Topological Indices on Line Graph of Different Chemical Structures

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A Post Graduate Thesis submitted to the name of Department of Mathematics as partial fulfillment of the requirement for the award of degree of MS Mathematics

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Declaration

I Minahil ijaz, CIIT/FA21-RMT-003/LHR, hereby state that my MS thesis titled "Topological indices on line graph of different chemical structures" is my own work and has not been submitted previously by me for taking any degree from this University "COMSATS University Islamabad, Lahore Campus" or anywhere else in the country/world. At any time if my statement is found to be incorrect even after my Graduate the university has the right to withdraw my MS degree.

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Certificate

It is certified that Minahil ijaz, CIIT/FA21-RMT-003/LHR has carried out all the work related to this thesis under my supervision at the Department of Mathematics, COMSATS University Islamabad, Lahore Campus and the work fulfills the requirement for award of PhD degree.

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DEDICATION

To My Parents and All Family

ACKNOWLEDGEMENTS

Praise to be ALLAH, the Cherisher and Lord
of the World, Most gracious and Most Merciful

First and foremost, I would like to thank ALLAH Almighty (the most beneficent and most merciful) for giving me the strength, knowledge, ability and opportunity to undertake this research study and to preserve and complete it satisfactorily. Without countless blessing of ALLAH Almighty, this achievement would not have been possible. May His peace and blessings be upon His messenger Hazrat Muhammad (PBUH), upon his family, companions and whoever follows him. My insightful gratitude to Hazrat Muhammad (PBUH) Who is forever a track of guidance and knowledge for humanity as a whole. In my journey towards this degree, I have found a teacher, an inspiration, a role model and a pillar of support in my life, my kind.

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ABSTRACT

Topological indices on line graph of different chemical structures

A topological index is a numerical measure that characterizes certain inherent properties or features (boiling point, stability and melting point, heat of creation and freezing point, and so on) of a Molecular graph representing some chemical compounds. These indices define topology and typically hold Graph invariant mathematical characteristics. The term ”molecular descriptor” refers to the process of turning chemical data from chemical compounds into meaningful numerical values. These molecular descriptors are commonly used in the investigation of quantitative structure-activity connections that provide insight on animated effects based on chemical structures. This study aims to investigate topological indices based on degrees, including Randic index, Sum connectivity index, Harmonic index, First Zagreb, second zagreb and third zagreb indices, Augmented zagreb index, Hyper zagreb index, Atom bond connectivity index (ABC), Geometric arithmetic index (GA), Inverse sum indeg index (ISI) and The fourth iteration of the Atom bond connectivity index, the fifth iteration of the Geometric arithmetic index, and the Sanskruti index for line graph of Polythiophene Network.

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Chapter 1

Introduction

1.1 Introduction

A new area called ”cheminformatics” integrates ideas from chemistry, mathematics, and some physical characteristics of chemical substances.Cheminformatics sheds light on how to mathematically describe molecules based on their physical features, including traits like boiling point.Chemical graphs are graphs that are especially used in mathematics to illustrate chemical structures. Chemical compounds and their structural features are shown graphically. The topological characteristics of chemical structures are the focus of the specialized field of mathematical chemistry known as chemical graph theory. In order to analyze and grasp chemical substances from a mathematical perspective, graph theory is used.Influential researchers were the first to present chemical graph theory, which studies the mathematical features of molecular structures. It is well known that Arthur Cayley was a pioneer in W. Böhm, who developed molecular docking using graph theory and algorithms. Their collective efforts have significantly advanced our comprehension of molecular structures and properties.The process of transforming chemical molecular data into meaningful numerical outcomes is known as a molecular descriptor.The topological index, also referred to as the connectivity index, is a type of molecular descriptor. A topological index is a numerical parameter that characterizes certain properties (such as connectivity, boiling point, stability, and melting point) of a molecular graph, which represents chemical compounds.

Chapter 1 will cover various aspects, including inscriptions, fundamental concepts, and descriptions related to graph theory and chemical graphs. Chapter 2 will focus on essential molecular descriptors that are based on the degree of vertices in Graph G.

In chapters 3 and 4, we will delve into the study of chemical graphs and line graphs, as well as explore their applications in determining results related to the subdivision of chemical networks.

Chapter 5 will be dedicated to presenting our conclusions based on the results obtained.

Chapter 6 will contain a list of references cited throughout the study.

1.2 Basic Definitions

Graph theory (GT) is subdivision of mathematics which deals with the study about the connection between the lines.Let's consider a graph G with a set of vertices denoted as $V(G)$ and a set of edges denoted as $E(G)$ given as

$$\begin{aligned} V(G) &= v_{11}, v_{22}, v_{33}, \ldots\ldots. v_n \\ E(G) &= v_{11}v_{22}, v_{22}v_{33}, v_{33}v_{44}, \ldots\ldots v_{n-11}v_n \end{aligned}$$

The term **finite graph** refers to a graph having a finite number of edges and vertices. If the quantity of edges and vertices is infinite than the graph is said to be **Infinite graph**. Such as

$$V(G) = v_{11}v_{22}, v_{22}v_{33}, v_{33}v_{44}, \ldots\ldots$$
$$E(G) = v_{11}v_{22}, v_{22}v_{33}, v_{33}v_{44}, \ldots\ldots$$

The cardinality of a set refers to the number of elements it contains. Cardinality of the set of vertices V(G) is known as **order** of (G). The **size** of the set $E(G)$ in graph G is referred to as the count of elements in set of edges. A vertex with degree one is known as **Pendant vertex**. There are some different types of graph as follow

1.2.1 Simple Graph

A graph having only one edge between two vertices than the graph is known as simple graph. It is a graph without parallel edges and loops. Figure 1.1 shows a simple, directed and a finite graph having set of V(G) $v_{11}, v_{22}, v_{33}, v_{44}$

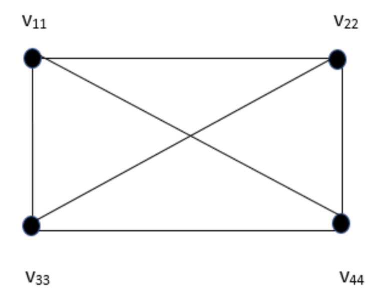

Figure 1.1: Simple Graph

1.2.2 Cyclic Graph and Acyclic graph

A cyclic graph is a type of graph that possesses at least one cycle within its structure with closed path having same starting and ending point. Figure 1.2 shows the cyclic graph with set of vertices $v_{11}, v_{22}, v_{33}, v_{44}, v_{55}$.

A graph that does not have any cycle in it is called non-cyclic graph also known as acyclic

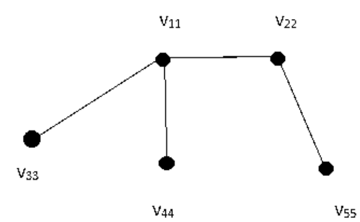

Figure 1.2: Cyclic Graph

graph. Figure 1.3 shows the acyclic graph having the set of V(G) $v_{11}, v_{22}, v_{33}, v_{44}, v_{55}$.

