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Mathematical Modeling to Compute Topological Indices of Some Polymers Using Graph Polynomials

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Abstract: Graph theory offers powerful tools for modeling, designing, analyzing, and understanding the features of chemical structures and networks. In this framework, atoms are represented as vertices and chemical bonds as edges, forming a molecular graph. This paper focuses on the chemical graphs of Styrene Acrylonitrile (SAN) and Acrylonitrile Butadiene Styrene (ABS). Styrene Acrylonitrile (SAN) copolymers have been available since 1940. Their increased toughness compared to styrene made them suitable for various applications. However, SAN's limitations led to the addition of rubber (butadiene) as a third monomer, giving rise to Acrylonitrile Butadiene Styrene (ABS) plastics. ABS copolymers were introduced in the 1950's and became popular due to their variability and ease of processing, establishing them as the most widely used engineering polymers. In this study, we compute several topological indices of the SAN and ABS chemical graphs using M-Polynomial and NM-Polynomial Methods. Specifically, we calculate the First Zagreb index, Second Zagreb index, Modified Second Zagreb index, Third Redefine Zagreb index, Symmetric Division index , General Randi´c index, Forgotten index, Inverse index, and Harmonic index. These indices are widely used in various fields, such as drug discovery, molecular modeling, and other molecular research areas. These indices enable the establishment of connections between specific physicochemical properties of chemical compounds, such as stability, boiling point, entropy, strain energy, and heat of formation.

Key words: Topological Indices; Chemical Properties; Graph Polynomial; Polymers Network.

1. Introduction:

The study of mathematical modeling of chemical events is the main focus of mathematical chemistry, which is the field of research that develops new mathematical applications to chemistry. Though it should not be confused with computational chemistry, mathematical chemistry is also occasionally referred to as computer chemistry. Trinajstić and Gutman in [26] gave a brief description of the historical development of mathematics and chemistry. In [2] Balaban, provided significant viewpoints of reflections about mathematical chemistry.

Graph theory is a discipline of mathematics that investigates graphs, which are mathematical structures used to model pairwise interactions between objects. A graph comprises of vertices (or nodes) connected by edges (or links). Graph theory explores various properties and types of graphs, including connectivity, traversal, and optimization problems. Applications range from computer science and network analysis to social sciences and biology.

Chemical graph theory applies the principles of graph theory to the study of chemical structures. In this context, molecules are represented as graphs where vertices correspond

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to atoms and edges represent bonds between them. By translating molecular structures into graphs, various topological indices can be derived. These indices serve as descriptors for predicting molecular properties like boiling points, stability, reactivity, and biological activity, see [20] and [30].

Topological indices are numerical values derived from the structure of chemical graphs that represent molecules which are primarily used in cheminformatics and quantitative structure-activity relationship (QSAR) studies. The concept emerged in the 1970s, with notable contributions from chemists like Zefirov and Gutman, who aimed to correlate molecular structure with chemical properties. The first widely recognized topological index is the Wiener index which was introduced by Hermann Wiener in 1947 [29], which measures the sum of distances between all pairs of vertices in a graph. This paved the way for the development of various other indices, such as the Zagreb indices in [8] and the Randi´c index in [19], each capturing different structural features.

In this paper, we explore the M-Polynomial and NM-Polynomial methods to analyze the topological indices of Styrene Acrylonitrile and Acrylonitrile Butadiene Styrene polymers structures. These polynomials are a fundamental tools in graph theory with a wide range of applications. A well-known example of a distancebased topological index is the Hosoya polynomial [10]. Deutsch and Klav Zar [4] proposed the M-polynomial which is essential for obtaining the degree-based topological indices in closed form. The topological indices for line graphs of chain silicate networks and H-naphthalenic nanotubes using M-polynomial was described in [11]. In [18], Mondal et al. defined NM-polynomial and compute the topological indices of crystallographic structures. Saharia and Dutta explored the neighborhood M-polynomial of graph operations, focusing on its applications in nanostructures and addressing cycle-related graph in [24]. Chamua et al. investigated the Mpolynomial and neighborhood M-polynomial related to specific drug structures, namely azacitidine, decitabine, and guadecitabine in [3]. Recently in [12], Irfan et al. computed neighborhood degree based topological indices of Nanotube via direct application of NM-Polynomial. In [1] Amer et al. compute degree based indices of bornon triangular nanotubes, Munir et al in [16] use M-polynomial to find indices of polyhex nanotubes, Yasin et al. in [17] used both M-polynomial and NM-polynomials to compute indices of biopolymers and in [21] Siddiqui et al. compute indices of certain networks.

Let $G(V, E)$ be a graph with vertex set V and edge set E. For a graph G, the degree of a vertex a, denoted by ζ_a, is the nuber of edges connected to a. The neighborhood degree sum of a, denoted by $n\zeta_a$, is the sum of the degrees of all vertices adjacent to a (i.e., all neighboring vertices of a). In this paper we compute several well-known topological indices based on these definitions. In Table 1, there are degree-based and neighbourhood degree sum-based expressions of topological indices.

Definition 1. [7] The M-Polynomial of a graph G is defined as

$$M(G;u,v) = \sum_{p\le q} k_{pq}(G)u^p v^q,$$

where k_{pq} is the total number of edges of type ab such that the degrees of vertices a and b are p and q, respectively.

Definition 2. [27] Let G be a graph. The following equation represents the NM-Polynomial:

$$NM(G;u,v) = \sum_{p\le q} l_{pq}(G)u^p v^q,$$

where l_{pq} is the total number of edges of type ab such that the neighbourhood degrees sum of vertices a and b are p and q, respectively.

Table 1: Degree-based and Neighbourhood Degree-based Topological indices.

Topological Indices	Degree-based	Neighbourhood Degree-based
First zagreb index (M_1) [8]	$\sum_{ab\in E(G)} \zeta_a + \zeta_b$	$\sum_{ab\in E(G)} n_{\zeta_a} + n_{\zeta_b}$
Second zagreb index (M_2) [8]	$\sum_{ab\in E(G)} \zeta_a\zeta_b$	$\sum_{ab\in E(G)} n_{\zeta_a} n_{\zeta_b}$
Modified Second Zagreb index (M_2^m) [15]	$\sum_{ab\in E(G)} 1/(\zeta_a\zeta_b)$	$\sum_{ab\in E(G)} 1/(n_{\zeta_a} n_{\zeta_b})$
Redfined Third Zagreb index $(ReZG_3)$ [6]	$\sum_{ab\in E(G)} (\zeta_a + \zeta_b)(\zeta_a\zeta_b)$	$\sum_{ab\in E(G)} (n_{\zeta_a} + n_{\zeta_b})(n_{\zeta_a} n_{\zeta_b})$
Symmetric division index (SDD) [28]	$\sum_{ab\in E(G)} (\zeta_a^2 + \zeta_b^2)/(\zeta_a\zeta_b)$	$\sum_{ab\in E(G)} (n_{\zeta_a}^2 + n_{\zeta_b}^2)/(n_{\zeta_a} n_{\zeta_b})$
General Randic index (R_α) [19]	$\sum_{ab\in E(G)} (\zeta_a\zeta_b)^\alpha$	$\sum_{ab\in E(G)} (n_{\zeta_a} n_{\zeta_b})^\alpha$
Forgotten index (F) [13]	$\sum_{ab\in E(G)} \zeta_a^2 + \zeta_b^2$	$\sum_{ab\in E(G)} n_{\zeta_a}^2 + n_{\zeta_b}^2$
Inverse index (I) [23]	$\sum_{ab\in E(G)} (\zeta_a\zeta_b)/(\zeta_a + \zeta_b)$	$\sum_{ab\in E(G)} (n_{\zeta_a} n_{\zeta_b})/(n_{\zeta_a} + n_{\zeta_b})$
Harmonic index (H) [9]	$\sum_{ab\in E(G)} 2/(\zeta_a + \zeta_b)$	$\sum_{ab\in E(G)} 2/(n_{\zeta_a} + n_{\zeta_b})$

Polynomials provide an easy and direct way to compute topological indices of graphs because they encode structural information in a compact and systematic form. Instead of computing indices separately through complex summations or iterative methods, polynomial representations such as the M-polynomial, Zagreb polynomials, and Hosoya polynomial allow indices to be derived through simple algebraic manipulations. By substituting appropriate values or performing basic differentiation and integration, multiple indices can be extracted efficiently,making polynomials a powerful tool for graph-based analysis in chemistry, network theory, and related fields. The indices listed in Table can be derived using various polynomials. The M-polynomial and NM-polynomial based expressions of the indices are expressed in Table 2.

Table 2: M-Polynomial and NM-Polynomial of Topological Indices.

