Computations of topological invariants of some types of dendrimers

by

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Abstract

Graph theory plays a vital part in the world of natural as well as chemical and biological sciences. One of the purposes of chemical graph theory is to highlight the primary and foremost role of the graph theory in the study of physico-chemical reactions, biological activities and in identifying structural properties of molecular graphs etc. Polynomials and topological indices are used to achieve the desired properties of molecular graphs.

In this dissertation, first we will discuss the topological properties of Triazine based dendrimer. The study involved computation of various eccentricity based indices and polynomials, specifically, eccentric-connectivity index, eccentricity based Zagreb indices, augmented eccentric-connectivity index, total eccentric-connectivity index, and others. Further calculations of counting polynomials and M-polynomial will also be performed for the molecular graph of this dendrimer.

Considering Phosphorus based dendrimer, we will figure out the M-polynomial, counting polynomials and eccentricity based indices i.e., modified eccentricity index and its corresponding polynomial, second Zagreb eccentricity index and eccentric-connectivity polynomials, etc. Likewise, a Porphyrin-cored dendrimer will also be used and all the indices mentioned above and few polynomials of molecular graph of this dendrimer will also be calculated.

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My parents and Husband,

for their support and prayers

Introduction

Graph theory has diversified applications in different fields, such as Chemistry, Computer technology, and Biochemistry, etc. Chemical structures are manipulated by using chemical graph theory. Many chemical structural problems can be fixed by the involvement of concepts of graph theory, where vertices corresponds to atoms and edges to bonds.

The first chapter is an amalgam of background, introduction and some important classes of graphs as well as it also includes introduction of chemical graph theory and other basic concepts of graph theory.

In the second chapter, we will discuss some renowned topological indices including counting polynomials, distance and degree based topological indices. We will give brief introduction of distance based indices namely, Wiener index, eccentricity-connectivity index, Balaban index, etc. Some degree based indices like, Randić index, geometric arithmetic index and Zagreb indices, etc. We will also discuss different types of polynomials, like counting polynomials and M-polynomial.

In last three chapters, we will calculate some eccentricity based indices and polynomials. In chapter three of the thesis, we will consider triazine based dendrimer and in chapter four we consider phosphorus containing dendrimer Cyclotriphosphazene. In the last chapter, we will compute some invariants of molecular graph of Porphyrin-cored dendrimer.

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Chapter 1

Basic definitions and terminologies

The graph theory is the mathematical theory of applications and properties of graphs. This theory is widely used in different fields like Biochemistry, Computer Sciences, Networking, Operations Research, etc.

1.1 Founder of graph theory

In 1736, a mathematician named Euler published his paper in terms of graph theory which was based on the solution of the Königsberg Bridges. The Königsberg city was located on the Pregel river. The city had seven bridges which connect the two big islands with city. Initially, people were confused with the fact that "Is there any walk exists through which they can move all the bridges at once"? Later, Euler considered this problem and he gave the proposal that such a path can exist if there were only even number of bridges linked with the city. But the land area was attached with odd number of bridges, so Euler proved that such path did not exist. Later on, he considered the bridges as edges and landmasses as nodes, and he introduced that there exists an Eulerian circuit and the problem was solved. The Königsberg bridge problem graph is shown in the Figure 1.1.

1.2 Graphs

A graph G has a set of vertices $V(G) = \{v_1, v_2, \ldots, v_n\}$ and a set of edges $E(G) = \{e_1, e_2, ..., e_m\}$, where n represents the number of vertices in the graph also known as order of graph and m represents the size of the graph. An edge of a graph G

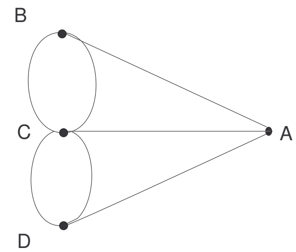

Figure 1.1: Königsberg Bridges graphs.

whose end vertices are u and v is denoted as uv. An edge having same starting and ending vertex is called a loop. Two or more edges that are incident to the same two vertices are called multiple edges. In a graph G, the largest vertex degree is called the maximum degree of G and it is denoted by $\Delta(G)$, and the smallest vertex degree of graph is known as minimum degree and it is denoted by $\delta(G)$. A vertex having only one edge adjacent to it, is called a pendent vertex. If no edge adjacent to a vertex is called isolated vertex. The graph with no loop and multiple edges is known as simple graph.

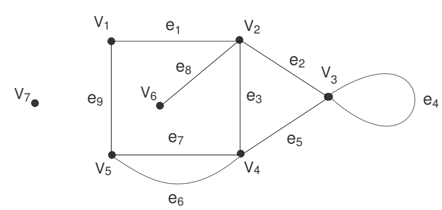

Figure 1.2: Graph.

A graph S is said to be the subgraph of G if the vertex set $V(S)$ of S is subset of $V(G)$ and edge set $E(S)$ of S is a subset of $E(G)$. If $V(G) = V(S)$, then the graph is called spanning subgraph. An induced subgraph F is formed from a subset of the vertices of G and all of the edges connecting pairs of vertices in that subset.

In a graph G, a u-v walk is any route through a graph from vertices and connecting edges. A walk may have same or different start or end vertices. A u-v walk is called a u-v trail when no edge is repeated. A walk u-v is called a u-v path when no edge and vertex is repeated. The number of edges in a path is called the path length. A u-v path is a cycle when there exist a uv edge between vertices u and v.

A graph G is connected if for every pair of vertices of G, there exists a path

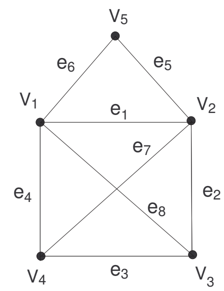

Figure 1.3: Simple graph.

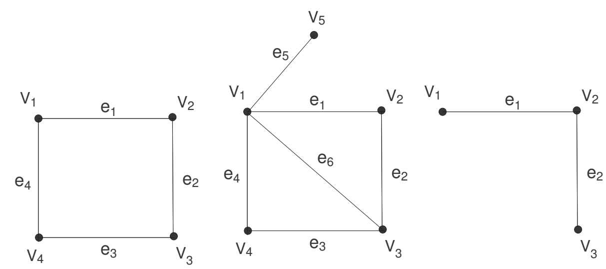

Figure 1.4: Subgraph, Spanning subgraph, Induced subgraph.

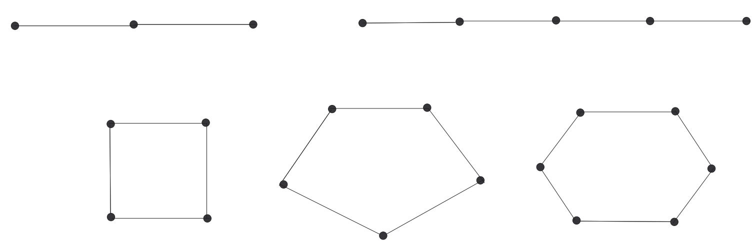

Figure 1.5: P_3, P_5, C_4, C_5, C_6.

between them. If there is any pair of vertices for which path does not exist is called disconnected graph.

Any edge uv in a graph, whose removal makes the graph disconnected, is called bridge or cut edge. Similarly any vertex in a graph G, whose removal disconnect the graph, is called cut vertex.

The distance between two vertices u and v is the shortest path between them and it is denoted as $d(u, v)$. The distance of a vertex u with any other vertex

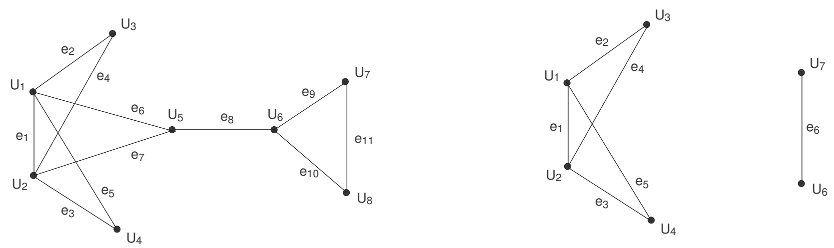

Figure 1.6: Connected graph and disconnected graph

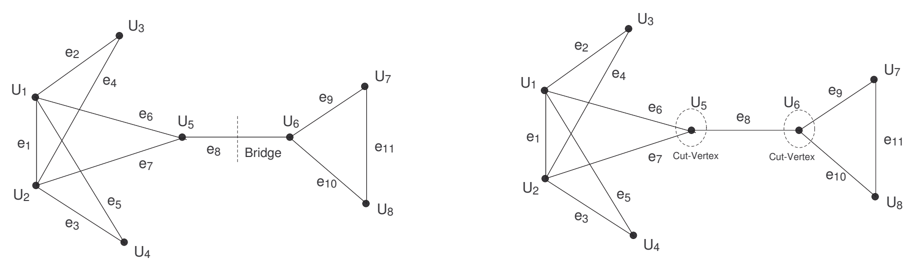

Figure 1.7: Bridge, Cut Vertices

which is farthest from u is called the eccentricity of u and denoted as $\varepsilon(u)$. The minimum eccentricity of graph is known as radius and is denoted as $rad(G)$ and defined as $rad(G) = \min\{\varepsilon(u) \mid u \in V(G)\}$. The diameter of the graph is the maximum distance between any two pair of vertices and it is denoted as $diam(G)$ and represented as $diam(G) = \max\{\varepsilon(u) \mid u \in V(G)\}$.

The degree of a vertex u is the number of edges incident with it and it is denoted by d_u. We also define degree sum of a vertex by $S_u = \sum_{v \in N_u} d_v$, where $N_u = \{u \in V(G) \mid uv \in E(G)\}$.

1.3 Some special types of Graphs

A graph having no cycle is called acyclic graph. A Tree T is a connected acyclic graph. The wheel graph W_n contains a cycle of $n-1$ order. In a wheel graph, every vertex of a cycle is connected with another vertex called hub and edges incident with hub are known as spokes. In a graph G, if there exists an edge between every two distinct vertices is known as complete graph denoted as K_n, where n is the order of graph and the number of edges in complete graph is given as $|E(K_n)| = \frac{n(n-1)}{2}$.

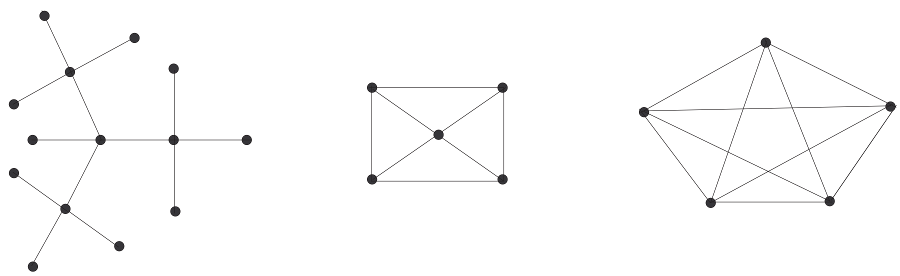

Figure 1.8: Tree, W_4, K_5.

A bipartite graph is a graph in which vertex set of G can be divided in two disjoint sets in such a way that no two vertices within the same set are connected by an edge. A bipartite graph is called complete bipartite if each vertex from one set is adjacent to each vertex of the other set and denoted by $K_{r,s}$, where r is the order of one vertex set and s is the order of other set of vertices. A complete bipartite graph is said to be a star graph if the order of one of the vertex set is 1.

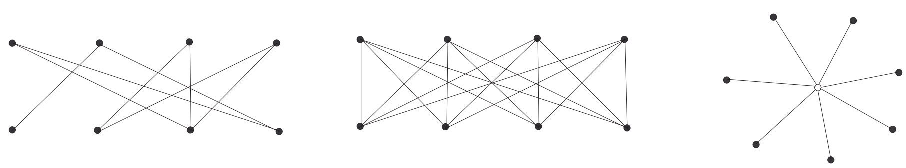

Figure 1.9: Bipartite Graph, $K_{4,4}$ S_7.

1.4 Chemical graph theory

Structures of chemical compounds in chemistry are very important to find boiling point and other physical characteristics. These structures can be represented by molecular graphs called chemical graph theory. The vertices of a graph reveal the atoms, of which, the compound is composed of, whereas the edges counts the number of bonds available within the structural formula.

Use of graph theory is gaining importance day by day in modeling the chemical structures. Molecular topology find application of graph theory by giving molecular graph representations of chemical structures. Physico-chemical property and isomerism depend on the mass of hydro-carbons, and the number of hydrogen and carbon items present in them. Moreover the number of covalent bonds present in the molecular structure require different energy consumption which lead to the estimation of boiling point and other characteristics.

However by using graph theory, the chemical structures are module into such form which do not involve hydrogen atoms and are termed as hydrogen depleted molecular graph.

Consider the structure of polyethylene terephthalate (commonly termed as polyester). In this compound, eight hydrogen atoms and four oxygen atoms are covalently bonded with ten carbon atoms. The molecular graph by deleting the hydrogen atoms(depleted molecular graph) is shown in Figure 1.4.

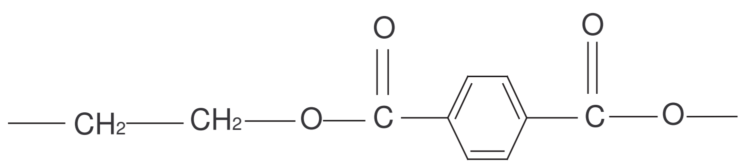

Figure 1.10: $C_{10}H_8O_4$

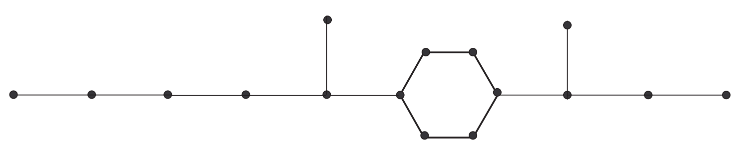

Figure 1.11: Depleted molecular graph

Chapter 2

Some topological invariants

There are hundreds of topological indices and it is very difficult to describe all of them. These are classified depending on graph parameters for example, degree and distance etc. We will define here some topological indices which are distance based and degree based. The degree based indices are those which are constructed by using the degree or valency of a vertex and the distance based indices are defined on the basis of distances of vertices in a graph. We discuss some types of degree based and distance based indices as this is not possible to cover all of them here.

