Degree and Distance Based Parameters of Certain Graph Structures

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CIIT/FA12-PMATH-006/LHR

PhD Thesis

In

Mathematics

COMSATS University Islamabad
Lahore Campus - Pakistan

Spring, 2019

COMSATS University Islamabad

Degree and Distance Based Parameters of Certain Graph Structures

A Thesis Presented to

COMSATS University Islamabad, Lahore Campus

In partial fulfillment

of the requirement for the degree of

PhD (Mathematics)

By

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CIIT/FA12-PMATH-006/LHR

Spring, 2019

Degree and Distance Based Parameters of Certain Graph Structures

A Post Graduate Thesis submitted to the department of Mathematics as partial fulfillment of the requirement for the award of Degree of PhD in Mathematics.

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DEDICATION

To My Parents and All Family

ACKNOWLEDGEMENTS

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 supervisor **Dr. Muhammad Faisal Nadeem**. He has been there providing his heartfelt support and guidance at all times and has given me invaluable guidance, inspiration and suggestions in my quest for knowledge.

Besides my supervisor, my sincere thanks also goes to **Dr. Muhammad Afzal Siddiqui,** for his intuitive comments and encouragement, but also for the hard questions which incented me to widen my research from various perspective**.**

It would be injustice if I omit to mention the names of my two close friends **Dr. Tanweer Ul Islam** and **Hafiz Muhammad Zia Akbar** who have, in their own ways, kept me going on my path to success, assisting me as per their abilities, in whatever manner possible and for ensuring that good times keep flowing.

Last but not the least, my acknowledgement would be incomplete without thanking the biggest source of my strength, my family. The blessings of my parents and the love and care of my wife and my siblings who never let things get dull or boring, have all made a tremendous contribution in helping me reach this stage in my life. I thank them for putting up with me in difficult moments where I felt stumped and for provoking me on to follow my dream of getting this degree.

May Allah bless them all (Ameen)

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ABSTRACT

Degree and Distance Based Parameters of Certain Graph Structures

Topological indices are a rapidly developing area of research in graph theory. There are various topological indices such as degree-based topological indices, spectrum-based topological indices and distance related topological indices. These topological indices correlate certain physico-chemical properties such as boiling point, stability of chemical compounds and many more. In this dissertation, we focus on degree based and spectrum based topological indices. Under the degree based topological indices, we study topological indices such Randic index, general Randic index, Zagreb index, general sum connectivity index, first and second multiple Zagreb indices, geometric index, atom bond connectivity index for para-line graphs of some chemical structures such as Phenylene, Anthracene, Benzenoid, Pentacene. Similarly, we study the spectrum based topological indices such as Estrada index for certain chemical graph structures such as Phenylene, Anthracene, Bi-smuth Tri-iodide, benzene ring embedded in P-type-surface in 2D network (BRE). Also we find the energy of above mentioned structures. We also discuss the notion of distance related parameters such as metric dimension and edge metric dimension. We compute the edge metric dimension for the barcycentric Subdivision of Cayley Graphs. Also we have studied the M-polynomial and entropy of generalized Sierpinski graphs.

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LIST OF SYMBOLS

$deg(v)$	Degree of a vertex v
$\delta(G)$	Minimum degree of graph
$\Delta(G)$	Minimum degree of graph
$N(x)$	Neighbourhood of x
$d(a,b)$	Distance between two vertices
C_n	Cycle graph
K_n	Complete graph
W_n	Wheel graph
$K_{m,n}$	Complete bipartite graph
$L(G)$	Line graph of G
$S(G)$	Subdivision of graph G
$L(S(G))$	Line graph of subdivision graph
$R_\alpha(G)$	Randic index
$M_\alpha(G)$	Zagreb index
$\chi_\alpha(G)$	General sum-connectivity index
$ABC(G)$	Atom-Bond connectivity index
$GA(G)$	Geometric arithmetic index
$ABC_4(G)$	Atom-Bond connectivity index of order 4
$GA_5(G)$	Geometric arithmetic index of order 5
$HM(G)$	Hyper-Zagreb index
$PM_1(G)$	1st multiple Zagreb index
$PM_2(G)$	2nd multiple Zagreb index
$M_1(G,p)$	1st Zagreb polynomials
$M_2(G,p)$	2nd Zagreb polynomials
$M_1II(G)$	1st Multiplicative Zagreb index
$M_2II(G)$	2nd Multiplicative Zagreb index
$AZIG$	Augmented Zagreb Index
$AZIIG$	Augmented Multiplicative Zagreb index
$^mM_2(G)$	2nd modified Zagreb index
$^mM_2II(G)$	2nd modified multiplicative Zagreb index
$H(G)$	Harmonic index
$I(G)$	Inverse sum index
$SSD(G)$	Symmetric division index
$I(G,W)$	Entropy of an edge weighted graph
$M(G,l,q)$	M-Polynomial of a graph G
$E(G)$	Energy of a graph G
$EE(G)$	Estrada index of a graph G
$dim(G)$	Metric dimension of a graph G
$edim(G)$	Edge metric dimension of a graph G

Chapter 1

Introduction

About 300 years ago, when no one was known about the subject of graph theory, at that time the problem of Seven Bridges of Konigsberg was arisen. Konigsberg was a city of Germany at that time and now it is a part of Russia situated on the Pregel river. This city contains seven bridges and it was connected with two islands via these seven bridges. The people of Konigsberg always thought that is there any possibility to cross all the seven bridges in one attempt without crossing the every bridge more than once. In 1736 [27], the person who had solved this problem was Leonhard Euler (1707-1783). Euler declared the conclusion about the problem that there is no way or it is impossible to cross these bridges in one attempt without crossing the bridges more than once. He used the dots (vertices) to express the landmasses and lines (edges) to express the seven bridges to solve this problem in a very simple way. He not only proved that it is impossible but also gave the reason why this is so. He explained this by defining the new term valance or degree of a vertex means the number of edges connected to a particular vertex. This notion leads to the birth of Eulerian graph. Actually this notion from Euler has opened the new area in the premises of mathematics named "Graph Theory". Graph theory is the branch of combinatorics. After 100 years, another invention made by Kirchhoff [57] in this field while he was working with electrical networks. Caley [11] and Sylvester [90] have proposed the properties of new class of graphs called trees. Graph theory has a close relationship with linear algebra another branch of mathematics. Another invention related to matrix theory and incidence matrix discovered by Poincare [80] in the premises of graph theory. The family of complete graph has been discovered by Mobious in 1840. In 1852, Gutherie developed the four color problem in theory of graphs.

Graph theory is a subject which is being applied now a days in many fields of sciences such as Computer science as networks, Chemistry as chemical graphs, Electrical Engineering as electrical circuits, Operation research as sewerage system, traffic flow, telephone lines. It is also used in optimization problem. There are several applications of graph theory which are very much helpful for mankind. Graph theory belongs to mathematics but its roots are penetrating in Economics, Biology, Statistics, Architecture, Communication, Management, Mechanical, Civil and Chemical engineering.

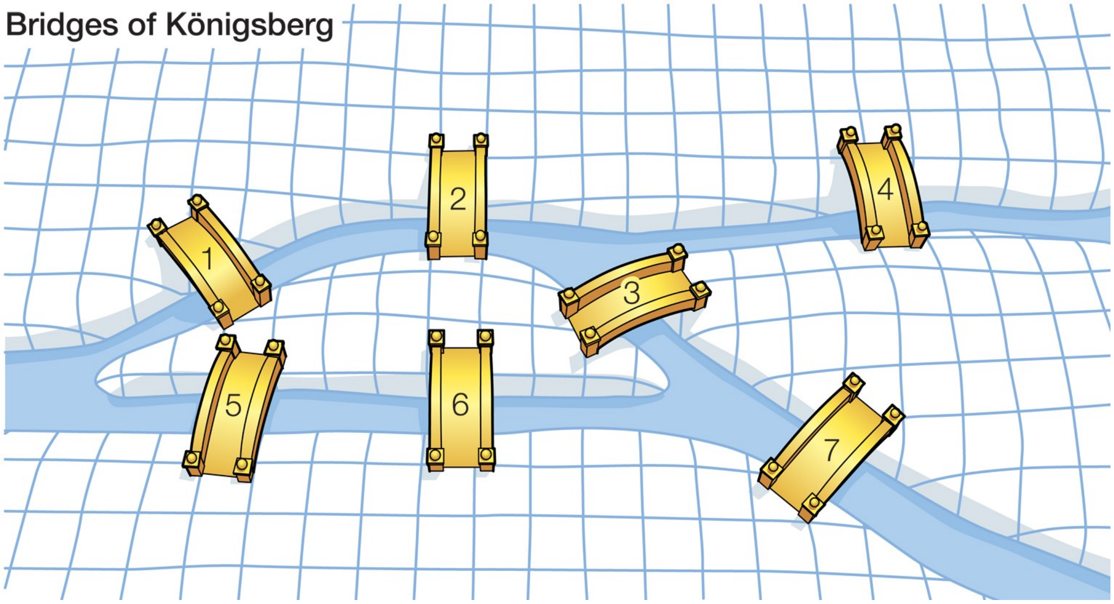

Figure 1.1: Konigsberg Bridge.

1.1 Application of Graph Theory in Diverse Areas

There are numerous applications in daily life where graph theory can be applied. Some of them are being mentioned here.

Traffic Signals

The vertex coloring techniques is being incorporated in traffic signals. The timing and pause between the red to green color is adjusted due to vertex coloring by giving chromatic number for the required number of cycles.

Clearance of Road Blockage

In hilly areas where in winters snow has blocked the roads and if you want to clean the roads then planning is needed to clear the roads by putting the salt on ice. This can be done by using Eulerian path or circuit in a quick way.

To Assign a Job to the Employees

The matching technique is used to assign the job to the employees. Softwares are used to optimize the job assignment.

Web Pages and Hyperlink

There are many search engines which are being used to search the information on internet. Hyperlink is used to link the web pages on internet. Every page represents as a vertex and the link between two pages serves as an edge.

Social Networks

In last decade social media has been getting much attention. It is a nice source to connect with friends and family. Multiple social media are working in the global world such as Facebook, Twitter, and Instagram. Users belongs to Facebook, Twitter, and Instagram are vertices and connection between them represent by an edges.

GPS System

GPS is a tracking system which is implemented to find the shortest routes between the two destinations. The destinations act as vertices and the connection between them act as an edge. Softwares are used to find the optimal route between the two destinations.

Google Map

Google Map is a wonderful application which is being used now a days, even a layman is using google map whenever he wants to go anywhere in the city, country and in the world without knowing the subject under which this system is working. Google Map actually find all the routes between two destinations and also mark the shortest route between them which is very beneficial application for all mankind. In google map the two destinations behave like a vertices and the routes between them are marked as edge. The software of google map provide the shortest route as a shortest path between two destinations.

1.2 Use of Graph Theory in Chemistry

Mathematics has the great ability to interlink itself with other subjects such as sciences and engineering. Graph theory is one of the richest outlet of mathematics which simplify the other subjects with the pictorial representation which helps to understand the topology of the object. Chemistry is the branch of science which has a close link with mathematics due to the subject of graph theory. The pictorial representation of chemical structures is connected with graph theory. Due to the close connection between chemistry and mathematics, a relatively new branch came into existence named chemical graph theory. Graph theory with respect to chemistry is an outlet of mathematics which relates the chemical substances to graphs. Chemical graph theory was started in late eighteen century. Chemical graph theory basically provides the atmosphere to unite the natural sciences and mathematics. For the first time graph theory had been used to represent the chemical aspects of certain chemical compounds by using the special type of graph such as Complete graph K_4. The vertices of graph represents the four species of chemical compounds and edges between them reflects the force which these compounds are exerting on each other in 1769 [16]. Chemical graph theory is being applied in enumerating the isomers, representing the chemical bonding, chemical documentation and also its use in chemical reaction networks and the most popular graph invariant such as topological indices.

1.3 Topological Descriptors: A Major Application of Chemical Graph Theory

Graph theory is basically used as a tool in chemistry. Chemical compounds are represented as graphs. Chemists use graph as graph invariants which is actually a numerical descriptors. This numerical parameters sometimes known as topological index. Topological index is just a number which can be generated by using the pictorial representation of the molecular graph. These numerical invariants can be generated by the adjacency matrix or distance matrix. Wiener was the first person who used the first graph invariants by using distance matrix in 1947 [95]. This index in these days is known as Wiener index. This index correlated well with the alkane'boiling point. For the best correlation and prediction of the molecular properties of molecules, topological indices have been implemented. The properties of molecules which are under investigation using topological indices are the physical properties such as boiling points, chemical properties such as reactivity, thermodynamic such as heat of formation , biochemical such as biological degradability , the pharmacological such as anesthetic behavior and toxicological such as toxicity. Some chemical compounds have various geometrical shapes such as polygonal shape, trees, path, and graphs. These shapes can be classified in terms of graphs by taking points as vertices and the connection between these points as a line called edges. The topological indices have been utilized in designing the drugs structure such as anti-cancer and anti-HIV. Fortunately mathematicians have successfully play their part by using the graph theory to analyze the drugs activity [32, 33]. Some topological descriptors such as Wiener index, Randic connectivity index, first Zagreb index, second Zagreb index and eccentric connectivity index have been employed to understand the drugs activity.

1.4 Application of Metric Dimension

Metric dimension has been proposed by Slater [88] and also investigated independently by "Harary and Melter" [43]. Metric dimension is a very devastating area of graph theory. Its role in daily life can change the direction of world and also its use in different field of sciences like biotechnology, technology, and engineering. Robots technology specifically is one of the finest application of graph theory [51]. Metric dimension is also applied in image processing and pattern recognition [55]. Mastermind game is a game of genius in which two players play and one of them is code setter and other is code breaker. In this game code setter selects a secret vector and a series of questions may be asked by the code breaker, each is a vector and the code setter answer the number of positions in which secret vector and questions meet. Navigation in networks have been studied by using the concept of graph. In the field of network, every place expressed as nodes in graph and relation between these nodes(places) expressed as edges. The places where we positioned a Robots are known as landmarks. The minimum number of robots requisite to trace the each node is known as metric dimension. For further study on metric dimension see [86, 87].

In literature, there are many other metric generators exist. one of them is edge metric dimension. In [54], the concept of edge metric dimension is explained explicitly. The results about edge metric dimension have been studied in literature, see [54, 78, 102].

In this thesis, we have tried to show the importance of the topological indices which are being used as a fundamental tool in different field of sciences such Chemistry, Biology, computer science etc. we have mustered up different aspects in one thesis such as degree and distance based parameters under these parameters we have discussed multiple topics such as degree based topological indices, M-Polynomial, Entropy, Energy of a graph , Estrada Index, Metric dimension and Edge metric dimension. Mostly we have picked the chemical structures which are useful in chemistry such as Pentacene, which is being used in nano silicon chip and Anthracene which is also used in Coaltar and many more.

Chapter 2

Preliminaries

This chapter contains the elementary notions of graph theory which are already given in the literature see [22, 93, 94].

2.1 Elements of Basic Graph Theory

Definition 2.1.1. [22]"A Graph $G = (V, E)$ of sets satisfying $E \subseteq [V]^2$, thus, the elements of E are 2-element subsets of V. The elements of V are called the vertices of a graph G and the elements of E are its edges."

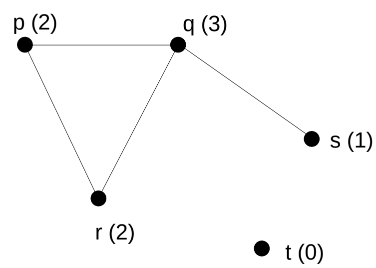

Figure 2.1: Graph

Definition 2.1.2. " **Finite graph** contains the finite number of vertices and edges."

Definition 2.1.3. "A graph G is **trivial** if it contains only an isolated vertex."

Figure 2.2: Trivial graph.

Definition 2.1.4. "The number of vertices in a vertex set and the number of edges in an edge set is called the **order** and **size** of G, respectively."

In Figure 2.1, the order and size of a graph G is 5 and 4, respectively.

Definition 2.1.5. " If two vertices having an edge between them then these vertices are called **adjacent vertices** and all those edges who have a common vertex are known as **adjacent edges**."

For example in Figure 2.1, vertex p is adjacent to vertex q because they have an edge between them and similarly r is adjacent to p because they also gave a common edge between them.
Similarly edges pq and pr are adjacent because they have a common vertex p between them and edges qr and qs are adjacent because q is a common vertex between them.

Definition 2.1.6. "If two vertices share more than one edge, then these edges are said to be **parallel edges**."

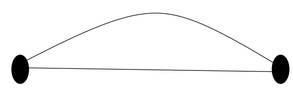

Figure 2.3: Parallel edges.

Definition 2.1.7. "If a single edge joins a vertex twice, then the edge is called a **loop**."

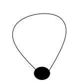

Figure 2.4: Loop.

Definition 2.1.8. " The count of the edges that connect with vertex is a **degree** of that vertex and is denoted by $deg(v)$ or $deg_G(v)$."

In Figure 2.1 the degree of each vertex is as follows: $deg_G(a) = 2, deg_G(b) = 3, deg_G(c) = 2, deg_G(d) = 1, deg_G(e) = 0$

Definition 2.1.9. "The minimum degree of a graph G is defined as the minimum number of edges connected to a vertex and is denoted by $\delta(G)$, where $\delta(G) = Min\{\text{deg(v)}|v \in V(G)\}$."
"The maximum degree of a graph G is defined as the maximum number of edges connected to a vertex and is denoted by $\Delta(G)$, where $\Delta(G) = Max\{\text{deg(v)}|v \in V(G)\}$."

Definition 2.1.10. The vertices are called **neighbors** of each other if they are adjacent.

In Figure 2.1 the vertex p has neighbors q and r, vertex q has neighbors p, r and s, vertex r has neighbors p and q, vertex s has neighbors q and vertex t has no neighbors.

Definition 2.1.11. $N(p)$ is the **neighborhood** of p if p contains all of its neighbors.

For instance, in Figure 2.1 $N(p) = \{q,r\}$, $N(q) = \{p,r,s\}$, $N(r) = \{q,r\}$, $N(s) = \{q\}$ and $N(t) = \Phi$

Definition 2.1.12. "The **degree sequence** of a graph is the list of vertex degrees, usually written in nonincreasing order, as $d_1 \geq d_2 \geq ... \geq d_n$."

In Figure 2.1, $(0,1,2,2,3)$ is the degree sequence of the graph G.

Lemma 2.1.1. *[22]"In any graph G the sum of all the vertex-degrees is an even number- in fact, twice the number of edges, since each edge contributes exactly 2 to the sum , namely*

$$2|E(G)| = \sum_{i=1}^{n} deg(p_i)$$

,

where (p_i) are the vertices of graph G, This result is known as the ***handshaking lemma****."*

Definition 2.1.13. "The **distance** between any two vertices a and b is defined as the shortest path length between a and b and it is denoted by $d(a,b)$."

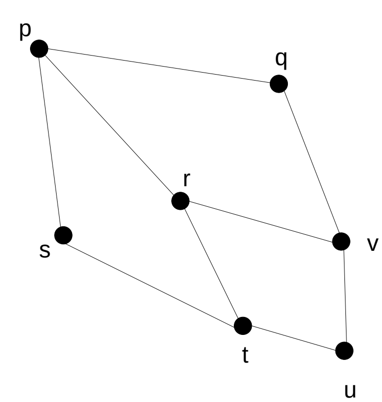

Figure 2.5: Graph with labled vertices.

The distances between some vertices of the above graphs are given below:
$d(p,q) = 1, d(p,r) = 1, d(p,s) = 1, d(p,t) = 2, d(p,v) = 2, d(p,u) = 3.$
Some of the terminologies in graph theory and in many other subjects belongs to Greek language. For instance, in graph theory the word Isomorphism falls in Greek language. The English meaning of this word is equal form or same form (isos means equal and morphe means form). Isomorphism [13] between two graphs is a beautiful phenomenon in graph theory.

Definition 2.1.14. [22]"Two graphs are **isomorphic** if two vertices in one graph are adjacent in such a way that their images are adjacent in other graph. In formal language, if p and q are not adjacent in one graph, then their images $f(p)$ and $f(q)$ must not be adjacent in other graph."

2.2 Some Renowned Graphs in Graph Theory

Some graphs are very much popular and have a strong impact in the field of graph theory.
Regular Graph[22]
"If all the vertices of G has same degree k, G is k-regular or simply regular."

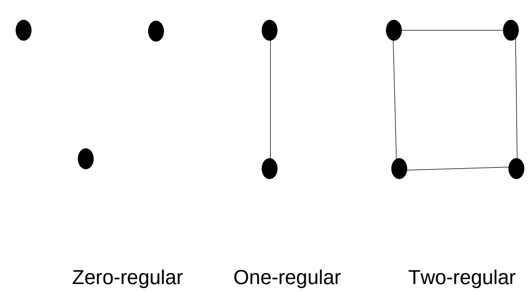

Figure 2.6: Regular graph.

Cycle Graph[94]
" A connected graph that is regular of degree 2 is a cycle graph. it is denoted by C_n with n vertices($n \geq 3$)."

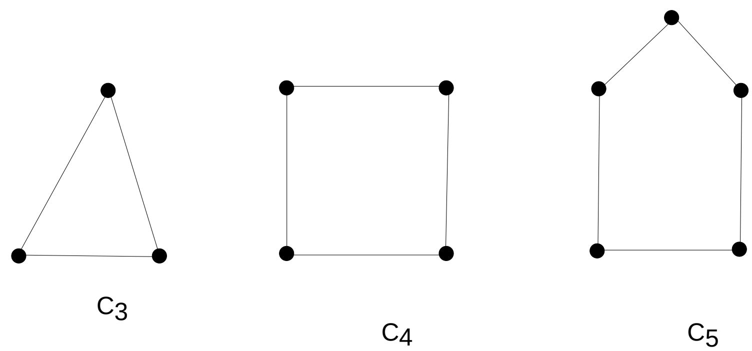

Figure 2.7: Cycle graph.

Complete Graph[94]

" A simple graph in which each pair of distinct vertices are adjacent is a complete graph and it is denoted by K_n with n vertices."

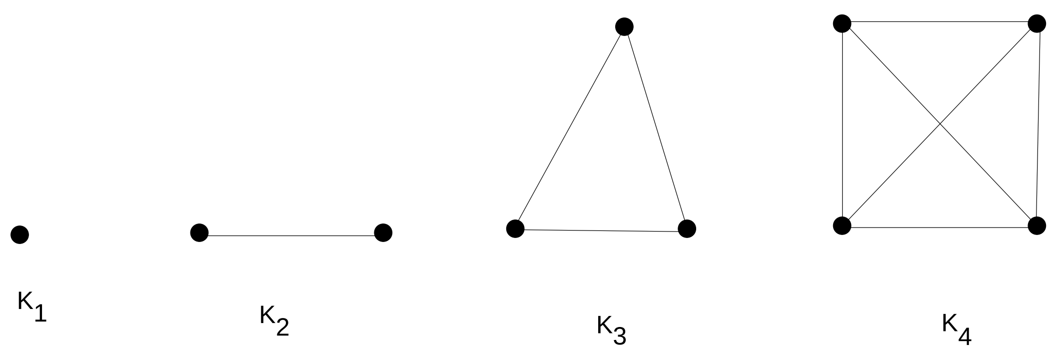

Figure 2.8: Complete graphs K_1,K_2,K_3,K_4 .

Wheel Graph[94]

The graph obtained from C_{n-1} by joining each vertex to a new vertex v is the Wheel graph on n vertices, denoted by W_n.

Wheel graphs are used in Computer networking[97].

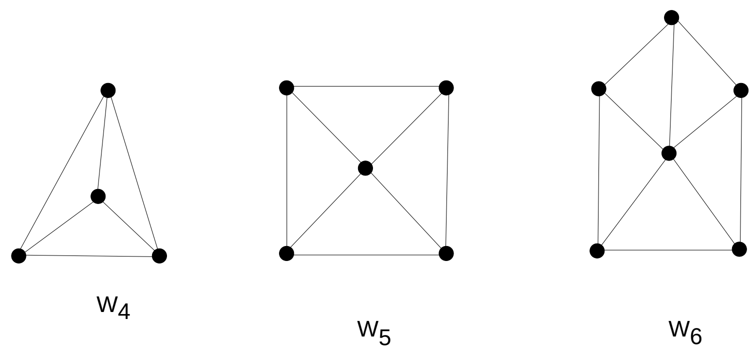

Figure 2.9: Wheel graph.

Bipartite Graph[94]

"If the vertex set of a graph G can be split into two disjoint sets A and B so that each edge of G joins a vertex of A and a vertex of B, then G is a bipartite graph." " Bipartite graphs are used in Coding theory to decode the words, which are , receives from the channel" [77].

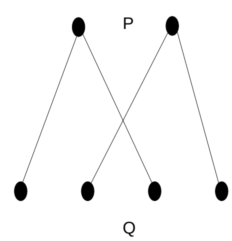

Figure 2.10: Bipartite graph.

Complete Bipartite Graph[94]

"A complete bipartite graph is a bipartite graph in which each vertex in A is joined to each vertex in B by just one edge."

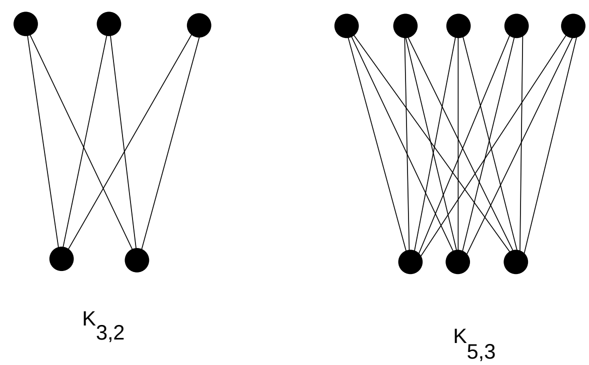

Figure 2.11: Complete bipartite graph.

Line Graph

"The line graph L(G) of a simple graph G is the graph whose vertices are in one-one correspondence with the edges of G, two vertices of L(G) being adjacent if and only if the corresponding edges of G are adjacent."

Line graphs are used in chemistry [77].

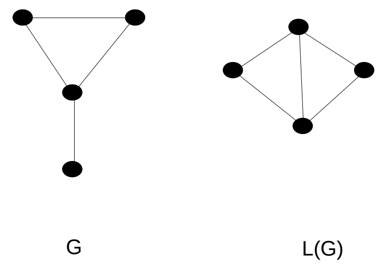

Figure 2.12: Graph and its line graph.

Sub division of a Graph

" if we subdivide every edge by inserting one vertex on every edge, this is called the sub division of graph and is denoted by $S(G)$."

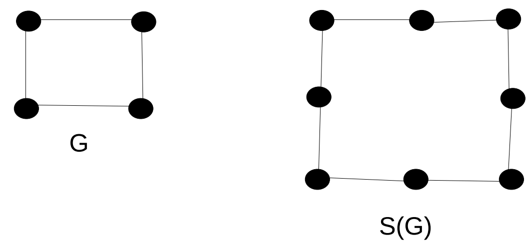

Figure 2.13: Graph and its Subdivision graph.

Para-Line Graph

“ The line graph of the subdivision graph is termed as the para-line graph of G which is denoted by $L(S(G))$”

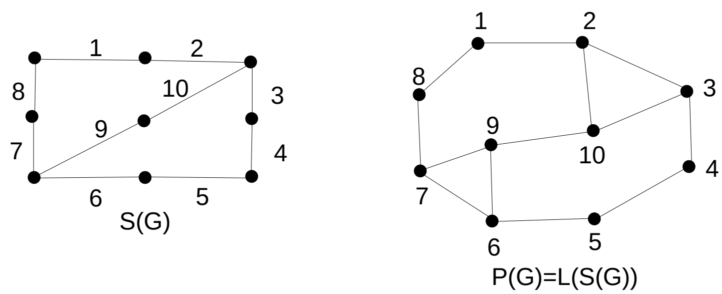

Figure 2.14: Subdivision of G and para-line graph of G

Chapter 3

Topological Indices

In the history of graph theory, graph can be expressed in quantitative terms by using different measures or indices. In this way, one can express the geometrical object in a unique real number which satisfy the geometric properties of that object. These measures in chemical graph theory represents as topological descriptors or molecular descriptors. For instance, chemists transform the chemical structure into a molecular graph, then find a numerical value by using topological indices. These topological indices are the numerical invariants of chemical graph. Hundreds of topological descriptors are existed in literature. But the first one was the Wiener index which was invented when Wiener was working on boiling points of alkane.

3.1 Topological Indices in Chemical Graph Theory

In chemical graph theory, chemical structure is transformed in the mathematical descriptions in such a way that both chemical and mathematical logic preserves. The way in which chemical structures is treated as graph is a very prominent methodology for understanding the nature of chemical structures and reactivity. By using this technique, graph theory delivers the pattern to the chemists by which chemist may get the qualitative predictions about the chemical structures. Topological descriptors are the numerical invariants of molecular graph. The advantage of topological index are that every chemical structure or species can be studied under topological indices and also topological index correlates well the physiochemical properties of the chemical structures.

3.2 Types of Topological Indices

The topological indices are of three types which we will discuss in this section. Major classes of topological indices or molecular descriptors are the following:

(1) Degree based molecular descriptors

(2) Spectrum based molecular descriptors

(3) Distance based molecular descriptors

3.2.1 Degree Based Molecular Descriptors

Degree based topological indices are much popular and much easier in their studies as compared to other topological indices. Technically, Randic index is a first degree based topological index which was conceived by Milan Randic in 1975 [81]. Randic himself picked its name as branching index, but after a short time its name has been changed to connectivity index by Randic. In recent day, its name has been again changed as Randic index by mostly authors due to the contribution of Randic. The index is demonstrated as $R = R(G) = \sum_{l,m \in V(G)} \frac{1}{\sqrt{(d_l)(d_m)}}$. Another topological index based on vertex degree has been considered as first degree based topological index named Zagreb index [82]. It was initially used totally in different purpose but with the passage of time it has been used as topological index. Randic index did not attract the audience of mathematics for twenty years but later storm came to attack on this index and hundreds of paper were published and multiple reviews on it two of them written by Randic himself.