No.	Topological Indices	Derived from b(u,v)=M(G;u,v)/ NM(G;u,v)
1	M_1	$(D_u + D_v)(b(u,v))_{u=v=1}$
2	M_2	$(D_u D_v)(b(u,v))_{u=v=1}$
3	M_2^n	$(F_u F_v)(b(u,v))_{u=v=1}$
4	$ReZG_3$	$[(D_u + D_v)(D_u D_v)](b(u,v))_{u=v=1}$
5	SDD	$(D_u F_v + D_v F_u)(b(u,v))_{u=v=1}$
6	R_α	$(D_u^\alpha D_v^\alpha)(b(u,v))_{u=v=1}$
7	F	$(D_u^2 + D_v^2)(b(u,v))_{u=v=1}$
8	I	$(F_u J D_u D_v)(b(u,v))_{u=v=1}$
9	H	$2(F_u J)(b(u,v))_{u=v=1}$

where

$$D_u = u\Big(\frac{\delta(b(u,v))}{\delta u}\Big), D_v = v\Big(\frac{\delta(b(u,v))}{\delta v}\Big), J(b(u,v)) = (b(u,v))\,|_{u=v},$$
$$F_u = \int_0^u \frac{b(u,v)\,|_{u=t}}{t} dt, F_v = \int_0^v \frac{b(u,v)\,|_{v=t}}{t} dt.$$

2. Styrene Acrylonitrile (SAN)

SAN is a resin that came into use in the 1930s and was developed by combining Styrene and Acrylonitrile to overcome the brittleness and limited chemical resistance of pure Styrene. By optimizing the polymerization process in the 1950s, manufacturers achieved a balance of properties that enhanced SAN's commercial viability. Composed primarily of Styrene (70–80)% and Acrylonitrile (20–30)%, SAN offers superior chemical resistance, dimensional stability, and impact resistance compared to its predecessor. For the more details of Polystyrene and Styrene copolymers look at [14] and [22]. In this section, we calculate both M-Polynomial and NMPolynomial for Styrene Acrylonitrile (SAN) and present our results. We also compare these indices numerically and graphically. The unit cell of Styrene Acrylonitrile (SAN) consists of Carbon (C), Hydrogen (H), and Carbon Nanotube (CN) where carbon, hydrogen and carbon nanotube are represented by vertices and bonds by edges. In SAN, there are $16n$ vertices and $17n-1$ edges, with n indicating the number of units. The chemical structure of Styrene Acrylonitrile is given in Figure 1 with its chemical graph of one unit and three units with carbon in green, hydrogen in blue, and carbon nanotube in yellow where red edges represents the connections between units. Table 3 and Table 4 are display the edge distribution of SAN for both degree-based and neighborhood degree-based edge partition respectively.

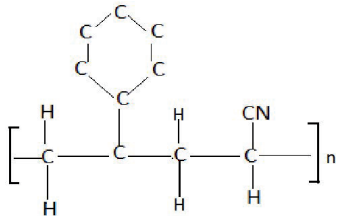
Table 3: Degree-based Edge Partition of Styrene Acrylonitrile Graph.

(ζ_u, ζ_v)	(1,3)	(1,4)	(2,2)	(2,3)	(3,3)	(3,4)	(4,4)
No. of edges	4	$6n-4$	$4n$	$2n$	$n+1$	$2n$	$2n-2$

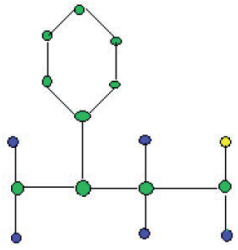
2.1 M-Polynomial of Styrene Acrylonitrile

The M-Polynomial of Styrene Acrylonitrile using degree-based edge partition in Table 3 is given as follows

$$\begin{aligned} M(G;u,v) &= \sum_{p\le q} k_{pq}(G) u^p v^q \\ &= |\,k_{1,3}\,|\,uv^3 + |\,k_{1,4}\,|\,uv^4 + |\,k_{2,2}\,|\,u^2v^2 + |\,k_{2,3}\,|\,u^2v^3 + |\,k_{3,3}\,|\,u^3v^3 + |\,k_{3,4}\,|\,u^3v^4 + |\,k_{4,4}\,|\,u^4v^4 \\ &= 4uv^3 + (6n-4)uv^4 + 4nu^2v^2 + 2nu^2v^3 + (n+1)u^3v^3 + 2nu^3v^4 + (2n-2)u^4v^4. \end{aligned} \quad (1)$$

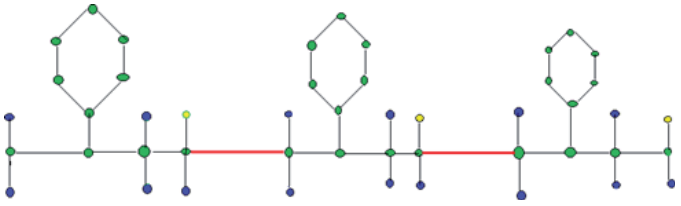


(a) Chemical Structure of SAN



(b) Chemical Graph of SAN

Figure 1: Molecular Configurations of Styrene Acrylonitrile (SAN).



(c) A Three Units Chain of SAN, with Each Unit Connected by Red Edges.

Table 4: Neighbourhood degree-based edge partition of Styrene Acrylonitrile graph for n ≥2.

$(n\zeta_a, n\zeta_b)$	No. of edges	$(n\zeta_a, n\zeta_b)$	No. of edges
(3,5)	2	(5,10)	1
(3,6)	2	(6,8)	1
(4,4)	$2n$	(7,10)	1
(4,5)	$2n$	(7,11)	$n-1$
(4,9)	$4n-4$	(8,11)	1
(4,10)	$2n-2$	(9,10)	$2n-1$
(4,8)	2	(9,11)	$2n-3$
(5,7)	$2n$		

By using Equation 1, the operators which are listed in Table 2 are as follows

$$D_u = u\left(\frac{\delta(b(u,v))}{\delta u}\right)$$
$$= u\frac{\delta}{\delta u}\left(4uv^3 + (6n-4)uv^4 + 4nu^2v^2 + 2nu^2v^3 + (n+1)u^3v^3 + 2nu^3v^4 + (2n-2)u^4v^4\right)$$
$$= 4uv^3 + (6n-4)uv^4 + 2(4n)u^2v^2 + 2(2n)u^2v^3 + 3(n+1)u^3v^3 + 3(2n)u^3v^4 + 4(2n-2)u^4v^4.$$

$$D_v = v\left(\frac{\delta(b(u,v))}{\delta v}\right)$$
$$= v\frac{\delta}{\delta v}\left(4uv^3 + (6n-4)uv^4 + 4nu^2v^2 + 2nu^2v^3 + (n+1)u^3v^3 + 2nu^3v^4 + (2n-2)u^4v^4\right)$$
$$= 3(4)uv^3 + 4(6n-4)uv^4 + 2(4n)u^2v^2 + 3(2n)u^2v^3 + 3(n+1)u^3v^3 + 4(2n)u^3v^4 + 4(2n-2)u^4v^4.$$

$$F_u = \int_0^u \frac{b(u,v)_{u=t}}{t}dt,$$

$$where\ \frac{b(u,v)_{u=t}}{t} = 4v^3 + (6n-4)v^4 + 4ntv^2 + 2ntv^3 + (n+1)t^2v^3 + 2nt^2v^4 + (2n-2)t^3v^4$$

$$F_u = (4)uv^3 + (6n-4)uv^4 + \frac{1}{2}(4n)u^2v^2 + \frac{1}{2}(2n)u^2v^3 + \frac{1}{3}(n+1)u^3v^3 + \frac{1}{3}(2n)u^3v^4 + \frac{1}{4}(2n-2)u^4v^4.$$

$$F_v = \int_0^v \frac{b(u,v)_{v=t}}{t}dt,$$

$$where\ \frac{b(u,v)_{v=t}}{t} = 4ut^2 + (6n-4)ut^3 + 4nu^2t + 2nu^2t^2 + (n+1)u^3t^2 + 2nu^3t^3 + (2n-2)u^4t^3$$

$$F_v = \frac{4}{3}uv^3 + \frac{1}{3}(6n-4)uv^4 + \frac{1}{2}(4n)u^2v^2 + \frac{1}{3}(2n)u^2v^3 + \frac{1}{3}(n+1)u^3v^3 + \frac{1}{4}(2n)u^3v^4 + \frac{1}{4}(2n-2)u^4v^4.$$

$$J(b(u,v)) = b(u,v)\,|_{u=v}$$
$$= 4u^4 + (6n-4)u^5 + 4nu^4 + 2nu^5 + (n+1)u^6 + 2nu^7 + (2n-2)u^8.$$

$$F_uJ = \int_0^u \frac{J(b(u,v))_{u=t}}{t}dt$$
$$= \frac{1}{4}(4)u^4 + \frac{1}{5}(6n-4)u^5 + \frac{1}{4}(4n)u^4 + \frac{1}{5}(2n)u^5 + \frac{1}{6}(n+1)u^6 + \frac{1}{7}(2n)u^7 + \frac{1}{8}(2n-2)u^8.$$

Theorem 1. Let G be the graphical network of Styrene Acrylonitrile then by using M-Polynomial the topological indices are

$$M_1(G) = 92n - 14$$
$$M_2(G) = 117n - 27$$
$$M_2^m(G) = 3.7361n - 0.013889$$
$$ReZG_3(G) = 722n - 234$$
$$R_\alpha(G) = 42.8271n - 6.07179$$
$$SDD(G) = 48.500n - 2$$
$$F(G) = 292n - 74$$
$$I(G) = 20.129n - 2.7000$$
$$H(G) = 6.6048n + 0.90000.$$

Proof: By using the results of M-polynomial of Styrene Acrylonitrile graph network and Table 2, we have

$$\begin{aligned} M_1(G) &= (D_u + D_v)(b(u,v))_{u=v=1} \\ &= 92n - 14. \\ M_2(G) &= (D_u D_v)(b(u,v))_{u=v=1} \\ &= 117n - 27. \\ M_2^m(G) &= (F_u F_v)(b(u,v))_{u=v=1} \\ &= 3.7361n - 0.013889. \end{aligned}$$

$$\begin{aligned} ReZG_3(G) &= [(D_u + D_v)(D_u D_v)](b(u,v))_{u=v=1} \\ &= 722n - 234. \\ SDD(G) &= (D_u F_v + D_v F_u)(b(u,v))_{u=v=1} \\ &= 48.500n - 2. \\ R_\alpha(G) &= (D_u^\alpha D_v^\alpha)(b(u,v))_{u=v=1} \\ &= 4 \cdot 3^\alpha + 4^\alpha(6n-4) + 4 \cdot (2^\alpha)^2 n + 2 \cdot 2^\alpha \cdot 3^\alpha n \\ &\quad + (3^\alpha)^2(n+1) + 2 \cdot 3^\alpha \cdot 4^\alpha n + (4^\alpha)^2(2n-2). \end{aligned}$$

$$For \ \alpha = \frac{1}{2}$$

$$\begin{aligned} R_{\frac{1}{2}}(G) &= 42.8271n - 6.07179. \\ F(G) &= (D_u^2 + D_v^2)(b(u,v))_{u=v=1} \\ &= 292n - 74. \\ I(G) &= (F_u J D_u D_v)(b(u,v))_{u=v=1} \\ &= 20.129n - 2.7000. \\ H(G) &= 2(F_u J)(b(u,v))_{u=v=1} \\ &= 6.6048n + 0.90000. \end{aligned}$$

