Spectrum of Engineering Sciences
ISSN (e) 3007-3138 (p) 3007-312X Volume 4, Issue 6, 2026

TOPOLOGICAL DESCRIPTORS OF LINE GRAPHS IN POLYMER SUPRAMOLECULAR NETWORKS

[1]Shama Sadiq, [*2]Farhan Ali, [3]Muhammad Ilyas, [4]Awais Maqsood, [5]Abdul Basit Butt

[1]Department of Mathematics, University of Management and Technology, Lahore 54770, Pakistan
[*2]School of Computer and IT, Beaconhouse National University, P.O. Box 53700 Lahore, Pakistan
[3]Department of software engineering, Superior University, Lahore 5400 Pakistan
[4]EE Deptt. SEN, University of Management and Technology, Lahore 54770, Pakistan
[5]EE Deptt. SEN, University of Management and Technology, Lahore 54770, Pakistan
[1]shamayasmeen36@gmail.com, [*2]farhan32748@gmail.com,
[3]muhammad.ilyas@superior.edu.pk, [4]awais.maqsood@umt.edu.pk,
[5]abdul.basit.butt05@gmail.com

DOI:-

Keywords
Topological indices; Line graph; Polymer Supramolecular Network

Article History
Received: 13 May, 2026
Accepted: 06 June, 2026
Published: 08 June, 2026

Corresponding Author: *

Farhan Ali

Abstract

This research provides the graph theoretical study for a polymer supramolecular network within the paradigm of deriving various degree-based topological invariants through the constructed line graph representation for the underlying supramolecular structure. Networks comprised of supramolecular structures, which are based on non-covalent bonds, are difficult to represent within the conventional graph representation paradigm because they are dynamic in nature and have non-covalent bonds within the network. The line graph transformation paradigm has been adopted with the supramolecular structure for a more appropriate representation of such complex systems' structure and connectivity within the underlying graph representation paradigm. These indices form the cornerstone of robust quantitative structure property relationship and quantitative structure activity relationship. The derivation of various important topological invariants, such as the Randić index, Zagreb index, and Harmonic index, provides the bridge for a quantitative relationship between the supramolecular network structures and various functional groups and behaviors within a deterministic paradigm for such complex networks and structures.

1. Introduction

Topological indices play an important role in chemical graph theory and mathematical chemistry, acting as tools to forecast physicochemical properties of numerous chemical structures. A topological index is specified as a numerical attribute allotted to a molecular graph, which remains unchanged under a graph isomorphism. These indices, being representative of specific structural features of molecular compounds, have experienced a surge in their applications and acceptances. The increased awareness of these indices is a result of their strong correlation to different chemical properties associated specifically with their molecular graphs. In addition, topological indices possess a pivotal contribution to quantitative structure property relationship (QSAR) and QSPR studies. Therefore, topological indices have proved to be essential for characterizing the structural features and bioactivity of chemical compounds. The importance of topological indices is as follows [1, 2, 3, 4], a topological index is a chemical descriptor presented by a number derived from a molecular compound's graph, which remains invariant after a specific transformation known as graph automorphism. The emergence of topological descriptors was associated with increased interest in computational chemistry, particularly owing to their ability to relate chemical compounds' structural features to quantitative chemical properties, often using non-traditional and non-obvious metrics.

Typically, classifications of topological indices occur in terms of distance, degree, and polynomial-based topological indices. Amongst all, degree-based topological indices have shown to be commonly used in a wide array of applications, thus highlighting the importance of chemical graphs in both theoretical and practical chemistry. The line graph, denoted as $L(G)$, is a graph such that the set of its vertices is in one-to-one correspondence with the set of edges in G. Two vertices, say g and h, in $L(G)$ are considered to be adjacent if they share a common endpoint in the original graph G [5, 6]. Separately, the Zagreb indices were initially proposed by Gutman and Trinajstic in 1972.

The M_1 [12] and the M_2 [12] are defined as:

$$M_1(G) = \sum_{gh \in E(G)} (d_g + d_h)$$

and

$$M_2(G) = \sum_{gh \in E(G)} (d_g \cdot d_h).$$

The M_3 index was initially conceptualized and introduced by Fath-Tabar [13]. The formal definition of this index is presented as follows:

$$M_3(G) = \sum_{gh \in E(G)} |d_g - d_h|.$$

In 2013, Shirdel et al. [21] proposed the *HM* index, a topological index derived from vertex degrees, which is formally defined as follows:

$$HM(G) = \sum_{gh \in E(G)} (d_g + d_h)^2.$$

Furtula, Gutman, and Ediz [9] conducted a study on the distinctions between Zagreb indices, revealing a strong correlation with the vertex-degree-based invariant designated as RM_2, which is formally defined as:

$$RM_2(G) = \sum_{gh \in E(G)} (d_g - 1)(d_h - 1).$$

In 2014, I. Gutman, B. Furtula, and C. Elphick [11] elucidated the relationship between the RM_2 index and the ordinary M_2 index, drawing an analogy in their structural derivation. Following this, the *RRR* index is formally defined as follows:

$$RRR(G) = \sum_{gh \in E(G)} \sqrt{((dg - 1)(dh - 1))}.$$

The index, which Bollobás and Erdős [16] first explored in 1998, is now widely recognized as the *R* index. It is also referred to by the alternative names mM_2 and the first-order overall index.

$$mM_2(G) = \sum_{gh \in E(G)} 1 / (d_g \cdot d_h).$$

In 2012, Ghorbani and Azimi [10] introduced several novel variants of Zagreb indices for a given graph G. Among these new indices are $PM_1(G)$ and $PM_2(G)$, which are categorized as follows:

$$PM_1(G) = \prod_{gh \in E(G)} (d_g + d_h),$$

and

$$PM_2(G) = \prod_{gh \in E(G)} (d_g \cdot d_h).$$

In 2009, Zhou and Trinajstić introduced the Sum-connectivity index (*SCI*), a topological index developed in response to Randić's concept of the product connectivity index. For a given graph G, the Sum-connectivity index is formally defined as follows [27]:

$$SCI(G) = \sum_{gh \in E(G)} 1/\sqrt{(dg + dh)}.$$

The Harmonic index represents a variant of the Randić index, originally introduced in 1975. For a given graph G, the Harmonic index, denoted as $H(G)$, is formally defined as follows [26]:

$H(G) = \sum_{gh \in E(G)} 2 / (d_g + d_h)$.