"The general Randic connectivity index of G is defined as [81]

$$R_\alpha(G) = \sum_{xy \in E(G)} (d_x d_y)^\alpha. \tag{3.2.1}$$

Where d_x and d_y are degrees of the end vertex, α represents a real number. If α is -1/2, then $R_{-1/2}(G)$ is said to be Randic connectivity index of G. Li and Zhao presented the first general Zagreb index in [68]:

$$M_\alpha(G) = \sum_{x \in V(G)} (d_x)^\alpha. \tag{3.2.2}$$

General sum-connectivity index $\chi_\alpha(G)$ has been invented [101]:

$$\chi_\alpha(G) = \sum_{xy \in E(G)} (d_x + d_y)^\alpha. \tag{3.2.3}$$

Estrada gave (ABC) index in [26]. The ABC index of graph G is expressed as

$$ABC(G) = \sum_{xy \in E(G)} \sqrt{\frac{d_x + d_y - 2}{d_x d_y}}. \tag{3.2.4}$$

Vukišević and Furtula announced the geometric arithmetic (GA)index in [92]. The geometric-arithmetic index, denoted by GA for graph G is presented by

$$GA(G) = \sum_{xy \in E(G)} \frac{2\sqrt{d_x d_y}}{d_x + d_y}. \tag{3.2.5}$$

Another index belongs to the 4th class of (ABC) index was invented by Ghorbani et al. in [35] as:

$$ABC_4(G) = \sum_{xy \in E(G)} \sqrt{\frac{S_x + S_y - 2}{S_x S_y}}. \tag{3.2.6}$$

Where $S_x = |N_x|$ and $S_y = |N_y|$ are cardinality of neighbourhood of vertex x and y. The fifth class of geometric-arithmetic index, denoted by GA_5 was presented by Graovac et al. in [36] as

$$GA_5(G) = \sum_{xy \in E(G)} \frac{2\sqrt{S_x S_y}}{S_x + S_y}. \tag{3.2.7}$$

In 2013, Hyper-Zagreb index has been introduced as

$$HM(G) = \sum_{xy \in E(G)} \left(d_x + d_y\right)^2 \tag{3.2.8}$$

Ghorbani and Azimi proposed two new types of Zagreb indices of a graph G in 2012. $PM_1(G)$, $PM_2(G)$, are the 1^{st} and 2^{nd} multiple Zagreb indices, $M_1(G,p)$ and $M_2(G,p)$, 1^{st} and 2^{nd} Zagreb polynomials, respectively, are presented as:

$$PM_1(G) = \prod_{xy \in E(G)} (d_x + d_y) \tag{3.2.9}$$

$$PM_2(G) = \prod_{xy \in E(G)} (d_x \times d_y) \tag{3.2.10}$$

$$M_1(G,p) = \sum_{xy\in E(G)} p^{(d_x+d_y)} \tag{3.2.11}$$

$$M_2(G,p) = \sum_{xy\in E(G)} p^{(d_x\times d_y)}, \tag{3.2.12}$$

1st and 2nd Multiplicative Zagreb Indices were determined by Consonni and Todeschini et al. in 2010 and are described as:

$$M_1II(G) = \prod_{L\in M(G)} \Big(d_x\Big)^2 \tag{3.2.13}$$

$$M_2II(G) = \prod_{x,y\in E(G)} \Big(d_x d_y\Big) \tag{3.2.14}$$

Gutman and Trinajstic proposed 2nd Zagreb Index in 1972 which are stated as:

$$M_2(G) = \sum_{x,y\in E(G)} \Big(d_x d_y\Big) \tag{3.2.15}$$

Furtula et al. was recognized Augmented Zagreb and Augmented Multiplicative Zagreb Index and described as:

$$AZIG = \sum_{x,y\in E(G)} \Big(\frac{d_x d_y}{d_x+d_y-2}\Big)^3 \tag{3.2.16}$$

$$AZI(II)G = \prod_{x,y\in E(G)} \Big(\frac{d_x d_y}{d_x+d_y-2}\Big)^3 \tag{3.2.17}$$

The authors introduced the 2nd modified and 2nd modified multiplicative Zagreb indices which stated as:

$$^mM_2(G) = \sum_{x,y\in E(G)} \Big(\frac{1}{d_x d_y}\Big) \tag{3.2.18}$$

$$^mM_2II(G) = \prod_{x,y\in E(G)} \Big(\frac{1}{d_x d_y}\Big) \tag{3.2.19}$$

This is another variant of Randic index. In 1987, Fajtlowicz proposed Harmonic index and stated:

$$H(G) = \sum_{x,y\in E(G)} \Big(\frac{2}{d_x+d_y}\Big) \tag{3.2.20}$$

Inverse Sum Index index is described as:

$$I(G) = \sum_{x,y \in E(G)} \Big(\frac{d_x d_y}{d_x + d_y} \Big) \tag{3.2.21}$$

Symmetric Division Index is described as:

$$SSD(G) = \sum_{x,y \in E(G)} \Big(\frac{min(d_x, d_y)}{max(d_x, d_y)} + \frac{max(d_x, d_y)}{min(d_x, d_y)} \Big) \tag{3.2.22}$$

3.2.2 Spectrum Based Molecular Descriptors

Topological indices based on spectrum play a key role in theoretical chemistry and nanotechnology. The connection of linear algebra and graph theory give rise to the new direction in the field of topological indices using adjacency matrix named as spectral graph theory. The basics of spectral graph theory can be found in [17, 18]. Indices based on spectrum has been generated by finding the eigen values of adjacency matrix. Estrada index $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$ was invented in 2000 when Estrada was working on the folding of protein molecules. A prominent application due to this index have been marked in chemical and non-chemical structures. This index is used in Huckel model of π – electron system in the field of theoretical chemistry [30, 31]. Energy of a molecule plays an important role in physics, chemistry and biology. In mathematics, the concept of energy is used in graph theory to help other subjects like chemistry. In graph theory, Nullity is the number of zeros extracted from the characteristic polynomials obtained from the adjacency matrix and inertia represents the positive and negative eigen values of the adjacency matrix. Energy is the sum of the absolute eigen values of its adjacency matrix. The mathematical representation of the energy is $E = \sum_{i=1}^{n} |\lambda_i|$.

Rank and nullity are also an important pillars of linear algebra. In a similar way rank and nullity are very important in the field of graph theory. Rank in the field of graph theory belongs to positive and negative inertia index of molecular structures. The sum of positive and negative inertia is called the rank. As both the fields are inter connected with the same concept. Also eigen values are very important in both fields. Eigen values have many applications in different fields like Economics, Mathematics, Graph theory etc. Because nullity plays a vital role in the stability of molecules so if nullity is zero this shows that the molecule is predicted to have a stable, closed-shell, electron configuration. If nullity is greater than zero, then the molecule is unstable, highly reactive, nonexistent, open-shell. In chemical graph theory we associate eigen values with the molecular structure. Every molecular structure can be represented as a square matrix with entries only $1's$ and $0's$. The main diagonal entries are all zero for this matrix. This also represents that the trace of every matrix obtained from a molecular structure is always zero. Consider the graph of the molecular structure and label that graph by G. Atoms represented by vertices and covalent bonds represented by edges. The adjacency matrix can be obtained from the molecular graph in such a way that edge between two vertices represented by 1, otherwise 0. Eigen values can be extracted from the characteristic polynomial of the graph G. Since the matrix is symmetric and symmetric matrix always has real eigen values so the positive eigen values $p(G)$ represent the positive inertia index while negative eigen values $n(G)$ represents negative inertia index and nullity $\eta(G)$ in graph theory reflects the stability of the molecule. Nullity is the number of zeros appear in the roots of characteristics polynomial. All the eigen values form a set called spectrum of G. The signature $s(G)$ of the graph G is just a number which is generated by the difference of the number of positive and negative eigen values .

3.2.3 Distance Based Molecular Descriptors

The first molecular descriptors based on distance was the invention of Harold Wiener in 1947 [95], when he was studying the boiling point of paraffin's and perceived the relationship with Wiener index. In the beginning, this notion was not appreciated and got attention from the chemists but with the passage of time, it was too much popular in molecular structure descriptor. The total count of distances between overall pair of vertices is known as Wiener index of G. This index is represented as $W(G) = \sum\limits_{l,m \in V(G)} d(l,m)$. The other famous distance based topological index is a Harary index. It is the sum of all the reciprocal distances between every pair of vertices. Harary was not the inventor of this index. Actually this name has been given in honor of Frank Harary on his 70th birthday in 1993 and is proposed independently by Plavšić [79] and by Ivanciuc [49]. The Harary index can be defined as $H(G) = \sum\limits_{l,m \in V(G)} \frac{1}{d(l,m)}$. The mathematical properties and applications of this index can be found in [19, 25, 70]. The next distance based topological index is eccentric connectivity index which is proposed by Sharma [85]. This index is defined as $\xi^c = \xi^c(G) = \sum\limits_{l \in V(G)} deg(l) \times \varepsilon(l)$. The eccentric connectivity index is being used now to mathematical model of biological activities and application can be seen in [23, 39, 64].

Chapter 4

Degree Based Topological Indices

4.1 Introduction

Various graph polynomials were established in the literature, some of them have been implemented in mathematical chemistry. For instance, Hosoya Polynomial [45] is the significant polynomial that has been used in the field of distance based molecular descriptors. The Wiener index can be generated by taking the first derivative of the Hosoya polynomial evaluated at 1. The other molecular descriptors named hyper-Wiener index [10] and the Tratch-Stankevich-Zefirov index can be found similarly [7, 42]. Also chemistry related polynomials are the matching polynomial [28, 40], the Zhang-Zhang polynomial (also known as the Clar covering polynomial) [15, 98, 99], the Schultz polynomial [44]. M-polynomial has been introduced by Deutsch and Klavžar in [20] they shown how degree based molecular descriptors can be computed from it.

The notion of the entropy of a graph has been proposed by Körner in [60]. The graph entropy is a functional depending on two parameters, the graph itself and a probability density function on its vertex set. This graph functional devised from the problem of source coding in information theory. The purpose of this functional is to study the minimum number of codewords requisited for representing an information source. Körner also studied the basic properties of the entropy of graph, see [61, 62]. Some results of this chapter are published in international journals [73, 74, 100].In this section, we have computed the M-polynomial and entropy of generalised Sierpinski graph.

Definition 4.1.1. The M-Polynomial of a graph G is defined [20] as

$$M(G,l,q) = \sum_{\delta \le g \le h \le \Delta} m_{gh}(G) l^g q^h, \tag{4.1.1}$$

where

$$\delta(G) = Min\{d_v | v \in V(G)\}$$

$$\Delta(G) = Max\{deg(v) | v \in V(G)\}$$

and $m_{gh}(G), g, h \ge 1$ is the number of edges uv of G such that $\{deg(u)(G), d(v)(G)\} =$

$\{g,h\}$

Definition 4.1.2. The entropy of an edge weighted graph $G(V,E,W)$, is defined [24] as:

$$I(G,W) = -\sum_{rs\in E(G)} (p_{rs})log(p_{rs})$$

where, V, E and W are the vertex set, edge set and the edge weight set, respectively.

Also,

$$p_{rs} = \frac{w(rs)}{\sum\limits_{rs\in E(G)} w(rs)}$$

and $w(rs) > 0$, is the weight of the edge rs.

For an edge $e = rs$ and any real number α, one defines as $w(e) = (d_r \times d_s)^{\alpha}$, where the degree of a vertex r is described as d_r, then the general Randic index in [65, 66, 67] is defined as:

$$R_{\alpha}(G) = \sum_{rs\in E(G)} (d_r \times d_s)^{\alpha}$$

The Relationship between $I(G,\alpha)$ and $R_{\alpha}(G)$

$$I(G,\alpha) = logR_{\alpha}(G) - \frac{\alpha}{R_{\alpha}(G)} \sum_{rs\in E(G)} ((d_r \times d_s)^{\alpha} log(d_r \times d_s))$$

has been established in [14].

4.2 Generalized Sierpinski Graphs

The sierpinski graph was introduce by Klavazar and Milutinovic [58] in 1997. The Sierpinski graph additionally called the sierpinski gasket or Sierpinski sieve. For further study on these graphs see [37]. It is named after the polished mathematician Wa claw Sierpinski. The Sierpinski sieve is a fractal described by Sierpinski in 1915 and It is also called the Sierpiński gasket or Sierpiński triangle.

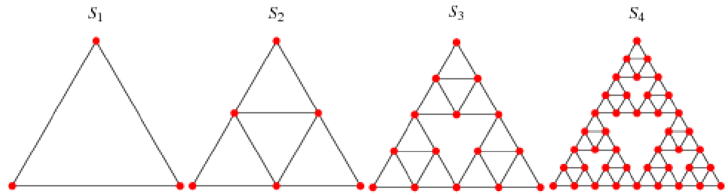

Figure 4.1: Sierpiński triangle

Let $G = (V, E)$ be a non-empty graph of order n. We represent the set by V^t, where V^t is the set of words of size t on alphabet V. The letters of a word p of length t are denoted by $p_1 p_2 p_3 ... p_t$. The chain of two words p and q is represented by pq. Klavazar and Milutinovic introduce the graph $S(K_n, t)$ whose vertex set V^t, where pq is an edge if and only if there exists $r \in \{1, 2, ..., t\}$ such that: (i) $p_s = q_s$, if $s < r$; (ii) $p_r \neq q_r$; (iii) $p_s = q_r$ and $q_s = p_r$ if $s > r$. When $n = 3$ then graphs are just called tower of Hanoi, later on, those graphs are named as Sierpinski graphs. The Sierpinski graphs have been generalised for any graph in [37]. In [37], they defined the t-th generalised Sierpinski graph of G and is represented as $S(G, t)$, the vertex set is V^t and the edge set, where pq is an edge if and only if there exists $r \in \{1, 2, ..., t\}$ such that: (i) $p_s = q_s$, if $s < r$; (ii) $p_r \neq q_r$ and $\{p_r, q_r\} \in E$; (iii) $p_s = q_r$ and $q_s = p_r$ if $s > r$. Let E_{pj} denotes the number of edges connecting the vertices of degree d_p and d_j.

In this graph G, the total number of vertices are $\frac{1}{6} \times 7^{n+1} - \frac{7}{6}$, in which there are three types of vertices namely two degree, three degree and four degree vertices. Moreover, the number of vertices of degree two, three and four are $\frac{343}{6} \times 7^{n-3} - \frac{1}{6}$, $\frac{539}{6} \times 7^{n-3} + \frac{7}{6}$

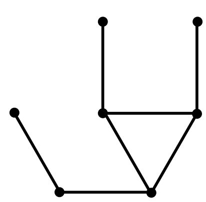

Figure 4.2: Graph G.

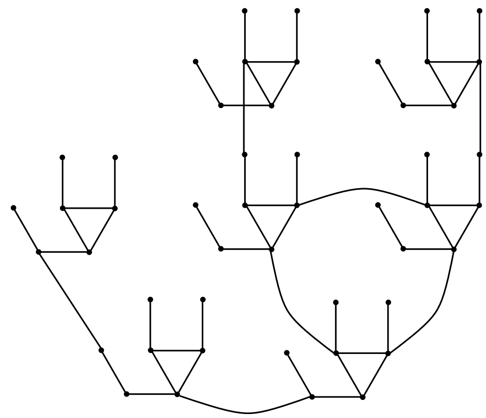

Figure 4.3: Sierpinski Graph of G, $S(G,2)$.

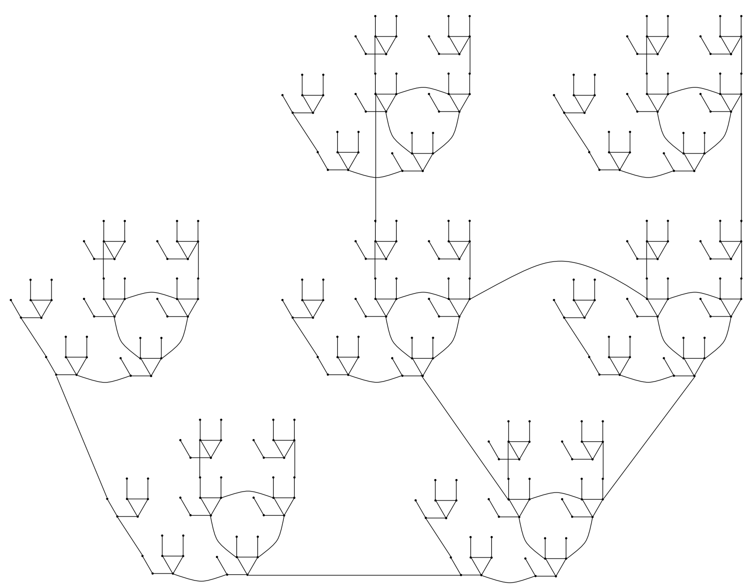

Figure 4.4: Sierpinski Graph of G, $S(G,3)$.

and $\frac{441}{6} \times 7^{n-3} - \frac{3}{2}$, respectively. Also the total number of edges are $\frac{2401}{6} \times 7^{n-3} - \frac{7}{6}$. To compute our main results we make a partite set of edges rely on degree of end vertices of each edge and represented in Table 4.1.

Table 4.1: The edge partition of graph G based on degree of end vertices of each edge

(d_p, d_j), where, $pj \in E(G)$	$E_{p,j}$	Number of Edges
$(1,2)$	$E_{(1,2)}$	$28 \times 7^{n-3}$
$(1,3)$	$E_{(1,3)}$	$\frac{329}{6} \times 7^{n-3} + \frac{1}{6}$
$(1,4)$	$E_{(1,4)}$	$\frac{119}{3} \times 7^{n-3} + \frac{1}{3}$
$(2,2)$	$E_{(2,2)}$	$\frac{14}{3} \times 7^{n-3} + \frac{1}{3}$
$(2,3)$	$E_{(2,3)}$	$\frac{98}{3} \times 7^{n-3} + \frac{1}{3}$
$(2,4)$	$E_{(2,4)}$	$\frac{133}{3} \times 7^{n-3} - \frac{4}{3}$
$(3,3)$	$E_{(3,3)}$	$\frac{105}{2} \times 7^{n-3} + \frac{1}{2}$
$(3,4)$	$E_{(3,4)}$	$77 \times 7^{n-3} + 2$
$(4,4)$	$E_{(4,4)}$	$\frac{133}{2} \times 7^{n-3} - \frac{7}{2}$

4.2.1 Results and Discussion on M-Polynomial of Generalized Sierpinski Graphs

First we will give our main results on topological indices with M-polynomial of generalized Sierpinski graphs. Consequently, in table explicit expressions for some degree based molecular discriptors are listed.

Table 4.2: Topological indices derived from M-polynomial

Topological indices	Derivation from $M(G,l,q)$
First Zagreb index	$M_1(G) = (D_l + D_q)(f(l,q))\|_{l=q=1}$
Second Zagreb index	$M_2(G) = (D_l D_q)(f(l,q))\|_{l=q=1}$
Second modified Zagreb index	${}^mM_2(G) = (\delta_l \delta_q)(f(l,q))\|_{l=q=1}$
General Randic' index,$\alpha \neq 0$	$R_\alpha(G) = (D_l^\alpha D_q^\alpha)(f(l,q))\|_{l=q=1}, \alpha \in N$
Inverse general Randic' index, $\alpha \neq 0$	$RR_\alpha(G) = (\delta_l^\alpha \delta_q^\alpha)(f(l,q))\|_{l=q=1}, \alpha \in N$
Symmetric division index	$SDD(G) = (D_l \delta_q + \delta_l D_q)(f(l,q))\|_{l=q=1}$
Harmonic index	$H(G) = 2\delta_l J(f(l,q))\|_{l=1}$
Inverse sum index	$I(G) = \delta_l J D_l D_q(f(l,q))\|_{l=1}$
Augmented Zagreb	$A(G) = \delta_l^3 Q_{-2} J D_l^3 D_q^3(f(l,q))\|_{l=1}$

where

$$
\begin{aligned}
D_l &= l\Big[\frac{\partial f(l,q)}{\partial l}\Big] \\
D_q &= q\Big[\frac{\partial f(l,q)}{\partial q}\Big] \\
\delta_l &= \int_0^l \Big[\frac{f(t,q)}{t}dt\Big] \\
\delta_q &= \int_0^q \Big[\frac{f(l,t)}{t}dt\Big] \\
J(f(l,q)) &= f(l,l) \\
Q_\alpha(f(l,q)) &= l^\alpha f(l,q)
\end{aligned}
$$

4.2.2 Relations of Topological Indices with M-polynomial of the Generalized Sierpinski Graphs

Theorem 4.2.1. *Consider the Sierpinski graph G, then its M-Polynomial is*

$$\begin{aligned} M(G,l,q) &= \Big(28\times 7^{n-3}\Big)l^1q^2+\Big(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\Big)l^1q^3+\Big(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^1q^4\\ &+ \Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^2q^3+\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)l^2q^4+\Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^3q^3\\ &+ \Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big)l^4q^4+\Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^2q^2++\Big(77\times 7^{n-3}+2\Big)l^3q^4 \end{aligned}$$

Proof. Let G be a Sierpinski graph, then from above discussion total number of vertices are $\frac{1}{6}\times 7^{n+1}-\frac{7}{6}$ and total number of edges are $\frac{2401}{6}\times 7^{n-3}-\frac{7}{6}$. Now the edges partition of Sierpinski graph are :

$|E_{\{1,2\}}| = |\{e = pj \in E(G|d_p = 1, d_j = 2\}| = 28\times 7^{n-3}$,

$|E_{\{1,3\}}| = |\{e = pj \in E(G|d_p = 1, d_j = 3\}| = \frac{329}{6}\times 7^{n-3}+\frac{1}{6}$,

$|E_{\{1,4\}}| = |\{e = pj \in E(G|d_p = 1, d_j = 4\}| = \frac{119}{3}\times 7^{n-3}+\frac{1}{3}$,

$|E_{\{2,2\}}| = |\{e = pj \in E(G|d_p = 2, d_j = 2\}| = \frac{14}{3}\times 7^{n-3}+\frac{1}{3}$,

$|E_{\{2,3\}}| = |\{e = pj \in E(G|d_p = 2, d_j = 3\}| = \frac{98}{3}\times 7^{n-3}+\frac{1}{3}$,

$|E_{\{2,4\}}| = |\{e = pj \in E(G|d_p = 2, d_j = 4\}| = \frac{133}{3}\times 7^{n-3}-\frac{4}{3}$,

$|E_{\{3,3\}}| = |\{e = pj \in E(G|d_p = 3, d_j = 3\}| = \frac{105}{2}\times 7^{n-3}+\frac{1}{2}$,

$|E_{\{3,4\}}| = |\{e = pj \in E(G|d_p = 3, d_j = 4\}| = 77\times 7^{n-3}+2$

$|E_{\{4,4\}}| = |\{e = pj \in E(G|d_p = 4, d_j = 4\}| = \frac{133}{2}\times 7^{n-3}-\frac{7}{2}$

Now apply definition of M-polynomial

$$\begin{aligned}
M(G,l,q) &= \sum_{g\leq h} m_{gh} l^g q^h \\
M(G,l,q) &= \sum_{1\leq 2} m_{12} l^1 q^2 + \sum_{1\leq 3} m_{13} l^1 q^3 + \sum_{1\leq 4} m_{14} l^1 q^4 + \sum_{2\leq 2} m_{22} l^2 q^2 \\
&+ \sum_{2\leq 3} m_{23} l^2 q^3 + \sum_{2\leq 4} m_{24} l^2 q^4 + \sum_{3\leq 3} m_{33} l^3 q^3 + \sum_{3\leq 4} m_{34} l^3 q^4 + \sum_{4\leq 4} m_{44} l^4 q^4 \\
M(G,l,q) &= |E_{\{1,2\}}| l^1 q^2 + |E_{\{1,2\}}| l^1 q^3 + |E_{\{1,4\}}| l^1 q^4 + |E_{\{2,2\}}| l^2 q^2 + |E_{\{2,3\}}| l^2 q^3 \\
&+ |E_{\{2,4\}}| l^2 q^4 + |E_{\{3,3\}}| l^3 q^3 + |E_{\{3,4\}}| l^3 q^4 + |E_{\{4,4\}}| l^4 q^4 \\
&= \Big(28\times 7^{n-3}\Big) l^1 q^2 + \Big(\frac{329}{6}\times 7^{n-3} + \frac{1}{6}\Big) l^1 q^3 + \Big(\frac{119}{3}\times 7^{n-3} + \frac{1}{3}\Big) l^1 q^4 \\
&+ \Big(\frac{98}{3}\times 7^{n-3} + \frac{1}{3}\Big) l^2 q^3 + \Big(\frac{133}{3}\times 7^{n-3} - \frac{4}{3}\Big) l^2 q^4 + \Big(\frac{105}{2}\times 7^{n-3} + \frac{1}{2}\Big) l^3 q^3 \\
&+ \Big(\frac{133}{2}\times 7^{n-3} - \frac{7}{2}\Big) l^4 q^4 + \Big(\frac{14}{3}\times 7^{n-3} + \frac{1}{3}\Big) l^2 q^2 + + \Big(77\times 7^{n-3} + 2\Big) l^3 q^4.
\end{aligned}$$

□

Proposition 4.2.2. *Let G be a Sierpinski graph, Then the topological indices are*

$$\begin{aligned}
M_1(G) &= \frac{7805}{3}\times 7^{n-3} - \frac{83}{3}. \\
M_2(G) &= \frac{6521}{2}\times 7^{n-3} - 33. \\
{}^m M_2(G) &= \frac{20377}{288}\times 7^{n-3} + \frac{11}{96}. \\
R_\alpha(G) &= 2^\alpha\Big(28\times 7^{n-3}\Big) + 3^\alpha\Big(\frac{329}{6}\times 7^{n-3} + \frac{1}{6}\Big) + 4^\alpha\Big(\frac{119}{3}\times 7^{n-3} + \frac{1}{3}\Big) \\
&+ 2^{2\alpha}\Big(\frac{14}{3}\times 7^{n-3} + \frac{1}{3}\Big) + 2^\alpha 3^\alpha\Big(\frac{98}{3}\times 7^{n-3} + \frac{1}{3}\Big) \\
&+ 2^\alpha 4^\alpha\Big(\frac{133}{3}\times 7^{n-3} - \frac{4}{3}\Big) + 3^{2\alpha}\Big(\frac{105}{2}\times 7^{n-3} + \frac{1}{2}\Big) \\
&+ 3^\alpha 4^\alpha\Big(77\times 7^{n-3} + 2\Big) + 4^{2\alpha}\Big(\frac{133}{2}\times 7^{n-3} + \frac{7}{2}\Big)
\end{aligned}$$

$$
\begin{aligned}
RR_{\alpha}(G) &= \frac{28}{2^{\alpha}}\times 7^{n-3}+\frac{1}{3^{\alpha}}\Big(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\Big)+\frac{1}{4^{\alpha}}\Big(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\Big)\\
&+ \frac{1}{2^{2\alpha}}\Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)+\frac{1}{3^{\alpha}2^{\alpha}}\Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)\\
&+ \frac{1}{2^{\alpha}4^{\alpha}}\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)+\frac{1}{3^{2\alpha}}\Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)\\
&+ \frac{1}{3^{\alpha}4^{\alpha}}\Big(77\times 7^{n-3}+2\Big)+\frac{1}{4^{2\alpha}}\Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big).\\
SDD(G) &= \frac{18445}{18}\times 7^{n-3}-\frac{65}{36}.\\
H(G) &= \frac{9461}{120}\times 7^{n-3}-\frac{247}{5040}.\\
I(G) &= \frac{68137}{120}\times 7^{n-3}-\frac{1751}{504}.\\
A(G) &= \frac{5287567733}{1296000}\times 7^{n-3}-\frac{47962067}{1296000}.
\end{aligned}
$$

Proof. Since by Theorem 1, we have

$$
\begin{aligned}
M(G,l,q) &= \Big(28\times 7^{n-3}\Big)l^1q^2+\Big(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\Big)l^1q^3+\Big(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^1q^4\\
&+ \Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^2q^3+\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)l^2q^4+\Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^3q^3\\
&+ \Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big)l^4q^4+\Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^2q^2++\Big(77\times 7^{n-3}+2\Big)l^3q^4.
\end{aligned}
$$