2.1 NM-Polynomial of Styrene Acrylonitrile

The NM-Polynomial of Styrene Acrylonitrile using neighbourhood degree-based edge partition in Table 4 is

$$\begin{aligned} NM(G;u,v) &= \sum_{p \le q} l_{pq}(G) u^p v^q \\ &= |\, l_{3,5} \,|\, u^3v^5 + |\, l_{3,6} \,|\, u^3v^6 + |\, l_{4,4} \,|\, u^4v^4 + |\, l_{4,5} \,|\, u^4v^5 + |\, l_{4,8} \,|\, u^4v^8 + |\, l_{4,9} \,|\, u^4v^9 + |\, l_{4,10} \,|\, u^4v^{10} + |\, l_{5,7} \,|\, u^5v^7 \\ &\quad + |\, l_{5,10} \,|\, u^5v^{10} + |\, l_{6,8} \,|\, u^6v^8 + |\, l_{7,10} \,|\, u^7v^{10} + |\, l_{7,11} \,|\, u^7v^{11} + |\, l_{8,11} \,|\, u^8v^{11} + |\, l_{9,10} \,|\, u^9v^{10} + |\, l_{9,11} \,|\, u^9v^{11} \\ &= 2u^3v^5 + 2u^3v^6 + 2nu^4v^4 + 2nu^4v^5 + 2u^4v^8 + (4n-4)u^4v^9 + (2n-2)u^4v^{10} + 2nu^5v^7 + u^5v^{10} \\ &\quad + u^6v^8 + u^7v^{10} + (n-1)u^7v^{11} + u^8v^{11} + (2n-1)u^9v^{10} + (2n-3)u^9v^{11}. \end{aligned} \tag{2}$$

By using Equation 2 the operators which are listed in Table 2 are as follows

$$\begin{aligned} D_u &= u\left(\frac{\delta(b(u,v))}{\delta u}\right) \\ &= 3(2)u^3v^5 + 3(2)u^3v^6 + 4(2n)u^4v^4 + 4(2n)u^4v^5 + 4(2)u^4v^8 + 4(4n-4)u^4v^9 \\ &\quad + 4(2n-2)u^4v^{10} + 5(2n)u^5v^7 + 5u^5v^{10} + 6u^6v^8 + 7u^7v^{10} + 7(n-1)u^7v^{11} \\ &\quad + 8u^8v^{11} + 9(2n-1)u^9v^{10} + 9(2n-3)u^9v^{11}. \end{aligned}$$

$$\begin{aligned} D_v &= v\left(\frac{\delta(b(u,v))}{\delta u}\right) \\ &= 5(2)u^3v^5 + 6(2)u^3v^6 + 4(2n)u^4v^4 + 5(2n)u^4v^5 + 8(2)u^4v^8 + 9(4n-4)u^4v^9 \\ &\quad + 10(2n-2)u^4v^{10} + 7(2n)u^5v^7 + 10u^5v^{10} + 8u^6v^8 + 10u^7v^{10} + 11(n-1)u^7v^{11} \\ &\quad + 11u^8v^{11} + 10(2n-1)u^9v^{10} + 11(2n-3)u^9v^{11}. \end{aligned}$$

$$F_u = \int_0^u \frac{b(u,v)_{u=t}}{t} dt,$$

$$\begin{aligned} where \ \frac{b(u,v)_{u=t}}{t} &= 2t^2v^5 + 2t^2v^6 + 2nt^3v^4 + 2nt^3v^5 + 2t^3v^8 + (4n-4)t^3v^9 + (2n-2)t^3v^{10} + 2nt^4v^7 \\ &\quad + t^4v^{10} + t^5v^8 + t^6v^{10} + (n-1)t^6v^{11} + t^7v^{11} + (2n-1)t^8v^{10} + (2n-3)t^8v^{11} \end{aligned}$$

$$F_u = \frac{1}{3}(2)u^3v^5 + \frac{1}{3}(2)u^3v^6 + \frac{1}{4}(2n)u^4v^4 + \frac{1}{4}(2n)u^4v^5 + \frac{1}{4}(2)u^4v^8 + \frac{1}{4}(4n-4)u^4v^9 + \frac{1}{4}(2n-2)u^4v^{10} + \frac{1}{5}(2n)u^5v^7 + \frac{1}{5}u^5v^{10} + \frac{1}{6}u^6v^8 + \frac{1}{7}u^7v^{10} + \frac{1}{7}(n-1)u^7v^{11} + \frac{1}{8}u^8v^{11} + \frac{1}{9}(2n-1)u^9v^{10} + \frac{1}{9}(2n-3)u^9v^{11}.$$

$$F_v = \int_0^v \frac{b(u,v)_{v=t}}{v}dv,$$

$$where\ \frac{b(u,v)_{v=t}}{t} = 2u^3t^4 + 2u^3t^5 + 2nu^4t^3 + 2nu^4t^4 + 2u^4t^7 + (4n-4)u^4t^8 + (2n-2)u^4t^9 + 2nu^5t^6 + u^5t^9 + u^6t^7 + u^7t^9 + (n-1)u^7t^{10} + u^8t^{10} + (2n-1)u^9t^9 + (2n-3)u^9t^{10}$$

$$F_v = \frac{1}{5}(2)u^3v^5 + \frac{1}{6}(2)u^3v^6 + \frac{1}{4}(2n)u^4v^4 + \frac{1}{5}(2n)u^4v^5 + \frac{1}{8}(2)u^4v^8 + \frac{(4n-4)}{9}u^4v^9 + \frac{(2n-2)}{10}u^4v^{10} + \frac{1}{7}(2n)u^5v^7 + \frac{1}{10}u^5v^{10} + \frac{1}{8}u^6v^8 + \frac{1}{10}u^7v^{10} + \frac{(n-1)}{11}u^7v^{11} + \frac{1}{11}u^8v^{11} + \frac{(2n-1)}{10}u^9v^{10} + \frac{(2n-3)}{11}u^9v^{11}.$$

$$Now,\ J(b(u,v)) = (b(u,v))|_{u=v} = 2u^8 + 2u^9 + 2nu^8 + 2nu^9 + 2u^{12} + (4n-4)u^{13} + (2n-2)u^{14} + 2nu^{12} + u^{15} + u^{14} + u^{17} + (n-1)u^{18} + u^{19} + (2n-1)u^{19} + (2n-3)u^{20}.$$

$$F_uJ = \int_0^u \frac{J(b(u,v))_{u=t}}{t}dt = \frac{1}{8}(2)u^8 + \frac{1}{9}(2)u^9 + \frac{1}{8}(2n)u^8 + \frac{1}{9}(2n)u^9 + \frac{1}{12}(2)u^{13} + \frac{(4n-4)}{13}u^{13} + \frac{(2n-2)}{14}u^{14} + \frac{1}{12}(2n)u^{12} + \frac{1}{15}u^{15} + \frac{1}{14}u^{14} + \frac{1}{17}u^{17} + \frac{(n-1)}{18}u^{18} + \frac{1}{19}u^{19} + \frac{(2n-1)}{19}u^{19} + \frac{(2n-3)}{20}u^{20}.$$

Theorem 2. Let G be the graphical network of Styrene Acrylonitrile then by using NM-Polynomial the topological indices are

$NM_1(G) = 234n - 54$
$NM_2(G) = 821n - 302$
$NM_2^m(G) = 0.49867n + 0.15791$
$ND_3(G) = 13214n - 6412$
$ND_5(G) = 37.217n - 3.5704$
$NR_\alpha(G) = 113.07392n - 25.4688$
$NF(G) = 1850n - 700$
$NI(G) = 54.720n - 12.900$
$NH(G) = 2.7005n + 0.35941.$

Proof: By using the results of NM-polynomial of Styrene Acrylonitrile graph network and Table 2, we have

$$NM_1(G) = (D_u + D_v)(b(u,v))_{u=v=1} = 234n - 54.$$

$$NM_2(G) = (D_uD_v)(b(u,v))_{u=v=1} = 821n - 302.$$

$$NM_2^m(G) = (F_uF_v)(b(u,v))_{u=v=1} = 0.49867n + 0.15791.$$

$$ND_3(G) = [(D_u + D_v)(D_uD_v)](b(u,v))_{u=v=1} = 13214n - 6412.$$

$$ND_5(G) = (D_uF_v + D_vF_u)(b(u,v))_{u=v=1} = 37.217n - 3.5704.$$

$$NR_\alpha(G) = (D_u^\alpha D_v^\alpha)(b(u,v))_{u=v=1} = 2\cdot5^\alpha\cdot3^\alpha + 2\cdot6^\alpha\cdot3^\alpha + 2\cdot(4^\alpha)^2n + 2\cdot5^\alpha\cdot4^\alpha n + 2\cdot8^\alpha\cdot4^\alpha + 9^\alpha\cdot4^\alpha(4n-4) + 10^\alpha\cdot4^\alpha(2n-2) + 2\cdot7^\alpha\cdot5^\alpha nn + 10^\alpha\cdot5^\alpha + 8^\alpha\cdot6^\alpha + 10^\alpha\cdot7^\alpha + 11^\alpha\cdot7^\alpha(n-1) + 11^\alpha\cdot8^\alpha + 10^\alpha\cdot9^\alpha(2n-1) + 11^\alpha\cdot9^\alpha(2n-3).$$

$For\ \alpha = \frac{1}{2}, we\ get$

$$NR_{\frac{1}{2}}(G) = 113.07392n - 25.4688.$$

$$NF(G) = (D_u^2 + D_v^2)(b(u,v))_{u=v=1} = 1850n - 700.$$

$$NI(G) = (F_u JD_u D_v)(b(u,v))_{u=v=1} n$$
$$= 54.720n - 12.900.$$
$$NH(G) = 2(F_u J)(b(u,v))_{u=v=1}$$
$$= 2.7005n + 0.35941.$$

The degree-based and neighborhood degree-based topological indices (TIs) of Styrene Acrylonitrile are calculated using both the M-polynomial and the NM-polynomial. The numerical results are presented in Tables 7 and 8, and their graphical representations are shown in Figure 6.