2.1 Distance based topological indices

Some important and well known distance based topological indices are as follow:
• Wiener index
• Eccentric connectivity index
• Total eccentricity index
• Eccentricity based Zagreb indices
• Augmented eccentric connectivity index

2.1.1 Wiener index

Harold Wiener [26] designed one of the oldest molecular description of simple connected graph of sodden hydrocarbons (alkanes). Wiener named it path number. He defined it as the sum of the number of bonds associating with all pairs of atoms. This path number now known as Wiener index and is denoted as W. The compactness of graph is more as the value of W is small. We define the Wiener index of graph G as:

$$M(G) = \sum_{(u,v)} d(u,v), \tag{2.1}$$

where (u,v) be any vertex pair from the set $V(G)$ and the distance between them is $d(u,v)$.

Wiener index is very important not just because it was the first topological index but also because it is very easy to calculate. Its major drawback is that the large number of different graphs have same value of Wiener index.

2.1.2 Eccentric connectivity index

Eccentric connectivity index was introduced by Sharma et al. [22]. It has been successfully used for the development of many mathematics models for the prediction of biological activities of various kinds. We can define eccentric connectivity index of G as:

$$\xi(G) = \sum_{u \in V(G)} \varepsilon(u) d_u. \tag{2.2}$$

The eccentric-connectivity polynomial for G is defined as:

$$ECP(G,y) = \sum_{u \in V(G)} y^{\varepsilon(u)} d_u. \tag{2.3}$$

If the degrees of vertices are not taken into account, then the total eccentric-connectivity index is defined as:

$$\varsigma(G) = \sum_{u \in V(G)} \varepsilon(u). \tag{2.4}$$

For a graph G, the total eccentricity-connectivity polynomial is

$$TECP(G,y) = \sum_{u \in V(G)} y^{\varepsilon(u)}. \tag{2.5}$$

2.1.3 Eccentricity based Zagreb indices

For a molecular graph G, Ghorbani and Hosseinzadeh [11] introduce some new versions of Zagreb indices which are expressed in terms of eccentricity. These indices are defined as:

$$M_1^{**}(G) = \sum_{u \in V(G)} (\varepsilon(u))^2, \tag{2.6}$$

$$M_2^{*}(G) = \sum_{uv \in E(G)} \varepsilon(u)\varepsilon(v). \tag{2.7}$$

2.1.4 Augmented eccentric-connectivity index

The generalization of the eccentric-connectivity index of G introduced by Gupta et al. [12], which is known as augmented eccentric-connectivity index and it is defined as:

$$^{A}\varepsilon(G) = \sum_{u \in V(G)} \frac{M(u)}{\varepsilon(u)}, \tag{2.8}$$

where $M(u)$ denotes the product of degrees of all neighbors of vertex u. The modified version of eccentric connectivity index is defined as:

$$\Lambda(G) = \sum_{u \in V(G)} S_u \varepsilon(u). \tag{2.9}$$

The edge version of eccentric-connectivity polynomial is defined as:

$$\Lambda(G) = \sum_{u \in V(G)} S_u y^{\varepsilon(u)}. \tag{2.10}$$

Xu et al. [27] introduced the edge version of eccentric-connectivity index of G and is defined as:

$$\varepsilon_e(G) = \sum_{g \in E(G)} d_g \varepsilon(g), \tag{2.11}$$

where the largest distance between the edge g with any other edge h in G is defined by $\varepsilon(g)$.

2.1.5 Balaban index

About 30 years ago, the Balaban index was introduced in [5]. It is also known as average distance sum connectivity index or distance connectivity index. This is also known as J index. We define Balaban index for G as follow:

$$J(G) = \frac{m}{\mu + 1} \sum_{uv \in E(G)} \frac{1}{\sqrt{\sigma_u \sigma_v}}, \tag{2.12}$$

where $\sigma_u = \sum\limits_{w \in V(G)} d(u,w)$ and $\mu = m - n + 1$ is known as cyclomatic number of G.

Balaban index has often used in different studies of QSAR and QSPR [4]. Balaban index and Wiener index are two most important kinds of indices for distance based topological indices.

2.2 Degree based topological indices

The topological indices which are based on degree of a vertex are known as degree based topological indices. They have strong application in drug design and pharmaceutical chemistry that's why they are very important. Resonance energy, boiling point and strain energy are some physico-chemical properties which are associated with degree based indices. Here we focuss on some very important degree based topological indices which are as:

- Randić index
- Sum connectivity index
- Zagreb indices
- Atom Bond connectivity index
- Geometric Arithmetic index

2.2.1 Randić index

Chemist Randić [21] introduced a topological index known as branching index in 1975. After some time, branching index turns into molecular connectivity index and afterwards it was referred as Randić index. The Randić index is defined as:

$$R_{-\frac{1}{2}}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}. \tag{2.13}$$

In 1998, the general Randić index was introduced by Bollobás et al. [6] and Amic et al. [1]. Theoretical chemist and mathematicians both have been widely studied it [18]. We define the general Randić index for G as follows:

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha. \tag{2.14}$$

Enthalpies of formation, boiling point, surface area, chromatographic retention times, etc [20] are some physico-chemical properties of alkanes which have very good correlation with Randić index. A large number of applications related to Randić index are reported in consequent years and mostly are related with medicinal and pharmacological issues.

2.2.2 Zagreb index

The dependence of total π electron on molecular structure was examined by Gutman et al. [15], more than 40 years ago. They conclude that two terms appear during the approximation of energy for total π electron. These two indices are as follows:

$$M_1(G) = \sum_{u \in V(G)} (d_u)^2 = \sum_{uv \in E(G)} (d_u + d_v). \tag{2.15}$$

$$M_2(G) = \sum_{uv \in E(G)} (d_u d_v). \tag{2.16}$$

Later on, Gutman and Trinajstić [14] continuously work on their ideas and expand their ideas about $M_1(G)$ and $M_2(G)$ and were finally named as first Zagreb group index and second Zagreb group index, respectively [13, 23].

Many work has been done in field of theoretical chemistry and researchers have been published large number of papers in this field.

2.2.3 Atom bond connectivity index

Atom bond connectivity (ABC) index is one of the famous connectivity topological index which was proposed by Estrada et al. [9]. The ABC index for G is defined as follows:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}. \tag{2.17}$$

Branched and cyclo-alkanes have some important physico-chemical properties like stability and strain energy which are correlated with ABC index.

We define five different forms of ABC index here for G. The generalized form of ABC index is:

$$ABC_k(G) = \sum_{uv \in E(G)} \sqrt{\frac{Q_u + Q_v - 2}{Q_u Q_v}}, \tag{2.18}$$

where the quantity Q_u is related to vertex u uniquely and $k \in \{1, 2, 3, 4, 5\}$.
• When $k = 1$ then $Q_v = d_v$ and $Q_u = d_u$

• If $k = 2$ then $Q_v = n_v$
• When $k = 3$ then $Q_v = m_v$ where m_v represents the set of all those edges of G which are lying closer to vertex v than u of the edge $e = uv$.
• If $k = 4$ then $Q_v = S_v$
• When $k = 5$ then $Q_v = \varepsilon(v)$

2.2.4 Geometric Arithmetic index

Vukičević et al. [25] introduced another famous topological index named as Geometric Arithmetic (GA) index. We define $GA(G)$ as follows:

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}. \tag{2.19}$$

Bioactivity is predicted by using the GA index of chemical compound. Entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation and centric factor are some properties of physico-chemical for which GA index is very important. GA index is more effective and give better result than Randić index.

We define some different forms of GA index. The generalized form of GA index is defined as:

$$GA_k(G) = \sum_{uv \in E(G)} \frac{2\sqrt{Q_u Q_v}}{Q_u + Q_v}, \tag{2.20}$$

where the quantity Q_u is related to vertex u uniquely and $k \in \{1, 2, 3, 4, 5\}$.
• If $k = 1$ then $Q_v = d_v$ and $Q_u = d_u$
• When $k = 2$ then $Q_v = n_v$
• When $k = 3$ then $Q_v = m_v$
• If $k = 4$ then $Q_v = \varepsilon(v)$
• When $k = 5$ then $Q_v = S_v$

2.3 Counting polynomials

A finite sequence of certain properties of a graph in graph theory can be applied in different areas of chemistry. These sequences such as k-independent edge set sequence or the sequence of distance degree form polynomials. These polynomials are known as counting polynomials. Hosaya [17] introduced the counting polynomials with independent edge set (Z-counting) and distance degree polynomials of G, which were initially named as Wiener and later on by Hosaya polynomials.

Let G be a molecular connected graph. The co-distant edges in the edge set $E(G)$ are $e = (x, y)$ and $f = (x^{'}, y^{'})$ shown by e co f, if for $k = \{0, 1, 2, ..., k\}$, where

$$d(x, x^{'}) = d(y, y^{'}) = k$$

and

$$d(x, y^{'}) = d(x^{'}, y) = k + 1$$

or vice versa. The relationship is satisfied for some edges of the connected graph as demonstrated below:

1. e co e
2. e co f $\Leftrightarrow$ f co e
3. e co f and f co j $\Rightarrow$ e co j.

However, the relationship depicted in (3), is not always necessarily considered valid. Consider

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

if the relation satisfies the (3), then the above equation shows the set of all edges of G which are co-distant to e. If all the elements validate the condition of relationship from $(1) - (3)$, $C(e)$ is called an orthogonal cut '*oc*' of the graph G. The graph is said to be a co-graph if and only if the set of edge $E(G)$ is the union of disjoint orthogonal cuts $C_1 \cup C_2 \cup C_3 \cup \cdots \cup C_k = E$. and $C_i \cap C_j = \emptyset$, for $i \neq j$ and $i, j = \{1, 2, 3, \ldots, k\}$.
If from the cut edge sequence, any two of the edges are codistant and related to the same face of the covering then such sequence is said to be a quasi-orthogonal cut '*qoc*' strip. This means that transitive relation is not necessarily followed. There are some counting polynomials
• Omega Polynomial
• Sadhana Polynomial
• PI Polynomial

2.3.1 Omega polynomial

A counting polynomial $\Omega(G, x)$ is known as Omega polynomial of graph G which was introduce by Diudea [8]. It is defined as:

$$\Omega(G, x) = \sum_{k} m(G, k) \times x^k, \tag{2.21}$$

where the number of '*qocs*' of length k is denoted by $m(G, k)$ and the sum is extended to the maximum length of '*qocs*' in G.

2.3.2 Sadhana polynomial

In any graph, Sadhana polynomial is defined on the opposite edge strips. Ashrafi et. al [2] introduced this polynomial. The Sadhana polynomial of graph G is denoted by $Sd(G, k)$ and it defined as:

$$Sd(G, x) = \sum_{k} m(G, k) \times x^{m-k}, \tag{2.22}$$

where the number of '*qocs*' of length k is denoted by $m(G, k)$ and m is the size of G. The equidistant edges in G counted by this polynomial.

2.3.3 PI polynomial

The PI polynomial is used for counting opposite edge strips in any graph. This polynomial of graph G is denoted by $PI(G, x)$, was introduced by Khadikar [19] and it is defined as:

$$PI(G, x) = \sum_{k} m(G, k) \times k \times x^{m-k}, \tag{2.23}$$

where the number of '*qocs*' of length k is denoted by $m(G, k)$. This polynomial is used for counting non-equidistant edges in G.

2.4 M-polynomial

Let G be a graph with vertex set V and edge set E. Let $m_{ij}(G)$, where $i, j \geq 1$ represents the number of edges $e = uv$ such that $d_u = i, d_v = j$, the $m_{ij}(G)$ quantities were first introduced and used in [7, 16]. The M-polynomial is defined as:

$$M(G;x,y) = \sum_{i \leq j} m_{ij}(G)x^i y^j. \tag{2.24}$$

Chapter 3

Topological indices and Polynomials of Triazine based dendrimer

In this chapter, we compute the topological indices and polynomials of Triazine based dendrimer. This dendrimer was synthesized by divergent method evading protection/deprotection or functional group interconversion. The full generations of this dendrimer were used as solubility enhancer of ketoprofen [10].

Let us denote the molecular graph of this dendrimer by $D_1(n)$, where the generations stage of $D_1(n)$ is represented by n. The number of vertices in the graph $D_1(n)$ is $\frac{2}{3}(5\times 2^{2n+4}+1)$ and number of edges is $7\times 2^{2n+3}+1$. We now partition the molecular graph of $D_1(n)$ into two parts, one of them is the core C and other is the subgraph $MS(n)$ of $D_1(n)$ having four similar branches with vertex set $V(D_1(n))-V(C)$.The dendrimer $D_1(n)$ with core and first generation are shown in Figure 3.1. It is enough to compute the required information for a set of representatives while computing the eccentricity based indices and polynomials of $D_1(n)$. First, we take one set of representatives from a set of vertices of the core of $D_1(n)$, which have the same degree, S_u, $M(u)$ and eccentricity for each u of the corresponding representative. For the core, these representatives are labeled by α_l, where $1 \leq l \leq 4$ as shown in Figure 3.1. This set of representatives with their degrees, S_u and $M(u)$, eccentricities and frequencies of occurrence are given in Table 3.1.