Now as shown in Table 4.2

$$
\begin{aligned}
M_1(G) &= (D_l+D_q)(f(l,q))|_{l=q=1}\\
D_lf(l,q) &= \Big(28\times 7^{n-3}\Big)l^1q^2+\Big(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\Big)l^1q^3+\Big(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^1q^4\\
&+ \Big(\frac{28}{3}\times 7^{n-3}+\frac{2}{3}\Big)l^2q^2+\Big(\frac{196}{3}\times 7^{n-3}+\frac{2}{3}\Big)l^2q^3+\Big(\frac{266}{3}\times 7^{n-3}-\frac{8}{3}\Big)l^2q^4\\
&+ \Big(\frac{315}{2}\times 7^{n-3}+\frac{3}{2}\Big)l^3q^3+\Big(231\times 7^{n-3}+2\Big)l^3q^4+\Big(\frac{532}{2}\times 7^{n-3}-\frac{28}{2}\Big)l^4q^4.
\end{aligned}
$$

$$
\begin{aligned}
D_q f(l,q) &= \Big(56\times 7^{n-3}\Big)l^1q^2 + \Big(\frac{329}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^1q^3 + \Big(\frac{476}{3}\times 7^{n-3}+\frac{4}{3}\Big)l^1q^4 \\
&+ \Big(\frac{28}{3}\times 7^{n-3}+\frac{2}{3}\Big)l^2q^2 + \Big(\frac{294}{3}\times 7^{n-3}+1\Big)l^2q^3 + \Big(\frac{532}{3}\times 7^{n-3}-\frac{16}{3}\Big)l^2q^4 \\
&+ \Big(\frac{315}{2}\times 7^{n-3}+\frac{3}{2}\Big)l^3q^3 + \Big(308\times 7^{n-3}+8\Big)l^3q^4 + \Big(266\times 7^{n-3}-14\Big)l^4q^4.
\end{aligned}
$$

substituting the values in $M_1(G)$

$$
\begin{aligned}
M_1(G) &= \Big|\Big((28\times 7^{n-3}\Big)l^1q^2 + \Big(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\Big)l^1q^3 + \Big(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^1q^4 \\
&+ \Big(\frac{28}{3}\times 7^{n-3}+\frac{2}{3}\Big)l^2q^2 + \Big(\frac{196}{3}\times 7^{n-3}+\frac{2}{3}\Big)l^2q^3 + \Big(\frac{266}{3}\times 7^{n-3}-\frac{8}{3}\Big)l^2q^4 \\
&+ \Big(\frac{315}{2}\times 7^{n-3}+\frac{3}{2}\Big)l^3q^3 + \Big(231\times 7^{n-3}+2\Big)l^3q^4 + \Big(\frac{532}{2}\times 7^{n-3}-\frac{28}{2}\Big)l^4q^4. \\
&+ (56\times 7^{n-3})l^1q^2 + \Big(\frac{329}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^1q^3 + \Big(\frac{476}{3}\times 7^{n-3}+\frac{4}{3}\Big)l^1q^4 \\
&+ \Big(\frac{28}{3}\times 7^{n-3}+\frac{2}{3}\Big)l^2q^2 + \Big(\frac{294}{3}\times 7^{n-3}+1\Big)l^2q^3 + \Big(\frac{532}{3}\times 7^{n-3}-\frac{16}{3}\Big)l^2q^4. \\
&+ \Big(\frac{315}{2}\times 7^{n-3}+\frac{3}{2}\Big)l^3q^3 + \Big(308\times 7^{n-3}+8\Big)l^3q^4 + \Big(266\times 7^{n-3}-14\Big)l^4q^4\Big|_{l=q=1} \\
M_1(G) &= \frac{7805}{3}\times 7^{n-3}-\frac{83}{3}.
\end{aligned}
$$

$$
\begin{aligned}
M_2(G) &= (D_lD_q)(f(l,q))|_{l=q=1} \\
D_lD_q &= \Big(56\times 7^{n-3}\Big)l^1q^2 + (\frac{329}{2}\times 7^{n-3}+\frac{1}{2})l^1q^3 + (\frac{476}{3}\times 7^{n-3}+\frac{4}{3})l^1q^4 \\
&+ \Big(\frac{56}{3}\times 7^{n-3}+\frac{4}{3}\Big)l^2q^2 + \Big(\frac{588}{3}\times 7^{n-3}+2)l^2q^3 + (\frac{1064}{3}\times 7^{n-3}-\frac{32}{3})l^2q^4 \\
&+ \Big(\frac{945}{2}\times 7^{n-3}+\frac{9}{2}\Big)l^3q^3 + \Big(924\times 7^{n-3}+24)l^3q^4 + (1064\times 7^{n-3}-56)l^4q^4
\end{aligned}
$$

$$
\begin{aligned}
M_2(G) &= \Big|\Big(56\times 7^{n-3}\Big)l^1q^2+\Big(\frac{329}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^1q^3+(\frac{476}{3}\times 7^{n-3}+\frac{4}{3})l^1q^4\\
&+ \Big(\frac{56}{3}\times 7^{n-3}+\frac{4}{3}\Big)l^2q^2+\Big(\frac{588}{3}\times 7^{n-3}+2\Big)l^2q^3+\Big(\frac{1064}{3}\times 7^{n-3}-\frac{32}{3}\Big)l^2q^4\\
&+ \Big(\frac{945}{2}\times 7^{n-3}+\frac{9}{2}\Big)l^3q^3+\Big(924\times 7^{n-3}+24\Big)l^3q^4+\Big(1064\times 7^{n-3}-56\Big)l^4q^4\Big|_{l=q=1}\\
M_2(G) &= \frac{6521}{2}\times 7^{n-3}-33.\\
{}^mM_2(G) &= (\delta_l\delta_q)(f(l,q))|_{l=q=1}\\
\delta_q f(l,q) &= \Big(14\times 7^{n-3}\Big)l^1q^2+\Big(\frac{329}{18}\times 7^{n-3}+\frac{1}{18}\Big)l^1q^3+\Big(\frac{119}{12}\times 7^{n-3}+\frac{1}{12}\Big)l^1q^4\\
&+ \Big(\frac{7}{3}\times 7^{n-3}+\frac{1}{6}\Big)l^2q^2+\Big(\frac{98}{9}\times 7^{n-3}+\frac{1}{9}\Big)l^2q^3+\Big(\frac{133}{12}\times 7^{n-3}-\frac{1}{3}\Big)l^2q^4\\
&+ \Big(\frac{105}{6}\times 7^{n-3}+\frac{1}{6}\Big)l^3q^3+\Big(\frac{77}{4}\times 7^{n-3}+\frac{1}{2}\Big)l^3q^4+\Big(\frac{133}{8}\times 7^{n-3}-\frac{7}{8}\Big)l^4q^4\\
\delta_l\delta_q &= \Big(14\times 7^{n-3}\Big)l^1q^2+\Big(\frac{329}{18}\times 7^{n-3}+\frac{1}{18}\Big)l^1q^3+\Big(\frac{119}{12}\times 7^{n-3}+\frac{1}{12}\Big)l^1q^4\\
&+ \Big(\frac{7}{6}\times 7^{n-3}+\frac{1}{12}\Big)l^2q^2+\Big(\frac{98}{18}\times 7^{n-3}+\frac{1}{18}\Big)l^2q^3+\Big(\frac{133}{24}\times 7^{n-3}-\frac{1}{6}\Big)l^2q^4\\
&+ \Big(\frac{105}{18}\times 7^{n-3}+\frac{1}{18}\Big)l^3q^3+\Big(\frac{77}{12}\times 7^{n-3}+\frac{1}{6}\Big)l^3q^4+\Big(\frac{133}{32}\times 7^{n-3}-\frac{7}{32}\Big)l^4q^4\\
{}^mM_2(G) &= \Big|\Big(14\times 7^{n-3}\Big)l^1q^2+\Big(\frac{329}{18}\times 7^{n-3}+\frac{1}{18}\Big)l^1q^3+\Big(\frac{119}{12}\times 7^{n-3}+\frac{1}{12}\Big)l^1q^4\\
&+ \Big(\frac{7}{6}\times 7^{n-3}+\frac{1}{12}\Big)l^2q^2+\Big(\frac{98}{18}\times 7^{n-3}+\frac{1}{18}\Big)l^2q^3+\Big(\frac{133}{24}\times 7^{n-3}-\frac{1}{6}\Big)l^2q^4\\
&+ \Big(\frac{105}{18}\times 7^{n-3}+\frac{1}{18}\Big)l^3q^3+\Big(\frac{77}{12}\times 7^{n-3}+\frac{1}{6}\Big)l^3q^4+\Big(\frac{133}{32}\times 7^{n-3}-\frac{7}{32}\Big)l^4q^4\Big|_{l=q=1}\\
{}^mM_2(G) &= \frac{20377}{288}\times 7^{n-3}+\frac{11}{96}.
\end{aligned}
$$

$$
\begin{aligned}
R_\alpha(G) &= (D_l^\alpha D_q^\alpha)(f(l,q))|_{l=q=1}\\
D_q^\alpha f(l,q) &= \Big(2^\alpha\times 28\times 7^{n-3}\Big)l^1q^2+3^\alpha\Big(\frac{329}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^1q^3\\
&+ 4^\alpha\Big(\frac{476}{3}\times 7^{n-3}+\frac{4}{3}\Big)l^1q^4+2^\alpha\Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^2q^2\\
&+ 3^\alpha\Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^2q^3+4^\alpha\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)l^2q^4\\
&+ 3^\alpha\Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^3q^3+4^\alpha\Big(77\times 7^{n-3}+2\Big)l^3q^4\\
&+ 4^\alpha\Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big)l^4q^4\\
D_l^\alpha D_q^\alpha f(l,q) &= \Big(2^\alpha 28\times 7^{n-3}\Big)l^1q^2+3^\alpha\Big(\frac{329}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^1q^3\\
&+ 4^\alpha\Big(\frac{476}{3}\times 7^{n-3}+\frac{4}{3}\Big)l^1q^4+2^{2\alpha}\Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^2q^2\\
&+ 2^\alpha 3^\alpha\Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^2q^3+2^\alpha 4^\alpha\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)l^2q^4\\
&+ 3^{2\alpha}\Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^3q^3+3^\alpha 4^\alpha\Big(77\times 7^{n-3}+2\Big)l^3q^4\\
&+ 4^{2\alpha}\Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big)l^4q^4
\end{aligned}
$$

substituting the values $D_l^\alpha D_q^\alpha f(l,q)$

$$
\begin{aligned}
R_\alpha(G) &= \Big|\Big(2^\alpha 28\times 7^{n-3}\Big)l^1q^2+3^\alpha\Big(\frac{329}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^1q^3+4^\alpha\Big(\frac{476}{3}\times 7^{n-3}+\frac{4}{3}\Big)l^1q^4\\
&+ 2^{2\alpha}\Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^2q^2+6^\alpha\Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^2q^3+8^\alpha\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)l^2q^4\\
&+ 3^{2\alpha}\Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^3q^3+12^\alpha\Big(77\times 7^{n-3}+2\Big)l^3q^4\\
&+ 4^{2\alpha}\Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big)l^4q^4\Big|_{l=q=1}\\
R_\alpha(G) &= 2^\alpha\times 28\times 7^{n-3}+3^\alpha\Big(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\Big)+4^\alpha\Big(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\Big)\\
&+ 2^{2\alpha}\Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)+2^\alpha 3^\alpha\Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)+2^\alpha 4^\alpha\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)\\
&+ 3^{2\alpha}\Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)+3^\alpha 4^\alpha\Big(77\times 7^{n-3}+2\Big)+4^{2\alpha}\Big(\frac{133}{2}\times 7^{n-3}+\frac{7}{2}\Big).
\end{aligned}
$$

$$
\begin{aligned}
RR_\alpha(G) &= (\delta_l^\alpha \delta_q^\alpha)(f(l,q))|_{l=q=1}\\
\delta_q^\alpha f(l,q) &= \Big(28\times 7^{n-3}\Big)\frac{l^1q^2}{2^\alpha}+\Big(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\Big)\frac{l^1q^3}{3^\alpha}+\Big(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^1q^4}{4^\alpha}\\
&+ \Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^2q^2}{2^\alpha}+(\frac{98}{3}\times 7^{n-3}+\frac{1}{3})\frac{l^2q^3}{3^\alpha}+\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)\frac{l^2q^4}{4^\alpha}\\
&+ \Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)\frac{l^3q^3}{3^\alpha}+(77\times 7^{n-3}+2)\frac{l^3q^4}{4^\alpha}+\Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big)\frac{l^4q^4}{4^\alpha}\\
\delta_l^\alpha\delta_q^\alpha f(l,q) &= \Big(28\times 7^{n-3}\Big)\frac{l^1q^2}{2^\alpha}+\Big(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\Big)\frac{l^1q^3}{3^\alpha}+\Big(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^1q^4}{4^\alpha}\\
&+ \Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^2q^2}{2^{2\alpha}}+\Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^2q^3}{2^\alpha 3^\alpha}+\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)\frac{l^2q^4}{2^\alpha 4^\alpha}\\
&+ \Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)\frac{l^3q^3}{3^{2\alpha}}+\Big(77\times 7^{n-3}+2\Big)\frac{l^3q^4}{3^\alpha 4^\alpha}+\Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big)\frac{l^4q^4}{4^{2\alpha}}.
\end{aligned}
$$

substituting the value in $RR_\alpha(G)$

$$
\begin{aligned}
RR_\alpha(G) &= \Big|\Big(28\times 7^{n-3}\Big)\frac{l^1q^2}{2^\alpha}+\Big(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\Big)\frac{l^1q^3}{3^\alpha}+\Big(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^1q^4}{4^\alpha}\\
&+ \Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^2q^2}{2^{2\alpha}}+\Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^2q^3}{2^\alpha 3^\alpha}+\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)\frac{l^2q^4}{2^\alpha 4^\alpha}\\
&+ \Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)\frac{l^3q^3}{3^{2\alpha}}+\Big(77\times 7^{n-3}+2\Big)\frac{l^3q^4}{3^\alpha 4^\alpha}+\Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big)\frac{l^4q^4}{4^{2\alpha}}\Big|_{l=q=1}\\
RR_\alpha(G) &= \frac{28}{2^\alpha}\times 7^{n-3}+\frac{1}{3^\alpha}\Big(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\Big)+\frac{1}{4^\alpha}\Big(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\Big)\\
&+ \frac{1}{2^{2\alpha}}\Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)+\frac{1}{6^\alpha}\Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)+\frac{1}{8^\alpha}\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)\\
&+ \frac{1}{3^{2\alpha}}\Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)+\frac{1}{12^\alpha}\Big(77\times 7^{n-3}+2\Big)+\frac{1}{4^{2\alpha}}\Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big).
\end{aligned}
$$

$$
\begin{aligned}
SDD(G) &= (\delta_q D_l + \delta_l D_q)(f(l,q))|_{l=q=1} \\
\delta_q D_l f(l,q) &= \Big(28\times 7^{n-3}\Big)\frac{l^1q^2}{2} + \Big(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\Big)\frac{l^1q^3}{3} + \Big(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^1q^4}{4} \\
&+ 2\Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^2q^2}{2} + 2\Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^2q^3}{3} + 2\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)\frac{l^2q^4}{4} \\
&+ 3\Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)\frac{l^3q^3}{3} + 3(77\times 7^{n-3}+2)\frac{l^3q^4}{4} + 4\Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big)\frac{l^4q^4}{4} \\
\delta_l D_q f(l,q) &= \Big(56\times 7^{n-3}\Big)l^1q^2 + \Big(\frac{329}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^1q^3 + \Big(\frac{476}{3}\times 7^{n-3}+\frac{4}{3}\Big)l^1q^4 \\
&= 2\Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^2q^2}{2} + 2\Big(\frac{294}{3}\times 7^{n-3}+1\Big)\frac{l^2q^3}{2} + \Big(\frac{532}{3}\times 7^{n-3}-\frac{16}{3}\Big)\frac{l^2q^4}{2} \\
&+ \Big(\frac{315}{2}\times 7^{n-3}+\frac{3}{2}\Big)\frac{l^3q^3}{3} + \Big(308\times 7^{n-3}+8\Big)\frac{l^3q^4}{3} + \Big(266\times 7^{n-3}-14\Big)\frac{l^4q^4}{4} \\
SDD(G) &= \Big|\Big(28\times 7^{n-3}\Big)\frac{l^1q^2}{2} + \Big(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\Big)\frac{l^1q^3}{3} + \Big(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^1q^4}{4} \\
&+ 2\Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^2q^2}{2} + 2\Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^2q^3}{3} + 2\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)\frac{l^2q^4}{4} \\
&+ 3\Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)\frac{l^3q^3}{3} + 3\Big(77\times 7^{n-3}+2\Big)\frac{l^3q^4}{4} + 4\Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big)\frac{l^4q^4}{4} \\
&+ \Big(56\times 7^{n-3}\Big)l^1q^2 + \Big(\frac{329}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^1q^3 + \Big(\frac{476}{3}\times 7^{n-3}+\frac{4}{3}\Big)l^1q^4 \\
&+ 2\Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^2q^2}{2} + 2\Big(\frac{294}{3}\times 7^{n-3}+1\Big)\frac{l^2q^3}{2} + \Big(\frac{532}{3}\times 7^{n-3}-\frac{16}{3}\Big)\frac{l^2q^4}{2} \\
&+ \Big(\frac{315}{2}\times 7^{n-3}+\frac{3}{2}\Big)\frac{l^3q^3}{3} + \Big(308\times 7^{n-3}+8\Big)\frac{l^3q^4}{3} \\
&+ \Big(266\times 7^{n-3}-14\Big)\frac{l^4q^4}{4}\Big|_{l=q=1} \\
SDD(G) &= \frac{18445}{18}\times 7^{n-3} - \frac{65}{36}.
\end{aligned}
$$

$$
\begin{aligned}
H(G) &= 2\delta_l J(f(l,q))|_{l=1} \\
J(f(l,q)) &= \Big(28\times 7^{n-3}\Big)l^3+\Big(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\Big)l^4+\Big(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^5 \\
&+ \Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^4+\Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^5+\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)l^6 \\
&+ \Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^6+\Big(77\times 7^{n-3}+2\Big)l^7+\Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big)l^8 \\
\delta_l J(f(l,q)) &= \Big(28\times 7^{n-3}\Big)\frac{l^3}{3}+\Big(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\Big)\frac{l^4}{4}+\Big(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^5}{5} \\
&+ \Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^4}{4}+\Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^5}{5}+\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)\frac{l^6}{6} \\
&+ \Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)\frac{l^6}{6}+\Big(77\times 7^{n-3}+2\Big)\frac{l^7}{7}+\Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big)\frac{l^8}{8} \\
H(G) &= \Big|2\Big(\Big(28\times 7^{n-3}\Big)\frac{l^3}{3}+\Big(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\Big)\frac{l^4}{4}+\Big(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^5}{5} \\
&+ \Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^4}{4}+\Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^5}{5}+\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)\frac{l^6}{6} \\
&+ \Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)\frac{l^6}{6}+\Big(77\times 7^{n-3}+2\Big)\frac{l^7}{7}+\Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big)\frac{l^8}{8}\Big)\Big|_{l=1} \\
H(G) &= \frac{9461}{120}\times 7^{n-3}-\frac{247}{5040}. \\
I(G) &= \delta_l J D_l D_q(f(l,q))|_{l=1} \\
JD_lD_qf(l,q) &= \Big(56\times 7^{n-3}\Big)l^3+\Big(\frac{329}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^4+\Big(\frac{476}{3}\times 7^{n-3}+\frac{4}{3}\Big)l^5 \\
&+ \Big(\frac{56}{3}\times 7^{n-3}+\frac{4}{3}\Big)l^4+\Big(\frac{588}{3}\times 7^{n-3}+2\Big)l^5+\Big(\frac{1064}{3}\times 7^{n-3}-\frac{32}{3}\Big)l^6 \\
&+ \Big(\frac{945}{2}\times 7^{n-3}+\frac{9}{2}\Big)l^6+\Big(924\times 7^{n-3}+24\Big)l^7+\Big(1064\times 7^{n-3}-56\Big)l^8 \\
\delta_l JD_lD_qf(l,q) &= \Big(56\times 7^{n-3}\Big)\frac{l^3}{3}+(\frac{329}{2}\times 7^{n-3}+\frac{1}{2})\frac{l^4}{4}+(\frac{476}{3}\times 7^{n-3}+\frac{4}{3})\frac{l^5}{5} \\
&+ \Big(\frac{56}{3}\times 7^{n-3}+\frac{4}{3}\Big)\frac{l^4}{4}+(\frac{588}{3}\times 7^{n-3}+2)\frac{l^5}{5}+(\frac{1064}{3}\times 7^{n-3}-\frac{32}{3})\frac{l^6}{6} \\
&+ \Big(\frac{945}{2}\times 7^{n-3}+\frac{9}{2}\Big)\frac{l^6}{6}+\Big(924\times 7^{n-3}+24\Big)\frac{l^7}{7}+\Big(1064\times 7^{n-3}-56\Big)\frac{l^8}{8}
\end{aligned}
$$

$$
\begin{aligned}
I(G) &= \Big|\Big(56\times 7^{n-3}\Big)\frac{l^3}{3}+\Big(\frac{329}{2}\times 7^{n-3}+\frac{1}{2}\Big)\frac{l^4}{4}+\Big(\frac{476}{3}\times 7^{n-3}+\frac{4}{3}\Big)\frac{l^5}{5}\\
&+ \Big(\frac{56}{3}\times 7^{n-3}+\frac{4}{3}\Big)\frac{l^4}{4}+\Big(\frac{588}{3}\times 7^{n-3}+2\Big)\frac{l^5}{5}+\Big(\frac{1064}{3}\times 7^{n-3}-\frac{32}{3}\Big)\frac{l^6}{6}\\
&+ \Big(\frac{945}{2}\times 7^{n-3}+\frac{9}{2}\Big)\frac{l^6}{6}+\Big(924\times 7^{n-3}+24\Big)\frac{l^7}{7}+\Big(1064\times 7^{n-3}-56\Big)\frac{l^8}{8}\Big|_{l=1}\\
I(G) &= \frac{68137}{120}\times 7^{n-3}-\frac{1751}{504}.\\
A(G) &= \delta_l^3 Q_2 J D_l^3 D_q^3(f(l,q))|_{l=1}\\
D_q^3 f(l,q) &= 2^3\Big(28\times 7^{n-3}\Big)l^1q^2+3^3\Big(\frac{329}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^1q^3+4^3\Big(\frac{476}{3}\times 7^{n-3}+\frac{4}{3}\Big)l^1q^4\\
&+ 2^3\Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^2q^2+3^3\Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^2q^3\\
&+ 4^3\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)l^2q^4+3^3\Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^3q^3\\
&+ 4^3\Big(77\times 7^{n-3}+2\Big)l^3q^4+4^3\Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big)l^4q^4\\
JD_l^3D_q^3 f(l,q) &= 2^3\Big(28\times 7^{n-3}\Big)l^3+3^3\Big(\frac{329}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^4+4^3\Big(\frac{476}{3}\times 7^{n-3}+\frac{4}{3}\Big)l^5\\
&+ 2^6\Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^4+6^3\Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^5+8^3\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)l^6\\
&+ 3^6\Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^6+12^3\Big(77\times 7^{n-3}+2\Big)l^7+4^6\Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big)l^8\\
Q_2JD_l^3D_q^3 &= 2^3\times 28\times 7^{n-3}l^1+3^3\Big(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\Big)l^2+4^3\Big(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^3\\
&+ 2^6\Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^2+6^3\Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)l^3+8^3\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)l^4\\
&+ 3^6\Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)l^4+12^3\Big(77\times 7^{n-3}+2\Big)l^5+4^6\Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big)l^6\\
\delta_l^3Q_2JD_l^3D_q^3 &= 2^3\times 28\times 7^{n-3}l^1+3^3\Big(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\Big)\frac{l^2}{2^3}+4^3\Big(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^3}{3^3}\\
&+ 2^6\Big(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^2}{2^3}+6^3\Big(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\Big)\frac{l^3}{3^3}+8^3\Big(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\Big)\frac{l^4}{4^3}\\
&+ 3^6\Big(\frac{105}{2}\times 7^{n-3}+\frac{1}{2}\Big)\frac{l^4}{4^3}+12^3\Big(77\times 7^{n-3}+2\Big)\frac{l^5}{5^3}+4^6\Big(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\Big)\frac{l^6}{6^3}
\end{aligned}
$$

$$
\begin{aligned}
A(G) &= \Big| 2^3 \times 28 \times 7^{n-3} l^1 + 3^3\Big(\frac{329}{6} \times 7^{n-3} + \frac{1}{6}\Big)\frac{l^2}{2^3} + 4^3\Big(\frac{119}{3} \times 7^{n-3} + \frac{1}{3}\Big)\frac{l^3}{3^3} \\
&+ 2^6\Big(\frac{14}{3} \times 7^{n-3} + \frac{1}{3}\Big)\frac{l^2}{2^3} + 6^3\Big(\frac{98}{3} \times 7^{n-3} + \frac{1}{3}\Big)\frac{l^3}{3^3} + 8^3\Big(\frac{133}{3} \times 7^{n-3} - \frac{4}{3}\Big)\frac{l^4}{4^3} \\
&+ 3^6\Big(\frac{105}{2} \times 7^{n-3} + \frac{1}{2}\Big)\frac{l^4}{4^3} + 12^3\Big(77 \times 7^{n-3} + 2\Big)\frac{l^5}{5^3} + 4^6\Big(\frac{133}{2} \times 7^{n-3} - \frac{7}{2}\Big)\frac{l^6}{6^3}\Big|_{l=1} \\
A(G) &= \frac{5287567733}{1296000} \times 7^{n-3} - \frac{47962067}{1296000}.
\end{aligned}
$$

□

4.2.3 Results and Discussion on Entropy of Generalized Sierpinski Graphs

Now we will give our main results on entropy of generalized Sierpinski graphs.

The aim of this section is to compute entropy (Relationship between $I(G,\alpha)$ and $R_\alpha(G)$) for the generalized Sierpinski graphs.

Table 4.3: The edge partition of graph G based on degree of end vertices of each edge.

(d_p, d_j), where, $pj \in E(G)$	Number of edges
$(1,2)$	$28 \times 7^{n-3}$
$(1,3)$	$\frac{329}{6} \times 7^{n-3} + \frac{1}{6}$
$(1,4)$	$\frac{119}{3} \times 7^{n-3} + \frac{1}{3}$
$(2,2)$	$\frac{14}{3} \times 7^{n-3} + \frac{1}{3}$
$(2,3)$	$\frac{98}{3} \times 7^{n-3} + \frac{1}{3}$
$(2,4)$	$\frac{133}{3} \times 7^{n-3} - \frac{4}{3}$
$(3,3)$	$\frac{105}{2} \times 7^{n-3} + \frac{1}{2}$
$(3,4)$	$77 \times 7^{n-3} + 2$
$(4,4)$	$\frac{133}{2} \times 7^{n-3} - \frac{7}{2}$
$Total$	$\frac{2401}{6} \times 7^{n-3} - \frac{7}{6}$

Theorem 4.2.3. *Let G be a generalized Sierpinski graph. Then the entropy of G is*

$$\begin{aligned}
I(G,\alpha) &= \log\Big[28\times 7^{n-3}\times 2^{\alpha}+\left(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\right)3^{\alpha}+\left(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\right)4^{\alpha}\\
&+ +\left(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\right)4^{\alpha}+\left(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\right)6^{\alpha}+\left(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\right)8^{\alpha}\\
&+ \left(\frac{105}{2}\times 7^{n-3}+\frac{1}{3}\right)9^{\alpha}+\left(77\times 7^{n-3}+2\right)12^{\alpha}+\left(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\right)16^{\alpha}\Big]\\
&- \alpha\left(\frac{\beta}{\gamma}\right)
\end{aligned}$$

where,

$$\begin{aligned}
\beta &= 28\times 7^{n-3}\times 2^{\alpha}\log(2^{\alpha})+\left(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\right)3^{\alpha}\log(3^{\alpha})\\
&+ \left(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\right)4^{\alpha}\log(4^{\alpha})+\left(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\right)4^{\alpha}\log(4^{\alpha})\\
&+ \left(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\right)6^{\alpha}\log(6^{\alpha})+\left(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\right)8^{\alpha}\log(8^{\alpha})\\
&+ \left(\frac{105}{2}\times 7^{n-3}+\frac{1}{3}\right)9^{\alpha}\log(9^{\alpha})+\left(77\times 7^{n-3}+2\right)12^{\alpha}\log(12^{\alpha})\\
&+ \left(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\right)16^{\alpha}\log(16^{\alpha})\\
\gamma &= 28\times 7^{n-3}\times 2^{\alpha}+\left(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\right)3^{\alpha}+\left(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\right)4^{\alpha}\\
&+ \left(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\right)4^{\alpha}+\left(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\right)6^{\alpha}+\left(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\right)8^{\alpha}\\
&+ \left(\frac{105}{2}\times 7^{n-3}+\frac{1}{3}\right)9^{\alpha}+\left(77\times 7^{n-3}+2\right)12^{\alpha}+\left(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\right)16^{\alpha}
\end{aligned}$$

and α is a real number.

Proof. The sierpinski graph is shown in Figure 4.4. Let $E_{p,j}$ denotes the number of edges connecting the vertices of degree d_p and d_j. In this graph G the total number of vertices are $\frac{2401}{6}\times 7^{n-3}-\frac{7}{6}$. The number of vertices of degree two three and four are $\frac{343}{6}\times 7^{n-3}-$

$\frac{1}{6}$, $\frac{539}{6} \times 7^{n-3} + \frac{7}{6}$,and $\frac{441}{6} \times 7^{n-3} - \frac{3}{2}$, respectively. The total number of edges of the generalised Sierpinski graph are $\frac{1}{6} \times 7^{n+1} - \frac{7}{6}$. The partite sets of edge rely on the degree of the end vertices of all edge as shown in Table 4.3. Since, the general Randić index is

$$R_\alpha(G) = \sum_{pj \in E(G)} (d_p d_j)^\alpha$$

This infers that

$$\begin{aligned}
R_\alpha(G) &= E_{1,2}\,(1\times 2)^\alpha + E_{1,3}\,(1\times 3)^\alpha + E_{1,4}\,(1\times 4)^\alpha + E_{2,2}\,(2\times 2)^\alpha + E_{2,3}\,(2\times 3)^\alpha \\
&+ E_{2,4}\,(2\times 4)^\alpha + E_{3,3}\,(3\times 3)^\alpha + E_{3,4}\,(3\times 4)^\alpha + E_{4,4}\,(4\times 4)^\alpha \\
R_\alpha(G) &= 28\times 7^{n-3} 2^\alpha + \left(\frac{329}{6} 7^{n-3} + 1/6\right) 3^\alpha + \left(\frac{119}{3}\times 7^{n-3} + \frac{1}{3}\right) 4^\alpha \\
&+ \left(14/3\times 7^{n-3} + \frac{1}{3}\right) 4^\alpha + \left(\frac{98}{3}\times 7^{n-3} + \frac{1}{3}\right) 6^\alpha \\
&+ \left(\frac{133}{3}\times 7^{n-3} - \frac{4}{3}\right) 8^\alpha + \left(\frac{105}{2}\times 7^{n-3} + \frac{1}{3}\right) 9^\alpha \\
&+ \left(77\times 7^{n-3} + 2\right) 12^\alpha + \left(\frac{133}{2}\times 7^{n-3} - \frac{7}{2}\right) 16^\alpha
\end{aligned}$$

The formula for the entropy is given as:

$$I(G,\alpha) = logR_\alpha(G) - \frac{\alpha}{R_\alpha(G)} \sum_{pj \in E(G)} ((d_p \times d_j)^\alpha log(d_p \times d_j))$$

after inserting the value of R_α, we get the following results

$$\begin{aligned}
I(G,\alpha) &= \log\Big[28\times 7^{n-3}\times 2^\alpha + \left(\frac{329}{6}\times 7^{n-3} + \frac{1}{6}\right) 3^\alpha + \left(\frac{119}{3}\times 7^{n-3} + \frac{1}{3}\right) 4^\alpha \\
&+ \left(\frac{14}{3}\times 7^{n-3} + \frac{1}{3}\right) 4^\alpha + \left(\frac{98}{3}\times 7^{n-3} + \frac{1}{3}\right) 6^\alpha + \left(\frac{133}{3}\times 7^{n-3} - \frac{4}{3}\right) 8^\alpha \\
&+ \left(\frac{105}{2}\times 7^{n-3} + \frac{1}{3}\right) 9^\alpha + \left(77\times 7^{n-3} + 2\right) 12^\alpha + \left(\frac{133}{2}\times 7^{n-3} - \frac{7}{2}\right) 16^\alpha\Big] \\
&- \alpha\Big(\frac{\beta}{\gamma}\Big)
\end{aligned}$$

where

$$
\begin{aligned}
\beta &= 28\times 7^{n-3}\times 2^{\alpha}\log(2^{\alpha})+\left(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\right)3^{\alpha}\log(3^{\alpha})\\
&+ \left(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\right)4^{\alpha}\log(4^{\alpha})+\left(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\right)4^{\alpha}\log(4^{\alpha})\\
&+ \left(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\right)6^{\alpha}\log(6^{\alpha})+\left(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\right)8^{\alpha}\log(8^{\alpha})\\
&+ \left(\frac{105}{2}\times 7^{n-3}+\frac{1}{3}\right)9^{\alpha}\log(9^{\alpha})+\left(77\times 7^{n-3}+2\right)12^{\alpha}\log(12^{\alpha})\\
&+ \left(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\right)16^{\alpha}\log(16^{\alpha})\\
\gamma &= 28\times 7^{n-3}\times 2^{\alpha}+\left(\frac{329}{6}\times 7^{n-3}+\frac{1}{6}\right)3^{\alpha}+\left(\frac{119}{3}\times 7^{n-3}+\frac{1}{3}\right)4^{\alpha}\\
&+ \left(\frac{14}{3}\times 7^{n-3}+\frac{1}{3}\right)4^{\alpha}+\left(\frac{98}{3}\times 7^{n-3}+\frac{1}{3}\right)6^{\alpha}+\left(\frac{133}{3}\times 7^{n-3}-\frac{4}{3}\right)8^{\alpha}\\
&+ \left(\frac{105}{2}\times 7^{n-3}+\frac{1}{3}\right)9^{\alpha}+\left(77\times 7^{n-3}+2\right)12^{\alpha}+\left(\frac{133}{2}\times 7^{n-3}-\frac{7}{2}\right)16^{\alpha}
\end{aligned}
$$

and α is a real number. □

4.3 Topological Indices of the Para-line Graphs of Some Chemical Structures

Ranjini (2011) designed the independent relations for the index which is presented by Schultz, they investigated subdivision of different graphs like helm, ladder, tadpole and wheel under the surveillance of Schultz index [83]. They also investigated the para-line graph of ladder, tadpole and wheel under Zagrib index in [82]. Su and Xu evaluate two indices of para-line graph of ladder, tadpole and wheel graphs, named ,the general sum-connectivity index and co-index in 2015 [89]. In [75], Nadeem et.al. computed ABC_4 and GA_5 index of the para-line graphs of the tadpole, wheel and ladder graphs. They examined some indices like R_α, M_α, χ_α, ABC, GA, ABC_4 and GA_5 indices of the para-line graph of lattice in $2D-$ nanotube and nanotorus $TUC_4C_8[p,q]$ in [76].

