Computing some topological indices of hetrofunctional dendrimer HFD(ei)

by

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Abstract

To predict the bioactivity of chemical compounds physicochemical properties and topological indices such as Wiener index, Szeged index, Randić index, Zagreb index, atom-bond connectivity (ABC) index and geometric-arithmetic (GA) index are rapidly used in the study of Quantitative Structure-Activity (QSAR) and Quantitative Structure-Property Relationship (QSPR).

To compute and study the topological indices of molecular graphs and nanostructures is a respected problem in both combinitorial chemistry and in theoretical nanoscience. In this thesis, we consider a hetrofuntional dendrimer HFD(ei) and compute its eccentricity based topological indices, namely eccentric connectivity index and eccentricity based Zagreb index.

Furthermore, we compute the nullity and number of Kekulé structure. If the Kekulé structure does not exist, we find the size of a maximum matching of HFD(ei). We also compute first version of atom-bond connectivity index (ABC), fourth version of atom bond connectivity index (ABC_4), first version of geometric-arithmetic index (GA), fifth version of geometric-arithmetic index (GA_5) and Randić index (R_α) for a hetrofunctional dendrimer HFD(ei).

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To My Papa G

Introduction

During the past two decades, there has been a considerable progress in the applications of algebraic graph theory in chemistry. Graph theory is concerned with manipulations of structures and structural informations. This involves classification of structures, that is, their grouping into smaller lots, characterization of structures, which can be accomplished by enumeration of selected structural invariants, and ordering of structurees, which implies a decision of which among two or more structures should be taken first in the sequence. The first two chapters of this thesis are devoted to some basic definitions and terminologies of graphs. In the first chapter, we define basic definitions of graph theory, after that we introduce chemical graph theory and some major types of chemical graphs that are commonly studied in chemical graph theory.

In the second chapter we give a brief history of some well-known topological indices mainly distance related topological indices, degree based topological indices, and counting based topological indices. In the class of distance based topological indices, we give a brief introduction of Wiener index, Harary index, Szeged index and Balaban index. In the class of degree based of topological indices, we discuss different types of degree based topological indices that are Randić index, sum connectivity index, Zagreb index and atom-bond connectivity index. In the counting related polynomials and topological indices, we give a brief introduction of counting polynomials and counting related indices that are Omega index, Sadhana index and Padmakar-Ivan (PI) index, to name of few.

In the third chapter, we consider a hetrofunctional dendrimer, HFD(ei) denoted by $D[n]$. We discuss its structure and compute eccentric connectivity index ($\xi(D[n])$) and eccentricity based Zagreb indices.

In the fourth chapter, we compute the nullity and number of Kekulé structures in a class of hetrofunctional dendrimer, HFD(ei). When there is no Kekulé structure, we find the size of a maximum matching in this dendrimer. Furthermore, we compute the first and fourth version of atom-bond connectivity index. We also calculate

the first and fifth version of geometric-arithmetic index and Randić index of this dendrimer.

A conclusion section highlighting the contribution made in this thesis with some possible open problems arising from the thesis is given at the end of this thesis.

Contents

Chapter 1

Fundamentals of Graph Theory

1.1 Introduction

In this chapter we discuss some basic concepts of graph theory. We first give a brief introduction and concept of some basic terminologies of graph theory. We also give some basic definitions of chemical graph theory.

1.2 History of graph theory

A Swiss mathematician Leonhard Paul Euler (1701-1783), also known as Euler, spent most of his life in Germany and Russia. He was the first mathematician who solved the first problem with the use of graph theory. The credit goes to him for creation of first graph to simulate a real time problem and situation to solve a problem which was said to be the toughest problem of that time.

1.2.1 The K*ö*nigsberg bridge problem

As by the name, this problem originated in the city of Königsberg located on the river Preger which is a part of Russia. This city is now named as Kaliningrad. By the way of seven bridges two islands were connected with the main-land. There existed a thought among people if there was any possible way to walk once and only once over all the bridges?

In 1736 one person came out with the solution in terms of graph theory. His name was Euler. He was the one to prove that it was impossible to walk through these seven bridges exactly one time. He formulated the problems in terms of graph theory. By removing all unnecessary features he abstracted the case of Königsberg. By using line segments as bridges and dots representing landmasses he drew a picture in which the line segments connected the dots.

Hence, the problem was clarified to the maximum extent. The problem can be simply seen now as the way of tracing the graph with a pencil without lifting it. It could be tried in all possible ways but soon one would come to know that it is impossible. Euler not only proved but also explained why it is impossible and what should be the attribute of the graphs so that its edge could be stretched across only once. He then came out with the concept of edges and nodes. The number of edges touching a given node is termed as degree of the node. Euler put forward that any graph could be traversed with each edge traversed absolutely once if and only if it had zero or exactly two nodes with odd degrees.

1.3 What is graph theory?

Graph theory is a branch of mathematics related to the study of graphs. This branch deals with mathematics and computer science simultaneously. In graph theory the term graph does not refer any data such as in line graph or bar graph. Here the term graph represents an ordered pair $G = (V(G), E(G))$. In this ordered pair, $V(G)$ is the set of vertices (nodes, points) and $E(G)$ represents the set of edges. If we want to establish a telephone network via cable that each telephone is reachable from others at minimum cost. If we want to decide the shortest route between two states. If a salesman want to travel in different cities in such a way that time should be minimize. These and there are so many other problems in daily life which involves graph theory. So, we can define a graph as a triple consisting a vertex set $V(G)$, edge set $E(G)$, and a relation that associate each edge with two vertices. In Fig.1.1, G is a graph with $E(G) = \{e_1, e_2, \cdots, e_7\}$ and $V(G) = \{v_1, v_2, \cdots, v_6\}$.

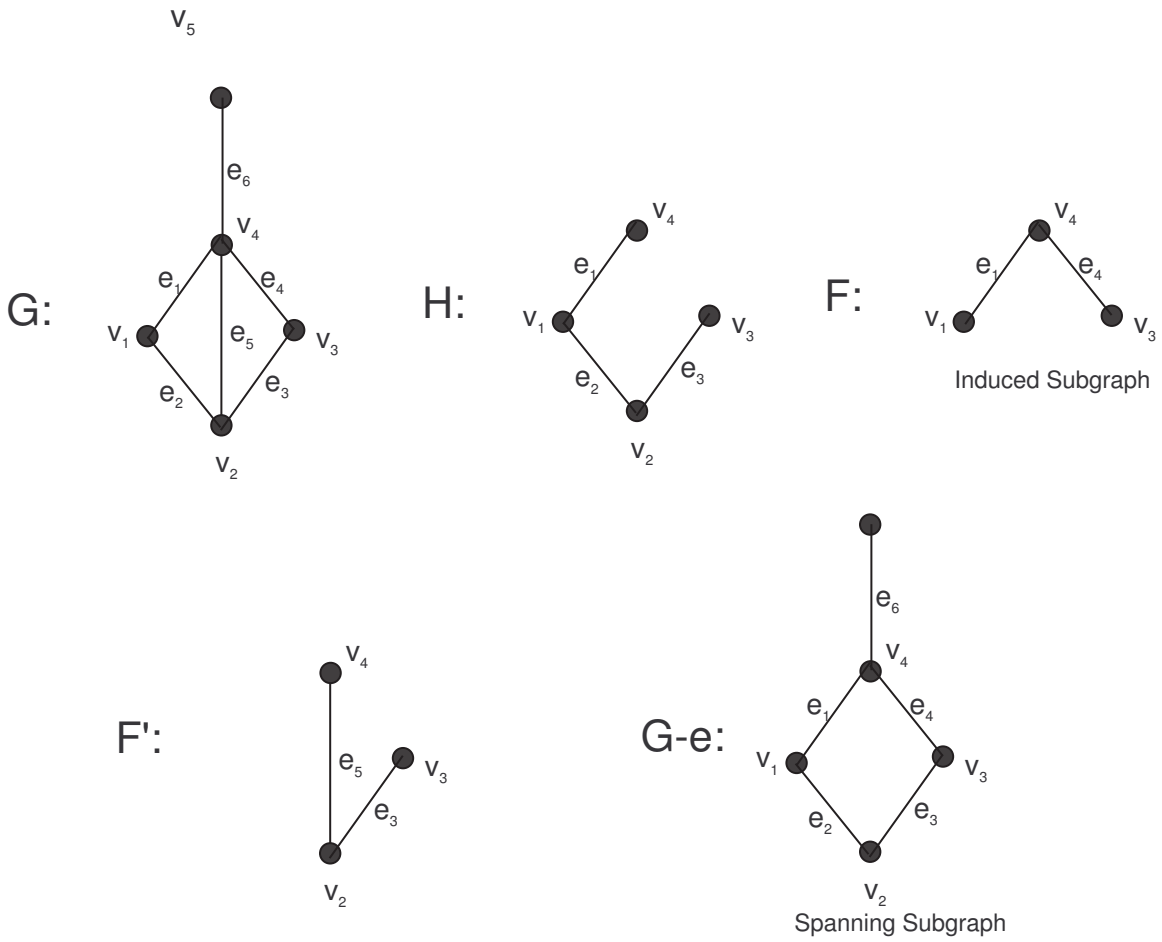

Figure 1.1: Graph G and its subgraphs.

A graph H is a subgraph of a graph G if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$, and is written as $H \subseteq G$. The subgraph H of a graph G is said to be a *proper* subgrah if $V(H)$ is a proper subset of $V(G)$ or $E(H)$ is a proper subset of $E(G)$. A subgraph H of a graph G is said to be a *spanning* subgraph of G if $V(H) = V(G)$. A subgraph F of a graph G is said to be an *induced* subgraph of G if $u, v \in V(F)$ and $uv \in E(G)$, then $uv \in E(F)$.

1.4 Basic concepts and definitions

An edge of a graph $G = (V(G), E(G))$ whose end points are u and v is called *uv-edge* or simply uv. An edge whose end vertices are same is called a *loop*. Two edges whose end points are same are called *multiple edges*. Two vertices u and v are end points of an edge then u is said to be *adjacent* to v or v is said to be adjacent to u. For a vertex $u \in V(G)$, the set of vertices adjacent to u is called *neighborhood* of u and is written as $N_G(u)$. The number of edges incident on a vertex u is called the *degree of vertex* u and is denoted by d_u or simply $d(u)$. Each loop counts twice in counting the degree of a graph.

Figure 1.2: a. A vertex, b. loop and c. multigraph

If the degree of a vertex is 0 then the vertex is called an *isolated vertex*. A vertex which has a degree 1 is called a *pendent vertex* or *end-vertex*. A graph that does not contain any loop and multiple edges is called a *simple graph*. A graph is said to be a *finite graph* if it contains finite number of vertices. A (u, v)-*path* on n vertices is a graph with vertex set $\{u = v_0, v_1, \ldots, v_n = v\}$ and edge set $\{v_i v_{i+1} \mid 0 \leq i \leq n-1\}$. The number of edges in path is called the *length* of a path. A graph G has a (u, v)-path, then the *distance* from u to v, written $d_G(u, v)$ or simply $d(u, v)$ is the least length of (u, v)-path. A graph is said to be a *connected graph* if, for every pair of vertices $u, v \in V(G)$ there exists a (u, v)-path otherwise, it is called *disconnected* graph. In a disconnected graph each maximal connected subgraph of G is called a *component*. A connected subgraph H' of a graph G is maximal if H' is not contained in any other connected subgraph of G. Obviously, connected graph consists of only one component. The eccentricity written as $ec(v)$ of a vertex v in a connected graph G is the maximum distance between v and any other vertex u of G.

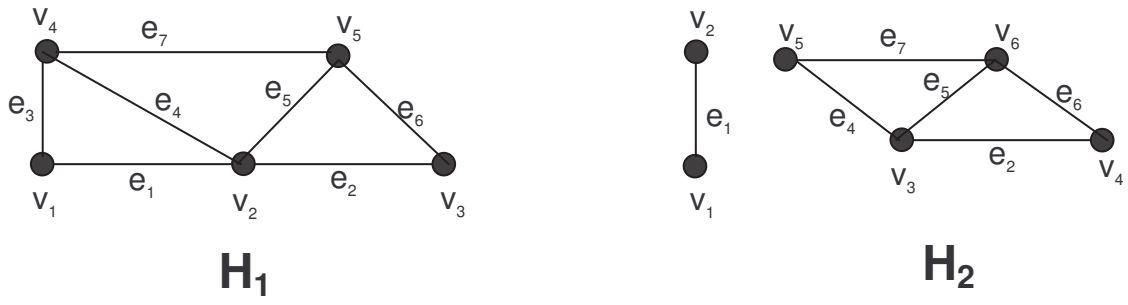

Figure 1.3: $\mathbf{H_1}$. Simple connected graph $\mathbf{H_2}$. Disconnected graph with two components.

Two graphs $G_1 = \big(V(G_1), E(G_1)\big)$ and $G_2 = \big(V(G_2), E(G_2)\big)$ are said to be *isomorphic* (written as $G_1 \cong G_2$) if there exist a mapping $f : V(G_1) \to V(G_2)$ which satisfy the following conditions:

1. f is a bijective function (one-to-one and onto),
2. for all vertices $u, v \in V$; $(u, v) \in E(G_1) \Leftrightarrow (f(u), f(v)) \in E(G_2)$.

The function f is called an isomorphism.

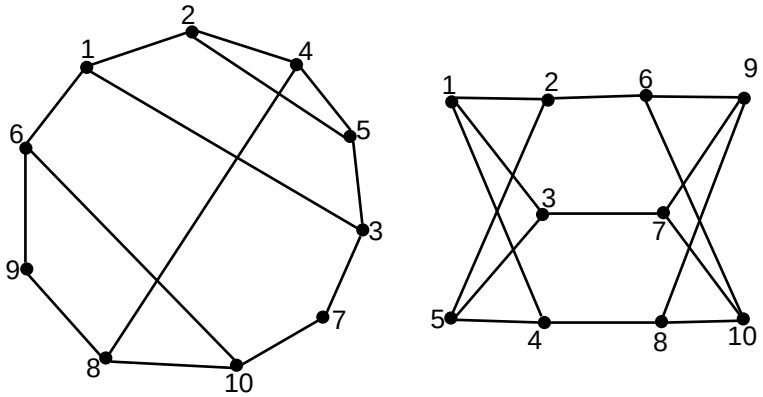

Figure 1.4: Two isomorphic graphs.

1.5 Some special classes of graphs

A *path* is a most simple class of a graph that is defined above. A path with $n+1$ vertices has n edeges and is denoted by P_n. A *cycle* is a simple graph whose vertices can be arranged in a cycle sequence such that every pair should be adjacent if they are consecutive in sequence. A cycle with n vertices is denoted C_n where n is called *lenght* of cycle. A cycle that consists on three vertices is called a *triangle*. A cycle that consists on four vertices is called a *quadrilateral*, a cycle which consists on five vertices is called a *pentagon* and a cycle with six vertices is called a *hexagon* and so on. A graph that does not contain any cycle is called an *acyclic* graph. A

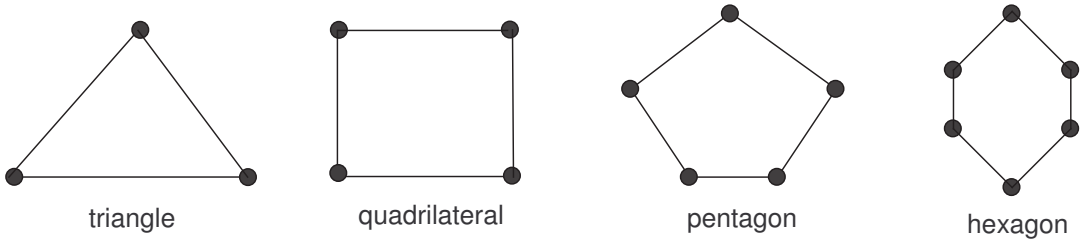

Figure 1.5:

connected acyclic graph is called a *tree* and is denoted by T. An acyclic graph is called a *forest*.

A simple graph G is said to be a *complete graph* in which each pair of distinct vertices from $V(G)$ is connected by a unique edge. A complete graph with n vertices is denoted by K_n.

A graph G is said to be a *bipartite graph* if its vertex set $V(G)$ can be partitioned in to two subsets X and Y in such a way that each edge has one end in X and other end in Y. The pair (X, Y) is called the bipartition of the bipartite graph. A bipartite graph with bipartition (X, Y) is represented as $G[X, Y]$. A graph $G[X, Y]$ is called a *complete bipartite* graph if each vertex in X is adjacent to each vertex of Y. A complete bipartite graph with bipartition (X, Y) is denoted by $K_{m,n}$, where $m = |X|$ and $n = |Y|$. A complete bipartite graph is said to be a *star* if $|X| = 1$ or $|Y| = 1$.

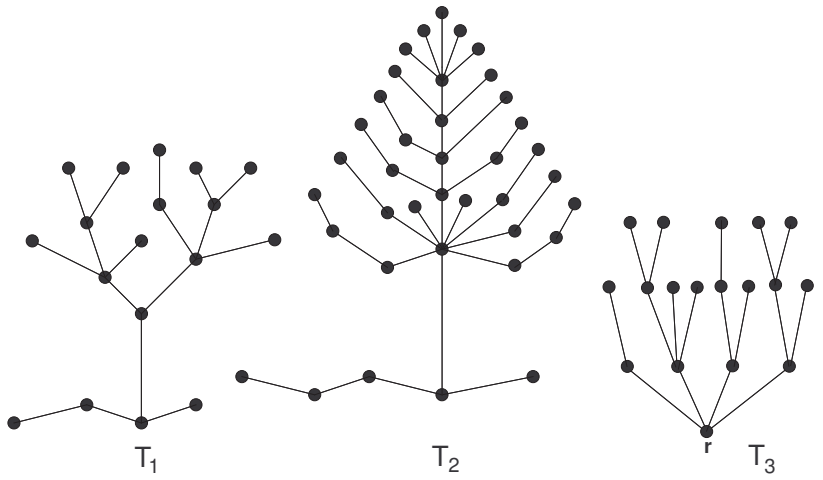

Figure 1.6: Tree.

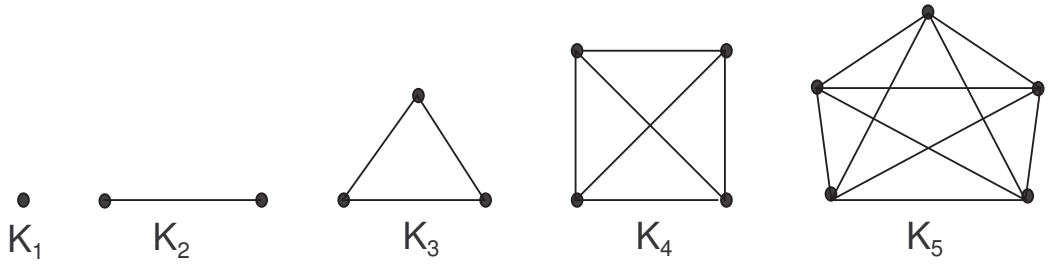

Figure 1.7: Complete graph $K_i (1 \leq i \leq 5)$.