3. Acrylonitrile Butadiene Styrene (ABS)

ABS was first synthesized in the 1940s through research efforts aimed at combining the properties of Acrylonitrile, Butadiene, and Styrene into a single polymer. ABS quickly gained popularity in the automotive industry for its ability to withstand impacts and chemical exposure, leading to its use in automotive trim, interior components, and exterior parts. Its versatility also finds applications in electronics, consumer goods, construction, and medical devices. It is the perfect material in any situation where exceptional colorfastness, sheen, and surface quality are needed. For parts that have to meet strict service specifications or can reduce weight, ABS is a very affordable material. For more details on the work related to ABS, read article [5] and [25]. In this section, we calculate both M-Polynomial and NM-Polynomial for Acrylonitrile Butadiene Styrene (ABS) and present our results. The unit cell of ABS consists of Carbon(C), Hydrogen(H), and Nitrogen(N), where cabon, hydrogen, and nitrogen are represented by vertices and their bonds are represented by edges. In Acrylonitrile Butadiene Styrene (ABS), there are $33n$ vertices and $34n-1$ edges, with n indicating the number of units. The chemical structure of Acrylonitrile Butadiene Styrene is shown in Figure 2 with its chemical graph of one unit and three units with carbon in green, hydrogen in blue, and carbon nanotube in yellow where red edges represents the connections between units. Table 2 and Table 6 display the edge distribution of ABC for degree-based and neighborhood degree-based respectively.

Table 5: Degree-based Edge Partition of Acrylonitrile Butadiene Styrene Graph.

(ζ_u, ζ_v)	(1,2)	(1,3)	(1,4)	(2,4)	(3,3)	(3,4)	(4,4)
No. of edges	n	$7n+4$	$10n-4$	n	$7n+1$	$3n$	$5n-2$

Table 6: Neighbourhood Degree-based Edge Partition of Acrylonitrile Butadiene Styrene (ABS) for n ≥2.

$(n\zeta_u, n\zeta_v)$	No. of edges	$(n\zeta_u, n\zeta_v)$	No. of edges
(2,5)	n	(6,11)	1
(3,5)	2	(7,7)	$4n$
(3,6)	2	(7,10)	$2n$
(3,7)	$5n+1$	(7,8)	1
(3,8)	$2n-1$	(8,8)	$n-1$
(4,9)	$4n-2$	(8,9)	$2n-1$
(4,10)	$5n-2$	(9,10)	$2n-1$
(4,11)	1	(10,10)	n
(4,12)	$n-1$	(10,11)	2
(5,7)	1	(10,12)	$3n-3$
(5,10)	n		

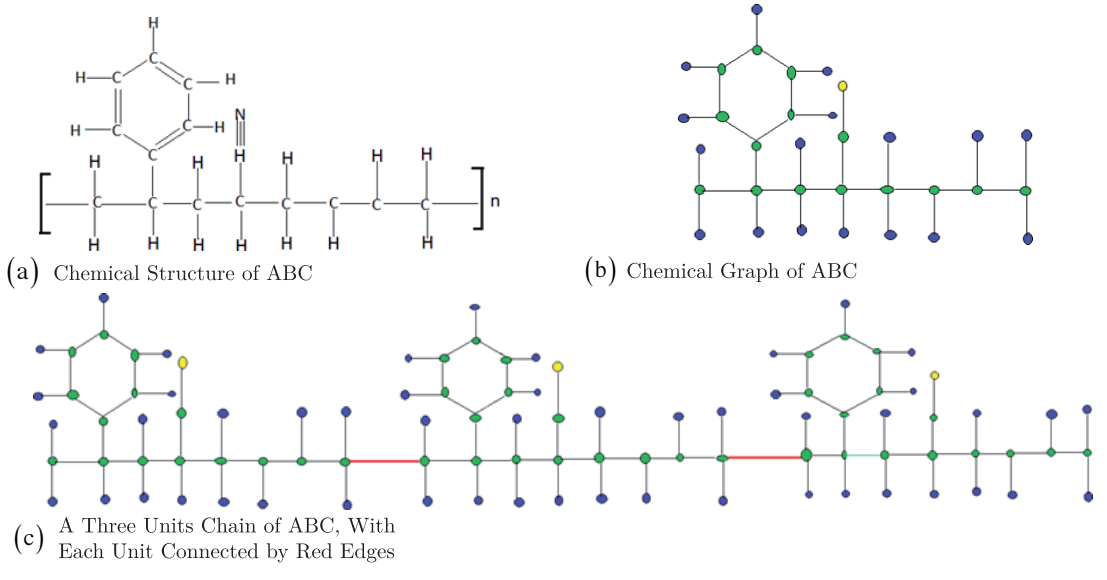


Figure 2: Molecular configurations of Acrylonitrile Butadiene Styrene (ABS).

3.1 M-Polynomial of Acrylonitrile Butadiene Styrene

The M-Polynomial of Acrylonitrile Butadiene Styrene using degree-based edge partition in Table 2 is

$$\begin{aligned} M(G;u,v) &= \sum_{p\le q} k_{pq}(G)u^p v^q \\ &= |\,k_{1,2}\,|\,uv^2 + |\,k_{1,3}\,|\,uv^3 + |\,k_{1,4}\,|\,uv^4 + |\,k_{2,4}\,|\,u^2v^4 + |\,k_{3,3}\,|\,u^3v^3 + |\,k_{3,4}\,|\,u^3v^4 + |\,k_{4,4}\,|\,u^4v^4 \\ &= nuv^2 + (7n+4)uv^3 + (10n-4)uv^4 + nu^2v^4 + (7n+1)u^3v^3 + 3nu^3v^4 + (5n-2)u^4v^4. \end{aligned} \tag{3}$$

Now by using Equation 3 the operators which are listed in Table 2 are as follows

$$\begin{aligned} D_u &= u\Big(\frac{\delta(b(u,v))}{\delta u}\Big) \\ &= u\frac{\delta}{\delta u}\Big(nuv^2 + (7n+4)uv^3 + (10n-4)uv^4 + nu^2v^4 + (7n+1)u^3v^3 + 3nu^3v^4 + (5n-2)u^4v^4\Big) \\ &= nuv^2 + (7n+4)uv^3 + (10n-4)uv^4 + 2nu^2v^4 + 3(7n+1)u^3v^3 + 3(3n)u^3v^4 + 4(5n-2)u^4v^4. \end{aligned}$$

$$\begin{aligned} D_v &= v\Big(\frac{\delta(b(u,v))}{\delta v}\Big) \\ &= v\frac{\delta}{\delta v}\Big(nuv^2 + (7n+4)uv^3 + (10n-4)uv^4 + nu^2v^4 + (7n+1)u^3v^3 + 3nu^3v^4 + (5n-2)u^4v^4\Big) \\ &= 2nuv^2 + 3(7n+4)uv^3 + 4(10n-4)uv^4 + 4nu^2v^4 + 3(7n+1)u^3v^3 + 4(3n)u^3v^4 + 4(5n-2)u^4v^4. \end{aligned}$$

$$F_u = \int_0^u \frac{b(u,v)_{u=t}}{t}dt,$$

$$where\ \frac{b(u,v)_{u=t}}{t} = nv^2 + (7n+4)v^3 + (10n-4)v^4 + ntv^4 + (7n+1)t^2v^3 + 3nt^2v^4 + (5n-2)t^3v^4$$

$$F_u = nuv^2 + (7n+4)uv^3 + (10n-4)uv^4 + \frac{1}{2}nu^2v^4 + \frac{1}{3}(7n+1)u^3v^3 + \frac{1}{3}(3n)u^3v^4 + \frac{1}{4}(5n-2)u^4v^4.$$

$$F_v = \int_0^v \frac{b(u,v)_{v=t}}{t}dt,$$

$$where\ \frac{b(u,v)_{v=t}}{t} = nut + (7n+4)ut^2 + (10n-4)ut^3 + nu^2t^3 + (7n+1)u^3t^2 + 3nu^3t^3 + (5n-2)u^4t^3$$

$$\begin{aligned} F_v &= \frac{1}{2}nuv^2 + \frac{1}{3}(7n+4)uv^3 + \frac{1}{4}(10n-4)uv^4 + \frac{1}{4}nu^2v^4 + \frac{1}{3}(7n+1)u^3v^3 + \frac{1}{4}(3n)u^3v^4 \\ &\quad + \frac{1}{4}(5n-2)u^4v^4. \end{aligned}$$

$$\begin{aligned} Now,\ J(b(u,v)) &= (b(u,v))\,|_{u=v} \\ &= nu^3 + (7n+4)u^4 + (10n-4)u^5 + nu^6 + (7n+1)u^9 + 3nu^7 + (5n-2)u^8. \end{aligned}$$

$$\begin{aligned} F_uJ &= \int_0^u \frac{J(b(u,v))_{u=t}}{t}dt \\ &= \frac{1}{3}nu^3 + \frac{1}{4}(7n+4)u^4 + \frac{1}{5}(10n-4)u^5 + \frac{1}{6}nu^6 + \frac{1}{9}(7n+1)u^9 + \frac{1}{7}(3n)u^7 + \frac{1}{8}(5n-2)u^8. \end{aligned}$$