In 2010, Vukičević and Gašperov introduced a novel class of molecular descriptors termed "discrete Adriatic indices," comprising 138 distinct descriptors. This development aimed to enhance various (QSPR) and (QSAR) methodologies. Among these, the Sum of Degrees Difference (SDI) index and the Inverse Sum Indegree (ISI) index are particularly notable as useful discrete Adriatic indices, formally defined as follows [24]:

$SDI(G) = \sum_{gh \in E(G)} (d_g^2 + d_h^2) / (d_g \times d_h)$,

and

$IS(G) = \sum_{gh \in E(G)} (d_g \times d_h) / (d_g + d_h)$.

Estrada and Torres [7] proposed the *ABC* index in 1998, and it is expressed as:

$$ABC(G) = \sum_{gh \in E(G)} \sqrt{((dg + dh - 2) / (dg \cdot dh))}.$$

In 2010, Boris Furtula and Graovac [14] introduced the Augmented Zagreb Index (*AZI*), a novel topological index whose development was inspired by the earlier work on the Atom-Bond Connectivity (*ABC*) index. Its definition is as follows:

$AZI(G) = \sum_{gh \in E(G)} [(d_g \cdot d_h) / (d_g + d_h - 2)]^3$.

In 2009, Vukičević and Furtula [15] introduced the Geometric-Arithmetic (*GA*) index, a topological descriptor that is formally defined as follows:

$$GA(G) = \sum_{gh \in E(G)} 2\sqrt{(dg \cdot dh)} / (dg + dh).$$

In 2015, Furtula and Gutman [8] put forth the *F*-index, described as:

$F(G) = \sum_{gh \in E(G)} [d_g^2 + d_h^2]$.

In 2017, V.R. Kulli [17] put forth the first and second GM (Gourava) indices, characterized by the definitions:

$GM_1 = \sum_{gh \in E(G)} [(d_g + d_h) + (d_g \cdot d_h)]$,

$GM_2 = \sum_{gh \in E(G)} (d_g + d_h) \cdot (d_g \cdot d_h)$.

In 2016, V. S. Shegehalli and R. Kanabur [20] put forth a new version of degree-based topological indices, with the following definitions:

$SK(G) = \sum_{gh \in E(G)} (d_g + d_h) / 2$,

$SK_1 = \sum_{gh \in E(G)} (d_g \cdot d_h) / 2$,

$SK_2 = \sum_{gh \in E(G)} [(d_g + d_h) / 2]^2$.

In 2008, Li and Shi [18] give value 1/2 to alpha, then *RR* is introduced which is defined as:

$$RR(G) = \sum_{gh \in E(G)} \sqrt{(dg \cdot dh)}.$$

In 2010, Vukičević [25] introduced the following bond additive discrete Adriatic indices:

$$MRD(G) = \sum_{gh \in E(G)} |\sqrt{dg} - \sqrt{dh}|,$$

$$MIRD(G) = \sum_{gh \in E(G)} |1/\sqrt{dg} - 1/\sqrt{dh}|,$$

$$MHD(G) = \sum_{gh \in E(G)} |2^{-dg} - 2^{-dh}|.$$

In 1975, M. Randić [19] introduced *RI* which is defined as:

$$RI(G) = \sum_{gh \in E(G)} 1 / \sqrt{(dg \cdot dh)} \quad (1.27)$$

2. Results and Discussion

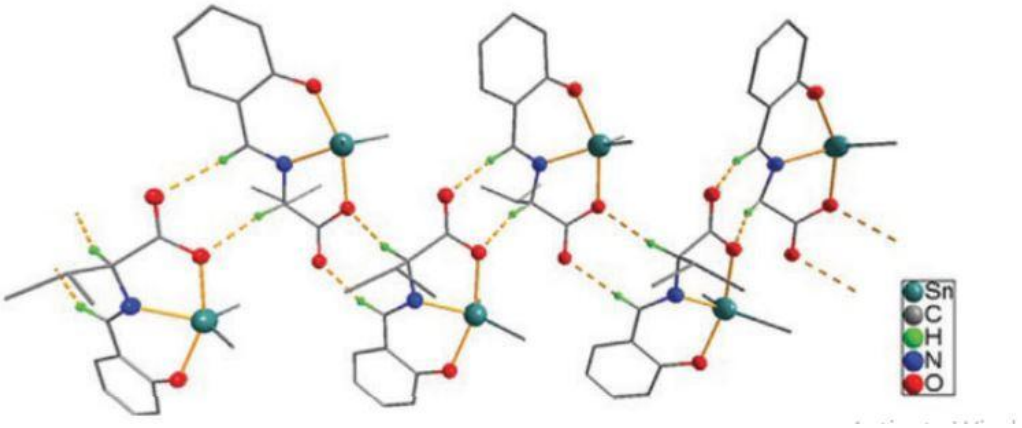

Figure 2.1. Structural Architecture of Supramolecular Polymer Networks.

The chemical composition of the polymer supramolecular network is presented in Figure 2.1. Specifically, Dialkyltin Complex-2 of N-salicylidene-L-valine (NsLv) is an organometallic complex where dialkyltin forms bonds with N-salicylidene-L-valine ligands. NsLv is particularly significant owing to its characteristic molecular structure and its augmented catalytic and cytotoxic efficacy. Originating from L-valine, a key amino acid integral to protein synthesis, NsLv is employed in

agricultural chemicals and therapeutic agents. Our next step involves developing the line graph corresponding to the polymer supramolecular network.