Figure 1.8: Complete birpartite graphs $K_{3,4}$ and $K_{1,4}$.

1.6 Chemical graph theory

A *molecular graph* or a *chemical graph* is a representation of the structural formula of a chemical compound in terms of graph theory. The vertices of a molecular graph correspond to the atoms of the compound and the edges correspond to chemical bonds between them [29].

Chemical graph theory is the topological branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena. The pioneers of the chemical graph theory are Alexandru Balaban, Ante Graovac, Ivan Gutman, Haruo Hosoya, Milan Randić and Nenad Trinajstić [40]. Model of a chemical system represents a chemical graph which is used to characterize the instructions among its components such as atoms, bonds, groups of atoms or molecules. A chemical graph with hydrogen molecule have the same topological properties as if it does not contain the hydrogen molecule. For example, consider the structure of benzene C_6H_6. Here, six hydrogen atoms are to complete their valency. It is convention in chemical graph theory to consider hydrogen depleted molecules because the hydrogen atoms are present their to complete the valancy of corbon items (Fig. 1.9). The molecular graph with hydrogen vertices deleted is called hydrogen depleted molecular graph or hydrogen suppressed molecular graph (Fig. 1.10).

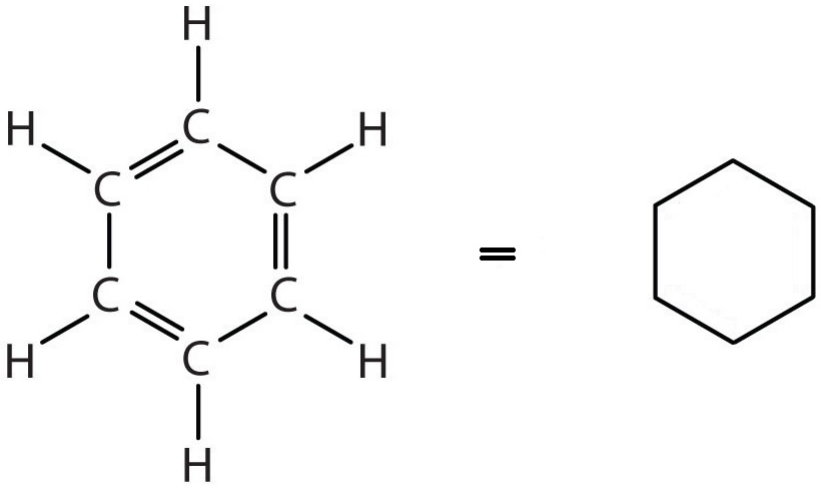

Figure 1.9: Hydrogen depleted graph of Benzene C_6H_6

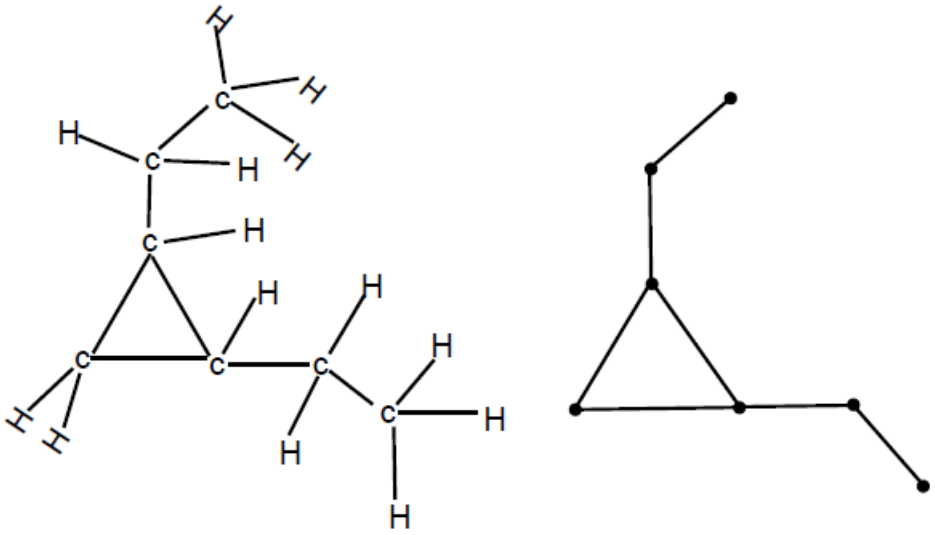

Figure 1.10: A chemical structure and its hydrogen depleted regresntation (molecular graph.

1.6.1 The first use of chemical graph theory

Much of the current panorama of graph theory has been erected on foundations that are essentially graph-theoretical in nature. Chemical graphs are now being used for many different purposes in all major branches of chemistry [5]. The present widespread usage of the chemical graph renders the origins of the earliest implicit application of graph theory of some considerable interest. Chemical graphs were first introduced in the latter half of the 18^{th} century. To understand the need for them at that time and the circumstances of their introduction into the chemical literature, it will be necessary to say something about the prevailing attitudes in chemistry. Chemical thinking in the 18^{th} century was steeped in Newtonian ideas, especially those pertaining to the internal structure of matter and the short-range forces existing between particles.

In 1687, Newton [10] himself had stated that all natural phenomena depend upon certain forces by which the particles of bodies, by some causes, are either mu-

tually impelled towards one another, and cohere in regular figures, or are repelled and recede from another.

The first chemical graph, clearly recognizable as such, were drawn by the Scottish chemist, William Cullen. In 1758, Cullen [47] started using so-called "affinity diagrams" in his lecture to represent the supposed forces, existing between pairs of molecules undergoing various chemical reactions. Unfortunately, these diagrams were used completely for illustrating his chemistry lecture notes, and none were ever published. Later on, Black [11] published similar diagrams those are used by Cullen in his lectures and claim falsely that he invented them. At the end of the 18^{th} century, such diagrams became commonplace in British chemistry textbooks of that period. Reproductions of two surviving diagrams, due to Cullen, are shown (Fig. 1.11).

The numbers (or, in some cases, symbols) appearing between pairs of re-

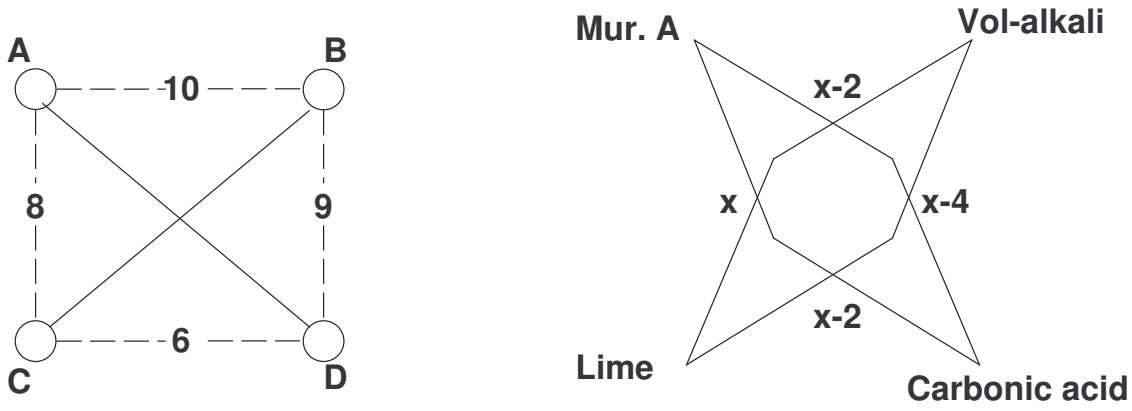

Figure 1.11: Examples of the first chemical graphs used by Cullen and Balck in 1758 to represent the interactions of chemical substances. The supposed forces between pairs of substances are indicated either in terms of numbers or symbols.

acting substances represent the magnitude of the gravitational attraction existing between the substances. It should be noted that these numbers have no physical basis whatsoever and thus express no more than a totally fictitious quantification of imagined forces acting between the substances concerned.

It was probably after seeing such diagrams that the Irish chemist William Higgins had the inspiration of representing the forces between the constituent components, that is the atoms, of molecules. It was most likely in the wake of seeing such graphs that the Irish scientist, William Higgins, had the motivation of speaking to the powers between the constituent parts, that is the iotas of particles. In a book published in 1789, Higgins [35] used a series of diagrams similar to those of Cullen to portray s number of different individual molecules. Examples of some of his diagrams, depicting the five oxides of nitrogen, are reproduced in (Fig. 1.12)

In these diagrams (Fig. 1.12), the nitrogen atom is always represented by the symbol P (standing for phlogisticated air) whereas the oxygen atoms are denoted by the symbols a through e. After Cullen, Higging inserted arbitrary numbers between the various pairs of atoms in a vain attempt to quantify the force of attraction between them. It is important to emphasize here that the lines joining pairs of atoms are not to be interpreted as chemical bonds in the modern sense. The concept of the chemical bond was developed only some three quarters of a century later. The spatial arrangement of atoms was also not understood at the time of Higgins, and so all of his representation are two-dimensional. Morover, in all of the diagrams in (Fig. 1.12), atoms are portrayed in topologically incorrect position. In spite of these evident drawbacks, however, the insight of Higgins were quite remarkable for his time.

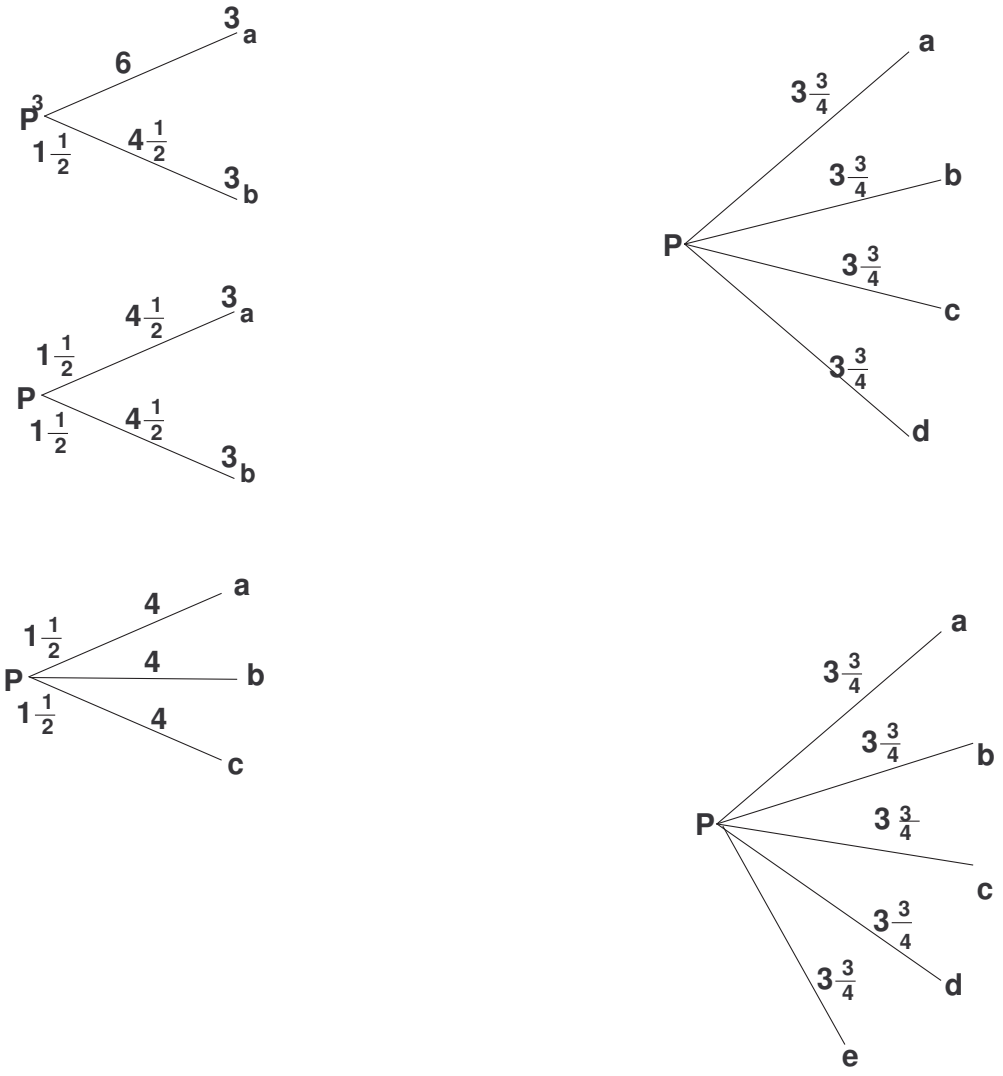

Figure 1.12: Reproduction of some of the first chemical graphs used by Higgins in 1789 to represen individual chemical species. Depicted here are the five oxide of nitrogen. The numbers indicate the supposed forces between pairs of atoms.

1.6.2 Equivalance between chemical and mathematical terms

It has been observed that chemist made use of graph theory unconsciously while writing organic chemical formulas and figuring out all constitutional isomers. Realizing this need, Balaban [8] introduced the chemical versus graph-theoretical vocabulary shown in Table 1.1.

Chemical Term	Mathematical (graph-theoretical) term
Atom	Vertex
Molecule	Molecular graph
Covalent bond	Edge
Acyclic hydrocarbon	Tree
Alternant structure	Bipartite graph
Valency of an atom	Vertex degree (number of lines at that vertex)
Skeletal structure	Hydrogen-depleted graph
Number of rings	Cyclomatic number
$[n]$Annulene	n-Vertex cycle
H*ü*ckel theory	Spectral theory
Topological matrix	Adjacency matrix
Energy level	Eigenvalue
Nonbonding level	Zero eigenvalue
Bonding level	Negative eigenvalue
Antibonding level	Positive eigenvalue
Secular polynomial	Characteristic polynomial
Kekulé resonance formula	Perfect matching, 1-factor

Table 1.1: Equivalence between chemical and mathematical terms in describing constitutional formulas (represented by a molecular graphs).

1.7 Types of chemical graphs

There are different types of chemical graphs. Some of most common chemical graphs that are studied frequently in graph theory are as follows.

1.7.1 Fullerene

A fullerene is a molecule of carbon in the form of a hollow sphere, ellipsoid, tube, and many other shapes. Spherical fullerenes are also called buckyballs and they resemble the balls used in football [28]. Cylindrical ones are called carbon nanotubes. Fullerenes are similar in structure to graphite, which is composed of stacked graphene sheets of linked hexagonal rings; but they may also contain pentagonal (or sometimes heptagonal) rings.

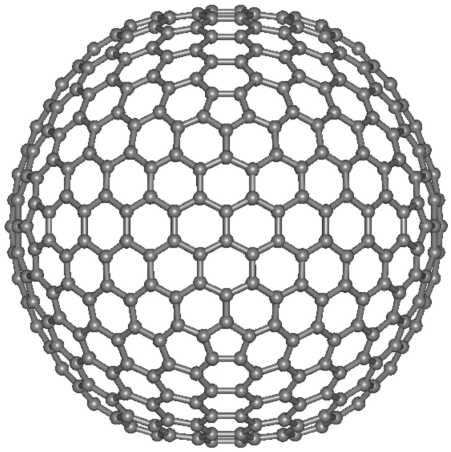

Figure 1.13: Fullerene C_{60}

Since the discovery of fullerenes in 1985 [37], structural variations on fullerenes have evolved well beyond the individual clusters themselves. Examples include

- Buckyball clusters
- Nanotubes
- Megatubes

- polymers
- nano "onions"
- linked "ball-and-chain" dimers
- fullerene rings

Fullerenes have been extensively used for several biomedical applications including the design of high-performance MRI contrast agents, X-Ray imaging contrast agents, photodynamic therapy and drug and gene delivery, summarized in several comprehensive reviews.

1.7.2 Nanotubes

A carbon nanotube is a tube-shaped material, made of carbon, having a diameter measuring on the nanometer scale [44]. A nanometer is one-billionth of a meter, or about one ten-thousandth of the thickness of a human hair. The graphite layer appears somewhat like a rolled-up chicken wire with a continuous unbroken hexagonal mesh and carbon molecules at the apexes of the hexagons.
Carbon nanotubes have many structures, differing in length, thickness, and in the type of helicity and number of layers. Although they are formed from essentially the same graphite sheet, their electrical characteristics differ depending on these variations, acting either as metals or as semiconductors.
As a group, carbon nanotubes typically have diameters ranging from less than 1 nm up to 50 nm. Their lengths are typically several microns, but recent advancements have made the nanotubes much longer, and measured in centimeters.
Carbon nanotubes can be categorized by their structures:

- Single-wall Nanotubes (SWNT)
- Multi-wall Nanotubes (MWNT)

A cylendrical shape nanotube with open ends is shown in following figure (Fig. 1.14)

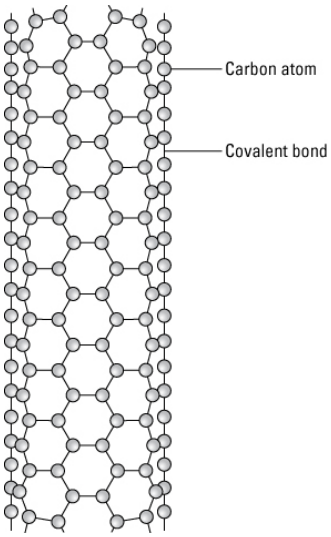

Figure 1.14: Carbon nanotube.

Carbon nanotube technology can be used for a wide range of applications that are as follows:

- Conductive plastics
- Structural composite materials
- Flat-panel displays
- Gas storage
- Antifouling paint
- Micro- and nano-electronics
- Radar-absorbing coating
- Technical textiles
- Ultra-capacitors
- Atomic Force Microscope (AFM) tips
- Batteries with improved lifetime

- Biosensors for harmful gases
- Extra strong fibers

1.7.3 Nanotorus

A nanotorus is theoretically described as carbon nanotube bent into a torus (doughnut shape) [43]. Nanotori are predicted to have many unique properties, such as magnetic moments 1000 times larger than previously expected for certain specific radii, or may be used as a black body whose emissivity or absorbance is almost of 1.0. Its properties vary widely depending on radius of the torus and radius of the tube. It is expected that the nanotorus has also have unique mechanical properties. A nanotorus is shown in the following (Fig. 1.15)

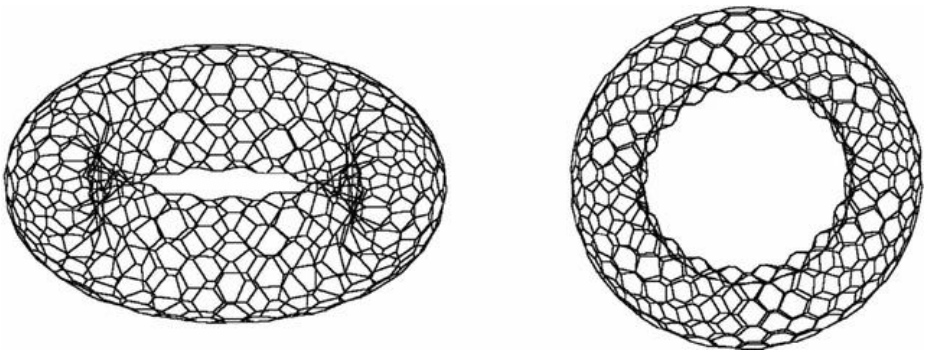

Figure 1.15: Nanotorus

1.7.4 Nanocones

Carbon nanocones are conical structures which are made predominantly from carbon and which have at least one dimension of the order one micrometer or smaller. Nanocones have height and base diameter of the same order of magnitude; this distinguishes them from tipped nanowires which are much longer than their diameter. Nanocones occur on the surface of natural graphite. Hollow carbon nanocones can also be produced by decomposing hydrocarbons with a plasma torch [18]. Electron microscopy reveals that the opening angle (apex) of the cones is not arbitrary, but has preferred values of approximately 20^o, 40^o, and 60^o.