For the subgraph $MS(n)$, these representatives are labeled by b_i, c_i, d_i, e_i, f_i, g_i and h_i, where $1 \leq i \leq n$ and a_m, $2 \leq m \leq n$ and we fix a_1 for $D_1(n)$ as shown in Figure 3.1. This set of representatives with their degrees, S_u, $M(u)$, eccentricities and frequencies are given in Table 3.2. For the sake of simplicity, we assume $\gamma = 7n + 7i$ in this chapter.

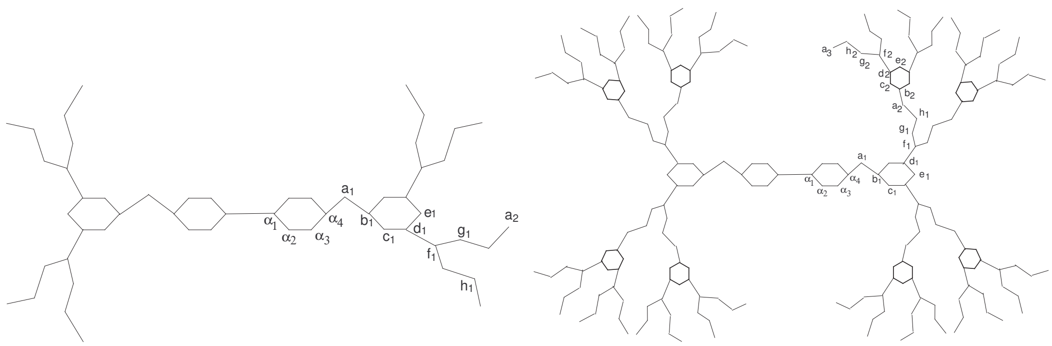

Figure 3.1: Core of $D_1(n)$ and first generation of $D_1(n)$.

3.1 The eccentricity-based indices and polynomials for the molecular graph $D_1(n)$

We compute the different eccentricity-based indices and their corresponding polynomials of molecular graph $D_1(n)$ with the help of Tables 3.1 and 3.2. In the following theorem, we determine the eccentric-connectivity index of the molecular graph.

Table 3.1: The set of representatives of core with their degrees, S_u, $M(u)$, eccentricities and frequencies.

Representative	Degree	S_u	$M(u)$	Eccentricity	Frequency
α_1	3	7	12	$7n+5$	2
α_2	2	5	6	$7n+6$	4
α_3	2	5	6	$7n+7$	4
α_4	3	6	8	$7n+8$	2

Theorem 3.1.1. *For the graph $D_1(n)$, the eccentric-connectivity index is given by*

$$\xi(D_1(n)) = \frac{(2^{2n+3} \times 147n + 42n + 2^{2n+1} \times 163 + 274)}{3}.$$

Proof. By using the values of Tables 3.1 and 3.2 in equation (2.2), the eccentric connectivity index of $D_1(n)$ can be written as follows:

$$\xi(D_1(n)) = \xi(C) + \xi(MS(n)) = \sum_{u\in V(C)} \varepsilon(u)d_u + \sum_{u\in V(MS(n))} \varepsilon(u)d_u$$
$$= (2\times 3)(7n+5) + (2\times 4)(7n+6) + (2\times 4)(7n+7) + (2\times 3)(7n+8)$$
$$+ (2\times 2)(7n+9) + (2^{2n+2})(14n+8) + (2^{2n+1})(14n+9)$$
$$+ \sum_{i=1}^{n}\Big((2^{2i-1}\times 3)(\gamma+3) + (2^{2i}\times 2)(\gamma+4) + (2^{2i}\times 3)(\gamma+5)$$
$$+ (2^{2i-1}\times 2)(\gamma+6) + (2^{2i}\times 3)(\gamma+6) + (2^{2i+1}\times 2)(\gamma+7)\Big)$$
$$+ \sum_{i=1}^{n-1}(2^{2i+1}\times 2)(\gamma+8) + \sum_{i=2}^{n}(2^{2i-1}\times 2)(\gamma+2).$$

After some calculations, we get

$$\xi(D_1(n)) = \frac{(2^{2n+3}\times 147n + 42n + 2^{2n+1}\times 163 + 274)}{3},$$

which proves the theorem. □

When the degrees of vertices are not taken into account, then by using the values of Tables 3.1 and 3.2 in (2.4), we have the following result.

Corollary 3.1.1. *For the graph $D_1(n)$, the total eccentric-connectivity index is given by*

$$\varsigma(D_1(n)) = \frac{(2^{2n+4}\times 105n + 2^{2n+1}\times 265 - 294n + 42n + 334)}{9}.$$

In the next theorem, the eccentric-connectivity polynomial for the molecular graph $D_1(n)$ has been derived.

Theorem 3.1.2. *For the graph $D_1(n)$, the eccentric-connectivity polynomial is given by*

$$ECP(D_1(n),y) = 2y^{7n+5}(2y^4+3y^3+4y^2+4y+3) + 2^{2n+1}y^{14n+9} + 2^{2n+2}y^{14n+8}$$
$$+ \frac{4y^{7n+8}(4y^{7n}-4y^7) + 4^n y^{7n+9}(4^n y^{7n}-4y^7)}{4y^7-1}$$
$$+ \frac{2y^{7n+10}(6y^2+4y+3)(4^n y^{7n}-1) + 16y^{7n+13}(y+1)(4^n y^{7n}-1)}{4y^7-1}.$$

Table 3.2: The set of representatives of subgraph $MS(n)$ of $D_1(n)$ with degrees, S_u, $M(u)$, eccentricities and frequencies.

Representative	Degree	S_u	$M(u)$	Eccentricity	Frequency
a_1	2	6	9	$7n+9$	2
a_i when $2 \leq i \leq n$	2	4	4	$7n+7i+2=\gamma+2$	2^{2i-1}
b_i	3	6	8	$\gamma+3$	2^{2i-1}
c_i	2	6	9	$\gamma+4$	2^{2i}
d_i	3	7	12	$\gamma+5$	2^{2i}
e_i	2	6	9	$\gamma+6$	2^{2i-1}
f_i	3	7	12	$\gamma+6$	2^{2i}
g_i	2	5	6	$\gamma+7$	2^{2i+1}
h_i when $i=n$	2	3	2	$14n+8$	2^{2n+1}
h_i when $i \neq n$	2	4	4	$\gamma+8$	2^{2i+1}
a_n+1 when $i=n$	1	2	2	$14n+9$	2^{2n+1}

Proof. By using the values of Tables 3.1 and 3.2 in equation (2.3), we have

$$\begin{aligned}
ECP(D_1(n),y) &= ECP(C,y)+ECP(MS(n),y)\\
&= \sum_{u\in V(C)} d_u y^{\varepsilon(u)} + \sum_{u\in V(MS(n))} d_u y^{\varepsilon(u)}\\
&= (3\times 2)y^{7n+5} + (2\times 4)y^{7n+6} + (2\times 4)y^{7n+7} + (3\times 2)y^{7n+8}\\
&+ (2\times 2)y^{7n+9} + (2\times 2^{2n+1})y^{14n+8} + (1\times 2^{2n+1})y^{14n+9}\\
&+ \sum_{i=1}^{n}\Big((3\times 2^{2i-1})y^{\gamma+3} + (2\times 2^{2i})y^{\gamma+4} + (3\times 2^{2i})y^{\gamma+5}\\
&+ (2\times 2^{2i-1})y^{\gamma+6} + (3\times 2^{2i})y^{\gamma+6} + (2\times 2^{2i+1})y^{\gamma+7}\Big)\\
&+ \sum_{i=1}^{n-1}(2\times 2^{2i+1})y^{\gamma+8} + \sum_{i=2}^{n}(2\times 2^{2i-1})y^{\gamma+2}.
\end{aligned}$$

After some calculation, we get the required result. □

By using the values of Tables 3.1 and 3.2 in (2.5), we have the following result.

Corollary 3.1.2. *For $D_1(n)$, the total eccentric-connectivity polynomial is given by*

$$
\begin{aligned}
TECP(D_1(n), y) &= 2y^{7n+5}(y^4 + y^3 + 2y^2 + 2y + 1) + 2^{2n+1}y^{14n+9} + 2^{2n+1}y^{14n+8} \\
&+ \frac{2y^{7n+8}(4y^{7n} - 4y^7)(y+1)}{4y^7 - 1} \\
&+ \frac{2y^{7n+10}(4y^4 + 3y^3 + 2y^2 + 2y + 1)(4^n y^{7n} - 1)}{4y^7 - 1}.
\end{aligned}
$$

In the next theorem, we compute the closed formula for the second Zagreb eccentricity index of molecular graph.

Theorem 3.1.3. *For the graph $D_1(n)$, the second Zagreb eccentricity index is given by*

$$
M_1^{**}(D_1(n)) = \frac{\begin{aligned}(2^{2n+5} \times 2205n^2 + 2^{2n+4} \times 2499n + 882n^2 + 14028n \\ + 2^{2n+1} \times 8005 + 2350)\end{aligned}}{27}
$$

Proof. By using the values of Tables 3.1 and 3.2 in equation (2.6), we compute the second Zagreb eccentricity index of $D_1(n)$ as follows:

$$
\begin{aligned}
M_1^{**}(D_1(n)) &= M_1^{**}(C) + M_1^{**}(MS(n)) = \sum_{v \in V(C)} [\varepsilon(v)]^2 + \sum_{v \in V(MS(n))} [\varepsilon(v)]^2 \\
&= 2(7n+5)^2 + 4(7n+6)^2 + 4(7n+7)^2 + 2(7n+8)^2 + 2(7n+9)^2 \\
&+ 2^{2n+1}(14n+8)^2 + 2^{2n+1}(14n+9)^2 + \sum_{i=1}^{n} \Big(2^{2i-1}(\gamma+3)^2 \\
&+ 2^{2i}(\gamma+4)^2 + 2^{2i}(\gamma+5)^2 + 2^{2i-1}(\gamma+6)^2 + 2^{2i}(\gamma+6)^2 \\
&+ 2^{2i+1}(\gamma+7)^2 \Big) + \sum_{i=1}^{n-1} 2^{2i+1}(\gamma+8)^2 + \sum_{i=2}^{n} 2^{2i-1}(\gamma+2)^2.
\end{aligned}
$$

After some calculations, we obtain

$$
M_1^{**}(D_1(n)) = \frac{\begin{aligned}(2^{2n+5} \times 2205n^2 + 2^{2n+4} \times 2499n + 882n^2 + 14028n \\ + 2^{2n+1} \times 8005 + 2350)\end{aligned}}{27}.
$$

This proves our theorem. □

Now, we compute the closed formula for the modified eccentric-connectivity index of molecular graph .

Theorem 3.1.4. *For the graph $D_1(n)$, the modified eccentric connectivity index is given by*

$$\Lambda(D_1(n)) = \frac{2(2^{2n+1} \times 1995n + 273n + 2^{2n+1} \times 521 + 1127)}{9}.$$

Proof. By using the values of Tables 3.1 and 3.2 in equation (2.9), we get

$$\begin{aligned}
\Lambda(D_1(n)) = \Lambda(C) + \Lambda(MS(n)) = &\sum_{u \in V(C)} S_u \varepsilon(u) + \sum_{u \in V(MS(n))} S_u \varepsilon(u) \\
&= (2 \times 7)(7n+5) + (4 \times 5)(7n+6) + (4 \times 5)(7n+7) + (2 \times 6)(7n+8) \\
&+ (2 \times 6)(7n+9) + (3 \times 2^{2n+1})(14n+8) + (2 \times 2^{2n+1})(14n+9) \\
&+ \sum_{i=1}^{n} \Big((2^{2i-1} \times 6)(\gamma+3) + (2^{2i} \times 6)(\gamma+4) + (2^{2i} \times 7)(\gamma+5) \\
&+ (2^{2i-1} \times 6)(\gamma+6) + (2^{2i} \times 7)(\gamma+6) + (2^{2i+1} \times 5)(\gamma+7) \Big) \\
&+ \sum_{i=1}^{n-1} (2^{2i+1} \times 4)(\gamma+8) + \sum_{i=2}^{n} (2^{2i-1} \times 4)(\gamma+2).
\end{aligned}$$

After some calculations, we obtain

$$\Lambda(D_1(n)) = \frac{2(2^{2n+1} \times 1995n + 273n + 2^{2n+1} \times 521 + 1127)}{9}.$$

The proof is complete. □

In the following theorem, we compute the closed formula for the modified eccentric-connectivity polynomial of molecular graph.

Theorem 3.1.5. *For the graph $D_1(n)$, the modified eccentric connectivity polynomial is given by*

$$\begin{aligned}
MECP(D_1(n), y) = &\, 2y^{7n+5}(12y^3 + 10y^2 + 10y + 7) + 2^{2n+1} y^{2(7n+4)}(2y+3) \\
&+ \frac{8y^{7n+8}(4^n y^{7n} - 4y^7) + 8y^{7n+9}(4^n y^{7n} - 4y^7)}{4y^7 - 1} \\
&+ \frac{4(10y^4 + 10y^3 + 7y^2 + 6y + 3) y^{7n+10}(4^n y^{7n} - 1)}{4y^7 - 1}.
\end{aligned}$$

Proof. By using the values of Tables 3.1 and 3.2 in equation (2.10), we compute the modified eccentric connectivity polynomial of $D_1(n)$ as:

$$\begin{aligned}
MECP(D_1(n), y) &= MECP(C, y) + MECP(MS(n), y) \\
&= \sum_{u \in V(C)} S_u y^{\varepsilon(u)} + \sum_{u \in V(MS(n))} S_u y^{\varepsilon(u)} \\
&= (2 \times 7)y^{7n+5} + (4 \times 5)y^{7n+6} + (4 \times 5)y^{7n+7} + (2 \times 6)y^{7n+8} \\
&+ (2 \times 6)y^{7n+9} + (3 \times 2^{2n+1})y^{14n+8} + (2 \times 2^{2n+1})y^{14n+9} \\
&+ \sum_{i=1}^{n} \Big((2^{2i-1} \times 6)y^{\gamma+3} + (2^{2i} \times 6)y^{\gamma+4} + (2^{2i} \times 7)y^{\gamma+5} \\
&+ (2^{2i-1} \times 6)y^{\gamma+6} + (2^{2i} \times 7)y^{\gamma+6} + (2^{2i+1} \times 5)y^{\gamma+7} \Big) \\
&+ \sum_{i=1}^{n-1} (2^{2i+1} \times 4)y^{\gamma+8} + \sum_{i=2}^{n} (2^{2i-1} \times 4)y^{\gamma+2}.
\end{aligned}$$

After some calculations, we obtain the required result. □

Now, we determine the augmented eccentric-connectivity index of molecular graph in next theorem.

