(f(r,t)\big) = \frac{1}{25}(4m+2n)r^5t^5 + \frac{1}{35}(4m+8)r^5t^7 + \frac{1}{40}(4m+4n-8)r^5t^8 + \frac{1}{63}(2m+4)r^7t^9 + \frac{1}{64}(2n-2)r^8t^8 + \frac{1}{72}(8m+4n-12)r^8t^9 + \frac{1}{81}(18mn-21m-n+10)r^9t^9,$

$D_r^{\varphi}D_t^{\varphi}\big(f(r,t)\big) = 25^{\varphi}(4m+2n)r^5t^5 + 35^{\varphi}(4m+8)r^5t^7 + 40^{\varphi}(4m+4n-8)r^5t^8 + 63^{\varphi}(2m+4)r^7t^9 + 64^{\varphi}(2n-2)r^8t^8 + 72^{\varphi}(8m+4n-12)r^8t^9 + 81^{\varphi}(18mn-21m-n+10)r^9t^9,$

$S_r^{\varphi}S_t^{\varphi}\big(f(r,t)\big) = \frac{1}{25^{\varphi}}(4m+2n)r^5t^5 + \frac{1}{35^{\varphi}}(4m+8)r^5t^7 + \frac{1}{40^{\varphi}}(4m+4n-8)r^5t^8 + \frac{1}{63^{\varphi}}(2m+4)r^7t^9 + \frac{1}{64^{\varphi}}(2n-2)r^8t^8 + \frac{1}{72^{\varphi}}(8m+4n-12)r^8t^9 + \frac{1}{81^{\varphi}}(18mn-21m-n+10)r^9t^9,$

$S_tD_r\big(f(r,t)\big) = 1(4m+2n)r^5t^5 + \frac{5}{7}(4m+8)r^5t^7 + \frac{5}{8}(4m+4n-8)r^5t^8 + \frac{7}{9}(2m+4)r^7t^9 + 1(2n-2)r^8t^8 + \frac{8}{9}(8m+4n-12)r^8t^9 + 1(18mn-21m-n+10)r^9t^9,$

$S_rD_t\big(f(r,t)\big) = 1(4m+2n)r^5t^5 + \frac{7}{5}(4m+8)r^5t^7 + \frac{8}{5}(4m+4n-8)r^5t^8 + \frac{9}{7}(2m+4)r^7t^9 + 1(2n-2)r^8t^8 + \frac{9}{8}(8m+4n-12)r^8t^9 + 1(18mn-21m-n+10)r^9t^9,$

$J\big(f(r,t)\big) = f(r,r) = (4m+2n)r^{10} + (4m+8)r^{12} + (4m+4n-8)r^{13} + (2m+4)r^{16} + (2n-2)r^{16} + (8m+4n-12)r^{17} + 9(18mn-21m-n+10)r^{18},$

$S_rJf(r,t) = \frac{1}{10}(4m+2n)r^{10} + \frac{1}{12}(4m+8)r^{12} + \frac{1}{13}(4m+4n-8)r^{13} + \frac{1}{16}(2m+4)r^{16} + \frac{1}{16}(2n-2)r^{16} + \frac{1}{17}(8m+4n-12)r^{17} + \frac{1}{18}(18mn-21m-n+10)r^{18}$,

$S_rJD_rD_tf(r,t) = \frac{25}{10}(4m+2n)r^{10} + \frac{35}{12}(4m+8)r^{12} + \frac{40}{13}(4m+4n-8)r^{13} + \frac{63}{16}(2m+4)r^{16} + \frac{64}{16}(2n-2)r^{16} + \frac{72}{17}(8m+4n-12)r^{17} + \frac{81}{18}(18mn-21m-n+10)r^{18}$,

$S_r^3Q_{-2}JD_r^3D_t^3f(r,t) = \left(\frac{25}{8}\right)^3(4m+2n)r^8 + \left(\frac{7}{2}\right)^3(4m+8)r^{10} + \left(\frac{40}{11}\right)^3(4m+4n-8)r^{11} + \left(\frac{9}{2}\right)^3(2m+4)r^{14} + \left(\frac{32}{7}\right)^3(2n-2)r^{14} + \left(\frac{24}{5}\right)^3(8m+4n-12)r^{15} + \left(\frac{81}{16}\right)^3(18mn-21m-n+10)r^{16}$,

$D_r^{\frac{1}{2}}Q_{-2}J\, S_r^{\frac{1}{2}}S_t^{\frac{1}{2}}f(r,t) = \frac{\sqrt{8}}{5}(4m+2n)r^8 + \frac{\sqrt{10}}{\sqrt{35}}(4m+8)r^{10} + \frac{\sqrt{11}}{\sqrt{40}}(4m+4n-8)r^{11} + \frac{\sqrt{14}}{3\sqrt{7}}(2m+4)r^{14} + \frac{\sqrt{14}}{8}(2n-2)r^{14} + \frac{\sqrt{15}}{3\sqrt{8}}(8m+4n-12)r^{15} + \frac{\sqrt{16}}{9}(18mn-21m-n+10)r^{16}$,

$$2S_rJD_r^{\frac{1}{2}}D_t^{\frac{1}{2}}f(r,t) = \frac{10}{10}(4m+2n)r^{10} + \frac{2\sqrt{35}}{12}(4m+8)r^{12} + \frac{2\sqrt{40}}{13}(4m+4n-8)r^{13} + \frac{2\sqrt{63}}{16}(2m+4)r^{16} + \frac{16}{16}(2n-2)r^{16} + \frac{2\sqrt{72}}{17}(8m+4n-12)r^{17} + \frac{18}{18}(18mn-21m-n+10)r^{18}$$

$$2D_rQ_{-2}Jf(r,t) = 2\cdot 8(4m+2n)r^8 + 2\cdot 10(4m+8)r^{10} + 2\cdot 11(4m+4n-8)r^{11} + 2\cdot 14(2m+4)r^{14} + 2\cdot 14(2n-2)r^{14} + 2\cdot 15(8m+4n-12)r^{15} + 2\cdot 16(18mn-21m-n+10)r^{16}$$