A nanocone is shown in the following (Fig.1.16). Carbon nanocones are produced

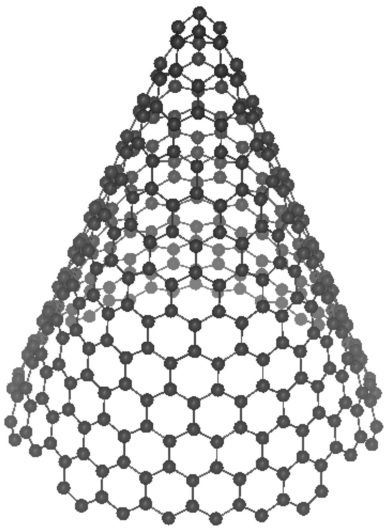

Figure 1.16: Nanocone .

in an industrial process that decomposes hydrocarbons into carbon and hydrogen with a plasma torch having a plasma temperature above 2000 ^{o}C.

1.7.5 Dendrimer

Dendrimers are repetitively branched molecules. The name comes from the Greek word $\delta\acute{\epsilon}\nu\delta\rho o\nu$ (dendron), which translates to tree. Synonymous terms for dendrimer include arborols and cascade molecules. However, dendrimer is currently internationally accepted term [2]. A dendrimer is typically symmetric around the core, and often adopts a spherical three-dimensional morphology. The word dendron is also encountered frequently. A dendron usually contains a single chemically addressable group called the focal point or core. The difference between dendrons and dendrimers is illustrated in the (Fig. 1.17), but the terms are typically encountered interchangeably.

Applications of dendrimers typically involve conjugating other chemical species to the dendrimer surface that can function as detecting agents (such as a dye

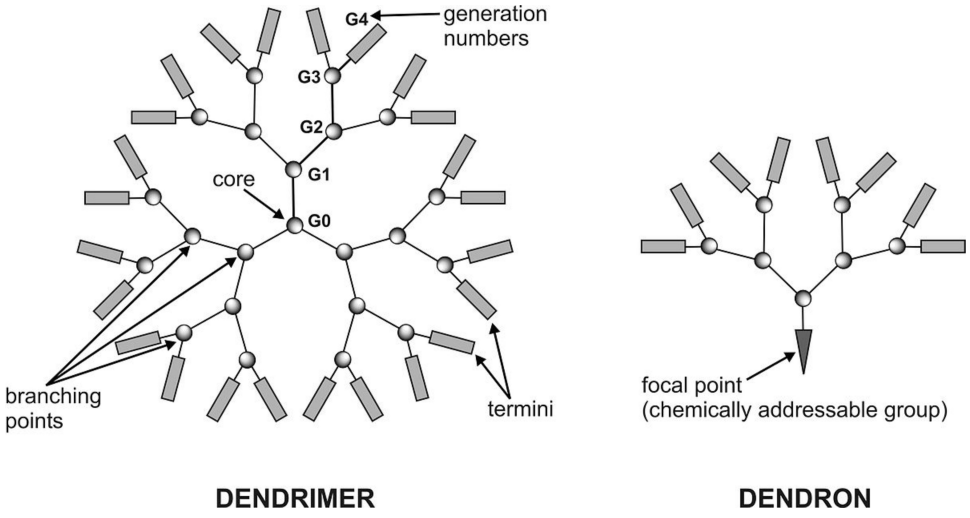

Figure 1.17: Dendrimer .

molecule), affinity ligands, targeting components, radioligands, imaging agents, or pharmaceutically active compounds. Dendrimers have very strong potential for these applications because their structure can lead to multivalent systems.

Chapter 2

Topological indices of molecular graphs

2.1 Introduction

In this chapter, we discuss the concept of topological indices and there types of indices that depend on different graph-theoretic parameters such as degree and distance. Moreover, we will also discuss some known results in the literature related to these topological indices.

2.2 Introduction to topological indices

In graph-theoretical terms, a *topological descriptor* is a single numeric number that represents a chemical structure. Topological descriptors are structural invariants that do not depende on the pictorial representation or the labeling of the graph. In the spit of loss of information by the projection in a single number of a structure, such descriptors found vast applications in the correlation and prediction of many molecular properties and also in test of association and isomorphisms. At the point when topological descriptor corresponds with a molecular property it can be named as *molecular index* or *topological index* (TI).

More than hundred of topological descriptors are proposed, such a large number of descriptors raises the question how to select the descriptor? So, following is the list of desirable attributes for a topological index.

- Explicit structural analysis
- A topological index has good correlation with at least one property
- Good discrimination of isomers
- They can be Locally described
- Generalizable to higher analogues
- Toplogical indices should be linearly independent
- Simplicity
- Not depend on physico-chemical properties
- Not trivially related to other indices
- Capability of construction
- Based on similar structural concepts
- Show a correct size-dependence
- Topological index should be gradualy change with gradual change in structures

2.3 Some major classes of topological indices

In literature, there are hundred of topological indices. It is very difficult to discuss all of them. We will classify them with respect to graph parameters such as degree and distance etc. Here, we define some degree based, distance based and counting related topological indices. The indices which are constructed by using the concept of valency or degree of the vertex in known as *degree based* indices. The

indices that are purely defined using the concept of distances in a graph are known as *distance based* indices. The indices that are based on counting polynomials are said to be *counting related* indices. In these classes, all types of indices can not be covered because there are some type of indices that are defined using both distance and degree of a graph, that is, degree distance index.

Here and on ward, G is considered to be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The distance between vertices u and v is denoted as $d_G(u, v)$ or simply $d(u, v)$ while $d(u)$ or d_u is the degree of a vertex $u \in V(G)$. We also define $\delta_G(u) = S_u = \sum_{v \in N_G(u)} d(v)$, where $N_G(u) = \{v \in V(G) \mid uv \in E(G)\}$.

2.4 Distance based topological indices

Distance based topological indices are defined on the ground of distance between two vertices in a connected graph. Some well known distance based topological indices are as follows:

- Wiener index
- Harary index
- Szeged index
- Balaban index, etc

2.4.1 Wiener Index

In 1947-48, Harold Wiener [51] proposed one of the first molecular descriptors of the topological nature of simple graph saturated hydrocarbons (alkanes). At that time Wiener called it the *path number*. He defined the path number as the sum of the number of bonds linking all pairs of atoms. Now a days, this molecular descriptor known as the *Wiener index*, and denoted by W. As the value of W is smaller the graph is more compact. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The Wiener index of graph G is defined as

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

where (u, v) be any ordered pair of vertices in G and $d(u, v)$ is the distance between vertices u and v.

It is difficult to compute all the distances in a graph having large number of edges and vertices, so researchers developed some special techniques to calculate these indices which reduced the computational complications of these indices.

Index W is important not just on the grounds that it was the first topological index to be invented, it is also important because it is easy to compute and it is entirely successful for some applications. Its fundamental disadvantage is its high degeneracy, that is, the way that numerous different graphs have the same W value.

2.4.2 Szeged Index

Szeged index was introduced by Gutman [24] and abrivated as Sz. It is a modified version of Wiener index for cycle molecules. It was named as Szeged index because it was conceived by Gutman at the Attila Jozsef University in Szeged.
Szeged index is more significant and power full than Wiener index in such a way that Wiener index only correlate the boiling point of branched alkanes, whereas the Szeged index associate the important physico-chemical property for both branched and cyclo-alkanes.

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. Consider two adjacent vertices u and v in G and let $e = uv$ be the edge between them. The set of all vertices of G lying closer to u than v is denoted by $B_u(e)$ and the set of all vertices lying closer to v then to u, is denoted by $B_v(e)$, that is

$$\begin{aligned} B_u(e) &= \{x \in V(G) \mid d(x, u) < d(x, v)\}, \\ B_v(e) &= \{x \in V(G) \mid d(x, v) < d(x, u)\}. \end{aligned}$$

Note that all the vertices which are at equidistant from u or v should be ignored. Now, define

$$n_u(e) = |B_u(e)| \text{ and } n_v(e) = |B_v(e)|.$$

The Szeged index can be defined as

$$Sz(G) = \sum_{e=uv \in E(G)} n_u(e) n_v(e).$$

2.4.3 Balaban index

The Balaban index was introduced about 30 years ago [7]. It is also called distance-connectivity index or average distance sum-connectivity index. It is a very particular molecular descriptor and molecule size or number of rings do not increase its value considerably. The *Balaban* index has very low degeneracy as compared to the Wiener index. This is also called J index. It is one of the most famous known graph invariant. It is a first index of a graph with very low degeneracy.

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The Balaban index is defined as follow:

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

where $\sigma_u = \sum_{w \in V(G)} d(u, w)$ and $\mu = m - n + 1$ is called the cyclomatic number of G where $m = |E(G)|$ and $n = |V(G)|$.

In the various studies of $QSAR$ and $QSPR$, *Balaban* index has been used frequently [4]. From the different kind of distance based topological indices, $Wiener$ index and *Balaban* index are two important indices.

2.5 Degree based topological indices

The degree based topological indices are based on the degree of the vertex. These type of indices are very important because of their applications in chemistry pharmaceutical and drug design. The degree based indices correlate many physico-chemical properties such as, strain energy, boiling point and resonance energy in more effective way with more foresight power. Now, we discuss some famous degree based topological indices which are as follows:

- Randić index
- Sum-connectivity index
- Zagreb index
- Atom-Bond Connectivity index
- Geometric-Arithmetic index, etc.

2.5.1 Randić index

In 1975, the chemist Milan Randić [39] proposed a topological index named as "branching index". It is suitable for calculating degree of the stretching of the carbon-atom skeleton of saturated of hydrocarbons. Later on, the branching index was renamed as "molecular connectivity index" and frequently referred as the Randić index.

For a graph G with vertex set $V(G)$ and edge set $E(G)$, the Randić index of G is defined as follows:

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

Here, d_u and d_v represent the degree of vertices u and v, respectively.

In 1998 Bollobás and Erdös [6] and Amic et al. [1] proposed general Randić index independently. Then it has been widely studied by both theoretical chemists and mathematicians [34].

For a graph G with vertex set $V(G)$ and edge set $E(G)$ the general randić index $R_\alpha(G)$ is the sum of $(d_u d_v)^\alpha$ over all edges $e = uv \in E(G)$ defined as

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

Randić index has a very good correlation with physico-chemical properties of alkanes: that is, enthalpies of formation, boiling point, chromatographic retention times, surface area, parameters in the Antoine equation for vapor pressure, etc [36].

In subsequent years, a large number of applications of Randić index are reported. Most of them related with the pharmacological and medicinal issues.

2.5.2 Zagreb index

More than 40 years ago, Gutman and Trinajstić [22] examined the dependence of total π-electron energy on molecular structure. They found that in the approximation for total π-electron energy the following two terms accour for a graph G with vertex set $V(G)$ and edge set $E(G)$

$$\begin{aligned} M_1 &= \sum_{u \in V(G)} (d_u)^2, \\ M_2 &= \sum_{uv \in E(G)} (d_u d_v). \end{aligned}$$

It was instantly perceived that M_1 and M_2 reflects the degree of stretching of molecular skeleton (and are thus responsible for the degree of π-electron energy with increasing branching). Later on, Gutman and Trinajstić [23] itself elaborated this point of view. Eventually, M_1 and M_2 were named the first Zagreb-Group index and second Zagreb-Group index, respectively. These names were later abbreviated into first Zagreb index and second Zagreb index [46].

Later on, after some more modifications made by Gutman and Trinajstić [33], the Zagreb index can be defined in such a way that for a graph G with vertex set $V(G)$ and edge set $E(G)$, the first Zagreb index is defined as:

$$M_1'(G) = \sum_{uv \in E(G)} (d_u + d_v).$$

The second Zagreb index is defined in same way as defined above. It is defined as the product of degree of end vertices of all edges of G, that is,

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

A lot of research has been done on these indices and their variants. In the field of theoretical chemistry, large number of paper has been published by the researchers of this interesting interdisciplinary area.

2.5.3 Atom-bond connectivity index

One of the famous connectivity topological index is atom-bond connectivity (ABC) index proposed by Estrada et al. [19]. Let G be a graph with vertex set

$V(G)$ and edge set $E(G)$, the ABC index is defined as follows:

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

ABC index is very efficient in correlating some important physico-chemical properties like strain energy as well as stability of both branched and cyclo-alkanes.

There are five versions of ABC index, which have been defined later on. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$ the generalized ABC index is defined as follows:

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

where $k \in \{1, 2, \cdots, 5\}$ and Q_u is the quantity which is uniquely related to the vertex u.

- When $k = 1$ then $Q_u = d_u$ and $Q_v = d_v$ where, d_u represents the degree of vertex u and d_v represents the degree of vertex v.

- When $k = 2$ then $Q_u = n_u$ where, n_u represents the number of vertices of G whose distances to vertex u are smaller than those to other vertex v of the edge $e = uv$.

- When $k = 3$ then $Q_u = m_u$ where, m_u represents the number of edges of G lying closer to vertex u than to v of the edge $e = uv$.

- When $k = 4$ then $Q_u = S_u$ where, $S_u = \sum_{v \in N_G(u)} d(v)$ and $N_G(u) = \{v \in V(G) \mid uv \in E(G)\}$.

- When $k = 5$ then $Q_u = ec(u)$ where, $ec(u) = \max_{v \in V(G)} d(u, v)$.

2.5.4 Geometric-arithmetic index

Now, we discuss another famous topological index, that is, *Geometric-Arithmetic* (GA) index which was introduced by Vukičević et al. [48]. Let G be a graph with

vertex set $V(G)$ and edge set $E(G)$. Then its GA index is defined as follows:

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

GA index is used to predict the bio-activity of chemical compounds. It is also important for physico-chemical properties such as entropy, enthalpy of vaporization, standard enthalpy of vaporization, enthalpy of formation, and a centric factor. GA index has more predictive power and somewhat better predictive power as compared to Randić index.

There are some versions of GA index which are defined consequently. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$, the generalized GA index is defined as follows:

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

where $k \in \{1, 2, \cdots, 5\}$ and Q_u is the quantity which is uniquely related to the vertex u.

- When $k = 1$ then $Q_u = d_u$ and $Q_v = d_v$ where, d_u represents the degree of vertex u and d_v represents the degree of vertex v.

- When $k = 2$ then $Q_u = n_u$ where, n_u represents the number of vertices of G whose distances to vertex u are smaller than those to other vertex v of the edge $e = uv$.

- When $k = 3$ then $Q_u = m_u$ where, m_u represents the number of edges of G lying closer to vertex u than to v of the edge $e = uv$.

- When $k = 4$ then $Q_u = ec(u)$ where, $ec(u) = \max\limits_{v \in V(G)} d(u, v)$.

- When $k = 5$ then $Q_u = S_u$ where, $S_u = \sum\limits_{v \in N_G(u)} d(v)$ and $N_G(u) = \{v \in V(G) \mid uv \in E(G)\}$.

2.6 Counting related polynomials and topological indices

2.6.1 Counting polynomials

Counting polynomials are those polynomials having at exponent the extent of a property partition and coefficients the multiplicity/occurrence of the corresponding partition. For a graph G, a counting polynomial is defined as:

$$P(G,x) = \sum_{k} m(G,k)x^k, \tag{2.1}$$

where the coefficients $m(G,k)$ can be calculated by various methods, techniques and algorithms. The expression (2.1) has been independently explained by Harary et al. [17]. The corresponding topological index of $P(G,x)$ is denoted by $P(G)$ and it is defined as follows:

$$P(G) = P'(G,x)|_{x=1} = \sum_{k} m(G,k) \times k,$$

where $P'(G,x)$ defined the first derivative of $P(G,x)$ with respect to x. A *moleculer/chemical graph* is a simple finite graph in which vertices denote the atoms and edges denote the chemical bonds in underlying chemical structure. A graph can be represented by a matrix, a sequence, a polynomial and by a numeric number (often called a topological index) which represents the whole graph and these representations are aimed to be uniquely defined for that graph.
Two edges $e = uv$ and $f = xy$ in $E(G)$ are said to be codistant, usually denoted by $e\ co\ f$, if

$$d(x,u) = d(y,v)$$

and

$$d(x,v) = d(y,u) = d(x,u) + 1 = d(y,v) + 1.$$

The relation "*co*" is reflexive as $e\ co\ e$ is true for all edges in G, also symmetric as if $e\ co\ f$ then $f\ co\ e$ for all $e, f \in E(G)$ but the relation "*co*" is not necessarily transitive [25]. Consider

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

If the relation is transitive on $C(e)$ also, then $C(e)$ is called an orthogonal cut. Let $e = uv$ and $f = xy$ be two edges of a graph G, which are opposite or topologically parallel, and this relation is denoted by $e\ op\ f$. A set of opposite edges, within the same face or ring, eventually forming a strip of adjacent faces/rings, is called an opposite edge strip *ops*, which is a quasi-orthogonal cut qoc (i.e. the transitivity relation is not necessarily obeyed). Note that "*co*" relation is defined in the whole graph while "*op*" is defined only in a face/ring. The length of *ops* is maximal irrespective of the string edge [25].

The following indices are examples of counting related topological indices.

- Omega polynomial / index
- Sadhana polynomial / index
- Padmakar-Ivan (PI) polynomial / index
- Non-Equidistance index, etc.

The construction is almost same for all indices which are mentioned above. All of them are defined on the base of counting the opposite edge strips ops defined above. We discuss two or three famous among them which are Omega, Sadhana and PI polynomials and their corresponding indices.

2.6.2 Omega index

Diudea [16] introduced the omega polynomial in 2006 on the ground of op strips. The Omega polynomial is proposed to describe cycle-containing molecular structures, particularly those associated with nanostructures. Let G be a graph. Then its Omega polynomial denoted by $\Omega(G, x)$ in x is defined as follows:

$$\Omega(G, x) = \sum_k m(G, k) \times x^k,$$

where $m(G, k)$ be the number of ops of length k.