Theorem 3. Let G be the graphical network of Acrylonitrile Butadiene Styrene then by using M-Polynomial the topological indices are

$$M_1(G) = 190n - 14$$
$$M_2(G) = 250n - 27$$
$$M_2^m(G) = 6.7986n + 0.31944$$
$$RezG_3(G) = 1608n - 234$$
$$SDD(G) = 101.08n - 5.6667$$
$$R_\alpha(G) = 87.75930n - 6.07179$$
$$F(G) = 626n - 74$$
$$I(G) = 40.893n - 2.7000$$
$$H(G) = 12.1626n + 0.12222.$$

Proof: By using the results of M-polynomial of Acrylonitrile Butadiene Styrene graph network and Table 2, we have

$$\begin{aligned} M_1(G) &= (D_u + D_v)(b(u,v))_{u=v=1} \\ &= 190n - 14. \\ M_2(G) &= (D_u D_v)(b(u,v))_{u=v=1} \\ &= 250n - 27. \end{aligned}$$

$$\begin{aligned} M_2^m(G) &= (F_u F_v)(b(u,v))_{u=v=1} \\ &= 6.7986n + 0.31944. \\ RezG_3(G) &= [(D_u + D_v)(D_u D_v)](b(u,v))_{u=v=1} \\ &= 1608n - 234. \\ SDD(G) &= (D_u F_v + D_v F_u)(b(u,v))_{u=v=1} \\ &= 101.08n - 5.6667. \\ R_\alpha(G) &= (D_u^\alpha D_v^\alpha)(b(u,v))_{u=v=1} \\ &= n \cdot 2^\alpha + 3^\alpha \cdot (7n+4) + 4^\alpha \cdot (10n-4) + 2^\alpha \cdot 4^\alpha \cdot n \\ &\quad + (3^\alpha)^2 \cdot (7n+1) + 3 \cdot 3^\alpha \cdot 4^\alpha \cdot n + (4^\alpha)^2 \cdot (5n-2). \end{aligned}$$

$For\ \ \alpha = \frac{1}{2}\ we\ get$

$$\begin{aligned} R_{\frac{1}{2}}(G) &= 87.75930n - 6.07179. \\ F(G) &= (D_u^2 + D_v^2)(b(u,v))_{u=v=1} \\ &= 626n - 74. \\ I(G) &= (F_u J D_u D_v)(b(u,v))_{u=v=1} \\ &= 40.893n - 2.7000 \\ H(G) &= 2(F_u J)(b(u,v))_{u=v=1} \\ &= 12.1626n + 0.12222. \end{aligned}$$

3.1 NM-Polynomial of Acrylonitrile Butadiene Styrene

The NM-Polynomial of Acrylonitrile Butadiene Styrene using degree-based edge partition in Table 6, is given as follows

$$\begin{aligned} NM(G;u,v) &= \sum_{p \le q} l_{pq}(G) u^p v^q \\ &= |\, l_{2,5} \,|\, u^2v^5 + |\, l_{3,5} \,|\, u^3v^5 + |\, l_{3,6} \,|\, u^3v^6 + |\, l_{3,7} \,|\, u^3v^7 + |\, l_{3,8} \,|\, u^3v^8 + |\, l_{4,9} \,|\, u^4v^9 + |\, l_{4,10} \,|\, u^4v^{10} + |\, l_{4,11} \,|\, u^4v^{11} \\ &\quad + |\, l_{4,12} \,|\, u^4v^{12} + |\, l_{5,7} \,|\, u^5v^7 + |\, l_{5,10} \,|\, u^5v^{10} + |\, l_{6,11} \,|\, u^6v^{11} + |\, l_{7,7} \,|\, u^7v^7 + |\, l_{7,8} \,|\, u^7v^8 + |\, l_{7,10} \,|\, u^7v^{10} \\ &\quad + |\, l_{8,8} \,|\, u^8v^8 + |\, l_{8,9} \,|\, u^8v^9 + |\, l_{9,10} \,|\, u^9v^{10} + |\, l_{10,10} \,|\, u^{10}v^{10} + |\, l_{10,11} \,|\, u^{10}v^{11} + |\, l_{10,12} \,|\, u^{10}v^{12} \\ &= nu^2v^5 + 2u^3v^5 + 2u^3v^6 + (5n+1)u^3v^7 + (2n-1)u^3v^8 + (4n-2)u^4v^9 + (5n-2)u^4v^{10} \\ &\quad + u^4v^{11} + (n-1)u^4v^{12} + u^5v^7 + nu^5v^{10} + u^6v^{11} + 4nu^7v^7 + 2nu^7v^8 + u^7v^{10} + (n-1)u^8v^8 \\ &\quad + (2n-1)u^8v^9 + (2n-1)u^9v^{10} + nu^{10}v^{10} + 2u^{10}v^{11} + (3n-3)u^{10}v^{12}. \end{aligned} \tag{4}$$

We apply Equation 4 to calculate these operators which are used Table 2 as

$$\begin{aligned} D_u &= 2nu^2v^5 + 3(2)u^3v^5 + 3(2)u^3v^6 + 3(5n+1)u^3v^7 + 3(2n-1)u^3v^8 + 4(4n-2)u^4v^9 + 4(5n-2)u^4v^{10} \\ &\quad + 4u^4v^{11} + 4(n-1)u^4v^{12} + 5u^5v^7 + 5nu^5v^{10} + 6u^6v^{11} + 7(4n)u^7v^7 + 7(2n)u^7v^8 + 7u^7v^{10} \\ &\quad + 8(n-1)u^8v^8 + 8(2n-1)u^8v^9 + 9(2n-1)u^9v^{10} + 10nu^{10}v^{10} + 10(2)u^{10}v^{11} + 10(3n-3)u^{10}v^{12}. \end{aligned}$$

$$\begin{aligned} D_v &= 5nu^2v^5 + 5(2)u^3v^5 + 6(2)u^3v^6 + 7(5n+1)u^3v^7 + 8(2n-1)u^3v^8 + 9(4n-2)u^4v^9 + 10(5n-2)u^4v^{10} \\ &\quad + 11u^4v^{11} + 12(n-1)u^4v^{12} + 7u^5v^7 + 10nu^5v^{10} + 11u^6v^{11} + 7(4n)u^7v^7 + 8(2n)u^7v^8 + 10u^7v^{10} \\ &\quad + 8(n-1)u^8v^8 + 9(2n-1)u^8v^9 + 10(2n-1)u^9v^{10} + 10nu^{10}v^{10} + 11(2)u^{10}v^{11} + 12(3n-3)u^{10}v^{12}. \end{aligned}$$

$$\begin{aligned} F_u &= \int_0^u \frac{b(u,v)_{u=t}}{t} dt \\ &= \frac{1}{2}nu^2v^5 + \frac{1}{3}(2)u^3v^5 + \frac{1}{3}(2)u^3v^6 + \frac{1}{3}(5n+1)u^3v^7 + \frac{1}{3}(2n-1)u^3v^8 + \frac{1}{4}(4n-2)u^4v^9 + \frac{1}{4}(5n-2)u^4v^{10} \\ &\quad + \frac{1}{4}u^4v^{11} + \frac{1}{4}(n-1)u^4v^{12} + \frac{1}{5}u^5v^7 + \frac{1}{5}nu^5v^{10} + \frac{1}{6}u^6v^{11} + \frac{1}{7}(4n)u^7v^7 + \frac{1}{7}(2n)u^7v^8 + \frac{1}{7}u^7v^{10} \\ &\quad + \frac{1}{8}(n-1)u^8v^8 + \frac{1}{8}(2n-1)u^8v^9 + \frac{1}{9}(2n-1)u^9v^{10} + \frac{1}{10}nu^{10}v^{10} + \frac{1}{10}(2)u^{10}v^{11} + \frac{1}{10}(3n-3)u^{10}v^{12}. \end{aligned}$$

$$J(b(u,v)) = (b(u,v))\,|_{u=v}$$
$$= nu^7 + 2u^8 + 2u^9 + (5n+1)u^{10} + (2n-1)u^{11} + (4n-2)u^{13} + (5n-2)u^{14} + u^{15} + (n-1)u^{16} + u^{12}$$
$$+nu^{15} + u^{17} + 4nu^{14} + (2n)u^{1}5 + u^{17} + (n-1)u^{16} + (2n-1)u^{17} + (2n-1)u^{19} + nu^{20} + 2u^{21}$$
$$+(3n-3)u^{22}.$$

$$F_uJ = \int_0^u \frac{J(b(u,v))_{u=t}}{t}dt$$
$$= \frac{1}{7}nu^7 + \frac{1}{8\cdot 2}u^8 + \frac{2}{9}u^9 + \frac{1}{10}(5n+1)u^{10} + \frac{1}{11}(2n-1)u^{11} + \frac{1}{13}(4n-2)u^{13} + \frac{1}{14}(5n-2)u^{14} + \frac{1}{15}u^{15}$$
$$+\frac{1}{16}(n-1)u^{16} + \frac{1}{12}u^{12} + \frac{1}{15}nu^{15} + \frac{1}{17}u^{17} + \frac{1}{14}(4n)u^{14} + \frac{1}{15}(2n)u^{15} + \frac{1}{17}u^{17} + \frac{1}{16}(n-1)u^{16}$$
$$+\frac{1}{17}(2n-1)u^{17} + \frac{1}{19}(2n-1)u^{19} + \frac{1}{20}nu^{20} + \frac{1}{20}u^{20} + \frac{1}{22}(3n-3)u^{22}.$$