$D_rQ_{-2}J(D_r+D_t)f(r,t) = 8\cdot 10(4m+2n)r^8 + 10\cdot 12(4m+8)r^{10} + 11\cdot 13(4m+4n-8)r^{11} + 14\cdot 16(2m+4)r^{14} + 14\cdot 16(2n-2)r^{14} + 15\cdot 17(8m+4n-12)r^{15} + 16\cdot 18(18mn-21m-n+10)r^{16}$,

$D_r^2Q_{-2}J(D_r^2+D_t^2)f(r,t) = 64\cdot 50(4m+2n)r^8 + 100\cdot 74(4m+8)r^{10} + 121\cdot 89(4m+4n-8)r^{11} + 196\cdot 130(2m+4)r^{14} + 196\cdot 128(2n-2)r^{14} + 225\cdot 145(8m+4n-12)r^{15} + 256\cdot 162(18mn-21m-n+10)r^{16}$.

The above results are obtained by using the conditions of M-Polynomial with its derivatives, and the partition Table 2.

Hence the proof.

2.4 Neighbourhood Degree Sum-Based Entropy Measures for β-Graphene

Theorem 3. If Γ is a β-Graphene system, then NM-entropy measures of$\Gamma$are given as follows

1. $NENT_{NM_1}(\Gamma) = log\ log\ (324mn - 70m + 154n)\ - \frac{1}{324mn-70m+154n}[(4m+2n)(10)\ log\ log\ (10)\ + (4m+8)(12)\ log\ log\ (12)\ + (4m+4n-8)(13)\ log\ log\ (13)\ + (2m+4)(16)\ log\ log\ (16)\ + (2n-2)(16)\ log\ log\ (16)\ + (8m+4n-12)(17)\ log\ log\ (17)\ + (18mn - 21m - n + 10)(18)\ log\ log\ (18)\ ]$

$$= log(324mn - 70m + 154n) - \left(\frac{-273.7788m + 408.7804n + 2.8232 + 936.4896mn}{324mn - 70m + 154n}\right)$$

2. $NENT_{NM_2}(\Gamma) = log\ log\ (1458mn - 599m + 545n + 30)\ - \frac{1}{1458mn-599m+545n+30}[(4m + 2n)(25)\ log\ log\ (25)\ + (4m+8)(35)\ log\ log\ (35)\ + (4m+4n-8)(40)\ log\ log\ (40)\ + (2m+4)(63)\ log\ log\ (63)\ + (2n-2)(64)\ log\ log\ (64)\ + (8m+4n-12)(72)\ log\ log\ (72)\ + (18mn - 21m - n + 10)(81)\ log\ log\ (81)\ ]$

$$= log(1458mn - 599m + 545n + 30) - \left(\frac{-3079.6186m + 2159.2464n + 191.1532 + 6407.0352mn}{1458mn - 599m + 545n + 30}\right)$$

3. $NENT_{NM_2^m}(\Gamma) = log\ log\ (\left(\frac{2437}{9450}\right)m + \left(\frac{16489}{64800}\right)n + \left(\frac{2}{9}\right)mn + \frac{1597}{90720})\ - \frac{1}{\left(\frac{2437}{9450}\right)m+\left(\frac{16489}{64800}\right)n+\left(\frac{2}{9}\right)mn+\frac{1597}{90720}}\left[(4m+2n)\left(\frac{1}{25}\right)log\left(\frac{1}{25}\right) + (4m+8)\left(\frac{1}{35}\right)log\left(\frac{1}{35}\right) + (4m+4n-8)\left(\frac{1}{40}\right)log\left(\frac{1}{40}\right) + (2m+4)\left(\frac{1}{63}\right)log\left(\frac{1}{63}\right) + (2n-2)\left(\frac{1}{64}\right)log\left(\frac{1}{64}\right) + (8m+4n-12)\left(\frac{1}{72}\right)log\left(\frac{1}{72}\right) + (18mn - 21m - n + 10)\left(\frac{1}{81}\right)log\left(\frac{1}{81}\right)\right]$

$$= log\left(\left(\frac{2437}{9450}\right)m + \left(\frac{16489}{64800}\right)n + \left(\frac{2}{9}\right)mn + \frac{1597}{90720}\right) - \left(\frac{-.7576449840m - .9397022176n - 0.376835284e - 1 - .9765333333mn}{\left(\frac{2437}{9450}\right)m + \left(\frac{16489}{64800}\right)n + \left(\frac{2}{9}\right)mn + \frac{1597}{90720}}\right)$$