Theorem 3.1.6. *For the graph $D_1(n)$, the augmented eccentric connectivity index is given by*

$$\begin{aligned}
{}^{A}\varepsilon(D_1(n)) &= \frac{24}{7n+5} + \frac{24}{7n+6} + \frac{24}{7n+7} + \frac{16}{7n+8} + \frac{18}{7n+9} \\
&+ \left(\frac{16}{7n+10} + \cdots + \frac{2^{2n+2}}{14n+3} \right) + \left(\frac{36}{7n+11} + \cdots + \frac{9 \times 2^{2n}}{14n+4} \right) \\
&+ \left(\frac{48}{7n+12} + \cdots + \frac{3 \times 2^{2n+2}}{14n+5} \right) + \left(\frac{18}{7n+13} + \cdots + \frac{9 \times 2^{2n-1}}{14n+6} \right) \\
&+ \left(\frac{48}{7n+13} + \cdots + \frac{3 \times 2^{2n+2}}{14n+6} \right) + \left(\frac{48}{7n+14} + \cdots + \frac{3 \times 2^{2n+2}}{14n+7} \right) \\
&+ \left(\frac{32}{7n+15} + \cdots + \frac{2^{2n+1}}{14n+1} \right) + \left(\frac{32}{7n+16} + \cdots + \frac{2^{2n+1}}{14n+2} \right).
\end{aligned}$$

Proof. By using the values of Tables 3.1 and 3.2 in equation (2.8), we compute the augmented eccentric connectivity index of $D_1(n)$ as:

$$
\begin{aligned}
{}^{A}\varepsilon(D_1(n)) ={}^{A}\varepsilon(C) +{}^{A}\varepsilon(MS(n)) &= \sum_{u\in V(C)} \frac{M(u)}{\varepsilon(u)} + \sum_{u\in V(MS(n))} \frac{M(u)}{\varepsilon(u)} \\
&= \frac{2\times 12}{7n+5} + \frac{4\times 6}{7n+6} + \frac{4\times 6}{7n+7} + \frac{2\times 8}{7n+8} + \frac{2\times 9}{7n+9} + \frac{2\times 2^{2n+1}}{14n+9} \\
&+ \frac{2\times 2^{2n+1}}{14n+8} + \sum_{i=1}^{n}\left(\frac{8\times 2^{2n-1}}{\gamma+3} + \frac{9\times 2^{2n}}{\gamma+4} + \frac{12\times 2^{2n}}{\gamma+5} + \frac{9\times 2^{2n-1}}{\gamma+6}\right. \\
&\left.+ \frac{12\times 2^{2n}}{\gamma+6} + \frac{6\times 2^{2n+1}}{\gamma+7}\right) + \sum_{i=1}^{n-1}\left(\frac{4\times 2^{2i+1}}{\gamma+8}\right) + \sum_{i=2}^{n}\left(\frac{4\times 2^{2i-1}}{\gamma+2}\right).
\end{aligned}
$$

After some calculations, we obtain the required result. □

Table 3.3: The edge partition of core of $D_1(n)$ with respect to the representatives of pairs of end vertices, eccentricity and degree of each edge and their frequencies.

Representative	Eccentricity	Frequency	Eccentricity of an edge	Degree of an edge
$[\alpha_1, \alpha_1]$	$[7n+5, 7n+5]$	1	$7n+3$	4
$[\alpha_1, \alpha_2]$	$[7n+5, 7n+6]$	4	$7n+4$	3
$[\alpha_2, \alpha_3]$	$[7n+6, 7n+7]$	4	$7n+5$	2
$[\alpha_3, \alpha_4]$	$[7n+7, 7n+8]$	4	$7n+6$	3
$[\alpha_4, a_1]$	$[7n+8, 7n+9]$	2	$7n+7$	3

In the next theorem, we determine the closed formula for the third Zagreb eccentricity index of the molecular graph.

Theorem 3.1.7. *For the graph $D_1(n)$, the third Zagreb eccentricity index is given by*

$$
M_2^*(D_1(n)) = \frac{\begin{aligned}(2^{2n+3}\times 3087n^2 + 2^{2n+2}\times 3423n + 2^{2n+2}\times 1249 + 441n^2 \\ + 5754n + 1133)\end{aligned}}{9}.
$$

Table 3.4: The edge partition of $MS(n)$ with respect to the representatives of pairs of end vertices, eccentricity and degree of each edge and their frequencices.

Representative	Eccentricity	Frequency	Eccentricity of an edge	Degree of an edge
$[a_i, b_i]$	$[\gamma+2, \gamma+3]$	2^{2i-1}	$\gamma+1$	3
$[b_i, c_i]$	$[\gamma+3, \gamma+4]$	2^{2i}	$\gamma+2$	3
$[c_i, d_i]$	$[\gamma+4, \gamma+5]$	2^{2i}	$\gamma+3$	3
$[d_i, e_i]$	$[\gamma+5, \gamma+6]$	2^{2i}	$\gamma+4$	3
$[d_i, f_i]$	$[\gamma+5, \gamma+6]$	2^{2i}	$\gamma+4$	4
$[f_i, g_i]$	$[\gamma+6, \gamma+7]$	2^{2i+1}	$\gamma+5$	3
$[g_i, h_i]$	$[\gamma+7, \gamma+8]$	2^{2i+1}	$\gamma+6$	2
$[h_i, a_{i+1}]$ when $i = n$	$[14n+8, 14n+9]$	2^{2n+1}	$14n+7$	1
$[h_i, a_{i+1}]$ when $i \neq n$	$[\gamma+8, \gamma+9]$	2^{2i+1}	$\gamma+7$	2

Proof. By using the values of Tables 3.3 and 3.4 in equation (2.7), we compute the third Zagreb eccentricity index of $D_1(n)$ as follows:

$$M_2^*(D_1(n)) = M_2^*(C) + M_2^*(MS(n)) = \sum_{uv\in E(C)} [\varepsilon(u)\varepsilon(v)] + \sum_{uv\in E(MS(n))} [\varepsilon(u)\varepsilon(v)]$$

$$= (7n+5)(7n+5) + 4(7n+5)(7n+6) + 4(7n+6)(7n+7)$$

$$+ 4(7n+7)(7n+8) + 2(7n+8)(7n+9) + 2^{2n+1}(14n+8)(14n+9)$$

$$+ \sum_{i=1}^{n} \Big(2^{2i-1}(\gamma+2)(\gamma+3) + 2^{2i}(\gamma+3)(\gamma+4) + 2^{2i}(\gamma+4)(\gamma+5)$$

$$+ 2^{2i}(\gamma+5)(\gamma+6) + 2^{2i}(\gamma+5)(\gamma+6) + 2^{2i+1}(\gamma+6)(\gamma+7)$$

$$+ 2^{2i+1}(\gamma+7)(\gamma+8)\Big) + \sum_{i=1}^{n-1} 2^{2i+1}(\gamma+8)(\gamma+9).$$

After some calculations, we have

$$M_2^*(D_1(n)) = \frac{(2^{2n+3}\times 3087n^2 + 2^{2n+2}\times 3423n + 2^{2n+2}\times 1249 + 441n^2 + 5754n + 1133)}{9}.$$

This proves our theorem. □

Finally, we now determine the explicit formula for the edge version of eccentric-connectivity index for the molecular graph $D_1(n)$.

Theorem 3.1.8. *For the graph $D_1(n)$, the edge version of eccentric connectivity index is given by*

$$\varepsilon_e(D_1(n)) = 2(2^{2n+2} \times 63n + 14n + 2^{2n} \times 33 + 67).$$

Proof. By using the values of Tables 3.3 and 3.4 in equation (2.11), the edge version of eccentric connectivity index of $D_1(n)$ can be written as follows:

$$\begin{aligned}\varepsilon_e(D_1(n)) &= \varepsilon_e(C) + \varepsilon_e(MS(n)) = \sum_{f\in E(C)} d_f\varepsilon(f) + \sum_{f\in E(MS(n))} d_f\varepsilon(f)\\ &= (4\times 1)(7n+3) + (4\times 3)(7n+4) + (2\times 4)(7n+5) + (3\times 4)(7n+6)\\ &+ (3\times 2)(7n+7) + (1\times 2^{2n+1})(14n+7) + \sum_{i=1}^{n}\Big((3\times 2^{2i-1})(\gamma+1)\\ &+ (3\times 2^{2i})(\gamma+2) + (3\times 2^{2i})(\gamma+3) + (3\times 2^{2i})(\gamma+4) + (4\times 2^{2i})(\gamma+4)\\ &+ (3\times 2^{2i+1})(\gamma+5) + (2\times 2^{2i+1})(\gamma+6)\Big) + \sum_{i=1}^{n-1}(2\times 2^{2i+1})(\gamma+7).\end{aligned}$$

After some calculations, we get

$$\varepsilon_e(D_1(n)) = 2(2^{2n+2} \times 63n + 14n + 2^{2n} \times 33 + 67).$$

This gives the required result. □

3.2 M-Polynomial

In this section, we will calculate the M-polynomial of $D_1(n)$. The partition set of edges with their frequencies for $D_1(n)$ is given in Table 3.5.

Theorem 3.2.1. *For the graph $D_1(n)$, the M-polynomial is given by*

$$\begin{aligned}M(D_1(n),x,y) &= 2^{2n+3}xy^2 + \frac{2}{3}(-2+5\times 2^{2n+2})x^2y^2 + \frac{2}{3}(4+11\times 2^{2n+2})x^2y^3\\ &+ \frac{1}{3}(-1+4^{n+2})x^3y^3.\end{aligned}$$

Table 3.5: The set of edge representatives with their frequencies of $D_1(n)$.

Representative	Frequency
$(1,2)$	2^{2n+3}
$(2,2)$	$\frac{2}{3}(-2+5\times 2^{2n+2})$
$(2,3)$	$\frac{2}{3}(4+11\times 2^{2n+2})$
$(3,3)$	$\frac{1}{3}(-1+4^{n+2})$

Proof. By using the values of Table 3.5 in equation (2.24), the M-polynomial of $D_1(n)$ can be written as follows:

$$M(D_1(n),x,y) = \sum_{i\leq j} m_{ij}(D_1(n))x^i y^j$$

$$= 2^{2n+3}xy^2 + \frac{2}{3}(-2+5\times 2^{2n+2})x^2y^2 + \frac{2}{3}(4+11\times 2^{2n+2})x^2y^3 + \frac{1}{3}(-1+4^{n+2})x^3y^3.$$

The proof is complete. □

3.3 Counting polynomials

In this section of the chapter, we will calculate counting polynomials for $D_1(n)$, for this we first find the qocs for $D_1(n)$. The strips are shown in Figure 3.3 and Table 3.6 represents the order and lengths of qocs.

Table 3.6: Lengths, Representations and Frequencies of qocs.

Representative	length	Frequency
C_1	1	$(-7+5\times 2^{2n+3})$
C_2	2	$2(2+2^{2n+2})$

Theorem 3.3.1. *For the graph $D_1(n)$, the Omega polynomial is given by*

$$\Omega(D_1(n),x) = (-7+5\times 2^{2n+3})x + 2(2+2^{2n+2})x^2.$$

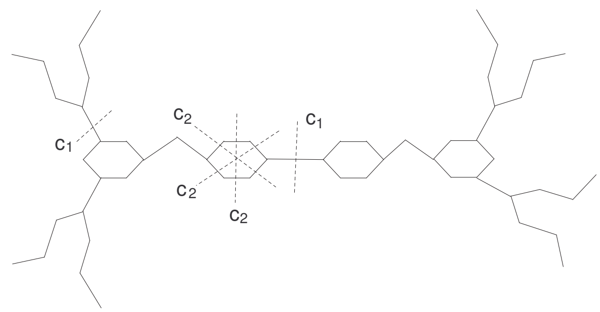

Figure 3.2: Core of $D_1(n)$

Proof. We calculate the Omega polynomial by using the values of Table 3.6 in equation (2.21) as follows:

$$\Omega(D_1(n),x) = (-7+5\times 2^{2n+3})x + 2(2+2^{2n+2})x^2.$$

Which is the required result. □

Theorem 3.3.2. *For the graph $D_1(n)$, the Sadhana polynomial is given by*

$$Sd(D_1(n),x) = (-7+5\times 2^{2n+3})x^{7\times 2^{2n+3}} + (4+2^{2n+3})x^{7\times 2^{2n+3}-1}.$$

Proof. Substitute the values of Table 3.6 into equation (2.22), then we have

$$\begin{aligned} Sd(D_1(n),x) &= (-7+5\times 2^{2n+3})x^{1+7\times 2^{2n+3}-1} + 2(2+2^{2n+2})x^{1+7\times 2^{2n+3}-2} \\ &= (-7+5\times 2^{2n+3})x^{7\times 2^{2n+3}} + (4+2^{2n+3})x^{7\times 2^{2n+3}-1}. \end{aligned}$$

The proof is complete. □

Theorem 3.3.3. *For the graph $D_1(n)$, the PI polynomial is given by*

$$PI(D_1(n),x) = (-7+5\times 2^{2n+3})x^{7\times 2^{2n+3}} + (8+2^{2n+4})x^{7\times 2^{2n+3}-1}.$$

Proof. By using Table 3.6, we substitute the values in equation (2.23) as follows:

$$\begin{aligned} PI(D_1(n),x) &= (-7+5\times 2^{2n+3})x^{1+7\times 2^{2n+3}-1} + 4(2+2^{2n+2})x^{1+7\times 2^{2n+3}-2} \\ &= (-7+5\times 2^{2n+3})x^{7\times 2^{2n+3}} + (8+2^{2n+4})x^{7\times 2^{2n+3}-1}. \end{aligned}$$

After some calculations, we obtain the required result. □

Chapter 4

Topological indices and polynomials of Cyclotriphosphazene dendrimer

Dendrimers, that can be applied for the magnetic behavior study of species which are paramagnetic, are micro molecules made for better specialized individual characteristics. Here we are focussing phosphorus containing dendrimer Cyclotriphosphazene (N_3P_3) which have stable end groups and these are studied by EPR temperature spectrum [3]. Let the molecular graph of this dendrimer be $D_2(n)$, where the generations stage of $D_2(n)$ is represented by n. The core and first generation of $D_2(n)$ are shown in Figure 4.1.