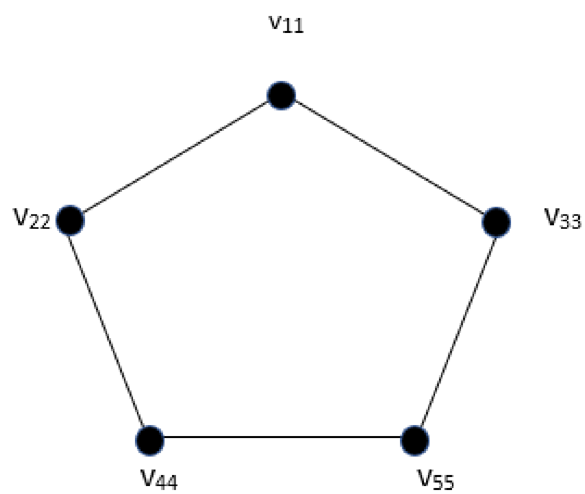

Figure 1.3: Acyclic Graph

1.2.3 Connected and Disconnected Graph

If every pair of vertices in graph G is connected by a path, then G is said to be connected. If any of the vertex is not connected than the graph is called disconnected graph. Figure 1.4 shows connected graph with a set V(G) $v_{11}, v_{22}, v_{33}, v_{44}$. In the figure Each pair of vertices clearly has a route (edge) connecting them. Figure 1.5 shows disconnected graph with a set of vertices $v_{11}, v_{22}, v_{33}, v_{44}, v_{55}$. In the figure it is clear that there is no path between $v_{33}v_{44}$ andv_4v_5. So, it is considered a disconnected graph.

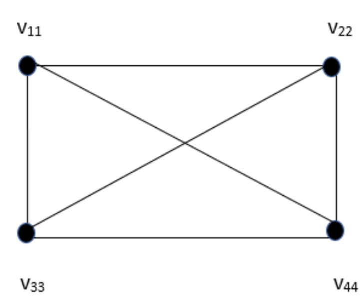

Figure 1.4: Connected Graph

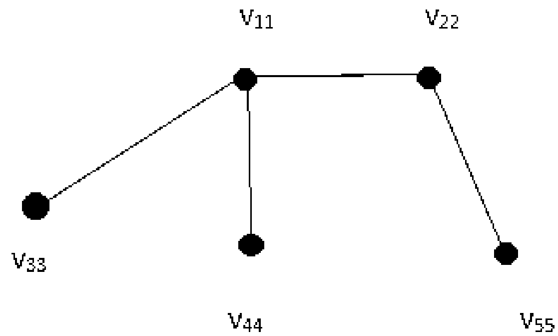

Figure 1.5: Disconnected Graph

1.2.4 Operations on Graphs

1.2.5 Union

A new graph is formed by the union of two graphs. For example, let $G_1 and G_2$ be two graphs, and their union will be $G_1 \cup G_2$.

$$
\begin{aligned}
V(G_1 \cup G_2) &= V(G_1) \cup V(G_2) \\
and\ E(G_1 \cup G_2) &= E(G_1) \cup E(G_2).
\end{aligned}
$$

Union of two graphs is shown in Figure 1.6

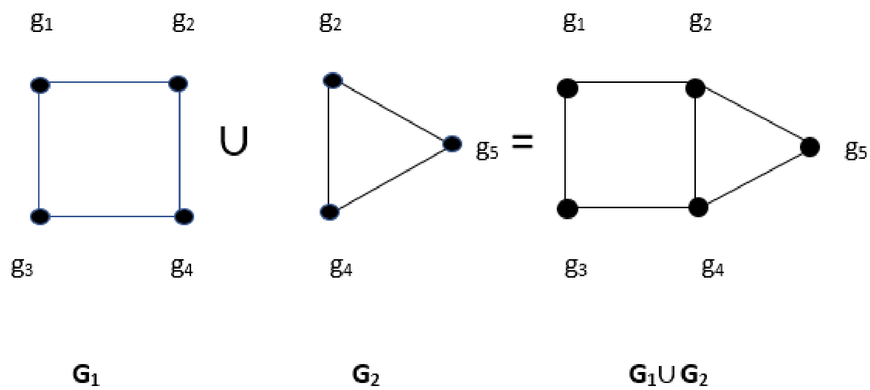

Figure 1.6: Union G_1 and G_2

1.2.6 Intersection

Intersection of two graphs is also a graph. Such as $G_1 and G_2$ be two graphs their intersection will be $G_1 \cap G_2$. Intersection is shown in Figure 1.7

$$
\begin{aligned}
V(G_1 \cap G_2) &= V(G_1) \cap V(G_2) \\
and\ E(G_1 \cap G_2) &= E(G_1) \cap E(G_2)
\end{aligned}
$$

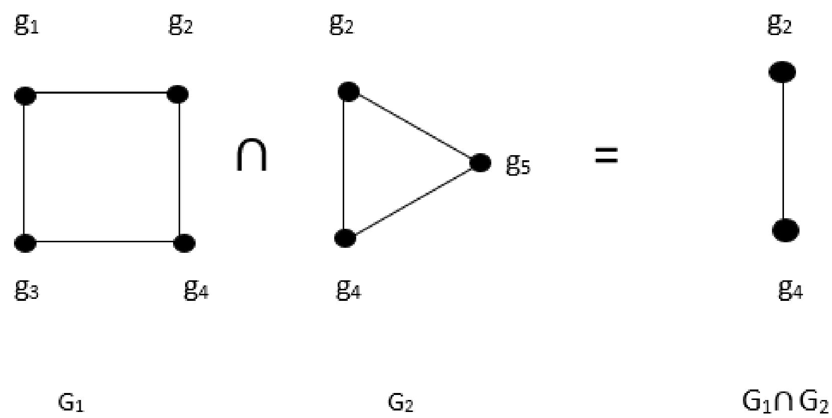

Figure 1.7: Intersection of G_1 and G_2

1.2.7 Sum

Sum of two graphs is also a graph. If G_1 and G_2 be two graph and intersection in set of vertices is empty $(V(G_1) \cup V(G_2) = \phi)$ than the sum is defined as $G_1 + G_2$ where sum of vertices is $V(G_1) + V(G_2)$ and sum of edges is contained by connecting every vertex of G_1 to each and every vertex of G_2. Sum of these two graphs is shown in Figure 1.8