The corresponding index of $\Omega(G,x)$ is Omega index $\Omega(G)$ and it is defined as follows:

$$\Omega(G) = \Omega'(G,x)|_{x=1} = \sum_k m(G,k) \times k.$$

Where $\Omega'(G,x)$ defined the first derivative of $\Omega(G,x)$ with respect to x.

2.6.3 Sadhana index

The Sadhana polynomial is based on counting opposite edge strips in any graph. This polynomial counts equidistant edges in a graph G [15]. Let G be a graph. Then Sadhana polynomial denoted by $Sd(G,x)$ is defined as follows:

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

where $m(G,k)$ be the number of ops of length k and $e = |E(G)|$ is the edge set cardinality of G.

The corresponding index of $Sd(G,x)$ id Sadhana index $Sd(G)$, and it is defined as follows:

$$Sd(G) = Sd'(G,x)|_{x=1} = \sum_k m(G,k) \times e - k.$$

Where $Sd'(G,x)$ defined the first derivative of $Sd(G,x)$ with respect to x.

2.6.4 PI index

The PI polynomial is also based on counting opposite edge strips in any graph. This polynomial counts non-equidistant edges in a graph G [15]. Let G be a graph. Then PI polynomial denoted by $PI(G,x)$ is defined as follows:

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

where $m(G,k)$ be the number of ops of length k and $e = |E(G)|$ is the edge set cardinality of G.

The corresponding index of $PI(G,x)$ is PI index $PI(G)$, and it is defined as follows:

$$PI(G) = PI'(G,x)|_{x=1} = \sum_k m(G,k) \times k \times e - k.$$

Where $PI'(G,x)$ defined the first derivative of $PI(G,x)$ with respect to x.

2.7 Application of topological indices

- Topological indices are numerical parameters of a graph which characterize its topology and are usually graph invariant.

- Topological indices are used in the development of quantitative structure-activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure.

- In the QSAR /QSPR study, physicochemical properties and topological indices such as Szeged index, Wiener index, Randić index, Zagreb index, ABC index are used to predict bioactivity of the chemical compounds.

- Topological indices correlates physico-chemical properties (Boiling point, stability, strain energy, entropy,enthalpy of vaporization, enthalpy of formation etc) of certain chemical compounds.

Topological indices play a vital role in QSAR /QSPR study. They correlate the certain physico-chemical properties of chemical compounds specially organic compounds. The chemical significance of some topological indices in mathematical chemistry is following.

- Randić index has been closely correlated with many chemical properties and found to parallel the boiling point and Kovats constants. In addition, the Randić index appears to predict the boiling points of alkanes more closely, and only it takes into account the bonding or adjacency degree among carbons in alkanes.

- Szeged index correlates the physico-chemical properties of both cyclic and branched alkanes.

- The atom-bond connectivity (ABC) index provides a good model for the stability of linear and branched alkanes as well as the strain energy of cycloalkanes.

- Wiener index is considered to represent a measure compactness of the molecules.

- Wiener index also show that the Wiener index number is closely correlated with the boiling points of alkane molecules. Later work on quantitative structureactivity relationships shows that it is also correlated with other quantities including the parameters of its critical point,the density, surface tension, and viscosity of its liquid phase,and the van der Waals surface area of the molecule.

- For certain physico-chemical properties, the predictive power of GA index is somewhat better than predictive power of the Randić connectivity index.

- The counting polynomials are useful in topological description of benzenoid structures as well as in counting some single number descriptors, also called topological indices. The qoc strips could account for the helicity of nanotubes and nanotori.

Chapter 3

Eccentricity based topological indices of a hetrofunctional dendrimerg

3.1 Introduction

Dendrimers, have attracted attention for their drug-delivery applications because of the ease of their synthesis, the ability to achieve well-defined shapes and sizes and their chemical diversity. Because of dendrimers' interior void space and surface functional groups, they are well-suited for use as carrier molecules in drug delivery. Topological indices are very helpful in drug designing and have very wide application. Now So, we consider a hetrofunctional dendrimer (HFD(ei)-G3-e-(allyl)_16-i-(hydroxyl)_28) and compute some eccentricity based topological indices. All the work in this chapter has been published in an international journal [21].

3.2 Eccentircity based Topological indices

These types of indices are based on the eccentricity of vertex u, where $u \in V(G)$.

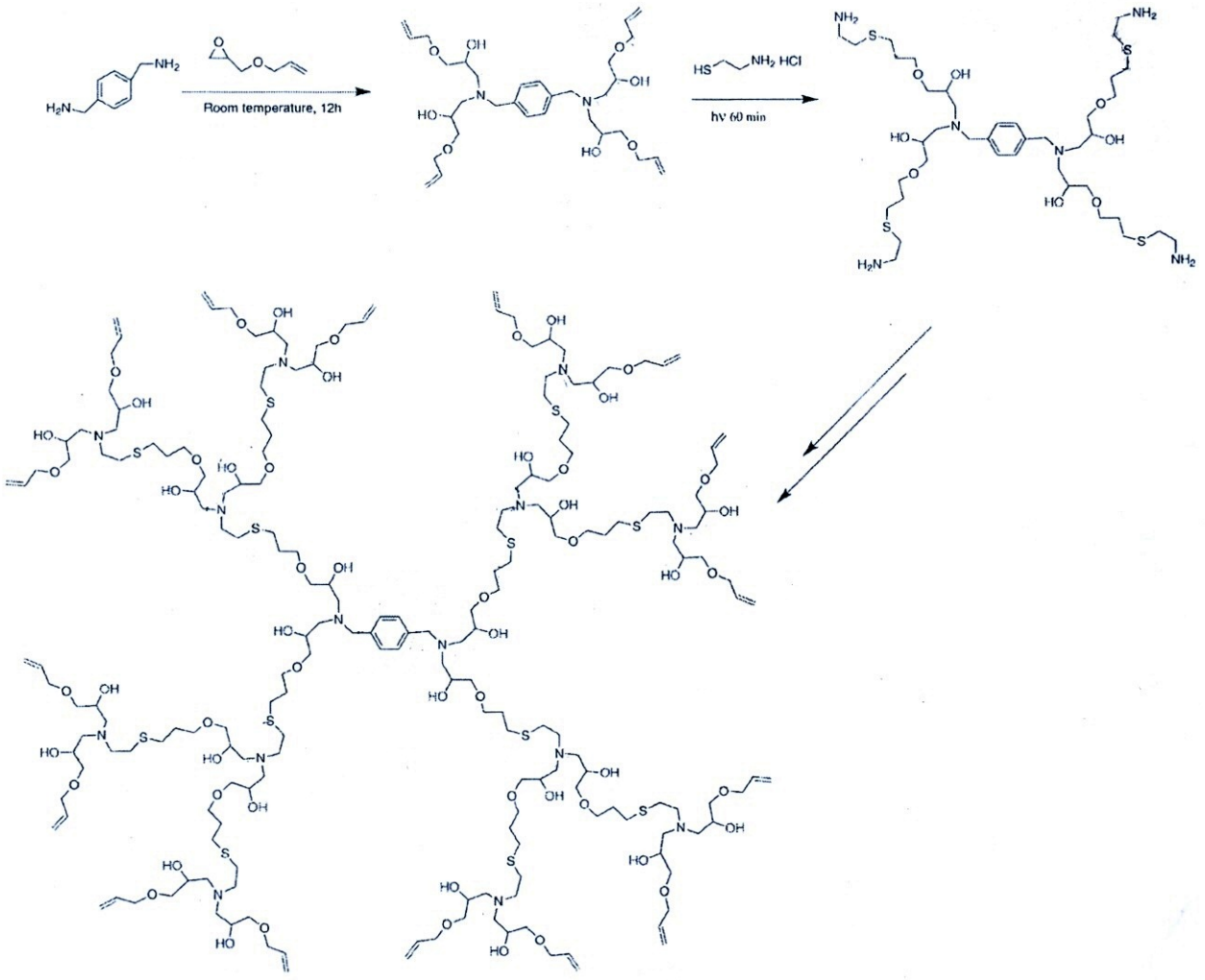

Figure 3.1: A dendrimer HFD(ei)-G3-e-(allyl)_16-i-(hydroxyl)_28 [50]

3.2.1 Eccentric connectivity index

Sharma et al. [45] introduced the eccentric connectivity index. Now a days it is used for mathematical modeling of biological activities of diverse nature.
Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. The eccentric connectivity index can be defined as

$$\xi(G) = \sum_{u \in V(G)} d(u)ec(u),$$

where $d(u)$ represent the degree of vertex u and $ec(u)$ represents the eccentricity of vertex u.

3.2.2 Eccentircity based Zagreb indices

Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajstic [26] as discussed in Chapter 2. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. Zagreb index are defined as:

$$\begin{aligned} M_1(G) &= \sum_{v \in V(G)} (d(v))^2, \\ M_2(G) &= \sum_{uv \in E(G)} d(u)d(v). \end{aligned}$$

Some new versions of Zagreb indices of a molecular graph G that are exprssed in terms of eccentricity are introduced by Ghorbani and Hosseinzadeh [27]. They are defined as follows

$$M_1^{**}(G) = \sum_{v \in V(G)} (ec(v))^2, \tag{3.1}$$

$$M_2^{*}(G) = \sum_{uv \in E(G)} ec(u)ec(v), \tag{3.2}$$

Where $ec(u)$ represents the eccentricity of a vertex $u \in V(G)$.

3.3 HFD(ei) dendrimer

HFD [50] are considered as state-of-art macromolecules having a large number of potential applications. With respect to positions of hetrofunctional group in HFD,

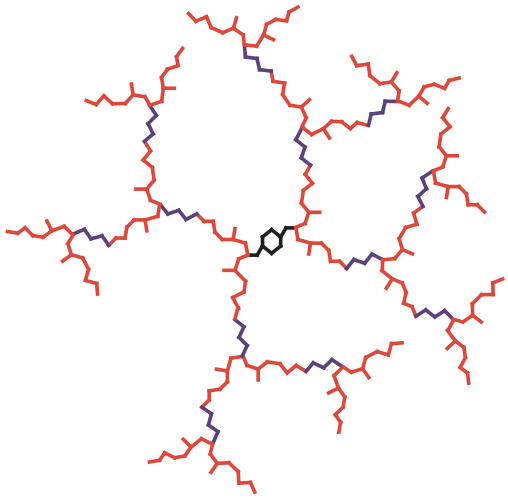

Figure 3.2: $D[n]$ with $n = 6$.

there are following three possibilities: external (e); internal (i); or combination of external and internal (ei). We select a HFD(ei)-G3-e(allyl)_16-i-(hydroxyl)_28 denoted by $D[n]$ and is shown in Fig. 3.2 which is an HFD with internal hydroxyl and peripheral allyl group. The graphs corresponding to different growth stages are shown in Fig. 3.3−3.4. It is evident that order and size of $D[n]$ are equal.

The order and size of $D[n]$ is given below:

$$\text{order of } D[n] = \text{size of } D[n] = \begin{cases} 16 \times 2^{t+1} + 8 \times 2^t - 38 & \text{if } n = 2t,\ t \geq 1 \\ 24 \times 2^{t+1} - 38 & \text{if } n = 2t+1,\ t \geq 0. \end{cases}$$

3.4 The eccentric connectivity index

This section is devoted to compute the eccentric connectivity index of the dendrimer $D[n]$ shown in Fig. 3.3−3.4.

Theorem 3.4.1. *The eccentric connectivity index of $D[n]$ for $n = 2t+1$ where $t \geq 0$ is given by*

$$\xi(D[n]) = 2112t \times 2^t - 936 \times 2^t - 836t + 1036.$$

Proof. Using the symmetry of the nanostar dendrimer $D[n]$, we use only one branch of $D[n]$ as labeled in Fig. 3.3−3.4. We take one representative from a set of vertices

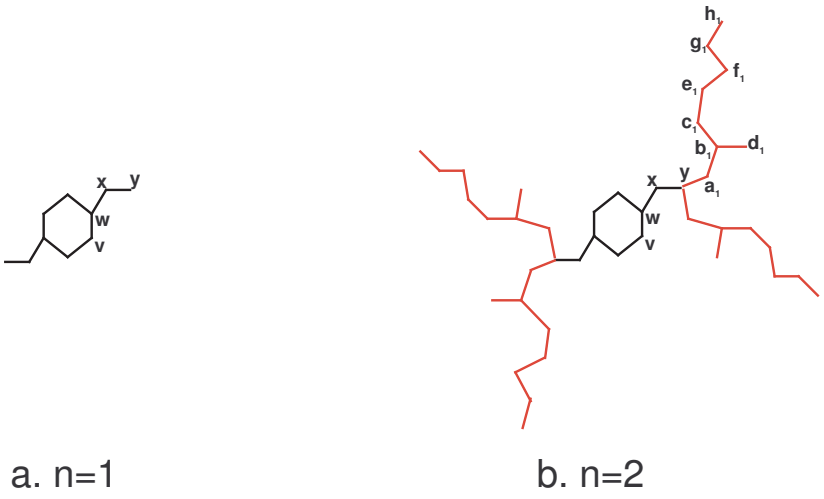

Figure 3.3: $D[n]$ with the core $n = 1$ and $n = 2$.

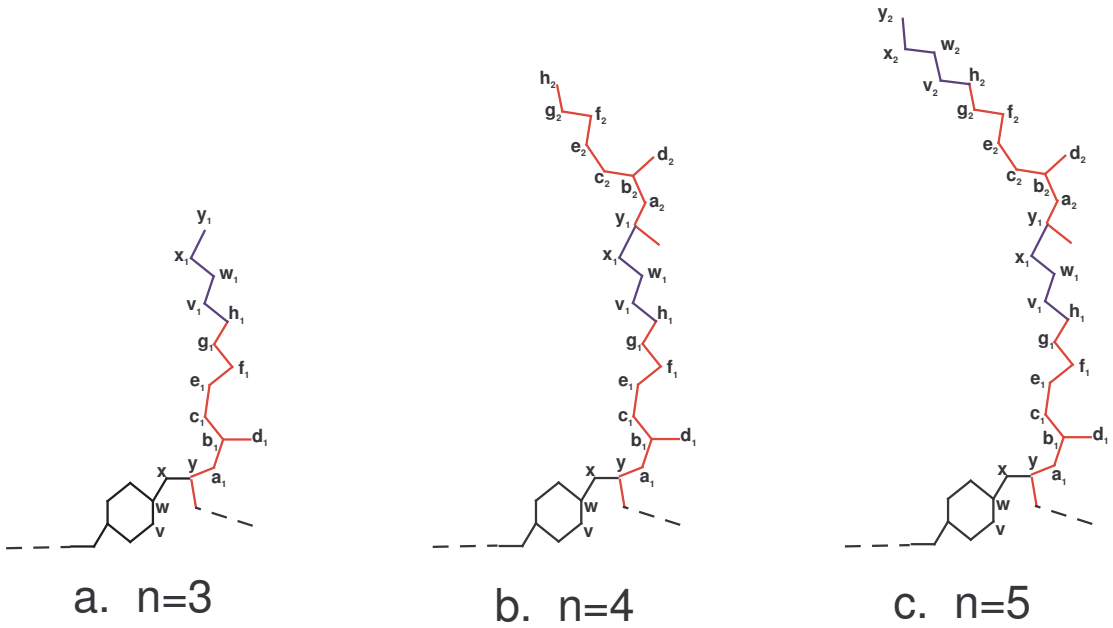

Figure 3.4: $D[n]$ with $n = 3, 4$ and 5.

which have same degree and eccentricity. These representatives are labeled by v, w, x, y, a_i, b_i, c_i, d_i, e_i, f_i, g_i, h_i, v_i, w_i, x_i, y_i. Here we have $1 \leq i \leq \frac{n-1}{2}$ when $n \geq 3$. The representatives of vertices of $D[n]$ with their degrees, eccentricities and frequencies of occurrence are given as follows.

Repersentative	Degree	Eccentricity	Frequency
v	2	$11t+4$	4
w	3	$11t+5$	2
x	2	$11t+6$	2
y $(n=1)$	1	7	2
y $(n \neq 1)$	3	$11t+7$	2

Table 3.1: The vertices introduced for the core (first generation) with their degree, eccentricity and frequency for $n \geq 1$, where n is odd.

Representative	Degree	Eccentricity	Frequency
a_i	2	$11t+11i-3$	2^{i+1}
b_i	3	$11t+11i-2$	2^{i+1}
c_i	2	$11t+11i-1$	2^{i+1}
d_i	1	$11t+11i-1$	2^{i+1}
e_i	2	$11t+11i$	2^{i+1}
f_i	2	$11t+11i+1$	2^{i+1}
g_i	2	$11t+11i+2$	2^{i+1}
h_i	2	$11t+11i+3$	2^{i+1}

Table 3.2: The vertices introduced at second generation with their degree, eccentricity and frequency for $n \geq 3$, where n is odd.

Representative	Degree	Eccentricity	Frequency
v_i	2	$11t + 11i + 4$	2^{i+1}
w_i	2	$11t + 11i + 5$	2^{i+1}
x_i	2	$11t + 11i + 6$	2^{i+1}
$y_i(i = t)$	1	$11t + 11i + 7$	2^{i+1}
$y_i(i \neq t)$	3	$11t + 11i + 7$	2^{i+1}

Table 3.3: The vertices introduced at third generation with their degree, eccentricity and frequency for $n \geq 3$, where n is odd.

