Polynomials and indices of some molecular graphs

by

Sabeel-e-Hafi

A dissertation submitted in partial fulfillment of the requirements
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Supervised by

Dr. Rashid Farooq

School of Natural Sciences
National University of Sciences and Technology
Islamabad, Pakistan

FORM TH-4

National University of Sciences & Technology

MASTER'S THESIS WORK

We hereby recommend that the dissertation prepared under our supervision by: SABEEL-E-HAFI, Regn No. NUST201463615MSNS78014F Titled: Polynomials and Indices of some Molecular Graphs be accepted in partial fulfillment of the requirements for the award of **M.Phil** degree.

Examination Committee Members

1. Name: DR. MATLOOB ANWAR Signature: _____
2. Name: DR. MUHAMMAD ISHAQ Signature: _____
3. Name: _____ Signature: _____
4. Name: DR. NASIR REHMAN Signature: _____

Supervisor's Name: DR. RASHID FAROOQ Signature: _____

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Abstract

Graph theory provides chemists a large number of useful tools. A large number of molecular properties like physico-chemical properties, thermodynamic properties, chemical reactivity and biological activity, are determined by chemical applications of graph theory. These properties can be characterized by some polynomials and a certain class of graph invariants referred to as topological indices. The mathematical models relating biological activities and chemical properties of chemical structures are, respectively, known as quantitative structure-activity relationships ($QSAR$) and quantitative structure-property relationships ($QSPR$). To predict the chemical and physical properties of chemical compounds, topological indices has played a vital role in the study of ($QSAR$) and ($QSPR$). Polynomials have a great importance in resonance theory, Kekules and Dewar structures and in finding many topological indices.

The aim of this thesis is to compute the polynomials and indices of some molecular graphs. We consider the SiO_2 layer structure and compute the counting polynomials, M-polynomial, Zagreb polynomials and some degree based indices, namely harmonic index, versions of Zagreb indices, general Randić index, inverse sum index, etc. We also consider two infinite families of fullerenes and compute the counting polynomials, M-polynomial and counting based indices.

Furthermore we consider a structure of dendrimer D_n and compute the counting polynomials, counting based indices, M-polynomial and Zagreb polynomials. We also compute the degree based indices, namely first Zagreb index, second Zagreb index, hyper-Zagreb index, first multiple Zagreb index and second multiple Zagreb index for the dendrimer structure.

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Dedicated to

My Loving Parents,
Brothers
&
Sisters

Introduction

Graph theory is applied in different branches of mathematics and science. It is growing rapidly because of its diverse applications in different fields like chemistry, biology, biochemistry, electrical engineering and computers applications, etc. It is classified into algebraic graph theory and spectral graph theory. Applications of algebraic graph theory in chemistry have made a remarkable progress. The branch of mathematics which is a combination of graph theory and chemistry is called chemical graph theory. Graphs are the mathematical structures having set of vertices and the edges joining these vertices. Graphs are used to model many problems of practical interest. In chemical graph theory, graphs are used to model the chemical compounds, where the vertices are the atoms and the edges are the bonds of the compound. Many chemical and physical properties of the chemical structures can be found by their modeling with the help of graphs. These properties can be characterized by some polynomials and indices. In this thesis some chemical structures are considered and the polynomials and indices are computed for these structures.

The first chapter of this thesis gives fundamentals of graph theory. We give basic definitions of graph theory, after that molecular topology, and a brief history of some topological indices is given. We give a brief introduction of distance based indices like Wiener index, Szeged index and Gutman index, Harary index, etc., and degree based indices like Zagreb indices, Randić index, harmonic index, etc. We also discuss the polynomials like characteristic polynomial, counting polynomials, M-polynomial, Zagreb polynomials, etc.

In the second chapter, we consider a SiO_2 layer structure, denoted by $SiO_2(p, q)$. We discuss the structure of SiO_2 layer structure and compute some counting polynomials, M-polynomial, Zagreb polynomials and the corresponding topological indices for SiO_2 layer structure.

In the third chapter, compute same counting polynomials, M-polynomial and the corresponding topological indices for two infinite families of fullerenes. In the fourth chapter, we consider a dendrimer structure and compute same counting polynomials, M-polynomial Zagreb polynomials and the corresponding topological indices for the dendrimer structure.

Contents

Chapter 1

Fundamentals of Graph Theory

1.1 Introduction

Graph theory is a discrete mathematical structure. It is related to different branches of Mathematics. It is widely used in different subjects like Physics, Chemistry, Computers, Operational Research, Communication Science, etc. It was born when a mathematician named Euler solved the problem of the Königsberg Bridges. Königsberg city was situated on the River Pregel. The city had two big islands which were connected through seven bridges. It is said that the people of Königsberg wondered whether they can go for a walk in the city by passing over each bridge exactly once and return to their starting point. No one found such a path and so they thought that no such path existed. This problem then was considered by Euler and he subsequently solved the problem. He said for such a walk to exist, the land area must have an even number of bridges linked with them. But as there are an odd number of bridges attached to a land area, the person will get stuck eventually. Hence, Euler proved that this kind of a path cannot exist. Later he defined Eulerian circuit and gave the solution of this problem. The graph of the Königsberg bridge problem is shown in Fig. 1.1.

The invention of this graph by Euler and his later work lead to the fundamental ideas of graph theory, which is now a major area of research.

1.2 Graphs

A *graph* G is a diagram or (a mathematical structure), which is a collection of a non empty finite set $V(G)$ of points, called *vertices*, and a set $E(G)$ of some lines joining unordered pairs of distinct points, called *edges*. The number of the vertices in set $V(G)$ is called the *order* of the graph G and the number of the edges in set $E(G)$ is called the *size* of the graph G. If $e \in E(G)$ is an edge joining the vertices

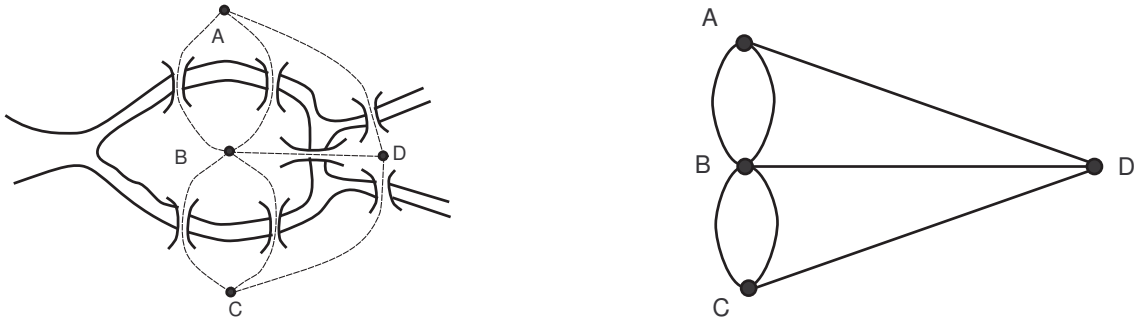

Figure 1.1: Seven bridges of Königsberg city and its graph

$x, y \in V(G)$ then we write $e = xy$ and x, y are called endpoints of e. The two edges having same endpoints are called *multiple edges*. An edge with same end vertices is called a *loop*. An edge is said to be *incident* with its endpoints. A vertex which has no incident edge is called *isolated vertex*. A graph is shown in the Fig. 1.2.

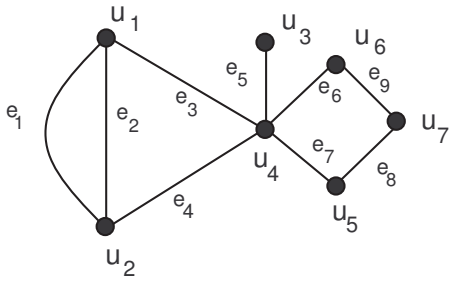

Figure 1.2: A graph

A graph which has no loops and multiple edges is known as a *simple graph*. A simple graph is shown in Fig. 1.3.

In any graph G, the number of edges incident with a vertex u is called the *degree* of the vertex u. It is usually denoted as $d(u)$ or $d_G(u)$. The vertex with even (odd) degree is called *even (odd) vertex*. The maximum vertex degree in the graph G is called *maximum degree* of the graph G, denoted as $\Delta(G)$, and the minimum vertex degree in the graph G is called the *minimum degree* of the graph G, denoted as $\delta(G)$. The vertex having degree 1 is referred to as *pendent* vertex or *leaf*. The vertex having degree 0 is called *isolated vertex*. In a simple graph G of order r, $\Delta(G) \leq r - 1$. Hence we have $0 \leq d_G(u) \leq r - 1$ for any vertex $u \in V(G)$. If $\Delta(G) = \delta(G) = r$, the graph G is known as *r-regular* graph.

The theorem stated below gives the degree sum formula for any graph, known as *The First Theorem of Graph Theory*.

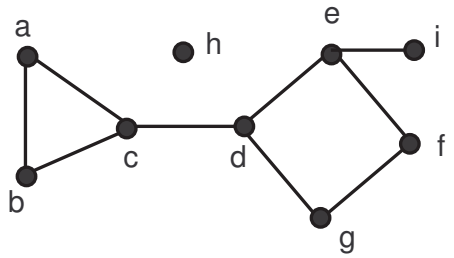

Figure 1.3: A simple graph G_1

Theorem 1.2.1. ([16]) *If G is any graph of size m, then*

$$\sum_{v \in V(G)} d_G(v) = 2(e(G)).$$

A graph H is called a *subgraph* of a graph G if vertex set of H is contained in vertex set of G and edge set of H is contained in edge set of G. If the vertex set of H and G are equal, that is, $V(H) = V(G)$ then the subgraph H is said to be *spanning subgraph* of G. If $V_1 \subset V(G)$, a *subgraph H induced by V_1*, denoted as $H[V_1]$, is a graph with $V(H) = V_1$ and contains all edges of G which have both ends in V_1.

A u, v-*walk* in a graph G is a sequence of vertices with the starting vertex u and the end vertex v such that the consecutive vertices in the sequence are adjacent. A u, v-*trail* is a u, v-walk in which no edge is repeated. A u, v-*path* is a u, v-walk in which no vertex is repeated. A path of order n is denoted by P_n. A closed trail having length 3 or more is called *circuit*. Similarly, A *cycle* is obtained from a u, v-path by joining u and v by an edge uv. A cycle of order n is denoted as C_n. The length of smallest cycle in the graph is known as the *girth* of the graph. The girth of the graph is undefined if there is no cycle in the graph.

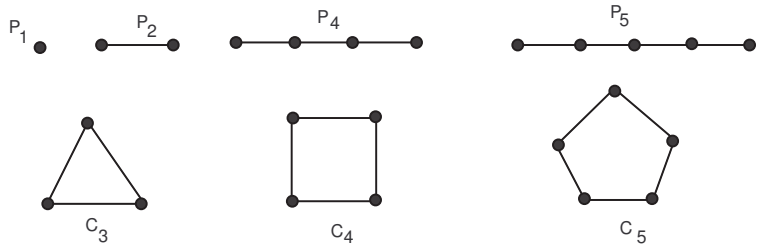

Figure 1.4: Paths and Cycles

Two graphs G and H are said to be *isomorphic* if there is a bijective map ϕ from

$V(G)$ to $V(H)$ such that $uv \in E(G)$ if and only if $\phi(u)\phi(v) \in E(H)$ and we write $G \cong H$. G and H are said to be *nonisomorphic* if they are not isomorphic and we write $G \ncong H$. Isomorphism produces an equivalence relation. Some isomorphic graphs are shown in the Fig. 1.5. Since isomorphism is an equivalence relation so it

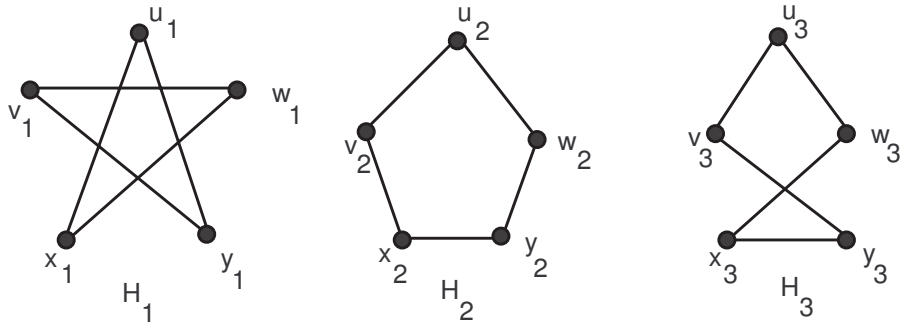

Figure 1.5: Isomorphic graphs

is apparent that the two isomorphic graphs must have:
i). an equal number of the edges,
ii). the same number of vertices with a given degree,
iii). an equal number of vertices.
But the converse is not true, that is, these conditions are not sufficient. The two graphs having same number of vertices, equal number of edges, and equal number of vertices with given degree may not be isomorphic as shown in the Fig. 1.6. The number of edges in a path is the length of path. The length of the shortest

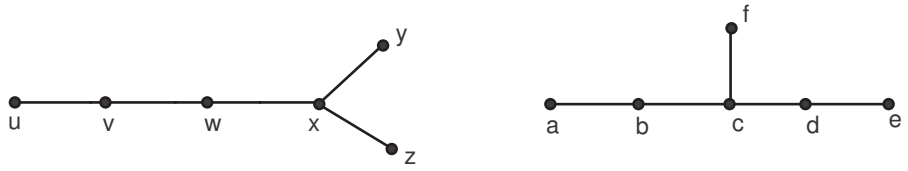

Figure 1.6: Two nonisomorphic graphs

path between the two vertices u and v is known as the *distance* between them and is denoted as $d(u, v)$. If no such path exists then $d(u, v) = \infty$. A u, v-*geodesics* is the path of length $d(u, v)$. The *eccentricity* $ecc(v)$ of a vertex v in a graph G is the distance between v and the vertex x which is farthest from v, that is, $ecc(v) = \max\{d(v, x) \mid x \in V(G)\}$. The maximum distance between any two vertices of G is the *diameter* of the graph. It is denoted as $diam(G)$. So $diam(G) =$

$\max\{ecc(v) \mid v \in V(G)\}$. The *radius* of a graph G is the minimum distance between any two vertices of G, that is, $rad(G) = \min\{ecc(v) \mid v \in V(G)\}$. The *central vertices* are the vertices having minimum eccentricities.

A graph G is said to be *connected* if for every pair u, v of distinct vertices in G there exists a u, v-path in G. A graph which is not connected is said to be *disconnected*. A *cut-vertex* is a vertex in the graph G, whose removal disconnects the graph G. Similarly, an edge whose removal from graph G disconnects the graph, is known as *cut-edge* or *bridge*.