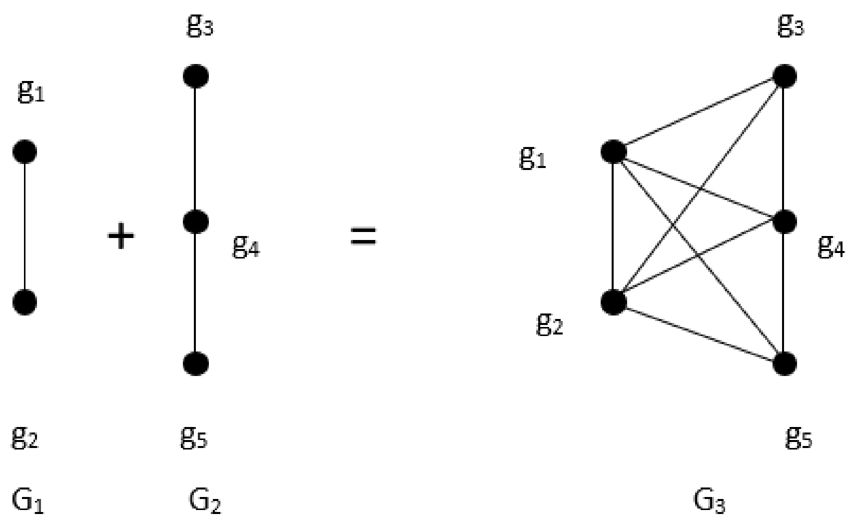

Figure 1.8: Sum of Two Graphs

1.2.8 Degree of a vertex

The vertex degree in a graph denotes the count of edges incident to that vertex. If a vertex has a loop, its degree is 2. A graph is considered regular when every vertex has the same degree. In Figure 1.9, the degree of vertex u_1 is $\xi_u 1(G) = 3$, and the degrees of vertices u_2, u_3, and u_4 are also 3, indicating that graph is regular graph.

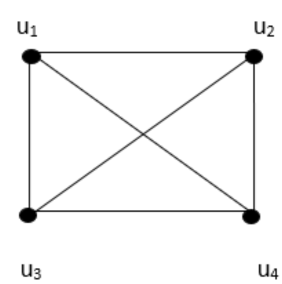

Figure 1.9: Degree of a vertex

1.2.9 Sum of degrees of vertices (δ_u)

The sum of the degrees of a vertex is represented by S_u and is defined as the sum of the degrees of all its neighboring vertices.

$$\delta_u = \sum_{v \in \mathrm{NG}(u)} \xi(v)$$

Where,

$$N_G(u) = v \in V(G)uv \in E(G)$$

Consider a finite graph G, where u_1 is a vertex. The degree of u_1, denoted as $\deg(u_1)$, is determined by summing the degrees of all vertices adjacent to u_1. In this particular case, u_2, u_3, and u_4 are adjacent to u_1, based on the definition of adjacency. Sum of the degrees of the vertex u_1 is 9 [1], is illustrated in the accompanying figure 1.10

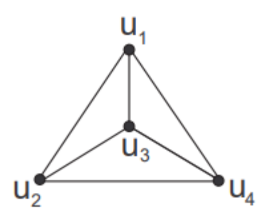

Figure 1.10: Sum of Degree of a Vertex

1.2.10 chemical compounds

The chemical compounds that consist of at least one oxygen atom and another atom in their chemical formula are known as oxides. Oxides are ions of oxygen, specifically $O^{-}2$, where -2 represents the oxidation state. On the other hand, compounds containing anionic silicon compounds are referred to as silicates. Many silicates are classified as oxides.SiO_4 contains four oxygen ions and one silicon ion. These compounds are composed of silicate anions, which are balanced by different cations. Minerals are also encompassed within the category of silicates.

1.2.11 Molecular or Chemical Graphs

A graph, often referred to as a molecular or chemical graph, represents a molecular networkwhere the vertices (nodes) are carbon atoms and the edges are covalent bonds between them corresponding carbon atoms within an organic molecule. This modeling approach is commonly used for representing molecules or chemical compounds.

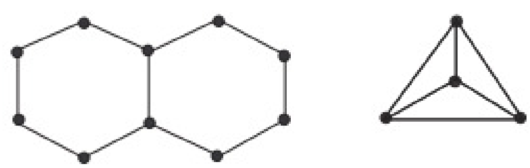

Figure 1.11: Chemical Graph

Chapter 2

Topological indices

2.1 Introduction

The numerical parameter known as a topological index is obtained by molecular graphs of various chemical structures with the aid of mathematics. Chemical graph theory, a significant field in mathematical chemistry, encompasses diverse topological indices. These indices prove beneficial for studying the properties of numerous chemical compounds. They associates with the chemical structure's composition, aiming to correlate it with various physio chemical properties, biological activity, chemical reactivity, or characteristics. Designing topological indices to transform a molecular graph to a numerical value which characterize its topology. They contribute to the study of Quantitative Structure-Activity Relationships and Quantitative Structure-Property Relationships , which predict the biological activities and properties of chemical compounds [2].

2.2 Types of Topological indices

There are different types of topological indices that can be classified as follows:

- Degree-based topological indices: These indices are determined by the degrees of vertices in a graph
- Distance-based topological indices: These indices are calculated based on the distances between vertices within a graph.
- Topological indices based on counting associated graphs and polynomials: These indices involve counting specific types of graphs or polynomials associated with the given graph.

2.3 Degree base topological indices

Among these indices, The most crucial and significant is the degree-based topological index.

In this thesis, we focused on investigating topological indices for the line graph of the polythiophene. We computed various indices, including the Randic index, sum connectivity index, harmonic index, first, second, and third Zagreb indices, augmented Zagreb index, hyper Zagreb index, atom-bond connectivity index, geometric-arithmetic index, and inverse sum indeg index as vertex degree-based topological indices. Furthermore, we calculated the fourth version of the atom-bond connectivity index, fifth version of the geometric-arithmetic index, and the Sanskurti index as vertex neighborhood sum degree-based topological indices.

If ξ_m and ξ_n denote the degrees of vertices m and n in graph G, respectively, and there is an edge $mn \in E(G)$, then the third chapter presents various topological indices based on vertex degrees. These indices are computed using the following formulas:

2.3.1 Randic Index

Milan Randi introduced the Randic index [3] in 1975, which has become a commonly employed tool in cheminformatics for examining compounds. This index, defined as Randic Index:

$$R(G) = \sum_{mn \in E(G)} \frac{1}{\sqrt{\xi_m \xi_n}}$$

2.3.2 Sum Connectivity Index

Zhou and Trinajsic put out a proposal in 2009 that the sum-connectivity index [4], using Randic's description of the product connectivity index as a foundation. The graph G's sum-connectivity index is defined as

$$SCI(G) = \sum_{mn \in E(G)} \frac{2}{\xi_m + \xi_n}$$

2.3.3 Harmonic Index

Fajtlowicz introduced the Harmonic index in 1987 [5], which has since been widely studied and applied in various fields is defined as

$$H(G) = \sum_{mn \in E(G)} (\frac{2}{\xi_m + \xi_n})$$

Extensive research has shown a significant correlation between the Harmonic index and both the Randic index and the sum-connectivity index.