4. $NENT_{NHM}(\Gamma) = log\ log\ (5832mn - 2328m + 2220n + 84)\ - \frac{1}{5832mn-2328m+2220n+84}[(4m+2n)(100)\ log\ log\ (100)\ + (4m+8)(144)\ log\ log\ (144)\ + (4m+4n-8)(169)\ log\ log\ (169)\ + (2m+4)(256)\ log\ log\ (256)\ + (2n-2)(256)\ log\ log\ (256)\ + (8m+4n-12)(289)\ log\ log\ (289)\ + (18mn - 21m - n + 10)(324)\ log\ log\ (324)\ ]$

$$= log(5832mn - 2328m + 2220n + 84) - \left(\frac{-15220.2744m + 11905.3064n + 707.5792 + 33713.6256mn}{5832mn - 2328m + 2220n + 84}\right)$$

5. $NENT_{NA}(\Gamma) = log\ log\ \left(\left(\frac{4782969}{2048}\right)mn - \left(\frac{798535392483}{681472000}\right)m + \left(\frac{176959019139103}{233744896000}\right)n + \frac{11934914516533}{116872448000}\right) - \frac{1}{\left(\frac{4782969}{2048}\right)mn - \left(\frac{798535392483}{681472000}\right)m + \left(\frac{176959019139103}{233744896000}\right)n + \frac{11934914516533}{116872448000}}\Big[(4m + 2n)\left(\frac{25}{8}\right)^3 log\ log\ \left(\frac{25}{8}\right)^3 + (4m + 8)\left(\frac{35}{10}\right)^3 log\ log\ \left(\frac{35}{10}\right)^3 + (4m + 4n - 8)\left(\frac{40}{11}\right)^3 log\ log\ \left(\frac{40}{11}\right)^3 + (2m + 4)\left(\frac{63}{14}\right)^3 log\ log\ \left(\frac{63}{14}\right)^3 + (2n - 2)\left(\frac{64}{14}\right)^3 log\ log\ \left(\frac{64}{14}\right)^3 + (8m + 4n - 12)\left(\frac{72}{15}\right)^3 log\ log\ \left(\frac{72}{15}\right)^3 + (18mn - 21m - n + 10)\left(\frac{81}{16}\right)^3 log\ log\ \left(\frac{81}{16}\right)^3\Big]$

$$= log\left(\left(\frac{4782969}{2048}\right)mn - \left(\frac{798535392483}{681472000}\right)m + \left(\frac{176959019139103}{233744896000}\right)n + \frac{11934914516533}{116872448000}\right) - \frac{-6658.292895m + 2328.656416n + 829.875339 + 9964.129511mn}{\left(\frac{4782969}{2048}\right)mn - \left(\frac{798535392483}{681472000}\right)m + \left(\frac{176959019139103}{233744896000}\right)n + \frac{11934914516533}{116872448000}}$$

6. $NENT_{NABC}(\Gamma) = log\ log\ (ABC(\Gamma)) - \frac{1}{ABC(\Gamma)}\Big[(4m + 2n)\left(\sqrt{\frac{8}{25}}\right) log\ log\ \left(\sqrt{\frac{8}{25}}\right) + (4m + 8)\left(\sqrt{\frac{10}{35}}\right) log\ log\ \left(\sqrt{\frac{10}{35}}\right) + (4m + 4n - 8)\left(\sqrt{\frac{11}{40}}\right) log\ log\ \left(\sqrt{\frac{11}{40}}\right) + (2m + 4)\left(\sqrt{\frac{14}{63}}\right) log\ log\ \left(\sqrt{\frac{14}{63}}\right) + (2n - 2)\left(\sqrt{\frac{14}{64}}\right) log\ log\ \left(\sqrt{\frac{14}{64}}\right) + (8m + 4n - 12)\left(\sqrt{\frac{15}{72}}\right) log\ log\ \left(\sqrt{\frac{15}{72}}\right) + (18mn - 21m - n + 10)\left(\sqrt{\frac{16}{81}}\right) log\ log\ \left(\sqrt{\frac{16}{81}}\right)\Big]$

7. $NENT_{NGA}(\Gamma) = log\ log\ (NGA(\Gamma)) - \frac{1}{NGA(\Gamma)}\Big[(4m + 2n)(1)\ log\ log\ (1) + (4m + 8)\left(\frac{2\sqrt{35}}{12}\right) log\ log\ \left(\frac{2\sqrt{35}}{12}\right) + (4m + 4n - 8)\left(\frac{2\sqrt{40}}{13}\right) log\ log\ \left(\frac{2\sqrt{40}}{13}\right) + (2m + 4)\left(\frac{2\sqrt{63}}{16}\right) log\ log\ \left(\frac{2\sqrt{63}}{16}\right) + (2n - 2)(1)\ log\ log\ (1) + (8m + 4n - 12)\left(\frac{2\sqrt{72}}{17}\right) log\ log\ \left(\frac{2\sqrt{72}}{17}\right) + (18mn - 21m - n + 10)(1)\ log\ log\ (1)\Big]$

8. $NENT_{NAG_1}(\Gamma) = log\ log\ (AG_1(\Gamma)) - \frac{1}{AG_1(\Gamma)}\Big[(4m + 2n)(1)\ log\ log\ (1) + (4m + 8)\left(\frac{12}{2\sqrt{35}}\right) log\ log\ \left(\frac{12}{2\sqrt{35}}\right) + (4m + 4n - 8)\left(\frac{13}{2\sqrt{40}}\right) log\ log\ \left(\frac{13}{2\sqrt{40}}\right) + (2m + 4)\left(\frac{16}{2\sqrt{63}}\right)$