1.3 Graph representation

Any graph G can be represented by matrices. A graph can either be represented by adjacency matrix or incidence matrix. The *adjacency matrix* of a graph G is the matrix $A(G) = [a_{ij}]$ of order $n \times n$, where a_{ij} is 1 if there is an edge between the two vertices v_i and v_j, otherwise zero. The adjacency matrix of the graph G in Fig. 1.2 is given below:

$$A(G) = \begin{pmatrix} 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 \end{pmatrix}$$

The entries on the principal diagonal represents the loops. If the graph is simple, every entry on the principal diagonal is 0. The adjacency matrix is a symmetric matrix. The sum of any row i or column j gives the degree of vertex v_i or v_j.

The *incidence matrix* of a graph G is a matrix $B(G) = [b_{ij}]$ of order $n \times m$, where b_{ij} is 1 if the vertex v_i and e_j are incident, otherwise zero. The incidence matrix of the graph G in Fig. 1.2 is given below:

$$B(G) = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix}$$

1.4 Some common classes of graphs

There are certain kinds of graphs. Some of them are defined below:

A *wheel* graph is a graph W_n, which is obtained from a cycle graph C_{n-1} by connecting a new vertex to all vertices of C_{n-1}. The new vertex added is known as *hub* and the edges of a wheel which are incident with the hub are called *spokes*. A

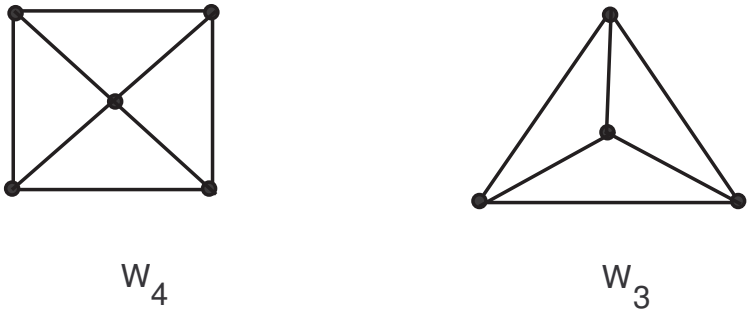

Figure 1.7: Wheel graphs

complete graph is a simple graph in which every two distinct vertices are adjacent. A complete graph of order p is denoted by K_p. Since there is an edge between every two distinct vertices of K_p, therefore the number of edges in K_p is $\binom{p}{2}$, that is,

$$E(K_p) = \binom{p}{2} = \frac{p(p-1)}{2}.$$

So the complete graph K_6 has 15 edges. Since there is an edge between every pair of the vertices, therefore K_p is $(p-1)$-regular graph. Some complete graphs are shown in the Fig. 1.8.

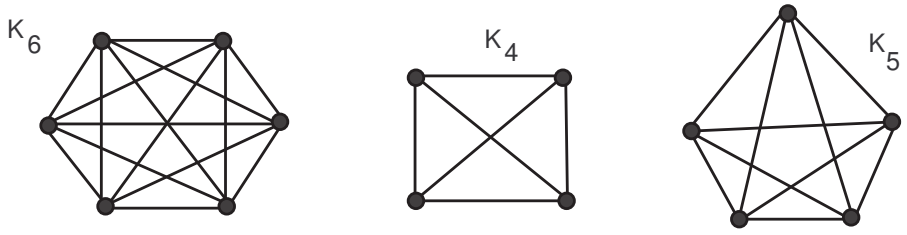

Figure 1.8: Some complete graphs

A *complement* graph $\overline{G}$ of a graph G is a graph with $V(\overline{G}) = V(G)$, such that e is an edge in $\overline{G}$ if and only if e is not an edge in G. A graph and its complement

both need not to be connected. At least one of them must be connected. If G is a graph of order n and size m, then the order and size of $\overline{G}$ are respectively, n and $\binom{n}{2} - m$. If G is disconnected graph, then $\overline{G}$ is connected.

A *bipartite* graph is a graph, whose vertex set can be partitioned into two subsets, such that every edge of G joins the vertices in the two subsets. The subsets, then are called *partite sets* or *bipartition* of the graph. Similarly, a graph G is said to be *k-partite* if vertex set $V(G)$ is the union of k independent sets. A characterization of the bipartite graphs is given in the theorem given below:

Theorem 1.4.1. ([26]) *A graph G is bipartite if and only if it contains no odd cycle.*

In a bipartite graph with partite sets A and B, to construct a cycle with starting vertex in A, we need to visit both partite sets A and B, because vertices in one partite set can not be adjacent. So every time we return back to the partite set A, we pass through an even number of edges.

A graph with two partite set, in which each vertex of one partite set is adjacent with each of the vertices of the other partite set is known as *complete bipartite graph*. A complete bipartite graph having p vertices in one partite set and q vertices in other partite set is denoted as $K(p, q)$. In Fig. 1.9, bipartite and complete bipartite graphs are shown.

A circuit containing all the edges of a graph G is called an *Eulerian circuit*. A graph which contains an Eulerian circuit is called *Eulerian graph*. Therefore an Eulerian circuit in a connected graph G is a closed trail that contains all edges of G. Following theorem gives a characterization of Eulerian graphs.

Theorem 1.4.2. ([16]) *The following statements are equivalent for a connected graph G.*
(1) *G is Eulerian.*
(2) *$E(G)$ is the union of edge-disjoint cycles in G.*
(3) *The degree of every vertex in G is even.*

A *hamiltonian cycle* is a cycle in a graph G, passing through all vertices of G. A *hamiltonian graph* is a graph which contains a hamiltonian cycle. In the Fig. 1.11 a hamiltonian graph with hamiltonian cycle *uvwzyxu* and a non-hamiltonian graph are shown. There is no characterization known for hamiltonian graphs, but some of the conditions are stated below:

Theorem 1.4.3. ([16]) *Let G be a simple n-vertex graph, where $n \geq 3$, such that $deg(x) + deg(y) \geq n$ for each pair of non-adjacent vertices x and y, then G is hamiltonian.*

Theorem 1.4.4. ([39]) *If G is a simple graph with at least three vertices and $\delta(G) \geq \frac{|G|}{2}$, then G is hamiltonian.*

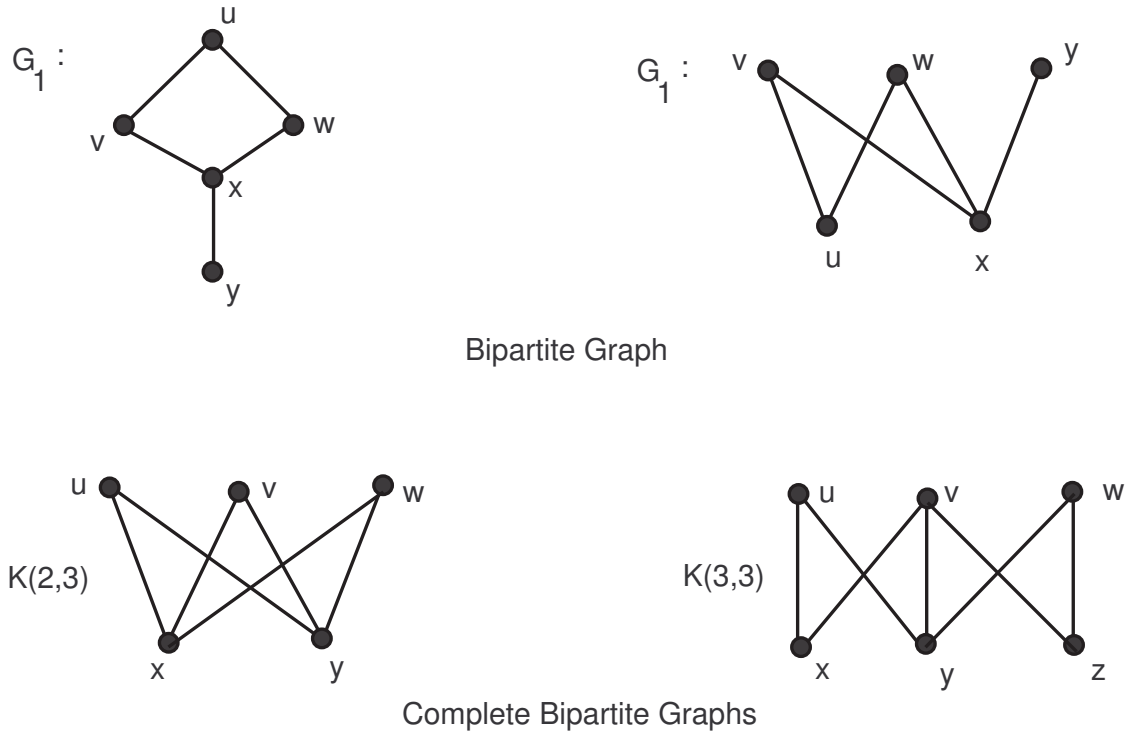

Figure 1.9: Bipartite and Complete bipartite graphs

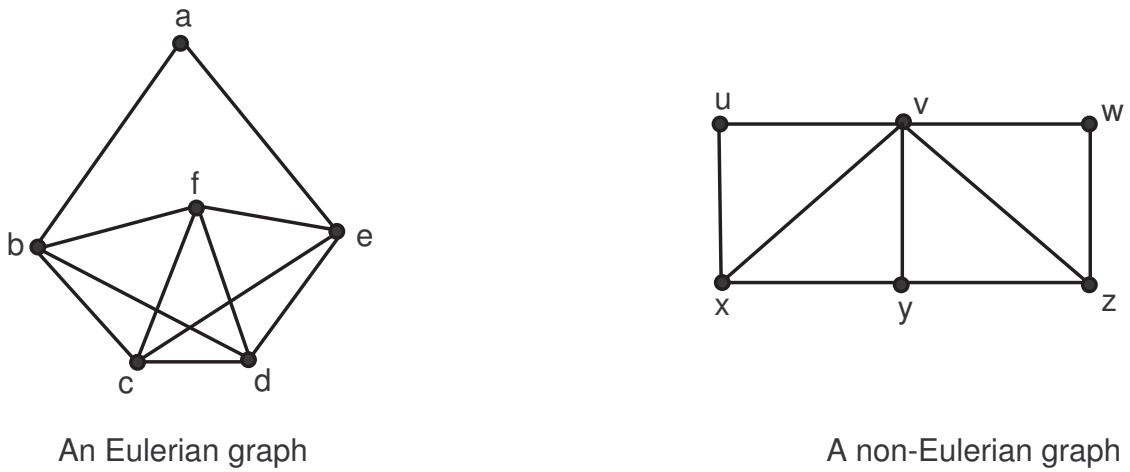

Figure 1.10: Eulerian and non-eulerian graphs

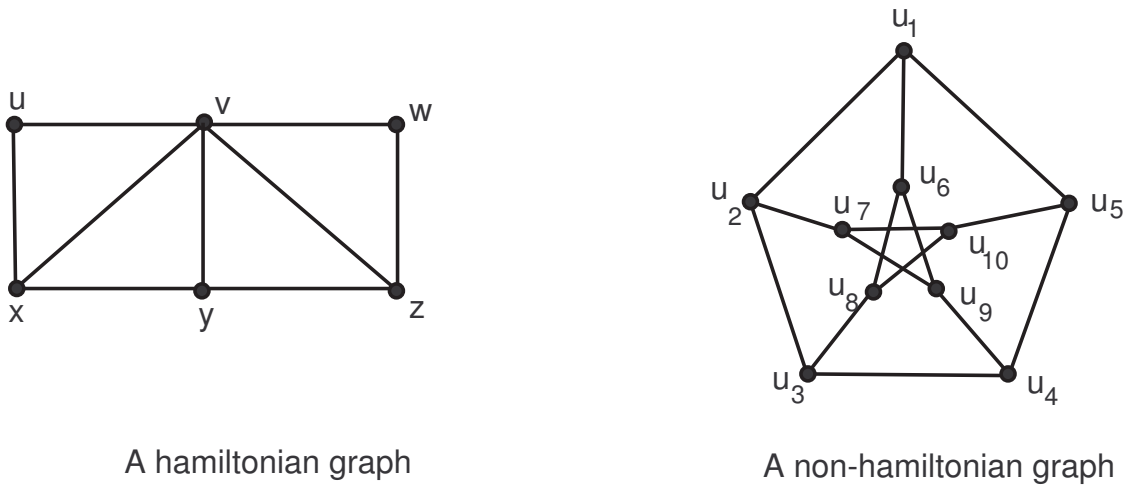

Figure 1.11: Hamiltonian and non-hamiltonian graphs

An *acyclic* graph is a graph G having no cycles. The acyclic graphs are also referred as *forests*. A connected acyclic graph G is called *tree*. Hence the graph in the Fig. 1.12 is a tree. Usually T is used for trees instead of G. A tree T is a star

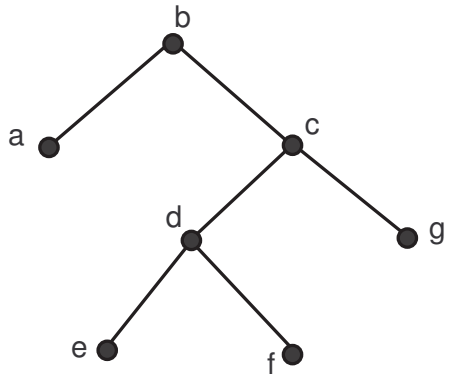

Figure 1.12: A tree

if $T \cong K(1,5)$. A *double star* is a tree having exactly two vertices which are not pendant vertices. A tree of order three or more is called *caterpillar*, if the removal of pendent vertices produces a path, called *spine* of the caterpillar. If a vertex in a tree T is selected as the root of T the tree then T is called a *rooted tree*. For a tree T of order n and size m, we have $m = n - 1$.

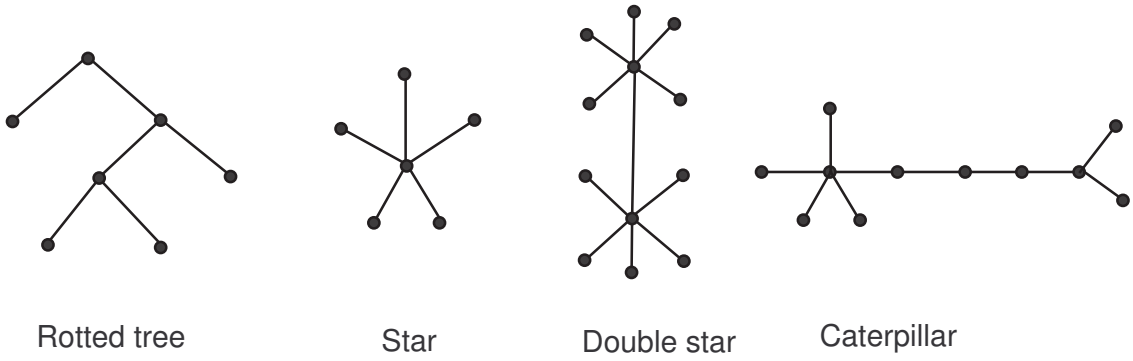

Figure 1.13: Rooted tree, star, double star and caterpillar

1.5 Chemical graph theory

Graph theory is one of the fastest growing branch of mathematics. It has been used and accepted in different branches of science. Molecular topology or chemical graph theory is the applications of graph theory in the fields where the molecular structures matters. The importance of chemistry in the branches of science is because most of the chemical information is associated with the chemical structures that may be uniquely indexed. In other branches of science the use of words is needed to explain but in chemistry it can be done by means of formulas. Molecular topology or chemical graph theory is not only equal as the other branches of chemistry but also is necessary for the understanding of chemical structures. The importance of graph theory in chemistry is mainly due to the phenomenon of isomerism. Finding and defining the isomers is a graph-theoretical problem. The adjacency matrix for the graphs of conjugated hydrocarbons in Hückel molecular orbital theory corresponds to the Hückel matrix [5]. Topological characterization of chemical structures allows the classification of molecules and modeling unknown structures with desired properties.