2.3.4 The Zagreb First, Second and Third Indices

Gutman and Trinajsti introduced the Zagreb indices in 1972 [6, 7]. Various terms have been used to refer to the Zagreb index in literature, including the Zagreb group indices [8, 9] , the Zagreb group parameters, and commonly, the Zagreb indices [10, 11]. The first, second, and third Zagreb indices are denoted as **First Index:**

$$M_1(G) = \sum_{mn \in E(G)} (\xi_m + \xi_n)$$

Second Index:

$$M_2(G) = \sum_{mn \in E(G)} (\xi_m \xi_n)$$

Third Index:
Third Zagreb index was porposed in 2011 to complement the previously defined first and second Zagreb indices [12]. It is defined as

$$M_3(G) = \sum_{mn \in E(G)} |\xi_m - \xi_n|$$

by using values from table 3.1

2.3.5 Augmented Zagreb Index

By Furtula et al., Augmented Zagreb index was first presented [13], presenting the following formulation

$$AZI(G) = \sum_{mn \in E(G)} (\frac{\xi_m \xi_n}{\xi_m + \xi_n - 2})^3$$

2.3.6 Hyper Zagreb Index

The Hyper Zagreb index, a new degree-based topological index, was released in 2013 [14]. Its definition is

$$HM(G) = \sum_{mn \in E(G)} (\xi_m + \xi_n)^2$$

In 2015, M.R. Farahani [15] calculated the Hyper-Zagreb index for a hexagonal nanotube.

2.3.7 Atom Bond Connectivity Index

“E. Estrada et al. introduced the atom-bond connectivity index in 1998” [16]. In subsequent research conducted in 2008, this index exhibited a strong correlation with the heat of formation of alkanes [17]. The atom-bond connectivity index is defined as follows

$$ABC(G) = \sum_{mn \in E(G)} \sqrt{\frac{\xi_m + \xi_n - 2}{\xi_m \xi_n}}$$

2.3.8 Geometric Arithmetic Index

The first Geometric-Arithmetic (GA) index was established by D. Vukicevic and B. Furtula in 2009 [18]. The GA index is defined as follows

$$GA(G) = \sum_{mn \in E(G)} 2\sqrt{\frac{\xi_m \xi_n}{\xi_m + \xi_n}}$$

2.3.9 Inverse sum indeg Index

"The inverse sum indeg index has been recognized as a meaningful predictor of the total surface area of octane isomers"[19]. The index known as the inverse sum indeg index is defined as follows

$$ISI(G) = \sum_{mn \in E(G)} \sqrt{\frac{\xi_m \xi_n}{\xi_m + \xi_n}}$$

2.4 Vertex Neighborhood Sum Degree Based Topological Indices

Let δ_m and δ_n represent the neighborhood sum degrees of adjacent nodes m and n in graph G, respectively. Furthermore, if $mn \in E(G)$, the fourth chapter of this study presents various formulae for neighborhood degree-based topological indices. These indices are based on vertex neighborhood sum degree and will be computed as follows

2.4.1 4^{th} version of Atom Bond Connectivity Index

In their study, Ghorbani and colleagues (Ghorbani et al., 2010) introduced the fourth iteration of the ABC index, providing a definition for this version as follows
ABC_4 Index:

$$ABC_4(G) = \sum_{mn \in E(G)} \sqrt{\frac{\delta_m + \delta_n - 2}{\delta_m \delta_n}}$$

2.4.2 5^{th} version of Geometric Arithmetic Index

"The fifth version of the GA index was proposed by Graovac et al."[21] Defined by
GA_5 Index:

$$GA_5(G) = \sum_{mn \in E(G)} \frac{2\sqrt{\delta_m \delta_n}}{\delta_m + \delta_n}$$

where

$$\delta_m = \sum_{n \in N_G(m)} d(n) \text{ and } N_G(m) = n \in V(G), mn \in E(G)$$

2.4.3 Sanskruti Index

The Sanskruti Index [22] was defined as

Sanskruti Index:

$$S(G) = \sum_{mn \in E(G)} \left(\frac{\delta_m \delta_n}{\delta_m + \delta_n - 2} \right)^3$$

In this chapter, we present all the formulae that are computed within this thesis. The calculations for two types of topological indices are performed: vertex degree-based indices in Chapter 3, and vertex neighborhood sum degree-based indices in Chapter 4. These calculations specifically apply to the line graph of polythiophene.

Chapter 3

Vertex Degree Based Topological Indices on Line Graph of Polythiophene Network

3.1 Introduction

In this section, we conducted calculations for vertex Topological indices based on the degrees of vertices are calculated on the line graph of Polythiophene Network. Polythiophene Network Chemoinformatics is a relatively new interdisciplinary field that combines elements of chemistry, mathematics, and other information sciences[23]. Its primary focus is on the collection, storage, processing, and analysis of chemical data. Polythiophene is the polymer constructed from repetitive units of thiophene monomers. Thiophene is heterocyclic aromatic compound with a five membered ring that includes four carbon atoms and one sulfur atom.A polythiophene network is a three-dimensional interconnected structure formed by the interaction and bonding of polythiophene molecules or polymer chains [24]. This network can arise through different mechanisms, including chemical cross-linking, physical entanglement, or intermolecular interactions.The chemical formula of a polythiophene network is $(C_4H_2S)_n$, here "n" represents the number units or monomers in the polymer chain forming the network [25]. One unit of polythiophene network is (C_4H_2S) and two units of polythiophene network $(C_4H_2S)_2$ are shown as follow

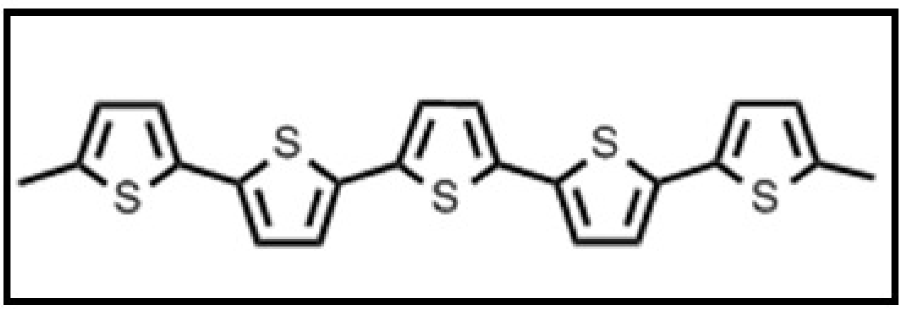

Figure 3.1: Chemical structure of polythiophene $(C_4H_2S)_5$

3.2 Planner Graph of Polythiophene Network

With the help of the chemical structures in graph theory we are able to construct the planner graph of different chemical structures. Figure 3.2 shows the planner of Polythiophene Network which

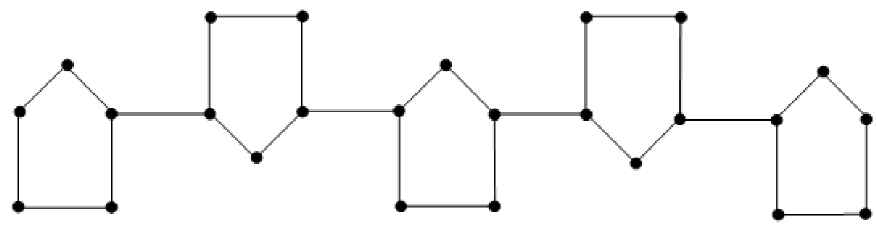

Figure 3.2: Planner Graph of Polythiophene Network $(C_4H_2S)_5$

3.3 Line Graph

In graph theory, by given graph G, we can create a new graph H, denoted as $L(G)$, which is commonly known as line graph of G. A line graph of a graph G is formed by introducing a vertex for each edge in G. In the resulting graph $H = L(G)$, two vertices are connected by an edge if and only if the corresponding edges in G share a common endpoint. Line Graph of Polythiophene Network represented by $L(PLY_n)$ for $n = 5$ is shown in figure 3.3