4.3.1 Topological Indices of Triangular Benzenoid

The molecular graph of triangular benzenoid is shown in Figure 4.5 and is denoted by T_n. There are n^2+4n+1 vertices and $\frac{3(n^2+3n)}{2}$ edges in T_n. In order to calculate the number of edges of the line graph, the following lemma is important for us.

Lemma 4.3.1. *[94] Let G be a graph. Then* $|E(L(G))| = \sum_{u\in V(G)} \frac{d_u^2}{2} - |E(G)|$ *where* $L(G)$ *is the line graph of G.*

Theorem 4.3.2. *Let* G^* *be the para-line graph of* T_n*. Then*

1. $R_\alpha(G^*) = 4^\alpha(3n+9) + 6^{\alpha+1}(n-1) + \frac{3}{2}9^\alpha(3n+4)(n-1)$.

2. $\chi_\alpha(G^*) = 4^\alpha(3n+9) + 5^\alpha(6n-6) + \frac{3}{2}6^\alpha(3n+4)(n-1)$.

3. $ABC(G^*) = 3n^2 + \left(\frac{9\sqrt{2}}{2}+1\right)n + \frac{3\sqrt{2}}{2} - 4$.

4. $GA(G^*) = \frac{9}{2}n^2 + \left(\frac{12\sqrt{6}}{5}+\frac{9}{2}\right)n + 3 - \frac{12\sqrt{6}}{5}$

Proof. The subdivision graph $S(T_n)$ contains $3n^2+9n$ edges and $\frac{1}{2}(5n^2+17n+2)$ vertices among which $\frac{1}{2}(3n^2+15n+6)$ vertices are of degree 2 and remaining n^2+n-2 vertices are of degree 3. Hence by Lemma 4.3.1 the total number of edges of G^* are $\frac{1}{2}(9n^2+21n-6)$. The edge set $E(G^*)$ divides into three edge partitions based on degrees of the end vertices, i.e. $E(G^*) = E_1(G^*) \cup E_2(G^*) \cup E_3(G^*)$. The edge partition $E_1(G^*)$ contains $3n+9$ edges uv,where $d_u = d_v = 2$, the edge partition $E_2(G^*)$ contains $6n-6$ edges uv, where $d_u = 2$ and $d_v = 3$, and the edge partition $E_3(G^*)$ contains $\frac{3}{2}(3n+4)(n-1)$ edges uv, where $d_u = d_v = 3$. From Formulas 3.2.1, 3.2.3, 3.2.4 and 3.2.5, we obtain the required results. □

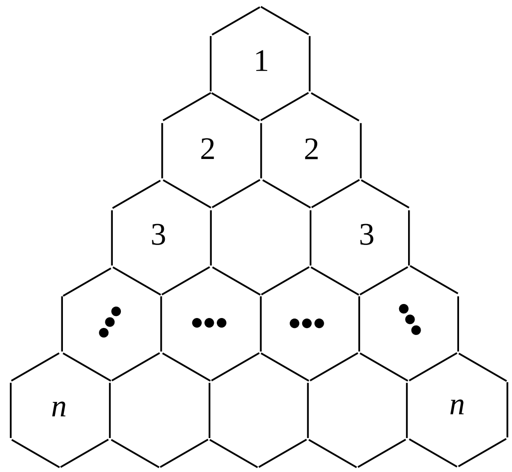

Figure 4.5: Triangular benzenoid.

Theorem 4.3.3. *Let G^* be the para-line graph of T_n. Then*

$$M_\alpha(G^*) = 2^{\alpha+1}(3n+3) + 3^{\alpha+1}(n^2+n-2)$$

.

Proof. The graph G^* is shown in Figure 4.6. In G^* there are total $3(n^2+3n)$ vertices among which $6(n+1)$ vertices are of degree 2 and $3(n^2+n-2)$ vertices are of degree 3. Hence we get $M_\alpha(G^*)$ by using Formula 3.2.2. $\square$

Theorem 4.3.4. *Let G^* be the para-line graph of T_n. Then*

1.

$$\begin{aligned} ABC_4(G^*) &= 2n^2 + \left(\frac{6\sqrt{2}}{5} + \frac{3\sqrt{110}}{10} + \frac{3\sqrt{14}}{8} + \frac{\sqrt{30}}{2} - \frac{10}{3}\right)n + \frac{9\sqrt{6}}{4} + \frac{3\sqrt{35}}{5} \\ &- \frac{12\sqrt{2}}{5} - \frac{3\sqrt{110}}{10} - \frac{3\sqrt{14}}{8} - \frac{\sqrt{30}}{2} + \frac{4}{3}. \end{aligned}$$

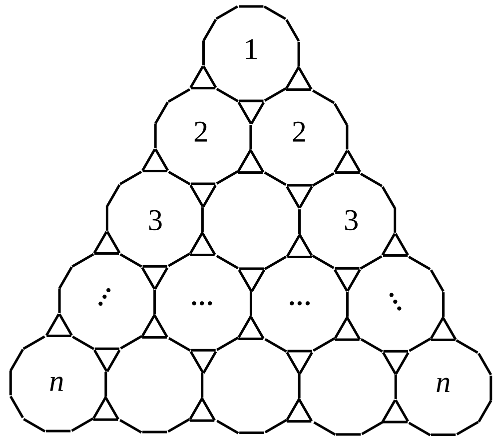

Figure 4.6: Para line graph of triangular benzenoid.

2.

$$GA_5(G^*) = \frac{9}{2}n^2 + \left(\frac{24\sqrt{10}}{13} - \frac{3}{2} + \frac{72\sqrt{2}}{17}\right)n + \frac{8\sqrt{5}}{3} - \frac{24\sqrt{10}}{13} - \frac{72\sqrt{2}}{17} + 3.$$

Proof. If we consider an edge partition based on degree sum of neighbors of end vertices then the edge set $E(G^*)$ can be divided into seven edge partitions $E_i(G^*)$, $i = 4, 5, \ldots, 10$, i.e. $E(G^*) = \cup_{i=4}^{10} E_i(G^*)$. The edge partition $E_4(G^*)$ contains 9 edges uv, where $S_u = S_v = 4$, the edge partition $E_5(G^*)$ contains 6 edges uv, where $S_u = 4$ and $S_v = 5$, the edge partition $E_6(G^*)$ contains $3n-6$ edges uv, where $S_u = S_v = 5$, the edge partition $E_7(G^*)$ contains $6n-6$ edges uv, where $S_u = 5$ and $S_v = 8$, the edge partition $E_8(G^*)$ contains $3n-3$ edges uv, where $S_u = S_v = 8$, the edge partition $E_9(G^*)$ contains $6n-6$ edges uv, where $S_u = 8$ and $S_v = 9$, and the edge partition $E_{10}(G^*)$ contains $\frac{3}{2}(n-1)(3n-2)$ edges uv, where $S_u = S_v = 9$. From Formulas 3.2.6 and 3.2.7, we obtain the required results. □

4.3.2 Topological Indices of the Para-line Graph of Linear Parallelogram Benzenoid

The molecular graph of linear parallelogram benzenoid is shown in Figure4.7 and is denoted by $P_{m,n}$. There are $2mn + 2m + 2n$ vertices and $3mn + 2n + 2m - 1$ edges in $P_{m,n}$.

Theorem 4.3.5. *Let G^* be the para-line graph of $P_{m,n}$. Then*

1. $R_\alpha(G^*) = 4^\alpha(2m+2n+8) + 6^\alpha(4m+4n-8) + 9^\alpha(9mn-2m-2n-5)$.

2. $\chi_\alpha(G^*) = 4^\alpha(2m+2n+8) + 5^\alpha(4m+4n-8) + 6^\alpha(9mn-2m-2n-5)$.

3. $ABC(G^*) = \left(6m + 3\sqrt{2} - \frac{4}{3}\right)n + \left(3\sqrt{2} - \frac{4}{3}\right)m - \frac{10}{3}$.

4. $GA(G^*) = \left(9m + \frac{8\sqrt{6}}{5}\right)n + \frac{8\sqrt{6}}{5}m + 3 - \frac{16\sqrt{6}}{5}$.

Proof. The subdivision graph $S(P_{m,n})$ of $P_{m,n}$ contains $6mn+4m+4n-2$ edges and $5mn+4m+4n-1$ vertices among which $3mn+4m+4n+1$ vertices are of degree 2 and remaining $2mn-2$ vertices are of degree 3. Hence by Lemma 4.3.1 the total number of edges of G^* are $9mn+4m+4n-5$. The edge set $E(G^*)$ divides into three edge edge sets based on degrees of the end vertices, i.e. $E(G^*) = E_1(G^*) \cup E_2(G^*) \cup E_3(G^*)$. The edge set $E_1(G^*)$ contains $2m+2n+8$ edges uv, where $d_u = d_v = 2$, the edge set $E_2(G^*)$ contains $4m+4n-8$ edges uv, where $d_u = 2$ and $d_v = 3$, and the edge set $E_3(G^*)$ contains $9mn-2m-2n-5$ edges uv, where $d_u = d_v = 3$. From Formulas 3.2.1, 3.2.3, 3.2.4 and 3.2.5, we obtain the required results. $\square$

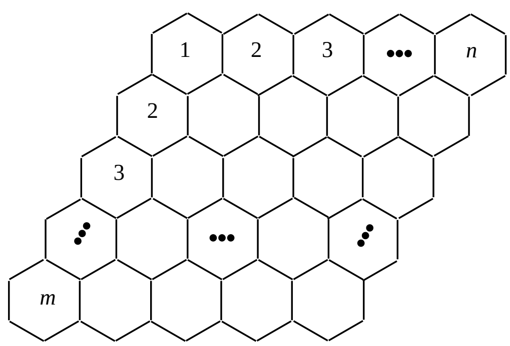

Figure 4.7: Linear parallelogram benzenoid.

Theorem 4.3.6. *Let G^* be the para-line graph of $P_{m,n}$. Then*

$$M_\alpha(G^*) = 2^{\alpha+2}(m+n+1) + 3^{\alpha+1}(2mn-2)$$

.

Proof. The graph G^* is shown in Figure 4.8. In G^* there are total $6mn+4m+4n-2$ vertices among which $4m+4n+4$ vertices are of degree 2 and $6mn-6$ vertices are of degree 3. Hence we get $M_\alpha(G^*)$ by using Formula 3.2.2. □

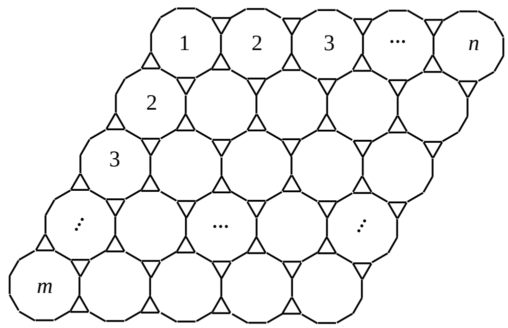

Figure 4.8: Para-line graph of linear parallelogram benzenoid.

Theorem 4.3.7. *Let G^* be the para-line graph of $P_{m,n}$. Then*

$$\begin{aligned}
ABC_4(G^*) &= \left(4m+\frac{4\sqrt{2}}{5}+\frac{\sqrt{14}}{4}+\frac{\sqrt{110}}{5}+\frac{\sqrt{30}}{3}-\frac{32}{9}\right)n \\
&+ \left(\frac{4\sqrt{2}}{5}+\frac{\sqrt{14}}{4}+\frac{\sqrt{110}}{5}-\frac{32}{9}+\frac{\sqrt{30}}{3}\right)m-\frac{\sqrt{14}}{2}+2\sqrt{6} \\
&+ \frac{4\sqrt{35}}{5}-\frac{16\sqrt{2}}{5}-\frac{2\sqrt{110}}{5}-\frac{2\sqrt{30}}{3}+\frac{28}{9}. \\
GA_5(G^*) &= \left(9m+\frac{48\sqrt{2}}{17}-4+\frac{16\sqrt{10}}{13}\right)n+\left(\frac{16\sqrt{10}}{13}-4+\frac{48\sqrt{2}}{17}\right)m+3 \\
&+ \frac{32\sqrt{5}}{9}-\frac{96\sqrt{2}}{17}-\frac{32\sqrt{10}}{13}.
\end{aligned}$$

Proof. If we consider an edge partition based on degree sum of neighbors of end vertices, then the edge set $E(G^*)$ can be divided into seven edge partite sets $E_i(G^*)$, $i=4,5,\ldots,10$, i.e. $E(G^*)=\cup_{i=4}^{10}E_i(G^*)$.The edge partition $E_4(G^*)$ contains 8 edges uv, where $S_u=S_v=4$, the edge partition $E_5(G^*)$ contains 8 edges uv, where $S_u=4$ and $S_v=5$, the edge partition $E_6(G^*)$ contains $2m+2n-8$ edges uv, where $S_u=S_v=5$, the edge partition

$E_7(G^*)$ contains $4m+4n-8$ edges uv, where $S_u=5$ and $S_v=8$, the edge partition $E_8(G^*)$ contains $2m+2n-4$ edges uv, where $S_u=S_v=8$, the edge partition $E_9(G^*)$ contains $4m+4n-8$ edges uv, where $S_u=8$ and $S_v=9$, and the edge partition $E_{10}(G^*)$ contains $9mn-8m-8n+7$ edges uv, where $S_u=S_v=9$. From Formulas 3.2.6 and 3.2.7, we obtain the required results. □

4.3.3 Topological Indices of Para-line Graph of Linear Anthracene

The molecular graph of linear Anthracene is shown in Figure 4.9 and it is denoted by T_s. There are $14s$ vertices and $18s-2$ edges in T_s.

Table 4.4: Distribution of edges with respect to degree of end vertices of every edge

Sr. No.	$E_{(d_p,d_q)}$	Number of edges
1	$E_{(2,2)}$	$6s+10$
2	$E_{(2,3)}$	$12s-4$
3	$E_{(3,3)}$	$30s-16$

Table 4.5: Distribution of edges w.r.t neighbour sum of every vertex of Anthracene

Sr. No.	$S_{(p,q)}$	Number of edges
1	$S_{(4,4)}$	10
2	$S_{(4,5)}$	4
3	$S_{(5,5)}$	$6s-4$
4	$S_{(5,8)}$	$12s-4$
5	$S_{(8,8)}$	$4s$
6	$S_{(8,9)}$	$16s-8$
7	$S_{(9,9)}$	$10s-8$

Theorem 4.3.8. *Let G^* be the para-line graph of T_s. Then*

$$M_\alpha(G^*) = (12s+8)2^{\alpha+2} + (24s-12)3^{\alpha+1}$$

Proof. The graph G^* is shown in Figure 4.10. In G^*, the total count of the vertices is $48s-10$ which is the sum of degree 2 and degree 2 vertices $8+12s$, $24s-12$, respectively.

As

$$M_\alpha(G^*) = (12s+8)2^{\alpha+2} + 3^{\alpha+1}(24s-12)$$

. $\square$

Theorem 4.3.9. *Let G^* be the para-line graph of T_s. Then*

1. $R_\alpha(G^*) = (6s+10)4^\alpha + (12s-4)6^\alpha + (30s-16)9^\alpha$.

2. $\chi_\alpha(G^*) = (6s+10)4^\alpha + (12s-4)5^\alpha + (30s-16)6^\alpha$.

3. $ABC(G^*) = \left(9\sqrt{2}+20\right)s + 3\sqrt{2} - \frac{32}{3}$.

4. $GA(G^*) = \left(36 + \frac{24}{5}\sqrt{6}\right)s - 6 - 8/5\sqrt{6}$.

Proof. The total count of edges of G^* is $74s-10$. The set of edges of G^* is represented as $E(G^*)$ which is disjoint union of three edge sets based on degrees of the end vertices, i.e. $E(G^*) = E_1(G^*) \cup E_2(G^*) \cup E_3(G^*)$. The first set $E_1(G^*)$ contains the edges of this type $E_{(2,2)} = 6s+10$ and the second set $E_2(G^*)$ holds the edges $E_{(2,3)} = 12s-4$ and the third set $E_3(G^*)$ includes the edges $E_{(3,3)} = 30s-16$, where $(2,2)$, $(2,3)$ and $(3,3)$ represents the degree of end vertices, respectively. From Formulas (3.2.1), (3.2.3), (3.2.4) and (3.2.5) and using Table 4.4, we get the desired results. $\square$

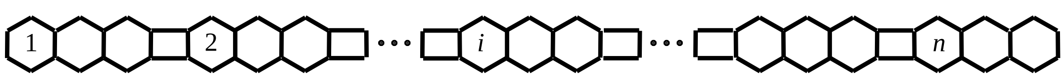

Figure 4.9: Linear Anthracene.

Theorem 4.3.10. *Let G^* be the para-line graph of T_s. Then*

$$\begin{aligned} ABC_4(G^*) &= \left(3/5\sqrt{110}+\frac{12}{5}\sqrt{2}+4/3\sqrt{30}+\frac{40}{9}+1/2\sqrt{14}\right)s+5/2\sqrt{6} \\ &+ 2/5\sqrt{35}-8/5\sqrt{2}-2/3\sqrt{30}-1/5\sqrt{110}-\frac{32}{9}. \\ GA_5(G^*) &= \left(20+\frac{48}{13}\sqrt{10}+\frac{192}{17}\sqrt{2}\right)s-2+\frac{16}{9}\sqrt{5}-\frac{16}{13}\sqrt{10}-\frac{96}{17}\sqrt{2}. \end{aligned}$$

Proof. Suppose the graph of Anthracene contains three hexagon connected with a square expanded vertically and horizontally. Let the edge $e_{(p,q)}$ represents the count of edges connecting the vertices of degree d_p and d_q. The graph of Anthracene holds the following edges shown in the Table 4.5:

$$ABC_4(G)=\sum_{pq\in E(G)}\sqrt{\frac{S_p+S_q-2}{S_pS_q}}$$

$$\begin{aligned} ABC_4(G^*) &= S_{(4,4)}\times\sqrt{\frac{4+4-2}{4\times 4}}+S_{(4,5)}\times\sqrt{\frac{4+5-2}{4\times 5}}+S_{(5,5)}\times\sqrt{\frac{5+5-2}{5\times 5}} \\ &+ S_{(5,8)}\times\sqrt{\frac{5+8-2}{5\times 8}}+S_{(8,8)}\times\sqrt{\frac{8+8-2}{8\times 8}}+S_{(8,9)}\times\sqrt{\frac{8+9-2}{8\times 9}} \\ &+ S_{(9,9)}\times\sqrt{\frac{9+9-2}{9\times 9}}. \end{aligned}$$

By using Table 4.5, we obtain the required results.

$$\begin{aligned} ABC_4(G^*) &= \left(3/5\sqrt{110}+\frac{12}{5}\sqrt{2}+4/3\sqrt{30}+\frac{40}{9}+1/2\sqrt{14}\right)s+5/2\sqrt{6}+2/5\sqrt{35} \\ &- 8/5\sqrt{2}-2/3\sqrt{30}-1/5\sqrt{110}-\frac{32}{9}. \end{aligned}$$

Similarly,

$$GA_5(G)=\sum_{pq\in E(G)}\frac{2\sqrt{S_pS_q}}{S_p+S_q}$$

$$
\begin{aligned}
GA_5(G) &= S_{(4,4)}\times 2\sqrt{\frac{4\times 4}{4+4}}+S_{(4,5)}\times 2\sqrt{\frac{4\times 5}{4+5}}+S_{(5,5)}\times 2\sqrt{\frac{5\times 5}{5+5}}\\
&+ S_{(5,8)}\times 2\sqrt{\frac{5\times 8}{5+8}}+S_{(8,8)}\times 2\sqrt{\frac{8\times 8}{8+8}}+S_{(8,9)}\times 2\sqrt{\frac{8\times 9}{8+9}}\\
&+ S_{(9,9)}\times 2\sqrt{\frac{9\times 9}{9+9}}.
\end{aligned}
$$

After simplification, we obtained the required result

$$
GA_5(G^*) = \left(20+\frac{48}{13}\sqrt{10}+\frac{192}{17}\sqrt{2}\right)s-2+\frac{16}{9}\sqrt{5}-\frac{16}{13}\sqrt{10}-\frac{96}{17}\sqrt{2}.
$$

□

Theorem 4.3.11. *Let G^* be the para-line graph of T_s. Then*

1. $HM(G^*) = 1404s - 636.$
2. $PM_1(G^*) = 4^{6s+10}5^{12s-4}6^{30s-16}.$
3. $PM_2(G^*) = 4^{6s+10}6^{12s-4}9^{30s-16}.$

Proof. Let G^* be the para-line graph of linear Anthracene. The edge set $E(G^*)$ on the basis of degree of end vertices is represented as the union of three partite sets i.e. $E(G^*) = E_1(G^*)\cup E_2(G^*)\cup E_3(G^*)$. The cardinality of first set $E_1(G^*)$, second set $E_2(G^*)$ and third set $E_3(G^*)$ is denoted as $E_{(2,2)}$, $E_{(2,3)}$ and $E_{(3,3)}$, respectively. The first disjoint edge set holds $E_{(2,2)} = 6s+10$ edges, the second disjoint set holds $E_{(2,3)} = 12s-4$ edges and the third disjoint set holds $E_{(3,3)} = 30s-16$ edges. Since,

By using Table 4.4, we get the following results.

$$
\begin{aligned}
\text{“}HM(G^*) &= \sum_{pq\in E(G)} \left(d_p+d_q\right)^2\\
HM(G^*) &= \sum_{pq\in E_1(G)} \left[d_p+d_q\right]^2+\sum_{pq\in E_2(G)} \left[d_p+d_q\right]^2+\sum_{pq\in E_3(G)} \left[d_p+d_q\right]^2\text{”}
\end{aligned}
$$

$$
\begin{aligned}
\text{“}HM(G^*) &= 16\times E_{(2,2)}+25\times E_{(2,3)}+36\times E_{(3,3)}\\
&= 16(6s+10)+25(12s-4)+36(30s-16)\\
HM(G^*) &= 1404\,s-636.\\
PM_1(G^*) &= \prod_{pq\in E(G)}(d_p+d_q)\\
PM_1(G^*) &= \prod_{pq\in E_1(G)}(d_p+d_q)\times\prod_{pq\in E_2(G)}(d_p+d_q)\times\prod_{pq\in E_3(G)}(d_p+d_q)\text{”}\\
\text{“}PM_1(G^*) &= 4^{E_{(2,2)}}\times 5^{E_{(2,3)}}\times 6^{E_{(3,3)}}\\
&= 4^{6s+10}\times 5^{12s-4}\times 6^{30s-16}\\
PM_1(G^*) &= 4^{6s+10}\times 5^{12s-4}\times 6^{30s-16}.\\
PM_2(G^*) &= \prod_{pq\in E(G)}(d_p\times d_q)\\
PM_2(G^*) &= \prod_{pq\in E_1(G)}(d_p\times d_q)\times\prod_{pq\in E_2(G)}(d_p\times d_q)\times\prod_{pq\in E_3(G)}(d_p\times d_q)\\
PM_2(G^*) &= 4^{E_{(2,2)}}\times 6^{E_{(2,3)}}\times 9^{E_{(3,3)}}\\
&= 4^{6s+10}\times 6^{12s-4}\times 9^{30s-16}.\text{”}
\end{aligned}
$$

□

Theorem 4.3.12. *Let G^* be the para-line graph of T_s. Then*

1. $M_1(G^*,a)=(6\,s+10)\,a^4+(12\,s-4)\,a^5+(30\,s-16)\,a^6.$

2. $M_2(G^*,a)=(6\,s+10)\,a^4+(12\,s-4)\,a^6+(30\,s-16)\,a^9.$

Proof. By using Table 4.4, we get

$$
\begin{aligned}
M_1(G^*,a) &= \sum_{pq\in E(G)} a^{(d_p+d_q)} \\
M_1(G^*,a) &= \sum_{pq\in E_1(G)} a^{(d_p+d_q)} + \sum_{pq\in E_2(G)} a^{(d_p+d_q)} + \sum_{pq\in E_3(G)} a^{(d_p+d_q)} \\
&= \sum_{pq\in E_1(G)} a^4 + \sum_{pq\in E_2(G)} a^5 + \sum_{pq\in E_3(G)} a^6 \\
&= E_{(2,2)} \times a^4 + E_{(2,3)} \times a^5 + E_{(3,3)} \times a^6 \\
&= (6s+10)\,a^4 + (12s-4)\,a^5 + (30s-16)\,a^6. \\
M_2(G^*,a) &= \sum_{pq\in E(G)} a^{(d_p\times d_q)} \\
M_2(G^*,a) &= \sum_{pq\in E_1(G)} a^{(d_p\times d_q)} + \sum_{pq\in E_2(G)} a^{(d_p\times d_q)} + \sum_{pq\in E_3(G)} a^{(d_p\times d_q)} \\
&= \sum_{pq\in E_1(G)} a^4 + \sum_{pq\in E_2(G)} a^6 + \sum_{pq\in E_3(G)} a^9 \\
&= E_{2,2} \times a^4 + E_{2,3} \times a^6 + E_{3,3} \times a^9 \\
&= (6s+10)\,a^4 + (12s-4)\,a^6 + (30s-16)\,a^9.
\end{aligned}
$$

Hence proved. □

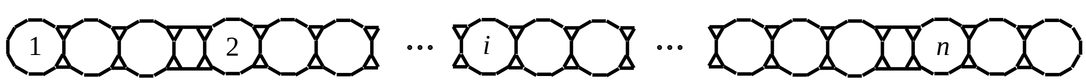

Figure 4.10: Para-line graph of linear anthracene.

4.3.4 Topological Indices of Para-line Graph of Multiple Anthracene

The molecular graph of multiple Anthracene is shown in Figure 4.11 and it is denoted by $T_{r,s}$. There are $22rs$ vertices and $33rs-2r-5s$ edges in $T_{r,s}$.

Table 4.6: Edge distribution of multiple Anthracene w.r.t. degree of end vertices

Sr. No.	$E_{(d_p,d_q)}$	Count of edges
1	$E_{(2,2)}$	$6r+6s+4$
2	$E_{(2,3)}$	$4r+12s-8$
3	$E_{(3,3)}$	$63rs-20r-33s+4$

Table 4.7: The edge partition of the graph of multiple Anthracene

Sr. No.	$S_{(p,q)}$	Count of edges
1	$S_{(4,4)}$	$2r+8$
2	$S_{(4,5)}$	$4r$
3	$S_{(5,5)}$	$6s-4$
4	$S_{(5,8)}$	$12s-4r-8$
5	$S_{(8,8)}$	$4s$
6	$S_{(8,9)}$	$8r+16s-16$
7	$S_{(9,9)}$	$63rs-28r-53s+20$

Theorem 4.3.13. *Let G^* be the para-line graph of $T_{r,s}$. Then*

$$M_\alpha(G^*) = (2r+3s)2^{\alpha+2} + 3^{\alpha+1}(14rs-4r-6s)$$

.

Proof. The graph G^* is shown in Figure 4.12. In G^*, the total count of the vertices is $63rs-10r-15s$ which is the sum of $8r+12s$ (vertices of degree 2) and $42rs-12r-18s$ (vertices of degree 3). Hence proved. □

Theorem 4.3.14. *Let G^* be the para-line graph of $T_{r,s}$. Then*

1. $R_\alpha(G^*) = (6s+6r+4)4^\alpha + (4r+12s-8)6^\alpha + (63rs-20r-33s+4)9^\alpha$.

2. $\chi_\alpha(G^*) = (6s+6r+4)4^\alpha + (4r+12s-8)5^\alpha + (63rs-20r-33s+4)6^\alpha$.

Proof. The total number of edges and vertices of subdivision graph of multiple Anthracene $S(T_{r,s})$ are $63rs-10r-15s$ and $198rs-20r-50$, respectively. The vertices are sub divided in the following way: The count of vertices of degree two is $8r+12s$ and the count of vertices of degree three is $42rs-12r-18s$. The total count of edges of G^* are $63rs-10r-15s$. The set of edges $E(G^*)$ bifurcates into three edge categories based on degrees of the end vertices,i.e. $E(G^*) = E_1(G^*) \cup E_2(G^*) \cup E_3(G^*)$. The edge partite set $E_1(G^*)$ holds $E_{(2,2)} = 6r+6s+4$ edges, where $E_{(2,2)}$ represents the edge whose both vertices have degree 2. The edge partite set $E_2(G^*)$ holds $E_{(2,3)} = 4r+12s-8$ edges, where $E_{(2,3)}$ represents the edge whose one vertex has degree 2 and second vertex has 3 and the edge partite set $E_3(G^*)$ holds $E_{(3,3)} = 63rs-20r-33s+4$ edges, where $E_{(3,3)}$ represents the edge whose both vertex has degree 3. From Formulas (3.2.1), (3.2.3), (3.2.4) and (3.2.5), Hence desired result is obtained. □

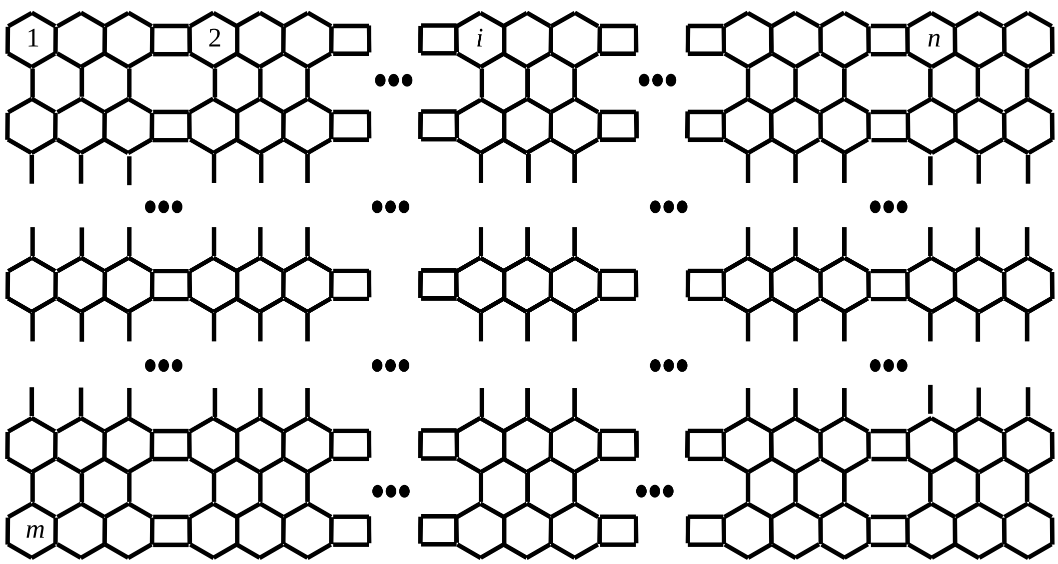

Figure 4.11: Multiple Anthracene.