Molecules and molecular compounds are modeled by molecular graphs. A model that is used to characterize a chemical compound is called *chemical graph*. A *molecular graph* is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds [5]. In Fig. 1.14, a chemical structure of Adeninie (DNA) and its molecular graph is shown. Hydrogen atoms are not considered usually in molecular graphs in which case the molecular graphs are known as hydrogen depleted molecular graph [5].

Isomers are the chemical compounds which have same molecular formula but different chemical structure such as n-butane and iso-butane. Molecular graphs helps

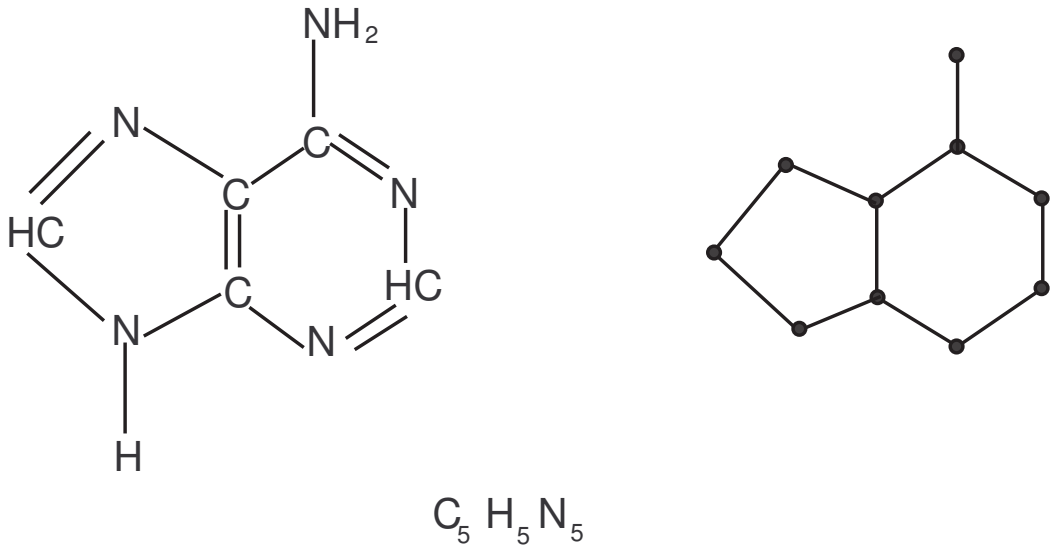

Figure 1.14: A chemical structure and its hydrogen depleted molecular graph

in distinguishing between isomers [5]. These graphs does not give any information about the 3-D arrangement of the bonds. Similarly, a chemical reaction can be modeled by a reaction graph. In a reaction graph the vertices are chemical compounds and edges are the reaction paths. Within this thesis, only molecular graphs are considered. A molecular graph can be described by numerous ways such as by a polynomial, a sequence of numbers, a derived number called a topological index, or a matrix [5].

1.5.1 Topological indices

Topological index is a single number that represents the chemical structure. Topological indices are the graph invariants which characterize the topology of a graph [5]. The mathematical models relating biological activities of a chemical structures are known as quantitative structure-activity relationships ($QSAR$) and quantitative structure-property relationships ($QSPR$). Topological indices are used in the development of quantitative structure-activity relationships ($QSAR$) and quantitative structure-property relationships ($QSPR$). Topological indices play a vital role in $QSAR$ and $QSPR$ study. To establish a correlation model between the structures of chemical compounds and the corresponding properties, it is required to numerically code the structures of chemical compounds. Hence, the task in $QSAR/QSPR$ researches is to transfer the molecular graph into numerical format. There are many techniques for this purpose, in which the popular ones are topological indices. They correlate some physical and chemical properties of compounds. They are also used

in testing the isomorphism. Some characteristics of topological indices are given below:
1). They directly interpret the chemical structure.
2). They discriminate between the isomers.
3). They correlate at least with one property of the chemical compound.
4). They are simple, defined locally, and are based on known concepts.
5). They can be generalized to higher analogues.
6). They are linearly independent.
7). They are not related to other indices trivially and show a correct dependence on size.
8). The construction of these indices is efficient and is not be based on physico-chemical properties.
9). They change gradually with the gradual change in the structures.

Different molecular properties are correlated with these descriptors. A correlation was found for the properties like boiling points, heat of combustion, enthalpy of formation, octane number and many biological properties. Many such descriptors have been proposed and tested. Wiener [38] was the first who introduced the first topological index while he was studying boiling point of paraffin. He named this index as path number and later on, it was renamed as Wiener index [9]. There are two main classes of topological indices which are:
• distance based topological indices.
• degree based topological indices.
Consider a graph G with vertex set $V(G)$ and edge set $E(G)$. Let order and size of the graph G be n and m, respectively. Some of the distance based and degree based indices for the graph G are defined in this section.

Distance based topological indices

Distance-based indices are defined by using the distances in the graph. Some of these topological indices are defined below:
For a molecular graph graph G, the Wiener index, denoted by $W(G)$, and is defined as

$$W(G) = \frac{1}{2} \sum_{u,v \in V(G)} d(u, v), \tag{1.1}$$

where $d(u, v)$ is the distance between u and v. This index correlate the boiling points of different molecular structures.

Another important index, the Szeged index, introduced by Gutman [20] correlate

chemical structures with their physico-chemical properties. It is defined as

$$Sz(G) = \sum_{uv \in E(G)} n_u(uv) n_v(uv), \tag{1.2}$$

where $n_u(uv)$ and $n_v(uv)$ are respectively the number of the vertices of G lying closer to u than v and the number of vertices lying closer to v then to u. It is to be noted that the vertices that are equidistance from u and v are not considered. Important physico-chemical properties which were modeled using Szeged index are molar volume, density, molecular weight, svan der Waals volume, boiling point, vapor pressure, dipole moments, and polarizability etc. Szeged index was also used in the modeling of some spectroscopic parameters such as edgeshift in the extended X-ray absorption fine structure spectroscopy, isomer shift, infrared group frequency and chemical shifts in nuclear magnetic resonance spectroscopy, etc [25].

Schultz [34] introduced an index, Schultz index to characterize the alkanes by an integer. This index is defined as

$$S(G) = \sum_{u,v \in V(G)} d(u,v)(d_G(u) + d_G(v)). \tag{1.3}$$

Schultz index and Wiener index are closely related for certain classes of chemical graphs. It was shown that for a tree T of order n [28], the Schultz index is given by

$$S(G) = 4W(G) - n(n-1).$$

Klavžar and Gutman [27] proposed the Schultz index of second kind. This index is known as Gutman index, and is defined as

$$Gut(G) = \sum_{u,v \in V(G)} d(u,v)(d_G(u) d_G(v)). \tag{1.4}$$

Plavšić et al. [31] introduced a new distance based index, namely, the Harary number $H(G)$. This index is defined as

$$H(G) = \frac{1}{2} \sum_{u,v \in V(G)} \frac{1}{d(u,v)}. \tag{1.5}$$

This index is suitable to predict the enthalpies of sublimation of carboxylic acids.

Degree based topological indices

The degree based indices for a graph are defined by using the degree of a vertex in that graph. Generally a degree-based topological index of a graph G is defined as

$$I(G) = \sum_{uv \in E(G)} f(d_G(u), d_G(v)),$$

where $f = f(x, y)$ is a function appropriately selected for possible chemical applications [18]. Some degree based indices are defined below:

Gutman and Trinajstić [19] introduced the *Zagreb indices*, denoted by $M_1(G)$ and $M_2(G)$, respectively. They are defined as

$$M_1(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v)), \tag{1.6}$$

$$M_2(G) = \sum_{uv \in E(G)} (d_G(u) d_G(v)). \tag{1.7}$$

These indices are used in the topological formula for finding the total π-electron energy.

Nikolić et al. [30] proposed the *second modified Zagreb index* denoted by $M_2^*(G)$, and is defined as

$$M_2^*(G) = \sum_{uv \in E(G)} \frac{1}{d_G(u) d_G(v)}. \tag{1.8}$$

Randić [32] introduced branching index R, called the *Randić index* and is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_G(u) d_G(v)}}. \tag{1.9}$$

Randić index is suitable for measuring the extent of branching of the carbon-atom of saturated hydrocarbons. Later, Bollobás and Erdös [2] generalized this index for any real number α, which was then called the *general Randić index*. It is defined as

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_G(u) d_G(v))^\alpha. \tag{1.10}$$

Another degree based index, the *symmetric division degree index* was introduced by Vukičevic and Gašperov [36], denoted by $SDD(G)$, and is defined as

$$SDD(G) = \sum_{uv \in E(G)} \frac{d_G(u)^2 + d_G(v)^2}{d_G(u) d_G(v)}. \tag{1.11}$$

Zhong [41] proposed the degree based index, *harmonic index*, denoted by $H(G)$, and is defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_G(u) + d_G(v)}. \tag{1.12}$$

The degree based index, *inverse sum index* was introduced by Vukičevic and Gašperov [36], denoted by $ISI(G)$, and is defined as

$$ISI(G) = \sum_{uv \in E(G)} \frac{d_G(u) d_G(v)}{d_G(u) + d_G(v)}. \tag{1.13}$$

Furtula et al. [11] introduced the *augmented Zagreb index*, denoted by $AZI(G)$, and is defined as

$$AZI(G) = \sum_{uv \in E(G)} \left(\frac{d_G(u) d_G(v)}{d_G(u) + d_G(v) - 2} \right)^3. \tag{1.14}$$

Shirdel et al. [33] defined a new version of Zagreb index, called *hyper Zagreb index*, $HM(G)$ as

$$HM(G) = \sum_{uv \in E(G)} (d_G(u) + d_G(v))^2. \tag{1.15}$$

Ghorbani and Azimi [14] defined two versions of Zagreb indices. The first multiple Zagreb index $PM_1(G)$ and second multiple Zagreb index $PM_2(G)$ of a graph G are defined as

$$PM_1(G) = \prod_{uv \in E(G)} (d_G(u) + d_G(v)), \tag{1.16}$$

$$PM_2(G) = \prod_{uv \in E(G)} (d_G(u) \times d_G(v)). \tag{1.17}$$

1.5.2 Polynomials

There are two main route by which polynomials enter in chemical graph theory. First, by Hückel theory and second, chemical applications of graph theory often encounters finite sequences of certain graph invariants and with these sequences one can introduce a polynomial [5]. In Quantum Chemistry, the early Hückel theory calculates the levels of π electron energy of the molecular orbitals, in conjugated hydrocarbons, as zeros of the polynomials. The extent of branching in the skeleton of a molecule is reflected by the coefficients and zeros of the polynomials. They are also related to the number of kekules and Dewar structures of the appropriate conjugated molecules. Polynomials are of great importance in resonance theory. They are use in measures of related topological indices. Some of these polynomials are defined in this section.

Characteristic polynomial

The *characteristic polynomial* of a graph G is defined as

$$\varphi(G, x) = det(xI - A(G)), \tag{1.18}$$

where $A(G)$ is the adjacency matrix. The characteristic polynomials of two isomorphic graphs coincide but if the two graphs have same characteristic polynomials then its not necessary that they are isomorphic. Characteristic polynomial of a graph G is independent of labeling of vertices.

Counting polynomials

Finite sequences of certain graph invariants are encountered in chemical applications of graph theory. With these sequences a polynomial can be introduced. This type of polynomial is known as *counting polynomial*. Counting polynomials were introduced by Hosoya with his Z-counting and the distance degree polynomials and were initially called Wiener and later Hosoya polynomials [22].

Consider a sequence $C = (C_0, C_1, C_2, \cdots, C_k)$. Instead of $k+1$ distinct quantities C_p, $p = 0, 1, 2, \cdots, k$, a single quantity can be introduced, which is defined as

$$C_0 + C_1 x + C_2 x^2 + \ldots + C_k x^k = \sum_{p=0}^{k} C_p x^k \tag{1.19}$$

Same information as the sequence C is contained in the polynomial (1.19). However, sometimes it is easy to deal with a polynomial instead of a sequence. The sequences of graph invariants have some properties which cannot be discovered without examining graph polynomials of form (1.19). A counting polynomial is defined as

$$P(G, x) = \sum_{k} m(G, k) x^k, \tag{1.20}$$

and the corresponding index is defined as

$$P(G) = \frac{d}{dx}(P(G, x))|_{x=1} = \sum_{k} m(G, k) \times k, \tag{1.21}$$

where $m(G, k)$ is the frequency of occurrence of the property partitions of G, of length k.

Two edges $e_1 = x_1 y_1$ and $e_2 = x_2 y_2$ in $E(G)$ are said to be *codistant*, denoted by e_1 *co* e_2, if for $k = 0, 1, 2, 3, \ldots$,

$$d(x_1, x_2) = d(y_1, y_2) = k,$$

and

$$d(x_1, y_2) = d(y_1, x_2) = k + 1.$$

or vice versa. For some edges of a connected graph G, the relation "*co*" is reflexive as e *co* e is true for all edges e in G. Also it is symmetric as if e_1 *co* e_2 then e_2 *co* e_1 for all $e_1, e_2 \in E(G)$. However, the relation "*co*" is not necessarily transitive [7].

Consider

$$C(e) = \{f \in E(G) : e \; co \; f\}.$$

If the relation "*co*" is transitive on $C(e)$ also, then $C(e)$ is called an *orthogonal cut*. The graph is called *co-graph* if and only if the set $E(G)$ is the union of disjoint

orthogonal cuts, that is, there are orthogonal cuts $C_1, C_2, \cdots, C_k$ satisfying $\bigcup_{i=1}^{k} C_i = E(G)$ and $C_i \cap C_j = \phi$ for $i \neq j$ [7].

If any two consecutive edges of a cut edge sequence are codistant and belong to the same face of the covering, such a sequence is called a qausi-orthogonal cut "qoc" strip. The transitivity is not required [7].