$\log\log\left(\frac{16}{2\sqrt{63}}\right) + (2n-2)(1)\log\log(1) + (8m+4n-12)\left(\frac{17}{2\sqrt{72}}\right)\log\log\left(\frac{17}{2\sqrt{72}}\right) + (18mn - 21m - n + 10)(1)\log\log(1)\Big]$

9. $NENT_{NF_1}(\Gamma) = \log\log(2916mn - 1130m + 1130n + 24) - \frac{1}{2916mn-1130m+1130n+24}[(4m+2n)(50)\log\log(50) + (4m+8)(74)\log\log(74) + (4m+4n-8)(89)\log\log(89) + (2m+4)(130)\log\log(130) + (2n-2)(128)\log\log(128) + (8m+4n-12)(145)\log\log(145) + (18mn-21m-n+10)(162)\log\log(162)]$

$$= \log(2916mn - 1130m + 1130n + 24) - \left(\frac{-6615.1380m + 5293.5484n + 223.5860 + 14835.4416mn}{2916mn - 1130m + 1130n + 24}\right)$$

10. $NENT_{NF_2}(\Gamma) = \log\log(118098mn - 74571m + 30017n + 8086) - \frac{1}{118098mn-74571m+30017n+8086}[(4m+2n)(625)\log\log(625) + (4m+8)(1225)\log\log(1225) + (4m+4n-8)(1600)\log\log(1600) + (2m+4)(3969)\log\log(3969) + (2n-2)(4096)\log\log(4096) + (8m+4n-12)(5184)\log\log(5184) + (18mn-21m-n+10)(6561)\log\log(6561)]$

$$= \log(118098mn - 74571m + 30017n + 8086) - \left(\frac{-6.922733326\times10^5 m + 2.431043232\times10^5 n + 83203.5944 + 1.037939702\times10^6 mn}{118098mn - 74571m + 30017n + 8086}\right)$$

11. $NENT_{N\chi}(\Gamma) = \log\log(N\chi(\Gamma)) - \frac{1}{N\chi(\Gamma)}\Big[(4m+2n)\left(\frac{1}{\sqrt{10}}\right)\log\log\left(\frac{1}{\sqrt{10}}\right) + (4m+8)\left(\frac{1}{\sqrt{12}}\right)\log\log\left(\frac{1}{\sqrt{12}}\right) + (4m+4n-8)\left(\frac{1}{\sqrt{13}}\right)\log\log\left(\frac{1}{\sqrt{13}}\right) + (2m+4)\left(\frac{1}{\sqrt{16}}\right)\log\log\left(\frac{1}{\sqrt{16}}\right) + (2n-2)\left(\frac{1}{\sqrt{16}}\right)\log\log\left(\frac{1}{\sqrt{16}}\right) + (8m+4n-12)\left(\frac{1}{\sqrt{17}}\right)\log\log\left(\frac{1}{\sqrt{17}}\right) + (18mn-21m-n+10)\left(\frac{1}{\sqrt{18}}\right)\log\log\left(\frac{1}{\sqrt{18}}\right)\Big]$

12. $NENT_{NReZ\Gamma_1}(\Gamma) = \log\log\left(\left(\frac{146}{35}\right)m + \left(\frac{274}{35}\right)n + \left(\frac{516}{35}\right)mn\right) - \frac{1}{\left(\frac{146}{35}\right)m+\left(\frac{274}{35}\right)n+\left(\frac{516}{35}\right)mn}\Big[(4m+2n)\left(\frac{10}{25}\right)\log\log\left(\frac{10}{25}\right) + (4m+8)\left(\frac{12}{35}\right)\log\log\left(\frac{12}{35}\right) + (4m+4n-8)\left(\frac{13}{40}\right)\log\log\left(\frac{13}{40}\right) + (2m+4)\left(\frac{16}{63}\right)\log\log\left(\frac{16}{63}\right) + (2n-2)\left(\frac{16}{64}\right)\log\log\left(\frac{16}{64}\right) + (8m+4n-12)\left(\frac{17}{72}\right)\log\log\left(\frac{17}{72}\right) + (18mn-21m-n+10)\left(\frac{18}{81}\right)\log\log\left(\frac{18}{81}\right)\Big]$

$$= log\left(\left(\frac{146}{35}\right)m + \left(\frac{274}{35}\right)n + \left(\frac{516}{35}\right)mn\right) - \left(\frac{-.798715906m - 3.916313112n + 0.34553969e - 1 - 6.016399999mn}{\left(\frac{146}{35}\right)m + \left(\frac{274}{35}\right)n + \left(\frac{516}{35}\right)mn}\right)$$

13. $NENT_{NReZG_2}(\Gamma) = log\ log\ (\left(\frac{1309}{18}\right)n + 121mn - \left(\frac{451}{18}\right)m) - \frac{1}{\left(\frac{1309}{18}\right)n+121mn-\left(\frac{451}{18}\right)m}\Big[(4m + 2n)\left(\frac{25}{10}\right) log\ log\ \left(\frac{25}{10}\right) + (4m+8)\left(\frac{35}{12}\right) log\ log\ \left(\frac{35}{12}\right) + (4m+4n-8)\left(\frac{40}{13}\right) log\ log\ \left(\frac{40}{13}\right) + (2m+4)\left(\frac{63}{16}\right) log\ log\ \left(\frac{63}{16}\right) + (2n-2)\left(\frac{64}{16}\right) log\ log\ \left(\frac{64}{16}\right) + (8m+4n-12)\left(\frac{72}{17}\right) log\ log\ \left(\frac{72}{17}\right) + (18mn - 21m - n + 10)\left(\frac{81}{18}\right) log\ log\ \left(\frac{81}{18}\right)\Big]$

$$= ln\left(\left(\frac{1309}{18}\right)n + 121mn - \left(\frac{451}{18}\right)m\right) - \left(\frac{-46.95207065m + 47.19060362n + 2.12647952 + 121.8321000mn}{\left(\frac{1309}{18}\right)n + 121mn - \left(\frac{451}{18}\right)m}\right)$$