When $n = 1$ then $t = 0$. Using Table 3.1, the eccentric connectivity index of $\xi(D[1])$ can be written as follows:

$$\begin{aligned}
\xi(D[1]) &= \sum_{u \in D[n]} d(u)ec(u) \\
&= (4 \times 2 \times 4) + (2 \times 3 \times 5) + (2 \times 2 \times 6) + (2 \times 1 \times 7) \\
&= 100 \\
&= 2112(0) \times 2^0 - 936 \times 2^0 - 836(0) + 1036.
\end{aligned}$$

When $n = 3$ then $t = 1$. Using Tables 3.1 and 3.2, the eccentric connectivity index of $D[3]$ can be written as follows:

$$\begin{aligned}
\xi(D[3]) &= \sum_{u \in D[n]} d(u)ec(u) \\
&= \Big((4 \times 2 \times 15) + (2 \times 3 \times 16) + (2 \times 2 \times 17) + (2 \times 3 \times 18)\Big) \\
&\quad + \Big((4 \times 2 \times 19) + (4 \times 3 \times 20) + (4 \times 2 \times 21) + (4 \times 1 \times 21) \\
&\quad + (4 \times 2 \times 22) + (4 \times 2 \times 23) + (4 \times 2 \times 24) + (4 \times 2 \times 25)\Big) \\
&\quad + \Big((4 \times 2 \times 26) + (4 \times 2 \times 27) + (4 \times 2 \times 28) + (4 \times 1 \times 29)\Big) \\
&= 2552 \\
&= 2112(1) \times 2^1 - 936 \times 2^1 - 836(1) + 1036.
\end{aligned}$$

When $n \geq 5$, then using Tables 3.1−3.3, the eccentric connectivity index is obtained as follows:

$$\begin{aligned}
\xi(D[n]) &= \sum_{u \in D[n]} d(u)ec(u) \\
&= \Big((2\times 4)\times(11t+4)+(3\times 2)\times(11t+5)+(2\times 2)\times(11t+6) \\
&\quad +(3\times 2)\times(11t+7)\Big)+\Bigg(\sum_{i=1}^{t}\Big(2\times 2^{i+1}\times(11t+11i-3) \\
&\quad +3\times 2^{i+1}\times(11t+11i-2)+2\times 2^{i+1}\times(11t+11i-1) \\
&\quad +2^{i+1}\times(11t+11i-1)+2\times 2^{i+1}\times(11t+11i) \\
&\quad +2\times 2^{i+1}\times(11t+11i+1)+2\times 2^{i+1}\times(11t+11i+2) \\
&\quad +2\times 2^{i+1}\times(11t+11i+3)\Big)\Bigg)+\Bigg(\sum_{i=1}^{t}\Big(2\times 2^{i+1}\times(11t+11i+4) \\
&\quad +2\times 2^{i+1}\times(11t+11i+5)+2\times 2^{i+1}\times(11t+11i+6)\Big) \\
&\quad +\sum_{i=1}^{t-1}\Big(3\times 2^{i+1}\times(11t+11i+7)\Big)+\Big(1\times 2^{t+1}\times(22t+7)\Big)\Bigg) \\
&= 2112t\times 2^{t}-936\times 2^{t}-836t+1036.
\end{aligned}$$

The proof is complete. □

Theorem 3.4.2. *The eccentric connectivity index of $D[n]$, for $n = 2t$, where $t \geq 1$ is given by*

$$\xi(D[n]) = 1760t\times 2^{t}-1336\times 2^{t}-836\times t+1340.$$

Proof. Using the symmetry of the nanostar dendrimer $D[n]$, we use only one branch of $D[n]$ as labeled in Fig. 3.3−3.4. We take one representative from a set of vertices which have same degree and eccentricity. These representatives are labeled by v, w, x, y, a_i, b_i, c_i, d_i, e_i, f_i, g_i, h_i. Here, we have $1 \leq i \leq \frac{n}{2}$.

Representative	Degree	Eccentricity	Frequency
v	2	$11t$	4
w	3	$11t+1$	2
x	2	$11t+2$	2
y	3	$11t+3$	2

Table 3.4: The vertices introduced for the core (first generation) with their degree, eccentricity and frequency for $n \geq 2$, where n is even.

Representative	Degree	Eccentricity	Frequency
a_i	2	$11t+11i-7$	2^{i+1}
b_i	3	$11t+11i-6$	2^{i+1}
c_i	2	$11t+11i-5$	2^{i+1}
d_i	1	$11t+11i-5$	2^{i+1}
e_i	2	$11t+11i-4$	2^{i+1}
f_i	2	$11t+11i-3$	2^{i+1}
g_i	2	$11t+11i-2$	2^{i+1}
$h_i(i=t)$	1	$11t+11i-1$	2^{i+1}
$h_i(i\neq t)$	2	$11t+11i-1$	2^{i+1}

Table 3.5: The vertices introduced at second generation with their degree, eccentricity and frequency for $n \geq 2$, where n is even.

When $n = 2$ then $t = 1$. Using Table 3.4, we get

$$\begin{aligned}
\xi(D[2]) &= \sum_{u\in V(D[n])} d(u)ec(u) \\
&= \Big((4\times 2\times 11)+(2\times 3\times 12)+(2\times 2\times 13)+(2\times 3\times 14)\Big) \\
&\quad +\Big((4\times 2\times 15)+(4\times 3\times 16)+(4\times 2\times 17)+(4\times 1\times 17) \\
&\quad +(4\times 2\times 18)+(4\times 2\times 19)+(4\times 2\times 20)+(4\times 1\times 21)\Big) \\
&= 1352 \\
&= 1760(1)\times 2^1 - 1336\times 2^1 - 836\times 1 + 1340.
\end{aligned}$$

Now we take the representative from a set of vertices which are introduce at $n = 3$ and have same degree and eccentricity also. These representatives are labeled v_i,w_i,x_i,y_i. Here $1 \leq i \leq t-1$ and $t = \frac{n}{2}$.

Representative	Degree	Eccentricity	Frequency
v_i	2	$11t + 11i$	2^{i+1}
w_i	2	$11t + 11i + 1$	2^{i+1}
x_i	2	$11t + 11i + 2$	2^{i+1}
y_i	3	$11t + 11i + 3$	2^{i+1}

Table 3.6: The vertices introduced at third generation with their degree, eccentricity and frequency for $n \geq 4$, where n is even.

When $n \geq 4$, then using Tables 3.4–3.6, the eccentric connectivity index of $D[n]$ can be written as follows.

$$\begin{aligned}
\xi(D[n]) &= \sum_{u \in D[n]} d(u)ec(u) \\
&= \Big(2 \times 4 \times 11t + (3 \times 2) \times (11t + 1) + (2 \times 2) \times (11t + 2) + (3 \times 2) \\
&\quad \times (11t + 3)\Big) + \Bigg(\sum_{i=1}^{t} \Big(2 \times 2^{i+1} \times (11t + 11i - 7) + 3 \times 2^{i+1} \times (11t + 11i - 6) \\
&\quad + 2 \times 2^{i+1} \times (11t + 11i - 5) + 1 \times 2^{i+1} \times (11t + 11i - 5) + 2 \times 2^{i+1} \\
&\quad \times (11t + 11i - 4) + 2 \times 2^{i+1} \times (11t + 11i - 3) + 2 \times 2^{i+1} \times (11t + 11i - 2)\Big) \\
&\quad + \sum_{t=1}^{t-1} \Big(2 \times 2^{i+1} \times (11t + 11i - 1)\Big) + \big(1 \times 2^{t+1} \times (22t - 1)\big)\Bigg) \\
&\quad + \Bigg(\sum_{i=1}^{t-1} \Big(2 \times 2^{i+1} \times (11t + 11i) + 2 \times 2^{i+1} \times (11t + 11i + 1) \\
&\quad + 2 \times 2^{i+1} \times (11t + 11i + 2) + 3 \times 2^{i+1} \times (11t + 11i + 3)\Big)\Bigg) \\
&= 1760t \times 2^t - 1336 \times 2^t - 836 \times t + 1340.
\end{aligned}$$

The proof is complete. □

3.5 Eccentricity based Zagreb indices

This section deals with some eccentricity based Zagreb indices defined in equations (3.1) and (3.2).

Theorem 3.5.1. *The second Zagreb eccentricity index M_1^* of $D[n]$, for $n = 2t+1$, where $t \geq 0$ is given by*

$$M_1^*(D[n]) = 23232t^2 \times 2^t - 19536t \times 2^t - 4598t^2 + 16196 \times 2^t + 10912t - 15912.$$

Proof. When $n = 1$ then $t = 0$. We use Table 3.1 to get

$$\begin{aligned} M_1^*(D[1]) &= \sum_{v \in V(D[1])} (ec(v))^2 \\ &= 4 \times (4)^2 + 2 \times (5)^2 + 2 \times (6)^2 + 2 \times (7)^2 \\ &= 284 \\ &= 23232(0^2) \times 2^0 - 19536(0) \times 2^0 - 4598(0^2) + 16196 \times 2^0 \\ &\quad +10912(0) - 15912. \end{aligned}$$

When $n = 3$ then $t = 1$. We use Table 3.1 and Table 3.2 to get

$$\begin{aligned} M_1^*(D[3]) &= \sum_{v \in V(D[3])} (ec(v))^2 \\ &= \Big(4 \times (15)^2 + 2 \times (16)^2 + 2 \times (17)^2 + 2 \times (18)^2\Big) + \Big(4 \times (19)^2 \\ &\quad +4 \times (20)^2 + 4 \times (21)^2 + 4 \times (21)^2 + 4 \times (22)^2 + 4 \times (23)^2 + 4 \times (24)^2 \\ &\quad +4 \times (25)^2\Big) + \Big(4 \times (26)^2 + 4 \times (27)^2 + 4 \times (28)^2 + 4 \times (29)^2\Big) \\ &= 30186 \\ &= 23232(1^2) \times 2^1 - 19536(1) \times 2^1 - 4598(1^2) + 16196 \times 2^1 + 10912(1) \\ &\quad -15912. \end{aligned}$$

When $n \geq 5$, then we use Tables 3.1−3.3 to get

$$\begin{aligned}
M_1^*(D[n]) &= \sum_{v \in V(D[n])} (ec(v))^2 \\
&= \Big(4 \times (11t+4)^2 + 2 \times (11t+5)^2 + 2 \times (11t+6)^2 + 2 \times (11t+7)^2\Big) \\
&\quad + \Bigg(\sum_{i=1}^{t} \Big(2^{i+1} \times (11t+11i-3)^2 + 2^{i+1} \times (11t+11i-2)^2 \\
&\quad + 2^{i+1} \times (11t+11i-1)^2 + 2^{i+1} \times (11t+11i-1)^2 + 2^{i+1} \times (11t+11i)^2 \\
&\quad + 2^{i+1} \times (11t+11i+1)^2 + 2^{i+1} \times (11t+11i+2)^2 \\
&\quad + 2^{i+1} \times (11t+11i+3)^2\Big)\Bigg) + \Bigg(\sum_{i=1}^{t} \Big(2^{i+1} \times (11t+11i+4)^2 \\
&\quad + 2^{i+1} \times (11t+11i+5)^2 + 2^{i+1} \times (11t+11i+6)^2\Big) \\
&\quad + \sum_{i=1}^{t-1} \Big(2^{i+1} \times (11t+11i+7)^2\Big) + \Big(2^{t+1} \times (22t+7)^2\Big)\Bigg) \\
&= 23232t^2 \times 2^t - 19536t \times 2^t - 4598t^2 + 16196 \times 2^t + 10912t - 15912.
\end{aligned}$$

The proof is complete. □

Theorem 3.5.2. *The second Zagreb-eccentricity index M_1^* of $D[n]$, for $n = 2t$, where $t \geq 1$ is given by*

$$M_1^*(D[n]) = 19360t^2 \times 2^t - 28512t \times 2^t - 4598t^2 + 20488 \times 2^t + 14256t - 20488. \quad (3.3)$$

Proof. When $n = 2$ then $t = 1$. Using Table 3.4, we get

$$\begin{aligned}
M_1^*(D[2]) &= \sum_{v \in V} [ec(v)]^2 \\
&= \Big(4 \times (11)^2 + 2 \times (12)^2 + 2 \times (13)^2 + 2 \times (14)^2\Big) + \Big(4 \times (15)^2 + 4 \times (16)^2 \\
&\quad + 4 \times (17)^2 + 4 \times (17)^2 + 4 \times (18)^2 + 4 \times (19)^2 + 4 \times (20)^2 + 4 \times (21)^2\Big) \\
&= 11824 \\
&= 19360(1^2) \times 2^1 - 28512(1) \times 2^1 - 4598(1^2) + 20488 \times 2^1 + 14256(1) - 20488.
\end{aligned}$$

When $n \geq 4$, the using Tables 3.4−3.6, we get

$$\begin{aligned}
M_1^*(D[n]) &= \sum_{v \in V(D[n])} (ec(v))^2 \\
&= \Big(4 \times (11t)^2 + 2 \times (11t+1)^2 + 2 \times (11t+2)^2 + 2 \times (11t+3)^2\Big) + \\
&\quad \Bigg(\sum_{i=1}^{t} \Big(2^{i+1} \times (11t+11i-7)^2 + 2^{i+1} \times (11t+11i-6)^2 + \\
&\quad 2^{i+1} \times (11t+11i-5)^2 + 2^{i+1} \times (11t+11i-5)^2 + \\
&\quad 2^{i+1} \times (11t+11i-4)^2 + 2^{i+1} \times (11t+11i-3)^2 + \\
&\quad 2^{i+1} \times (11t+11i-2)^2\Big) + \sum_{i=1}^{t-1} \Big(2^{i+1} \times (11t+11i-1)^2\Big) \\
&\quad + \big(1 \times 2^{t+1} \times (22t-1)^2\big)\Bigg) + \Bigg(\sum_{i=1}^{t-1} \Big(2^{i+1} \times (11t+11i)^2 + \\
&\quad 2^{i+1} \times (11t+11i+1)^2 + 2^{i+1} \times (11t+11i+2)^2 + \\
&\quad 2^{i+1} \times (11t+11i+3)^2\Big)\Bigg) \\
&= 19360t^2 \times 2^t - 28512t \times 2^t - 4598t^2 + 20488 \times 2^t + 14256t - 20488.
\end{aligned}$$

The proof is complete. □

Theorem 3.5.3. *The third Zagreb eccentricity index $M_2^*(D[n]$ of $D[n]$ for $n = 2t+1$, is given by*

$$M_2^*(D[n]) = \begin{cases} 256 & \text{if } t = 0, \\ 23232t^2 \times 2^t - 20592t \times 2^t - 4598t^2 & \\ +16640 \times 2^t + 11396t - 16384. & \text{if } t \geq 1. \end{cases}$$

Proof. Using the symmetry of the nanostar dendrimer $D[n]$, we use only one branch of $D[n]$ as labeled in Fig. 6-10. We take one representative from a set of vertices which have same degree and eccentricity. These representatives are labeled by u, v, w, x, y, a_i, b_i, c_i, d_i, e_i, f_i, g_i, h_i.

When $n = 1$ then $t = 0$. We use Table 3.1 to compute M_2^* as follows:

$$\begin{aligned} M_2^*(D[1]) &= \sum_{uv \in E} ec(u)ec(v) \\ &= 2 \times (4 \times 4) + 4 \times (4 \times 5) + 2 \times (5 \times 6) + 2 \times (6 \times 7) \\ &= 256. \end{aligned}$$

When $n = 3$, we have $t = 1$, Using Table 3.1 and Table 3.2, we compute M_2^* as follows:

$$\begin{aligned} M_2^*(D[3]) &= \sum_{uv \in E} ec(u)ec(v) \\ &= \Big(2 \times (15 \times 15) + 4 \times (15 \times 16) + 2 \times (16 \times 17) + 2 \times (7 \times 18)\Big) \\ &\quad + \Big(4 \times (18 \times 19) + 4 \times (19 \times 20) + 4 \times (20 \times 21) + 4 \times (20 \times 21) \\ &\quad + 4 \times (21 \times 22) + 4 \times (22 \times 23) + 4 \times (23 \times 24) + 4 \times (24 \times 25)\Big) \\ &\quad + \Big(4 \times (25 \times 26) + 4 \times (26 \times 27) + 4 \times (28 \times 29)\Big) \\ &= 28974. \end{aligned}$$

When $n \geq 5$, we use Tables 3.1−3.3 to compute M_2^* as follows:

$$\begin{aligned} M_2^*(D[n]) &= \sum_{uv \in E} ec(u)ec(v) \\ &= 2 \times (11t + 4) \times (11t + 4) + 4 \times (11t + 4) \times (11t + 5) + \\ &\quad 2 \times (11t + 5) \times (11t + 6) + 2 \times (11t + 6) \times (11t + 7) \\ &\quad + 4 \times (11t + 7) \times (11t + 8) + 2^2 \times (11t + 8) \times (11t + 9) + \\ &\quad 2^3 \times (11t + 9) \times (11t + 10) + 2^2 \times (11t + 10) \times (11t + 11) + \\ &\quad 2^2 \times (11t + 11) \times (11t + 12) + 2^2 \times (11t + 12) \times (11t + 13) \\ &\quad + 2^2 \times (11t + 13) \times (11t + 14) + 2^2 \times (11t + 14) \times (11t + 15) + \\ &\quad 2^2 \times (11t + 15) \times (11t + 16) + 2^2 \times (11t + 16) \times (11t + 17) + \\ &\quad 2^2 \times (11t + 17) \times (11t + 18) + \\ &\quad \sum_{i=1}^{t-1} \Big(2^{i+2} \times (11t + 11i + 7) \times (11t + 11(i + 1) - 3) + \\ &\quad 2^{i+2} \times (11t + 11(i + 1) - 3) \times (11t + 11(i + 1) - 2) + \end{aligned}$$

$$
\begin{aligned}
& 2^{i+3} \times (11t + 11(i+1) - 2) \times (11t + 11 \times (i+1) - 1) + \\
& 2^{i+2} \times (11t + 11(i+1) - 1) \times (11t + 11(i+1)) + \\
& 2^{i+2} \times (11t + 11(i+1)) \times (11t + 11(i+1) + 1) + \\
& 2^{i+2} \times (11t + 11(i+1) + 1) \times (11t + 11(i+1) + 2) + \\
& 2^{i+2} \times (11t + 11(i+1) + 2)(11t + 11(i+1) + 3) + \\
& 2^{i+2} \times (11t + 11(i+1) + 3) \times (11t + 11(i+1) + 4) + \\
& 2^{i+2} \times (11t + 11(i+1) + 4) \times (11t + 11(i+1) + 5) + \\
& 2^{i+2} \times (11t + 11(i+1) + 5) \times (11t + 11(i+1) + 6) + \\
& 2^{i+2} \times (11t + 11(i+1) + 6) \times (11t + 11(i+1) + 7)\Big) \\
= \; & 23232t^2 \times 2^t - 20592t \times 2^t - 4598t^2 + 16640 \times 2^t + 11396t - 16384.
\end{aligned}
$$

This completes the proof. □

Theorem 3.5.4. *The third Zagreb eccentricity index of $D[n]$ for $n = 2t$ where $t \geq 1$ is given by*

$$
M_2^*(D[n]) = \begin{cases} 11214 & \text{if } n = 2, \\ 19360t^2 \times 2^t - 29392t \times 2^t - 4598t^2 + 21136 \times 2^t & \\ +14740t - 21136. & \text{if } n > 2. \end{cases}
$$

Proof. When $n = 2$ then $t = 1$. We have

$$
\begin{aligned}
M_2^*(D[2]) &= \sum_{uv \in E(D[2])} ec(u)ec(v) \\
&= 2 \times (11 \times 11) + 4 \times (11 \times 12) + 2 \times (12 \times 13) + 2 \times (13 \times 14) \\
&\quad +4 \times (14 \times 15) + 4 \times (15 \times 16) + 8 \times (17 \times 18) + 4 \times (17 \times 18) \\
&\quad +4 \times (18 \times 19) + 4 \times (19 \times 20) + 4 \times (20 \times 21) \\
&= 11214.
\end{aligned}
$$