Denote by $m(G,k)$ the number of qocs of length k. A counting polynomial, namely, *Omega polynomial*, denoted by $\Omega(G,x)$, was introduced by Diudea [7] and is defined as

$$\Omega(G,x) = \sum_k m(G,k) \times x^k, \tag{1.22}$$

where the summation runs up to the maximum length of qocs in G. The corresponding *Omega index* is given by

$$\Omega(G) = \frac{d}{dx}(\Omega(G,x))|_{x=1} = \sum_k m(G,k) \times k. \tag{1.23}$$

The *Sadhana polynomial* is defined on the opposite edge strips in any graph. This polynomial counts codistant edges in G and was introduced by Ashrafi et al. [1], denoted by $Sd(G,x)$, and is defined as:

$$Sd(G,x) = \sum_k m(G,k) \times x^{m-k}, \tag{1.24}$$

where m is the size of G, and $m(G,k)$ is the number of qocs of length k. The corresponding *Sadhana index* is given by

$$Sd(G) = \frac{d}{dx}(Sd(G,x))|_{x=1} = \sum_k m(G,k) \times (m-k). \tag{1.25}$$

The *PI polynomial* is defined by Khadikar [23] based on counting opposite edge strips in any graph. This polynomial counts non-codistant edges in G. The *PI polynomial* denoted by $PI(G,x)$ is defined as

$$PI(G,x) = \sum_k m(G,k) \times k \times x^{m-k}. \tag{1.26}$$

The corresponding *PI index* is given by

$$PI(G) = \frac{d}{dx}(PI(G,x))|_{x=1} = \sum_k k \times m(G,k) \times (m-k). \tag{1.27}$$

M-polynomial

Let $G = (V, E)$ be a graph. Let $m_{ij}(G)$, $i, j \geq 1$, be the number of edges $e = uv$ of G such that $\{d_G(u), d_G(v)\} = \{i, j\}$. The quantities $m_{ij}(G)$ were first introduced and applied in [17]. The M-polynomial of G is introduced by Deutsch and Klavžar [8], and is defined as

$$M(G; x, y) = \sum_{i \leq j} m_{ij}(G) x^i y^j. \tag{1.28}$$

For some connected graphs, M-polynomial is useful in finding some degree based indices like Zagreb indices, general Randić index, harmonic index augmented Zagreb index, inverse sum index, etc.

Hosoya polynomial

Hosoya [22] introduced a distance based polynomial known as Hosoya polynomial. It is defined as

$$H(G, x) = \sum_{k \geq 0} d(G, k) x^k, \tag{1.29}$$

where $d(G, k)$ is the number of pairs of vertices of G, which are at distance k. $d(G, 1)$ is equal to the size of the graph G, and $d(G, 0)$ is equal to the order of the graph G. The first derivative of Hosoya polynomial, $H(G, x)$ at $x = 1$ gives the famous index, Wiener index, that is,

$$\frac{d}{dx}(H(G, x))|_{x=1} = W(G) \tag{1.30}$$

Hyper-Wiener index is given as

$$\frac{d}{dx}(H(G, x))|_{x=1} + \frac{1}{2}\frac{d^2}{dx^2}(H(G, x))|_{x=1} = WW(G) \tag{1.31}$$

Some other distance-based topological indices can also be derived from Hosoya polynomial.

Zagreb polynomials

Fath-Tabar [12] introduced the first and second Zagreb polynomials. The first Zagreb polynomial $M_1(G, x)$ of a graph G is defined as

$$M_1(G, x) = \sum_{uv \in E(G)} x^{d_G(u) + d_G(v)}. \tag{1.32}$$

The second Zagreb polynomial $M_2(G, x)$ of a graph G is defined as

$$M_2(G, x) = \sum_{uv \in E(G)} x^{d_G(u) \times d_G(v)}. \tag{1.33}$$

Chapter 2

Polynomials and Indices of SiO_2 Layer Structure

Silicates are of the utmost importance as raw materials, mass produced items and are considered one of the most abundant class of minerals on the earth [29]. The variety and abundance of silicates is due to the nature of the silicon atom, specifically the stability of the silicon when it bonds with the oxygen atom. The formula unit SiO_4^{4-} is the building block of all silicate structures. This formula unit consists of a central silicon atom which is surrounded by four oxygen atoms and forms a tetrahedron. These tetrahedrons link to self-similar tetrahedrons, sharing corner oxygens of the tetrahedron and form amazing but complicated structures. The silicate tetrahedrons combine in different ways and form single units, double units, chains, sheets, rings and framework structures.

The structure of the formula unit SiO_4^{4-} is shown in the Fig. 2.1. The SiO_4^{4-} tetrahedron combines with the other similar SiO_4^{4-} tetrahedrons and form different structures. In the structure considered in this chapter, these tetrahedrons combine together and form octagons. A single octagon is shown in the Fig. 2.2. In the similar way, the SiO_4^{4-} units combine and forms SiO_2 layer structure.

In this chapter, the molecular graph of SiO_2 layer structure is considered. Furthermore, p and q are respectively the number of octagons in the rows and the columns in the $SiO_2(p, q)$ structure. The graph of $SiO_2(p, q)$ layer structure is shown in Fig. 2.3. The order and size of the $SiO_2(p, q)$ structure are $n(SiO_2(p, q)) = 3pq + 4p + 4q + 5$ and $e(SiO_2(p, q)) = 4(pq + p + q + 1)$, respectively.

We compute Omega, Sadhana and PI polynomials by using standard cut method of SiO_2 layer structure. Furthermore, we compute M-polynomial and the topological indices derived from above mentioned polynomials. Ghorbani et al. computed Omega and Sadhana polynomials of an infinite family of fullerenes [15]. Diudea et al. studied the Omega type polynomials in phenacenes [6]. The following section

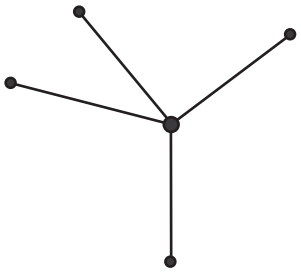

Figure 2.1: Formula unit SiO_4^{4-}

Figure 2.2: Octagon in SiO_2 layer structure

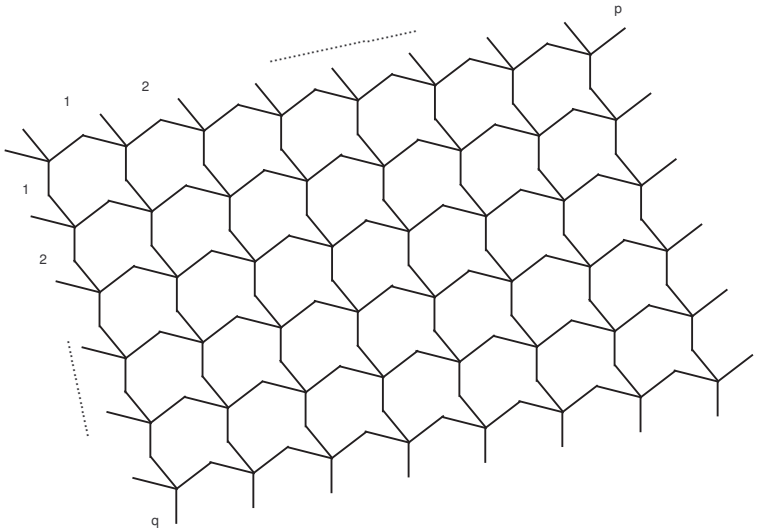

Figure 2.3: $SiO_2(p, q)$ layer structure

gives all polynomials and indices defined by (1.22)−(1.27) for the $SiO_2(p, q)$ layer structure.

2.1 Counting polynomials and corresponding indices

The following theorem gives the Omega, Sadhana and PI polynomials of $SiO_2(p, q)$ layer structure.

Theorem 2.1.1. *The Omega, Sadhana and PI polynomials of $SiO_2(p, q)$ structure are respectively given by:*

$$\begin{aligned} \Omega(SiO_2(p,q),x) &= 2x(qx^p + px^q + p + q + 2), \\ Sd(SiO_2(p,q),x) &= 2qx^{4pq+3p+4q+3} + 2px^{4pq+4p+3q+3} + (2q+2p+4)x^{4pq+4p+4q+3}, \end{aligned}$$

$$PI(SiO_2(p,q),x) = 2q(p+1)x^{4pq+3p+4q+3} + 2p(q+1)x^{4pq+4p+3q+3} + (2q+2p+4)x^{4pq+4p+4q+3}.$$

Proof. We use the standard cut-method to compute our results. We define two horizontal cuts $\{C_i \mid 1 \leq i \leq q\}$ and $\{C_i' \mid 1 \leq i \leq q\}$, two vertical cuts $\{\widehat{C}_i \mid 1 \leq i \leq p\}$, $\{\widehat{C}_i' \mid 1 \leq i \leq p\}$ and the cuts through pendent edges are denoted by $\{\widetilde{C}_i \mid 1 \leq i \leq 2q+2p+4\}$. There are $2p+2q+4$ pendent edges in $SiO_2(p,q)$ layer structure. The cuts are shown in Fig. 2.4.

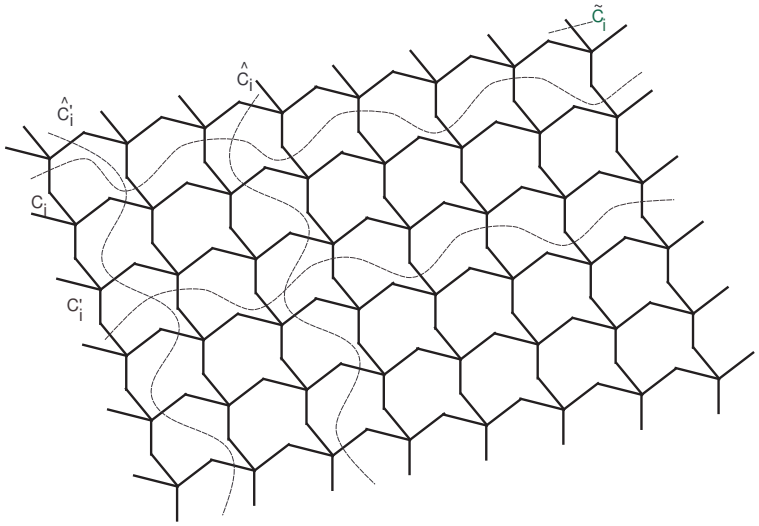

Figure 2.4: Dotted lines show the cuts in $SiO_2(p,q)$ layer structure

It is easily seen that C_i, C_i', $i = 1,2,3,....q$ and $\widehat{C}_i$, $\widehat{C}_i'$, $i = 1,2,3,....p$ are qocs. The length and the number of qocs for SiO_2 layer structure are given in Table 2.1.

Types of *qoc*	Length of qoc	No. of *qoc*
C_i	$p+1$	q
C_i'	$p+1$	q
$\widehat{C}_i$	$q+1$	p
$\widehat{C}_i'$	$q+1$	p
$\widetilde{C}_i$	1	$2p+2q+4$

Table 2.1: Types of qocs, length of qocs and number of qocs in SiO_2 layer structure.

First we compute the Omega polynomial for $SiO_2(p,q)$ layer structure. Substituting the values from Table 2.1 in equation (1.22), we get

$$\Omega(SiO_2(p,q),x) = qx^{p+1} + qx^{p+1} + px^{q+1} + px^{q+1} + (2p+2q+4)x^1.$$

After simplifying the above expression, we get

$$\Omega(SiO_2(p,q),x) = 2x(qx^p + px^q + p + q + 2).$$

Next we find the expression for the Sadhana polynomial for the $SiO_2(p,q)$ layer structure. Substituting the values from Table 2.1 in equation (1.24), we get

$$\begin{aligned} Sd(SiO_2(p,q),x) \quad &= qx^{4(pq+p+q+1)-(p+1)} + qx^{4(pq+p+q+1)-(p+1)} + px^{4(pq+p+q+1)-(q+1)} \\ &+px^{4(pq+p+q+1)-(q+1)} + (2p+2q+4)x^{4(pq+p+q+1)-1}. \end{aligned}$$

After simplifying the above expression, we obtain

$$Sd(SiO_2(p,q),x) = 2qx^{4pq+3p+4q+3} + 2px^{4pq+4p+3q+3} + (2q+2p+4)x^{4pq+4p+4q+3}.$$

Next we compute the expression for the PI polynomial. Substituting the values from Table 2.1 in equation (1.26), we get

$$\begin{aligned} PI(SiO_2(p,q),x) \quad &= q(p+1)x^{4(pq+p+q+1)-(p+1)} + q(p+1)x^{4(pq+p+q+1)-(p+1)} \\ &+p(q+1)x^{4(pq+p+q+1)-(q+1)} + p(q+1)x^{4(pq+p+q+1)-(q+1)} \\ &+(2p+2q+4)(1)x^{4(pq+p+q+1)-1}. \end{aligned}$$

After simplifying the above expression, we get

$$\begin{aligned} PI(SiO_2(p,q),x) \quad &= 2q(p+1)x^{4pq+3p+4q+3} + 2p(q+1)x^{4pq+4p+3q+3} \\ &+(2q+2p+4)x^{4pq+4p+4q+3}. \end{aligned}$$

This completes the proof. □

Next we find the indices derived from the polynomials computed in the Theorem 2.1.1.

Corollary 2.1.1. *The Omega, Sadhana and PI indices of $SiO_2(p,q)$ layer structure are given below:*

$$\begin{aligned} \Omega(G) &= 4pq + 4p + 4q + 4, \\ Sd(G) &= 16p^2q + 16pq^2 + 16p^2 + 44pq + 16q^2 + 28p + 28q + 12, \\ PI(G) &= 16p^2q^2 + 30p^2q + 30pq^2 + 16p^2 + 56pq + 16q^2 + 28p + 28q + 12. \end{aligned}$$

Proof. Using Theorem 2.1.1 and the equation (1.23), the Omega index is given by:

$$\Omega(G) = 2q(p+1) + 2p(q+1) + 2(p+q+2).$$

After simplifying the above expression, we get

$$\Omega(G) = 4pq + 4p + 4q + 4.$$

Next we compute the Sadhana index. Using Theorem 2.1.1 and the equation (1.25), we have

$$\begin{aligned} Sd(G) \quad &= 2q(4pq + 3p + 4q + 3) + 2p(4pq + 4p + 3q + 3) \\ &+(2q + 2p + 4)(4pq + 4p + 4q + 3). \end{aligned}$$

After simplifying the above expression, we get

$$Sd(G) = 16p^2q + 16pq^2 + 16p^2 + 44pq + 16q^2 + 28p + 28q + 12.$$

Next we give the expression for the PI index. Using Theorem 2.1.1 and the equation (1.27), we have

$$\begin{aligned} PI(G) \quad &= 2q(p+1)(4pq + 3p + 4q + 3) + 2p(q+1)(4pq + 4p + 3q + 3) \\ &+(2q + 2p + 4)(4pq + 4p + 4q + 3). \end{aligned}$$

After simplifying the above expression, we get

$$PI(G) = 16p^2q^2 + 30p^2q + 30pq^2 + 16p^2 + 56pq + 16q^2 + 28p + 28q + 12.$$

The proof is complete. □

2.2 M-Polynomial and some degree based indices

This section gives the M-polynomial defined by (1.28) for the silicate network.