14. $NENT_{NReZG_3}(\Gamma) = log\ log\ (26244mn - 14050m + 8066n + 1076) - \frac{1}{26244mn-14050m+8066n+1076}[(4m + 2n)(250)\ log\ log\ (250) + (4m + 8)(420)\ log\ log\ (420) + (4m + 4n - 8)(520)\ log\ log\ (520) + (2m + 4)(1008)\ log\ log\ (1008) + (2n - 2)(1024)\ log\ log\ (1024) + (8m + 4n - 12)(1224)\ log\ log\ (1224) + (18mn - 21m - n + 10)(1458)\ log\ log\ (1458)]$

$$= log(26244mn - 14050m + 8066n + 1076) - \left(\frac{-1.108067064 \times 10^5 m + 54153.1980n + 9750.1632 + 1.911822912 \times 10^5 mn}{26244mn - 14050m + 8066n + 1076}\right)$$

Where $NABC(\Gamma), NMGA(\Gamma), NAG_1(\Gamma)$ and $N\chi(\Gamma)$ can be represented as $NABC(\Gamma) = \left(\frac{34}{15}\right)\sqrt{2}m + \left(\frac{4}{5}\right)\sqrt{2}n + \left(\frac{4}{7}\right)\sqrt{2}\sqrt{7}m + \left(\frac{25}{28}\right)\sqrt{2}\sqrt{7} + \left(\frac{1}{5}\right)\sqrt{2}\sqrt{5}\sqrt{11}m + \left(\frac{1}{5}\right)\sqrt{2}\sqrt{5}\sqrt{11}n - \left(\frac{2}{5}\right)\sqrt{2}\sqrt{5}\sqrt{11} + \left(\frac{4}{3}\right)\sqrt{2} + \left(\frac{1}{4}\right)\sqrt{2}\sqrt{7}n + \left(\frac{2}{3}\right)\sqrt{2}\sqrt{5}\sqrt{3}m + \left(\frac{1}{3}\right)\sqrt{2}\sqrt{5}\sqrt{3}n - s\sqrt{2}\sqrt{5}\sqrt{3} + 8mn - \left(\frac{28}{3}\right)m - \left(\frac{4}{9}\right)n + \frac{40}{9}$ $,NMGA(\Gamma) = 18mn - 17m + 3n + \left(\frac{2}{3}\right)\sqrt{7}\sqrt{5}m + \left(\frac{4}{3}\right)\sqrt{7}\sqrt{5} + \left(\frac{16}{13}\right)\sqrt{2}\sqrt{5}m + \left(\frac{16}{13}\right)\sqrt{2}\sqrt{5}n - \left(\frac{32}{13}\right)\sqrt{2}\sqrt{5} + \left(\frac{3}{4}\right)\sqrt{7}m + \left(\frac{3}{2}\right)\sqrt{7} + 8 + \left(\frac{96}{17}\right)\sqrt{2}m + \left(\frac{48}{17}\right)\sqrt{2}\,n - \left(\frac{144}{17}\right)\sqrt{2}, NMAG_1 = 18mn - 17m + 3n + \left(\frac{24}{35}\right)\sqrt{7}\sqrt{5}m + \left(\frac{48}{35}\right)\sqrt{7}\sqrt{5} + \left(\frac{13}{10}\right)\sqrt{2}\sqrt{5}m + \left(\frac{13}{10}\right)\sqrt{2}\sqrt{5}n - \left(\frac{13}{5}\right)\sqrt{2}\sqrt{5} + \left(\frac{16}{21}\right)\sqrt{7}m + \left(\frac{32}{21}\right)\sqrt{7} + 8 + \left(\frac{17}{3}\right)\sqrt{2}m + \left(\frac{17}{6}\right)\sqrt{2}n - \left(\frac{17}{2}\right)\sqrt{2}$ and $NM\chi(\Gamma) = \left(\frac{2}{5}\right)\sqrt{2}\sqrt{5}m + \left(\frac{1}{5}\right)\sqrt{2}\sqrt{5}n + \left(\frac{2}{3}\right)\sqrt{3}m + \left(\frac{4}{3}\right)\sqrt{3} + \left(\frac{4}{13}\right)\sqrt{13}m + \left(\frac{4}{13}\right)\sqrt{13}n - \left(\frac{8}{13}\right)\sqrt{13} + \left(\frac{1}{2}\right)m + \frac{1}{2} + \left(\frac{1}{2}\right)n + \left(\frac{8}{17}\right)\sqrt{17}m + \left(\frac{4}{17}\right)\sqrt{17}n - \left(\frac{12}{17}\right)\sqrt{17} + 3\sqrt{2}mn - \left(\frac{7}{2}\right)\sqrt{2}m - \left(\frac{1}{6}\right)\sqrt{2}n + \left(\frac{5}{3}\right)\sqrt{2}.$

2.5 Comparative analysis for β-Graphene

In this section, the analytical expressions of the neighbourhood degree sum-based indices derived in Theorem 2 and Theorem 3 are represented as 3D plots. These plots help the reader visually interpret and understand the behaviour of the indices with respect to the variables that define the molecular structure. In addition, the results of Theorem 2 have also been represented as comparison plots where all the neighbourhood degree sum-based indices are plotted in the same graph against the same structural variables. These comparison plots provide a graphical representation of how the indices vary with respect to each other and the molecular structure. These plots are presented in Figure 2 and Figure 3.