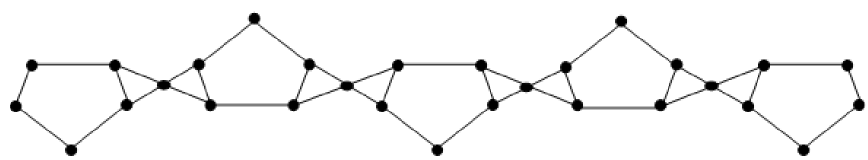

Figure 3.3: line Graph of Polythiophene Network $(C_4H_2S)_5$

3.4 Degree Based Topological Indices on $L(PLY_n)$

Network $L(PLY_n)$ depending on calculation based on the summation of the degrees of the vertices associated with each edge. The types of edges based on vertex degrees of $L(PLY_n)$, where $n \geq 1$ are shown in table 3.1.Now we computed the topological indices based on vertex degrees include the Randić index, sum connectivity index, harmonic index, first, second, and third Zagreb indices, augmented Zagreb index, hyper Zagreb index, atom-

(ξ_m, ξ_n), **where** $mn \in E(G)$	**No. of edges E(G)**
(2,2)	4
(2,3)	2n
(3,3)	3n-4
(3,4)	4n-4

Table 3.1: Edge partitioned for Line Graph of Polythiophene

bond connectivity index, geometric-arithmetic index and inverse sum indeg index.

3.5 Related Theorems and Results

3.5.1 Theorem

Let $G = L(PLY_n)$ where $n \geq 1$ then Randic Index is

$$R(G) = n\left(1 + \frac{2}{\sqrt{6}} + \frac{2}{2\sqrt{3}}\right) + \left(2 - \frac{4}{3} - \frac{2}{\sqrt{3}}\right)$$

Proof

Randic Index:

$$R(G) = \sum_{mn \in E(G)} \frac{1}{\sqrt{\xi_m \xi_n}}$$

by using values from table 3.1

$$\begin{aligned}
R(G) &= 4\frac{1}{\sqrt{2\times 2}} + (2n)\frac{1}{\sqrt{2\times 3}} + \\
&\quad (3n-4)\frac{1}{\sqrt{3\times 3}} + (4n-4)\frac{1}{\sqrt{3\times 4}} \\
&= 2 + \frac{2n}{\sqrt{6}} + \frac{3n-4}{\sqrt{9}} + \frac{4n-4}{\sqrt{12}} \\
&= 2 + \frac{2n}{\sqrt{6}} + \frac{3n}{\sqrt{9}} - \frac{4}{\sqrt{9}} + \frac{4n}{2\sqrt{3}} - \frac{4}{2\sqrt{3}} \\
&= n\left(1 + \frac{2}{\sqrt{6}} + \frac{2}{2\sqrt{3}}\right) + \left(2 - \frac{4}{3} - \frac{2}{\sqrt{3}}\right)
\end{aligned}$$

3.5.2 Theorem

Let $G = L(PLY_n)$ where $n \geq 1$ then sum connectivity Index is

$$SCI(G) = n\left(\frac{2}{\sqrt{5}} + \frac{3}{\sqrt{6}} + \frac{4}{\sqrt{7}}\right) + \left(2 - \frac{4}{\sqrt{6}} - \frac{4}{\sqrt{7}}\right)$$

Proof

Sum Connectivity Index:

$$SCI(G) = \sum_{mn \in E(G)} \frac{2}{\xi_m + \xi_n}$$

by using values from table 3.1

$$\begin{aligned} SCI(G) &= 4\frac{1}{\sqrt{2+2}} + 2n\frac{1}{\sqrt{2+3}} + (3n-4)\frac{1}{\sqrt{3+3}} + (4n-4)\frac{1}{\sqrt{3+4}} \\ &= \frac{4}{\sqrt{4}} + \frac{2n}{\sqrt{5}} + \frac{3n-4}{\sqrt{6}} + \frac{4n-4}{\sqrt{7}} \\ &= 2 + \frac{2n}{\sqrt{5}} + \frac{3n}{\sqrt{6}} - \frac{4}{\sqrt{6}} + \frac{4n}{\sqrt{7}} - \frac{4}{\sqrt{7}} \\ &= n\left(\frac{2}{\sqrt{5}} + \frac{3}{\sqrt{6}} + \frac{4}{\sqrt{7}}\right) + \left(2 - \frac{4}{\sqrt{6}} - \frac{4}{\sqrt{7}}\right) \end{aligned}$$

3.5.3 Theorem

Let $G = L(PLY_n)$ where $n \geq 1$ then Harmonic Index is

$$H(G) = n\left(\frac{4}{5} + 1\right) + \left(2 - \frac{4}{3}\right)$$

Proof.

Harmonic Index:

$$H(G) = \sum_{mn \in E(G)} \left(\frac{2}{\xi_m + \xi_n}\right)$$

by using values from table 3.1

$$\begin{aligned} H(G) &= 4\frac{2}{2+2}+2n\frac{2}{2+3}+(3n-4)\frac{2}{3+3}+(4n-4)\frac{2}{3+4} \\ &= 2+\frac{4n}{5}+n-\frac{8}{3} \\ &= n\left(\frac{4}{5}+1\right)+\left(2-\frac{4}{3}\right) \end{aligned}$$

3.5.4 Theorem

Let $G = L(PLY_n)$ where $n \geq 1$ then First, Second and Third Zagreb Indices are

First Index:

$$M_1(G) = 56n - 36$$

Second Index:

$$M_2(G) = 87n - 68$$

Third Index:

$$M_3(G) = 6n - 4$$

Proof

First Index:

$$M_1(G) = \sum_{mn \in E(G)} (\xi_m + \xi_n)$$

by using values from table 3.1

$$\begin{aligned} M_1(G) &= 4(2+2)+2n(2+3)+(3n-4)(3+3)+(4n-4)(3+4) \\ &= 16+10n+18n-24+28n-28 \\ &= 56n-36 \end{aligned}$$

Second Index:

$$M_2(G) = \sum_{mn \in E(G)} (\xi_m \xi_n)$$

by using values from table 3.1

$$\begin{aligned} M_2(G) &= 4(2\times 2)+2n(2\times 3)+(3n-4)(3\times 3)+(4n-4)(3\times 4) \\ &= 16+12n+27n-36+48n-48 \\ &= 87n-68 \end{aligned}$$

Third Index:

$$M_3(G)=\sum_{mn\in E(G)} |\xi_m-\xi_n|$$

by using values from table 3.1

$$\begin{aligned} M_3(G) &= 4\,|2-2|+2n\,|2-3|+(3n-4)\,|3-3|+(4n-4)\,|3-4| \\ &= 0+2n(1)+0+(4n-4)(1) \\ &= 2n+4n-4 \\ &= 6n-4 \end{aligned}$$