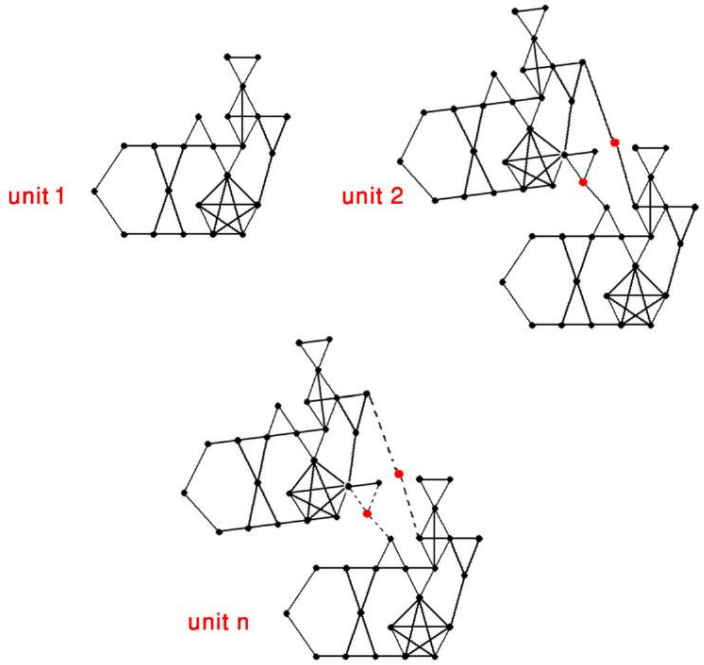

Figure 2.2. Line graph (G) of complex-2.

Table 2.1. *Edge partition of line graph of polymer supramolecular network*

(d_g, d_h)	Number of Edges	(d_g, d_h)	Number of Edges	(d_g, d_h)	Number of Edges
(2,2)	3n	(2,3)	3n	(2,4)	n+1
(2,5)	2n+1	(3,3)	2n−1	(3,4)	8n−4
(3,5)	2n+4	(4,4)	3n	(3,6)	n−1
(4,5)	7n−2	(4,6)	6n−3	(5,5)	3n+1
(5,6)	3n	(6,6)	n−1		

Theorem 2.1. Given that G denotes the line graph of a polymer supramolecular network, the *SCI* can be expressed as $SCI(G) = 16.3n - 1.63$.

Proof.

Equation (1.10) presents the definition of the *SCI* formula. By using Table 2.1:

$SCI(G) = 3n/\sqrt{4} + 3n/\sqrt{5} + (n+1)/\sqrt{6} + (2n+1)/\sqrt{7} + (2n-1)/\sqrt{6}$
$+ (8n-4)/\sqrt{7} + (2n+4)/\sqrt{8} + (n-1)/\sqrt{9} + 3n/\sqrt{8} + (7n-2)/\sqrt{9}$
$+ (6n-3)/\sqrt{10} + (3n+1)/\sqrt{10} + 3n/\sqrt{11} + (n-1)/\sqrt{12},$
$= 16.3n - 1.63.$

□

Theorem 2.2. Given that G denotes the line graph of a polymer supramolecular network, the M_1 can be expressed as $M_1(G) = 362n - 48$.

Proof.

Equation (1.1) presents the definition of the M_1 formula. By using Table 2.1:

$M_1(G) = (3n)(2+2) + (3n)(2+3) + (n+1)(2+4) + (2n+1)(2+5)$
$+ (2n-1)(3+3) + (8n-4)(3+4) + (2n+4)(3+5) + (3n)(4+4)$
$+ (7n-2)(4+5) + (6n-3)(4+6) + (3n+1)(5+5) + (3n)(5+6)$
$+ (n-1)(3+6) + (n-1)(6+6),$
$= 362n - 48.$

□

Theorem 2.3. The M_2 can be written as follows, where G represents the line graph of a polymer supramolecular network: $M_2(G) = 753n - 120$.

Proof.

The M_2 formula definition is shown in equation (1.2). By using Table 2.1:

$M_2 = (3n)(2\times2) + (3n)(2\times3) + (n+1)(2\times4) + (2n+1)(2\times5)$
$+ (2n-1)(3\times3) + (8n-4)(3\times4) + (2n+4)(3\times5) + (n-1)(3\times6)$
$+ (3n)(4\times4) + (7n-2)(4\times5) + (6n-3)(4\times6) + (3n+1)(5\times5)$
$+ (3n)(5\times6) + (n-1)(6\times6),$
$= 753n - 120.$

□

Theorem 2.4. The M_3 can be written as follows, where G represents the line graph of a polymer supramolecular network: $M_3(G) = 48n - 2$.

Proof.

The M_3 formula definition is shown in equation (1.3). By using Table 2.1:

$M_3 = (3n)|2-3| + (n+1)|2-4| + (2n+1)|2-5| + (2n-1)|3-3| + (8n-4)|3-4|$
$+ (2n+4)|3-5| + (7n-2)|4-5| + (6n-3)|4-6| + (3n)|5-6| + (n-1)|3-6|,$
$= 48n - 2.$

□

Theorem 2.5. The PM_1 can be written as follows, where G represents the line graph of a polymer supramolecular network:

Proof.

$PM_1(G) = 4^{3n} \times 5^{3n} \times 6^{3n} \times 7^{10n-3} \times 8^{5n+4} \times 9^{8n-3} \times 10^{9n-2} \times 11^{3n} \times 12^{n-1}.$

The definition of the PM_1 formula is shown in equation (1.8). By using Table 2.1:

$PM_1 = [2+2]^{3n} \times [2+3]^{3n} \times [2+4]^{n+1} \times [2+5]^{2n+1} \times [3+3]^{2n-1} \times [3+4]^{8n-4} \times [3+5]^{2n+4} \times [4+4]^{3n} \times [4+5]^{7n-2} \times [4+6]^{6n-3} \times [5+5]^{3n+1} \times [5+6]^{3n} \times [3+6]^{n-1} \times [6+6]^{n-1},$
$= 4^{3n} \times 5^{3n} \times 6^{3n} \times 7^{10n-3} \times 8^{5n+4} \times 9^{8n-3} \times 10^{9n-2} \times 11^{3n} \times 12^{n-1}.$

□

Theorem 2.6. The PM_2 can be written as follows, where G represents the line graph of a polymer supramolecular network:

Proof.

$PM_2(G) = 4^{3n} \times 6^{3n} \times 8^{n+1} \times 10^{2n+1} \times 9^{2n-1} \times 12^{8n-1} \times 15^{2n+4} \times 16^{3n} \times 20^{7n-2} \times 24^{6n-3} \times 25^{3n+1} \times 30^{3n} \times 18^{n-1} \times 36^{n-1}.$

The definition of the PM_2 formula is shown in equation (1.9). By using Table 2.1:

$PM_2 = [2\times2]^{3n} \times [2\times3]^{3n} \times [2\times4]^{n+1} \times [2\times5]^{2n+1} \times [3\times3]^{2n-1} \times [3\times4]^{8n-4} \times [3\times5]^{2n+4} \times [4\times4]^{3n} \times [4\times5]^{7n-2} \times [4\times6]^{6n-3} \times [5\times5]^{3n+1} \times [5\times6]^{3n} \times [3\times6]^{n-1} \times [6\times6]^{n-1}.$

□

Theorem 2.7. The HM can be written as follows, where G represents the line graph of a polymer supramolecular network: $HM(G) = 3096n - 478$.