Theorem 4.3.15. *Let G^* be the para-line graph of $T_{r,s}$. Then*

$$\begin{aligned}
ABC_4(G^*) &= \left(28\,r + 1/2\,\sqrt{14} + \frac{12}{5}\,\sqrt{2} + 3/5\,\sqrt{110} + 4/3\,\sqrt{30} - \frac{212}{9}\right)s \\
&+ \left(1/2\,\sqrt{6} + 1/5\,\sqrt{110} + 2/5\,\sqrt{35} - \frac{112}{9} + 2/3\,\sqrt{30}\right)r \\
&+ 2\,\sqrt{6} - 8/5\,\sqrt{2} - 2/5\,\sqrt{110} - 4/3\,\sqrt{30} + \frac{80}{9}. \\
GA_5(G^*) &= \left(\frac{80}{13}\,\sqrt{10} + 99\,r + \frac{288}{17}\,\sqrt{2} - 69\right)s \\
&+ \left(-26 + \frac{16}{13}\,\sqrt{10} + \frac{16}{9}\,\sqrt{5} + \frac{96}{17}\,\sqrt{2}\right)r - \frac{192}{17}\,\sqrt{2} - \frac{32}{13}\,\sqrt{10} + 24.
\end{aligned}$$

Proof. Let the degree sum of neighbours of end vertices p and q is represented as $S_(p,q)$. Suppose the set of edges $E(G^*)$ can be distributed into seven disjoint edge sets $E_i(G^*)$, $i = 4,5,\ldots,10$, i.e. $E(G^*) = \cup_{i=4}^{10} E_i(G^*)$. The edge partite set $E_4(G^*)$ contains $S_{(p,q)} = (4,4) = 2r+8$ edges, the edge partite set $E_5(G^*)$ contains $(S_(p,q) = (4,5) = 4r$ edges, the edge partite set $E_6(G^*)$ contains $S_(p,q) = (5,5) = 6s-4$ edges, the edge partite set $E_7(G^*)$ contains $S_{(p,q)} = (5,8) = 12s+4r-8$ edges, the edge partite set $E_8(G^*)$ contains $S_{(p,q)} = (8,8) = 4s$ edges, the edge partite set $E_9(G^*)$ contains $S_{(p,q)} = (8,9) = 8r+16s-16$ edges, and the edge partite set $E_{10}(G^*)$ contains $S_{(p,q)} = (9,9) = 63rs-28r-53s+20$ edges. From Formulas (3.2.6) and (3.2.7), the required result is obtained. $\square$

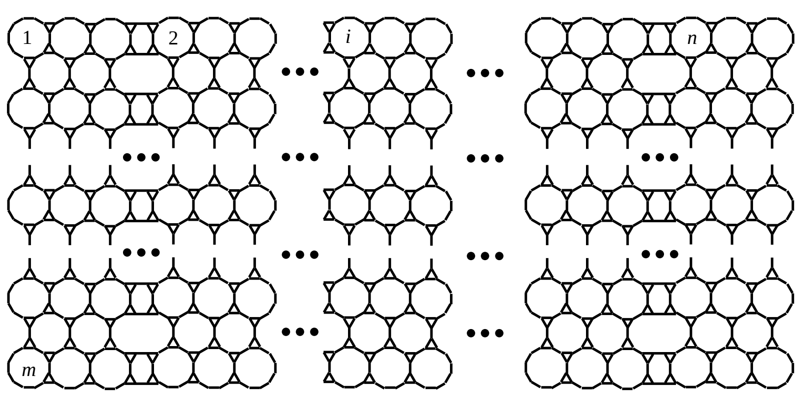

Figure 4.12: Para-line graph of multiple Anthracene.

We find the following indices $HM(G)$, $PM_1(G)$, $PM_2(G)$, Zagreb polynomials $M_1(G,a)$, $M_2(G,a)$ by computation for chemical structures of multiple-Anthracene.

Theorem 4.3.16. *Let G^* be the para-line graph of $T_{r,s}$.Then*

1. $HM(G^*) = 2268\,rs - 596\,r - 864\,s - 40$.
2. $PM_1(G^*) = 4^{6s+6r+4}5^{4r+12s-8}6^{63rs-20r-33s+4}$.
3. $PM_2(G^*) = 4^{6s+6r+4}6^{4r+12s-8}9^{63rs-20r-33s+4}$.
4. $M_1(G^*,a) = (6s+6r+4)\,a^4 + (4r+12s-8)\,a^5 + (63rs-20r-33s+4)\,a^6$.
5. $M_2(G^*,a) = (6s+6r+4)\,a^4 + (4r+12s-8)\,a^6 + (63rs-20r-33s+4)\,a^9$.

Proof. Let G^* be the para-line graph of multiple Anthracene. The edge set $E(G^*)$ on the basis of degree of end vertices is represented as the union of the three partite sets i.e. $E(G^*) = E_1(G^*) \cup E_2(G^*) \cup E_3(G^*)$. The cardinality of first set $E_1(G^*)$, second set $E_2(G^*)$ and third set $E_3(G^*)$ is denoted as $|E_{(2,2)}|$, $|E_{(2,3)}|$ and $|E_{(3,3)}|$, respectively. The first disjoint edge set holds $E_{(2,2)} = 8r + 12s$ edges, the second disjoint set holds $E_{(2,3)} = 42rs + 12r - 18s$ edges and the third disjoint set holds $E_{(3,3)} = 63rs - 20r - 33s + 4$ edges. Since, By using Table 4.4, we get the following results.

$$
\begin{aligned}
\text{``}HM(G^*) &= \sum_{pq\in E(G)} \left(d_p + d_q\right)^2 \\
HM(G^*) &= \sum_{pq\in E_1(G)} \left[d_p + d_q\right]^2 + \sum_{pq\in E_2(G)} \left[d_p + d_q\right]^2 + \sum_{pq\in E_3(G)} \left[d_p + d_q\right]^2 \\
HM(G^*) &= 16 \times E_{(2,2)} + 25 \times E_{(2,3)} + 36 \times E_{(3,3)} \\
&= 16(6s + 6r + 4) + 25(12s + 4r - 8) + 36(63rs - 20r - 33s + 4). \\
HM(G^*) &= 2268\,rs - 596\,r - 864\,s - 40.
\end{aligned}
$$

$$
\begin{aligned}
PM_1(G^*) &= \prod_{pq\in E(G)} (d_p+d_q) \\
PM_1(G^*) &= \prod_{pq\in E_1(G)} (d_p+d_q) \times \prod_{pq\in E_2(G)} (d_p+d_q) \times \prod_{pq\in E_3(G)} (d_p+d_q)\text{''} \\
PM_1(G^*) &= 4^{E_{(2,2)}} \times 5^{E_{(2,3)}} \times 6^{E_{(3,3)}} \\
&= 4^{6s+6r+4} \times 5^{12s+4r-8} \times 6^{63rs-20r-33s+4}.
\end{aligned}
$$

$$
\begin{aligned}
\text{``}PM_2(G^*) &= \prod_{pq\in E(G)} (d_p \times d_q) \\
PM_2(G^*) &= \prod_{pq\in E_1(G)} (d_p \times d_q) \times \prod_{pq\in E_2(G)} (d_p \times d_q) \times \prod_{pq\in E_3(G)} (d_p \times d_q)\text{''} \\
PM_2(G^*) &= 4^{e_{(2,2)}} \times 6^{e_{(2,3)}} \times 9^{e_{(3,3)}} \\
&= 4^{6s+6r+4} \times 6^{12s+4r-8} \times 9^{63rs-20r-33s+4}.
\end{aligned}
$$

$$
\begin{aligned}
M_1(G^*,a) &= \sum_{pq\in E(G)} a^{(d_p+d_q)} \\
M_1(G^*,a) &= \sum_{pq\in E_1(G)} a^{(d_p+d_q)} + \sum_{pq\in E_2(G)} a^{(d_p+d_q)} + \sum_{pq\in E_3(G)} a^{(d_p+d_q)} \\
&= \sum_{pq\in E_1(G)} a^4 + \sum_{pq\in E_2(G)} a^5 + \sum_{pq\in E_3(G)} a^6 \\
&= E_{(2,2)} \times a^4 + E_{(2,3)} \times a^5 + E_{(3,3)} \times a^6 \\
&= (6s+6r+4)\,a^4 + (4r+12s-8)\,a^5 + (63rs-20r-33s+4)\,a^6.
\end{aligned}
$$

$$
\begin{aligned}
M_2(G,a) &= \sum_{pq\in E(G)} a^{(d_p\times d_q)} \\
M_2(G,a) &= \sum_{pq\in E_1(G)} a^{(d_p\times d_q)} + \sum_{pq\in E_2(G)} a^{(d_p\times d_q)} + \sum_{pq\in E_3(G)} a^{(d_p\times d_q)} \\
&= \sum_{pq\in E_1(G)} a^4 + \sum_{pq\in E_2(G)} a^6 + \sum_{pq\in E_3(G)} a^9 \\
&= E_{(2,2)} \times a^4 + E_{(2,3)} a^6 + E_{(3,3)} \times a^9 \\
&= (6s+6r+4)\,a^4 + (4r+12s-8)\,a^6 + (63rs-20r-33s+4)\,a^9.
\end{aligned}
$$

Which completes the proof. $\square$

4.3.5 Topological Indices of the Para-line Graph of Linear Pentacene

In this sub section, we have figured R_α, M_α, χ_α, ABC, GA, ABC_4, GA_5, PM_1, PM_2, $M_1(G,x)$, and $M_1(G,x)$ indices of the para-line graph of linear Pentacene and multiple Pentacene.

The molecular graph of linear Pentacene is shown in Figure 4.13 and it is denoted by T_n. There are $22n$ vertices and $28n-2$ edges in T_n.

Theorem 4.3.17. *Let G^* be the para-line graph of T_n. Then*

$$M_\alpha(G^*) = (5n+2)2^{\alpha+2} + 3^{\alpha+1}(12n-4)$$

Proof. The graph G^* is shown in Figure 4.14. In G^* there are total $56n-4$ vertices among which $20n+8$ vertices are of degree 2 and $36n-12$ vertices are of degree 3. As

$$M_\alpha(G^*) = (5n+2)2^{\alpha+2} + 3^{\alpha+1}(12n-4)$$

$\square$

Theorem 4.3.18. *Let G^* be the para-line graph of T_n. Then*

1. $R_\alpha(G^*) = (10n+10)4^\alpha + (20n-4)6^\alpha + (44n-16)9^\alpha$.
2. $\chi_\alpha(G^*) = (10n+10)4^\alpha + (20n-4)5^\alpha + (44n-16)6^\alpha$.
3. $ABC(G^*) = \left(15\sqrt{2} + \frac{88}{3}\right)n + 3\sqrt{2} - \frac{32}{3}$.
4. $GA(G^*) = \left(54 + 8\sqrt{6}\right)n - 6 - \frac{8}{5}\sqrt{6}$.

Proof. The total cardinality of edge set of G^* is $74n-10$. The edge set $E(G^*)$ is partitioned in the following three disjoint edge sets depends on the degrees of the end vertices, i.e. $E(G^*) = E_1(G^*) \cup E_2(G^*) \cup E_3(G^*)$. The edge partite set $E_1(G^*)$ holds $10n+10$ edges xy, where $d_x = d_y = 2$, the edge partite set $E_2(G^*)$ holds $20n-4$ edges xy, where $d_x = 2$ and $d_y = 3$, and the edge partite set $E_3(G^*)$ holds $44n-16$ edges xy, where $d_x = d_y = 3$. From Formulas (3.2.1), (3.2.3), (3.2.4) and (3.2.5), we get the desired results. □

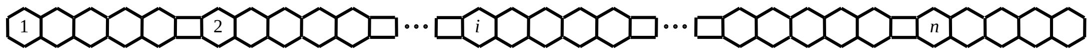

Figure 4.13: Linear Pentacene.

Theorem 4.3.19. *Let G^* be the para-line graph of T_n. Then*

$$\begin{aligned}
ABC_4(G^*) &= \left(\sqrt{110}+4\sqrt{2}+2\sqrt{30}+\frac{16}{3}+\sqrt{14}\right)n \\
&+ 5/2\sqrt{6}+\frac{2}{5}\sqrt{35}-\frac{8}{5}\sqrt{2}-\frac{2}{3}\sqrt{30}-\frac{1}{5}\sqrt{110}-\frac{32}{9} \\
GA_5(G^*) &= \left(30+\frac{80}{13}\sqrt{10}+\frac{288}{17}\sqrt{2}\right)n \\
&- 2+\frac{16}{9}\sqrt{5}-\frac{16}{13}\sqrt{10}-\frac{96}{17}\sqrt{2}.
\end{aligned}$$

Proof. If we suppose an edge collection depends on degree sum of neighbours of end vertices then the set of edges $E(G^*)$ can be distributed into seven disjoint sets of edges $E_i(G^*)$, $i = 4,5,\ldots,10$, i.e. $E(G^*) = \cup_{i=4}^{10} E_i(G^*)$. The edge collection $E_4(G^*)$ holds 10 edges xy, where $S_x = S_y = 4$, the edge collection $E_5(G^*)$ holds 4 edges xy, where $S_x = 4$ and $S_y = 5$, the edge collection $E_6(G^*)$ holds $10n-4$ edges xy, where $S_x = S_y = 5$, the edge collection $E_7(G^*)$ holds $20n-4$ edges xy, where $S_x = 5$ and $S_y = 8$, the edge collection $E_8(G^*)$ holds $8n$ edges xy, where $S_x = S_y = 8$, the edge collection $E_9(G^*)$ holds $24n-8$ edges xy, where $S_x = 8$ and $S_y = 9$, and the edge collection $E_{10}(G^*)$ holds $12n-8$ edges xy, where $S_x = S_y = 9$. From Formulas 3.2.6 and 3.2.7, we obtain the required results. □

Theorem 4.3.20. *Let G^* be the para-line graph of T_n. Then*

1. $HM(G^*) = 2124n - 636$.

2. $PM_1(G^*) = 4^{10n+10} \times 5^{20n-4} \times 6^{44n-16}$.

3. $PM_2(G^*) = 4^{10n+10} \times 6^{20n-4} \times 9^{44n-16}$.

Proof. Let G^* be the para-line graph of linear pentacene. The edge set $E(G^*)$ is distributed in three categories which depends on the degree of end vertices. The first disjoint edge set $E_1(G^*)$ holds 10n+10 edges xy, where $d_x = d_y = 2$. The second disjoint set $E_2(G^*)$ holds 20n-4 edges xy, where $d_x = 2, d_y = 3$.The third disjoint set $E_3(G^*)$ holds 44n-16 edges xy, where $d_x = d_y = 3$. Now, $|E_1(G)| = e_{2,2}$, $|E_2(G)| = e_{2,3}$ and $|E_3(G)| = e_{3,3}$. Since,

$$
\begin{aligned}
HM(G^*) &= \sum_{xy\in E(G)} \left(d_x + d_y\right)^2 \\
HM(G^*) &= \sum_{xy\in E_1(G)} \left[d_x + d_y\right]^2 + \sum_{xy\in E_2(G)} \left[d_x + d_y\right]^2 + \sum_{xy\in E_3(G)} \left[d_x + d_y\right]^2 \\
HM(G^*) &= 16|E_1(G)| + 25|E_2(G)| + 36|E_3(G)| \\
&= 16(10n+10) + 25(20n-4) + 36(44n-16). \\
HM(G^*) &= 2124n - 636.
\end{aligned}
$$

$$
\begin{aligned}
PM_1(G^*) &= \prod_{xy\in E(G)} (d_x + d_y) \\
PM_1(G^*) &= \prod_{xy\in E_1(G)} (d_x + d_y) \times \prod_{xy\in E_2(G)} (d_x + d_y) \times \prod_{xy\in E_3(G)} (d_x + d_y) \\
PM_1(G^*) &= 4^{|E_1(G)|} \times 5^{|E_2(G)|} \times 6^{|E_3(G)|} \\
&= 4^{10n+10} \times 5^{20n-4} \times 6^{44n-16} \\
PM_1(G^*) &= 4^{10n+10} \times 5^{20n-4} \times 6^{44n-16}. \\
PM_2(G^*) &= \prod_{xy\in E(G)} (d_x \times d_y) \\
PM_2(G^*) &= \prod_{xy\in E_1(G)} (d_x \times d_y) \times \prod_{xy\in E_2(G)} (d_x \times d_y) \times \prod_{xy\in E_3(G)} (d_x \times d_y) \\
PM_2(G^*) &= 4^{|E_1(G)|} \times 6^{|E_2(G)|} \times 9^{|E_3(G)|} \\
&= 4^{10n+10} \times 6^{20n-4} \times 9^{44n-16}.
\end{aligned}
$$

□

Theorem 4.3.21. *Let G^* be the para-line graph of T_n. Then*

1. $M_1(G^*, p) = (10n+10)\,p^4 + (20n-4)\,p^5 + (44n-16)\,p^6$.

2. $M_2(G^*, p) = (10n+10)\,p^4 + (20n-4)\,p^6 + (44n-16)\,p^9$.

Proof.

$$
\begin{aligned}
M_1(G^*,p) &= \sum_{xy\in E(G)} p^{(d_x+d_y)} \\
M_1(G^*,p) &= \sum_{xy\in E_1(G)} p^{(d_x+d_y)} + \sum_{xy\in E_2(G)} p^{(d_x+d_y)} + \sum_{xy\in E_3(G)} p^{(d_x+d_y)} \\
M_1(G^*,p) &= \sum_{xy\in E_1(G)} p^4 + \sum_{xy\in E_2(G)} p^5 + \sum_{xy\in E_3(G)} p^6 \\
M_1(G^*,p) &= |E_1(G)|p^4 + |E_2(G)|p^5 + |E_3(G)|p^6 \\
M_1(G^*,p) &= (10n+10)\,p^4 + (20n-4)\,p^5 + (44n-16)\,p^6.
\end{aligned}
$$

$$
\begin{aligned}
M_2(G^*,p) &= \sum_{xy\in E(G)} p^{(d_x\times d_y)} \\
M_2(G^*,p) &= \sum_{xy\in E_1(G)} p^{(d_x\times d_y)} + \sum_{xy\in E_2(G)} p^{(d_x\times d_y)} + \sum_{xy\in E_3(G)} p^{(d_x\times d_y)} \\
M_2(G^*,p) &= \sum_{xy\in E_1(G)} p^4 + \sum_{xy\in E_2(G)} p^6 + \sum_{xy\in E_3(G)} p^9 \\
M_2(G^*,p) &= |E_1(G)|p^4 + |E_2(G)|p^6 + |E_3(G)|p^9 \\
M_2(G^*,p) &= (10n+10)\,p^4 + (20n-4)\,p^6 + (44n-16)\,p^9.
\end{aligned}
$$

Hence proved.

□

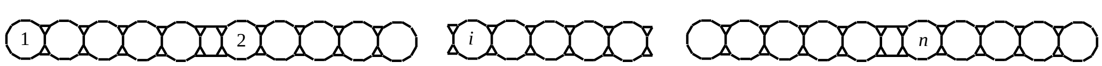

Figure 4.14: Paraline graph of linear Pentacene.

4.3.6 Topological Indices of the Para-line Graph of Multiple Pentacene

The molecular graph of multiple pentacene is shown in Figure 4.15 and it is denoted by $T_{m,n}$. There are $22mn$ vertices and $33mn-2m-5n$ edges in $T_{m,n}$.

Theorem 4.3.22. *Let G^* be the para-line graph of $T_{m,n}$. Then*

$$M_\alpha(G^*) \;=\; (5n+2)2^{\alpha+2}+3^{\alpha+1}(12n-4)$$

Proof. The graph G^* is shown in Figure 4.15 In G^* there are total $56n-4$ vertices among which $20n+8$ degree 2 vertices and $36n-12$ degree 3 vertices. Hence we get $M_\alpha(G^*)$ by using Formula 3.2.2. □

Theorem 4.3.23. *Let G^* be the para-line graph of $T_{m,n}$. Then*

$$\begin{aligned}
R_\alpha(G^*) &= (10n+6m+4)\,4^\alpha+(4m+20n-8)\,6^\alpha+(99mn-20m-55n+4)\,9^\alpha\;. \\
\chi_\alpha(G^*) &= (10n+6m+4)\,4^\alpha+(4m+20n-8)\,5^\alpha+(99mn-20m-55n+4)\,6^\alpha 5. \\
ABC_4(G^*) &= \left(\sqrt{110}+4\sqrt{2}+2\sqrt{30}+\frac{16}{3}+\sqrt{14}\right)n \\
&+\; 5/2\sqrt{6}+\frac{2}{5}\sqrt{35}-\frac{8}{5}\sqrt{2}-\frac{2}{3}\sqrt{30}-\frac{1}{5}\sqrt{110}-\frac{32}{9}. \\
GA_5(G^*) &= \left(30+\frac{80}{13}\sqrt{10}+\frac{288}{17}\sqrt{2}\right)n-2+\frac{16}{9}\sqrt{5}-\frac{16}{13}\sqrt{10}-\frac{96}{17}\sqrt{2}.
\end{aligned}$$

Proof. The subdivision graph of multiple Pentacene $S(T_{m,n})$ holds $99mn-10m-25n$ edges and $198mn-20m-50$ vertices in total. The division of the vertices is as follows: The number of vertices of degree two are $8m+20n$ and the number of vertices of degree three are $66mn-12m-30n$. The cardinality of edge set E of G^* are $99mn-20m-55n+4$. The edge set $E(G^*)$ splits into three edge categories depends on the degrees of the end vertices, i.e. $E(G^*)=E_1(G^*)\cup E_2(G^*)\cup E_3(G^*)$. The edge partite set $E_1(G^*)$ holds $10n+6m+4$ edges xy, where $d_x=d_y=2$, the edge partite set $E_2(G^*)$ holds $4m+20n-8$ edges xy, where $d_x=2$ and $d_y=3$, and the edge partite set $E_3(G^*)$ holds $99mn-20m-55n+4$ edges xy, where $d_x=d_y=3$. From Formulas (3.2.1), (3.2.3), (3.2.4) and (3.2.5), Hence desired result is obtained. □

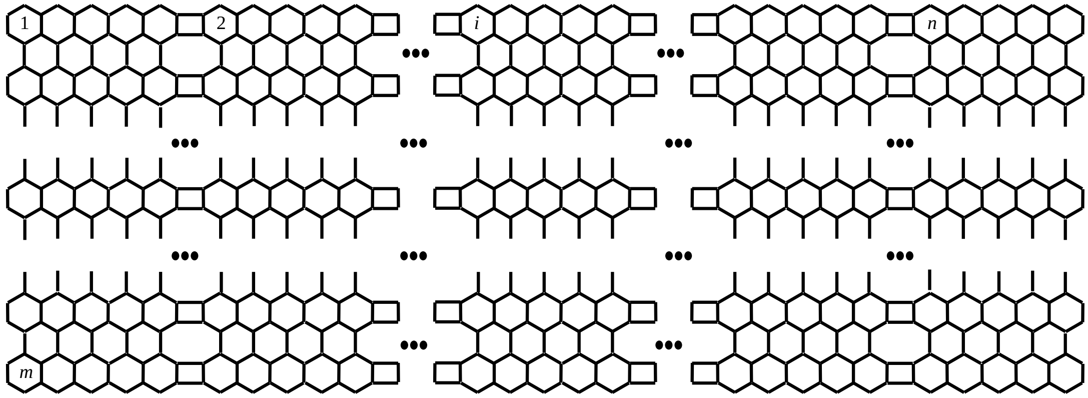

Figure 4.15: Multiple Pentacene.

Theorem 4.3.24. *Let G^* be the para-line graph of multiple Pentacene $T_{m,n}$. Then*

$$\begin{aligned}
ABC_4(G^*) &= \left(44m+\sqrt{14}+4\sqrt{2}+\sqrt{110}+2\sqrt{30}-\frac{116}{3}\right)n \\
&+ \left(1/2\sqrt{6}+1/5\sqrt{110}+2/5\sqrt{35}-\frac{112}{9}+2/3\sqrt{30}\right)m \\
&+ 2\sqrt{6}-8/5\sqrt{2}-2/5\sqrt{110}-4/3\sqrt{30}+\frac{80}{9}. \\
GA_5(G^*) &= \left(\frac{80}{13}\sqrt{10}+99m+\frac{288}{17}\sqrt{2}-69\right)n \\
&+ \left(-26+\frac{16}{13}\sqrt{10}+\frac{16}{9}\sqrt{5}+\frac{96}{17}\sqrt{2}\right)m \\
&- \frac{192}{17}\sqrt{2}-\frac{32}{13}\sqrt{10}+24.
\end{aligned}$$

Proof. If the edge partition under consideration depends on degree sum of neighbours of end vertices, then the set of edges $E(G^*)$ can be classified into seven disjoint edge sets $E_i(G^*), i=4,5,\ldots,10$, i.e. $E(G^*)=\cup_{i=4}^{10}E_i(G^*)$. The edge partite set $E_4(G^*)$ holds $2m+8$ edges xy, where $S_x=S_y=4$, the edge partite set $E_5(G^*)$ holds $4m$ edges xy, where $S_x=4$ and $S_y=5$, the edge partite set $E_6(G^*)$ holds $10n-4$ edges xy, where $S_x=S_y=5$, the edge partite set $E_7(G^*)$ holds $20n+4m-8$ edges xy, where $S_x=5$ and $S_y=8$, the edge partite set $E_8(G^*)$ holds $8n$ edges xy, where $S_x=S_y=8$, the edge partite set $E_9(G^*)$ holds $8m+24n-16$ edges xy, where $S_x=8$ and $S_y=9$, and the edge partite set $E_{10}(G^*)$ holds $99mn-28m-87n+20$ edges xy, where $S_x=S_y=9$. From Formulas (3.2.6) and (3.2.7), the required result is obtained. □

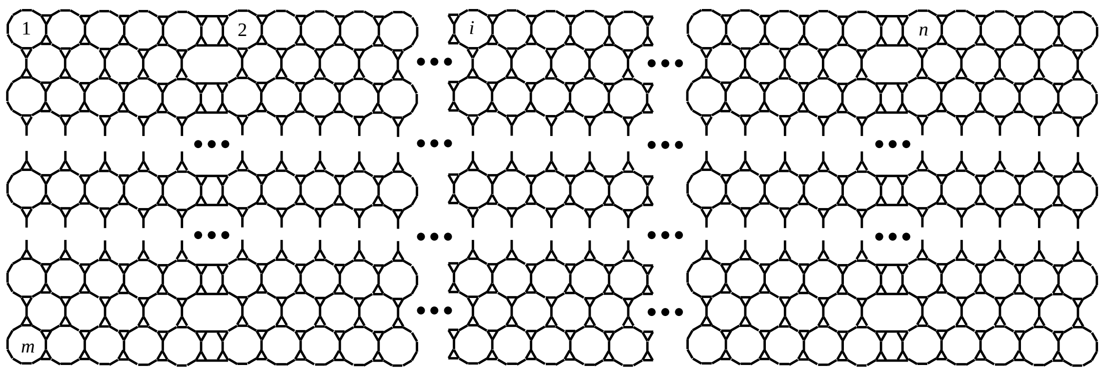

Figure 4.16: Para-line graph of multiple Pentacene.

We find the following indices $HM(G)$, $PM_1(G)$, $PM_2(G)$, Zagreb polynomials $M_1(G,x)$, $M_2(G,x)$ by computation for chemical structures of multiple-pentacene.