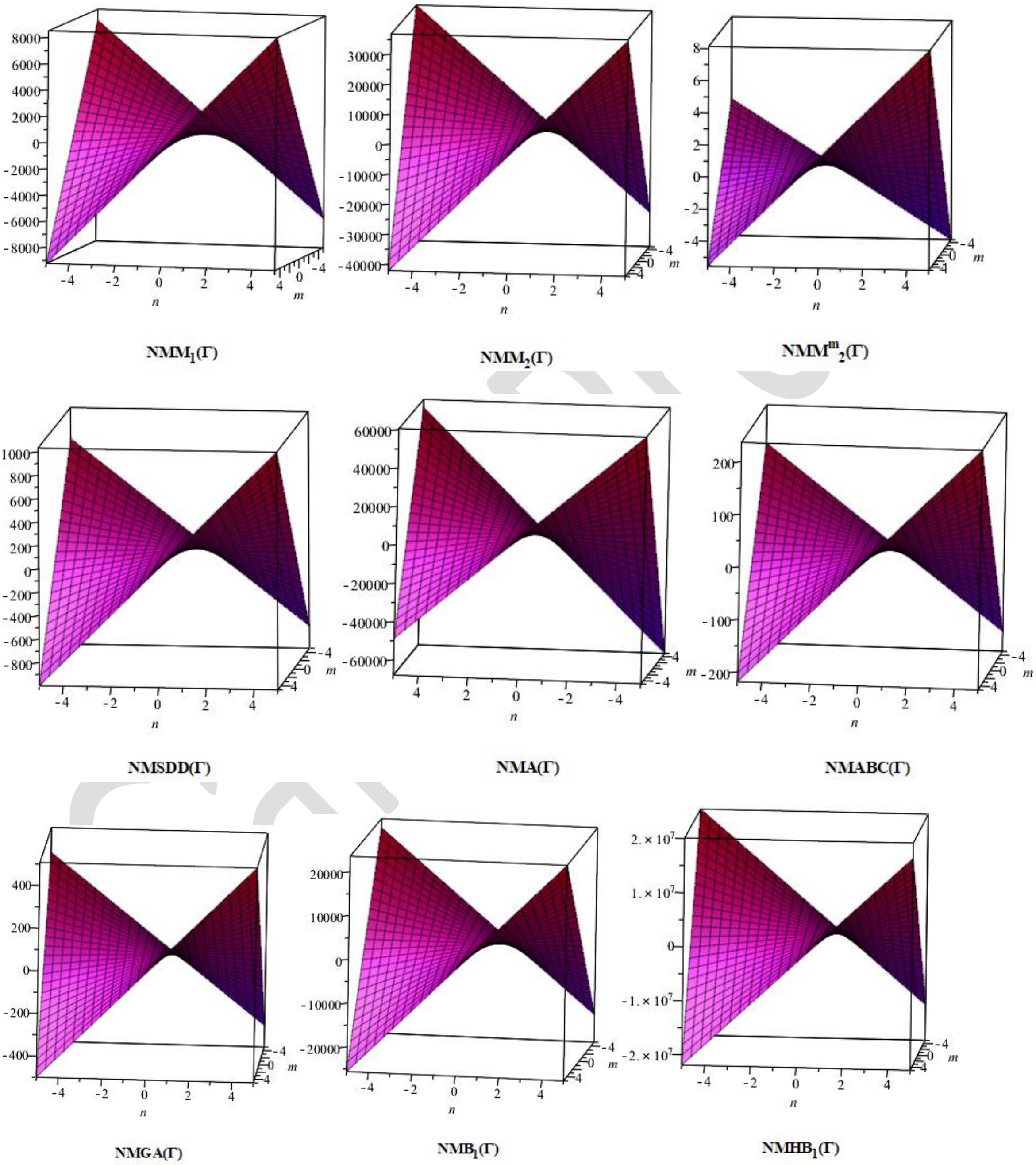

Figure 2: *3D plots for Theorem 2*

Table 3: *Comparison Table for Theorem 2.*

$m=n$	$NMM_1(\Gamma)$	$NMM_2(\Gamma)$	$NMM_2^m(\Gamma)$	$NMR_\alpha(\Gamma)$	$NMRR_\alpha(\Gamma)$	$NMSDD(\Gamma)$	$NMH(\Gamma)$
1	408	1434	0.75	202.61	4.65	61.75	4.62
2	1464	5754	1.93	728.58	13.26	196.30	13.18
3	3168	12990	3.55	1578.53	25.88	402.85	25.75
4	5520	23142	5.62	2752.49	42.49	681.40	42.31
5	8520	36210	8.13	4250.45	63.10	1032.00	62.88

Table 4: *Comparison Table for Theorem 2.*

$m=n$	$NMI(\Gamma)$	$NMA(\Gamma)$	$NMABC(\Gamma)$	$NMGA(\Gamma)$	$NMB_1(\Gamma)$	$NMB_2(\Gamma)$	$NMHB_1(\Gamma)$
1	100.62	2022.83	15.30	29.79	1104	4992	509712
2	362.61	8614.42	46.61	95.48	4008	20268	2464404
3	786.59	19876.87	93.91	197.17	8712	45912	5912088
4	1372.57	35810.19	157.22	334.86	15216	81924	10852764
5	2120.55	56414.37	236.53	508.56	23520	128304	17286432