Proof.

The HM formula definition is shown in equation (1.4). By using Table 2.1:

$HM(G) = (3n)(2+2)^2 + (3n)(2+3)^2 + (n+1)(2+4)^2 + (2n+1)(2+5)^2$
$+ (2n-1)(3+3)^2 + (8n-4)(3+4)^2 + (2n+4)(3+5)^2 + (3n)(4+4)^2$
$+ (7n-2)(4+5)^2 + (6n-3)(4+6)^2 + (3n+1)(5+5)^2$
$+ (3n)(5+6)^2 + (n-1)(3+6)^2 + (n-1)(6+6)^2,$
$= 3096n - 478.$

□

Theorem 2.8. The H of a polymer supramolecular network can be written as follows, where G represents the line graph: $H(G) = 2111n/252 - 199/210$.

Proof.

The H formula is defined in equation (1.11). By using Table 2.1:

$H(G) = 2(3n)/(2+2) + 2(3n)/(2+3) + 2(n+1)/(2+4) + 2(2n+1)/(2+5) + 2(2n-1)/(3+3)$
$+ 2(8n-4)/(3+4) + 2(2n+4)/(3+5) + 2(n-1)/(3+6) + 2(3n)/(4+4) + 2(7n-2)/(4+5)$
$+ 2(6n-3)/(4+6) + 2(3n+1)/(5+5) + 2(3n)/(5+6) + 2(n-1)/(6+6),$
$= 2111n/252 - 199/210.$

□

Theorem 2.9. The ABC can be written as follows, where G represents the line graph of a polymer supramolecular network: $ABC(G) = 29.16n - 4.02$.

Proof.

The ABC formula definition is shown in equation (1.14). By using Table 2.1:

$ABC(G) = (3n)\sqrt{((2+2-2)/(2\times 2))} + (3n)\sqrt{((2+3-2)/(2\times 3))} + (n+1)\sqrt{((2+4-2)/(2\times 4))} + (2n+1)\sqrt{((2+5-2)/(2\times 5))} + (2n-1)\sqrt{((3+3-2)/(3\times 3))} + (8n-4)\sqrt{((3+4-2)/(3\times 4))} + (2n+4)\sqrt{((3+5-2)/(3\times 5))} + (n-1)\sqrt{((3+6-2)/(3\times 6))} + (3n)\sqrt{((4+4-2)/(4\times 4))} + (7n-2)\sqrt{((4+5-2)/(4\times 5))} + (6n-3)\sqrt{((4+6-2)/(4\times 6))} + (3n+1)\sqrt{((5+5-2)/(5\times 5))} + (3n)\sqrt{((5+6-2)/(5\times 6))} + (n-1)\sqrt{((6+6-2)/(6\times 6))},$
$= 29.16n - 4.02.$

□

Theorem 2.10. The GA can be written as follows, where G represents the line graph of a polymer supramolecular network: $GA(G) = 43.88n - 5.02$.

Proof.

The GA formula is defined in equation (1.16). By using Table 2.1:

$GA(G) = 2(3n)\sqrt{(2\times 2)/(2+2)} + 2(3n)\sqrt{(2\times 3)/(2+3)} + 2(n+1)\sqrt{(2\times 4)/(2+4)} + 2(2n+1)\sqrt{(2\times 5)/(2+5)} + 2(2n-1)\sqrt{(3\times 3)/(3+3)} + 2(8n-4)\sqrt{(3\times 4)/(3+4)} + 2(2n+4)\sqrt{(3\times 5)/(3+5)} + 2(n-1)\sqrt{(3\times 6)/(3+6)} + 2(3n)\sqrt{(4\times 4)/(4+4)} + 2(7n-2)\sqrt{(4\times 5)/(4+5)} + 2(6n-3)\sqrt{(4\times 6)/(4+6)} + 2(3n+1)\sqrt{(5\times 5)/(5+5)} + 2(3n)\sqrt{(5\times 6)/(5+6)} + 2(n-1)\sqrt{(6\times 6)/(6+6)},$
$= 43.88n - 5.02.$

□

Theorem 2.11. The mM_2 can be written as follows, where G represents the line graph of a polymer supramolecular network: $mM_2(G) = 3.3n - 0.46$.

Proof.

The definition of the mM_2 formula is shown in equation (1.7). By using Table 2.1:

$mM_2(G) = (3n)/(2\times 2) + (3n)/(2\times 3) + (n+1)/(2\times 4) + (2n+1)/(2\times 5) + (2n-1)/(3\times 3) + (8n-4)/(3\times 4) + (2n+4)/(3\times 5) + (n-1)/(3\times 6) + (3n)/(4\times 4) + (7n-2)/(4\times 5) + (6n-3)/(4\times 6) + (3n+1)/(5\times 5) + (3n)/(5\times 6) + (n-1)/(6\times 6),$
$= 3.3n - 0.46.$

□

Theorem 2.12. Given that G denotes the line graph of a polymer supramolecular network, the RM_2 can be expressed as $RM_2(G) = 436n - 77$.

Proof.

The definition of the RM_2 formula is shown in equation (1.5). By using Table 2.1:

$RM_2(G) = (3n)[(2-1)(2-1)] + (3n)[(2-1)(3-1)] + (n+1)[(4-1)(2-1)] + (2n+1)[(2-1)(5-1)] + (2n-1)[(3-1)(3-1)] + (8n-4)[(3-1)(4-1)] + (2n+4)[(3-1)(5-1)] + (7n-2)[(4-1)(5-1)] + (6n-3)[(4-1)(6-1)] + (3n)[(5-1)(6-1)] + (n-1)[(3-1)(6-1)],$
$= 436n - 77.$

□

Theorem 2.13. The *RRR* can be written as follows, where G represents the line graph of a polymer supramolecular network: $RRR(G) = 132.25n - 19.44$.

Proof.