Theorem 4. Let G be the graphical network of Acrylonitrile Butadiene Styrene then by using NM-Polynomial the topological indices are

$$NM_1(G) = 492n - 52$$
$$NM_2(G) = 1761n - 288$$
$$NM_2^m(G) = 0.91634n + 0.15730$$
$$ND_3(G) = 2253n - 340$$
$$ND_5(G) = 83.979n - 3.5998$$
$$NR_\alpha(G) = 235.27n - 29.236$$
$$NF(G) = 4048n - 670$$
$$NI(G) = 112.76n - 11.594$$
$$NH(G) = 5.0190n + 0.34935.$$

Proof: By using the results of M-polynomial of Acrylonitrile Butadiene Styrene graph network and Table 2, we have

$$NM_1(G) = (D_u + D_v)(b(u,v))_{u=v=1}$$
$$= 492n - 52.$$
$$NM_2(G) = (D_uD_v)(b(u,v))_{u=v=1}$$
$$= 1761n - 288.$$
$$NM_2^m(G) = (F_uF_v)(b(u,v))_{u=v=1}$$
$$= 0.91634n + 0.15730.$$
$$ND_3(G) = [(D_u + D_v)(D_uD_v)](b(u,v))_{u=v=1}$$
$$= 2253n - 340.$$
$$ND_5(G) = (D_uF_v + D_vF_u)(b(u,y))_{u=v=1}$$
$$= 83.979n - 3.5998.$$
$$NR_\alpha(G) = (D_u^\alpha D_v^\alpha)(b(u,v))_{u=v=1}$$
$$= 5^\alpha 2^\alpha n + 2\cdot 5^\alpha 3^\alpha + 2\cdot 6^\alpha 3^\alpha + 7^\alpha 3^\alpha(5n+1)$$
$$+8^\alpha 3^\alpha(2n-1) + 4^\alpha 9^\alpha(4n-2) + 4^\alpha 10^\alpha(5n-2)$$
$$+4^\alpha 11^\alpha + 4^\alpha 12^\alpha(n-1) + 7^\alpha 5^\alpha + 5^\alpha 10^\alpha n + 6^\alpha 11^\alpha$$
$$+4\cdot(7^\alpha)^2 n + 2\cdot 7^\alpha 8^\alpha n + 10^\alpha 7^\alpha + (8^\alpha)^2(n-1)$$
$$+8^\alpha 9^\alpha(2n-1) + 10^\alpha 9^\alpha(2n-1) + (10^\alpha)^2 nn$$
$$+2\cdot 10^\alpha 11^\alpha + 10^\alpha 12^\alpha(3n-3).$$

$For\ \ \alpha = \frac{1}{2},\ we\ get$
$$NR_{\frac{1}{2}}(G) = 235.27n - 29.236.$$
$$NF(G) = (D_u^2 + D_v^2)(b(u,v))_{u=v=1}$$
$$= 4048n - 670.$$
$$NI(G) = (F_uJD_uD_v)(b(u,v))_{u=1}$$
$$= 112.76n - 11.594.$$
$$NH(G) = 2(F_uJ)(b(u,v))_{u=1}$$
$$= 5.0190n + 0.34935.$$

Table 7: Results for the M-Polynomial of Styrene Acrylonitrile Parameters as a Function of n.

n	$M_1(G)$	$M_2(G)$	$M_2^m(G)$	$ReZG_3(G)$	$SDD(G)$	$F(G)$	$I(G)$	$H(G)$	$R_{\frac{1}{2}}(G)$
1	78	90	3.7222	488	46.500	218	17.4290	7.5048	36.7553
2	170	207	7.4583	1210	95.000	510	37.5580	14.1096	79.58241
3	262	324	11.1944	1932	143.500	802	57.6870	20.7144	122.40951
4	354	441	14.9306	2654	192.000	1094	77.8160	27.3192	165.23661
5	446	558	18.6667	3376	240.500	1386	97.9450	33.9240	208.06371
6	538	675	22.4028	4098	289.000	1678	118.0740	40.5288	250.89081
7	630	792	26.1389	4820	337.500	1970	138.2030	47.1336	293.71791
8	722	909	29.8750	5542	386.000	2262	158.3320	53.7384	336.54501
9	814	1026	33.6111	6264	434.500	2554	178.4610	60.3432	379.3721
10	906	1143	37.3472	6986	483.000	2846	198.5900	66.9480	422.1992

The degree-based and neighborhood degree-based topological indices (TIs) of Acrylonitrile Butadiene Styrene are calculated using both the M-polynomial and the NM-polynomial. The numerical results are presented in Tables 9 and 10, and their graphical representations are shown in Figure 7.

Table 8: Results for the NM-Polynomial of Styrene Acrylonitrile Parameters as a Function of n.

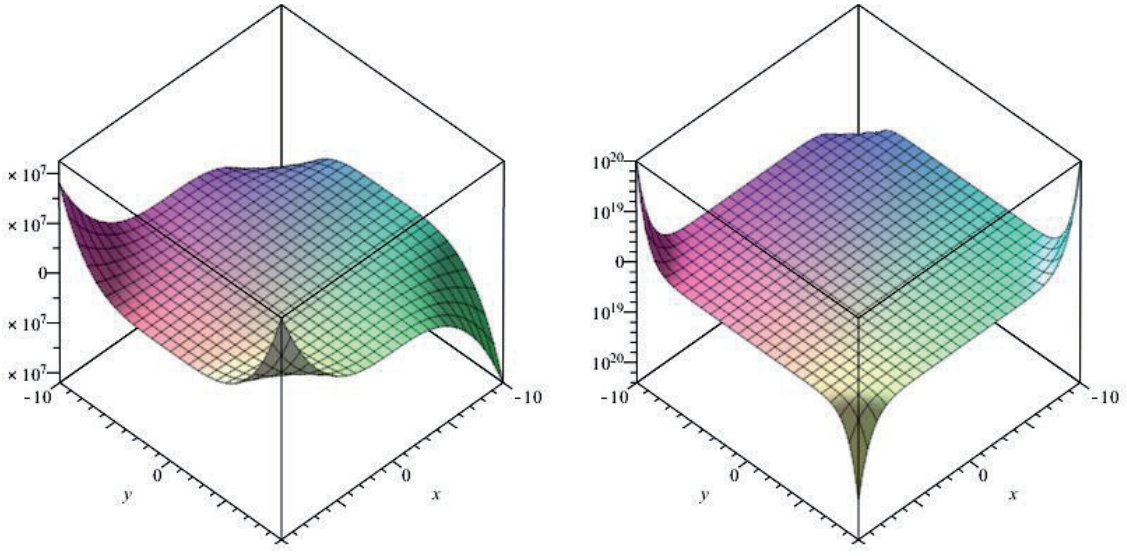
n	$NM_1(G)$	$NM_2(G)$	$NM_2^m(G)$	$ND_3(G)$	$ND_5(G)$	$NR_{\frac{1}{2}}(G)$	$NF(G)$	$NI(G)$	$NH(G)$
1	180	519	0.65658	6802	33.6466	87.60512	1150	41.82	3.05991
2	414	1340	1.15525	20016	70.8646	200.6790	3000	96.54	5.76041
3	648	2161	1.65392	33230	108.083	313.7529	4850	151.26	8.46091
4	882	2982	2.15259	46444	145.301	426.8268	6700	205.98	11.1614
5	1116	3803	2.65126	59658	182.518	539.9008	8550	260.7	13.8619
6	1350	4624	3.14993	72872	219.736	652.9747	10400	315.42	16.5624
7	1584	5445	3.6486	86086	256.953	766.0486	12250	370.14	19.2629
8	1818	6266	4.14727	99300	294.171	879.1225	14100	424.86	21.9634
9	2052	7087	4.64594	112514	331.388	992.1964	15950	479.58	24.6639
10	2286	7908	5.14461	125728	368.606	1105.2703	17800	534.3	27.3644

Table 9: Results for the M-Polynomial of Acrylonitrile Butadiene Styrene Parameters as a Function of n.

n	$M_1(G)$	$M_2(G)$	$M_2^m(G)$	$RezG_3(G)$	$SDD(G)$	$R_{\frac{1}{2}}(G)$	$F(G)$	$I(G)$	$H(G)$
1	176	223	7.1180	1374	95.4133	81.68750	552	38.193	12.2848
2	366	473	14.2366	2982	196.4933	169.4468	1178	79.086	24.4464
3	556	723	21.3552	4590	297.5733	257.2061	1804	119.979	36.6080
4	746	973	28.4738	6198	398.6533	344.9654	2430	160.872	48.7696
5	936	1223	35.5924	7806	499.7333	432.7247	3056	201.765	60.9312
6	1126	1473	42.7110	9414	600.8133	520.4840	3682	242.658	73.0928
7	1316	1723	49.8296	11022	701.8933	608.2433	4308	283.551	85.2544
8	1506	1973	56.9482	12630	802.9733	696.0026	4934	324.444	97.4160
9	1696	2223	64.0668	14238	904.0533	783.7619	5560	365.337	109.578
10	1886	2473	71.1854	15846	1005.133	871.5212	6186	406.230	121.740