When $n \geq 4$ then using Tables 3.4−3.6, we have

$$\begin{aligned}
M_2^*(D[n]) &= \sum_{uv \in E(D[n])} ec(u)ec(v) \\
&= 2 \times (11t) \times (11t) + 4 \times (11t) \times (11t+1) + 2 \times (11t+1) \times (11t+2) \\
&\quad +2 \times (11t+2) \times (11t+3) + 4 \times (11t+3) \times (11t+4) \\
&\quad + \sum_{i=1}^{t-1} \Big(2^{i+1} \times (11t+11i-7) \times (11t+11i-6) \\
&\quad +2^{i+2} \times (11t+11i-6) \times (11t+11i-5) + 2^{i+1} \times (11t+11i-5) \\
&\quad \times (11t+11i-4) + 2^{i+1} \times (11t+11i-4) \times (11t+11i-3) \\
&\quad +2^{i+1} \times (11t+11i-3) \times (11t+11i-2) \\
&\quad +2^{i+1} \times (11t+11i-2) \times (11t+11i-1) + 2^{i+1} \times (11t+11i-1) \\
&\quad \times (11t+11i) + 2^{i+1} \times (11t+11i) \times (11t+11i+1) \\
&\quad +2^{i+1} \times (11t+11i+1) \times (11t+11i+2) + 2^{i+1} \times (11t+11i+2) \\
&\quad \times (11t+11i+3) + 2^{i+2} \times (11t+11i+3) \times (11t+11(i+1)-7) \Big) \\
&\quad +2^{t+1} \times (11t+11t-7) \times (11t+11t-6) + 2^{t+2} \times (11t+11t-6) \\
&\quad \times (11t+11t-5) + 2^{t+1} \times (11t+11t-5) \times (11t+11t-4) \\
&\quad +2^{t+1} \times (11t+11t-4) \times (11t+11t-3) + 2^{t+1} \times (11t+11t-3) \\
&\quad \times (11t+11t-2) + 2^{t+1} \times (11t+11t-2) \times (11t+11t-1) \\
&= 19360t^2 \times 2^t - 29392t \times 2^t - 4598t^2 + 21136 \times 2^t + 14740t - 21136.
\end{aligned}$$

This completes the proof. □

Representative	Eccentricity	Frequency
$[u, v]$	$[11t + 4, 11t + 4]$	2
$[v, w]$	$[11t + 4, 11t + 5]$	2^2
$[w, x]$	$[11t + 5, 11t + 6]$	2
$[x, y]$	$[11t + 6, 11t + 7]$	2
$[y, a_1]$	$[11t + 7, 11t + 8]$	2^2
$[a_1, b_1]$	$[11t + 8, 11t + 9]$	2^2
$[b_1, c_1]$	$[11t + 9, 11t + 10]$	2^3
$[c_1, e_1]$	$[11t + 10, 11t + 11]$	2^2
$[e_1, f_1]$	$[11t + 11, 11t + 12]$	2^2
$[f_1, g_1]$	$[11t + 12, 11t + 13]$	2^2
$[g_1, h_1]$	$[11t + 13, 11t + 14]$	2^2
$[h_1, v_1]$	$[11t + 14, 11t + 15]$	2^2
$[v_1, w_1]$	$[11t + 15, 11t + 16]$	2^2
$[w_1, x_1]$	$[11t + 16, 11t + 17]$	2^2
$[x_1, y_1]$	$[11t + 17, 11t + 18]$	2^2
$[y_i, a_{i+1}]$	$[11t + 11i + 7, 11t + 11(i + 1) - 3]$	2^{i+2}
$[a_{i+1}, b_{i+1}]$	$[11t + 11(i + 1) - 3, 11t + 11(i + 1) - 2]$	2^{i+2}
$[b_{i+1}, c_{i+1}]$	$[11t + 11(i + 1) - 2, 11t + 11(i + 1) - 1]$	2^{i+3}
$[c_{i+1}, e_{i+1}]$	$[11t + 11(i + 1) - 1, 11t + 11(i + 1)]$	2^{i+2}
$[e_{i+1}, f_{i+1}]$	$[11t + 11(i + 1), 11t + 11(i + 1) + 1]$	2^{i+2}
$[f_{i+1}, g_{i+1}]$	$[11t + 11(i + 1) + 1, 11t + 11(i + 1) + 2]$	2^{i+2}
$[g_{i+1}, h_{i+1}]$	$[11t + 11(i + 1) + 2, 11t + 11(i + 1) + 3]$	2^{i+2}
$[h_{i+1}, v_{i+1}]$	$[11t + 11(i + 1) + 3, 11t + 11(i + 1) + 4]$	2^{i+2}
$[v_{i+1}, w_{i+1}]$	$[11t + 11(i + 1) + 4, 11t + 11(i + 1) + 5]$	2^{i+2}
$[w_{i+1}, x_{i+1}]$	$[11t + 11(i + 1) + 5, 11t + 11(i + 1) + 6]$	2^{i+2}
$[x_{i+1}, y_{i+1}]$	$[11t + 11(i + 1) + 6, 11t + 11(i + 1) + 7]$	2^{i+2}

Table 3.7: The edge partition of $D[n]$, with respect to the representatives of pair of end-vertices and their frequency of occurrence. The eccentricities are taken from Table 3.1, Table 3.2 and Table 3.3, Here n is odd, $t = \frac{n-1}{2}$, $1 \leq i \leq t - 1$

Representative	Eccentricity	Frequency
$[u, v]$	$[11t, 11t]$	2
$[v, w]$	$[11t, 11t + 1]$	2^2
$[w, x]$	$[11t + 1, 11t + 2]$	2
$[x, y]$	$[11t + 2, 11t + 3]$	2
$[y, a_1]$	$[11t + 3, 11t + 4]$	2^2
$[a_i, b_i]$	$[11t + 11i - 7, 11t + 11i - 6]$	2^{i+1}
$[b_i, c_i]$	$[11t + 11i - 6, 11t + 11i - 5]$	2^{i+2}
$[c_i, e_i]$	$[11t + 11i - 5, 11t + 11i - 4]$	2^{i+1}
$[e_i, f_i]$	$[11t + 11i - 4, 11t + 11i - 3]$	2^{i+1}
$[f_i, g_i]$	$[11t + 11i - 3, 11t + 11i - 2]$	2^{i+1}
$[g_i, h_i]$	$[11t + 11i - 2, 11t + 11i - 1]$	2^{i+1}
$[h_i, v_i]$	$[11t + 11i - 1, 11t + 11i]$	2^{i+1}
$[v_i, w_i]$	$[11t + 11i, 11t + 11i + 1]$	2^{i+1}
$[w_i, x_i]$	$[11t + 11i + 1, 11t + 11i + 2]$	2^{i+1}
$[x_i, y_i]$	$[11t + 11i + 2, 11t + 11i + 3]$	2^{i+1}
$[y_i, a_{i+1}]$	$[11t + 11i + 3, 11t + 11(i + 1) - 7]$	2^{i+2}
$[a_t, b_t]$	$[22t - 7, 22t - 6]$	2^{t+1}
$[b_t, c_t]$	$[22t - 6, 22t - 5]$	2^{t+2}
$[c_t, e_t]$	$[22t - 5, 22t - 4]$	2^{t+1}
$[e_t, f_t]$	$[22t - 4, 22t - 3]$	2^{t+1}
$[f_t, g_t]$	$[22t - 3, 22t - 2]$	2^{t+1}
$[g_t, h_t]$	$[22t - 2, 22t - 1]$	2^{t+1}

Table 3.8: The edge partition of $D[n]$ with respect to the representatives of pair of end-vertices and their frequency of occurrence. The eccentricities are taken from Table 3.4, Table 3.5 and Table 3.6. Here n is even, $t = \frac{n}{2}$, $1 \leq i \leq t - 1$

Chapter 4

Degree-based topological indices of a hetrofunctional dendrimer

4.1 Introduction

In this chapter, we compute the nullity and number of Kekulé structures in a class of hetrofunctional dendrimer (HFD)ei (Fig. 3.2). When there is no Kekulé structure, we find the size of a maximum matching in this dendrimer. Furthermore, we compute the first and fifth version of geometric-arithmetic index and Randić index of this dendrimer. All these work has been submitted in a international journal for publish [38].

4.2 Basic definition

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. A subset $M \subseteq E(G)$ is called a matching if no two edges in M share an end-vertex. A vertex $v \in V(G)$ is said to be M-saturated if v is incident with an edge in M. Otherwise, v is said to be M-unsaturated. The matching M is called perfect if it saturates all the vertices of G. A path in G is said to be M-alternating if its edges alternately lie in M and $E(G) \setminus M$. An M-alternating path is said to be M-augmenting path if both of its ends are M-unsaturated. Perfect matchings correspond to Kekulé structures in

molecular graphs, which play an important role in analysis of the resonance energy and stability of hydro-carbon compounds [33]. The organic compounds without any Kekulé structure are known to chemically unstable. Thus study of Kekulé structures of chemical compounds is very important as it explains their physico chemical properties [42].

The anti-Kekulé number of a connected graph G, denoted by $ak(G)$, is the minimum number of edges which must be deleted from G to obtain a connected subgraph that does not contain any Kekulé structure. Obviously, when a graph G does not contain any Kekulé structure then $ak(G) = 0$. If it is not possible to find a connected spanning subgraph of G without any Kekulé structure then $ak(G) = \infty$.

The adjacency matrix $A(G) = [a_{ij}]_{n\times n}$ of a graph G is defined by

$$a_{ij} = \begin{cases} 1 & \text{if } v_iv_j \in E(G) \\ 0 & \text{otherwise} \end{cases} \quad (\forall v_i, v_j \in V(G)).$$

The eigenvalues of $A(G)$ are called the eigenvalues of the graph G. Similarly the spectrum of the graph G is the multiset of eigenvalues of $A(G)$. The nullity $\eta(G)$ of graph G is the multiplicity of the eigenvalue zero in the spectrum of G. The graph G is singular if $\eta(G) > 0$ and non-singular otherwise. In [14], Collatz and Sinogowitz posed the problem of characterizing singular graphs. Since then, the theory of nullity of graphs has stimulated much research because of its noteworthy applications in chemistry. The role of nullity of graphs in chemistry was first recognized by Gutman [13].

4.3 The Kekulé structures and maximum matchings in $D[n]$

In this next section, we find the number of Kekulé structures in the dendrimer $D[n]$. When there is no Kekulé structure in $D[n]$, we find a maximum matching in it and give the size of this maximum matching for any stage n (≥ 1).

We first give the following lemma.

Lemma 4.3.1. *For $n = 1$, there are two Kekulé structures in $D[n]$.*

Figure 4.1: Two distinct perfect matchings in $D[n]$ with $n = 1$, where thick edges represent a matching.

Proof. Consider the matchings represented by the thick edges in Fig. 4.1-(a) and Fig. 4.1-(b). There is only one hexagon in $D[1]$ and a hexagon has exactly two Kekulé structures. Thus $D[1]$ has two Kekule structures. □

In the next lemma, we show that $D[n]$ contains no Kekule structure when n exceeds 1.

Lemma 4.3.2. *For $n \geq 2$, $D[n]$ has no Kekulé structure.*

Proof. From the structure of $D[n]$, we see that if n is even then $D[n]$ contains a path P_7 whose end vertices have degree 1 in $D[n]$. Denote by $v_1, v_2, \cdots, v_7$ the vertices of P_7. Then $d(v_1) = d(v_7) = 1$, $d(v_2) = 3$ and all other internal vertices of P_7 has degree 2 in $D[n]$. If M is a perfect matching in $D[n]$ then $v_1v_2 \in M$. Since $1 \leq d(v_i) \leq 2$ for $i \in \{3, 4, \cdots, 7\}$, P_7 has one M-unsaturated vertex which contradicts the fact that M is a perfect matching.

If n is odd then $D[n]$ contains a path P_{11}. By similar arguments as given above, one can show that $D[n]$ has no perfect matching. Thus $D[n]$ has no Kekulé structure.

Observation 1: Consider a tree T_n on n-vertices, $n \geq 7$, shown in Fig. 4.4 such that

(i) $d(x, y)$ and $d(z, w)$ are odd.

(ii) $d(y, z)$ is even.

Then from the construction of T_n, we can easily see that the size of a maximum matching in T_n is $\lfloor \frac{n}{2} \rfloor - 1$.

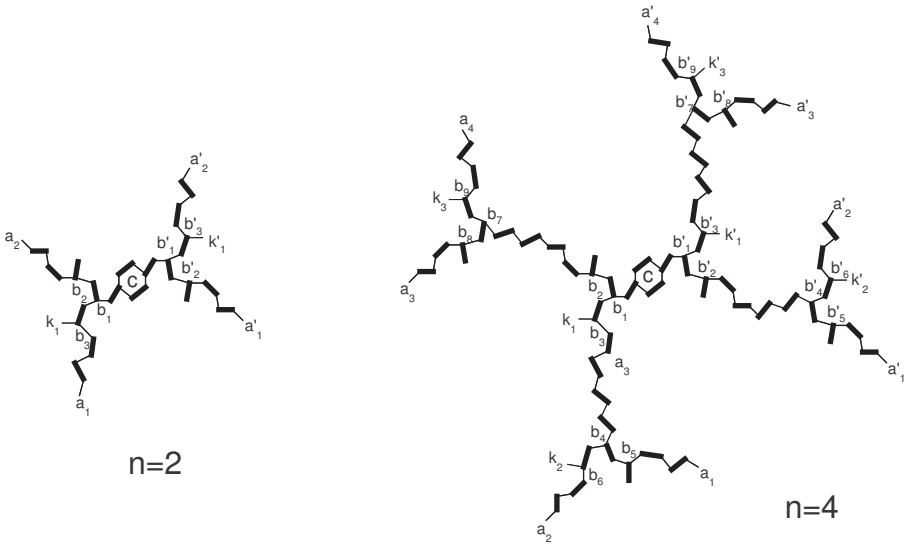

Figure 4.2: $D[n]$ with $n = 2$ and $n = 4$. The thick edges represent a matching.

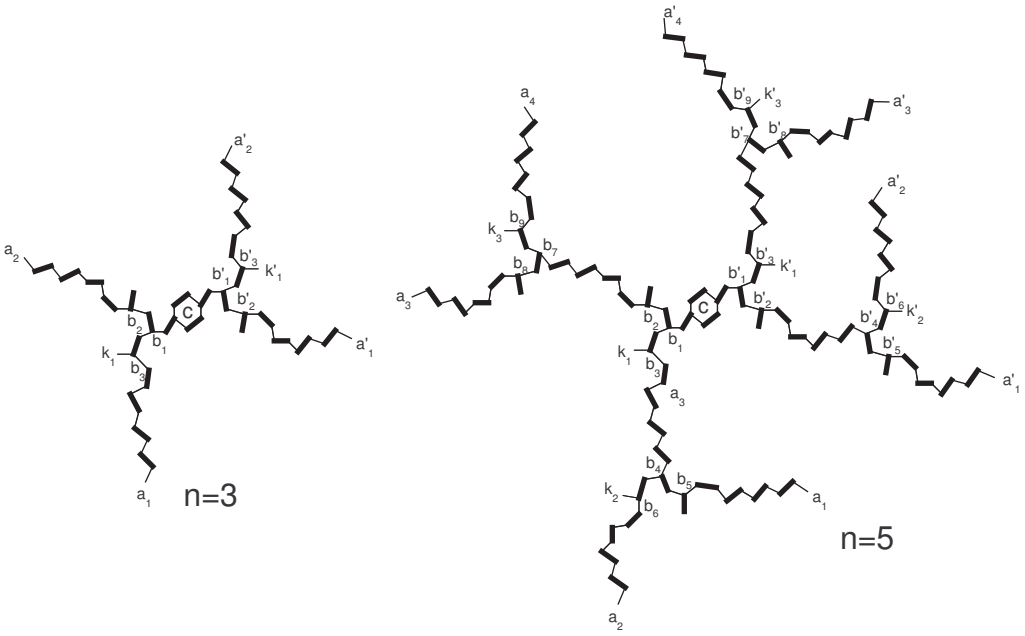

Figure 4.3: $D[n]$ with $n = 3$ and $n = 5$. The thick edges represent a matching M.

Figure 4.4: A tree T_n, $n \geq 7$.

Observation 2: Let T_{n_1} and T_{n_2} be two trees that satisfies (i) and (ii) of Observation 1, where $n_1, n_2 \geq 7$. We join T_{n_1} with T_n at vertex x and T_{n_2} with T_n at vertex w and the resulting tree, say $T_{n+n_1+n_2}$, is shown in Fig. 4.5. Then the size of a maximum matching in $T_{n+n_1+n_2}$ is $\lfloor \frac{n}{2} \rfloor + \lfloor \frac{n_1}{2} \rfloor + \lfloor \frac{n_2}{2} \rfloor - 3$.

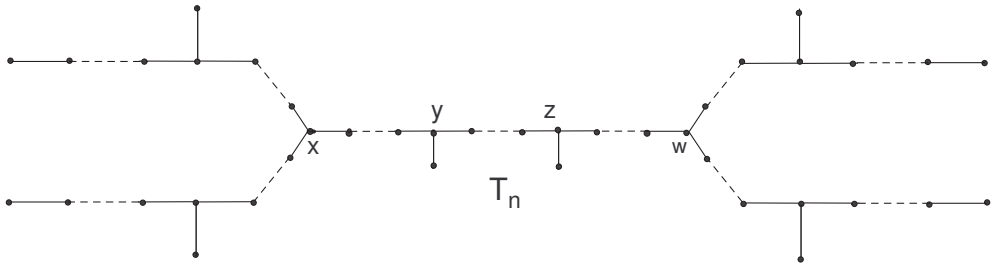

Figure 4.5: Joining of T_{n_1} and T_{n_2} with T_n.

Let M denotes a matching in $D[n]$ formed by the thick edges shown in Fig. 4.3. In the next theorem, we show that M represents a maximum matching in $D[n]$. Moreover, we give the size of this maximum matching. □

Theorem 4.3.1. *The size of the maximum matching M in $D[n]$ is given by*

$$|M| = \begin{cases} 18 \times 2^t - 18 & \text{if } n = 2t \\ 11 \times 2^{t+1} - 18 & \text{if } n = 2t+1, \end{cases}$$

where $t \geq 1$ is an integer.