The *RRR* formula definition is shown in equation (1.6). By using Table 2.1:

$RRR(G) = (3n)\sqrt{((2-1)(2-1))} + (3n)\sqrt{((2-1)(3-1))} + (n+1)\sqrt{((4-1)(2-1))} + (2n+1)\sqrt{((2-1)(5-1))} + (2n-1)\sqrt{((3-1)(3-1))} + (8n-4)\sqrt{((3-1)(4-1))} + (2n+4)\sqrt{((3-1)(5-1))} + (7n-2)\sqrt{((4-1)(5-1))} + (6n-3)\sqrt{((4-1)(6-1))} + (3n)\sqrt{((5-1)(6-1))} + (n-1)\sqrt{((3-1)(6-1))},$
$= 132.25n - 19.44.$

□

Theorem 2.14. The *AZI* can be written as follows, where G represents the line graph of a polymer supramolecular network: $AZI(G) = 796.53n - 148.96$.

Proof.

The *AZI* formula definition is shown in equation (1.15). By using Table 2.1:

$AZI(G) = (3n)((2\times2)/(2+2-2))^3 + (3n)((2\times3)/(2+3-2))^3 + (n+1)((2\times4)/(2+4-2))^3$
$+ (2n+1)((2\times5)/(2+5-2))^3 + (2n-1)((3\times3)/(3+3-2))^3 + (8n-4)((3\times4)/(3+4-2))^3$
$+ (2n+4)((3\times5)/(3+5-2))^3 + (n-1)((3\times6)/(3+6-2))^3 + (3n)((4\times4)/(4+4-2))^3$
$+ (7n-2)((4\times5)/(4+5-2))^3 + (6n-3)((4\times6)/(4+6-2))^3 + (3n+1)((5\times5)/(5+5-2))^3$
$+ (3n)((5\times6)/(5+6-2))^3 + (n-1)((6\times6)/(6+6-2))^3,$
$= 796.53n - 148.96.$

□

Theorem 2.15. The *SDI* can be written as follows, where G represents the line graph of a polymer supramolecular network: $SDI(G) = 95.94n - 11.97$.

Proof.

The *SDI* formula definition is shown in equation (1.12). By using Table 2.1:

$SDI(G) = (3n)(2^2+2^2)/(2\times2) + (3n)(2^2+3^2)/(2\times3) + (n+1)(2^2+4^2)/(2\times4)$
$+ (2n+1)(2^2+5^2)/(2\times5) + (2n-1)(3^2+3^2)/(3\times3) + (8n-4)(3^2+4^2)/(3\times4)$
$+ (2n+4)(3^2+5^2)/(3\times5) + (n-1)(3^2+6^2)/(3\times6) + (3n)(4^2+4^2)/(4\times4)$
$+ (7n-2)(4^2+5^2)/(4\times5) + (6n-3)(4^2+6^2)/(4\times6) + (3n+1)(5^2+5^2)/(5\times5)$
$+ (3n)(5^2+6^2)/(5\times6) + (n-1)(6^2+6^2)/(6\times6),$
$= 95.94n - 11.97.$

□

Theorem 2.16. The *ISI* can be written as follows, where G represents the line graph of a polymer supramolecular network: $ISI(G) = 87.89n - 12.23$.

Proof.

The *ISI* formula definition is shown in equation (1.13). By using Table 2.1:

$ISI(G) = (3n)(2\times2)/(2+2) + (3n)(2\times3)/(2+3) + (n+1)(2\times4)/(2+4) + (2n+1)(2\times5)/(2+5)$
$+ (2n-1)(3\times3)/(3+3) + (8n-4)(3\times4)/(3+4) + (2n+4)(3\times5)/(3+5) + (n-1)(6\times3)/(6+3)$
$+ (3n)(4\times4)/(4+4) + (7n-2)(4\times5)/(4+5) + (6n-3)(4\times6)/(4+6) + (3n+1)(5\times5)/(5+5)$
$+ (3n)(5\times6)/(5+6) + (n-1)(6\times6)/(6+6),$
$= 87.689n - 12.23.$

□

Theorem 2.17. If G represents the line graph of a supramolecular network of polymers, then *F* can be written as follows: $F(G) = 1590n - 238$.

Proof.

This definition of the *F* formula is shown in equation (1.17). By using Table 2.1:

$F(G) = (3n)(8) + (3n)(13) + (n+1)(20) + (2n+1)(29) + (2n-1)(18)$
$+ (8n-4)(25) + (2n+4)(34) + (3n)(32) + (7n-2)(41) + (6n-3)(52)$
$+ (3n+1)(50) + (3n)(61) + (n-1)(45) + (n-1)(72),$
$= 1590n - 238.$

□

Theorem 2.18. The *SK* can be written as follows, where G represents the line graph of a polymer supramolecular network: $SK(G) = 181n - 24$.

Proof.

With equation (1.20), the *SK* formula is defined. By using Table 2.1:

$SK(G) = (3n)(4/2) + (3n)(5/2) + (n+1)(6/2) + (2n+1)(7/2)$
$+ (2n-1)(6/2) + (8n-4)(7/2) + (2n+4)(8/2) + (3n)(8/2)$
$+ (7n-2)(9/2) + (6n-3)(10/2) + (3n+1)(10/2) + (3n)(11/2)$
$+ (n-1)(9/2) + (n-1)(12/2),$
$= 181n - 24.$

□

Theorem 2.19. The SK_1 can be written as follows, where G represents the line graph of a polymer supramolecular network: $SK_1(G) = 753n/2 - 60$.

Proof.

The SK_1 formula definition is shown in equation (1.21). By using Table 2.1:

$SK_1(G) = (3n)(4/2) + (3n)(6/2) + (n+1)(8/2) + (2n+1)(10/2)$
$+ (2n-1)(9/2) + (8n-4)(12/2) + (2n+4)(15/2) + (3n)(16/2)$
$+ (7n-2)(20/2) + (6n-3)(24/2) + (3n+1)(25/2) + (3n)(30/2)$
$+ (n-1)(36/2) + (n-1)(18/2),$
$= 753n/2 - 60.$

□

Theorem 2.20. The SK_2 can be written as follows, where G represents the line graph of a polymer supramolecular network: $SK_2(G) = 15403n/4 - 779$.

Proof.