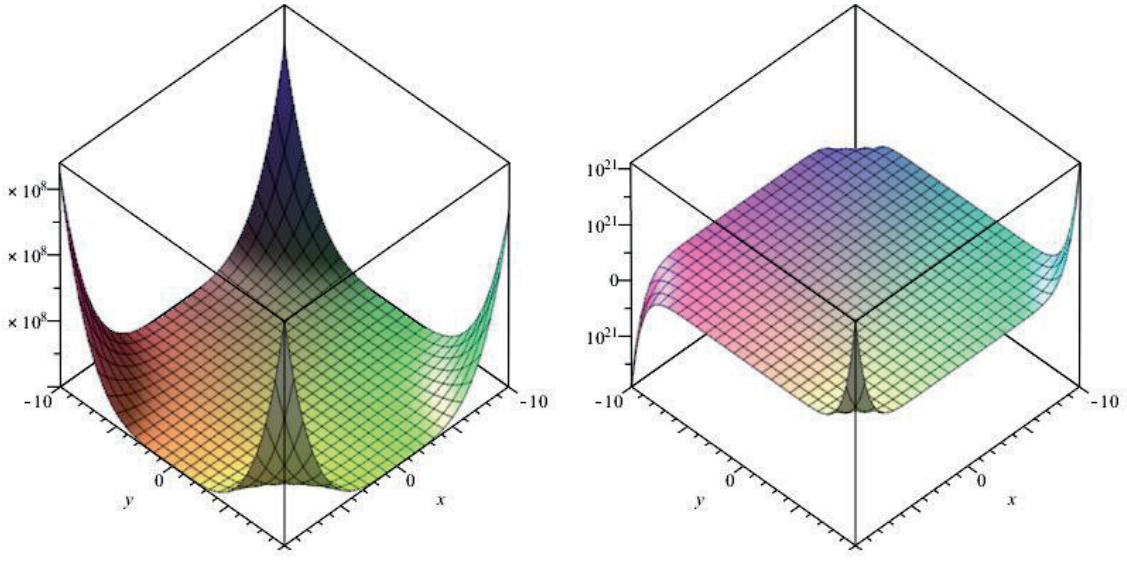
Table 10: Results for the NM-Polynomial of Acrylonitrile Butadiene Styrene Parameters as a Function of n.

n	$NM_1(G)$	$NM_2(G)$	$NM_2^m(G)$	$ND_3(G)$	$ND_5(G)$	$NR_{\frac{1}{2}}(G)$	$NF(G)$	$NI(G)$	$NH(G)$
1	440	1473	1.07364	1913	80.3792	206.034	3378	101.166	5.36835
2	880	3234	1.99098	4566	164.3594	441.304	7426	213.922	10.38735
3	1320	4995	2.90832	7219	248.3396	676.574	11474	326.678	15.40635
4	1760	6756	3.82566	9872	332.3198	911.844	15522	439.434	20.42535
5	2200	8517	4.74300	12525	416.3000	1147.114	19570	552.190	25.44435
6	2640	10278	5.66034	15078	500.2802	1382.384	23618	664.946	30.46335
7	3080	12039	6.57768	17631	584.2604	1617.654	27666	777.702	35.48235
8	3520	13800	7.49502	20184	668.2406	1852.924	31714	890.458	40.50135
9	3960	15561	8.41236	22737	752.2208	2088.194	35762	1003.214	45.52035
10	4400	17322	9.32970	25290	836.2010	2323.464	39810	1115.970	50.53935



(a) A1 (b) A2

Figure 3: (A1) 3D Plot of M-Polynomial as Defined in Equation 1, (A2) 3D Plot of NM-Polynomial as Defined in Equation 2 for Styrene Acrylonitrile.



(a) A3 (b) A4

Figure 4: (A3) 3D Plot of M-Polynomial as Defined in Equation 3, (A4) 3D Plot of NM-Polynomial as Defined in Equation 4 for Acrylonitrile Butadiene Styrene.

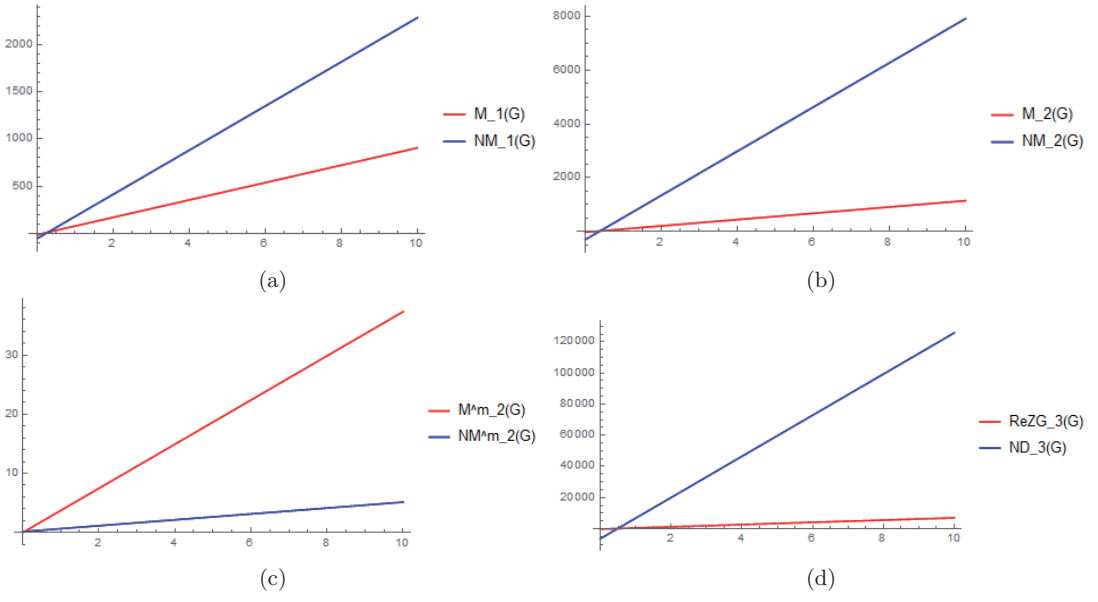


Figure 5: Comparison between M-Polynomial and NM-Polynomial for Styrene Acrylonitrile.

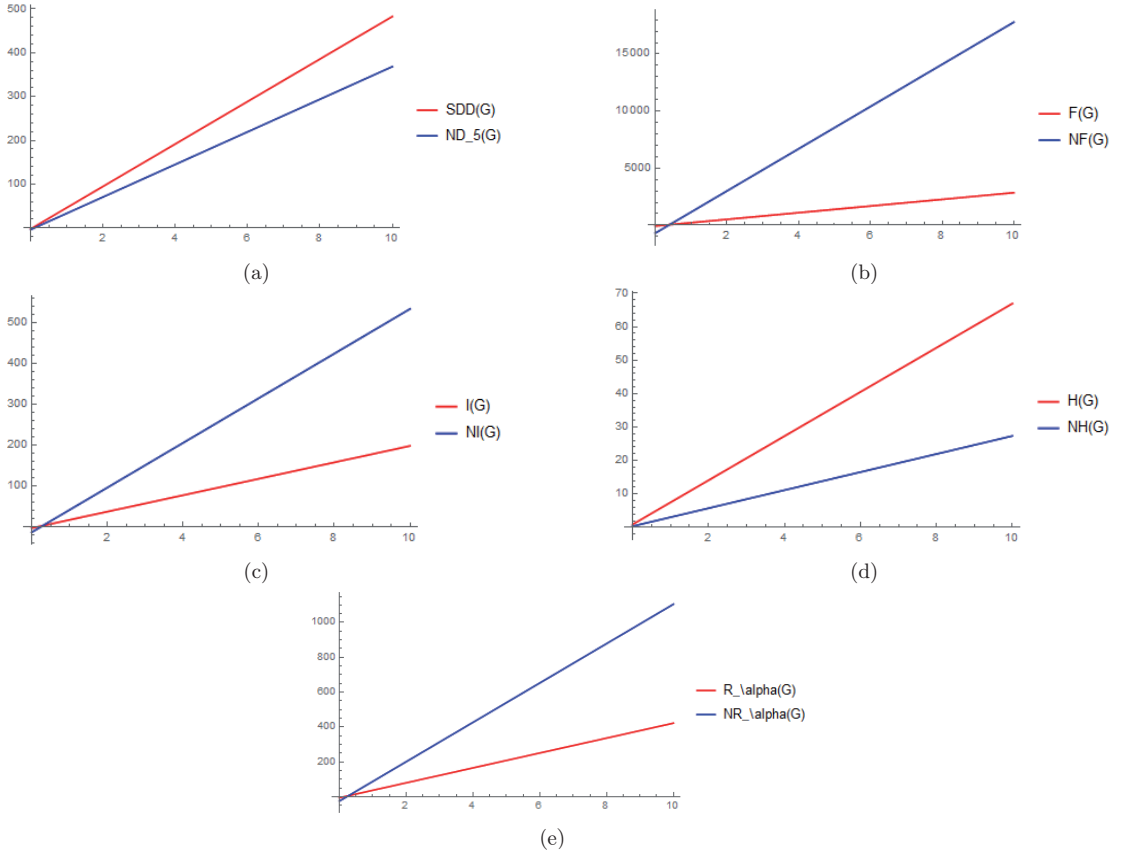


Figure 6: Comparison between M-Polynomial and NM-Polynomial for Styrene Acrylonitrile.