Let $f(x, y)$ be a differentiable function of two variables. Deutsch and Klavžar [8] defined the operators D_x, D_y, S_x, S_y, J and Q_α on $f(x, y)$ as follows:

$$D_x(f(x,y)) = x\frac{\partial f(x,y)}{\partial x},$$

$$D_y(f(x,y)) = y\frac{\partial f(x,y)}{\partial y},$$

$$S_x(f(x,y)) = \int_0^x \frac{f(t,y)}{t}dt,$$

$$S_y(f(x,y)) = \int_0^y \frac{f(x,t)}{t} dt,$$
$$J(f(x,y)) = f(x,x),$$
$$Q_\alpha(f(x,y)) = x^\alpha f(x,y),$$

where $\alpha \neq 0$.

Deutsch and Klavžar [8] gave the expressions for degree based indices (1.6) – (1.14), using M-polynomial. Table 2.2 gives these expressions. The set of positive integers and the set of negative integers are denoted by $\mathbb{Z}^+$ and $\mathbb{Z}^-$, respectively.

Topological indices	$\boldsymbol{f(x,y)}$	**Derivation from M-Polynomial**
$M_1(G)$	$x+y$	$(D_x + D_y)(M(G;x,y))\|_{x=y=1}$
$M_2(G)$	xy	$(D_x D_y)(M(G;x,y))\|_{x=y=1}$
$M_2^*(G)$	$\frac{1}{xy}$	$(S_x S_y)(M(G;x,y))\|_{x=y=1}$
$R_\alpha(G)$ $(\alpha \in \mathbb{Z}^+)$	$(xy)^\alpha$	$(D_x^\alpha D_y^\alpha)(M(G;x,y))\|_{x=y=1}$
$R_\alpha(G)$ $(\alpha \in \mathbb{Z}^-)$	$(xy)^\alpha$	$(S_x^{-\alpha} S_y^{-\alpha})(M(G;x,y))\|_{x=y=1}$
$SDD(G)$	$\frac{x^2+y^2}{xy}$	$(D_x S_y + D_y S_x)(M(G;x,y))\|_{x=y=1}$
$H(G)$	$\frac{2}{x+y}$	$2S_x J(M(G;x,y))\|_{x=1}$
$ISI(G)$	$\frac{xy}{x+y}$	$S_x J D_x D_y(M(G;x,y))\|_{x=1}$
$AZI(G)$	$(\frac{xy}{x+y-2})^3$	$S_x^3 Q_{-2} J D_x^3 D_y^3(M(G;x,y))\|_{x=1}$

Table 2.2: Expressions for degree based topological indices [8].

Now we give the formula for computing the M-polynomial of the $SiO_2(p,q)$ layer structure.

Theorem 2.2.1. *The M-polynomial of $SiO_2(p,q)$ layer structure is given below:*

$$M(SiO_2(p,q);x,y) = (2p+2q+4)xy^4 + (4pq+2p+2q)x^2y^4.$$

Proof. The number of edges uv of $SiO_2(p,q)$ layer structure such that $\{d_G(u), d_G(v)\} = \{i,j\}$ are given below:

$$m_{11} = m_{12} = m_{13} = m_{22} = m_{23} = m_{33} = m_{34} = m_{44} = 0,$$

and

$$m_{14} = 2p + 2q + 4, m_{24} = 4pq + 2p + 2q.$$

Substituting the above values of m_{ij} in equation (1.28), we get

$$\begin{aligned} M(SiO_2(p,q);x,y) &= (0)xy^1 + (0)xy^2 + (0)xy^3 + (2p+2q+4)xy^4 + (0)x^2y^2 \\ &\quad +(4pq+2p+2q)x^2y^3 + (0)x^2y^4 + (0)x^3y^3 + (0)x^3y^4 \\ &\quad +(0)x^4y^4. \end{aligned}$$

After simplifying the above expression, we get

$$M(SiO_2(p,q);x,y) = (2p+2q+4)xy^4 + (4pq+2p+2q)x^2y^4.$$

This gives the required expression. □

The following corollary is an easy consequence of Theorem 2.2.1, which gives the degree based indices derived from the M-polynomial.

Corollary 2.2.1. *First Zagreb index, second Zagreb index, second modified Zagreb index, general Randić index, symmetric division degree index, harmonic index, inverse sum index, and augmented Zagreb index derived from M-polynomial of SiO_2 layer structure are respectively given below:*

$$\begin{aligned} M_1(SiO_2(p,q)) &= 24pq + 22p + 22q + 20, \\ M_2(SiO_2(p,q)) &= 32pq + 24p + 24q + 16, \\ M_2^*(SiO_2(p,q)) &= \frac{3}{4}p + \frac{3}{4}q + \frac{1}{2}pq + 1, \\ R_\alpha(SiO_2(p,q)) &= 4^\alpha(2p+2q+4) + 8^\alpha(4pq+2p+2q), \alpha \in \mathbb{Z}^+ \\ R_\alpha(SiO_2(p,q)) &= \frac{1}{4^{-\alpha}}(2p+2q+4) + \frac{1}{8^{-\alpha}}(4pq+2p+2q), \alpha \in \mathbb{Z}^- \\ SDD(SiO_2(p,q)) &= 10pq + \frac{27}{2}p + \frac{27}{2}q + 17, \\ H(SiO_2(p,q)) &= \frac{22}{15}p + \frac{22}{15}q + \frac{4}{3}pq + \frac{8}{5}, \\ ISI(SiO_2(p,q)) &= \frac{64}{15}p + \frac{64}{15}q + \frac{16}{3}pq + \frac{16}{5}, \\ AZI(SiO_2(p,q)) &= \frac{560}{27}p + \frac{560}{27}q + \frac{256}{27} + 32pq. \end{aligned}$$

Proof. First we compute first Zagreb index. Using Theorem 2.2.1 and Table 2.2, we have

$$\begin{aligned} M_1(SiO_2(p,q)) &= (D_x + D_y)((2p+2q+4)xy^4 + (4pq+2p+2q)x^2y^4)|_{x=y=1} \\ &= (2p+2q+4)xy^4 + 2(4pq+2p+2q)x^2y^4 + 4(2p+2q+4)xy^4 \end{aligned}$$

$$
\begin{aligned}
& +4(4pq+2p+2q)x^2y^4|_{x=y=1} \\
= \; & (2p+2q+4)+2(4pq+2p+2q)+4(2p+2q+4) \\
& +4(4pq+2p+2q) \\
= \; & 24pq+22p+22q+20.
\end{aligned}
$$

Using Theorem 2.2.1 and Table 2.2, second Zagreb index for the $SiO_2(p,q)$ layer structure is given by:

$$
\begin{aligned}
M_2(SiO_2(p,q)) &= (D_xD_y)((2p+2q+4)xy^4+(4pq+2p+2q)x^2y^4)|_{x=y=1} \\
&= 4(2p+2q+4)xy^4+(2)(4)(4pq+2p+2q)x^2y^4|_{x=y=1} \\
&= 4(2p+2q+4)+(2)(4)(4pq+2p+2q) \\
&= 32pq+24p+24q+16.
\end{aligned}
$$

Again using Theorem 2.2.1 and Table 2.2, the expression for second modified Zagreb index for the $SiO_2(p,q)$ layer structure is given by:

$$
\begin{aligned}
M_2^*(SiO_2(p,q)) &= (S_xS_y)((2p+2q+4)xy^4+(4pq+2p+2q)x^2y^4))|_{x=y=1} \\
&= \frac{1}{4}(2p+2q+4)xy^4+(\frac{1}{4})(\frac{1}{2})(4pq+2p+2q)x^2y^4|_{x=y=1} \\
&= \frac{1}{4}(2p+2q+4)+(\frac{1}{4})(\frac{1}{2})(4pq+2p+2q) \\
&= \frac{3}{4}p+\frac{3}{4}q+\frac{1}{2}pq+1.
\end{aligned}
$$

Next we compute the expression for general Randic index $R_\alpha(G)$ for $\alpha \in \mathbb{Z}^+$ corresponding to the function $f(x,y)=(xy)^\alpha$. Using Theorem 2.2.1 and Table 2.2, we have

$$
\begin{aligned}
R_\alpha(SiO_2(p,q)) &= (D_x^\alpha D_y^\alpha)((2p+2q+4)xy^4+(4pq+2p+2q)x^2y^4))|_{x=y=1} \\
&= (2p+2q+4)x(4^\alpha)y^4+(4pq+2p+2q)(2^\alpha)x^2(4^\alpha)y^4))|_{x=y=1} \\
&= (2p+2q+4)(4^\alpha)+(4pq+2p+2q)(2^\alpha)(4^\alpha) \\
&= 4^\alpha(2p+2q+4)+8^\alpha(4pq+2p+2q).
\end{aligned}
$$

Next we compute the expression for general Randic index $R_\alpha(G)$ for $\alpha \in \mathbb{Z}^-$ corresponding to the function $f(x,y)=(xy)^\alpha$. Using Theorem 2.2.1 and Table 2.2, we have

$$
\begin{aligned}
R_\alpha(SiO_2(p,q)) &= (S_x^{-\alpha}S_y^{-\alpha})((2p+2q+4)xy^4+(4pq+2p+2q)x^2y^4))|_{x=y=1}, \\
&= (2p+2q+4)\frac{1}{4^{-\alpha}}xy^4+(4pq+2p+2q)(\frac{1}{2^{-\alpha}})x^2(\frac{1}{4^{-\alpha}})y^4|_{x=y=1}, \\
&= (2p+2q+4)\frac{1}{4^{-\alpha}}+(4pq+2p+2q)(\frac{1}{2^{-\alpha}})(\frac{1}{4^{-\alpha}}),
\end{aligned}
$$

$$= \frac{1}{4^{-\alpha}}(2p+2q+4)+\frac{1}{8^{-\alpha}}(4pq+2p+2q).$$

Again using Theorem 2.2.1 and Table 2.2, the expression for symmetric division degree index for the $SiO_2(p,q)$ layer structure is given by:

$$\begin{aligned}
SDD(SiO_2(p,q)) &= (D_xS_y+D_yS_x)((2p+2q+4)xy^4+(4pq+2p+2q)x^2y^4))|_{x=y=1}\\
&= \frac{1}{4}(2p+2q+4)xy^4+\frac{2}{4}(4pq+2p+2q)x^2y^4+4(2p+2q+4)xy^4\\
&+ (4pq+2p+2q)\frac{4}{2}x^2y^4|_{x=y=1}\\
&= \frac{1}{4}(2p+2q+4)+\frac{2}{4}(4pq+2p+2q)+4(2p+2q+4)\\
&+ \frac{4}{2}(4pq+2p+2q)\\
&= 10pq+\frac{27}{2}p+\frac{27}{2}q+17.
\end{aligned}$$

Next we compute the expression for harmonic index for the $SiO_2(p,q)$ layer structure. Using Theorem 2.2.1 and Table 2.2, we have

$$\begin{aligned}
H(SiO_2(p,q)) &= 2S_xJ((2p+2q+4)xy^4+(4pq+2p+2q)x^2y^4))|_{x=1}\\
&= 2(\frac{1}{5}(2p+2q+4)x^5+\frac{1}{6}(4pq+2p+2q)x^6)|_{x=1}\\
&= 2(\frac{1}{5}(2p+2q+4)+\frac{1}{6}(4pq+2p+2q))\\
&= \frac{22}{15}p+\frac{22}{15}q+\frac{4}{3}pq+\frac{8}{5}.
\end{aligned}$$

Next we compute the expression for inverse sum index for the $SiO_2(p,q)$ layer structure. Using Theorem 2.2.1 and Table 2.2, we have

$$\begin{aligned}
ISI(SiO_2(p,q)) &= S_xJD_xD_y((2p+2q+4)xy^4+(4pq+2p+2q)x^2y^4))|_{x=1}\\
&= (4(\frac{1}{5})(2p+2q+4)x^5+4(2)(\frac{1}{6})(4pq+2p+2q)x^6)|_{x=1}\\
&= (4(\frac{1}{5})(2p+2q+4)+4(2)(\frac{1}{6})(4pq+2p+2q))\\
&= \frac{64}{15}p+\frac{64}{15}q+\frac{16}{3}pq+\frac{16}{5}.
\end{aligned}$$

Next we compute the expression for augmented Zagreb index $AZI(G)$ for the $SiO_2(p,q)$ layer structure. Using Theorem 2.2.1 and Table 2.2, we have

$$AZI(SiO_2(p,q)) = S_x^3Q_{-2}JD_x^3D_y^3((2p+2q+4)xy^4+(4pq+2p+2q)x^2y^4)|_{x=1}$$

$$
\begin{aligned}
&= ((\frac{1}{3^3})(4^3)(2p+2q+4)x^3 + (\frac{1}{4^3})(4^3)(2^3)(4pq+2p+2q)x^4)|_{x=1} \\
&= \frac{560}{27}p + \frac{560}{27}q + \frac{256}{27} + 32pq.
\end{aligned}
$$

The proof is complete. □

2.3 Zagreb polynomials and indices

The following theorem gives the Zagreb polynomials defined by (1.32)-(1.33) and Zagreb indices defined by (1.15)-(1.17) of the SiO_2 layer structure.

Theorem 2.3.1. *The formulae for Zagreb polynomials and Zagreb indices of $SiO_2(p,q)$ are given below:*

$$
\begin{aligned}
M_1(SiO_2(p,q),x) &= (2p+2q+4)x^5 + (4pq+2p+2q)x^6, \\
M_2(SiO_2(p,q),x) &= (2p+2q+4)x^4 + (4pq+2p+2q)x^8, \\
HM(SiO_2(p,q)) &= 144pq + 122p + 122q + 100, \\
PM_1(SiO_2(p,q)) &= 240p^2q + 240pq^2 + 120p^2 + 720pq + 120q^2 + 240p + 240q, \\
PM_2(SiO_2(p,q)) &= 256p^2q + 256pq^2 + 128p^2 + 768pq + 128q^2 + 256p + 256q.
\end{aligned}
$$

Proof. The edge partition based on the degrees of end vertices of each edge of graph of SiO_2 layer structure is given in Table 2.3. Using this table the Zagreb polynomials and indices can be computed as follows:

The first Zagreb polynomial $M_1(SiO_2(p,q),x)$ can be obtained by substituting the values from Table 2.3 in equation (1.32) as follows:

$$
\begin{aligned}
M_1(SiO_2(p,q),x) &= (2p+2q+4)x^{1+4} + (4pq+2p+2q)x^{2+4} \\
&= (2p+2q+4)x^5 + (4pq+2p+2q)x^6.
\end{aligned}
$$

The second Zagreb polynomial $M_2(SiO_2(p,q),x)$ can be obtained by substituting the values from Table 2.3 in equation (1.33) as follows:

$$
\begin{aligned}
M_2(SiO_2(p,q),x) &= (2p+2q+4)x^{1\times 4} + (4pq+2p+2q)x^{2\times 4} \\
&= (2p+2q+4)x^4 + (4pq+2p+2q)x^8.
\end{aligned}
$$

The hyper Zagreb index $HM(SiO_2(p,q))$ can be obtained by substituting the values from Table 2.3 in equation (1.15) as follows:

$$
\begin{aligned}
HM(SiO_2(p,q)) &= (2p+2q+4)(1+4)^2 + (4pq+2p+2q)(2+4)^2 \\
&= 144pq + 122p + 122q + 100.
\end{aligned}
$$

$(d_G(u), d_G(v))$, where $uv \in E(G)$	No. of edges
$(1, 4)$	$2p + 2q + 4$
$(2, 4)$	$4pq + 2p + 2q$

Table 2.3: Edge partition of SiO_2 layer structure based on degrees of end vertices of each edge.