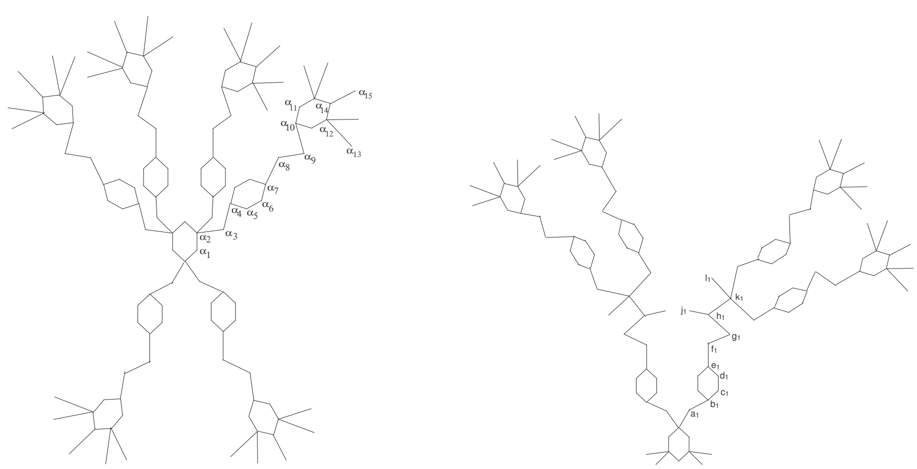

Figure 4.1: Core of $D_2(n)$ and one branch of first generation of $D_2(n)$.

The size and order of the graph $D_2(n)$ are $6(9 \times 2^{n+2} - 13)$ and $9(-8 + 11 \times 2^n)$, respectively. We divide the molecular graph $D_2(n)$ into two parts, one is core and other is the subgraph $H(n)$ of $D_2(n)$. The degrees, S_u, $M(u)$ and eccentricity for each u for the core and subgraph $H(n)$ of $D_2(n)$ are shown in Table 4.1 and Table 4.2 respectively. For simplicity, we assume $\gamma = 9n + 9i$.

4.1 The eccentricity-based indices and polynomials for the molecular graph $D_2(n)$

In this chapter, we will compute some eccentricity based indices and their corresponding polynomials for molecular graph $D_2(n)$ by using the values of Table 4.1 and 4.2. In the following theorem, we determine the eccentric-connectivity index of $D_2(n)$.

Table 4.1: The set of representatives of the core with their degrees, S_u, $M(u)$, eccentricities and frequencies.

Representative	Degree	S_u	$M(u)$	Eccentricity	Frequency
α_1	2	8	16	$9n+15$	3
α_2	4	8	16	$9n+14$	3
α_3	2	7	12	$9n+15$	$3\times 2^{n+1}$
α_4	3	6	8	$9n+16$	$3\times 2^{n+1}$
α_5	2	5	6	$9n+17$	$3\times 2^{n+2}$
α_6	2	5	6	$9n+18$	$3\times 2^{n+2}$
α_7	3	6	8	$9n+19$	$3\times 2^{n+1}$
α_8	2	5	6	$9n+20$	$3\times 2^{n+1}$
α_9	2	5	6	$9n+21$	$3\times 2^{n+1}$
α_{10}	3	6	8	$9n+22$	$3\times 2^{n+1}$
α_{11}	2	7	12	$9n+23$	$3\times 2^{n+2}$
α_{12}	4	7	6	$9n+24$	$3\times 2^{n+2}$
α_{13}	1	4	4	$9n+25$	$3\times 2^{n+3}$
α_{14}	3	9	16	$9n+25$	$3\times 2^{n+1}$
α_{15}	1	3	3	$9n+26$	$3\times 2^{n+1}$

Table 4.2: The set of representatives of the subgraph $H(n)$ of $D_2(n)$ with degrees, S_u, $M(u)$, eccentricities and frequencies.

Representative	Degree	S_u	$M(u)$	Eccentricity	Frequency
a_i	2	7	12	$9n+9i+6=\gamma+6$	3×2^i
b_i	3	6	8	$\gamma+7$	3×2^i
c_i	2	5	6	$\gamma+8$	$3\times 2^{i+1}$
d_i	2	5	6	$\gamma+9$	$3\times 2^{i+1}$
e_i	3	6	8	$\gamma+10$	3×2^i
f_i	2	5	6	$\gamma+11$	3×2^i
g_i	2	5	6	$\gamma+12$	3×2^i
h_i	3	7	8	$\gamma+13$	3×2^i
j_i	1	3	3	$\gamma+14$	3×2^i
k_i	4	8	12	$\gamma+14$	3×2^i
l_i	1	4	4	$\gamma+15$	3×2^i

Theorem 4.1.1. *For the graph $D_2(n)$, the eccentric-connectivity index is given by*

$$\xi(D_2(n)) = 18(2^{n+2}\times 79 - 78n + 2^n\times 303n + 1).$$

Proof. By using the values of Tables 4.1 and 4.2 in equation (2.2), the eccentric connectivity index of $D_2(n)$ can be written as follows:

$$\begin{aligned}
\xi(D_2(n)) = \xi(C) + \xi(H(n)) &= \sum_{u\in V(C)} \varepsilon(u)d_u + \sum_{u\in V(H(n))} \varepsilon(u)d_u \\
&= (2\times 3)(9n+15) + (3\times 4)(9n+14) + (3\times 2^{n+1}\times 2)(9n+15) \\
&+ (3\times 2^{n+1}\times 3)(9n+16) + (2\times 2^{n+2}\times 3)(9n+17) \\
&+ (2\times 2^{n+2}\times 3)(9n+18) + (3\times 2^{n+1}\times 3)(9n+19) \\
&+ (2\times 2^{n+1}\times 3)(9n+20) + (2\times 2^{n+1}\times 3)(9n+21) \\
&+ (3\times 2^{n+1}\times 3)(9n+22) + (2\times 2^{n+2}\times 3)(9n+23) \\
&+ (4\times 2^{n+2}\times 3)(9n+24) + (1\times 2^{n+3}\times 3)(9n+25) \\
&+ (3\times 2^{n+1}\times 3)(9n+25) + (1\times 2^{n+1}\times 3)(9n+26) \\
&+ \sum_{i=1}^{n} \Big((2\times 2^i\times 3)(\gamma+6) + (3\times 2^i\times 3)(\gamma+7) + (2\times 2^{i+1}\times 3)(\gamma+8)
\end{aligned}$$

$$+ (2 \times 2^{i+1} \times 3)(\gamma + 9) + (3 \times 2^i \times 3)(\gamma + 10) + (3 \times 2^i \times 2)(\gamma + 11)$$
$$+ (2 \times 2^i \times 3)(\gamma + 12) + (3 \times 2^i \times 3)(\gamma + 13) + (1 \times 2^i \times 3)(\gamma + 14)$$
$$+ (4 \times 2^i \times 3)(\gamma + 14) + (1 \times 2^i \times 3)(\gamma + 15)\Big).$$

After some calculations, we get

$$\xi(D_2(n)) = 18(2^{n+2} \times 79 - 78n + 2^n \times 303n + 1),$$

which proves the theorem. □

When the degrees of vertices are not taken into account, then by using the values of Tables 4.1 and 4.2 in (2.4), we have the following result.

Corollary 4.1.1. *For the graph $D_2(n)$, the total eccentric-connectivity index is given by*

$$\varsigma(D_2(n)) = 9(2^{n+2} \times 69n + 2^{n+1} \times 149 - 72n - 3).$$

In the next theorem, the eccentric-connectivity polynomial for the molecular graph $D_2(n)$ has been derived.

Theorem 4.1.2. *For the graph $D_2(n)$, the eccentric-connectivity polynomial is given by*

$$\begin{aligned} ECP(D_2(n), y) &= 6y^{9n+14}(y + 2) + 3 \times 2^{n+1}y^{9n+15}(y^{11} + 7y^{10} + 8y^9 + 4y^8 + 3y^7 \\ &+ 2y^6 + 2y^5 + 3y^4 + 4y^3 + 4y^2 + 3y + 2) \\ &+ \frac{6(2y^5 + 3y^4 + 4y^3 + 4y^2 + 3y + 2) \times y^{9n+15}(2^n y^{9n} - 1)}{2y^9 - 1} \\ &+ \frac{6(y^3 + 5y^2 + 3y + 2) \times y^{9n+21}(2^n y^{9n} - 1)}{2y^9 - 1}. \end{aligned}$$

Proof. By using the values of Tables 4.1 and 4.2 in (2.3), we have

$$\begin{aligned} ECP(D_2(n), y) &= ECP(C, y) + ECP(H(n), y) = \sum_{u \in V(C)} d_u y^{\varepsilon(u)} + \sum_{u \in V(H(n))} d_u y^{\varepsilon(u)} \\ &= (2 \times 3)y^{9n+15} + (4 \times 3)y^{9n+14} + (2 \times 3 \times 2^{n+1})y^{9n+15} \\ &+ (3 \times 3 \times 2^{n+1})y^{9n+16} + (2 \times 3 \times 2^{n+2})y^{9n+17} + (2 \times 3 \times 2^{n+2})y^{9n+18} \end{aligned}$$

$$
\begin{aligned}
&+ (3 \times 3 \times 2^{n+1})y^{9n+19} + (2 \times 3 \times 2^{n+1})y^{9n+20} + (2 \times 3 \times 2^{n+1})y^{9n+21} \\
&+ (3 \times 3 \times 2^{n+1})y^{9n+22} + (2 \times 3 \times 2^{n+2})y^{9n+23} + (4 \times 3 \times 2^{n+2})y^{9n+24} \\
&+ (1 \times 3 \times 2^{n+3})y^{9n+25} + (3 \times 3 \times 2^{n+1})y^{9n+25} + (1 \times 3 \times 2^{n+1})y^{9n+26} \\
&+ \sum_{i=1}^{n} \Big((2 \times 3 \times 2^{i})y^{\gamma+6} + (3 \times 3 \times 2^{i})y^{\gamma+7} + (2 \times 3 \times 2^{i+1})y^{\gamma+8} \\
&+ (2 \times 3 \times 2^{i+1})y^{\gamma+9} + (3 \times 3 \times 2^{i})y^{\gamma+10} + (2 \times 3 \times 2^{i})y^{\gamma+11} \\
&+ (2 \times 3 \times 2^{i})y^{\gamma+12} + (3 \times 3 \times 2^{i})y^{\gamma+13} + (1 \times 3 \times 2^{i})y^{\gamma+14} \\
&+ (4 \times 3 \times 2^{i})y^{\gamma+14} + (1 \times 3 \times 2^{i})y^{\gamma+15} \Big).
\end{aligned}
$$

After some calculations, we get the required result. □

By using the values of Tables 4.1 and 4.2 in (2.5), we have the following result.

Corollary 4.1.2. *For the graph $D_2(n)$, the total eccentric-connectivity polynomial is given by*

$$
\begin{aligned}
TECP(D_2(n), y) = {} & 3y^{9n+14}(y+1) + 3 \times 2^{n+1} y^{9n+15}(y^{11} + 5y^{10} + 2y^{9} + 2y^{8} + y^{7} \\
& + y^{6} + y^{5} + y^{4} + 2y^{3} + 2y^{2} + y + 1) \\
& + \frac{6(y^3 + 2y^2 + y + 1) \times y^{9n+21}(2^n y^{9n} - 1)}{2y^9 - 1} \\
& + \frac{6(y+1)(y^2+1)^2 \times y^{9n+15}(2^n y^{9n} - 1)}{2y^9 - 1}.
\end{aligned}
$$

In the next theorem, we compute the closed formula for the second Zagreb eccentricity index of molecular graph.