Theorem 4.3.25. *Let G^* be the para-line graph of multiple Anthracene $T_{m,n}$.Then*

1. $HM(G^*)=3564mn-596m-1440n-40.$

2. $PM_1(G^*)=4^{10n+6m+4}\times 5^{4m+20n-8}\times 6^{99mn-20m-55n+4}.$

3. $PM_2(G^*)=4^{10n+6m+4}\times 6^{4m+20n-8}\times 9^{99mn-20m-55n+4}.$

4. $M_1(G^*,p)=(10n+6m+4)\,p^4+(4m+20n-8)\,p^5+(99mn-20m-55n+4)\,p^6.$

5. $M_2(G^*,p)=(10n+6m+4)\,p^4+(4m+20n-8)\,p^6+(99mn-20m-55n+4)\,p^9.$

Proof. Let G^* be the graph. The edge set $E(G^*)$ classified into three edge categories based on degree of end vertices. The first edge partite set $E_1(G)$ holds $10n+6m+4$ edges xy, where $d_x=d_y=2$. The second edge partite set $E_2(G)$ holds $4m+20n-8$ edges xy, where $d_x=2$, $d_y=3$. The third edge partite set $E_3(G)$ holds $99mn-20m-55n+4$ edges xy, where $d_x = 3,\ d_y = 3$. It is simple to observe that $|E_1(G)| = e_{2,2}$, $|E_2(G)| = e_{2,3}$ and $|E_3(G)| = e_{3,3}$. Since,

$$\begin{aligned}
HM(G^*) &= \sum_{xy\in E(G)} \left(d_x + d_y\right)^2 \\
HM(G^*) &= \sum_{xy\in E_1(G)} \left[d_x + d_y\right]^2 + \sum_{xy\in E_2(G)} \left[d_x + d_y\right]^2 + \sum_{xy\in E_3(G)} \left[d_x + d_y\right]^2 \\
HM(G^*) &= 16|E_1(G)| + 25|E_2(G)| + 36|E_3(G)| \\
&= 16(10n + 6m + 4) + 25(20n + 4m - 8) \\
&= 36(99mn - 20m - 55n + 4). \\
HM(G^*) &= 3564\,mn - 596\,m - 1440\,n - 40. \\
PM_1(G^*) &= \prod_{xy\in E(G)} (d_x + d_y) \\
PM_1(G^*) &= \prod_{xy\in E_1(G)} (d_x + d_y) \times \prod_{xy\in E_2(G)} (d_x + d_y) \times \prod_{xy\in E_3(G)} (d_x + d_y) \\
PM_1(G^*) &= 4^{|E_1(G)|} \times 5^{|E_2(G)|} \times 6^{|E_3(G)|} \\
&= 4^{10n+6m+4} \times 5^{20n+4m-8} \times 6^{99mn-20m-55n+4}.
\end{aligned}$$

Now, since

$$\begin{aligned}
PM_2(G^*) &= \prod_{xy\in E(G)} (d_x \times d_y) \\
PM_2(G^*) &= \prod_{xy\in E_1(G)} (d_x \times d_y) \times \prod_{xy\in E_2(G)} (d_x \times d_y) \times \prod_{xy\in E_3(G)} (d_x \times d_y)
\end{aligned}$$

$$
\begin{aligned}
PM_2(G^*) &= 4^{|E_1(G)|} \times 6^{|E_2(G)|} \times 9^{|E_3(G)|} \\
&= 4^{10n+6m+4} \times 6^{20n+4m-8} \times 9^{99mn-20m-55n+4}. \\
M_1(G^*,p) &= \sum_{xy\in E(G)} p^{(d_x+d_y)} \\
M_1(G^*,p) &= \sum_{xy\in E_1(G)} p^{(d_x+d_y)} + \sum_{xy\in E_2(G)} p^{(d_x+d_y)} + \sum_{xy\in E_3(G)} p^{(d_x+d_y)} \\
M_1(G^*,p) &= \sum_{xy\in E_1(G)} p^4 + \sum_{xy\in E_2(G)} p^5 + \sum_{xy\in E_3(G)} p^6 \\
M_1(G^*,p) &= |E_1(G)|p^4 + |E_2(G)|p^5 + |E_3(G)|p^6 \\
M_1(G^*,p) &= (10n+6m+4)\,p^4 + (4m+20n-8)\,p^5 + (99mn-20m-55n+4)\,p^6. \\
M_2(G,p) &= \sum_{xy\in E(G)} p^{(d_x\times d_y)} \\
M_2(G,p) &= \sum_{xy\in E_1(G)} p^{(d_x\times d_y)} + \sum_{xy\in E_2(G)} p^{(d_x\times d_y)} + \sum_{xy\in E_3(G)} p^{(d_x\times d_y)} \\
M_2(G^*,p) &= \sum_{xy\in E_1(G)} p^4 + \sum_{xy\in E_2(G)} p^6 + \sum_{xy\in E_3(G)} p^9 \\
M_2(G^*,p) &= |E_1(G)|p^4 + |E_2(G)|p^6 + |E_3(G)|p^9 \\
M_2(G^*,p) &= (10n+6m+4)\,p^4 + (4m+20n-8)\,p^6 + (99mn-20m-55n+4)\,p^9.
\end{aligned}
$$

This completes the proof. $\square$

Chapter 5

Spectrum Based Topological Indices

Spectrum based topological indices are much popular these days and they are used in the field of molecular orbital theory to study unsaturated compounds. Afterwards it was noticed that these spectral indices generalised to any compound and also found application in modeling physico-chemical properties of molecules. Spectral indices are basically defined for the eigen values of the square matrix of the graph of molecular structures. The notion of graph energy has been proposed by Gutman in [69].“ If G is a graph on n vertices and $\lambda_1, \lambda_2, \lambda_3, ..., \lambda_n$ are its eigen values, then the energy of graph G is $E = \sum_{i=1}^{q} |\lambda_i|$.” As a whole, all the eigen values of the graph G are called spectrum of G. These eigen values have a close correspondence with the molecular orbital energy levels of π-electrons in conjugated hydrocarbons. There are many form of energies in the literature that has been investigated such as Laplacian energy, distance energy etc.
In this section, we discuss the process of finding the energy and Estrada index of the Phenylene and Anthracene by using the computational methods. In first step, we use HyperChem to draw the molecular graph of our chemical structures. In second step, from the graph drawn by HyperChem we construct an adjacency matrix by using TopoCluj. In third step, we find the energy with the help of MATLAB which is represented in Table 5.1. In fourth step, we construct the curve (polynomial) of degree two with the help of cftoolbox of MATLAB. The results obtained from this data are displayed in Table 5.2. In Table 5.3 and 5.4, we have find the errors between the exact and estimated values extracted from the curve for energy and Estrada index of Phenylene. We have also calculated the inertia index, nullity and signature of the Phenylene which are displayed in Table 5.5. Similar process has been used for Anthracene. In Table 5.6 and 5.7, we have found the polynomials by using the above techniques and also in Table 5.8 and 5.9 we have calculated the errors of the exact and estimated values of the energy and Estrada index of Anthracene. At the end in Table 5.10 we have displayed the inertia index, nullity and signature of Anthracene.

5.1 Energy and Estrada Index of Some Chemical Structures

In this section, we have computed the energy and Estrada index, inertia, nullity and signature for some chemical structures such as Phenylene, Anthracene, Bismuth Tri-iodide and

Benzene Ring Embedded in P-type-surface in 2D network(BRE).

5.1.1 Energy and Estrada Index of the Phenylene

In this section we will study the energy, Estrada index, nullity, inertia and signature of Phenylene. We will also show the comparison between exact and estimated values of energy and Estrada index of Phenylene.

Proposition 5.1.1. *Let P be the graph of Phenylene, then the energy and Estrada index of P is given by*

$$\begin{aligned} E(P) = -6\times10^{-6}m^2n^2 - 0.0002n^2m + 0.0007n^2 + 0.0005nm^2 \\ +8.8999nm - 0.4393n - 0.0007m^2 - 0.5161m + 0.0729 \end{aligned} \tag{5.1.1}$$

$$\begin{aligned} EE(P) = -6\times10^{-11}m^2n^2 + 6\times10^{-9}n^2m + 6\times10^{-9}n^2 + 0.0017nm^2 \\ +18.831nm - 1.1281n - 0.0015m^2 - 0.7436m - 3.2623. \end{aligned} \tag{5.1.2}$$

The two curves which are representing the energy and Estrada index of the graph are given by Equations (5.1.1) and (5.1.2), respectively. The equation of the energy of the graph has been obtained for Phenylene and the Estrada index of the Phenylene has been generated. We have observed that exact value of energy of Phenylene is always greater than the estimated values of energy of Phenylene, i.e. $E_{ext}(P) > E_{ast}(P)$, where E_{ext} represents the exact value of energy and E_{ast} represents the estimated value of energy. Also error is always positive between the exact and estimated values of energy of Phenylene, i.e. error>0.

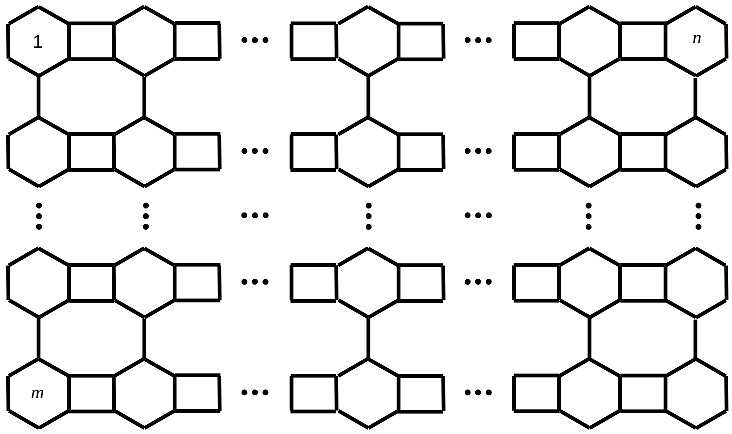

Figure 5.1: Phenylene.

Similarly, we have observed that exact value of Estrada index of Phenylene is always less than the estimated values of Estrada index of Phenylene, i.e. $EE_{ext}(P) < EE_{ast}(P)$, where EE_{ext} represents the exact value of Estrada index and EE_{ast} represents the estimated value of Estrada index.

In Table 5.1 for every curve, the value of m and n ranges from 1 to 10.

Table 5.1: The quadratic curves for the energy and Estrada index of Phenylene.

(m,n)	Energy(E(P))	Estrada Index(EE(P))
$(1,n)$	$-0.0009n^2+8.4872n-0.4467$	$-9\times10^{-9}n^2+18.089n-4.3925$
$(2,n)$	$0.0027n^2+17.354n-1.0234$	$6\times10^{-8}n^2+35.724n-3.9426$
$(3,n)$	$-0.0001n^2+26.226n-1.4013$	$1\times10^{-9}n^2+55.789n-5.9133$
$(4,n)$	$-0.0011n^2+35.143n-1.9339$	$3\times10^{-8}n^2+74.234n-6.2703$
$(5,n)$	$-0.0004n^2+44.12n-2.6087$	$3\times10^{-8}n^2+93.085n-7.0307$
$(6,n)$	$-0.0008n^2+52.982n-3.0532$	$4\times10^{-8}n^2+111.93n-7.7911$
$(7,n)$	$-0.0011n^2+61.888n-3.5766$	$4\times10^{-8}n^2+130.78n-8.5516$
$(8,n)$	$-0.0014n^2+70.793n-4.1001$	$5\times10^{-8}n^2+149.63n-9.312$
$(9,n)$	$-0.0016n^2+79.698n-4.6236$	$5\times10^{-8}n^2+168.48n-10.072$
$(10,n)$	$-0.0019n^2+88.604n-5.147$	$6\times10^{-8}n^2+187.34n-10.833$

In this table, we have shown the quadratic curves which is extracted from the coefficient of the above equations

Table 5.2: Quadratic curves extracted from the equations shown in Table 5.1

	Energy(E(P))	Estrada Index(EE(P))
n^2	$-6\times10^{-6}m^2-0.0002m+0.0007$	$-6\times10^{-11}m^2+6\times10^{-9}m+6\times10^{-9}$
n	$0.0005m^2+8.8999m-0.4393$	$0.0017m^2+18.831m-1.1281$
1	$-0.0007m^2-0.5161m+0.0729$	$-0.0015m^2-0.7436m-3.2623$

The error between the exact values and estimated values of energy and Estrada index are shown in the Tables 5.3 and 5.4. Also the nullity, signature and positive and negative eigen values are presented in Table 5.5.

Table 5.3: The exact $E_{ext}(P)$ and estimated values $E_{ast}(P)$ of the energy of Phenylene

(m,n)	E_{ext}(P)	E_{ast}(P)	Error
$(10,1)$	84.51	84.21	0.3
$(10,2)$	172.99	172.69	0.3
$(10,3)$	261.4	261.17	0.23
$(10,4)$	349.96	349.66	0.3
$(10,5)$	438.61	438.15	0.46
$(10,6)$	527.166	526.66	0.506
$(10,7)$	615.43	615.17	0.26
$(10,8)$	704.113	703.69	0.423
$(10,9)$	792.63	792.22	0.41
$(10,10)$	881.11	880.74	0.37

Table 5.4: $EE_{ext}(P)$ and $EE_{ast}(P)$ values of Estrada index of Phenylene

(m,n)	EE_{ext}(P)	EE_{ast}(P)	Error
$(10,1)$	176.5041333	176.51413	-0.01
$(10,2)$	363.8355	363.8555	-0.02
$(10,3)$	551.1702333	551.2074	-0.0372
$(10,4)$	738.5094444	738.5593	-0.0499
$(10,5)$	925.8424944	925.9112	-0.0687
$(10,6)$	1113.177561	1113.2631	-0.0851
$(10,7)$	1300.512628	1300.6150	-0.102
$(10,8)$	1487.847694	1487.9669	-0.1189
$(10,9)$	1675.182761	1675.3188	-0.1358
$(10,10)$	1862.517828	1862.6707	-0.1527

Table 5.5: The inertia, nullity and signature of Phenylene

P=Phenylene	$p(P)$	$n(P)$	$\eta(P)$	$s(P)$
$(8,1)$	24	24	0	0
$(8,2)$	48	48	0	0
$(8,3)$	72	72	0	0
$(8,4)$	96	96	0	0
$(8,5)$	120	120	0	0
$(8,6)$	144	144	0	0
$(8,7)$	168	168	0	0
$(8,8)$	192	192	0	0
$(8,9)$	216	216	0	0
$(8,10)$	240	240	0	0
$8,11)$	264	264	0	0
$8,12)$	288	288	0	0

5.1.2 Energy and Estrada Index of Anthracene

In this section, we will study the energy, Estrada index, nullity, inertia and signature of Anthracene. We will also show the comparison between exact and estimated values of energy and Estrada index of Anthracene.

Proposition 5.1.2. *Let A be the graph of Anthracene. Then the energy and Estrada index of A is given by*

$$\begin{aligned} E(A) = &-2\times10^{-8}m^2n^2 - 2\times10^{-7}n^2m + 5\times10^{-6}n^2 + 2\times10^{-5}nm^2 \\ &+21.432nm + 20.789n - 4\times10^{-5}m^2 - 1.4874m - 1.5503. \end{aligned} \tag{5.1.3}$$

$$\begin{aligned} EE(A) = &-3\times10^{-15}m^2n^2 + 2\times10^{-14}n^2m - 1\times10^{-13}n^2 + 3\times10^{-14}nm^2 \\ &+94.388nm + 40.903n - 7\times10^{-15}m^2 - 41.225m + 49.611. \end{aligned} \tag{5.1.4}$$

Table 5.6: Quadratic curves for the energy and Estrada index of Anthracene.

(m,n)	Energy$(E(A))$	Estrada index$(EE(A))$
$(1,n)$	$7\times10^{-6}n^2+42.356n-3.2224$	$3\times10^{-14}n^2+135.29n+8.3861$
$(2,n)$	$3\times10^{-6}n^2+63.382n-4.1488$	$-1\times10^{-13}n^2+229.68n-32.84$
$(3,n)$	$9\times10^{-6}n^2+85.212n-6.1953$	$-1\times10^{-13}n^2+324.07n-74.066$
$(4,n)$	$3\times10^{-6}n^2+106.53n-7.5104$	$-3\times10^{-13}n^2+418.46n-115.29$
$(5,n)$	$4\times10^{-6}n^2+127.94n-8.9824$	$-2\times10^{-13}n^2+512.85n-156.52$
$(6,n)$	$4\times10^{-6}n^2+149.38n-10.476$	$1\times10^{-13}n^2+607.23n-197.74$
$(7,n)$	$3\times10^{-6}n^2+170.82n-11.965$	$6\times10^{-14}n^2+701.62n-238.97$
$(8,n)$	$3\times10^{-6}n^2+192.25n-13.453$	$-5\times10^{-13}n^2+796.01n-280.2$
$(9,n)$	$2\times10^{-6}n^2+213.68n-14.941$	$2\times10^{-13}n^2+890.4n-321.42$
$(10,n)$	$2\times10^{-6}n^2+235.11n-16.429$	$-5\times10^{-13}n^2+984.79n-362.65$

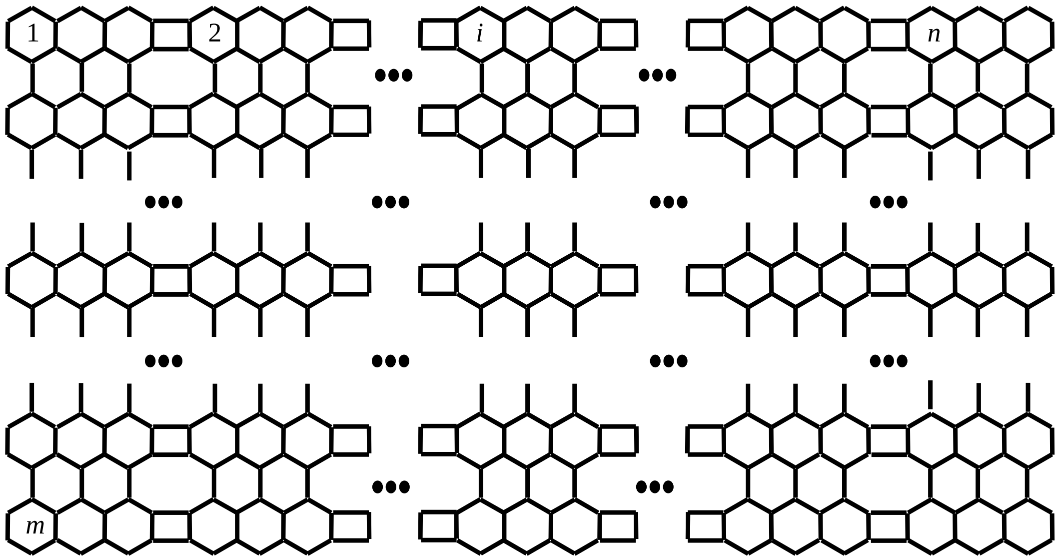

Figure 5.2: Multiple Anthracene.

Table 5.7: Quadratic curves extracted from the equations in Table 5.6

	Energy$(E(A))$	Estrada index$(EE(A))$
n^2	$-2\times10^{-8}m^2-2\times10^{-7}m+5\times10^{-6}$	$-3\times10^{-15}m^2+2\times10^{-14}m-1\times10^{-13}$
n	$2\times10^{-5}m^2+21.432m+20.789$	$3\times10^{-14}m^2+94.388m+40.903$
1	$-4\times10^{-5}m^2-1.4874m-1.5503$	$-7\times10^{-5}m^2-41.225m+49.611$

The errors of energy and Estrada index have been found in the Tables 5.8 and 5.9 and also the signature, nullity and positive and negative eigen values in Table 5.10

Table 5.8: The $E_{ext}(A)$ and $E_{ast}(A)$ values of the energy of the Anthracene

(m,n)	E_{ext}(A)	E_{ast}(A)	Error
$(10,1)$	218.7247	218.6827	0.042
$(10,2)$	453.8533	453.7937	0.0596
$(10,3)$	688.9118	688.9047	0.0071
$(10,4)$	924.0977	924.0157	0.082
$(10,5)$	1159.1496	1159.1267	0.0229
$(10,6)$	1394.247	1394.2377	0.0093
$(10,7)$	1629.359	1629.3487	0.0103
$(10,8)$	1864.472	1864.4597	0.0123
$(10,9)$	2099.585	2099.5707	0.0143
$(10,10)$	2334.697	2334.6818	0.0152

Table 5.9: The $EE_{ext}(A)$ and $EE_{ast}(A)$ values of the Estrada index of the Anthracene

(m,n)	EE_{ext}(A)	EE_{ast}(A)	Error
$(10,1)$	622.138	622.137	0.001
$(10,2)$	1606.922	1606.92	0.002
$(10,3)$	2591.707	2591.703	0.004
$(10,4)$	3576.493	3576.486	0.007
$(10,5)$	4561.279	4561.269	0.01
$(10,6)$	5546.065	5546.052	0.013
$(10,7)$	6530.85	6530.835	0.015
$(10,8)$	7515.636	7515.618	0.018
$(10,9)$	8500.422	8500.401	0.021
$(10,10)$	9485.207	9485.184	0.023

Table 5.10: The inertia, nullity and signature of Anthracene

G=Anthracene	$p(G)$	$n(G)$	$\eta(G)$	$s(G)$
$(8,1)$	35	35	0	0
$(8,2)$	70	70	0	0
$(8,3)$	105	105	0	0
$(8,4)$	140	140	0	0
$(8,5)$	175	175	0	0
$(8,6)$	210	210	0	0
$(8,7)$	280	280	0	0
$(8,8)$	315	315	0	0
$(8,9)$	350	350	0	0
$(8,10)$	385	385	0	0
$8,11)$	420	420	0	0
$8,12)$	455	455	0	0

We have observed that exact value of energy of Anthracene is always greater than the estimated values of energy of Anthracene, i.e. $E_{ext}(A) > E_{ast}(A)$. Also Error is always positive between the exact and estimated values of energy of Anthracene, i.e. error>0. Similarly, we have observed that exact value of Estrada index of Anthracene is always greater than the estimated values of Estrada index of Anthracene, i.e. $EE_{ext}(A) > EE_{ast}(A)$

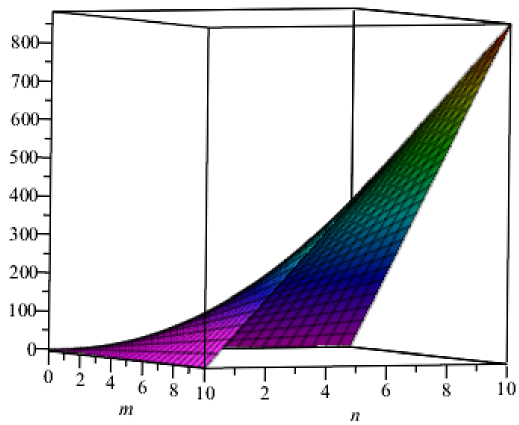

Figure 5.3: Energy of Phenylene.

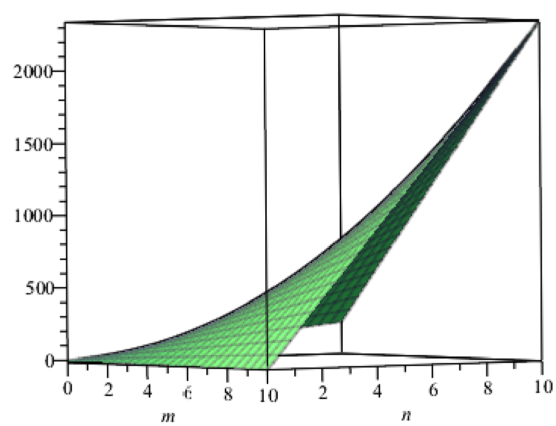

Figure 5.4: Energy of Anthracene.

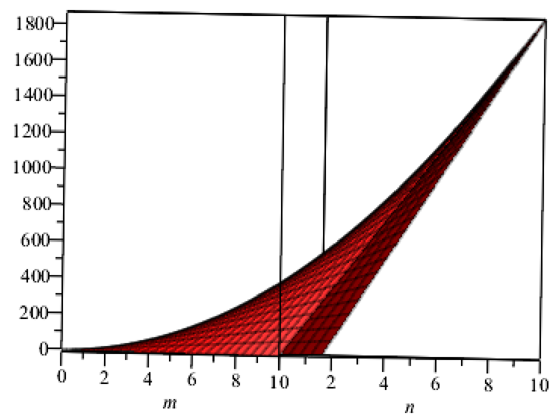

Figure 5.5: Estrada index of Phenylene.

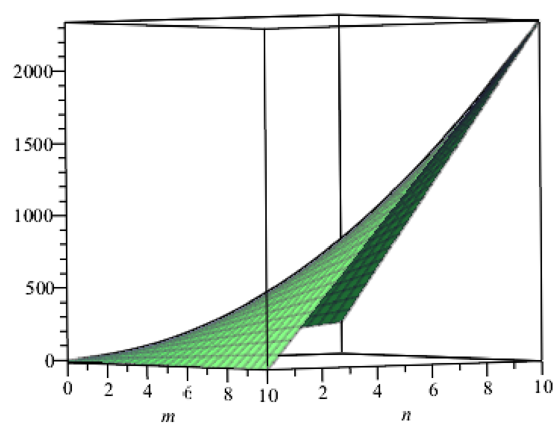

Figure 5.6: Estrada index of Anthracene.

5.1.3 Energy and Estrada Index of Bismuth Tri-Iodide

In this section, we describe the way how we find the energy and Estrada index of certain graphs using computational methods. The computational method has been done in few steps. In first step, we draw the molecular graph of chemical structures using HyperChem.

In second step, with the help of TopoCluj we generate an adjacency matrix. In third step, we use MATLAB to find the eigen values of the adjacency matrix. In fourth step, by using cftoolbox of MATLAB, we develop the polynomial of degree 2 presented in the Equations (5.1.5) and (5.1.6). From the Equations (5.1.5) and (5.1.6), we have generated energy equations shown in Table 5.11. In Table 5.13 and 5.14, we have evaluated the errors for energy and Estrada index of Bismuth Tri-iodide by taking the difference between the exact and estimated values of polynomial of degree 2. We also have examined the inertia, nullity and signature of the Bismuth Tri-iodide which are displayed in Table 5.15. Similar procedure has been implemented for Benzene Ring Embedded in P-type-surface in 2D network. In Table 5.16 and 5.17, we have manipulated the polynomials of degree 2 by performing the above techniques and then in Table 5.18 and 5.19 we have observed the errors of the exact and estimated values of the energy and Estrada index of Benzene Ring Embedded in P-type-surface in 2D network. At the end in Table 5.20, we have showed the inertia index, nullity and signature of Benzene Ring Embedded in P-type-surface in 2D network. Now we will discuss the energy, Estrada index, nullity, inertia and signature of

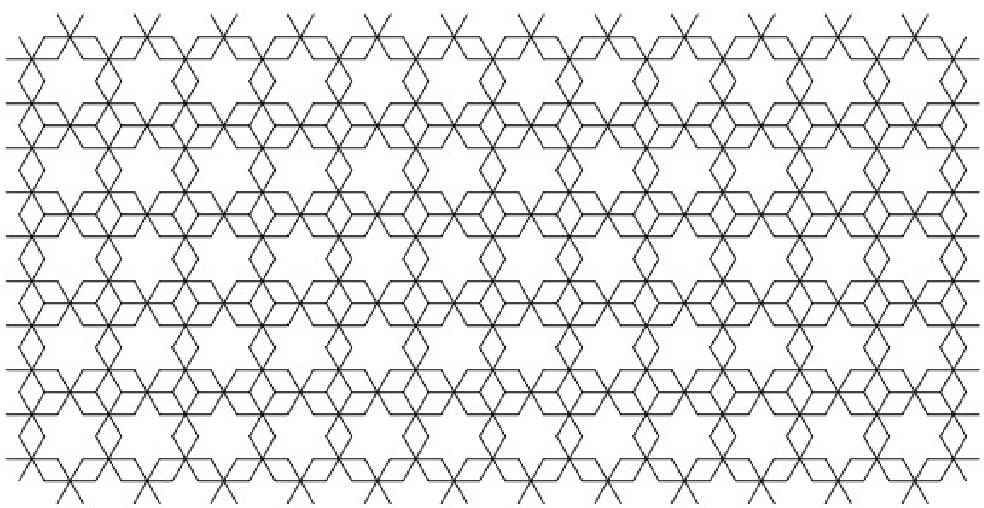

Figure 5.7: Bismuth Tri-iodide.

Bismuth Tri-iodide. We will also demonstrate the comparison between exact and estimated values of energy and Estrada index of Bismuth Tri-iodide.

Proposition 5.1.3. *Let B be the graph of Bismuth Tri-iodide. Then the energy and Estrada* *index of B is given by*

$$E(B) = 7\times 10^{-9}m^2n^2 - 9\times 10^{-5}n^2m + 0.0003n^2 - 0.0003nm^2 + 13.794nm + 9.5506n - 0.0014m^2 + 5.1553m - 0.3239. \tag{5.1.5}$$

$$EE(B) = 3.167m^2n^2 - 15.839n^2m + 19.009n^2 - 12.672nm^2 + 110.86nm - 44.392n + 9.498m^2 - 32.462m + 57.857. \tag{5.1.6}$$

The two second order polynomials which are displaying the energy and Estrada index of the Bismuth Tri-iodide are given by equations (5.1.5) and (5.1.6), respectively. These equations provide the data for any unit of graph. We have observed that exact value of energy of Bismuth Tri-iodide is always less than the estimated values of energy of Bismuth Tri-iodide, i.e. $E_{ext}(B) < E_{ast}(B)$, where E_{ext} represents the exact value of energy and E_{ast} estimated value of energy respectively. Also error is always positive between the exact and estimated values of energy of Bismuth Tri-iodide, i.e. error>0. Similarly, We have observed that exact value of Estrada index of Bismuth Tri-iodide is always greater than the estimated values of Estrada index of Bismuth Tri-iodide, i.e. $EE_{ext}(B) > EE_{ast}(B)$, where EE_{ext} and EE_{ast} represents the exact and estimated value of Estrada index, respectively. In Table 5.11, the value of m and n ranges from 1 to 10.

Table 5.11: Equations for the Energy and Estrada index of Bismuth Tri-iodide.

(m,n)	Energy(E(B))	Estrada Index(EE(B))
$(1,n)$	$2.10\times10^{-4}n^2+23.3443n+4.83$	$6.342n^2-176.2n+34.887$
$(2,n)$	$1.28\times10^{-4}n^2+19.86n+9.9811$	$0.009n^2-103.35n+30.918$
$(3,n)$	$3\times10^{-5}n^2+50.9299n+15.1294$	$-99.986n^2+244.16n-154.057$
$(4,n)$	$-5\times10^{-5}n^2+64.7218n+20.2749$	$-293.643n^2+866.33n-520.038$
$(5,n)$	$-1.49\times10^{-4}n^2+78.5131n+25.4456$	$-580.962n^2+1763.16n-1067.025$
$(6,n)$	$-2.39\times10^{-4}n^2+92.3038n+30.5575$	$-961.943n^2+2934.65n-1795.018$
$(7,n)$	$-3.29\times10^{-4}n^2+106.1233n+35.6946$	$-1436.586n^2+4380.8n-2704.017$
$(8,n)$	$-4.19\times10^{-4}n^2+119.9218n+40.8289$	$-2004.891n^2+6101.61n-3794.022$
$(9,n)$	$-5.09\times10^{-4}n^2+133.7209n+45.9604$	$-2666.858n^2+8097.08n-5065.033$
$(10,n)$	$-5.99\times10^{-4}n^2+147.5206n+51.0891$	$-3422.487n^2+10367.21n-6517.05$

Table 5.12: Equations extracted from the coefficient shown in Table 5.11

	Energy(E(B))	Estrada Index(EE(B))
n^2	$7\times10^{-9}m^2-9\times10^{-5}m+0.0003$	$3.167m^2-15.839m+19.009$
n	$-0.0003m^2+13.794m+9.5506$	$-12.672m^2+110.86m-44.392$
1	$-0.0014m^2+5.1553m-0.3239$	$9.498m^2-32.462m+57.857$

Also the error between the exact values and estimated values of energy and Estrada index are shown in the Tables 5.13 and 5.14 below.