The first multiple Zagreb index $PM_1(SiO_2(p, q))$ can be obtained by substituting the values from Table 2.3 in equation (1.16) as follows:

$$\begin{aligned} PM_1(SiO_2(p,q)) &= (2p + 2q + 4)(1 + 4) \times (4pq + 2p + 2q)(2 + 4) \\ &= 240p^2q + 240pq^2 + 120p^2 + 720pq + 120q^2 + 240p + 240q. \end{aligned}$$

The second multiple Zagreb index $M_1(SiO_2(p, q))$ can be obtained by substituting the values from Table 2.3 in equation (1.17) as follows:

$$\begin{aligned} PM_2(SiO_2(p,q)) &= (2p + 2q + 4)(1 \times 4) \times (4pq + 2p + 2q)(2 \times 4) \\ &= 256p^2q + 256pq^2 + 128p^2 + 768pq + 128q^2 + 256p + 256q. \end{aligned}$$

This completes the proof. □

Chapter 3

Polynomials and Indices of Fullerenes

A fullerene is a carbon molecule in the shape of a hollow sphere or an ellipsoid. It is a 3-regular plane graph all of whose faces are of lengths k and 6. The only values of k for which a $(k, 6)$-fullerene exists is for $k = 3, 4$ and 5. All the faces of an ordinary fullerene have lengths 5 and 6. Kroto et al. [24] discovered a fullerene molecule and named it the buckminster fullerene. The $(3, 6)$-fullerenes have received attention because of the similarity of their structure with ordinary fullerenes. For further details on the properties of $(3, 6)$-fullerenes, the reader is referred to [10, 40]. In this chapter, we consider two infinite families of $(3, 6)$-fullerenes and denote them as $F_1(n)$ and $F_2(n)$, respectively (See Fig. 3.1). The order of $F_1(n)$ and $F_2(n)$ is $8n + 12$ and $12n + 16$, respectively.

We compute counting polynomials and their related indices defined by $(1.22)-(1.27)$ for these fullerenes.

3.1 Counting polynomials and corresponding indices

The vital task in computing the counting polynomials of Fullerenes $F_1(n)$ and $F_2(n)$ is to find the qoc's of these fullerenes. The distinct qoc's with respect to their lengths in $F_1(n)$ are presented in Fig. 3.2 and Table 3.1, respectively. The qoc's in $F_2(n)$ behave differently for even and odd values of n. The distinct qoc's in $F_2(n)$ and their lengths, for odd n, are presented in Fig. 3.3 and Table 3.2, respectively. In the same fashion, the lengths of distinct qoc's in $F_2(n)$, for even n, are shown in Table 3.3.

The following theorem gives the Omega, Sadhana and PI polynomials of $F_1(n)$

Theorem 3.1.1. *The Omega, Sadhana and PI polynomials of $F_1(n)$ network are given by:*

$$\Omega(F_1(n), x) = x^{2n+3} + x^{n+1} + x^{n+2} + 2x^{2n+3} + 2x^{2n+2} + 2x,$$

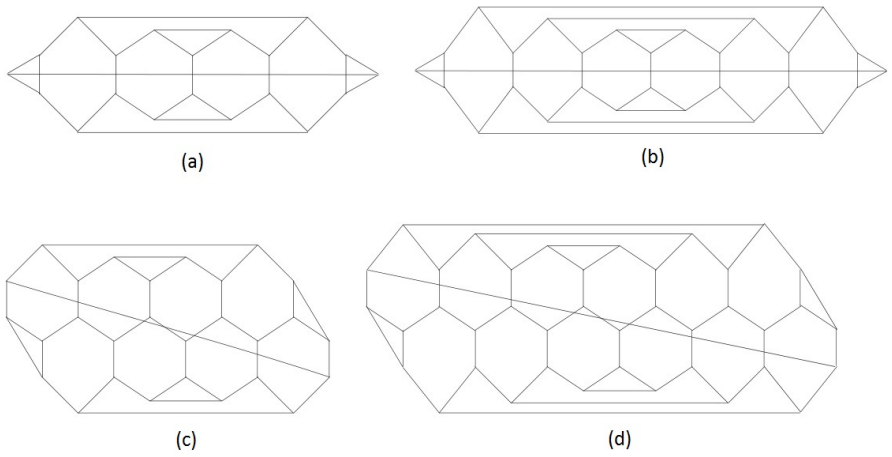

Figure 3.1: The fullerene graphs $F_1(n)$ for $n = 1$ and $n = 2$ are shown in (a) and (b), respectively. The fullerenes $F_2(n)$ for $n = 1$ and $n = 2$ are shown in (c) and (d), respectively

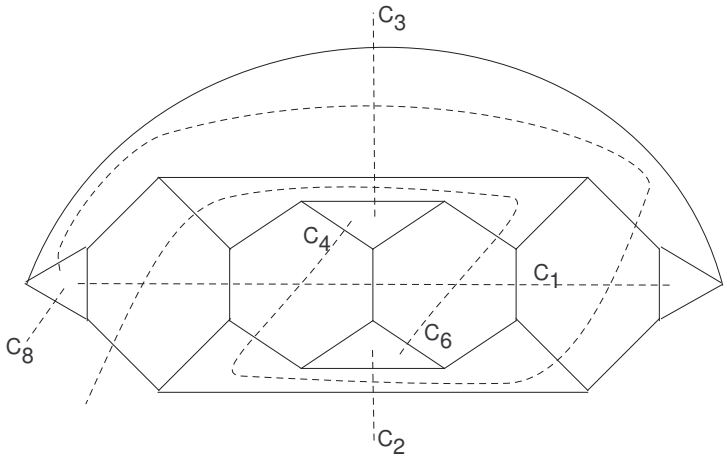

Figure 3.2: The dotted lines show the qoc in $F_1(n)$ for $n = 1$

Types of *qoc*	Length of qoc	No. of *qoc*
C_1	$2n+3$	1
C_2	$n+1$	1
C_3	$n+2$	1
C_4	$2n+3$	2
C_6	$2n+2$	2
C_8	1	2

Table 3.1: Types of qoc, length of qoc and number of qoc in $F_1(n)$.

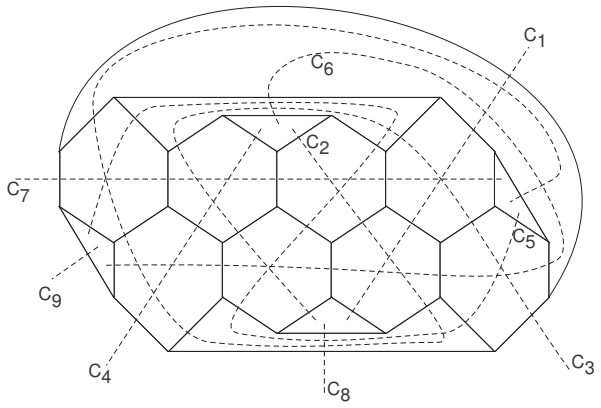

Figure 3.3: The dotted lines show the qoc in $F_2(n)$ for $n = 1$

Types of *qoc*	Length of qoc	No. of *qoc*
C_1	$\frac{3n+5}{2}$	1
C_2	$3n+4$	1
C_3	$3n+3$	1
C_4	$\frac{3n+3}{2}$	1
C_5	$3n+4$	1
C_6	$3n+4$	1
C_7	$2n+3$	1
C_8	$n+1$	1
C_9	1	1

Table 3.2: Types of qoc, length of qoc and number of qoc in $F_2(n)$, for odd n.

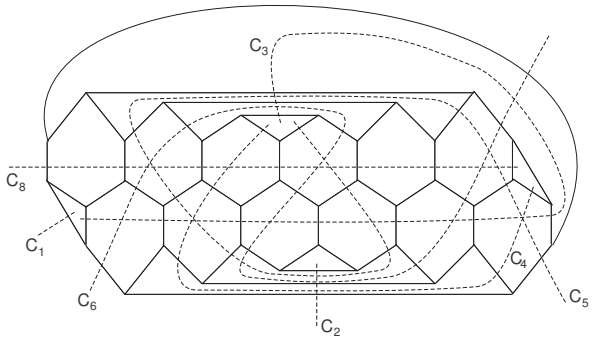

Figure 3.4: The dotted lines show the qoc in $F_2(n)$ for $n = 2$

Types of *qoc*	Length of qoc	No. of *qoc*
C_1	1	1
C_2	$n+1$	1
C_3	$3n+4$	1
C_4	$\frac{3}{2}n+2$	2
C_5	$3n+3$	1
C_6	$3n+4$	2
C_8	$2n+3$	1

Table 3.3: Types of qoc, length of qoc and number of qoc in $F_2(n)$, for even n.

$$\begin{aligned} Sd(F_1(n),x) &= x^{10n+15}+x^{11n+17}+x^{11n+16}+2x^{10n+15}+2x^{10n+16}+2x^{12n+17}, \\ PI(F_1(n),x) &= (2n+3)x^{10n+15}+(n+1)x^{11n+17}+(n+2)x^{11n+16}+(4n+6)x^{10n+15} \\ &\quad +(4n+4)x^{10n+16}+2x^{12n+17}. \end{aligned}$$

Proof. The qoc's $C_1, C_2, \cdots, C_6$ of the graph $F_1(n)$ and their lengths are shown in Fig. 3.2 and Table 3.1, respectively. Substituting these in equation (1.22), we get

$$\begin{aligned} \Omega(F_1(n),x) &= x^{2n+3}+x^{n+1}+x^{n+2}+2x^{2n+3}+2x^{2n+2}+2x \\ &= x^{2n+3}+x^{n+1}+x^{n+2}+2x^{2n+3}+2x^{2n+2}+2x. \end{aligned}$$

The Sadhana polynomial of $F_1(n)$ can be obtained by substituting the values from Table 3.1 in equation (1.24), as follows.

$$\begin{aligned} Sd(F_1(n),x) &= x^{(12n+18)-(2n+3)}+x^{(12n+18)-(n+1)}+x^{(12n+18)-(n+2)}+2x^{(12n+18)-(2n+3)} \\ &\quad +2x^{(12n+18)-(2n+2)}+2x^{(12n+18)-1} \\ &= x^{10n+15}+x^{11n+17}+x^{11n+16}+2x^{10n+15}+2x^{10n+16}+2x^{12n+17}. \end{aligned}$$

The PI polynomial is obtained by substituting the values from Table 3.1 in equation (1.26).

$$\begin{aligned} PI(F_1(n),x) &= (2n+3)x^{(12n+18)-(2n+3)}+(n+1)x^{(12n+18)-(n+1)} \\ &\quad +(n+2)x^{(12n+18)-(n+2)}+2(2n+3)x^{(12n+18)-(2n+3)} \\ &\quad +2(2n+2)x^{(12n+18)-(2n+2)}+2(1)x^{(12n+18)-1} \\ &= (2n+3)x^{10n+15}+(n+1)x^{11n+17}+(n+2)x^{11n+16}+(4n+6)x^{10n+15} \\ &\quad +(4n+4)x^{10n+16}+2x^{12n+17}. \end{aligned}$$

This completes the proof. □

Next we find the indices derived from the polynomials computed in the Theorem 3.1.1.

Corollary 3.1.1. *The Omega, Sadhana and PI indices of $F_1(n)$ are given below:*

$$\begin{aligned} \Omega(F_1(n)) &= 12n+18, \\ Sd(F_1(n)) &= 96n+144, \\ PI(F_1(n)) &= 122n^2+374n+282. \end{aligned}$$

Proof. Using Theorem 3.1.1 and equation (1.21), and performing some calculations, the Omega, Sadhana and PI indices are obtained as follows.

$$\begin{aligned} \Omega(F_1(n)) &= (2n+3)+(n+1)+(n+2)+2(2n+3)+2(2n+2)+2 \\ &= 12n+18. \\ Sd(F_1(n)) &= (10n+15)+(11n+17)+(11n+16)+2(10n+15)+2(10n+16) \\ &\quad +2(12n+17) \\ &= 96n+144. \\ PI(F_1(n)) &= (2n+3)(10n+15)+(n+1)(11n+17)+(n+2)(11n+16) \\ &\quad +2(2n+3)(10n+15)+2(2n+2)(10n+16)+2(1)(12n+17) \\ &= 122n^2+374n+282. \end{aligned}$$

The proof is complete. □

Theorem 3.1.2. *Let n be an odd integer, then the Omega, Sadhana and PI polynomials of $F_2(n)$ network are given by:*

$$\begin{aligned} \Omega(F_2(n),x) &= x^{\frac{3n+5}{2}}+x^{3n+3}+x^{\frac{3n+3}{2}}+3x^{3n+4}+x^{2n+3}+x^{n+1}+x, \\ Sd(F_2(n),x) &= x^{\frac{33n+43}{2}}+x^{15n+21}+x^{\frac{33n+45}{2}}+3x^{15n+20}+x^{16n+21}+x^{17n+23} \\ &\quad +x^{18n+23}, \\ PI(F_2(n),x) &= (\frac{3n+5}{2})x^{\frac{33n+43}{2}}+(3n+3)x^{15n+21}+(\frac{3n+3}{2})x^{\frac{33n+45}{2}} \\ &\quad +3(3n+4)x^{15n+20}+(2n+3)x^{16n+21}+(n+1)x^{17n+23}+x^{18n+23}. \end{aligned}$$

Proof. The qoc's $C_1, C_2, \cdots, C_9$ in $F_2(n)$, for odd n, are shown in Fig. 3.3. The lengths of these qoc's are shown in Table 3.2. Substituting these values in equation (1.22), we get

$$\begin{aligned} \Omega(F_2(n),x) &= x^{\frac{3n+5}{2}}+x^{3n+4}+x^{3n+3}+x^{\frac{3n+3}{2}}+x^{3n+4}+x^{3n+4}+x^{2n+3}+x^{n+1}+x^1 \\ &= x^{\frac{3n+5}{2}}+x^{3n+3}+x^{\frac{3n+3}{2}}+3x^{3n+4}+x^{2n+3}+x^{n+1}+x. \end{aligned}$$

The expression for the Sadhana polynomial for $F_2(n)$ is obtained by substituting the values from Table 3.2 in equation (1.24), we get

$$\begin{aligned} Sd(F_2(n),x) &= x^{(18n+24)-(\frac{3n+5}{2})} + x^{(18n+24)-(3n+4)} + x^{(18n+24)-(3n+3)} + x^{(18n+24)-(\frac{3n+3}{2})} \\ &\quad + x^{(18n+24)-(3n+4)} + x^{(18n+24)-(3n+4)} + x^{(18n+24)-(2n+3)} + x^{(18n+24)-(n+1)} \\ &\quad + x^{(18n+24)-1} \\ &= x^{\frac{33n+43}{2}} + x^{15n+21} + x^{\frac{33n+45}{2}} + 3x^{15n+20} + x^{16n+21} + x^{17n+23} + x^{18n+23}. \end{aligned}$$