3.5.5 Theorem

Let $G=L(PLY_n)$ where $n\geq 1$ then Augmented Zagreb Index is

$$AZI(G)=n\left(16+\frac{2187}{64}+\frac{6912}{125}\right)+\left(32-\frac{2916}{64}-\frac{6912}{125}\right)$$

Proof

AZI(G) Index :

$$AZI(G)=\sum_{mn\in E(G)} (\frac{\xi_m\xi_n}{\xi_m+\xi_n-2})^3$$

By using the values of table 3.1

$$
\begin{aligned}
AZI(G) &= 4(\frac{2\times 2}{2+2-2})^3 + 2n(\frac{2\times 2}{2+3-2})^3 \\
&\quad +(3n-4)(\frac{3\times 3}{3+3-2})^3 + (4n-4)(\frac{3\times 4}{3+4-2})^3 \\
&= 4(8) + 2n(8) + (3n-4)(\frac{729}{64}) + (4n-4)(\frac{1728}{125}) \\
&\quad 32 + 16n + \frac{2187}{654}n - \frac{2916}{64} + \frac{6912}{125} - \frac{6912}{125}n \\
AZI(G) &= n\left(16 + \frac{2187}{64} + \frac{6912}{125}\right) + \left(32 - \frac{2916}{64} - \frac{6912}{125}\right)
\end{aligned}
$$

3.5.6 Theorem

Let $G = L(PLY_n)$ where $n \geq 1$ then Hyper Zagreb Index is

$$HM(G) = 354n - 276$$

proof

HM(G) Index : By using the values of table 3.1

$$
\begin{aligned}
HM(G) &= \sum_{mn\in E(G)} (\xi_m + \xi_n)^2 \\
HM(G) &= 4(2+2)^2 + 2n(2+3)^2 + (3n-4)(3+3)^2 + (4n-4)(3+4)^2 \\
&= 4(16) + 2n(25) + (3n-4)(36) + (4n-4)(49) \\
&= 64 + 50n + 108n - 144 + 196n - 196 \\
HM(G) &= 354n - 276
\end{aligned}
$$

3.5.7 Theorem

Let $G = L(PLY_n)$ where $n \geq 1$ then Atom Bond Connectivity Index is

$$ABC(G) = n\left(2 + \frac{2}{\sqrt{2}} + 2\frac{\sqrt{5}}{\sqrt{3}}\right) + \left(\frac{4}{\sqrt{2}} - \frac{8}{3} - 2\frac{\sqrt{5}}{\sqrt{3}}\right)$$

Proof

ABC(G) Index :

$$ABC(G) = \sum_{mn \in E(G)} \sqrt{\frac{\xi_m + \xi_n - 2}{\xi_m \xi_n}}$$

By using the values of table 3.1

$$\begin{aligned}
ABC(G) &= 4\sqrt{\frac{2+2-2}{2\times 2}} + 2n\sqrt{\frac{2+3-2}{2\times 3}} + (3n-4)\sqrt{\frac{3+3-2}{3\times 3}} \\
&\quad +(4n-4)\sqrt{\frac{3+4-2}{3\times 4}} \\
&= 4\sqrt{\frac{2}{4}} + 2n\sqrt{\frac{3}{6}} + (3n-4)\sqrt{\frac{4}{9}} + (4n-4)\sqrt{\frac{5}{12}} \\
&= \frac{4}{\sqrt{2}} + \frac{2n}{\sqrt{2}} + 3n(\frac{2}{3}) - 4(\frac{2}{3}) + 4n(\sqrt{\frac{5}{12}}) - 4(\sqrt{\frac{5}{12}}) \\
&= \frac{4}{\sqrt{2}} + \frac{2n}{\sqrt{2}} + 2n - (\frac{8}{3}) + 4n(\sqrt{\frac{5}{12}}) - 4(\sqrt{\frac{5}{12}}) \\
ABC(G) &= n\left(2 + \frac{2}{\sqrt{2}} + 2\frac{\sqrt{5}}{\sqrt{3}}\right) + \left(\frac{4}{\sqrt{2}} - \frac{8}{3} - 2\frac{\sqrt{5}}{\sqrt{3}}\right)
\end{aligned}$$

3.5.8 Theorem

Let $G = L(PLY_n)$ where $n \geq 1$ then Geometric Arithmetic Index is

$$GA(G) = n(3 + \frac{\sqrt{6}}{5} + 16\frac{\sqrt{3}}{7}) - 16\frac{\sqrt{3}}{7}$$

Proof

GA(G) Index :

$$GA(G) = \sum_{mn \in E(G)} 2\sqrt{\frac{\xi_m \xi_n}{\xi_m + \xi_n}}$$

By using the values of table 3.1

$$\begin{aligned}
GA(G) &= (4)\frac{2\sqrt{2\times 2}}{2+2}+(2n)\frac{2\sqrt{2\times 3}}{2+3}+(3n-4)\frac{2\sqrt{3\times 3}}{3+3} \\
&\quad +(4n-4)\frac{2\sqrt{3\times 4}}{3+4} \\
&= 2\sqrt{4}+4n\frac{\sqrt{6}}{5}+(3n-4)\frac{2\sqrt{9}}{6}+(4n-4)\frac{2\sqrt{12}}{7} \\
&= 4+4n\frac{\sqrt{6}}{5}+3\frac{(3n-4)}{3}+4(4n-4)\frac{\sqrt{3}}{7} \\
&= 4+4n\frac{\sqrt{6}}{5}+3n-4+16n\frac{\sqrt{3}}{7}-16n\frac{\sqrt{3}}{7}
\end{aligned}$$

3.5.9 Theorem

Let $G = L(PLY_n)$ where $n \geq 1$ then The Inverse Sum Indeg Index is

$$ISI(G) = n\left(\frac{12}{5}+\frac{9}{2}+\frac{48}{7}\right)+\left(-2-\frac{48}{7}\right)$$

Proof

ISI(G) Index :

$$ISI(G) = \sum_{mn\in E(G)} \sqrt{\frac{\xi_m \xi_n}{\xi_m+\xi_n}}$$

By using the values of table 3.1

$$\begin{aligned}
ISI(G) &= 4\left(\frac{2\times 2}{2+2}\right)+2n\left(\frac{2\times 3}{2+3}\right)+(3n-4)\left(\frac{3\times 3}{3+3}\right)+(4n-4)\left(\frac{3\times 4}{3+4}\right) \\
&= 4+n\frac{12}{5}+n\frac{9}{2}-6+n\frac{48}{7}-\frac{48}{7} \\
ISI(G) &= n\left(\frac{12}{5}+\frac{9}{2}+\frac{48}{7}\right)+\left(-2-\frac{48}{7}\right)
\end{aligned}$$

Chapter 4

Vertex Neighborhood Sum Degree Based Topological Indices on Line Graph of Polythiophene Network

4.1 Introduction

In this chapter, some topological indices for Line Graph of Polythiophene Network which are based on vertex neighborhood sum degree are calculated. Vertex Neighborhood Sum Degree Based Topological Indices on $L(PLY_n)$ Let $L(PLY_n)$ be Line graph of Polythiophene Network as shown in Figure 3.3. We calculated vertex neighborhood sum degree based topological indices of our Graph $L(PLY_n)$. Now with the help of these degree sum of neighbor edges type and number of these edges, we computed the neighborhood sum degree of vertices based topological indices namely, the $4th$ version of atom bond connectivity index, the 5th version of geometric arithmetic index and the sanskruti index.