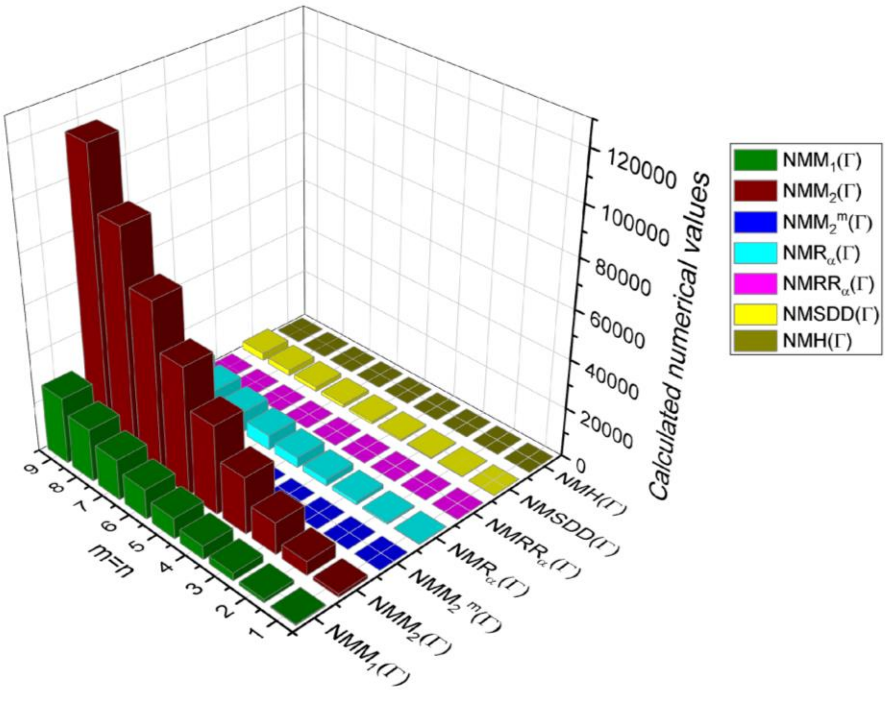

Figure 3: *3D Plots for Table 3.*

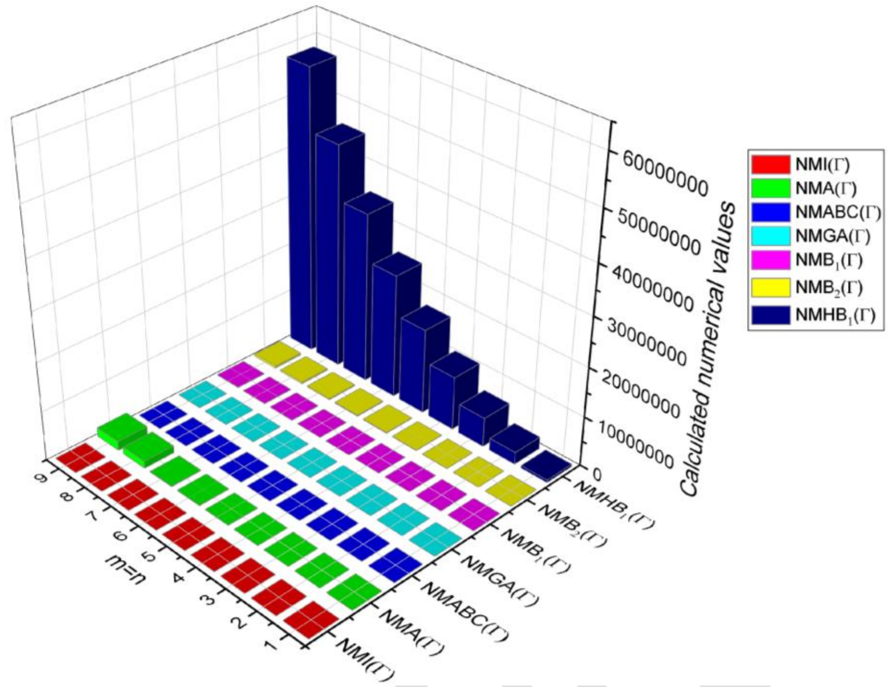

Figure 4: *3D Plots for Table 4.*

Table 5: *Comparison Table for Theorem 3*

$m=n$	$NENT_{M_{1(\Gamma)}}$	$NENT_{M_{2(\Gamma)}}$	$NENT_{{M_2}^m{}_{(\Gamma)}}$	$NENT_{HM_{(\Gamma)}}$	$NENT_{A_{(\Gamma)}}$	$NENT_{ABC_{(\Gamma)}}$	$NENT_{GA_{(\Gamma)}}$
1	3.38	3.31	3.32	3.31	4.42	3.40	3.40
2	4.54	4.49	4.46	4.49	5.34	4.56	4.56
3	5.27	5.23	5.18	5.23	6.00	5.28	5.29
4	5.80	5.77	5.72	5.77	6.49	5.81	5.82
5	6.22	6.20	6.15	6.20	6.89	6.23	6.23