The SK_2 formula definition is shown in equation (1.22). By using Table 2.1:

$SK_2(G) = (3n)(4/2)^2 + (3n)(6/2)^2 + (n+1)(8/2)^2 + (2n+1)(10/2)^2$
$+ (2n-1)(9/2)^2 + (8n-4)(12/2)^2 + (2n+4)(15/2)^2 + (3n)(16/2)^2$
$+ (7n-2)(20/2)^2 + (6n-3)(24/2)^2 + (3n+1)(25/2)^2 + (3n)(30/2)^2$
$+ (n-1)(36/2)^2 + (n-1)(18/2)^2,$
$= 15403n/4 - 779.$

□

Theorem 2.21. The GM_1 can be written as follows, where G represents the line graph of a polymer supramolecular network: $GM_1(G) = 1115n - 168$.

Proof.

The GM_1 formula definition is shown in equation (1.18). By using Table 2.1:

$GM_1(G) = (3n)(4+4) + (3n)(5+6) + (n+1)(6+8) + (2n+1)(7+10)$
$+ (2n-1)(6+9) + (8n-4)(7+12) + (2n+4)(8+15) + (3n)(8+16)$
$+ (7n-2)(9+20) + (6n-3)(10+24) + (3n+1)(10+25) + (3n)(11+30)$
$+ (n-1)(9+18) + (n-1)(12+36),$
$= 1115n - 168.$

□

Theorem 2.22. The GM_2 can be written as follows, where G represents the line graph of a polymer supramolecular network: $GM_2(G) = 6764n - 1216$.

Proof.

The GM_2 formula definition is shown in equation (1.19). By using Table 2.1:

$GM_2(G) = (3n)(4\times4) + (3n)(5\times6) + (n+1)(6\times8) + (2n+1)(7\times10)$
$+ (2n-1)(6\times9) + (8n-4)(7\times12) + (2n+4)(8\times15) + (3n)(8\times16)$
$+ (7n-2)(9\times20) + (6n-3)(10\times24) + (3n+1)(10\times25) + (3n)(11\times30)$
$+ (n-1)(9\times18) + (n-1)(12\times36),$
$= 6764n - 1216.$

□

Theorem 2.23. The *RR* can be written as follows, where G represents the line graph of a polymer supramolecular network: $RR(G) = 178.29n - 24.25$.

Proof.

The *RR* formula is defined in equation (1.23). By using Table 2.1:

$RR(G) = (3n)\sqrt{4} + (3n)\sqrt{6} + (n+1)\sqrt{8} + (2n+1)\sqrt{10} + (2n-1)\sqrt{9}$
$+ (8n-4)\sqrt{12} + (2n+4)\sqrt{15} + (3n)\sqrt{16} + (7n-2)\sqrt{20} + (6n-3)\sqrt{24}$
$+ (3n+1)\sqrt{25} + (3n)\sqrt{30} + (n-1)\sqrt{18} + (n-1)\sqrt{36},$
$= 178.29n - 24.25.$

□

Theorem 2.24. The *RI* of a polymer supramolecular network, where G represents the line graph, can be written as follows: $RI(G) = 12.23n - 1.03$.

Proof.

The *RI* formula definition is shown in equation (1.27). By using Table 2.1:

$RI(G) = 3n/\sqrt{4} + 3n/\sqrt{6} + (n+1)/\sqrt{8} + (2n+1)/\sqrt{10} + (2n-1)/\sqrt{9}$
$+ (8n-4)/\sqrt{12} + (2n+4)/\sqrt{15} + 3n/\sqrt{16} + (7n-2)/\sqrt{20} + (6n-3)/\sqrt{24}$
$+ (3n+1)/\sqrt{25} + 3n/\sqrt{30} + (n-1)/\sqrt{18} + (n-1)/\sqrt{36},$
$= 12.23n - 1.03.$

□

Theorem 2.25. The *MRD* can be written as follows, where G represents the line graph of a polymer supramolecular network: $MRD(G) = 11.94n - 0.8$.

Proof.

The *MRD* formula definition is shown in equation (1.24). By using Table 2.1:

$MRD(G) = (3n)|\sqrt{2} - \sqrt{3}| + (n+1)|\sqrt{2} - \sqrt{4}| + (2n+1)|\sqrt{2} - \sqrt{5}|$
$+ (8n-4)|\sqrt{3} - \sqrt{4}| + (2n+4)|\sqrt{3} - \sqrt{5}| + (7n-2)|\sqrt{4} - \sqrt{5}|$
$+ (6n-3)|\sqrt{4} - \sqrt{6}| + (3n)|\sqrt{5} - \sqrt{6}| + (n-1)|\sqrt{3} - \sqrt{6}|,$
$= 11.94n - 0.8.$

□

Theorem 2.26. The *MHD* can be written as follows, where G represents the line graph of a polymer supramolecular network: $MHD(G) = 2.36n + 0.21$.

Proof.
The *MHD* formula definition is shown in equation (1.26). By using Table 2.1:

$$MHD(G) = (3n)|2^{-2} - 2^{-3}| + (n+1)|2^{-2} - 2^{-4}| + (2n+1)|2^{-2} - 2^{-5}| + (8n-4)|2^{-3} - 2^{-4}| + (2n+4)|2^{-3} - 2^{-5}| + (7n-2)|2^{-4} - 2^{-5}| + (6n-3)|2^{-4} - 2^{-6}| + (3n)|2^{-5} - 2^{-6}| + (n-1)|2^{-3} - 2^{-6}|,$$

$$= 2.36n + 0.21.$$

□

Theorem 2.27. The *MIRD* can be written as follows, where G represents the line graph of a polymer supramolecular network: $MIRD(G) = 3.24n + 0.11$.