(δ_m, δ_n), where $mn \in E(G)$	No. of edges E(G)
(4,4)	5 for n = 1
(4,5)	4 for $n \geq 2$
(5,9)	4 for $n \geq 2$
(6,9)	2(n-2) for$n \geq 2$
(9,9)	2 for$n \geq 2$
(9,10)	2(n-2) for$n \geq 2$
(9,12)	2n for$n \geq 2$
(10,10)	n-2 for$n \geq 2$
(10,12)	2(n-2) for$n \geq 2$

Table 4.1: Edge partitioned for Line Graph of Polythiophene Network $L(PLY_n)$ based on degree sum of neighbors of end vertices of each edge

4.2 Related Theorems and Results

4.2.1 Theorem

Let $G = L(PLY_n)$, then its ABC_4 index is

$$ABC_4 = \begin{cases} \frac{5\sqrt{6}}{4}, & \text{if } n = 1 \\ n\left(\frac{2\sqrt{13}}{3\sqrt{6}} + \frac{2\sqrt{7}}{3\sqrt{10}} + \frac{\sqrt{19}}{3\sqrt{3}} + \frac{3\sqrt{2}}{10} + \frac{2\sqrt{5}}{\sqrt{30}}\right) + & \\ \left(\frac{2\sqrt{7}}{\sqrt{5}} + \frac{8\sqrt{3}}{3\sqrt{5}} + \frac{8}{9} - \frac{4\sqrt{13}}{3\sqrt{6}} - \frac{4\sqrt{17}}{3\sqrt{10}} - \frac{6\sqrt{2}}{10} - \frac{4\sqrt{5}}{\sqrt{30}}\right), & \text{if } n \geq 2 \end{cases}$$

Proof

ABC_4 Index:

$$ABC_4(G) = \sum mn \in E(G)\sqrt{\frac{\delta_m + \delta_n - 2}{\delta_m \delta_n}}$$

By using the value of table 4.1

for n=1

$$
\begin{aligned}
ABC_4(G) &= 5\sqrt{\frac{4+4-2}{4\times 4}} \\
&= 5\sqrt{\frac{6}{16}} \\
ABC_4(G) &= 5\frac{\sqrt{6}}{4} \\
& forn \geq 2, \\
ABC_4(G) &= 4\sqrt{\frac{4+5-2}{4\times 5}}+4\sqrt{\frac{5+9-2}{5\times 9}}+2(n-2)\sqrt{\frac{6+9-2}{6\times 9}}+ \\
& 2\sqrt{\frac{9+9-2}{9\times 9}}+2(n-2)\sqrt{\frac{9+10-2}{9\times 10}}+2n\sqrt{\frac{9+12-2}{9\times 12}}+ \\
& (n-2)\sqrt{\frac{10+10-2}{10\times 10}}+2(n-2)\sqrt{\frac{10+12-2}{10\times 12}} \\
&= 4\sqrt{\frac{7}{20}}+4\sqrt{\frac{12}{45}}+2(n-2)\sqrt{\frac{13}{54}}+2\sqrt{\frac{16}{81}}+2(n-2)\sqrt{\frac{17}{90}}+ \\
& 2n\sqrt{\frac{19}{108}}+(n-2)\sqrt{\frac{18}{100}}+2(n-2)\sqrt{\frac{20}{120}} \\
&= 2\sqrt{\frac{7}{5}}+4\frac{2\sqrt{3}}{3\sqrt{5}}+(2n-4)\frac{\sqrt{13}}{3\sqrt{6}}+2\frac{4}{9}+(2n-4)\frac{\sqrt{17}}{3\sqrt{10}}+ \\
& 2n\frac{\sqrt{19}}{6\sqrt{3}}+(n-2)\frac{3\sqrt{2}}{10}+(2n-4)\sqrt{\frac{1}{6}} \\
&= 2\sqrt{\frac{7}{5}}+\frac{8\sqrt{3}}{3\sqrt{5}}+\frac{2n\sqrt{13}}{3\sqrt{6}}-\frac{4\sqrt{13}}{3\sqrt{6}}+\frac{8}{9}+\frac{2n\sqrt{17}}{3\sqrt{10}}-\frac{4\sqrt{17}}{3\sqrt{10}} \\
& +\frac{n\sqrt{19}}{3\sqrt{3}}+\frac{3n\sqrt{2}}{10}-\frac{6\sqrt{2}}{10}+2n\sqrt{\frac{1}{5}}-4\sqrt{\frac{1}{6}} \\
&= n\left(\frac{2\sqrt{13}}{3\sqrt{6}}+\frac{2\sqrt{7}}{3\sqrt{10}}+\frac{\sqrt{19}}{3\sqrt{3}}+\frac{3\sqrt{2}}{10}+\frac{2\sqrt{5}}{\sqrt{30}}\right)+ \\
& \left(\frac{2\sqrt{7}}{\sqrt{5}}+\frac{8\sqrt{3}}{3\sqrt{5}}+\frac{8}{9}-\frac{4\sqrt{13}}{3\sqrt{6}}-\frac{4\sqrt{17}}{3\sqrt{10}}-\frac{6\sqrt{2}}{10}-\frac{4\sqrt{1}}{\sqrt{6}}\right)
\end{aligned}
$$

4.2.2 Theorem

Let $G = L(PLY_n)$, then its $GA_5(G)$ index is equal to

$$GA_5(G) = \begin{cases} 5, & \text{if } n = 1 \\ n\left(\frac{4\sqrt{6}}{5} + \frac{12\sqrt{10}}{91} + \frac{8\sqrt{3}}{7} + \frac{2\sqrt{22}}{11} + 1\right) + & \\ \left(\frac{16\sqrt{5}}{9} + \frac{12\sqrt{5}}{7} + \frac{8\sqrt{6}}{5} - \frac{24\sqrt{10}}{19} - \frac{4\sqrt{22}}{11}\right), & \text{if } n \geq 2 \end{cases}$$

Proof

$GA_5(G)$ Index:

$$GA_5(G) = \sum_{mn \in E(G)} \frac{2\sqrt{\delta_m \delta_n}}{\delta_m + \delta_n}$$