Proof. Let $n = 2$. Then from Fig. 4.2, one can see that there are two copies of a tree T_{17} each of which joined with one pendent vertex of $D[1]$. The tree T_{17} satisfies (i) and (ii) of observation 1. By Observation 1, the size of a maximum matching in

T_{17} is $\lfloor\frac{17}{2}\rfloor - 1$. The size of maximum matching M in $D[2]$ is

$$\begin{aligned} |M| &= 2\big(\lfloor\frac{17}{2}\rfloor - 1\big) + 4 \\ &= 18 \\ &= 18 \times 2^1 - 18. \end{aligned} \tag{4.1}$$

Let $n = 3$. Then from Fig. 4.3, we note that there are two copies of a tree T_{25} each of which is joined with one pendent vertex of $D[1]$. The tree T_{25} satisfies (i) and (ii) of Observation 1. By Observation 1, the size of a maximum matching in T_{25} is $\lfloor\frac{25}{2}\rfloor - 1$. Thus, the size of maximum matching M is $D[3]$ is

$$\begin{aligned} |M| &= 2\big(\lfloor\frac{25}{2}\rfloor - 1\big) + 4 \\ &= 26 \\ &= 11 \times 2^{1+1} - 18. \end{aligned} \tag{4.2}$$

Let $n = 4$. Then from Fig. 4.2, we note that there are four copies of a tree T_{17} each of which is joined with one of pendent vertex of two copies of a tree T_{25}. The graph obtained after joining two copies of T_{17} with T_{25} satisfies the condition of Observation 2. Thus by Observation 2, the size of maximum matching in the join of two copies of T_{17} and T_{25} is $\lfloor\frac{25}{2}\rfloor + 2\lfloor\frac{17}{2}\rfloor - 3$. Thus the size of maximum matching M in $D[4]$ is

$$\begin{aligned} |M| &= 2\big(\lfloor\frac{25}{2}\rfloor + 2\lfloor\frac{17}{2}\rfloor - 3\big) + 4 \\ &= 54 \\ &= 18 \times 2^2 - 18. \end{aligned} \tag{4.3}$$

Let $n = 5$. Then from Fig. 4.3, we observe that there are four copies of a tree T_{25} each of which is joined with one pendent vertex of two copies of a tree T_{25}. By similar arguments used to find the size of a maximum matching in D[4], we conclude that the size of a maximum matching M in $D[5]$ is given by

$$\begin{aligned} |M| &= 2\big(3\lfloor\frac{25}{2}\rfloor - 3\big) + 4 \\ &= 70 \\ &= 11 \times 2^{2+1} - 18. \end{aligned} \tag{4.4}$$

Since the growth of $D[n]$ is systematic, from (4.1) and (4.3), we conclude that when $n = 2t$, $t = 1, 2, ...$, the size of a maximum matching M in $D[n]$ is given by

$$|M| = 18 \times 2^t - 18.$$

From (4.2) and (4.4), we observe that when $n = 2t + 1$, where $t = 1, 2, ...$, the size of a maximum matching M in $D[n]$ is given by:

$$|M| = 11 \times 2^{t+1} - 18.$$

This proves the required assertion. □

From Theorem 4.3.1, we have the following result.

Corollary 4.3.1. *The anti-Kekulé number of $D[n]$ for $n \geq 2$ is 0.*

4.4 The nullity of hetrofunctional dendrimers $D[n]$

In this section, we calculate the nullity of the hetrofunctional dendrimers $D[n]$. Let M be the maximum matching in the graph $D[n]$ as shown in Fig. 4.2 and Fig. 4.3. The next lemma is useful in calculating the nullity of bipartite graphs.

Lemma 4.4.1 (Cvetkovic, Gutman [12])**.** *If a bipartite graph G with $n \geq 1$ vertices does not contain any cycle of length $r \equiv 0(\text{mod}4)$, then $\eta(G) = |V| - 2|M|$, where $|M|$ is the size of its maximum matching.*

The following lemma is useful in finding nullity of graphs with pendent vertices.

Lemma 4.4.2 (Cvetkovic, Gutman [13])**.** *Let v be a pendant vertex in a graph G and u be the vertex adjacent to v. Then $\eta(G) = \eta(G - u - v)$, where $G - u - v$ is the graph obtained from G by deleting the vertices u and v.*

The nullity of a path and cycle is computed as follows.

Lemma 4.4.3 (Cvetkovic, Gutman [13])**.** *(i) The eigenvalues of the path P_n are of the form $2\cos(\frac{k\pi}{n+1})$, where $k = 1, \ldots, n$. Thus,*

$$\eta(P_n) = \begin{cases} 1 & \text{if } n \text{ is odd} \\ 0 & \text{if } n \text{ is even.} \end{cases}$$

(ii) The eigenvalues of the cycle C_n are $2\cos(\frac{2k\pi}{n})$, where $k = 0, 1, \ldots, n-1$. Thus

$$\eta(C_n) = \begin{cases} 2 & \text{if } n \equiv 0(\text{mod}4) \\ 0 & \text{otherwise.} \end{cases}$$

The following lemma states that the sum of the nullities of components of a graph is equal to nullity of graph.

Lemma 4.4.4 (Gutman, Borovicanin [32])**.** *Let $G = \bigcup_{i=1}^{t} G_i$, where G_i, for each $i = 1, \ldots, t$, are connected components of G. Then $\eta(G) = \sum_{i=1}^{t} \eta(G_i)$.*

Next theorem gives the nullity of $D[n]$.

Theorem 4.4.1. *The nullity of $D[n]$ is given by*

$$\eta(D[n]) = \begin{cases} 0 & \text{if } n = 1 \\ 4 \times 2^t - 2 & \text{if } n \geq 2, \end{cases}$$

where $t = \lfloor \frac{n}{2} \rfloor$.

Proof. Note that $D[1]$ is a bipartite graph and does not contain any cycle of length $r \equiv 0(\text{ mod } 4)$. Also, the size of maximum matching in $D[1]$ is 5. Thus, Lemma 4.4.1 gives

$$\eta(D[1]) = 0$$

Now, let $n \geq 2$. Again $D[n]$ is a bipartite graph for each $n \geq 2$ and does not contain any cycle of length of $r \equiv 0(\text{mod}4)$. By Theorem 4.3.1, the size of a maximum matching in $D[n]$ is $18 \times 2^t - 18$ when $n = 2t$ and $11 \times 2^{t+1} - 18$ when $n = 2t + 1$. When $n = 2t$, Lemma 4.4.1 gives

$$\begin{aligned} \eta(D[n]) &= \big(16 \times 2^{t+1} + 8 \times 2^t - 38\big) - \big(18^t - 18\big) \\ &= 4 \times 2^t - 2. \end{aligned}$$

When $n = 2t + 1$, Lemma 4.4.1 yields

$$\begin{aligned} \eta(D[n]) &= \big(24 \times 2^{t+1} - 38\big) - 2\big(11 \times 2^{t+1} - 18\big) \\ &= 4 \times 2^t - 2. \end{aligned}$$

This proves the assertion. □

4.5 Some degree based topological indices of hetrofunctional dendrimers

This section deals with some degree based topological indices of the dendrimer $D[n]$. Let G be a simple connected graph with vertex set $V(G)$ and the edge set $E(G)$. The degree of vertex $v \in V(G)$ is denoted by d_v. Also, define $S_u = \sum_{v \in N_G(u)} d_v$, where $N_G(u) = \{v \in V(G) | uv \in E(G)\}$. Introduced by Estarada et al. [20], the atom bond connectivity index (hencefourth, $ABC - Index$) is defined by

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}. \tag{4.5}$$

Recently, Ghorbani et al. [30] introduced the fourth version of $ABC - Index$ defined by

$$ABC_4(G) = \sum_{uv \in E(G)} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}}. \tag{4.6}$$

Another well-known connectivity topological descriptor is the geometric-arithmetic index (henceforth, $GA - index$), which was introduced by Vukičević and Furtula [49] and is defined by

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}. \tag{4.7}$$

Graovac et al. [31] proposed the fifth version of $GA - index$, which is defined by

$$GA_5(G) = \sum_{uv \in E(G)} \frac{2\sqrt{S_u S_v}}{S_u + S_v}. \tag{4.8}$$

With each edge uv, we associate two pairs (d_u, d_v) and (S_u, S_v). The edge partition of the dendrimer $D[n]$ with respect to degrees of the end-vertices of edges and with respect to the sum of degrees of the neighbours of end-vertices of edges is given by Table 4.1 and Table 4.2, respectively.

4.5.1 Results for ABC and ABC_4-Index

Now, we compute the ABC and ABC_4-indices of the dendrimer $D[n]$ using the edge partition shown in Tables 4.1 −4.2.

(d_u, d_v)	Number of edges
$(1,2)$	2^{t+1}
$(2,3)$	$\sum_{i=1}^{t} 2^i + \sum_{i=0}^{t}(2^i \times 6)$
$(2,2)$	$2 + \sum_{i=2}^{t+1}(2^i \times 3) + \sum_{i=2}^{t}(2^i \times 4)$ if $n = 2t$
$(2,2)$	$2 + \sum_{i=2}^{t+1}(2^i \times 3) + \sum_{i=1}^{t}(2^{i+1} \times 4)$ if $n = 2t+1$
$(1,3)$	$\sum_{i=1}^{t} 2^{i+1}$

Table 4.1: (d_u, d_v)-type edge partion of $D[n]$, for $n \geq 3$ and $t = \lfloor \frac{n}{2} \rfloor$.

(S_u, S_v)	Number of edges
$(5,5)$	$\sum_{i=0}^{t} 2^{i+1}$
$(5,6)$	$3 \times 2^{t+1} - 4$
$(6,6)$	$4 + \sum_{i=1}^{t} 2^{i+1}$
$(5,3)$	$\sum_{i=1}^{t} 2^{i+1}$
$(5,4)$	$3 \times 2^{t+1} - 8$
$(4,4)$	$\sum_{i=1}^{t} 2^{i+1} + \sum_{i=1}^{t-1}(4 \times 2^{i+1})$ if $n = 2t$
$(4,4)$	$\sum_{i=1}^{t}(5 \times 2^{i+1})$ if $n = 2t+1$
$(4,3)$	2^{t+1}
$(3,2)$	2^{t+1}

Table 4.2: (S_u, S_v)-type edge partion of $D[n]$, for $n \geq 3$ and $t = \lfloor \frac{n}{2} \rfloor$.

Theorem 4.5.1. *The atom-bond connectivity index of $D[n]$, for $n = 2t+1$, where $t \geq 0$ is given by*

$$ABC(D[n]) = 22\sqrt{2} \times 2^t - 17\sqrt{2} + \frac{4}{3}\sqrt{6} \times 2^t - \frac{4}{3}\sqrt{6}.$$

Proof. We use equation (4.5) and the edge partitions in Table 4.1.

For $n = 1$, we have

$$\begin{aligned} ABC(D[1]) &= \sum_{uv \in D(1)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\ &= 2 \times \sqrt{\frac{1+2-2}{1\times 2}} + 6 \times \sqrt{\frac{2+3-2}{2\times 3}} + 2 \times \sqrt{\frac{2+2-2}{2\times 2}} \\ &= 5\sqrt{2} \\ &= 22\sqrt{2} \times 2^0 - 17\sqrt{2} + \frac{4}{3}\sqrt{6} \times 2^0 - \frac{4}{3}\sqrt{6}. \end{aligned}$$

For $n \geq 3$, we have

$$\begin{aligned} ABC(D[n]) &= \sum_{uv \in D(n)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\ &= 2^{t+1} \times \sqrt{\frac{1+2-2}{1\times 2}} + \Big(\sum_{i=1}^{t} 2^i + \sum_{i=0}^{t} (2^i \times 6) \Big) \times \sqrt{\frac{2+3-2}{2\times 3}} \\ &\quad + \Big(2 + \sum_{i=2}^{t+1} (2^i \times 3) + \sum_{i=1}^{t} 2^{i+1} \times 4) \Big) \times \sqrt{\frac{2+2-2}{2\times 2}} \\ &\quad + \sum_{i=1}^{t} 2^{i+1} \times \sqrt{\frac{1+3-2}{1\times 3}} \\ &= 22\sqrt{2} \times 2^t - 17\sqrt{2} + \frac{4}{3}\sqrt{6} \times 2^t - \frac{4}{3}\sqrt{6}. \end{aligned}$$

This completes the proof. □

Theorem 4.5.2. *The atom-bond connectivity index of $D[n]$, for $n = 2t$, where $t \geq 1$ is given by*

$$ABC(D[n]) = 18\sqrt{2} \times 2^t - 17\sqrt{2} + \frac{4}{3}\sqrt{6} \times 2^t - \frac{4}{3}\sqrt{6}. \tag{4.9}$$

Proof. We use equation (4.5) and the edge partitions in Table 4.1.

For $n = 2$, we have

$$\begin{aligned} ABC(D[2]) &= \sum_{uv\in D(2)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\ &= 4 \times \sqrt{\frac{1+2-2}{1\times 2}} + 20 \times \sqrt{\frac{2+3-2}{2\times 3}} + 14 \times \sqrt{\frac{2+2-2}{2\times 2}} \\ &\quad +14 \times \sqrt{\frac{1+3-2}{1\times 3}} \\ &= 19\sqrt{2} + \frac{4}{3}\sqrt{6} \\ &= 18\sqrt{2} \times 2^1 - 17\sqrt{2} + \frac{4}{3}\sqrt{6} \times 2^1 - \frac{4}{3}\sqrt{6}. \end{aligned}$$

For $n \geq 4$, we have

$$\begin{aligned} ABC(D[n]) &= \sum_{uv\in D(n)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}} \\ &= 2^{t+1} \times \sqrt{\frac{1+2-2}{1\times 2}} + \Big(\sum_{i=1}^{t} 2^i + \sum_{i=0}^{t} (2^i \times 6)\Big) \times \sqrt{\frac{2+3-2}{2\times 3}} \\ &\quad +\Big(2 + \sum_{i=2}^{t+1} (2^i \times 3) + \sum_{i=2}^{t} 2^i \times 4)\Big) \times \sqrt{\frac{2+2-2}{2\times 2}} \\ &\quad + \sum_{i=1}^{t} 2^{i+1} \times \sqrt{\frac{1+3-2}{1\times 3}} \\ &= 18\sqrt{2} \times 2^t - 17\sqrt{2} + \frac{4}{3}\sqrt{6} \times 2^t - \frac{4}{3}\sqrt{6}. \end{aligned}$$

This completes the proof. □

Theorem 4.5.3. *The fourth atom-bond connectivity index of $D[n]$, for $n = 2t + 1$, where $t \geq 0$ is given by*

$$ABC_4(D[n]) = \begin{cases} \frac{9}{5}\sqrt{2} + \frac{2}{5}\sqrt{30} + \frac{2}{3}\sqrt{3} & \text{if } t = 0, \\ \frac{1}{15}\Bigg(2^{\frac{2t+1}{2}} \times \Big(9\sqrt{15} + 22\sqrt{5} + 75\sqrt{3} + 39\Big) + \\ 2^t \times \Big(5\sqrt{15} - 9\sqrt{35}\Big) - 6\sqrt{30} - 12\sqrt{10} - 12\sqrt{35}\Bigg) - \\ 5\sqrt{6} - \frac{4}{5}\sqrt{2}. & \text{if } t \geq 1. \end{cases}$$

Proof. When $n = 1$, the fourth atom-bond connectivity index of $D[1]$ can be written as follows:

$$\begin{aligned} ABC_4(D[1]) &= \sum_{uv\in E(D[n])} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} \\ &= 2 \times \sqrt{\frac{5+5-2}{5\times 5}} + 4 \times \sqrt{\frac{5+6-2}{5\times 6}} + 2 \times \sqrt{\frac{6+4-2}{6\times 4}} \\ &\quad +2 \times \sqrt{\frac{4+2-2}{4\times 2}}. \\ &= \frac{9}{5}\sqrt{2} + \frac{2}{5}\sqrt{30} + \frac{2}{3}\sqrt{3}. \end{aligned}$$

When $n \geq 3$, using Table 4.2, the fourth atom-bond connectivity index of $D[n]$ can be written as follows:

$$\begin{aligned} ABC_4(D[n]) &= \sum_{uv\in E(D[n])} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} \\ &= \sum_{i=0}^{t} 2^{i+1} \times \sqrt{\frac{5+5-2}{5\times 5}} + \big(3\times 2^{t+1} - 4\big) \times \sqrt{\frac{5+6-2}{5\times 6}} \\ &\quad +\big(4 + \sum_{i=1}^{t} 2^{i+1}\big) \times \sqrt{\frac{6+6-2}{6\times 6}} + \sum_{i=1}^{t} 2^{i+1} \times \sqrt{\frac{5+3-2}{5\times 3}} \\ &\quad +\big(3\times 2^{t+1} - 8\big) \times \sqrt{\frac{5+4-2}{5\times 4}} + \big(\sum_{i=1}^{t} 5\times 2^{i+1}\big) \times \sqrt{\frac{4+4-2}{4\times 4}} \\ &\quad +2^{t+1} \times \sqrt{\frac{4+3-2}{4\times 3}} + 2^{t+1} \times \sqrt{\frac{3+2-2}{3\times 2}} \\ &= \frac{1}{15}\Bigg(2^{\frac{2t+1}{2}} \times \Big(9\sqrt{15} + 22\sqrt{5} + 75\sqrt{3} + 39\Big) + 2^t \times \Big(5\sqrt{15} - 9\sqrt{35}\Big) \\ &\quad -6\sqrt{30} - 12\sqrt{10} - 12\sqrt{35}\Bigg) - 5\sqrt{6} - \frac{4}{5}\sqrt{2}. \end{aligned}$$

This completes the proof. □

Theorem 4.5.4. *The fourth atom-bond connectivity index of $D[n]$, for $n = 2t$,*

where $t \geq 1$ is given by

$$ABC_4(D[n]) = \begin{cases} \frac{22}{5}\sqrt{2} + \frac{4}{5}\sqrt{30} + \frac{32}{15}\sqrt{10} + \frac{2}{5}\sqrt{35} + \sqrt{6} + \frac{2}{3}\sqrt{15} & \text{if } t = 1, \\ \frac{1}{15}\Bigg(2^{\frac{2t+1}{2}} \times \Big(9\sqrt{15} + 22\sqrt{5} + 45\sqrt{3} + 39\Big) + \\ 2^t \times \Big(5\sqrt{15} - 9\sqrt{35}\Big) - 6\sqrt{30} - 12\sqrt{10} - 12\sqrt{35}\Bigg) - \\ 5\sqrt{6} - \frac{4}{5}\sqrt{2}. & \text{if } t \geq 2. \end{cases}$$

Proof. When $n = 2$, the fourth atom-bond connectivity index of $D[2]$ can be written as follows:

$$\begin{aligned} ABC_4(D[2]) &= \sum_{uv \in E(D[n])} \sqrt{\frac{S_u + S_v - 2}{S_u S_v}} \\ &= 6 \times \sqrt{\frac{5+5-2}{5\times 5}} + 8 \times \sqrt{\frac{5+6-2}{5\times 6}} + 8 \times \sqrt{\frac{6+6-2}{6\times 6}} \\ &\quad +4 \times \sqrt{\frac{5+3-2}{5\times 3}} + 4 \times \sqrt{\frac{5+4-2}{5\times 4}} + 4 \times \sqrt{\frac{4+4-2}{4\times 4}} \\ &\quad +4 \times \sqrt{\frac{3+2-2}{3\times 2}} + 4 \times \sqrt{\frac{4+3-2}{4\times 3}} \\ &= \frac{22}{5}\sqrt{2} + \frac{4}{5}\sqrt{30} + \frac{32}{15}\sqrt{10} + \frac{2}{5}\sqrt{35} + \sqrt{6} + \frac{2}{3}\sqrt{15}. \end{aligned}$$

When $n \geq 4$, using Table 4.2, the fourth atom-bond connectivity index of $D[n]$ can be written as follows:

$$
\begin{aligned}
ABC_4(D[n]) &= \sum_{uv\in E(D[n])} \sqrt{\frac{S_u+S_v-2}{S_uS_v}} \\
&= \sum_{i=0}^{t} 2^{i+1}\times\sqrt{\frac{5+5-2}{5\times 5}} + \big(3\times 2^{t+1}-4\big)\times\sqrt{\frac{5+6-2}{5\times 6}} \\
&\quad +\big(4+\sum_{i=1}^{t}2^{i+1}\big)\times\sqrt{\frac{6+6-2}{6\times 6}} + \sum_{i=1}^{t}2^{i+1}\times\sqrt{\frac{5+3-2}{5\times 3}} \\
&\quad +\big(3\times 2^{t+1}-8\big)\times\sqrt{\frac{5+4-2}{5\times 4}} + \big(\sum_{i=1}^{t}2^{i+1}+\sum_{i=1}^{t-1}(4\times 2^{i+1})\big) \\
&\quad \times\sqrt{\frac{4+4-2}{4\times 4}} + 2^{t+1}\times\sqrt{\frac{4+3-2}{4\times 3}} + 2^{t+1}\times\sqrt{\frac{3+2-2}{3\times 2}} \\
&= \frac{1}{15}\Bigg(2^{\frac{2t+1}{2}}\times\Big(9\sqrt{15}+22\sqrt{5}+45\sqrt{3}+39\Big) + 2^{t}\times\Big(5\sqrt{15}-9\sqrt{35}\Big) \\
&\quad -6\sqrt{30}-12\sqrt{10}-12\sqrt{35}\Bigg) - 5\sqrt{6}-\frac{4}{5}\sqrt{2}.
\end{aligned}
$$

The proof is complete. □

4.5.2 Results for GA and GA_5-Index

Now, we compute the GA and GA_5-indices of the dendrimer $D[n]$ using the edge partitions shown in Tables 1-2.