Theorem 4.1.3. *For the graph $D_2(n)$, the second Zagreb eccentricity index is given by*

$$M_1^{**}(D_2(n)) = 3(2^{n+4} \times 7295n^2 + 2^{n+3} \times 2097n - 1944n^2 - 162n + 2^{n+1} \times 11641 - 4053).$$

Proof. By using the values of Tables 4.1 and 4.2 in (2.6), we compute the second Zagreb eccentricity index of $D_2(n)$ as follows:

$$
\begin{aligned}
M_1^{**}(D_2(n)) = M_1^{**}(C) + M_1^{**}(H(n)) &= \sum_{v \in V(C)} [\varepsilon(v)]^2 + \sum_{v \in V(H(n))} [\varepsilon(v)]^2 \\
&= 3(9n+15)^2 + 3(9n+14)^2 + (3 \times 2^{n+1})(9n+15)^2
\end{aligned}
$$

$$+ (3 \times 2^{n+1})(9n+16)^2 + (3 \times 2^{n+2})(9n+17)^2 + (3 \times 2^{n+2})(9n+18)^2$$
$$+ (3 \times 2^{n+1})(9n+19)^2 + (3 \times 2^{n+1})(9n+20)^2 + (3 \times 2^{n+1})(9n+21)^2$$
$$+ (3 \times 2^{n+1})(9n+22)^2 + (3 \times 2^{n+2})(9n+23)^2 + (3 \times 2^{n+2})(9n+24)^2$$
$$+ (3 \times 2^{n+3})(9n+25)^2 + (3 \times 2^{n+1})(9n+25)^2 + (3 \times 2^{n+1})(9n+26)^2$$
$$+ \sum_{i=1}^{n} \Big((3 \times 2^{i})(\gamma+6)^2 + (3 \times 2^{i})(\gamma+7)^2 + (3 \times 2^{i+1})(\gamma+8)^2$$
$$+ (3 \times 2^{i+1})(\gamma+9)^2 + (3 \times 2^{i})(\gamma+10)^2 + (3 \times 2^{i})(\gamma+11)^2$$
$$+ (3 \times 2^{i})(\gamma+12)^2 + (3 \times 2^{i})(\gamma+13)^2 + (3 \times 2^{i})(\gamma+14)^2$$
$$+ (3 \times 2^{i})(\gamma+14)^2 + (3 \times 2^{i})(\gamma+15)^2 \Big).$$

After some calculations, we obtain

$$M_1^{**}(D_2(n)) = 3(2^{n+4} \times 7295n^2 + 2^{n+3} \times 2097n - 1944n^2 - 162n + 2^{n+1} \times 11641 - 4053),$$

that proves our theorem. □

Now, we compute the closed formula for the modified eccentric-connectivity index of molecular graph.

Theorem 4.1.4. *For the graph $D_2(n)$, the modified eccentric connectivity index is given by*

$$\Lambda(D_2(n)) = 6(2^n \times 2277n - 567n + 2^{n+1} \times 1229 + 21).$$

Proof. By using the values of Tables 4.1 and 4.2 in (2.9), we compute the modified eccentric connectivity index of $D_2(n)$ in the following way:

$$\Lambda(D_2(n)) = \Lambda(C) + \Lambda(H(n)) = \sum_{u \in V(C)} S_u \varepsilon(u) + \sum_{u \in V(H(n))} S_u \varepsilon(u)$$
$$= (8 \times 3)(9n+15) + (8 \times 3)(9n+14) + (7 \times 3 \times 2^{n+1})(9n+15)$$
$$+ (6 \times 3 \times 2^{n+1})(9n+16) + (5 \times 3 \times 2^{n+2})(9n+17)$$
$$+ (5 \times 3 \times 2^{n+2})(9n+18) + (6 \times 3 \times 2^{n+1})(9n+19)$$
$$+ (5 \times 3 \times 2^{n+1})(9n+20) + (5 \times 3 \times 2^{n+1})(9n+21)$$
$$+ (6 \times 3 \times 2^{n+1})(9n+22) + (7 \times 3 \times 2^{n+2})(9n+23)$$
$$+ (7 \times 3 \times 2^{n+2})(9n+24) + (4 \times 3 \times 2^{n+3})(9n+25)$$
$$+ (9 \times 3 \times 2^{n+1})(9n+25) + (3 \times 3 \times 2^{n+1})(9n+26)$$

$$+\sum_{i=1}^{n}\Big((7\times 3\times 2^{i})(\gamma+6)+(6\times 3\times 2^{i})(\gamma+7)+(5\times 3\times 2^{i+1})(\gamma+8)$$
$$+(5\times 3\times 2^{i+1})(\gamma+9)+(6\times 3\times 2^{i})(\gamma+10)+(5\times 3\times 2^{i})(\gamma+11)$$
$$+(5\times 3\times 2^{i})(\gamma+12)+(7\times 3\times 2^{i})(\gamma+13)+(3\times 3\times 2^{i})(\gamma+14)$$
$$+(8\times 3\times 2^{i})(\gamma+14)+(4\times 3\times 2^{i})(\gamma+15)\Big).$$

After some calculations, we obtain

$$\Lambda(D_2(n))=6(2^{n}\times 2277n-567n+2^{n+1}\times 1229+21).$$

The proof is complete. □

In the following theorem, we compute the closed formula for the modified eccentric-connectivity polynomial of molecular graph.

Theorem 4.1.5. *For the graph $D_2(n)$, the modified eccentric connectivity polynomial is given by*

$$\begin{aligned}MECP(D_2(n),y)&=24y^{9n+14}(y+1)+2^{n+1}\times y^{9n+15}(9y^{11}+75y^{10}+42y^{9}+42y^{8}\\&+18y^{7}+15y^{6}+15y^{5}+18y^{4}+30y^{3}+30y^{2}+18y+21)\\&+\frac{6(5y^{5}+6y^{4}+10y^{3}+10y^{2}+6y+7)y^{9n+15}(2^{n}y^{9n}-1)}{2y^{9}-1}\\&+\frac{6(4y^{3}+11y^{2}+7y+5)y^{9n+21}(2^{n}y^{9n}-1)}{2y^{9}-1}.\end{aligned}$$

Proof. By using the values of Tables 4.1 and 4.2 in (2.10), we compute the modified eccentric connectivity polynomial of $D_2(n)$ in the following way:

$$\begin{aligned}MECP(D_2(n),y)&=MECP(C,y)+MECP(H(n),y)\\&=\sum_{u\in V(C)}S_u y^{\varepsilon(u)}+\sum_{u\in V(H(n))}S_u y^{\varepsilon(u)}\\&=(8\times 3)y^{9n+15}+(8\times 3)y^{9n+14}+(7\times 3\times 2^{n+1})y^{9n+15}\\&+(6\times 3\times 2^{n+1})y^{9n+16}+(5\times 3\times 2^{n+2})y^{9n+17}\\&+(5\times 3\times 2^{n+2})y^{9n+18}+(6\times 3\times 2^{n+1})y^{9n+19}\\&+(5\times 3\times 2^{n+1})y^{9n+20}+(5\times 3\times 2^{n+1})y^{9n+21}\end{aligned}$$

$$+ (6 \times 3 \times 2^{n+1})y^{9n+22} + (7 \times 3 \times 2^{n+2})y^{9n+23} + (7 \times 3 \times 2^{n+2})y^{9n+24}$$
$$+ (4 \times 3 \times 2^{n+3})y^{9n+25} + (9 \times 3 \times 2^{n+1})y^{9n+25} + (3 \times 3 \times 2^{n+1})y^{9n+26}$$
$$+ \sum_{i=1}^{n} \Bigg((7 \times 3 \times 2^{i})(y^{\gamma+6}) + (6 \times 3 \times 2^{i})(y^{\gamma+7}) + (5 \times 3 \times 2^{i+1})(y^{\gamma+8})$$
$$+ (5 \times 3 \times 2^{i+1})(y^{\gamma+9}) + (6 \times 3 \times 2^{i})(y^{\gamma+10}) + (5 \times 3 \times 2^{i})(y^{\gamma+11})$$
$$+ (5 \times 3 \times 2^{i})(y^{\gamma+12}) + (7 \times 3 \times 2^{i})(y^{\gamma+13}) + (3 \times 3 \times 2^{i})(y^{\gamma+14})$$
$$+ (8 \times 3 \times 2^{i})(y^{\gamma+14}) + (4 \times 3 \times 2^{i})(y^{\gamma+15}) \Bigg).$$

After some calculations, we obtain the required result. □

Now, we determine the augmented eccentric-connectivity index of molecular graph in next theorem.

Theorem 4.1.6. *For the graph $D_2(n)$, the augmented eccentric connectivity index is given by*

$$\begin{aligned} {}^{A}\varepsilon(D_2(n)) = {} & \frac{48}{9n+15} + \frac{48}{9n+14} + \frac{36 \times 2^{n+1}}{9n+15} + \frac{24 \times 2^{n+1}}{9n+16} + \frac{18 \times 2^{n+2}}{9n+17} \\ & + \frac{18 \times 2^{n+2}}{9n+18} + \frac{24 \times 2^{n+1}}{9n+19} + \frac{18 \times 2^{n+1}}{9n+20} + \frac{18 \times 2^{n+1}}{9n+21} + \frac{24 \times 2^{n+1}}{9n+22} \\ & + \frac{36 \times 2^{n+2}}{9n+23} + \frac{18 \times 2^{n+2}}{9n+24} + \frac{12 \times 2^{n+3}}{9n+25} + \frac{48 \times 2^{n+1}}{9n+25} + \frac{9 \times 2^{n+1}}{9n+26} \\ & + \left(\frac{72}{9n+15} + \cdots + \frac{36 \times 2^{n}}{18n+6} \right) + \left(\frac{48}{9n+16} + \cdots + \frac{24 \times 2^{n}}{18n+7} \right) \\ & + \left(\frac{72}{9n+17} + \cdots + \frac{18 \times 2^{n+1}}{18n+8} \right) + \left(\frac{72}{9n+18} + \cdots + \frac{18 \times 2^{n+1}}{18n+9} \right) \\ & + \left(\frac{48}{9n+19} + \cdots + \frac{24 \times 2^{n}}{18n+10} \right) + \left(\frac{36}{9n+20} + \cdots + \frac{18 \times 2^{n}}{18n+11} \right) \\ & + \left(\frac{36}{9n+21} + \cdots + \frac{18 \times 2^{n}}{18n+12} \right) + \left(\frac{48}{9n+22} + \cdots + \frac{24 \times 2^{n}}{18n+13} \right) \\ & + \left(\frac{18}{9n+23} + \cdots + \frac{9 \times 2^{n}}{18n+14} \right) + \left(\frac{72}{9n+23} + \cdots + \frac{36 \times 2^{n}}{18n+14} \right) \\ & + \left(\frac{24}{9n+24} + \cdots + \frac{12 \times 2^{n}}{18n+15} \right). \end{aligned}$$

Proof. By using the values of Tables 4.1 and 4.2 in (2.8), we compute the augumented eccentric connectivity index of $D_2(n)$ in the following way:

$$
\begin{aligned}
{}^{A}\varepsilon(D_2(n)) ={}^{A} \varepsilon(C) +{}^{A} \varepsilon(H(n)) &= \sum_{u\in V(C)} \frac{M(u)}{\varepsilon(u)} + \sum_{u\in V(H(n))} \frac{M(u)}{\varepsilon(u)} \\
&= \frac{3\times 16}{9n+15} + \frac{3\times 16}{9n+14} + \frac{3\times 2^{n+1}\times 12}{9n+15} + \frac{3\times 2^{n+1}\times 8}{9n+16} + \frac{3\times 2^{n+2}\times 6}{9n+17} \\
&+ \frac{3\times 2^{n+2}\times 6}{9n+18} + \frac{3\times 2^{n+1}\times 8}{9n+19} + \frac{3\times 2^{n+1}\times 6}{9n+20} + \frac{3\times 2^{n+1}\times 6}{9n+21} \\
&+ \frac{3\times 2^{n+1}\times 8}{9n+22} + \frac{3\times 2^{n+2}\times 12}{9n+23} + \frac{3\times 2^{n+2}\times 6}{9n+24} + \frac{3\times 2^{n+3}\times 4}{9n+25} \\
&+ \frac{3\times 2^{n+1}\times 16}{9n+25} + \frac{3\times 2^{n+1}\times 3}{9n+26} + \sum_{i=1}^{n}\Big(\frac{3\times 2^{i}\times 12}{\gamma+6} + \frac{3\times 2^{i}\times 8}{\gamma+7} \\
&+ \frac{3\times 2^{i+1}\times 6}{\gamma+8} + \frac{3\times 2^{i+1}\times 6}{\gamma+9} + \frac{3\times 2^{i}\times 8}{\gamma+10} + \frac{3\times 2^{i}\times 6}{\gamma+11} + \frac{3\times 2^{i}\times 6}{\gamma+12} \\
&+ \frac{3\times 2^{i}\times 8}{\gamma+13} + \frac{3\times 2^{i}\times 3}{\gamma+14} + \frac{3\times 2^{i}\times 12}{\gamma+14} + \frac{3\times 2^{i}\times 4}{\gamma+15}\Big).
\end{aligned}
$$

After some calculations, we obtain the required result. □

4.2 Counting polynomials

To calculate these polynomials, we first find qocs for $D_2(n)$. The cuts of core are represented in Figure 4.3. The qocs C_1, C_2, C_3, C_4 along with their lengths and frequencies are given in Table 4.3. We will calculate the counting polynomials by using the following theorems.

Theorem 4.2.1. *For the graph $D_2(n)$, the Omega polynomial is given by*

$$\Omega(D_2(n), x) = 12(-4 + 9\times 2^{n})x + 3(-5 + 9\times 2^{n+1})x^2.$$

Proof. For Omega polynomial, substitute the values of Table 4.3 in (2.21), then we have

$$
\begin{aligned}
\Omega(D_2(n), x) &= 12(-4 + 9\times 2^{n})x + (-5 + 9\times 2^{n+1})x^2 + (-5 + 9\times 2^{n+1})x^2 \\
&+ (-5 + 9\times 2^{n+1}x^2) \\
&= 12(-4 + 3^2\times 2^{n})x + 3(-5 + 3^2\times 2^{n+1})x^2.
\end{aligned}
$$

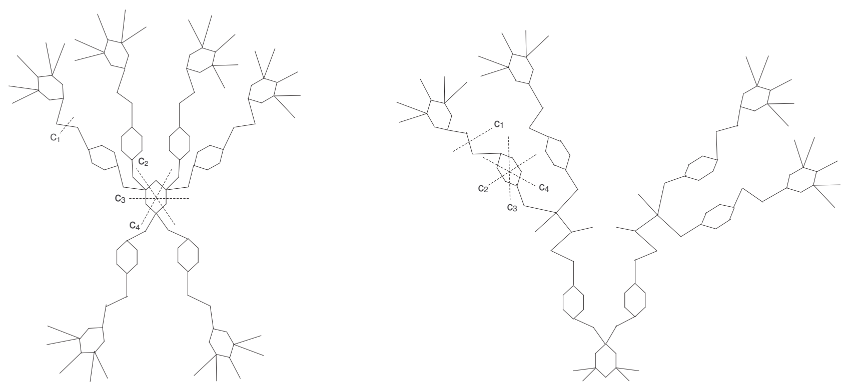

Figure 4.2: Qocs for Core and qocs for first generation of $D_2(n)$.