By using the value of table 4.1

for $n = 1$

$$\begin{aligned} GA_5(G) &= 5\frac{2\sqrt{4\times 4}}{4+4} \\ &= \frac{10\sqrt{16}}{8} \\ &= \frac{10\times 4}{8} \\ &= \frac{10\times 4}{8} \\ &= \frac{40}{8} \\ &= 5 \end{aligned}$$

for $n \geq 2$

$$\begin{aligned}
GA_5(G) &= 4\frac{2\sqrt{4\times 4}}{4+5}+4\frac{2\sqrt{5\times 9}}{5+9}+2(n-2)\frac{2\sqrt{6\times 9}}{6+9}+\\
&\quad 2\frac{2\sqrt{9\times 9}}{9+9}+2(n-2)\frac{2\sqrt{9\times 10}}{9+10}+2n\frac{2\sqrt{9\times 12}}{9+12}\\
&\quad +(n-2)\frac{2\sqrt{10\times 10}}{10+10}+2(n-2)\frac{2\sqrt{10\times 12}}{10+12}\\
&= 8\frac{\sqrt{20}}{9}+8\frac{\sqrt{45}}{14}+4(n-2)\frac{\sqrt{54}}{15}+4\frac{\sqrt{81}}{18}+\\
&\quad 4(n-2)\frac{\sqrt{90}}{19}+4n\frac{\sqrt{108}}{21}+2(n-2)\frac{\sqrt{100}}{20}\\
&\quad +4(n-2)\frac{\sqrt{22}}{22}\\
&= 8\frac{\sqrt{20}}{9}+8\frac{\sqrt{45}}{14}+4n\frac{\sqrt{54}}{15}-8\frac{\sqrt{54}}{15}+4\frac{9}{18}+\\
&\quad 4n\frac{\sqrt{90}}{19}-8\frac{\sqrt{90}}{19}+4n\frac{\sqrt{108}}{21}+2n\frac{10}{20}-4\frac{10}{20}+\\
&\quad 4n\frac{\sqrt{22}}{22}-4n\frac{\sqrt{22}}{22}\\
&= n\left(\frac{4\sqrt{54}}{15}+\frac{12\sqrt{10}}{91}+\frac{24\sqrt{3}}{21}+\frac{4\sqrt{22}}{22}+1\right)+\\
&\quad \left(\frac{16\sqrt{5}}{9}+\frac{24\sqrt{5}}{14}+2-\frac{24\sqrt{6}}{15}-\frac{24\sqrt{10}}{19}-\frac{8\sqrt{22}}{22}\right)\\
&= n\left(\frac{4\sqrt{6}}{5}+\frac{12\sqrt{10}}{91}+\frac{8\sqrt{3}}{7}+\frac{2\sqrt{22}}{11}+1\right)+\\
&\quad \left(\frac{16\sqrt{5}}{9}+\frac{12\sqrt{5}}{7}+\frac{8\sqrt{6}}{5}-\frac{24\sqrt{10}}{19}-\frac{4\sqrt{22}}{11}\right)
\end{aligned}$$

4.2.3 Theorem

Let $G = L(PLY_n)$, then its Sanskruti index is equal to

$$S(G) = \begin{cases} \frac{2560}{27}, & \text{if } n = 1 \\ n(\frac{4\sqrt{6}}{5}+\frac{12\sqrt{10}}{91}+\frac{8\sqrt{3}}{7}+\frac{2\sqrt{22}}{11}+1)+ & \\ (\frac{16\sqrt{5}}{9}+\frac{12\sqrt{5}}{7}+\frac{8\sqrt{6}}{5}-\frac{24\sqrt{10}}{19}-\frac{4\sqrt{22}}{11}), & \text{if } n \geq 2 \end{cases}$$

Proof

Sanskruti Index:

$$S(G) = \sum_{mn \in E(G)} \left(\frac{\delta_m \delta_n}{\delta_m + \delta_n - 2} \right)^3$$

for $n = 1$

$$\begin{aligned} S(G) &= 5\left(\frac{4\times 4}{4+4-2}\right)^3 \\ &= 5\left(\frac{16}{6}\right)^3 \\ &= 5\left(\frac{8}{3}\right)^3 \\ &= 5\left(\frac{512}{27}\right) \\ &= \frac{2560}{27} \end{aligned}$$

for $n \geq 2$

$$\begin{aligned}
S(G) &= 4\left(\frac{4\times5}{4+5-2}\right)^3+4\left(\frac{5\times9}{5+9-2}\right)^3+2(n-2)\left(\frac{6\times9}{6+9-2}\right)^3+\\
&\quad 2\left(\frac{9\times9}{9+9-2}\right)^3+2(n-2)\left(\frac{9\times10}{9+10-2}\right)^3+2n\left(\frac{9\times12}{9+12-2}\right)^3\\
&\quad +(n-2)\left(\frac{10\times10}{10+10-2}\right)^3+2(n-2)\left(\frac{10\times12}{10+12-2}\right)^3\\
&= 4\left(\frac{20}{7}\right)^3+4\left(\frac{45}{12}\right)^3+2(n-2)\left(\frac{54}{13}\right)^3+2\left(\frac{81}{16}\right)^3+2(n-2)\left(\frac{90}{17}\right)^3+\\
&\quad 2n\left(\frac{108}{19}\right)^3+(n-2)\left(\frac{100}{18}\right)^3+2(n-2)\left(\frac{120}{20}\right)^3\\
&= 4\left(\frac{8000}{343}\right)+4\left(\frac{3375}{64}\right)+2(n-2)\left(\frac{157464}{2197}\right)+2\left(\frac{531441}{4096}\right)+\\
&\quad 2(n-2)\left(\frac{729000}{4913}\right)+2n\left(\frac{1259712}{6859}\right)+(n-2)\left(\frac{125000}{729}\right)\\
&\quad +2(n-2)(216)\\
&= \frac{32000}{343}+\frac{13500}{64}+\frac{314934}{2197}n-\frac{629868}{2197}+\frac{1062882}{4096}+\frac{1458000}{4913}n-\\
&\quad \frac{2916000}{4913}+\frac{2519424}{6859}n+\frac{125000}{729}n-\frac{125000}{729}+432n-864\\
&= n\left(\frac{314934}{2197}+\frac{1458000}{4913}+\frac{2519424}{6859}+\frac{125000}{729}+432\right)+\\
&\quad \left(\frac{32000}{343}+\frac{3375}{16}+\frac{531441}{2048}-\frac{52489}{183}-\frac{2916000}{4913}-\frac{25000}{729}-864\right)
\end{aligned}$$

This completes the proof.

All above are the topological indices for Line Graph of the Polythiophene Network that were based on vertex neighborhood sum degree.There are several other vertex neighbourhood sum degree-based topological indices that are not covered by this thesis.These topological indices must be relevant to graphs that are finite, simple, and undirected with no loops and no multiple edges, but not to graphs with isolated vertices.We computed all of the degree-based topological indices covered in our third chapter since the graph under consideration here satisfies all of the requirements.

Chapter 5

Conclusion

In this thesis, we computed a few neighbourhood sum degree-based topological indices and degree-based topological indices on a line graph of polythiophene network.By utilising topological indices, we discovered some new results and discussed about how to build chemical graphs.An ongoing issue with chemical networks and art/design sciences is the research of new architectural structures. Future work will focus on the sketching of new graphs and networks (webs), as well as the discussion of topological indices that are useful for comprehending the topologies of these new structures.

Chapter 6

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