Table 6: *Comparison Table for Theorem 3*

$m = n$	$NENT_{AG_{1(\Gamma)}}$	$NENT_{F_{1(\Gamma)}}$	$NENT_{F_{2(\Gamma)}}$	$NENT_{\chi(\Gamma)}$	$NENT_{REZG_{1(\Gamma)}}$	$NENT_{REZG_{2(\Gamma)}}$	$NENT_{REZG_{3(\Gamma)}}$
1	3.40	3.31	3.08	6.80	3.69	4.39	3.21
2	4.56	4.50	4.35	8.41	4.82	5.52	4.42
3	5.29	5.24	5.13	9.35	5.53	6.22	5.18
4	5.82	5.77	5.70	10.00	6.05	6.74	5.73
5	6.23	6.20	6.13	10.51	6.47	7.16	6.17

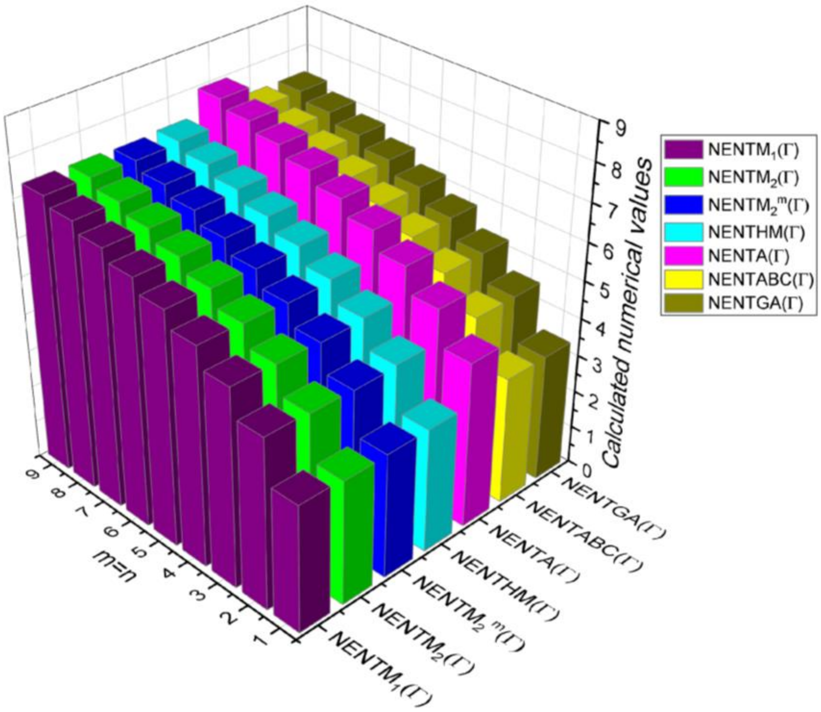

Figure 5: *3D Plots for Table 5.*

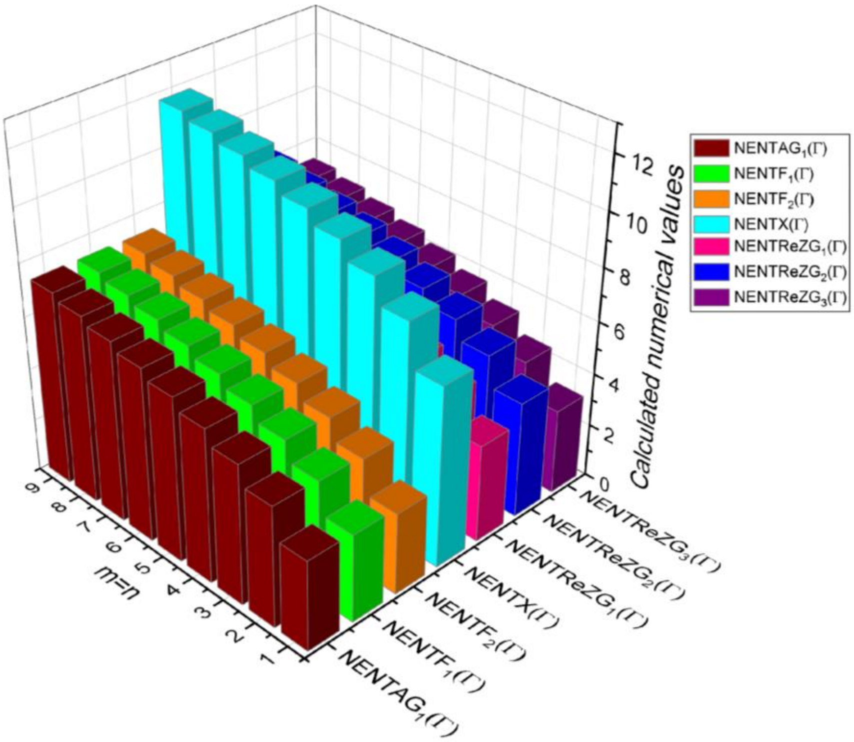

Figure 6:*3D Plots for Table 6.*

3 Conclusion

In this article, the closed form analytical expressions of neighbourhood sum degree-based indices of graphene have been derived using M-Polynomial. The computed indices are presented as individual 3D plots and comparison plots for a convenient interpretation of the mathematical expressions. The neighbourhood sum degree-based entropy measures have also been calculated for the three types of graphene structures. These indices are also visualised as 3D plots to corroborate the dependence of the indices on the underlying molecular structure. These indices have not been studied before for these structures; hence, this study is one of a kind. This study will enable future researchers to explore more topological indices for these fascinating structures.

4 Declarations

4.1 Competing Interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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