Proof.
The *MIRD* formula definition is shown in equation (1.25). By using Table 2.1:

$$MIRD(G) = (3n)|1/\sqrt{2} - 1/\sqrt{3}| + (n+1)|1/\sqrt{2} - 1/\sqrt{4}| + (2n+1)|1/\sqrt{2} - 1/\sqrt{5}| + (8n-4)|1/\sqrt{3} - 1/\sqrt{4}| + (2n+4)|1/\sqrt{3} - 1/\sqrt{5}| + (7n-2)|1/\sqrt{4} - 1/\sqrt{5}| + (6n-3)|1/\sqrt{4} - 1/\sqrt{6}| + (3n)|1/\sqrt{5} - 1\sqrt{6}| + (n-1)|1/\sqrt{3} - 1/\sqrt{6}|,$$

$$= 3.24n + 0.11.$$

□

3. Graphical Comparison

Topological indices, in the context of chemistry, hold significant value and serve as a criterion for assessing the quantitative aspects of different chemical compounds to a specific level. Moreover, the calculation of topological indices for any chemical compound is feasible, irrespective of the level of intricacy, and the possibility of predictions in the context of chemical and physical characteristics exists. On a specific note, the domain of drug designing and discovery holds prime value for topological indices in the context of chemistry.

In the same way, the bioactivity of a substance, which could be in terms of its toxic potential or its affinity towards a particular protein, is also subject to being predicted, and this, in turn, increases the possibility of remedial compounds.

Moreover, topological indices have been found to provide a reliable framework for the classification of chemical substances or for identifying structural similarities between various chemical compounds or entities. This approach also applies to the classification of various chemical compounds or substances based on structural properties or patterns. This classification bears promise for introducing new substances or compounds with requisite properties, as well as new compound entities with beneficial properties.

Moreover, topological indices can be applied in other artificial intelligence models, and this is not limited to QSAR models but rather for the purpose of predicting specific chemical properties found in compounds. Thus, based on the aforementioned factors, it can be comprehended and established that topological indices represent an efficient tool that can be employed in chemistry, facilitating the establishment and determination of compound qualities or characteristics through neat and easily understandable concepts, whereby chemical compounds can be pictorially represented, thus facilitating the easy identification and detection of specific components or qualities associated with these compounds, particularly those qualities or components that cannot be easily deduced or established with reference to the molecular formula composition, as depicted in Figures 3.1, 3.2, and 3.3.

It is worth noting that among the most effective tools in the analysis, prediction, or even discovery of the compounds of chemistry in the subject of chemistry is the representation of the compound in the form of a graph in the subject of chemistry. Tables 3.1, 3.2 and 3.3 show a numerical comparison of calculated results.

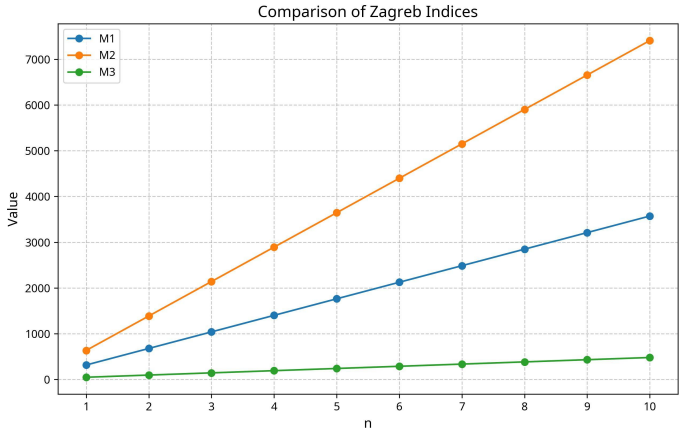

Figure 3.1. Comparative analysis of Zagreb indices of line graph (G) of polymer supramolecular network.

Table 3.1. *Comparison table of Zagreb indices of line graph of polymer supramolecular network.*

n	M_1	M_2	M_3
1	314	633	46
2	676	1386	94
3	1038	2139	142
4	1400	2892	190
5	1762	3645	238
6	2124	4398	286
7	2486	5151	334
8	2848	5904	382
9	3210	6657	430
10	3572	7410	478

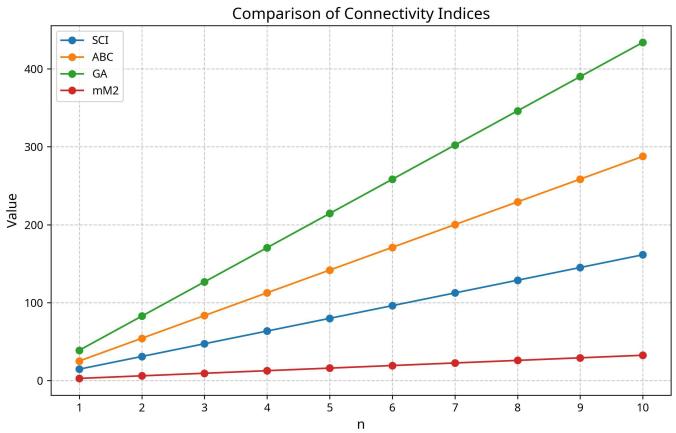

Figure 3.2. Comparative analysis of SCI, ABC, nM_2 and GA index of line graph (G) of polymer supramolecular network.

Table 3.2. *Comparison table of Connectivity indices of line graph (G) of polymer supramolecular network.*

n	*SCI*	*ABC*	*GA*	mM_2
1	14.67	25.14	38.86	2.84
2	30.97	54.30	82.74	6.14
3	47.27	83.46	126.62	9.44
4	63.57	112.62	170.50	12.74
5	79.87	141.78	214.38	16.04
6	96.17	170.94	258.26	19.34
7	112.47	200.10	302.14	22.64
8	128.77	229.26	346.02	25.94
9	145.07	258.42	389.90	29.24
10	161.37	287.58	433.78	32.54

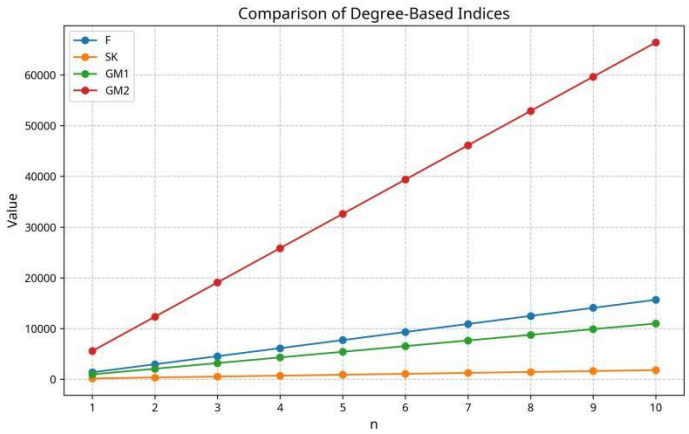

Figure 3.3. Comparative analysis of F, SK, GM_1 and GM_2 index of line graph (G) of polymer supramolecular network.