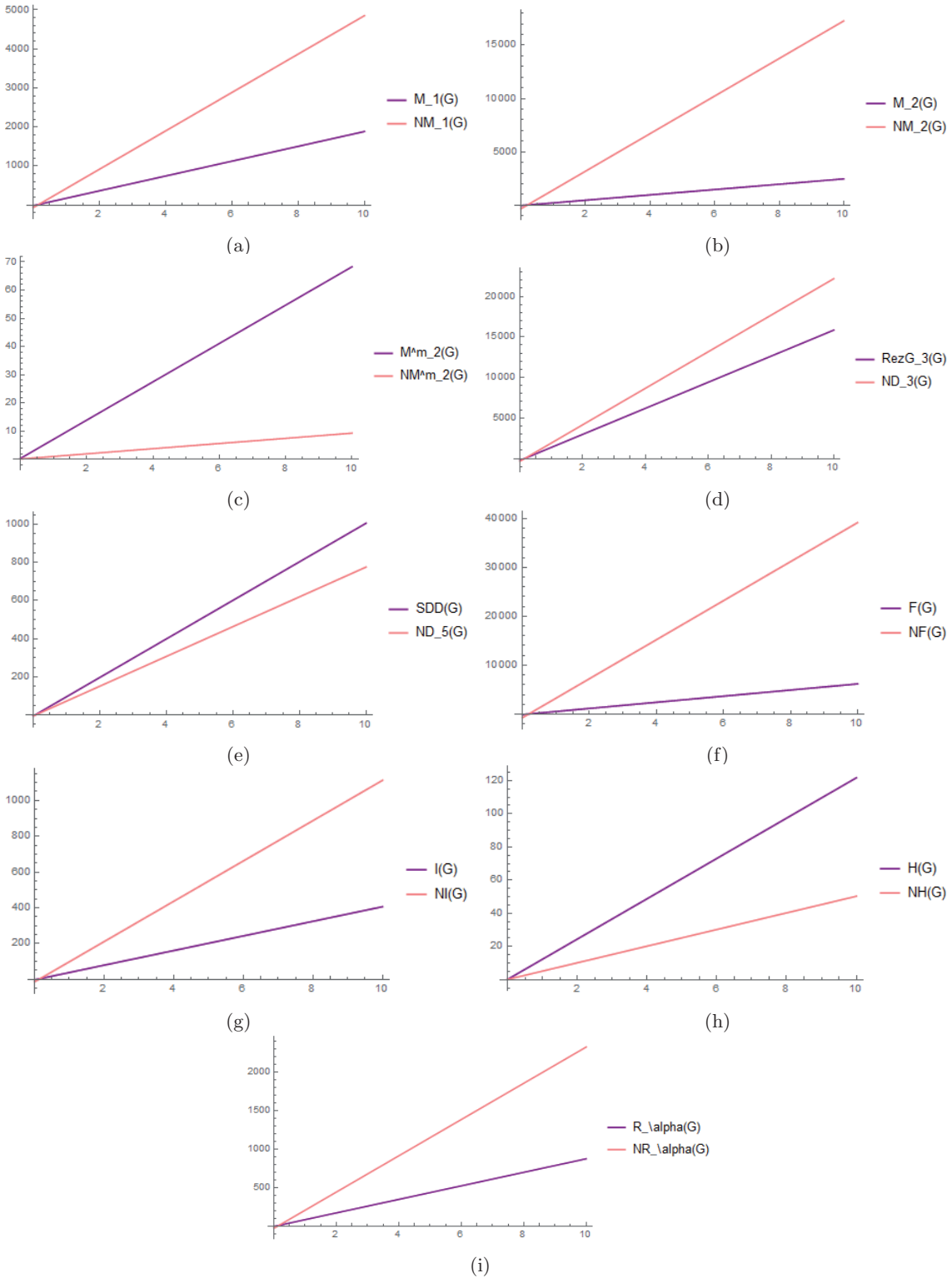


Figure 7: Comparison between M-Polynomial and NM-Polynomial for Acrylonitrile Butadiene Styrene.

4. Conclusion

We have computed the degree-based and neighborhood degree-based topological indices (TIs) of Styrene Acrylonitrile and Acrylonitrile Butadiene Styrene using both the M-polynomial and the NM-polynomial. The results from both tools are identical. These outcomes will be helpful in addressing numerous issues in the field of chemical analysis. The indices are particularly useful for studying molecular structures in chemistry, as they enable the prediction of compounds' physical and chemical properties. Furthermore, these indices can provide valuable insights into the influence and interconnectedness of individuals within a network in social network analysis. The numerical results are presented in Tables 7, 8, 9 and 10, and their graphical representations are shown in Figures 6 and 7.

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References

[1] Amer, A., Naeem, M., Rehman, H., Irfan, M., Saleem, M. S., & Yang, H. (2020). Edge version of topological degree-based indices of boron triangular nanotubes. Journal of Information and Optimization Sciences, 41(4), 973-990.

[2] Balaban, A. T. (2005). Reflections about mathematical chemistry. Foundations of Chemistry, 7, 289-306.

[3] Chamua, M., Moran, R., Pegu, A., & Bharali, A. (2022). M-polynomial and neighborhood M-polynomial of some concise drug structures: Azacitidine, Decitabine, and Guadecitabine. Journal of Molecular Structure, 1263, 133197.

[4] Deutsch, E., & Klavžar, S. (2014). M-polynomials and degree-based topological indices. Journal of Mathematical Chemistry, 53(7), 1614-1625.

[5] Donald, A. M., & Kramer, E. J. (1982). Plastic deformation mechanisms in poly(acrylonitrile-butadienestyrene) [ABS]. Journal of Materials Science, 17, 1765-1772.

[6] Furtula, B. A., & Gutman, I. (2011). A third version of the Zagreb index. International Journal of Chemical Modeling, 3, 1-17.

[7] Gutman, I., & Randić, M. (2014). M-polynomials and degree-based topological indices. Journal of Mathematical Chemistry, 52(2), 399-411.

[8] Gutman, I., & Trinajstić, N. (1972). Graph theory and molecular orbitals. I. Graph theoretical parameters in describing the topology of molecules. Chemistry, 27(9), 10-20.

[9] Gutman, I. (1998). The harmonic index. Mathematical and Computational Chemistry, 24(2), 227-229.

[10] Hosoya, H. (1988). On some counting polynomials in chemistry. Discrete Applied Mathematics, 19, 239-257.

[11] Irfan, M., Rehman, H., Almusawa, H., Rasheed, S., & Baloch, I. A. (2021). M-polynomials and topological indices for line graphs of chain silicate network and H-naphtalenic nanotubes. Journal of Mathematics, 1-11.

[12] Irfan, M., Yasmeen, F., Aziz, S., & Mukhtar, M. (2024). Neighborhood degree-based topological indices of nanotube via direct and NM-polynomial. International Journal of Quantum Chemistry, 124(17), e27474.

[13] Kiran Kumar, M. R. S., Prasad, B. T. K. V., & Srinivas, K. M. S. R. V. (2021). A novel forgotten topological index and its applications in chemical graph theory. International Journal of Mathematical and Computational Sciences, 15(4), 145-150.

[14] Maul, J., Frushour, B. G., Kontoff, J. R., Eichenauer, H., Ott, K. H., & Schade, C. (2007). Polystyrene and styrene copolymers. Ullmann's Encyclopedia of Industrial Chemistry, 29, 475-522.

[15] Miličevič, A., Nikolić, S., & Trinajstić, N. (2004). On modified second Zagreb index. Croatica Chemica Acta, 77(4), 1-9.

[16] Munir, M., Nazeer, W., Rafique, S., & Kang, S. M. (2016). M-polynomial and degree-based topological indices of polyhex nanotubes. Symmetry, 8(149).

[17] Mohammed Yasin, H., Suresh, M., Abebe, G. A., & Fufa, S. A. (2023). Results on certain biopolymers using M-polynomial and NM-polynomial of topological indices. Computational and Mathematical Methods in Medicine, 15.

[18] Mondal, S., Siddiqui, M. K., De, N., & Pal, A. (2021). Neighborhood M-polynomial of crystallographic structures. Biointerface Research in Applied Chemistry, 11, 9372–9381.

[19] Randić, M. (1975). Characterization of molecular branching. Journal of the American Chemical Society, 97, 6609–6615.

[20] Rücker, G., & Rücker, C. (1999). On topological indices, boiling points, and cycloalkanes. Journal of Chemical Information and Computer Sciences, 39(5), 788–802.

[21] Siddiqui, M. K., Naeem, M., Rahman, N. A., & Imran, M. (2016). Computing topological indices of certain networks. Journal of Optoelectronics and Advanced Materials, 18, 884–892.

[22] Satterthwaite, K. (2017). Plastics based on styrene. In Brydson's Plastics Materials, 311-328.

[23] Silva, G. A. L., & Al-Khayyal, N. A. (1994). The inverse index. Journal of Mathematical Chemistry, 16(1), 1-5.

[24] Saharia, G., & Dutta, S. (2024). Neighborhood M-polynomial of graph operations: Exploring nanostructure applications

and correcting cycle-related graph results. Iranian Journal of Mathematical Chemistry, 15(3), 155-174.

[25] Tiganis, B. E., Koutsoukos, P. G., & Papageorgiou, G. Z. (2002). Thermal degradation of acrylonitrilebutadiene-styrene (ABS) blends. Polymer Degradation and Stability, 76(3), 425-434.

[26] Trinajstić, N., & Gutman, I. (2002). Mathematical chemistry. Croatica Chemica Acta, 75, 329-356.

[27] Verma, A., & Mondal, S. (2019). Neighborhood M-polynomial and its applications. MATCH Communications in Mathematical and in Computer Chemistry, 81, 51-70.

[28] Vukičević, D., & Furtula, B. (2009). Topological index based on the ratios of geometrical means and sums of end-vertex degrees of edges. Journal of Mathematical Chemistry, 46(4), 1369-1376.

[29] Wiener, H. (1947). Structural determination of paraffin boiling points. Journal of the American Chemical Society, 69(17), 17-20.

[30] Yan, F., Shang, Q., Xia, S., Wang, Q., & Ma, P. (2015). Application of topological index in predicting ionic liquids densities by the quantitative structure–property relationship method. Journal of Chemical & Engineering Data, 60(3), 734–739.