Table 4.3: Lengths, Representations and Frequencies of qocs.

Representative	length	Frequency
C_1	1	$12(-4+9\times 2^n)$
C_2	2	$(-5+9\times 2^{n+1})$
C_3	2	$(-5+9\times 2^{n+1})$
C_4	2	$(-5+9\times 2^{n+1})$

Which is the required result. □

Theorem 4.2.2. *For the graph $D_2(n)$, the Sadhana polynomial is given by*

$$Sd(D_2(n),x) = 12(-4+3^2\times 2^n)x^{-79+3^3\times 2^{n+3}} + 3(-5+3^2\times 2^{n+1})x^{-80+3^3\times 2^{n+3}}.$$

Proof. By using the values of Table 4.3 in (2.22), we get the following result

$$\begin{aligned} Sd(D_2(n),x) &= 12(-4+9\times 2^n)x^{6(-13+3^2\times 2^{n+2})-1} + 3(-5+9\times 2^{n+1})x^{6(-13+3^2\times 2^{n+2})-2} \\ &= 12(-4+3^2\times 2^n)x^{-79+3^3\times 2^{n+3}} + 3(-5+3^2\times 2^{n+1})x^{-80+3^3\times 2^{n+3}}. \end{aligned}$$

This proves our theorem. □

Theorem 4.2.3. *For the graph $D_2(n)$, the PI polynomial is given by*

$$PI(D_2(n),x) = 12(-4+3^2\times 2^n)x^{-79+3^3\times 2^{n+3}} + 6(-5+3^2\times 2^{n+1})x^{-80+3^3\times 2^{n+3}}.$$

Proof. Using the values of Table 4.3 in (2.23), we have

$$\begin{aligned}PI(D_2(n),x) &= 12(-4+9\times 2^n)\times 1\times x^{6(-13+9\times 2^{n+2})-1} + 3(-5+9\times 2^{n+1})\\ &\quad \times 2\times x^{6(-13+9\times 2^{n+2})-2}\\ &= 12(-4+3^2\times 2^n)x^{-79+3^3\times 2^{n+3}} + 6(-5+3^2\times 2^{n+1})x^{-80+3^3\times 2^{n+3}}.\end{aligned}$$

The proof is complete. □

4.3 M-Polynomial

To compute M-polynomial for $D_2(n)$, we use the partition set of edges and their relevant frequencies provided in Table 4.4.

Table 4.4: Edge partition for $D_2(n)$.

Representative	Frequency
$(1,3)$	$6(-1+2^{n+1})$
$(1,4)$	$6(-1+5\times 2^n)$
$(2,2)$	$18(-1+2^{n+1})$
$(2,3)$	$6(-7+2^{n+4})$
$(2,4)$	$3\times 2^{n+3}$
$(3,4)$	$6(-1+3\times 2^n)$

Theorem 4.3.1. *For the graph $D_2(n)$, the M-Polynomial is*

$$\begin{aligned}M(D_2(n),x,y) &= 6(-1+2^{n+1})xy^3 + 6(-1+5\times 2^n)xy^4 + 18(-1+2^{n+1})x^2y^2\\ &\quad + 6(-7+2^{n+4})x^2y^3 + 3\times 2^{n+3}x^2y^4 + 6(-1+3\times 2^n)x^3y^4.\end{aligned}$$

Proof. By using the values of Tables 4.4 in (2.24), then we have

$$\begin{aligned}M(D_2(n),x,y) &= \sum_{i\le j} m_{ij}(D_2(n))x^iy^j\\ &= 6(-1+2^{n+1})xy^3 + 6(-1+5\times 2^n)xy^4 + 18(-1+2^{n+1})x^2y^2\\ &\quad + 6(-7+2^{n+4})x^2y^3 + 3\times 2^{n+3}x^2y^4 + 6(-1+3\times 2^n)x^3y^4.\end{aligned}$$

which proves the theorem. □

Chapter 5

Topological indices and Polynomials of Porphyrin-cored $2,2$-Bis (methylol) Propionic acid dendrimer

In this chapter, we will study different topological indices and polynomials of molecular graph of Porphyrin-cored 2,2-Bis (methylol) Propionic acid dendrimers. The synthesis and characterization of this dendrimer upto fifth generation are described in [24].

Let the molecular graph of this dendrimer be $D_3(n)$, where the generations stage of $D_3(n)$ is represented by n. The molecular graphs of $D_3(n)$ with core and first generation are shown in Figure 5.1. It is enough to compute the required information for a set of representatives while computing the eccentricity based indices and polynomials of $D_3(n)$. The order of graph $D_3(n)$ is $4(9+2^{n+3})$ and number of edges is $4(11+2^{n+3})$. We partition the molecular graph $D_3(n)$ into two parts, one of them is core C and other is subgraph $Z(n)$ of $D_3(n)$ having four similar branches with vertex set $V(D_3(n))-V(C)$. The sets of representatives from a set of vertices of the core and subgraph of $D_3(n)$, with their degrees, S_u, $M(u)$ and eccentricity for each u are given in Table 5.1 and 5.2, respectively. In this chapter we fix $\gamma = 4n + 4i$.

5.1 The eccentricity-based indices and polynomials for the molecular graph $D_3(n)$

By using the Tables 5.1 and 5.2, we calculate the different eccentricity-based indices and their corresponding polynomials. In the following theorem, we determine the

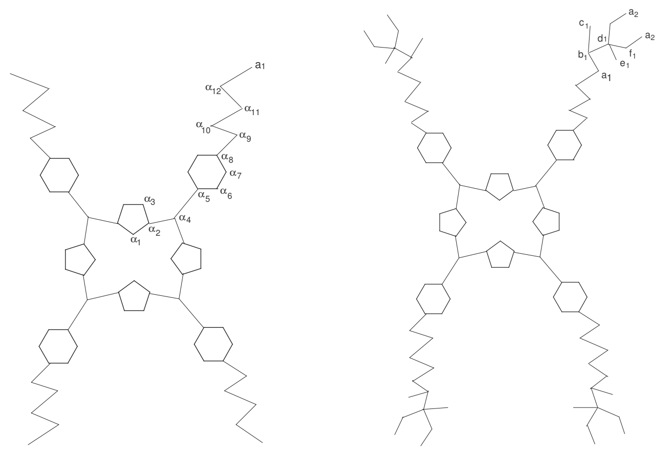

Figure 5.1: Core of $D_3(n)$ and first Generation of $D_3(n)$.

eccentric-connectivity index of $D_3(n)$.

Table 5.1: The set of representatives of the core with their degrees, S_u, $M(u)$, eccentricities and frequencies.

Representative	Degree	S_u	$M(u)$	Eccentricity	Frequency
α_1	2	6	9	$4n+15$	4
α_2	3	7	12	$4n+16$	8
α_3	2	5	6	$4n+16$	8
α_4	3	9	27	$4n+17$	4
α_5	3	7	12	$4n+18$	4
α_6	2	5	6	$4n+19$	8
α_7	2	5	6	$4n+20$	8
α_8	3	6	8	$4n+21$	4
α_9	2	5	6	$4n+22$	4
α_{10}	2	4	4	$4n+23$	4
α_{11}	2	4	4	$4n+24$	4
α_{12}	2	3	2	$4n+25$	4

Theorem 5.1.1. *For the graph $D_3(n)$, the eccentric-connectivity index is given by*

$$\xi(D_3(n)) = 16(2^{n+5} \times n + 22n + 2^n \times 81 + 101).$$

Table 5.2: The set of representatives of the subgraph $Z(n)$ of $D_3(n)$ with degrees, S_u, $M(u)$, eccentricities and frequencies.

Representative	Degree	S_u	$M(u)$	Eccentricity	Frequency
a_i when i=n+1	1	2	2	$8n+26$	2^{n+2}
a_i when $i \neq n+1$	2	5	6	$\gamma+22$	2^{i+1}
b_i	3	7	8	$\gamma+23$	2^{i+1}
c_i	1	3	3	$\gamma+24$	2^{i+1}
d_i	4	8	12	$\gamma+24$	2^{i+1}
e_i	1	4	4	$\gamma+25$	2^{i+1}
f_i	2	5	4	$\gamma+25$	2^{i+2}

Proof. By using the values of Tables 5.1 and 5.2 in (2.2), the eccentric connectivity index of $D_3(n)$ can be written as follows:

$$\begin{aligned}\xi(D_3(n)) = \xi(C) + \xi(Z(n)) = \sum_{u\in V(C)} \varepsilon(u)d_u + \sum_{u\in V(Z(n))} \varepsilon(u)d_u \\
&= (2\times 4)(4n+15) + (3\times 8)(4n+16) + (2\times 8)(4n+16) \\
&+ (3\times 4)(4n+17) + (3\times 4)(4n+18) + (2\times 8)(4n+19) \\
&+ (2\times 8)(4n+20) + (3\times 4)(4n+21) + (2\times 4)(4n+22) \\
&+ (2\times 4)(4n+23) + (2\times 4)(4n+24) + (2\times 4)(4n+25) \\
&+ (1\times 2^{n+2})(8n+26) + \sum_{i=1}^{n}\Big((2\times 2^{i+1})(\gamma+22) + (3\times 2^{i+1})(\gamma+23) \\
&+ (1\times 2^{i+1})(\gamma+24) + (4\times 2^{i+1})(\gamma+24) \\
&+ (1\times 2^{i+1})(\gamma+25) + (2\times 2^{i+2})(\gamma+25)\Big).\end{aligned}$$

After some calculations, we get

$$\xi(D_3(n)) = 16(2^{n+5}\times n + 22n + 2^n \times 81 + 101),$$

which proves the theorem. □

When the degrees of vertices are not taken into account, then by using the values of Tables 5.1 and 5.2 in (2.4), we have the following result.

Corollary 5.1.1. *For the graph $D_3(n)$, the total eccentric-connectivity index is given by*

$$\varsigma(D_3(n)) = 4(2^{n+6} \times n + 2^{n+1} \times 83 + 36n + 167).$$

In the next theorem, the eccentric-connectivity polynomial for the molecular graph $D_3(n)$ has been derived.

Theorem 5.1.2. *For the graph $D_3(n)$, the eccentric-connectivity polynomial is given by*

$$\begin{aligned} ECP(D_3(n), y) = {} & 4y^{4n+15}(2y^{10} + 2y^9 + 2y^8 + 2y^7 + 3y^6 + 4y^5 + 4y^4 \\ & + 3y^3 + 3y^2 + 10y + 2) + 2^{n+2}y^{2(4n+13)} \\ & + \frac{4(5y^3 + 5y^2 + 3y + 2) \times y^{4n+26}(2^n y^{4n} - 1)}{2y^4 - 1}. \end{aligned}$$

Proof. By using the values of Tables 5.1 and 5.2 in (2.3), we have

$$\begin{aligned} ECP(D_3(n), y) &= ECP(C, y) + ECP(Z(n), y) = \sum_{u \in V(C)} d_u y^{\varepsilon(u)} + \sum_{u \in V(Z(n))} d_u y^{\varepsilon(u)} \\ &= (2 \times 4)y^{4n+15} + (8 \times 3)y^{4n+16} + (8 \times 2)y^{4n+16} + (4 \times 3)y^{4n+17} \\ &+ (4 \times 3)y^{4n+18} + (8 \times 2)y^{4n+19} + (8 \times 2)y^{4n+20} + (4 \times 3)y^{4n+21} \\ &+ (4 \times 2)y^{4n+22} + (4 \times 2)y^{4n+23} + (4 \times 2)y^{4n+24} + (4 \times 2)y^{4n+25} \\ &+ (1 \times 2^{n+2})y^{8n+26} + \sum_{i=1}^{n} \Big((2 \times 2^{i+1})y^{\gamma+22} + (3 \times 2^{i+1})y^{\gamma+23} \\ &+ (1 \times 2^{i+1})y^{\gamma+24} + (4 \times 2^{i+1})y^{\gamma+24} + (1 \times 2^{i+1})y^{\gamma+25} \\ &+ (2 \times 2^{i+2})y^{\gamma+25} \Big). \end{aligned}$$

After some calculations, we get the required result. □

Use the values of Tables 5.1 and 5.2 in (2.5), we have the following result.

Corollary 5.1.2. *For the graph $D_3(n)$, the total eccentric-connectivity polynomial is given by*

$$\begin{aligned} TECP(D_3(n), y) = {} & 4y^{4n+15}(y^{10} + y^9 + y^8 + y^7 + y^6 + 2y^5 + 2y^4 + y^3 + y^2 + 4y + 1) \\ & + 2^{n+2}y^{2(4n+13)} + \frac{4(3y^3 + 2y^2 + y + 1)y^{4n+26}(2^n y^{4n} - 1)}{2y^4 - 1}. \end{aligned}$$

In the next theorem, we compute the closed formula for the second Zagreb eccentricity index of molecular graph .