Table 5.13: The $E_{ext}(B)$ and $E_{ast}(B)$ values of the energy of the Bismuth Tri-iodide

(m,n)	E_{ext}(B)	E_{ast}(B)	Error
$(3,1)$	65.996	66.05	0.054
$(3,2)$	116.924	116.989	0.065
$(3,3)$	167.849	167.919	0.07
$(3,4)$	218.775	218.849	0.074
$(3,5)$	269.7014	269.779	0.078
$(3,6)$	320.6268	320.709	0.082
$(3,7)$	371.552	371.64	0.088
$(3,8)$	422.4786	422.57	0.091
$(3,9)$	473.403	473.5	0.097
$(3,10)$	524.3288	524.431	0.102

Table 5.14: The $EE_{ext}(B)$ and $EE_{ast}(B)$ values of Bismuth Tri-iodide

(m,n)	EE_{ext}(B)	EE_{ast}(B)	Error
$(3,1)$	220.09	220.088	-0.002
$(3,2)$	394.22	394.213	-0.007
$(3,3)$	568.343	568.328	-0.015
$(3,4)$	742.4706667	742.433	-0.037
$(3,5)$	916.5971667	916.528	-0.069
$(3,6)$	1090.723667	1090.613	-0.111
$(3,7)$	1264.850167	1264.688	-0.162
$(3,8)$	1438.976667	1438.753	-0.224
$(3,9)$	1613.103167	1612.808	-0.297
$(3,10)$	1787.229667	1786.853	-0.377

Table 5.15: The inertia, nullity and signature of Bismuth Tri-iodide

B=Bismuth Tri-iodide	$p(B)$	$n(B)$	$\eta(B)$	$s(B)$
$(3,1)$	16	16	40	0
$(3,2)$	26	26	60	0
$(3,3)$	36	36	80	0
$(3,4)$	46	46	100	0
$(3,5)$	56	56	120	0
$(3,6)$	66	66	140	0
$(3,7)$	76	76	160	0
$(3,8)$	86	86	180	0
$(3,9)$	96	96	200	0
$(3,10)$	106	106	220	0
$(3,11)$	116	116	240	0
$(3,12)$	126	126	260	0

5.1.4 Energy and Estrada Index of the Benzene Ring Embedded in P-type-surface in 2D network(BRE)

In this sub section, we will study the energy, Estrada index, nullity, inertia and signature of BRE. We will also show the comparison between exact and estimated values of energy and Estrada index of BRE. we will use this notation BRE to represent (Benzene Ring Embedded in P-type-surface in 2D network) throughout this paper.

Proposition 5.1.4. *Let BRE be the graph of BRE. Then the energy and Estrada index of BRE is given by*

$$\begin{aligned} E(BRE) = 2\times 10^{-7}m^2n^2 - 2\times 10^{-5}n^2m + 2\times 10^{-5}n^2 - 0.01nm^2 \\ +35.2nm + 0.98n - 0.0085m^2 + 0.9773m - 0.1176. \end{aligned} \tag{5.1.7}$$

$$
\begin{aligned}
EE(BRE) = 0.0542\,m^2n^2 - 0.1387\,mn^2 - 0.0665\,n^2 - 0.0145\,m^2n \\
+70.062\,mn + 2.193\,n - 0.1985\,m^2 + 2.3475\,m - 1.994.
\end{aligned} \tag{5.1.8}
$$

Table 5.16: The quadratic curves suitable for the Energy and Estrada index of *BRE*.

m,n	Energy$(E(BRE))$	Estrada index$(EE(BRE))$
$(1,n)$	$\frac{1}{5000000}n^2 + 36.17n + 0.8682$	$-0.1510n^2 + 72.2405n + 0.1550$
$(2,n)$	$-\frac{3}{156250}n^2 + 71.34n + 1.8710$	$-0.1271n^2 + 142.2590n + 1.9070$
$(3,n)$	$-\frac{191}{5000000}n^2 + 106.49n + 2.8908$	$0.0052n^2 + 212.2485n + 3.2620$
$(4,n)$	$-\frac{71}{1250000}n^2 + 141.62n + 3.9276$	$0.2459n^2 + 282.2090n + 4.2200$
$(5,n)$	$-\frac{3}{40000}n^2 + 176.73n + 4.9814$	$0.5950n^2 + 352.1405n + 4.7810$
$(6,n)$	$-\frac{29}{312500}n^2 + 211.82n + 6.0522$	$1.0525n^2 + 422.0430n + 4.9450$
$(7,n)$	$-\frac{551}{5000000}n^2 + 246.89n + 7.1400$	$1.6184n^2 + 491.9165n + 4.7120$
$(8,n)$	$-\frac{159}{1250000}n^2 + 281.94n + 8.2448$	$2.2927n^2 + 561.7610n + 4.0820$
$(9,n)$	$-\frac{719}{5000000}n^2 + 316.97n + 9.3666$	$3.0754n^2 + 631.5765n + 3.0550$
$(10,n)$	$-\frac{1}{6250}n^2 + 351.98n + 10.5054$	$3.9665n^2 + 701.3630n + 1.6310$

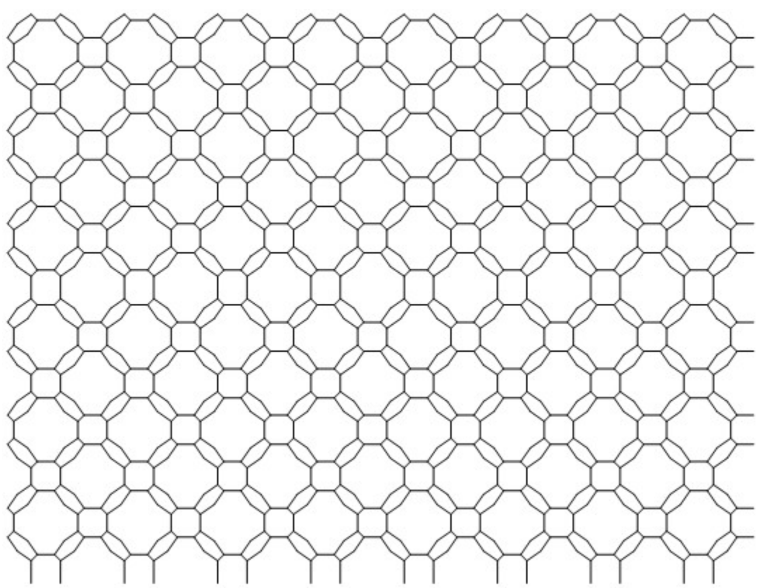

Figure 5.8: Benzene ring embedded in p-type-surface in 2D network(BRE).

Table 5.17: Equations extracted from the coefficient of the equations in Table 5.16

	Energy$(E(BRE))$	Estrada index$(EE(BRE))$
n^2	$2\times10^{-7}m^2-2\times10^{-5}m-2\times10^{-5}$	$0.0542m^2-0.1387m-0.0665$
n	$-0.01m^2+35.2m+0.98$	$-0.0145m^2+70.062m+2.193$
1	$-0.0085m^2+0.9773m-0.1176$	$-0.1985m^2+2.3475m-1.994$

The errors of energy and Estrada index have been found in the Tables 5.18 and 5.19 and inertia, signature and nullity in Table 5.20

Table 5.18: The $E_x(BRE)$ and $E_s(BRE)$ values of the energy of the BRE

(m,n)	E_{ext}(BRE)	E_{ast}(BRE)	Error
$(3,1)$	109.3768	109.3782	0.0014
$(3,2)$	215.8872	215.8908	0.0036
$(3,3)$	322.3614	322.3604	-0.001
$(3,4)$	428.834	428.8253	-0.0087
$(3,5)$	535.3054	535.1707	-0.1347
$(3,6)$	641.779	641.5113	-0.2677
$(3,7)$	748.2644533	747.809	-0.4554
$(3,8)$	854.7426876	854.0636	-0.679
$(3,9)$	961.2209219	960.2753	-0.9456
$(3,10)$	1067.699156	1066.444	-1.2551

Table 5.19: The $EE_{ext}(BRE)$ and $EE_{ast}(BRE)$ values of the Estrada index of the BRE

(m,n)	EE_{ext}(BRE)	EE_{ast}(BRE)	Error
$(3,1)$	215.519	215.515	−0.004
$(3,2)$	427.787	427.780	−0.007
$(3,3)$	640.066	640.054	−0.012
$(3,4)$	852.338	852.341	−0.002
$(3,5)$	1064.611	1064.634	0.023
$(3,6)$	1276.885	1276.940	−0.055
$(3,7)$	1489.158	1489.256	0.098
$(3,8)$	1701.432	1701.583	0.151
$(3,9)$	1913.705	1913.920	0.215
$(3,10)$	2125.979	2126.267	0.288

Table 5.20: The inertia, nullity and signature of BRE

BRE=Benzene Ring Embedded	$p(BRE)$	$n(BRE)$	$\eta(BRE)$	$s(BRE)$
$(3,1)$	39	39	2	0
$(3,2)$	76	76	2	0
$(3,3)$	113	113	2	0
$(3,4)$	150	150	2	0
$(3,5)$	187	187	2	0
$(3,6)$	224	224	2	0
$(3,7)$	261	261	2	0
$(3,8)$	298	298	2	0
$(3,9)$	335	335	2	0
$(3,10)$	372	372	2	0
$(3,11)$	409	409	2	0
$(3,12)$	446	446	2	0

We have observed that exact value of energy of BRE is less than for first two terms, the gradually increases from the estimated values of energy of BRE. Similarly, we have observed that exact value of Estrada index of BRE is less than the estimated values of Estrada index of BRE, for few terms, then suddenly behavior is changed for the remaining five values.

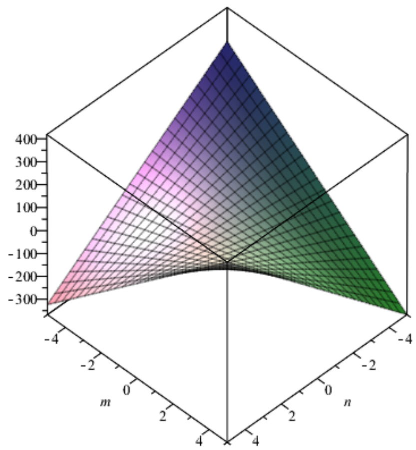

Figure 5.9: Energy of Bismuth Tri-iodide.

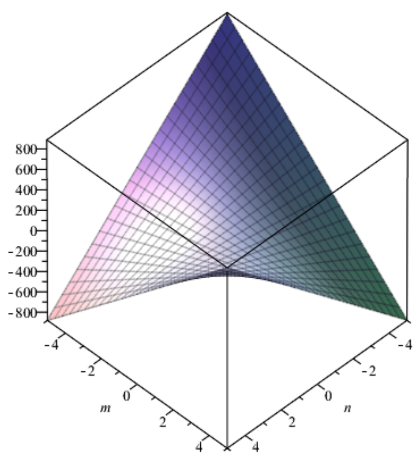

Figure 5.10: Energy of BRE.

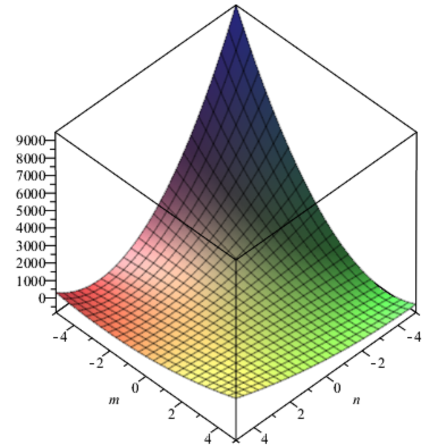

Figure 5.11: Estrada index Bismuth Tri-iodide.

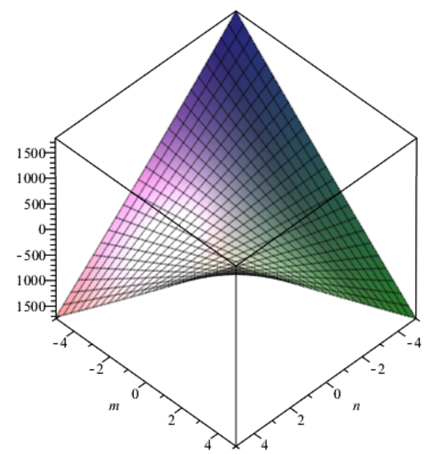

Figure 5.12: Estrada index *BRE*.

Chapter 6

Metric Dimension

6.1 Introduction

Distance based parameters in graph theory are getting high attention these days due to its effectiveness in daily life. One of them, namely, the metric dimension has addressed many investigations. The term metric dimension was introduced by Slater [88] and also studied by Harary and Melter independently [43]. Metric Dimension is much popular these days due to its vast application in daily life. Metric dimension is basically a distance based parameter which is applicable in different distance related problems such as robotic navigation, mastermind game and so many other fields.

6.1.1 Basic Terms Related to Distance Based Parameters

Definition 6.1.1. Let G be a simple finite connected graph and the distance from a to b is described as the shortest path length between these two vertices a and b and it is denoted by $d(a,b)$.

Definition 6.1.2. The eccentricity of a vertex b of a graph G, denoted by $e(b)$, is described as the maximum distance between a vertex to all other vertices of graph G.

Definition 6.1.3. Diameter is the maximum eccentricity between the overall vertices of graph G and is denoted by $diam(G)$.

Definition 6.1.4. Radius is the smallest distance of a fixed vertex among all the vertices of graph G and is denoted by $rad(G)$.

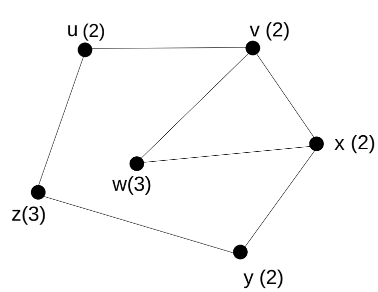

Figure 6.1: Graph with eccentricities of its vertices

The eccentricity of every vertex of a graph G is represented in the parenthesis shown above in the figure. The diameter and radius of the above graph G is 3 and 2, respectively.

Resolving Set and Metric Dimension

A vertex $y \in V(G)$ resolves a pair of vertices r, s if $d(y,r) \neq d(y,s)$. A set of vertices $Q \in V(G)$ resolves G if each pair of distinct vertices of G is resolved by some vertex in Q, then the set Q is said to be a resolving set of G. The set $Q = \{q_1, q_2, ..., q_m\}$ is an ordered set of distinct vertices. The smallest number of vertices in the resolving set is called a basis for G and this smallest number of vertices is the metric dimension of G, represented by $dim(G)$. The m-tuple $r(s/Q) = (d(s,q_1), d(s,q_2), d(s,q_3), ..., d(s,q_m))$ represents a vector, of a fixed vertex s with respect to the resolving set Q.

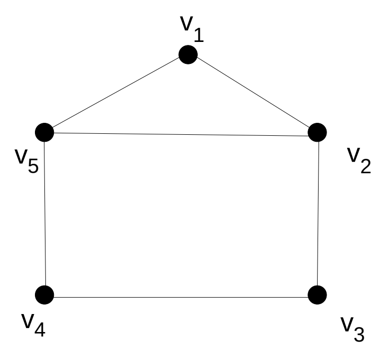

Figure 6.2: Graph whose metric dimension 2

The resolving set $Q = \{v_1, v_3\}$ is a basis for a graph G given above. The vertices of G with respect to the resolving set Q are $r(v_1/Q) = (0,2), r(v_2/Q) = (1,1), r(v_2/Q) = (2,0), r(v_4/Q) = (2,1), r(v_5/Q) = (1,2)$.

6.1.2 Some Renowned Results about Metric Dimensions

The metric dimension has a prominent role in the field of graph theory. There are so many results already exist in literature on this notion. Caceres and Hernando has introduced the metric dimension of cartesian product of graphs [9]. The metric dimension is NP-complete for planar graphs has been described by Diaz et al. [21]. In [8], Buczkowski has proposed a formula of metric dimensions of wheel graphs. The metric dimension of corona product graphs has been studied by Yero et al. [96]. Garey and Johnson has proved that finding the metric dimension of an arbitrary graph is an NP-complete problem [34]. In [91], Tomescu has studied the metric dimension of Jahangir Graph when he visited Jahangir's tomb in Lahore. Ali et al. has been studied the metric dimension of the mobius ladder [2]. Chartrand has observed the metric dimension and presented the notion of sharp lower bounds and greatest degree [13]. The metric dimension of regular bipartite graph has also been investigated by Bǎca [3]. In [29], Fernau et al. has computed the metric dimension of chain graphs. Siddiqui and Imran have investigated the metric dimension of wheel related graph and convex polytopes generated by wheel related graph [86, 87]. The metric dimension arises in many diverse areas, including navigation of robots [56], telecommunications [6], combinatorial optimization [84] and sonar and coast guard Loran [88] and applications to chemistry in [12, 13, 52]. Furthermore, this topic has some applications to problems of pattern recognition and image processing, some of which involve the use of hierarchical data structures [72]. Metric dimension of several interesting classes of graphs can be seen in [1, 4, 5, 9, 46, 47, 48, 63]. Let $G = (V,E)$ be a simple and connected graph. For a vertex $x \in V(G)$ distinguishes two vertices $y,z \in V(G)$ if $d_G(y,x) \neq d_G(z,x)$, where $d_G(x,y)$ denotes the length of the shortest path between the vertices x and y in G. A vertex set $R_1 \subseteq V(G)$ is a metric generator for G, if any pair of vertices of G is distinguished by at least one vertex of R_1 and R_1 is the resolving set of G. The minimum cardinality of any metric generator for G is the metric dimension of G, denoted by $dim(G)$. Let $R_1 = \{r_1, r_2, \ldots, r_s\}$ be an ordered set of vertices of G and let $x \in V(G)$, then the *representation* $r(x|R_1)$ of x with respect to R_1 is the s-tuple $(d_G(x,r_1), d_G(x,r_2), d_G(x,r_3), \ldots, d_G(x,r_s))$. Since the set R_1 has the minimum cardinality, therefore this is also known as the basis of G, and its cardinality is called the metric dimension or location number [8].

6.2 Edge Metric Dimensions

Edge metric dimension is recently proposed in [54]. In edge metric dimension, a natural question comes into our mind: are there some sets of vertices which uniquely identify all the edges of graph? The answer is yes. So it is our aim to study such sets for the barycentric subdivision of Cayley graph $Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2)$. Now we will introduce some basic terminologies regarding distance based parameters.

Similarly, for $x \in V(G)$ be a vertex and $e = yz \in E(G)$ be an edge. The distance between the vertex x and the edge e is given by $d_G(x,e) = \min\{d_G(x,y), d_G(x,z)\}$. A vertex $t \in V(G)$ distinguishes two edges $e, f \in E(G)$ if $d_G(t,e) \neq d_G(t,f)$. A set $R \subseteq V(G)$ is an edge metric generator for G if every two edges of G are distinguished by some vertex of R. The minimum cardinality of R is called the edge metric dimension and is denoted by $edim(G)$ [54]. Let $R = \{r_1, r_2, \ldots, r_t\}$ be an ordered set of vertices of G and let $e \in E(G)$, then the *representation* $r(e|R)$ of e with respect to R is the t-tuple $(d_G(e,r_1), d_G(e,r_2), d_G(e,r_3), \ldots, d_G(e,r_t))$. In addition, combined (mixed) form of these two parameters depicted above is of fascinate. A vertex $x \in V(G)$ distinguishes two elements (vertices or edges) $u, v \in V(G) \cup E(G)$ if $d_G(x,u) \neq d_G(x,v)$. A set $R^m \subseteq V(G)$ is a mixed metric generator for G if every two distinct elements (vertices or edges) of G are distinguished by some vertices of R^m. The smallest cardinality of R^m is the mixed metric dimension and is denoted by $mdim(G)$ [53]. Geometrically, an operation that splits an edge into two edges by inserting a new vertex into the interior of an edge is known as subdividing an edge. If we are performing a sequence of edge-subdivision operations, then it is called *Subdividing a graph G* and resulting graph is called a *subdivision of the graph G*. The subdivision of graph can be used to convert a general graph into a simple graph. If we subdividing each edge of the graph G, then this subdivision is called the *barycentric subdivision* of G. Gross and Yellen [38] proved the results that the barycentric subdivision of any graph is a simple and bipartite graph. A graph G is *planar* if it can be drawn in the plane without edge crossings. Subdivision of graphs play a very important role in characterization of planar graphs. A graph G is planar if and only if every subdivision of G is planar. Two graphs are said to be homeomorphic if they are subdivisions of same graph G. The next theorem gives a nice characterization of planar graphs.

Theorem 6.2.1. [38] *"A graph is planar if and only if it does not contain a subdivision of K_5 or $K_{3,3}$"*.

In this section, we study the edge metric dimension of barycentric subdivision of Cayley graphs $Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2)$. We prove that these subdivisions of Cayley graphs have constant edge metric dimension and only three vertices chosen appropriately suffice to resolve all the vertices of these subdivision of Cayley graphs $Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2)$. As expressed, there are a several graphs in which metric generator and edge metric generator are same. In this sense, one could believe that most likely any edge metric generator R is likewise a standard metric generator. In any case, this is again further far from the truth, despite the fact that there are a few families of graphs in which such actualities happen. Kelenc *et al.* [54] explained some comparison between the edge metric generator and standard metric generator in detailed. We show a few results concerning the edge metric dimension of graphs. The first importance result about the complexity is as follows:

Theorem 6.2.2. [54] *"Computing the edge metric dimension of graphs is NP-hard."*

The edge metric dimension of Cartesian product of two paths P_r and P_t with r and t vertices is determined in the following proposition.

Proposition 6.2.3. [54] *"Let G be the grid graph $G = P_r \square P_t$, with $r \geq t \geq 2$. Then $edim(G) = dim(G) = 2$."*

Kelenc *et al.* [54] proved in the next Proposition that the edge metric dimension of wheel graphs is unbounded and observe it is strictly larger than the value for the metric dimension, except in the case $W_{1,3}$. The wheel graph $W_{1,n}$ is the graph obtained from a cycle $C_n, n \geq 3$ by joining all vertices of C_n to an additional vertex. In [54], they determined the edge metric dimension of wheel graph $W_{1,n}$ in the following Proposition:

Proposition 6.2.4. [54] *" Let $W_{1,n}$ be a wheel graph. Then*

$$edim(W_{1,n}) = \begin{cases} n, & for\, n = 3,4 \\ n-1, & for\, n \geq 5 \end{cases} \text{"}$$

The fan graph $F_{1,n}$ is the graph obtained by joining each vertex of a path P_n, to an additional vertex. In the next proposition, the edge metric dimension of fan graph $F_{1,n}$ is determined.

Proposition 6.2.5. [54]*"Let $F_{1,n}$ be a fan graph. Then*

$$edim(F_{1,n}) = \begin{cases} n, & for\, n = 1,2,3 \\ n-1, & for\, n \geq 4 \end{cases} \text{"}$$

Kelenc *et al.* [54] also determined the edge metric dimension of path, cycle, complete graph, complete bipartite, cartesian product of cycles and bounds for some families of graphs.

6.3 The Edge Metric Dimension of Barcycentric Subdivision of Cayley Graphs $Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2)$

Let G be a semigroup, and let H be a nonempty subset of G. The Cayley graph $Cay(G,H)$ of G relative to H is defined as the graph with vertex set G and edge set $E(H)$ consisting of those ordered pairs (a,b) such that $ha = b$ for some $h \in H$. Cayley graphs of groups are significant both in group theory and in constructions of interesting graphs with nice properties. The Cayley graph $Cay(G,H)$ of a group G is symmetric or undirected if and only if $H = H^{-1}$. The Cayley graphs $Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2), n \geq 3$, is a 3-regular graph which is also known as the cartesian product $C_n \square P_2$ of a cycle of order n with a path of order 2. The Cayley graphs $Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2), n \geq 3$ consists of an inner n-cycle $a_1a_2a_3 \ldots a_na_1$, an outer n-cycle $x_1x_2x_3 \ldots x_nx_1$ and n spokes $a_ix_i, 1 \leq i \leq n$. This implies that the order and size of $Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2)$ is $2n$ and $3n$, respectively. The metric dimension of Cayley graphs $Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2)$ has been determined in [9] while the metric dimension of Cayley graphs $Cay(\mathbb{Z}_n : H)$ for all $n \geq 7$ and $H = \{\pm 1, \pm 3\}$ hase been determined in [50]. The barycentric subdivision graph $BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))$ can be obtained by splitting edges a_ia_{i+1} by inserting a new vertices b_i, splitting edges a_ix_i by inserting a new vertices c_i splitting edges x_ix_{i+1} by inserting a new vertices y_i. From this we observe that , $BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))$ contains $5n$ vertices among of these $3n$ vertices of degree 2 and $2n$ vertices of degree 3 and $6n$ edges. In the next theorem, we prove that the metric dimension of the barycentric subdivision $BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))$ of is constant and only three vertices appropriately chosen suffice to resolve all the vertices of the $BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))$.

Theorem 6.3.1. *Let $BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))$ be the barycentric subdivision of Cayley graphs $(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))$. Then $edim(BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))) = 3$ for every $n \geq 6$.*

Proof. We will prove the result by double inequalities. To prove edge metric dimension $edim(BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))) \leq 3$, we have the following cases: **Case 1.** When n is even.
Let $R = \{a_1, a_{\frac{n}{2}+1,a_n}\} \subset V(BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2)))$, we show that R is a resolving set for $BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))$ in this case. For this we give representations of any edge of $E(BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2)))$ with respect to R.
Representations for the edges of $BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))$ are

$$r(a_ib_i|R) = \begin{cases} (2i-2, n-2i+1, 2i), & \text{for } 1 \leq i \leq \frac{n}{2}-1 \\ (n-2, 1, n-1), & \text{for } i = \frac{n}{2} \\ (2n-2i+1, 2i-n-2, 2n-2i-1), & \text{for } \frac{n}{2}+1 \leq i \leq n-1 \\ (1, n-2, 0), & \text{for } i = n \end{cases}$$

and

$$r(b_ia_{i+1}|R) = \begin{cases} (2i-1, n-2i, 2i+1), & \text{for } 1 \leq i \leq \frac{n}{2}-1 \\ (n-1, 0, n-2), & \text{for } i = \frac{n}{2} \\ (2n-2i, 2i-n-1, 2n-2i-2), & \text{for } \frac{n}{2}+1 \leq i \leq n-1 \\ (0, n-1, 1), & \text{for } i = n \end{cases}$$

Representations for the set of interior edges of $BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))$ are

$$r(a_ic_i|R) = \begin{cases} (2i-2, n-2i+2, 2i), & \text{for } 1 \leq i \leq \frac{n}{2} \\ (2n-2i+2, 2i-n-2, 2n-2i), & \text{for } \frac{n}{2}+1 \leq i \leq n \end{cases}$$

and

$$r(c_ix_i|R) = \begin{cases} (2i-1, n-2i+3, 2i+1), & \text{for } 1 \leq i \leq \frac{n}{2} \\ (2n-2i+3, 2i-n-1, 2n-2i+1), & \text{for } \frac{n}{2}+1 \leq i \leq n \end{cases}$$

Representations for the edges on the outer cycle of $BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))$ are

$$r(x_iy_i|R) = \begin{cases} (2i, n-2i+3, 2i+2), & \text{for } 1 \leq i \leq \frac{n}{2}-1 \\ (n, 3, n+1), & \text{for } i = \frac{n}{2} \\ (2n-2i+3, 2i-n, 2n-2i+1), & \text{for } \frac{n}{2}+1 \leq i \leq n-1 \\ (3, n, 2), & \text{for } i = n \end{cases}$$

and

$$r(y_ix_{i+1}|R)=\begin{cases}(2i+1,n-2i+2,2i+3), & \text{for}\, 1\leq i\leq \frac{n}{2}-1\\ (n+1,2,n), & \text{for}\, i=\frac{n}{2}\\ (2n-2i+2,2i-n+1,2n-2i), & \text{for}\, \frac{n}{2}+1\leq i\leq n-1\\ (2,n+1,3), & \text{for}\, i=n\end{cases}$$

We note that there are no two edges having the same representations implying that $edim(BS(Cay(\mathbb{Z}_n\oplus\mathbb{Z}_2)))\leq 3$.

On the other hand, we show that $edim(BS(Cay(\mathbb{Z}_n\oplus\mathbb{Z}_2)))\geq 3$. Suppose on contrary that $edim(BS(Cay(\mathbb{Z}_n\oplus\mathbb{Z}_2)))=2$, then there are the following possibilities to be discussed.

(1) Both vertices are in the inner cycle. Here are the following subcases.

• Both vertices belong to the set $\{a_i : 1\leq i\leq n\}$. Without loss of generality, we can suppose that one resolving vertex is a_1. Suppose that the second resolving vertex is a_k $(2\leq k\leq \frac{n}{2}+1)$. Then for $2\leq k\leq \frac{n}{2}$, we have $r(a_1c_1|\{a_1,a_k\})=r(a_1b_n|\{a_1,a_k\})=(0,2k-2)$, and for $k=\frac{n}{2}+1$, we have $r(a_1b_1|\{a_1,a_{\frac{n}{2}+1}\})=r(a_1b_n|\{a_1,a_{\frac{n}{2}+1}\})=(0,n-1)$, a contradiction.

• Both vertices belong to the set $\{b_i : 1\leq i\leq n\}$. Without loss of generality, we can suppose that one resolving vertex is b_1. Suppose that the second resolving vertex is b_k $(2\leq k\leq \frac{n}{2}+1)$. Then for $2\leq k\leq \frac{n}{2}$, we have $r(a_1c_1|\{b_1,b_k\})=r(a_1b_n|\{(b_1,b_k\})=(1,2k-1)$, and for $k=\frac{n}{2}+1$, we have $r(a_1b_1|\{b_1,b_{\frac{n}{2}+1}\})=r(a_2b_1|\{b_1,b_{\frac{n}{2}+1}\})=(0,n-1)$, a contradiction.

• One vertex belong to the set $\{a_i : 1\leq i\leq n\}$ and the second vertex belong to the set $\{b_i : 1\leq i\leq n\}$. Without loss of generality, we can suppose that one resolving vertex is a_1. Suppose that the second resolving vertex is b_k $(1\leq k\leq \frac{n}{2}+1)$. Then for $1\leq k\leq \frac{n}{2}$, we have $r(a_1b_n|\{a_1,b_k\})=r(a_1c_1|\{a_1,b_k\})=(0,2k-1)$, and for $k=\frac{n}{2}+1$, we have $r(a_1b_1|\{a_1,b_{\frac{n}{2}+1}\})=r(a_1c_1|\{a_1,b_{\frac{n}{2}+1}\})=(0,n-1)$, a contradiction.

(2) Both vertices are in the interior vertices. Without loss of generality, we can suppose that one resolving vertex is c_1. Suppose that the second resolving vertex is c_k $(2\leq k\leq \frac{n}{2}+1)$. Then for $2\leq k\leq \frac{n}{2}+1$, we have $r(x_1c_1|\{c_1,c_k\})=r(a_1c_1|\{c_1,c_k\})=(0,2k-1)$, a contradiction.

(3) Both vertices are in the outer cycle. Due to the symmetry of the graph, this case is analogous to case **(1)**.

(4) One vertex is in the inner cycle and the other one is in the set of interior vertices. Here are the two subcases.