The expression for the PI polynomial can be computed by substituting the values from Table 3.2 in equation (1.26), we obtain

$$\begin{aligned} PI(F_2(n),x) &= (\frac{3n+5}{2})x^{(18n+24)-(\frac{3n+5}{2})} + (3n+4)x^{(18n+24)-(3n+4)} \\ &\quad + (3n+3)x^{(18n+24)-(3n+3)} + (\frac{3n+3}{2})x^{(18n+24)-(\frac{3n+3}{2})} \\ &\quad + (3n+4)x^{(18n+24)-(3n+4)} + (3n+4)x^{(18n+24)-(3n+4)} \\ &\quad + (2n+3)^{(18n+24)-(2n+3)} + (n+1)x^{(18n+24)-(n+1)} + (1)x^{(18n+24)-1} \\ &= (\frac{3n+5}{2})x^{\frac{33n+43}{2}} + (3n+3)x^{15n+21} + (\frac{3n+3}{2})x^{\frac{33n+45}{2}} \\ &\quad + 3(3n+4)x^{15n+20} + (2n+3)x^{16n+21} + (n+1)x^{17n+23} + x^{18n+23}. \end{aligned}$$

The proof is complete. □

Theorem 3.1.3. *Let n be an even integer. Then the Omega, Sadhana and PI polynomials of $F_2(n)$ network are given by:*

$$\begin{aligned} \Omega(F_2(n),x) &= x + x^{n+1} + 3x^{3n+4} + 2x^{\frac{3}{2}n+2} + x^{3n+3} + x^{2n+3}, \\ Sd(F_2(n),x) &= x^{18n+23} + x^{17n+23} + 3x^{15n+20} + 2x^{\frac{33}{2}n+22} + x^{15n+21} + x^{16n+21}, \\ PI(F_2(n),x) &= x^{18n+23} + (n+1)x^{17n+23} + 3(3n+4)x^{15n+20} + 2(\frac{3}{2}n+2)x^{\frac{33}{2}n+22} \\ &\quad + (3n+3)x^{15n+21} + (2n+3)x^{16n+21}. \end{aligned}$$

Proof. The qoc's $C_1, C_2, \cdots, C_7$ in $F_2(n)$, for even n, are shown in Fig. 3.4. The length and the number of qoc's are given in Table 3.3. Now we compute the Omega polynomial for $F_2(n)$ by substituting the values from Table 3.3 in equation (1.22), we get

$$\begin{aligned} \Omega(F_2(n),x) &= x^1 + x^{n+1} + x^{3n+4} + 2x^{\frac{3}{2}n+2} + x^{3n+3} + 2x^{3n+4} + x^{2n+3} \\ &= x + x^{n+1} + 3x^{3n+4} + 2x^{\frac{3}{2}n+2} + x^{3n+3} + x^{2n+3}. \end{aligned}$$

The expression for the Sadhana polynomial for $F_2(n)$ is obtained by substituting the values from Table 3.3 in equation (1.24), we get

$$Sd(F_2(n),x) = x^{(18n+24)-1} + x^{(18n+24)-(n+1)} + x^{(18n+24)-(3n+4)} + 2x^{(18n+24)-(\frac{3}{2}n+2)}$$

$$
\begin{aligned}
& +x^{(18n+24)-(3n+3)} + 2x^{(18n+24)-(3n+4)} + x^{(18n+24)-(2n+3)} \\
= \; & x^{18n+23} + x^{17n+23} + 3x^{15n+20} + 2x^{\frac{33}{2}n+22} + x^{15n+21} + x^{16n+21}.
\end{aligned}
$$

The expression for the PI polynomial can be computed by substituting the values from Table 3.3 in equation (1.26), we obtain

$$
\begin{aligned}
PI(F_2(n), x) = \; & x^{(18n+24)-1} + (n+1)x^{(18n+24)-(n+1)} + (3n+4)x^{(18n+24)-(3n+4)} \\
& +2(\frac{3}{2}n+2)x^{(18n+24)-(\frac{3}{2}n+2)} + (3n+3)x^{(18n+24)-(3n+3)} \\
& +2(3n+4)x^{(18n+24)-(3n+4)} + (2n+3)x^{(18n+24)-(2n+3)} \\
= \; & x^{18n+23} + (n+1)x^{17n+23} + 3(3n+4)x^{15n+20} + 2(\frac{3}{2}n+2)x^{\frac{33}{2}n+22} \\
& +(3n+3)x^{15n+21} + (2n+3)x^{16n+21}.
\end{aligned}
$$

This completes the proof. □

Next we find the indices derived from the polynomials computed in the Theorems (3.1.2)-(3.1.3).

Corollary 3.1.2. *Let n be an odd integer. Then the Omega, Sadhana and PI indices of $F_2(n)$ network are given by:*

$$
\begin{aligned}
\Omega(F_2(n)) &= 18n + 24, \\
Sd(F_2(n)) &= 144n + 152, \\
PI(F_2(n)) &= \frac{557}{2}n^2 + 748n + \frac{999}{2}.
\end{aligned}
$$

Proof. Using Theorem 3.1.2 and equation (1.21), and performing some calculations, the Omega, Sadhana and PI index is obtained as follows.

$$
\begin{aligned}
\Omega(F_2(n)) &= \frac{3n+5}{2} + (3n+3) + \frac{3n+3}{2} + 3(3n+4) + 2n + 3 + n + 1 + 1 \\
&= 18n + 24, \\
Sd(F_2(n)) &= \frac{33n+43}{2} + 15n + 21 + \frac{33n+45}{2} + 15n + 20 + 16n + 21 + 17n \\
&\quad +23 + 18n + 23 \\
&= 144n + 152, \\
PI(F_2(n)) &= (\frac{3n+5}{2})(\frac{33n+43}{2}) + (3n+3)(15n+21) + (\frac{3n+3}{2})(\frac{33n+45}{2}) \\
&\quad +3(3n+4)(15n+20) + (2n+3)(16n+21) + (n+1)(17n+23) \\
&\quad +(1)(18n+23) \\
&= \frac{557}{2}n^2 + 748n + \frac{999}{2}.
\end{aligned}
$$

The proof is complete. □

Corollary 3.1.3. *Let n be an even integer. Then the Omega, Sadhana and PI indices of $F_2(n)$ network are given by:*

$$\begin{aligned} \Omega(F_2(n)) &= 18n + 24, \\ Sd(F_2(n)) &= 144n + 192, \\ PI(F_2(n)) &= \frac{557}{2}n^2 + 748n + 500. \end{aligned}$$

Proof. Using Theorem 3.1.3 and equation (1.21), and performing some calculations, the Omega, Sadhana and PI index is obtained as follows:

$$\begin{aligned} \Omega(F_2(n)) &= 1 + (n+1) + (3n+4) + 2(\frac{3}{2}n + 2) + 2(3n+4) + (3n+3) + (2n+3) \\ &= 18n + 24, \\ Sd(F_2(n)) &= (18n+23) + (17n+23) + (15n+20) + 2(\frac{33}{2}n + 22) + 2(15n+20) \\ &\quad +(15n+21) + (16n+21) \\ &= 144n + 192, \\ PI(F_2(n)) &= (18n+23) + (n+1)(17n+23) + (3n+4)(15n+20) + 2(3/2n \\ &\quad +2)(\frac{33}{2}n + 22) + 2(3n+4)(15n+20) + (3n+3)(15n+21) \\ &\quad +(2n+3)(16n+21) \\ &= \frac{557}{2}n^2 + 748n + 500. \end{aligned}$$

This complete the proof. □

3.2 M-polynomials

This section gives the M-polynomial defined by (1.28) for $F_1(n)$ and $F_2(n)$ network.

Theorem 3.2.1. *The formula for M-polynomial of $F_1(n)$ is given below:*

$$M(F_1(n); x, y) = (12n + 18)x^3y^3.$$

Proof. Since m_{ij} is the number of edges uv of $F_1(n)$ such that $\{d_G(u), d_G(v)\} = \{i, j\}$ and $F_1(n)$ is a 3-regular graph so $m_{33} = 12n + 18$. The number of edges uv of $F_1(n)$ such that $\{d_G(u), d_G(v)\} = \{i, j\}$ are given below:

$$m_{11} = m_{12} = m_{13} = m_{14} = m_{22} = m_{23} = m_{24} = m_{34} = m_{44} = 0,$$

and

$$m_{33} = 12n + 18.$$

Substituting the values of m_{ij} in the equation (1.28), we get

$$\begin{aligned} M(F_1(n);x,y) &= (0)xy^1 + (0)xy^2 + (0)xy^3 + (0)xy^4 + (0)x^2y^2 + (0)x^2y^3 \\ &\quad +(0)x^2y^4 + (12n+18)x^3y^3 + (0)x^3y^4 + (0)x^4y^4 \\ &= (12n+18)x^3y^3. \end{aligned}$$

This completes the proof. □

Corollary 3.2.1. *The formula for M-polynomial of $F_2(n)$ is given below:*

$$M(F_2(n);x,y) = (18n+24)x^3y^3.$$

Proof. Since $m_{33} = 18n+24$. The number of edges uv of $F_2(n)$ such that $\{d_G(u), d_G(v)\} = \{i,j\}$ are given below:

$$m_{11} = m_{12} = m_{13} = m_{14} = m_{22} = m_{23} = m_{24} = m_{34} = m_{44} = 0,$$

and

$$m_{33} = 18n+24.$$

Substituting the values of m_{ij} in the equation (1.28), we get

$$\begin{aligned} M(F_2(n);x,y) &= (0)xy^1 + (0)xy^2 + (0)xy^3 + (0)xy^4 + (0)x^2y^2 + (0)x^2y^3 \\ &+ (0)x^2y^4 + (18n+24)x^3y^3 + (0)x^3y^4 + (0)x^4y^4 \\ &= (18n+24)x^3y^3. \end{aligned}$$

This completes the proof. □

Chapter 4

Polynomials and Indices of hypercore dendrimer

Dendrimers are 3-dimensional hyper-branched macromolecules synthetically manufactured with a well-defined structure. The structure of a dendrimer molecule begins with a central atom or a group of atoms which is called the central core. First dendrimes were synthesized step-by-step in an iterative process using a divergent approach starting from the core [3, 35]. Later on, a convergent synthetic approach was introduced in 1990 by Hawker et al. [13]. Dendrimers have a specific topology and have a large number of chain ends and functional groups. They can vary in stability, solubility, rigidity and flexibility due to the end functional groups [37]. The structural property relationships of dendritic molecules can be rationalized because they have structural homogeneity and regularity. Due to their large size and structure, they possess unusual physico-chemical properties which are not possessed by micromolecules [4]. Many dendrimers are synthesized by different techniques.

The hypercore dendrimer considered in this paper is synthesized by a repetitive addition and activation steps which increase the number of branches in the molecule. The growth of this dendrimer is from the central core to the periphery. The central core $1,1,1$- tris (4-hydroxyphenyl)ethane contains multiple copies of the functional group, namely hydroxy group, which reacts with and couples with an activated bifunctional branched structure linked to the central unit in the form of segments, called dendron, and give a protected hypercore dendrimer. The resulting protected hypercore is then activated by removing its benzyl groups by the catalytic hydrogenation and produce the first generation hypercore dendrimer (See Fig. 4.1). Further the first generation dendrimer D_1 couples with additional bifunctional monomer to give second generation dendrimer D_2. In the similar way the synthesized $(n-1)^{th}$ generation dendrimer D_{n-1} combines with the additional bifunctional monomer and give D_n and so on. With increase in generation number time required for completion of reaction also increases. In this chapter, we consider

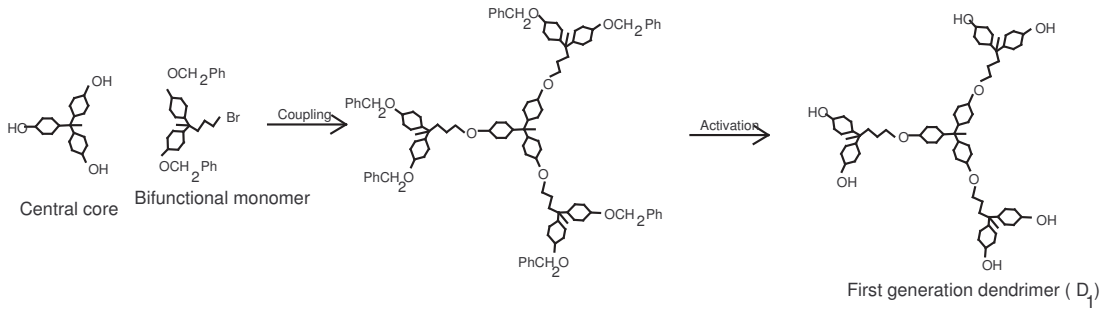

Figure 4.1: Synthetic strategy of dendrimer D_1

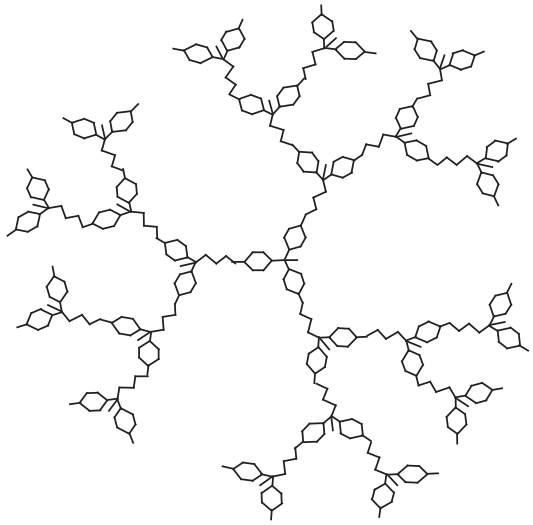

Figure 4.2: Third generation dendrimer D_3

the molecular graph, denoted by D_n, of the hypercore dendrimer shown in Figures 4.1 and 4.2. Here n denotes the different generations of the hypercore dendrimer and D_0 represents the central core. The order and size of D_n are respectively given by $57(2^n) - 34$ and $63(2^n) - 38$. We compute Omega polynomial, Sadhana polynomial, PI polynomial for D_n using the standard cut method. We also compute topological indices derived from these polynomials. Furthermore, we compute M-polynomial, Zagreb polynomials and Zagreb indices for D_n. Some properties of Zagreb polynomials for chemical structures have been studied in [21]. The following section gives counting polynomials and their related indices defined by $(1.22)-(1.27)$ for D_n.