Theorem 5.1.3. *For the graph $D_3(n)$, the second Zagreb eccentricity index is given by*

$$M_1^{**}(D_3(n)) = 4(2^{n+9} \times n^2 + 2^{n+5} \times 83n + 2^{n+2} \times 927 + 144n^2 + 1336n + 3007).$$

Proof. By using the values of Tables 5.1 and 5.2 in (2.6), we compute the second Zagreb eccentricity index of $D_3(n)$ as follows:

$$\begin{aligned} M_1^{**}(D_3(n)) = M_1^{**}(C) + M_1^{**}(Z(n)) &= \sum_{v\in V(C)} [\varepsilon(v)]^2 + \sum_{v\in V(Z(n))} [\varepsilon(v)]^2 \\ &= 4(4n+15)^2 + 8(4n+16)^2 + 8(4n+16)^2 + 4(4n+17)^2 + 4(4n+18)^2 \\ &+ 8(4n+19)^2 + 8(4n+20)^2 + 4(4n+21)^2 + 4(4n+22)^2 + 4(4n+23)^2 \\ &+ 4(4n+24)^2 + 4(4n+25)^2 + 2^{n+2}(8n+26)^2 + \sum_{i=1}^{n}\Big(2^{i+1}(\gamma+22)^2 \\ &+ 2^{i+1}(\gamma+23)^2 + 2^{i+1}(\gamma+24)^2 + 2^{i+1}(\gamma+24)^2 \\ &+ 2^{i+1}(\gamma+25)^2 + 2^{i+2}(\gamma+25)^2\Big). \end{aligned}$$

After some calculations, we obtain

$$M_1^{**}(D_3(n)) = 4(2^{n+9} \times n^2 + 2^{n+5} \times 83n + 2^{n+2} \times 927 + 144n^2 + 1336n + 3007),$$

that proves our theorem. □

Now, we compute the closed formula for the modified eccentric-connectivity index of molecular graph.

Theorem 5.1.4. *For the graph $D_3(n)$, the modified eccentric connectivity index is given by*

$$\Lambda(D_3(n)) = 4(2^{n+3} \times 39n + 204n + 2^n \times 789 + 905).$$

Proof. By using the values of Tables 5.1 and 5.2 in (2.9), we compute the modified eccentric connectivity index of $D_3(n)$ in the following way:

$$\begin{aligned} \Lambda(D_3(n)) = \Lambda(C) + \Lambda(Z(n)) &= \sum_{u\in V(C)} S_u\varepsilon(u) + \sum_{u\in V(Z(n))} S_u\varepsilon(u) \\ &= (6\times 4)(4n+15) + (7\times 8)(4n+16) + (5\times 8)(4n+16) \end{aligned}$$

$$+ (9\times 4)(4n+17) + (7\times 4)(4n+18) + (5\times 8)(4n+19) + (5\times 8)(4n+20)$$
$$+ (36\times 4)(4n+21) + (5\times 4)(4n+22) + (4\times 4)(4n+23) + (4\times 4)(4n+24)$$
$$+ (3\times 4)(4n+25) + (2\times 2^{n+2})(8n+26) + \sum_{i=1}^{n}\Big((5\times 2^{i+1})(\gamma+22)$$
$$+ (7\times 2^{i+1})(\gamma+23) + (3\times 2^{i+1})(\gamma+24) + (8\times 2^{i+1})(\gamma+24)$$
$$+ (4\times 2^{i+1})(\gamma+25) + (5\times 2^{i+2})(\gamma+25)\Big).$$

After some calculations, we obtain

$$\Lambda(D_3(n)) = 4(2^{n+3}\times 39n + 204n + 2^n\times 789 + 905),$$

The proof is complete. □

In the following theorem, we compute the closed formula for the modified eccentric-connectivity polynomial of molecular graph.

Theorem 5.1.5. *For the graph $D_3(n)$, the modified eccentric connectivity polynomial is given by*

$$\begin{aligned}\Lambda(D_3(n)) &= 4y^{4n+15}(3y^{10} + 4y^9 + 4y^8 + 5y^7 + 6y^6 + 10y^5 + 10y^4 + 7y^3\\ &\quad + 9y^2 + 24y + 6) + 2^{n+3}y^{2(4n+13)}\\ &\quad + \frac{4(14y^3 + 11y^2 + 7y + 5)y^{4n+26}(2^n y^{4n} - 1)}{2y^4 - 1}.\end{aligned}$$

Proof. By using the values of Tables 5.1 and 5.2 in (2.10), we compute the modified eccentric connectivity polynomial of $D_3(n)$ in the following way:

$$\begin{aligned}MECP(D_3(n), y) &= MECP(C, y) + MECP(Z(n), y)\\ &= \sum_{u\in V(C)} S_u y^{\varepsilon(u)} + \sum_{u\in V(Z(n))} S_u y^{\varepsilon(u)}\\ &= (6\times 4)y^{4n+15} + (8\times 7)y^{4n+16} + (8\times 5)y^{4n+16} + (4\times 9)y^{4n+17}\\ &\quad + (4\times 7)y^{4n+18} + (8\times 5)y^{4n+19} + (8\times 5)y^{4n+20} + (4\times 6)y^{4n+21}\\ &\quad + (4\times 5)y^{4n+22} + (4\times 4)y^{4n+23} + (4\times 4)y^{4n+24} + (4\times 3)y^{4n+25}\\ &\quad + (2\times 2^{n+2})y^{8n+26} + \sum_{i=1}^{n}\Big((5\times 2^{i+1})y^{\gamma+22} + (7\times 2^{i+1})y^{\gamma+23}\end{aligned}$$

$$+ (3 \times 2^{i+1})y^{\gamma+24} + (8 \times 2^{i+1})y^{\gamma+24} + (4 \times 2^{i+1})y^{\gamma+25} + (5 \times 2^{i+2})y^{\gamma+25}\Big).$$

After some calculations, we obtain the required result. □

Theorem 5.1.6. *For the graph $D_3(n)$, the augmented eccentric connectivity index is given by*

$$\begin{aligned}
{}^{A}\varepsilon(D_3(n)) = {} & \frac{36}{4n+15} + \frac{144}{4n+16} + \frac{108}{4n+17} + \frac{48}{4n+18} + \frac{48}{4n+19} + \frac{48}{4n+20} \\
& + \frac{32}{4n+21} + \frac{24}{4n+22} + \frac{16}{4n+23} + \frac{16}{4n+24} + \frac{8}{4n+25} + \frac{2^{n+3}}{8n+26} \\
& + \left(\frac{24}{4n+26} + \cdots + \frac{3 \times 2^{n+2}}{8n+22}\right) + \left(\frac{32}{4n+27} + \cdots + \frac{2^{n+4}}{8n+23}\right) \\
& + \left(\frac{12}{4n+28} + \cdots + \frac{3 \times 2^{n+1}}{8n+24}\right) + \left(\frac{48}{4n+28} + \cdots + \frac{3 \times 2^{n+3}}{8n+24}\right) \\
& + \left(\frac{16}{4n+29} + \cdots + \frac{2^{n+3}}{8n+25}\right) + \left(\frac{32}{4n+29} + \cdots + \frac{2^{n+4}}{8n+25}\right).
\end{aligned}$$

Proof. By using the values of Tables 5.1 and 5.2 in (2.8), we compute the augmented eccentric connectivity index of $D_3(n)$ in the following way:

$$\begin{aligned}
{}^{A}\varepsilon(D_3(n)) = {}^{A}\varepsilon(C) + {}^{A}\varepsilon(Z(n)) = {} & \sum_{u \in V(C)} \frac{M(u)}{\varepsilon(u)} + \sum_{u \in V(Z(n))} \frac{M(u)}{\varepsilon(u)} \\
= {} & \frac{9 \times 4}{4n+15} + \frac{12 \times 8}{4n+16} + \frac{6 \times 8}{4n+16} + \frac{27 \times 4}{4n+17} + \frac{12 \times 4}{4n+18} + \frac{6 \times 8}{4n+19} \\
& + \frac{6 \times 8}{4n+20} + \frac{4 \times 8}{4n+21} + \frac{6 \times 4}{4n+22} + \frac{4 \times 4}{4n+23} + \frac{4 \times 4}{4n+24} + \frac{2 \times 4}{4n+25} \\
& + \frac{2 \times 2^{n+2}}{4n+26} + \sum_{i=1}^{n} \Bigg(\frac{6 \times 2^{i+1}}{\gamma+22} + \frac{8 \times 2^{i+1}}{\gamma+23} + \frac{3 \times 2^{i+1}}{\gamma+24} + \frac{12 \times 2^{i+1}}{\gamma+24} \\
& + \frac{4 \times 2^{i+1}}{\gamma+25} + \frac{4 \times 2^{i+2}}{\gamma+25}\Bigg).
\end{aligned}$$

After some calculations, we obtain the required result. □

5.2 Counting polynomials

To compute the counting polynomials, we find the qocs for $D_3(n)$. The qocs along with their lengths and frequencies are given in Table 5.3 and the cuts for core and subgraph are shown in Figure 5.3.

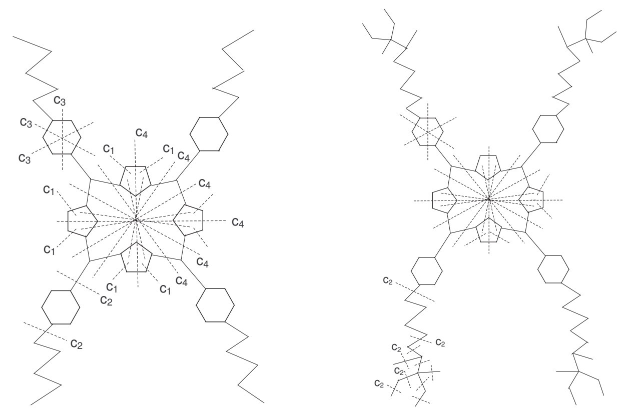

Figure 5.2: Qocs for Core and qocs for First Generation of $D_3(n)$.

Table 5.3: Qocs with their lengths and frequencies.

qocs	length	Frequency
C_1	1	8
C_2	1	$8(-1+2^{n+2})$
C_3	2	12
C_4	2	10

Theorem 5.2.1. *For the graph $D_3(n)$, the Omega polynomial is given by*

$$\Omega(D_3(n), x) = 2^{n+5}x + 22x^2.$$

Proof. The Figure 5.3 and Table 5.3 shows the qocs C_1, C_2, C_3, C_4 of the graph $D_3(n)$ and their lengths. Substitute the values of Table 5.3 in (2.21) we get

$$\begin{aligned}\Omega(D_3(n), x) &= 8x + 8(-1+2^{n+2})x + 12x^2 + 10x^2 \\ &= 2^{n+5}x + 22x^2.\end{aligned}$$

This gives the required result. □

Theorem 5.2.2. *For the graph $D_3(n)$, the Sadhana polynomial is given by*

$$Sd(D_3(n), x) = 2^{n+5}x^{43+2^{n+5}} + 22x^{42+2^{n+5}}.$$

Proof. To compute Sadhana polynomial, we use the values of Table 5.3 in (2.22) as,

$$\begin{aligned} Sd(D_3(n), x) &= 8x^{4(11+2^{n+3})-1} + 8(-1+2^{n+2})x^{4(11+2^{n+3}-1} + 12x^{4(11+2^{n+3})-2} \\ &+ 10x^{4(11+2^{n+3})-2} \\ &= 2^{n+5}x^{43+2^{n+5}} + 22x^{42+2^{n+5}}. \end{aligned}$$

The proof is complete. □

Theorem 5.2.3. *For the graph $D_3(n)$, the PI polynomial is given by*

$$PI(D_3(n), x) = 2^{n+5}x^{43+2^{n+5}} + 44x^{42+2^{n+5}}.$$

Proof. To compute this polynomial, we substitutes the values in (2.23)

$$\begin{aligned} PI(D_3(n), x) &= 8x^{4(11+2^{n+3})-1} + 8(-1+2^{n+2})x^{4(11+2^{n+3}-1} + 12 \times 2x^{4(11+2^{n+3})-2} \\ &+ 10 \times 2x^{4(11+2^{n+3})-2} \\ &= 2^{n+5}x^{43+2^{n+5}} + 44x^{42+2^{n+5}}. \end{aligned}$$

After some calculations, we obtain the required result. □

5.3 M-Polynomial

In this section, we will calculate the M-polynomial by using the values given in Table 5.4.

Theorem 5.3.1. *For the graph $D_3(n)$, the M-Polynomial is*

$$\begin{aligned} M(D_3(n), x, y) &= 2^{n+2}xy^2 + 4(-1+2^n)xy^3 + 4(-1+2^n)xy^4 + 4(5+2^n)x^2y^2 \\ &+ 4(8+2^n)x^2y^3 + 8(-1+2^n)x^2y^4 + 12x^3y^3 + 4(-1+2^n)x^3y^4. \end{aligned}$$

Proof. By using the values of Tables 5.4 in (2.24), we get

$$\begin{aligned} M(D_3(n), x, y) &= \sum_{i \le j} m_{ij}(D_3(n))x^iy^j. \\ &= 2^{n+2}xy^2 + 4(-1+2^n)xy^3 + 4(-1+2^n)xy^4 + 4(5+2^n)x^2y^2 \\ &+ 4(8+2^n)x^2y^3 + 8(-1+2^n)x^2y^4 + 12x^3y^3 + 4(-1+2^n)x^3y^4. \end{aligned}$$

which is the required result. □

Table 5.4: Edge partition of First Generation.

Representative	Frequency
$(1,3)$	$6(-1+2^{n+1})$
$(1,4)$	$6(-1+5\times 2^{n})$
$(2,2)$	$18(-1+2^{n+1})$
$(2,3)$	$6(-7+2^{n+4})$
$(2,4)$	$3\times 2^{n+3}$
$(3,4)$	$6(-1+3\times 2^{n})$

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