Table 3.3. *Comparison table of Degree-Based indices of line graph (G) of polymer supramolecular network.*

n	*F*	*SK*	GM_1	GM_2
1	1352	157	947	5548
2	2942	338	2062	12312
3	4532	519	3177	19076
4	6122	700	4292	25840
5	7712	881	5407	32604
6	9302	1062	6522	39368

n	F	SK	GM_1	GM_2
7	10892	1243	7637	46132
8	12482	1424	8752	52896
9	14072	1605	9867	59660
10	15662	1786	10982	66424

4. Conclusion and General Remarks

This study undertook a detailed topological assessment of the line graph associated with a polymer supramolecular network. Employing the graph-theoretic representation of the Dialkyltin Complex of N-salicylidene-L-valine, we determined a wide array of degree-based topological indices. These comprised the foundational Zagreb indices (first, second, and third), their multiplicative and altered versions, the hyper Zagreb index, and the augmented Zagreb index, along with other key descriptors such as the sum connectivity, harmonic, geometric-arithmetic, atom-bond connectivity, symmetric division deg, inverse sum, and forgotten topological indices.

Explicit closed-form equations for each index are provided, formulated as linear or multiplicative functions of the parameter n, which defines the network's repeating structural unit. These results yield a precise quantitative understanding of the network's structural design. Further graphical and numerical analyses, conducted with increasing values of n, reveal the differing growth characteristics and possible relationships among the various indices.

Funding: This research received no external funding.

Data Availability Statement: No data set is used in this study.

Declaration Statement: The authors declare no conflicts of interest.

References

[1] Balaban, A. T. (1979). Chemical graphs. Theoretica Chimica Acta, 53(4), 355–375.

[2] Balaban, A. T. (1988). Topological indices and their uses: a new approach for the coding of alkanes. Journal of Molecular Structure: THEOCHEM, 165(3–4), 243–253.

[3] Balaban, A. T., Motoc, I., Bonchev, D., & Mekenyan, O. (1983). Topological indices for structure-activity correlations. In Steric effects in drug design (pp. 21–55). Springer, Berlin, Heidelberg.

[4] Harren, T., Matter, H., Hessler, G., Rarey, M., & Grebner, C. (2022). Interpretation of Structure–Activity Relationships in Real-World Drug Design Data Sets Using Explainable Artificial Intelligence. Journal of Chemical Information and Modeling.

[5] Behzad, M., & Chartrand, G. (1966). An introduction to total graphs, coloring, line graphs. In Proc. Symp. Rome (pp. 31–33).

[6] Shirai, T. (2000). The spectrum of infinite regular line graphs. Transactions of the American Mathematical Society, 352(1), 115–132.

[7] Estrada, E., Torres, L., Rodriguez, L., & Gutman, I. (1998). An atom-bond connectivity index: modelling the enthalpy of formation of alkanes.

[8] Furtula, B., & Gutman, I. (2015). A forgotten topological index. Journal of Mathematical Chemistry, 53(4), 1184–1190.

[9] Furtula, B., Gutman, I., & Ediz, S. (2014). On difference of Zagreb indices. Discrete Applied Mathematics, 178, 83–88.

[10] Ghorbani, M., & Azimi, N. (2012). Note on multiple Zagreb indices. Iranian Journal of Mathematical Chemistry, 3(2), 137–143.

[11] Gutman, I., Furtula, B., & Elphick, C. (2014). Three new/old vertex-degree-based topological indices. MATCH Commun. Math. Comput. Chem, 72(24), 617–632.

[12] Gutman, I., & Trinajstić, N. (1972). Graph theory and molecular orbitals. Total electron energy of alternant hydrocarbons. Chemical Physics Letters, 17(4), 535–538.

[13] Fath-Tabar, G. H. (2011). Old and new Zagreb indices of graphs. MATCH Commun. Math. Comput. Chem, 65(1), 79–84.

[14] Furtula, B., Graovac, A., & Vukičević, D. (2010). Augmented Zagreb index. Journal of Mathematical Chemistry, 48(2), 370–380.
[15] Vukičević, D., & Furtula, B. (2009). Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges. Journal of Mathematical Chemistry, 46(4), 1369–1376.
[16] Nikolić, S., Kovačević, G., Miličević, A., & Trinajstić, N. (2003). The Zagreb indices 30 years after. Croatica Chemica Acta, 76(2), 113–124.
[17] Kulli, V. R. (2017). The Gourava indices and coindices of graphs. Annals of Pure and Applied Mathematics, 14(1), 33–38.
[18] Li, X., & Shi, Y. (2008). A survey on the Randić index. MATCH Commun. Math. Comput. Chem, 59(1), 127–156.
[19] Randić, M. (1975). Characterization of molecular branching. Journal of the American Chemical Society, 97(23), 6609–6615.
[20] Shigehalli, V., & Kanabur, R. (2016). New version of degree-based topological indices of certain nanotube. Journal of Mathematical Nanoscience, 6(1), 27–40.
[21] Shirdel, G. H., Rezapour, H., & Sayadi, A. M. (2013). The hyper-Zagreb index of graph operations.
[22] Tian, L., Wang, R., Zhang, J., Zhong, F., & Qiu, Y. (2020). Synthesis and structural characterization of dialkyltin complexes of N-salicylidene-L-valine. Main Group Metal Chemistry, 43(1), 138–146.
[23] Ghorbani, M., & Hosseinzadeh, M. A. (2010). Computing ABC4 index of nanostar dendrimers. Optoelectronics and Advanced Materials–Rapid Communications, 4 (September 2010), 1419–1422.
[24] Vukičević, D. (2011). Bond additive modeling 4. QSPR and QSAR studies of the variable Adriatic indices. Croatica Chemica Acta, 84(1), 87–91.
[25] Vukičević, D., & Gašperov, M. (2010). Bond additive modeling 1. Adriatic indices. Croatica Chemica Acta, 83(3), 243–260.
[26] Zhong, L. (2012). The harmonic index for graphs. Applied Mathematics Letters, 25(3), 561–566.
[27] Zhou, B., & Trinajstić, N. (2009). On a novel connectivity index. Journal of Mathematical Chemistry, 46(4), 1252–1270.