• One vertex is in the set $\{a_i : 1 \leq i \leq n\}$ and the other one is in the set of interior vertices $\{c_i : 1 \leq i \leq n\}$. Without loss of generality, we can suppose that one resolving vertex is a_1. Suppose that the second resolving vertex is c_k $(1 \leq k \leq \frac{n}{2}+1)$. Then for $k = 1$, we have $r(a_1b_1|\{a_1, c_1\}) = r(a_1b_n|\{a_1, c_1\}) = (0, 1)$. For $2 \leq k \leq \frac{n}{2}$, we have $r(a_1b_n|\{a_1, c_k\}) = r(a_1c_1|\{a_1, c_k\}) = (0, 2k-1)$ and for $k = \frac{n}{2}+1$, we have $r(a_1b_n|\{a_1, c_{\frac{n}{2}+1}\}) = r(a_1b_1|\{a_1, c_{\frac{n}{2}+1}\}) = (0, 2n)$, a contradiction.

• One vertex is in the set $\{b_i : 1 \leq i \leq n\}$ and the other one is in the set of interior vertices $\{c_i : 1 \leq i \leq n\}$. Without loss of generality, we can suppose that one resolving vertex is b_1. Suppose that the second resolving vertex is c_k $(1 \leq k \leq \frac{n}{2}+1)$. Then for $k = 1$, we have $r(x_1y_1|\{b_1, c_1\}) = r(x_1y_n|\{b_1, c_1\}) = (3, 1)$. For $2 \leq k \leq \frac{n}{2}$, we have $r(a_1c_1|\{b_1, c_k\}) = r(a_1b_n|\{b_1, c_k\}) = (1, 2k-1)$ and for $k = \frac{n}{2}+1$, we have $r(c_2x_2|\{b_1, c_{\frac{n}{2}+1}\}) = r(a_nb_n|\{b_1, c_{\frac{n}{2}+1}\}) = (2, n-1)$, a contradiction.

(5) One vertex is in the outer cycle and the other one is in the set of interior vertices. Due to the symmetry of the graph, this case is analogous to case **(4)**.

(6) One vertex is in the inner cycle and the other one is in the outer cycle. Here are the following subcases.

• One vertex is in the set $\{a_i : 1 \leq i \leq n\}$ and the other one is in the set $\{x_i : 1 \leq i \leq n\}$. Without loss of generality, we can suppose that one resolving vertex is a_1. Suppose that the second resolving vertex is x_k $(1 \leq k \leq \frac{n}{2}+1)$. Then for $k = 1$, we have $r(a_1b_1|\{a_1, x_1\}) = r(a_1b_n|\{a_1, x_1\}) = (0, 2)$. For $2 \leq k \leq \frac{n}{2}+1$, we have $r(a_1b_1|\{a_1, x_k\}) = r(a_1c_1|\{a_1, x_k\}) = (0, 2k-1)$, a contradiction.

• One vertex is in the set $\{a_i : 1 \leq i \leq n\}$ and the other one is in the set $\{y_i : 1 \leq i \leq n\}$. Without loss of generality, we can suppose that one resolving vertex is a_1. Suppose that the second resolving vertex is y_k $(1 \leq k \leq \frac{n}{2}+1)$. Then for $k = 1$, we have $r(a_1b_1|\{a_1, y_1\}) = r(a_1b_n|\{a_1, y_1\}) = (0, 3)$. For $2 \leq k \leq \frac{n}{2}$, we have $r(a_1b_1|\{a_1, y_k\}) = r(a_1c_1|\{a_1, y_k\}) = (0, 2k)$ and for $k = \frac{n}{2}+1$, we have $r(a_1b_1|\{a_1, y_{\frac{n}{2}+1}\}) = r(a_1c_1|\{a_1, y_{\frac{n}{2}+1}\}) = (0, n+1)$, a contradiction.

• One vertex is in the set $\{b_i : 1 \leq i \leq n\}$ and the other one is in the set $\{y_i : 1 \leq i \leq n\}$. Without loss of generality, we can suppose that one resolving vertex is b_1. Suppose that the second resolving vertex is y_k $(1 \leq k \leq \frac{n}{2}+1)$. Then for $k=1$, we have $r(a_1b_1|\{b_1,y_1\}) = r(a_2b_1|\{b_1,y_1\}) = (0,3)$. For $k=2$, we have $r(x_1y_1|\{b_1,y_2\}) = r(a_3c_3|\{b_1,y_2\}) = (3,2)$. For $3 \leq k \leq \frac{n}{2}+1$, we have $r(x_2y_2|\{b_1,y_k\}) = r(a_3c_3|\{b_1,y_k\}) = (3,2k-4)$, a contradiction.

Hence from above it follows that there is no resolving set with two vertices for $V(BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2)))$ implying that $edim(BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))) \neq 2$ in this case. Therefore, $edim(BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))) = 3$.

Case 2. When n is odd.

Let $R = \{a_1, b_{\lceil \frac{n}{2} \rceil}, a_n\} \subset V(BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2)))$, we show that R is a resolving set for $BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))$ in this case. For this we give representations of any edge of $E(BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2)))$ with respect to R.

Representations for the edges of of the inner cycle of $BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))$ are

$$r(a_ib_i|R) = \begin{cases} (2i-2, n+1-2i, 2i), & \text{for } 1 \leq i \leq \lceil \frac{n}{2} \rceil - 1 \\ (2i-2, n+1-2i, 2n-2i-1), & \text{for } i = \lceil \frac{n}{2} \rceil \\ (2n-2i+1, 2i-n-2, 2n-2i-1), & \text{for } \lceil \frac{n}{2} \rceil + 1 \leq i \leq n-1 \\ (1, n-2, 0), & \text{for } i = n. \end{cases}$$

and

$$r(b_ia_{i+1}|R) = \begin{cases} (2i-1, n-2i, 2i+1), & \text{for } 1 \leq i \leq \lceil \frac{n}{2} \rceil - 2 \\ (2i-1, n-2i, 2n-2i-2), & \text{for } i = \lceil \frac{n}{2} \rceil - 1 \\ (2n-2i, 2i-n-1, 2n-2i-2), & \text{for } \lceil \frac{n}{2} \rceil \leq i \leq n-1 \\ (0, n-1, 1), & \text{for } i = n \end{cases}$$

Representations for the edges on the outer cycle of $BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))$ are

$$r(x_iy_i|R) = \begin{cases} (2i, n+3-2i, 2i+2), & \text{for } 1 \le i \le \lceil \frac{n}{2} \rceil - 1 \\ (2i, n-2i+3, 2n-2i+1), & \text{for } i = \lceil \frac{n}{2} \rceil \\ (2n-2i+3, 2i-n, 2n-2i+1), & \text{for } \lceil \frac{n}{2} \rceil + 1 \le i \le n-1 \\ (3, n, 2), & \text{for } i = n \end{cases}$$

and

$$r(y_ix_{i+1}|R) = \begin{cases} (2i+1, n-2i+2, 2i+3), & \text{for } 1 \le i \le \lceil \frac{n}{2} \rceil - 2 \\ (2i+1, n-2i+2, 2n-2i), & \text{for } i = \lceil \frac{n}{2} \rceil - 1 \\ (2n-2i+2, 3, 2n-2i), & \text{for } i = \lceil \frac{n}{2} \rceil \\ (2n-2i+2, 2i-n+1, 2n-2i), & \text{for } \lceil \frac{n}{2} \rceil + 1 \le i \le n-1 \\ (2, n+1, 3), & \text{for } i = n \end{cases}$$

Representations for the set of interior edges of $BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))$ are

$$r(a_ic_i|R) = \begin{cases} (2i-2, n-2i+2, 2i), & \text{for } 1 \le i \le \lceil \frac{n}{2} \rceil - 1 \\ (2i-2, n-2i+2, 2n-2i), & \text{for } i = \lceil \frac{n}{2} \rceil \\ (2n-2i+2, 2i-n-2, 2n-2i), & \text{for } \lceil \frac{n}{2} \rceil + 1 \le i \le n \end{cases}$$

$$r(c_ix_i|R) = \begin{cases} (2i-1, n-2i+3, 2i+1), & \text{for } 1 \le i \le \lceil \frac{n}{2} \rceil - 1 \\ (2i-1, n-2i+3, 2n-2i+1), & \text{for } i = \lceil \frac{n}{2} \rceil \\ (2n-2i+3, 2i-n-1, 2n-2i+1), & \text{for } \lceil \frac{n}{2} \rceil + 1 \le i \le n \end{cases}$$

Again we see that there are no two vertices having the same representations which implies that $edim(BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))) \le 3$.

On the other hand, suppose that $edim(BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))) = 2$, then there are the same possibilities as in case (1) and contradictions can be deduced analogously. This implies that $edim(BS(Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2))) = 3$ in this case, which completes the proof.

□

Chapter 7

Conclusion and Open Problems

In this thesis first we have found the M-polynomial and entropy of generalized Sierpinski graphs of some particular graphs. We have also studied the degree based topological indices of paraline graphs such as Randic index, general Randic index, Zagreb index, general sum connectivity index, first and second multiple Zagreb indices, geometric index, atom bond connectivity index for para-line graphs of some chemical structures such as Phenylene, Anthracene, Benzenoid, and Pentacene. There are still other classes of generalized Sierpinski graphs and many chemical networks whose degree based topological, M-polynomials and entropy of line and paraline graphs are not found. Thus we give following open problems.

Open Problem 1.

Find the M-Polynomial for the line graph of other classes of generalized Sierpinski graphs.

Open Problem 2.

Find the entropy for the line graph and the para-line graph of generalized Sierpinski graphs.

In Chapter five, we studied Estrada index, Energy, Inertia, Nullity, and Signature of Phenylene, Anthracene, Bismuth Tri-iodide and BRE. The following inequalities $E_x(P) > E_s(P)$, $EE_x(P) > EE_s(P)$, $E_x(A) > E_s(A)$ and $EE_x(A) > EE_s(A)$ have been observed between exact and estimated values of energy of Phenylene and Anthracene.

Also $E_{ext}(B) > E_{est}(B)$, $EE_{ext}(B) > EE_{est}(B)$, $E_{ext}(BRE) > E_{est}(BRE)$ and $EE_{ext}\ (BRE) > EE_{est}(BRE)$ have been observed between exact and estimated values of energy of Bismuth Tri-iodide and BRE. One can also use the method used to find the spectrum based indices in this thesis to find the results for other chemical structures.

We use quadratic equations to estimates these results one can use other types of equations to find energy of the above mention structures and give better approximation than we found using quadratic equations.

Open Problem 3.

Use other types of equations to estimates the energy and Estrada index of other structures.

In chapter six, we have explained the notion of distance related parameters such as metric dimension and edge metric dimension and computed the edge metric dimension for the barcycentric subdivision of Cayley graph .

Chapter 8

References

[1] Ahmad, A., Baca, M., & Sultan, S. (2018). Minimal Doubly Resolving Sets of Necklace Graph. *Math. Rep*, 20, 123-129.

[2] Ali, M., Ali, G., Imran, M., Baig, A. Q., & Shafiq, M. K. (2012). On the metric dimension of Mobius ladders. *Ars Combinatoria*, 105, 403-410.

[3] Bača, M., Baskoro, E. T., Salman, A. N. M., Saputro, S. W., & Suprijanto, D. (2011). On metric dimension of regular bipartite graphs, *Bull. Math. Soc. Sci.Math. Roumanie* 54,15-28.

[4] Bailey, R. F., & Cameron, P. J. (2011). Base size, metric dimension and other invariants of groups and graphs. *Bull London Math Soc.* 43(2), 209-242.

[5] Bailey, R. F., & Meagher, K. (2010). On the metric dimension of Grassmann graphs, *Discret Math Theo Comput Sci.* 13(4), 97–104.

[6] Beerliova, Z., Eberhard, F., Erlebach, T., Hall, A., Hoffmann, M., Mihal'ak, M., & Ram, L. S. (2006). Network discovery and verification, *IEEE J. Sel. Area Comm.* 24, 2168–2181.

[7] Brückler, F. M., Došlic, T., Graovac, A., & Gutman, I. (2011). On a class of distance-based molecular structure descriptors. *Chem. phys. lett.* 503(4-6), 336-338.

[8] Buczkowski, P., Chartrand, G., Poisson, C., & Zhang, P. (2003). On k-dimensional graphs and their basis, *Periodica Math. Hung.* 46,9-15.

[9] Cáceres, J., Hernando, C., Mora, M., Pelayo, I. M., Puertas, M. L., Seara, C., & Wood, D. R. (2007). On the metric dimension of cartesian products of graphs. *SIAM J Discrete Math*, 21(2), 423-441.

[10] Cash, G. G. (2002). Relationship between the Hosoya polynomial and the hyper-Wiener index. *Appl. Math. Lett.*, 15(7), 893-895.

[11] Cayley, A. (1889—1897). On the theory of the analytical forms called trees. *Math. Papers*,Cambridge, 3, 242-–246.

[12] Chartrand, G., Eroh, L., Johnson, M. A., & Oellermann, O. R. (2000). Resolvability in graphs and the metric dimension of a graph. *Discrete Appl Math*, 105(1-3), 99-113.

[13] Chartrand, G., Poisson, C., & Zhang, P. (2000). Resolvability and the upper dimension of graphs. *Comput Math Appl.* 39(12), 19-28.

[14] Chen, Z., Dehmer, M., Emmert-Streib, F., & Shi, Y. (2015). Entropy of Weighted Graphs with Randi c Weights. *Entropy*, 17(6), 3710-3723.

[15] Chou, C. P., & Witek, H. A. (2014). Closed-form formulas for the Zhang-Zhang polynomials of benzenoid structures: chevrons and generalized chevrons. *MATCH Commun. Math. Comput. Chem*, 72, 105-124.

[16] Crosland, M. P. (1959). The use of diagrams as chemical 'equations' in the lecture notes of William Cullen and Joseph Black. *Ann Sci*, 15(2), 75-90.

[17] Cvetkovic, D., Doob, M, & H. Sachs, (1995). Spectra of Graphs-Theory and Application, third ed., Johann Ambrosius Barth Verlag, Heidelberg, Leipzig.

[18] Cvetkovic, D., Rowlinson, P., & Simic, S. (2001). An Introduction to the Theory of Graph Spectra London Mathematical Society Student Texts. Cambridge: Cambridge University Press.

[19] Das, K. C., Zhou, B., & Trinajstić, N. (2009). Bounds on Harary index. *J Math Chem*, 46(4), 1377-1393.

[20] Deutsch, E., & Klavžar, S. (2014). M-polynomial and degree-based topological indices. arXiv preprint arXiv:1407.1592.

[21] Díaz, J., Pottonen, O., Serna, M., & Van Leeuwen, E. J. (2012). On the complexity of metric dimension. In European Symposium on Algorithms . Springer, Berlin, Heidelberg. 419-430.

[22] Diestel, R. (2018) Graph theory. Springer Publishing Company, Incorporated.

[23] Dureja, H., Gupta, S., & Madan, A. K. (2008). Predicting anti-HIV-1 activity of 6-arylbenzonitriles: Computational approach using superaugmented eccentric connectivity topochemical indices. Journal of Molecular Graphics and Modelling, 26(6), 1020-1029.

[24] Eagle, N., Macy, M., & Claxton, R. (2010). Network diversity and economic development. *Science*, 328(5981), 1029-1031.

[25] Estrada, E., & Rodriguez, L. (1997). Matrix algebraic manipulation of molecular graphs. 2. Harary-and MTI-like molecular descriptors. *MATCH Commun. Math. Comput. Chem*, 35, 157-167.

[26] Estrada, E., Torres, L., Rodriguez, L., & Gutman, I. (1998). An atom-bond connectivity index: modelling the enthalpy of formation of alkanes. *Indian journal of chemistry*. Sect. A: Inorganic, physical, theoretical & analytical, 37(10), 849-855.

[27] Euler, L. (1927). Solutio problematic ad Geometrian situs pertinentis, Comm Acad Petropolitanae 8: 128-–140. Translated in: Speiser klassische Stücke der Mathematik, Zürich, 127-138.

[28] Farrell, E. J. (1979). An introduction to matching polynomials. *J. Combin. Theory Ser.* B, 27(1), 75-86.

[29] Fernau, H., Heggernes, P., van't Hof, P., Meister, D., & Saei, R. (2015). Computing the metric dimension for chain graphs. *Inform Process Lett*, 115(9), 671-676.

[30] Fowler, P. W., & Pisanski, T. (2010). HOMO-LUMO maps for chemical graphs. *MATCH Commun. Math. Comput. Chem*, 64(2), 373-390.

[31] Fowler, P. W., & Pisanski, T. (2010). HOMO-LUMO maps for fullerenes, *Acta Chim. Slov.*, 57(3), 513-517.

[32] Gao, W., Farahani, M. R., & Shi, L. (2016). Forgotten topological index of some drug structures. *Acta Medica Mediterr*, 32(1), 579-585.

[33] Gao, W., Wang, W., & Fara hani, M. R. (2016). Topological indices study of molecular structure in anticancer drugs. *J. Chem. NY*.

[34] Gary, M. R., & Johnson, D. S. (1979). Computers and Intractability: A Guide to the Theory of NP-completeness.

[35] Ghorbani, M., & Hosseinzadeh, M. A. (2010). Computing ABC4 index of nanostar dendrimers. *Optoelectron. Adv. Mater. Rapid Commun*, 4(9), 1419-1422.

[36] Graovac, A., Ghorbani, M., & Hosseinzadeh, M. A. (2011). Computing fifth geometric-arithmetic index for nanostar dendrimers. Journal of Mathematical Nanoscience, 1(1), 33-42.

[37] Gravier, S., Kovse, M., & Parreau, A. (2011) Generalized Sierpinski graphs. Poster, Euro-Comb11, Budapest.

[38] Gross, J. L., & Yellen, J. (2005). Graph theory and its applications. Chapman and Hall/CRC.

[39] Gupta, S., Singh, M., & Madan, A. K. (2002). Eccentric distance sum: A novel graph invariant for predicting biological and physical properties. J. Math. Anal. Appl., 275(1), 386-401.

[40] Gutman, I. (1977). The acyclic polynomial of a graph. *Publ. Inst. Math.(Beograd)(NS)*, 22(36), 63-69.

[41] Gutman, I., Ruščić, B., Trinajstić, N., & Wilcox Jr, C. F. (1975). Graph theory and molecular orbitals. XII. Acyclic polyenes. The Journal of Chemical Physics, 62(9), 3399-3405.

[42] Gutman, I., Zhang, Y., Dehmer, M., & Ilic, A. (2012). Altenburg, Wiener, and Hosoya polynomials. Distance in Molecular Graphs-Theory, Univ. Kragujevac, Kragujevac, 49-70.

[43] Harary, F., & Melter, R. A. (1976). On the metric dimension of a graph. *Ars Combinatoria*, 2(191-195), 1.

[44] Hassani, F., Iranmanesh, A., & Mirzaie, S. (2013). Schultz and modified Schultz polynomials of C100 fullerene. *MATCH Commun. Math. Comput. Chem*, 69, 87-92.

[45] Hosoya,H. On some counting polynomials in chemistry, *Discrete Appl. Math.* 19 (1988) 239–257

[46] Imran, M., Ahmad, A., Al-Mushayt, O., & Bokhary, S. A. U. H. (2015). On the metric dimension of barcycentric subdivision of Cayley graphs $Cay(\mathbb{Z}_n \oplus \mathbb{Z}_2)$, *Miskolc Math Notes* 16(2), 637-646.

[47] Imran, M., Ahmad, A., Semaničová–Feňovčíková, (2013). On classes of regular graphs with constant metric dimension. *Acta Math. Sci.*, 33(1), 187-206.

[48] Imran, S., Siddiqui, M., Imran, M., Hussain, M., Bilal, H., Cheema, I., ... & Saleem, Z. (2018). Computing the metric dimension of gear graphs. *Symmetry*, 10(6), 209.

[49] Ivanciuc, O., Balaban, T. S., & Balaban, A. T. (1993). Design of topological indices. Part 4. Reciprocal distance matrix, related local vertex invariants and topological indices. *J. Math. Chem.*, 12(1), 309-318.

[50] Javaid, I., Azhar, M. N., & Salman, M. (2012). Metric dimension and determining number of Cayley graphs. *World Applied Sciences Journal*, 18(12), 1800-1812.

[51] Javaid, I., Rahim, M. T., & Ali, K. (2008). Families of regular graphs with constant metric dimension. *Utilitas Mathematica*, 75, 21-34.

[52] Johnson, M. (1993). Structure-activity maps for visualizing the graph variables arising in drug design. *J. Biopharm. Stat.*, 3(2), 203-236.

[53] Kelenc, A., Kuziak, D., Taranenko, A., & Yero, I. G. (2017). Mixed metric dimension of graphs. *Appl Math Comput.*, 314, 429-438.

[54] Kelenc, A., Tratnik, N., & Yero, I. G. (2018). Uniquely identifying the edges of a graph: the edge metric dimension. *Discrete Appl. Math.*, 251, 204-220.

[55] Khuller, S., Raghavachari, B., & Rosenfeld, A., “Localization in Graphs,” Technical Report CS-Tr3326, University of Maryland at College Park, 1994.

[56] Khuller, S., Raghavachari, B., & Rosenfeld, A. (1996). Landmarks in graphs. *Discrete Appl. Math.*, 70(3), 217-229.

[57] Kirchhoff, G. (1847). Ueber die Auflösung der Gleichungen, auf welche man bei der Untersuchung der linearen Vertheilung galvanischer Ströme geführt wird. Annalen der Physik, 148(12), 497-508.

[58] Klavžar, S., & Milutinovič, U. (1997). Graphs S (n, k) and a variant of the Tower of Hanoi problem. *Czech. Math. J.*, 47(1), 95-104.

[59] Kobler, J., Schöning, U., & Torán, J. (1994). The graph isomorphism problem: its structural complexity.

[60] Körner, J. (1973, September). Coding of an information source having ambiguous alphabet and the entropy of graphs. In 6th Prague conference on information theory, 411-425.

[61] Körner, J. (1986). Fredman–Komlós bounds and information theory. *SIAM J. Algebraic Discrete Methods*, 7(4), 560-570.

[62] Körner, J., Simonyi, G., & Tuza, Z. (1992). Perfect couples of graphs. *Combinatorica*, 12(2), 179-192.

[63] Kratica, J., Kovačević-Vujčić, V., Čangalović, M., & Stojanović, M. (2012). Minimal doubly resolving sets and the strong metric dimension of some convex polytopes. *Appl Math Comput.*, 218(19), 9790-9801.

[64] Kumar, V., Sardana, S., & Madan, A. K. (2004). Predicting anti-HIV activity of 2, 3-diaryl-1, 3-thiazolidin-4-ones: computational approach using reformed eccentric connectivity index. *J. Mol. Model.*, 10(5-6), 399-407.

[65] Li, X., & Gutman, I. (2006). Mathematical Aspects of Randic–Type Molecular Structure Descriptors, Univ. Kragujevac, Kragujevac.Serbia.

[66] Li, X., Shi, Y., & Zhong, L. (2008). Minimum general Randic index on chemical trees with given order and number of pendent vertices. *MATCH Commun. Math. Comput. Chem*, 60, 539-554.

[67] Li, X., Shi, Y., & Xu, T. (2006). Unicyclic Graphs with Maximum General Randic Index for alpha¿ 0. *MATCH-Commun.Math. Co.*, 56(3), 557-570.

[68] Li, X., & Zhao, H. (2004). Trees with the first three smallest and largest generalized topological indices. *MATCH Commun. Math. Comput. Chem*, 50, 57-62.

[69] Li, X., Shi, Y., & Gutman, I. (2012). Graph energy. Springer Science & Business Media.

[70] Lučić, B., Miličević, A., Nikolić, S., & Trinajstić, N. (2002). Harary index-twelve years later. *Croat. chem. acta*, 75(4), 847-868.

[71] Manjusha, R., & Sunny Kuriakose, A. (2015). METRIC DIMENSION AND UNCERTAINTY OF TRAVERSING ROBOTS IN ANetwork. *International Journal on Applications of Graph Theory in Wireless Ad Hoc Networks and Sensor Networks* (GRAPH-HOC), 7, 2-3.

[72] Melter, R. A., & Tomescu, I. (1984). Metric bases in digital geometry. *Computer Vision, Graphics, and Image Proc.*, 25(1), 113-121.

[73] Mufti, Z. S., Zafar, S., Zahid, Z., & Nadeem, M. F. (2017). Study of the paraline graphs of certain Benzenoid structures using topological indices. *MAGNT Research Report*, 2017, 4 (3), 110-116.

[74] Mufti, Z. S., Nadeem, M. F., Gao, W., & Ahmad, Z. (2018). Topological study of the para-line graphs of certain pentacene via topological indices. *Open Chemistry*, 16(1), 1200-1206.

[75] Nadeem, M. F., Zafar, S., & Zahid, Z. (2015). On certain topological indices of the line graph of subdivision graphs. *Appl Math Comput.*, 271, 790-794.

[76] Nadeem, M. F., Zafar, S., & Zahid, Z. (2016). On topological properties of the line graphs of subdivision graphs of certain nanostructures. *Appl Math Comput.*, 273, 125-130.

[77] Patel, P., & Patel, C. (2013). Various graphs and their applications in real world. *International Journal of Engineering Research and Technology*, 2(12), 1499-1504.

[78] Peterin, I., & Yero, I. G. (2018). Edge metric dimension of some graph operations. arXiv preprint arXiv:1809.08900.

[79] Plavšić, D., Nikolić, S., Trinajstić, N., & Mihalić, Z. (1993). On the Harary index for the characterization of chemical graphs. *J. Math. Chem.*, 12(1), 235-250.

[80] Poincarè, H., (1901) Second complement à l0analysis situs. *Proc.Lond. Math. Soc.* 32 ,277–308.

[81] Randic, M. (1975). Characterization of molecular branching. *J. AM. CHEM. SOC.*, 97(23), 6609-6615.

[82] Ranjini, P. S., Lokesha, V., & Cangül, I. N. (2011). On the Zagreb indices of the line graphs of the subdivision graphs. *Appl Math Comput.*, 218(3), 699-702.

[83] Ranjini, P. S., Lokesha, V., Rajan, M. A., & Raju, M. P. (2011). On the Shultz index of the subdivision graphs. *Adv. Stud. Contemp. Math.*, 21(3), 279-290.

[84] SebSebö, A., & Tannier, E. (2004). On metric generators of graphs. *Math. Oper. Res.*, 29(2), 383-393.

[85] Sharma, V., Goswami, R., & Madan, A. K. (1997). Eccentric connectivity index: a novel highly discriminating topological descriptor for structure- property and structure-activity studies. *J. Chem. Inf. Comput. Sci.*, 37(2), 273-282.

[86] Siddiqui, H. M. A., & Imran, M. (2014). Computing the metric dimension of wheel related graphs. *Appl Math Comput.*, 242, 624-632.

[87] Imran, M., & Siddiqui, H. M. A. (2016). Computing the metric dimension of convex polytopes generated by wheel related graphs. Acta Mathematica Hungarica, 149(1), 10-30.

[88] Slater, P. J. (1975). Leaves of trees. *Congr. Numer*, 14(549-559), 37.

[89] Su, G., & Xu, L. (2015). Topological indices of the line graph of subdivision graphs and their Schur-bounds. *Appl Math Comput.*, 253, 395-401.

[90] Sylvester. JJ., (1909). On the geometrical forms called trees. Math. Papers, Cambridge University Press, 3, 640–641.

[91] Tomescu, I., & Javaid, I. (2007). On the metric dimension of the Jahangir graph. *B. Math. Soc. Sci. Math.*, 371-376.

[92] Vukičević, D., & Furtula, B. (2009). Topological index based on the ratios of geometrical and arithmetical means of end-vertex degrees of edges. *J. Math. Chem.*, 46(4), 1369-1376.

[93] West, D. B. (1996). Introduction to graph theory (Vol. 2). Upper Saddle River, NJ: Prentice hall.

[94] Wilson, R. J. (1979). Introduction to graph theory. Pearson Education India.

[95] Wiener, H. (1947). Structural determination of paraffin boiling points. *J. Am. Chem. Soc.*, 69(1), 17-20.

[96] Yero, I. G., Kuziak, D., & Rodríguez-Velázquez, J. A. (2011). On the metric dimension of corona product graphs. *Comput. Math. Appl.*, 61(9), 2793-2798.

[97] Zhang, Y., Liu, X., & Yong, X. (2009). Which wheel graphs are determined by their Laplacian spectra?. *Computers & Mathematics with Applications*, 58(10), 1887-1890.

[98] Zhang, H., Shiu, W. C., & Sun, P. K. (2012). A relation between Clar covering polynomial and cube polynomial. arXiv preprint arXiv:1210.5322.

[99] Zhang, H., & Zhang, F. (1996). The Clar covering polynomial of hexagonal systems I. Discrete applied mathematics, 69(1-2), 147-167.

[100] Zhang, Z., Mufti, Z. S., Nadeem, M. F., Ahmad, Z., Siddiqui, M. K., & Farahani, M. R. (2019). Computing Topological Indices for Para-Line Graphs of Anthracene. *Open Chemistry*, 17(1), 955-962.

[101] Zhou, B., & Trinajstić, N. (2010). On general sum-connectivity index. *J. Math. Chem.*, 47(1), 210-218.

[102] Zubrilina, N. (2018). On the edge dimension of a graph. *Discrete Math.*, 341(7), 2083-2088.

Appendix

List of Publications

1. Zhang, Z., Mufti, Z. S., Nadeem, M. F., Ahmad, Z., Siddiqui, M. K., & Farahani, M. R. (2019). Computing topological indices for para-line graphs of anthracene. Open Chem., 17(1), 955-962.

2. Mufti, Z. S., Nadeem, M. F., Gao, W., & Ahmad, Z. (2018). Topological study of the para-line graphs of certain pentacene via topological indices. Open Chem., 16(1), 1200-1206.

3. Mufti, Z. S., Zafar, S., Zahid, Z., & Nadeem, M. F. (2017). Study of the paraline graphs of certain benzenoid structures using topological indices. MAGNT Research Report, 2017, 4 (3), 110-116.

4. Mufti, Z. S, Nadeem, M. F, Ahmad, A., & Ahmad, Z. Computation of edge metric dimension of barycentric subdivision of Cayley graphs Italian Journal of Pure and Applied Mathematics (Accepted)

5. Mufti Z. S., Nadeem, M. F., Ahmad, Z, &Siddiqui, H.M.A, theoretical study of energy, inertia and nullity of phenylene and anthracene (Submitted)

6. Mufti, Z. S, Nadeem, M. F, Ahmad, A., & Ahmad, Z. Computing Certain Spectrum Based Topological Indices of Some Molecules (Submitted)

7. Mufti Z. S., Nadeem, M. F., Ahmad, Z, Siddiqui, H.M.A, & Siddiqui M. K, On degree based topological indices and entropy of generalized Sierpinski graphs (Submitted)