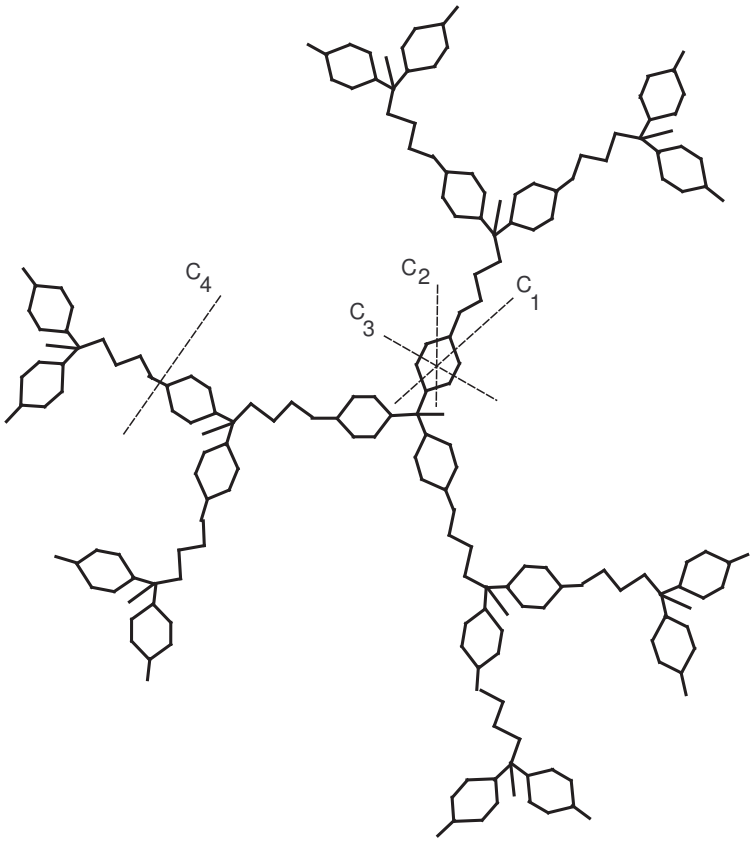

Figure 4.3: The dotted lines show the qoc in D_n for $n = 2$.

4.1 Counting polynomials and corresponding indices

To compute the counting polynomials of D_n, it is required to find the qocs in D_n. Different qocs in D_n are shown by dotted lines in Fig. 4.3. The length and the number of qocs in D_n are shown in Table 4.1.

The following theorem gives the Omega, Sadhana and PI polynomials of D_n

Theorem 4.1.1. *The Omega, Sadhana and PI polynomials of D_n, $n = 0, 1, 2, \cdots$, are given by:*

$$\begin{aligned} \Omega(D_n, x) &= 3(-3 + 6(2^n))x^2 + (-20 + 27(2^n))x, \\ Sd(D_n, x) &= 3(-3 + 6(2^n))x^{63(2^n)-40} + (-20 + 27(2^n))x^{63(2^n)-39}, \\ PI(D_n, x) &= 6(-3 + 6(2^n))x^{63(2^n)-40} + (-20 + 27(2^n))x^{63(2^n)-39}. \end{aligned}$$

Proof. The qocs of length 2 through the edges of each hexagon are denoted by C_1, C_2 and C_3. The qoc of length 1 through the edges not in any hexagon of the D_n is

Types of *qoc*	Length of qoc	No. of *qoc*
C_1	2	$-3+6(2^n)$
C_2	2	$-3+6(2^n)$
C_3	2	$-3+6(2^n)$
C_4	1	$-20+27(2^n)$

Table 4.1: Types of qoc, length of qoc and number of qoc in D_n.

denoted by C_4. From Table 4.1 and equation (1.22), we get

$$\begin{aligned}\Omega(D_n,x) &= (-3+6(2^n))x^2+(-3+6(2^n))x^2+(-3+6(2^n))x^2+(-20+27(2^n))x\\ &= 3(-3+6(2^n))x^2+(-20+27(2^n))x.\end{aligned}$$

The Sadhana polynomial of D_n can be obtained by substituting the values from Table 4.1 in equation (1.24) as follows:

$$\begin{aligned}Sd(D_n,x) &= (-3+6(2^n))x^{63(2^n)-38-2}+(-3+6(2^n))x^{63(2^n)-38-2}+\\ &\quad (-3+6(2^n))x^{63(2^n)-38-2}+(-20+27(2^n))x^{63(2^n)-38-1}\\ &= 3(-3+6(2^n))x^{63(2^n)-40}+(-20+27(2^n))x^{63(2^n)-39}.\end{aligned}$$

The PI polynomial is obtained by substituting the values from Table 4.1 in equation (1.26) as follows:

$$\begin{aligned}PI(D_n,x) &= 2(-3+6(2^n))x^{63(2^n)-38-2}+2(-3+6(2^n))x^{63(2^n)-38-2}\\ &\quad +2(-3+6(2^n))x^{63(2^n)-38-2}+(1)(-20+27(2^n))x^{63(2^n)-38-1}\\ &= 6(-3+6(2^n))x^{63(2^n)-40}+(-20+27(2^n))x^{63(2^n)-39}.\end{aligned}$$

This completes the proof. □

Next we find the indices derived from the polynomials computed in the Theorem 4.1.1.

Corollary 4.1.1. *The Omega, Sadhana and PI indices of D_n, $n=0,1,2,\cdots$, are given below:*

$$\begin{aligned}\Omega(D_n) &= 63(2^n)-38,\\ Sd(D_n) &= -3600(2^n)+1140+2835(2^n)^2,\\ PI(D_n) &= -4887(2^n)+1500+3969(2^n)^2.\end{aligned}$$

Proof. By Theorem 4.1.1 and equation (1.23), (1.25) and (1.27), the Omega, Sadhana and PI indices are respectively obtained as follows:

$$\begin{aligned}
\Omega(D_n) &= (2n+3)+(n+1)+(n+2)+2(2n+3)+2(2n+2)+2 \\
&= 63(2^n)-38. \\
Sd(D_n) &= 3(-3+6(2^n))(63(2^n)-40)+(63(2^n)-39).(-20+27(2^n)) \\
&= -3600(2^n)+1140+2835(2^n)^2. \\
PI(D_n) &= 6(-3+6(2^n))(63(2^n)-40)+(63(2^n)-39).(-20+27(2^n)) \\
&= -4887(2^n)+1500+3969(2^n)^2.
\end{aligned}$$

The proof is complete. □

4.2 M-polynomial

This section gives the M-polynomial defined by (1.28) of the dendrimer D_n.

Theorem 4.2.1. *The formula of M-polynomial for D_n, $n = 0, 1, 2, \cdots$, is given below:*

$$\begin{aligned}
M(D_n; x, y) &= (3(2^n))xy^3+(-2+3(2^n))xy^4+(-15+21(2^n))x^2y^2+(-15 \\
&\quad +27(2^n))x^2y^3+(-3+3(2^n))x^2y^4+(-3+6(2^n)))x^3y^4.
\end{aligned}$$

Proof. The possible values of m_{ij}, $i, j \geq 1$ for D_n are given by:

$$m_{11} = m_{12} = m_{33} = m_{44} = 0,$$

$$m_{13} = 3(2^n), \quad m_{14} = -2+3(2^n), \quad m_{22} = -15+21(2^n),$$
$$m_{23} = -15+27(2^n), \quad m_{24} = -3+3(2^n), \quad m_{34} = -3+6(2^n)).$$

By substituting the values of m_{ij} in equation (1.28), we obtain

$$\begin{aligned}
M(D_n; x, y) &= (0)xy^1+(0)xy^2+(3(2^n))xy^3+(-2+3(2^n))xy^4+(-15 \\
&\quad +21(2^n))x^2y^2+(-15+27(2^n))x^2y^3+(-3+3(2^n))x^2y^4 \\
&\quad +(0)x^3y^3+(-3+6(2^n)))x^3y^4+(0)x^4y^4 \\
&= (3(2^n))xy^3+(-2+3(2^n))xy^4+(-15+21(2^n))x^2y^2+(-15 \\
&\quad +27(2^n))x^2y^3+(-3+3(2^n))x^2y^4+(-3+6(2^n)))x^3y^4.
\end{aligned}$$

The proof is complete. □

$(d_G(u), d_G(v))$, $uv \in E(G)$	No. of edges
$(1,3)$	$3(2^n)$
$(1,4)$	$-2+3(2^n)$
$(2,2)$	$-15+21(2^n)$
$(2,3)$	$-15+27(2^n)$
$(2,4)$	$-3+3(2^n)$
$(3,4)$	$-3+6(2^n)$

Table 4.2: Edge partition of D_n based on degrees of end vertices of each edge.

4.3 Zagreb polynomials and Zagreb indices

The following theorem gives the Zagreb polynomials defined by (1.32)-(1.33) and Zagreb indices defined by (1.6)-(1.7), (1.15)-(1.17) of the dendrimer D_n.

Theorem 4.3.1. *The formulae of Zagreb polynomials and Zagreb indices for D_n, $n = 0, 1, 2, \cdots$, are given below:*

$$\begin{aligned}
M_1(D_n, x) &= (24(2^n)-15)x^4 + (30(2^n)-17)x^5 + (3(2^n)-3)x^6 + (6(2^n)-3)x^7,\\
M_2(D_n, x) &= 3(2^n)x^3 + (24(2^n)-17)x^4 + (27(2^n)-15)x^6 + (3(2^n)-3)x^8\\
&\quad +(6(2^n)-3)x^{12},\\
M_1(D_n) &= 306(2^n) - 184,\\
M_2(D_n) &= 363(2^n) - 218,\\
HM(D_n) &= 1536(2^n) - 920,\\
PM_1(D_n) &= -204120000(2^n) + 1571724000(2^n)^2 - 4780490400(2^n)^3\\
&\quad +7172776800(2^n)^4 - 5303037600(2^n)^5 + 1543147200(2^n)^6,\\
PM_2(D_n) &= -335923200(2^n) + 2586608640(2^n)^2 - 7867321344(2^n)^3\\
&\quad +11804341248(2^n)^4 - 8727284736(2^n)^5 + 2539579392(2^n)^6.
\end{aligned}$$

Proof. The edge partition based on the degrees of end vertices of each edge of D_n is given in Table 4.2. Using this table, we compute the Zagreb polynomials and indices. The first Zagreb polynomial $M_1(D_n, x)$ can be obtained by substituting the values from Table 4.2 in equation (1.32), as follows:

$$\begin{aligned}
M_1(D_n, x) &= (3(2^n))x^{1+3} + (-2+3(2^n))x^{1+4} + (-15+21(2^n))x^{2+2} + (-15\\
&\quad +27(2^n))x^{2+3} + (-3+3(2^n))x^{2+4} + (-3+6(2^n))x^{3+4}
\end{aligned}$$

$$= (24(2^n) - 15)x^4 + (30(2^n) - 17)x^5 + (3(2^n) - 3)x^6 + (6(2^n) - 3)x^7.$$

To obtain second Zagreb polynomial $M_2(D_n, x)$, we substitute the values from Table 4.2 in equation (1.33) as follows:

$$\begin{aligned} M_2(D_n, x) &= (3(2^n))x^{1\times3} + (-2 + 3(2^n))x^{1\times4} + (-15 + 21(2^n))x^{2\times2} + (-15 \\ &\quad +27(2^n))x^{2\times3} + (-3 + 3(2^n))x^{2\times4} + (-3 + 6(2^n))x^{3\times4} \\ &= 3(2^n)x^3 + (24(2^n) - 17)x^4 + (27(2^n) - 15)x^6 + (3(2^n) - 3)x^8 \\ &\quad +(6(2^n) - 3)x^{12}. \end{aligned}$$

We substitute the values from Table 4.2 in equation (1.6) to obtain first Zagreb index $M_1(D_n)$ as follows:

$$\begin{aligned} M_1(D_n) &= (3(2^n))(1 + 3) + (-2 + 3(2^n))(1 + 4) + (-15 + 21(2^n))(2 + 2) + (-15 \\ &\quad +27(2^n))(2 + 3) + (-3 + 3(2^n))(2 + 4) + (-3 + 6(2^n))(3 + 4) \\ &= 306(2^n) - 184. \end{aligned}$$

The second Zagreb index $M_2(D_n)$ can be obtained by substituting the values from Table 4.2 in equation (1.7) as follows:

$$\begin{aligned} M_2(D_n) &= (3(2^n))(1 \times 3) + (-2 + 3(2^n))(1 \times 4) + (-15 + 21(2^n))(2 \times 2) + (-15 \\ &\quad +27(2^n))(2 \times 3) + (-3 + 3(2^n))(2 \times 4) + (-3 + 6(2^n))(3 \times 4) \\ &= 363(2^n) - 218. \end{aligned}$$

We obtain hyper Zagreb index $HM(D_n)$ by substituting the values from Table 4.2 in equation (1.15) as follows:

$$\begin{aligned} HM(D_n) &= (3(2^n))(1 + 3)^2 + (-2 + 3(2^n))(1 + 4)^2 + (-15 + 21(2^n))(2 + 2)^2 \\ &\quad +(-15 + 27(2^n))(2 + 3)^2 + (-3 + 3(2^n))(2 + 4)^2 + (-3 + 6(2^n))(3 + 4)^2 \\ &= 1536(2^n) - 920. \end{aligned}$$

We obtain first multiple Zagreb index $PM_1(D_n)$ by substituting the values from Table 4.2 in equation (1.16) as follows:

$$\begin{aligned} PM_1(D_n) &= (3(2^n))(1 + 3) \times (-2 + 3(2^n))(1 + 4) \times (-15 + 21(2^n))(2 + 2) \times (-15 \\ &\quad +27(2^n))(2 + 3) \times (-3 + 3(2^n))(2 + 4) \times (-3 + 6(2^n))(3 + 4) \\ &= -204120000(2^n) + 1571724000(2^n)^2 - 4780490400(2^n)^3 \\ &\quad +7172776800(2^n)^4 - 5303037600(2^n)^5 + 1543147200(2^n)^6. \end{aligned}$$

The second multiple Zagreb index $M_1(D_n)$ can be obtained by substituting the values from Table 4.2 in equation (1.17), as follows.

$$PM_2(D_n) = (3(2^n))(1 \times 3) \times (-2 + 3(2^n))(1 \times 4) \times (-15 + 21(2^n))(2 \times 2) \times (-15$$

$$
\begin{aligned}
& +27(2^n))(2\times 3)\times(-3+3(2^n))(2\times 4)\times(-3+6(2^n))(3\times 4) \\
= \; & -335923200(2^n)+2586608640(2^n)^2-7867321344(2^n)^3 \\
& +11804341248(2^n)^4-8727284736(2^n)^5+2539579392(2^n)^6.
\end{aligned}
$$

This completes the proof. □

Appendix A – graph-theoretic symbols

$E(G)$	edge set of G
m	size of G
$V(G)$	vertex set of G
n	order of G
$d_G(u)$	degree of vertex u (in G)
$\delta(G)$	minimum degree of G
$\Delta(G)$	maximum degree of G
W_n	wheel graph
C_n	cycle on n vertices
$\overline{G}$	complement of G
K_p	complete graph on p vertices
$K_{p,q}$	complete bipartite graph with parts of cardinalities p and q
P_n	path on n vertices
T	tree

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