Theorem 4.5.5. *The geometric-arithmetic index of $D[n]$, for $n = 2t+1$ where $t \geq 0$ is given by*

$$
GA(D[n]) = \begin{cases}
\frac{4}{3}\sqrt{2}+\frac{12}{5}\sqrt{6}+2 & \text{if } t=0, \\
2^{\frac{2t+1}{2}}\times\Big(\frac{4}{3}+\frac{28}{5}\sqrt{3}\Big)+2^{t}\times\Big(28+2\sqrt{3}\Big)- & \\
\frac{16}{5}\sqrt{6}-2\sqrt{3}-26 & \text{if } t\geq 1.
\end{cases}
$$

Proof. When $n = 1$, the geometric-arithmetic index of $D[1]$ can be written as follows:

$$\begin{aligned} GA(D[1]) &= \sum_{uv \in D[n]} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\ &= 2 \times \frac{2\sqrt{1 \times 2}}{1+2} + 6 \times \frac{2\sqrt{2 \times 3}}{2+3} + 2 \times \frac{2\sqrt{2 \times 2}}{2+2} \\ &= \frac{4}{3}\sqrt{2} + \frac{12}{5}\sqrt{6} + 2. \end{aligned}$$

When $n \geq 3$, using Table 4.1, the geometric-arithmetic index of $D[n]$ can be written as follows:

$$\begin{aligned} GA(D[n]) &= \sum_{uv \in D[n]} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\ &= 2^{t+1} \times \frac{2\sqrt{1 \times 2}}{1+2} + \Big(\sum_{i=1}^{t} 2^i + \sum_{i=0}^{t} (2^i \times 6) \Big) \times \frac{2\sqrt{2 \times 3}}{2+3} + \\ &\quad \Big(2 + \sum_{i=2}^{t+1} (2^i \times 3) + \sum_{i=1}^{t} (2^{i+1} \times 4) \Big) \times \frac{2\sqrt{2 \times 2}}{2+2} + \Big(\sum_{i=1}^{t} 2^{i+1} \Big) \times \frac{2\sqrt{1 \times 3}}{1+3} \\ &= 2^{\frac{2t+1}{2}} \times \Big(\frac{4}{3} + \frac{28}{5}\sqrt{3} \Big) + 2^t \times \Big(28 + 2\sqrt{3} \Big) - \frac{16}{5}\sqrt{6} - 2\sqrt{3} - 26. \end{aligned}$$

This completes the proof. □

Theorem 4.5.6. *The geometric-arithmetic index of $D[n]$, for $n = 2t$, where $t \geq 1$ is given by*

$$GA(D[n]) = \begin{cases} \frac{8}{3}\sqrt{2} + 8\sqrt{6} + 14 + 2\sqrt{3} & \text{if } t = 1, \\ 2^{\frac{2t+1}{2}} \times \Big(\frac{4}{3} + \frac{28}{5}\sqrt{3} \Big) + 2^t \times \Big(20 + 2\sqrt{3} \Big) - & \\ \frac{16}{5}\sqrt{6} - 2\sqrt{3} - 26 & \text{if } t \geq 2. \end{cases}$$

Proof. When $n = 2$, the geometric-arithmetic index of $D[2]$ can be written as follows:

$$\begin{aligned} GA(D[2]) &= \sum_{uv \in D[n]} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\ &= 4 \times \frac{2\sqrt{1 \times 2}}{1+2} + 20 \times \frac{2\sqrt{2 \times 3}}{2+3} + 14 \times \frac{2\sqrt{2 \times 2}}{2+2} + 4 \times \frac{2\sqrt{1 \times 3}}{1+3} \\ &= \frac{8}{3}\sqrt{2} + 8\sqrt{6} + 14 + 2\sqrt{3}. \end{aligned}$$

When $n \geq 4$, using Table 4.1, the geometric-arithmetic index of $D[n]$ can be written as follows:

$$\begin{aligned} GA(D[n]) &= \sum_{uv \in D[n]} \frac{2\sqrt{d_u d_v}}{d_u + d_v} \\ &= 2^{t+1} \times \frac{2\sqrt{1\times 2}}{1+2} + \Big(\sum_{i=1}^{t} 2^i + \sum_{i=0}^{t}(2^i \times 6)\Big) \times \frac{2\sqrt{2\times 3}}{2+3} + \\ &\quad \Big(2 + \sum_{i=2}^{t+1}(2^i \times 3) + \sum_{i=2}^{t}(2^i \times 4)\Big) \times \frac{2\sqrt{2\times 2}}{2+2} + \Big(\sum_{i=1}^{t} 2^{i+1}\Big)\frac{2\sqrt{1\times 3}}{1+3} \\ &= 2^{\frac{2t+1}{2}} \times \Big(\frac{4}{3} + \frac{28}{5}\sqrt{3}\Big) + 2^t \times \Big(20 + 2\sqrt{3}\Big) - \frac{16}{5}\sqrt{6} - 2\sqrt{3} - 26, \end{aligned}$$

which is the required result. □

Theorem 4.5.7. *The fifth geometric-arithmetic index of $D[n]$, for $n = 2t+1$, where $t \geq 0$ is given by*

$$GA_5(D[n]) = \begin{cases} 2 + \frac{8}{11}\sqrt{30} + \frac{4}{5}\sqrt{6} + \frac{4}{3}\sqrt{2} & \text{if } t = 0, \\ 2^{\frac{2t+1}{2}} \times \Big(\frac{12}{11}\sqrt{15} + \frac{4}{5}\sqrt{3}\Big) + 2^t \times \Big(28 + \sqrt{15} + \frac{8}{3}\sqrt{5} + \frac{8}{7}\sqrt{3}\Big) & \\ -\frac{8}{11}\sqrt{30} - \frac{32}{9}\sqrt{5} - \sqrt{15} - 22 & \text{if } t \geq 1. \end{cases}$$

Proof. When $n = 1$, the fifth geometric-arithmetic index of $D[1]$ can be written as follows:

$$\begin{aligned} GA_5(D[1]) &= \sum_{uv \in D[n]} \frac{2\sqrt{S_u S_v}}{S_u + S_v} \\ &= 2 \times \frac{2\sqrt{5\times 5}}{5+5} + 4 \times \frac{2\sqrt{5\times 6}}{5+6} + 2 \times \frac{2\sqrt{6\times 4}}{6+4} + 2 \times \frac{2\sqrt{4\times 2}}{4+2} \\ &= 2 + \frac{8}{11}\sqrt{30} + \frac{4}{5}\sqrt{6} + \frac{4}{3}\sqrt{2}. \end{aligned}$$

When $n \geq 3$, using Table 4.2, the geometric-arithmetic index of $D[n]$ can be written as follows:

$$\begin{aligned}
GA_5(D[n]) &= \sum_{uv\in D[n]} \frac{2\sqrt{S_u S_v}}{S_u+S_v} \\
&= \Big(\sum_{i=0}^{t} 2^{i+1}\Big) \times \frac{2\sqrt{5\times 5}}{5+5} + \Big(3\times 2^{t+1}-4\Big) \times \frac{2\sqrt{5\times 6}}{5+6} \\
&\quad + \Big(4+\sum_{i=1}^{t} 2^{i+1}\Big) \times \frac{2\sqrt{6\times 6}}{6+6} + \Big(\sum_{i=1}^{t} 2^{i+1}\Big) \times \frac{2\sqrt{5\times 3}}{5+3} \\
&\quad + \Big(3\times 2^{t+1}-8\Big) \times \frac{2\sqrt{5\times 4}}{5+4} + \Big(\sum_{i=1}^{t} (5\times 2^{i+1})\Big) \times \frac{2\sqrt{4\times 4}}{4+4} \\
&\quad + \Big(2^{t+1}\Big) \times \frac{2\sqrt{4\times 3}}{4+3} + \Big(2^{t+1}\Big) \times \frac{2\sqrt{3\times 2}}{3+2} \\
&= 2^{\frac{2t+1}{2}} \times \Big(\frac{12}{11}\sqrt{15}+\frac{4}{5}\sqrt{3}\Big) + 2^t \times \Big(28+\sqrt{15}+\frac{8}{3}\sqrt{5}+\frac{8}{7}\sqrt{3}\Big) \\
&\quad - \frac{8}{11}\sqrt{30} - \frac{32}{9}\sqrt{5} - \sqrt{15} - 22.
\end{aligned}$$

This completes the proof. □

Theorem 4.5.8. *The fifth geometric-arithmetic index of $D[n]$, for $n = 2t$, where $t \geq 1$ is given by*

$$GA_5(D[n]) = \begin{cases} 18+\frac{16}{11}\sqrt{30}+\sqrt{15}+\frac{16}{9}\sqrt{5}+\frac{8}{5}\sqrt{6}+\frac{16}{7}\sqrt{3} & \text{if } t=1, \\ \\ 2^{\frac{2t+1}{2}} \times \Big(\frac{12}{11}\sqrt{15}+\frac{4}{5}\sqrt{3}\Big) + 2^t \times \Big(20+\sqrt{15}+\frac{8}{3}\sqrt{5}+\frac{8}{7}\sqrt{3}\Big) & \\ -\frac{8}{11}\sqrt{30}-\frac{32}{9}\sqrt{5}-\sqrt{15}-22 & \text{if } t\geq 2. \end{cases}$$

Proof. When $n = 2$, the fifth geometric-arithmetic index of $D[2]$ can be written as follows:

$$\begin{aligned}
GA_5(D[2]) &= \sum_{uv\in D[n]} \frac{2\sqrt{S_u S_v}}{S_u+S_v} \\
&= 6\times \frac{2\sqrt{5\times 5}}{5+5} + 8\times \frac{2\sqrt{5\times 6}}{5+6} + 8\times \frac{2\sqrt{6\times 6}}{6+6} + 4\times \frac{2\sqrt{5\times 3}}{5+3} \\
&\quad + 4\times \frac{2\sqrt{5\times 4}}{5+4} + 4\times \frac{2\sqrt{4\times 4}}{4+4} + 4\times \frac{2\sqrt{3\times 2}}{3+2} + 4\times \frac{2\sqrt{4\times 3}}{4+3} \\
&= 18+\frac{16}{11}\sqrt{30}+\sqrt{15}+\frac{16}{9}\sqrt{5}+\frac{8}{5}\sqrt{6}+\frac{16}{7}\sqrt{3}.
\end{aligned}$$

When $n \geq 4$, using Table 4.2, the geometric-arithmetic index of $D[n]$ can be written as follows:

$$\begin{aligned}
GA_5(D[n]) &= \sum_{uv \in D[n]} \frac{2\sqrt{S_u S_v}}{S_u + S_v} \\
&= \Big(\sum_{i=0}^{t} 2^{i+1}\Big) \times \frac{2\sqrt{5\times 5}}{5+5} + \Big(3\times 2^{t+1} - 4\Big) \times \frac{2\sqrt{5\times 6}}{5+6} \\
&\quad + \Big(4 + \sum_{i=1}^{t} 2^{i+1}\Big) \times \frac{2\sqrt{6\times 6}}{6+6} + \Big(\sum_{i=1}^{t} 2^{i+1}\Big) \times \frac{2\sqrt{5\times 3}}{5+3} \\
&\quad + \Big(3\times 2^{t+1} - 8\Big) \times \frac{2\sqrt{5\times 4}}{5+4} + \Big(\sum_{i=1}^{t} 2^{i+1} + \sum_{i=1}^{t-1}(4\times 2^{i+1})\Big) \\
&\quad \times \frac{2\sqrt{4\times 4}}{4+4} + \Big(2^{t+1}\Big) \times \frac{2\sqrt{4\times 3}}{4+3} + \Big(2^{t+1}\Big) \times \frac{2\sqrt{3\times 2}}{3+2} \\
&= 2^{\frac{2t+1}{2}} \times \Big(\frac{12}{11}\sqrt{15} + \frac{4}{5}\sqrt{3}\Big) + 2^t \times \Big(20 + \sqrt{15} + \frac{8}{3}\sqrt{5} + \frac{8}{7}\sqrt{3}\Big) \\
&\quad - \frac{8}{11}\sqrt{30} - \frac{32}{9}\sqrt{5} - \sqrt{15} - 22.
\end{aligned}$$

This completes the proof. □

4.6 Randić index

The very first and oldest degree based topological index is the Randić index, which was introduced by Milan Randić [41] in 1975. The Randić index of a graph $G = \big(V(G), E(G)\big)$ is defined as

$$R_{-\frac{1}{2}} = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}. \tag{4.10}$$

Later on, the general Randić index was introduced by Bollobas and Erdös [9] and Amic et al. [3] in 1988. The general Randić index of the graph is defined as

$$R_\alpha(G) = \sum_{uv \in E(G)} \big(d_u d_v\big)^\alpha, \tag{4.11}$$

where $\alpha \in \mathbb{R}$.

Theorem 4.6.1. *The Randić index is given by for $n = 2t + 1$, where $t \geq 0$ can be defined as*

$$R_\alpha(D[n]) = \begin{cases} 106 \times 2^{t+1} - 164 & \text{if } \alpha = 1, \\ 2^{\frac{2t+1}{2}} \times \left(14\sqrt{3} + \sqrt{2}\right) + 2^t \times \left(4\sqrt{3} + 56\right) - 8\sqrt{6} - 4\sqrt{3} - 52 & \text{if } \alpha = \frac{1}{2}, \\ 2^{2t+1} \times \frac{35}{6} - \frac{55}{6} & \text{if } \alpha = -1, \\ 2^{\frac{2t+1}{2}} \times \left(1 + \frac{7}{\sqrt{3}}\right) + 2^t \times \left(14 + \frac{4}{\sqrt{3}}\right) - \frac{4}{3}\sqrt{6} - \frac{4}{3}\sqrt{3} - 13 & \text{if } \alpha = -\frac{1}{2}. \end{cases}$$

Proof. We use the Table 4.1 to prove the result.

When $\alpha = 1$:

By using Table 4.1 and equation (4.11), we get:

$$\begin{aligned} R_1(D[n]) &= \sum_{uv \in E(D[n])} \left(d_u d_v\right)^1 \\ &= \Big(\sum_{i=1}^{t} 2^i + \sum_{i=0}^{t} (2^i \times 6)\Big) \times \left(2 \times 3\right)^1 + \Big(2 + \sum_{i=2}^{t+1} (2^i \times 3) + \sum_{i=1}^{t} (2^{i+1} \times 4)\Big) \\ &\quad \times \left(2 \times 2\right)^1 + \Big(\sum_{i=1}^{t} 2^{i+1}\Big) \times \left(1 \times 3\right)^1 + 2^{t+1} \times \left(1 \times 2\right)^1 \\ &= 106 \times 2^{t+1} - 164. \end{aligned}$$

When $\alpha = \frac{1}{2}$:

By using Table 4.1 and equation (4.11), we get:

$$\begin{aligned} R_{\frac{1}{2}}(D[n]) &= \sum_{uv \in E(D[n])} \left(d_u d_v\right)^{\frac{1}{2}} \\ &= \Big(\sum_{i=1}^{t} 2^i + \sum_{i=0}^{t} (2^i \times 6)\Big) \times \left(2 \times 3\right)^{\frac{1}{2}} + \Big(2 + \sum_{i=2}^{t+1} (2^i \times 3) + \sum_{i=1}^{t} (2^{i+1} \times 4)\Big) \\ &\quad \times \left(2 \times 2\right)^{\frac{1}{2}} + \Big(\sum_{i=1}^{t} 2^{i+1}\Big) \times \left(1 \times 3\right)^{\frac{1}{2}} + 2^{t+1} \times \left(1 \times 2\right)^{\frac{1}{2}} \\ &= 2^{\frac{2t+1}{2}} \times \left(14\sqrt{3} + \sqrt{2}\right) + 2^t \times \left(4\sqrt{3} + 56\right) - 8\sqrt{6} - 4\sqrt{3} - 52. \end{aligned}$$

When $\alpha = -1$:

By using Table 4.1 and equation (4.11), we get:

$$\begin{aligned} R_{-1}(D[n]) &= \sum_{uv\in E(D[n])} \big(d_u d_v\big)^{-1} \\ &= \Big(\sum_{i=1}^{t} 2^i + \sum_{i=0}^{t}(2^i\times 6)\Big)\times\big(2\times 3\big)^{-1} + \Big(2+\sum_{i=2}^{t+1}(2^i\times 3)+\sum_{i=1}^{t}(2^{i+1}\times 4)\Big) \\ &\quad \times\big(2\times 2\big)^{-1} + \Big(\sum_{i=1}^{t} 2^{i+1}\Big)\times\big(1\times 3\big)^{-1} + 2^{t+1}\times\big(1\times 2\big)^{-1} \\ &= 2^{t+1}\times\frac{35}{6}-\frac{55}{6}. \end{aligned}$$

When $\alpha=-\frac{1}{2}$:
By using Table 4.1 and equation (4.11), we get:

$$\begin{aligned} R_{-\frac{1}{2}}(D[n]) &= \sum_{uv\in E(D[n])} \big(d_u d_v\big)^{-\frac{1}{2}} \\ &= \Big(\sum_{i=1}^{t} 2^i + \sum_{i=0}^{t}(2^i\times 6)\Big)\times\big(2\times 3\big)^{-\frac{1}{2}} + \Big(2+\sum_{i=2}^{t+1}(2^i\times 3)+\sum_{i=1}^{t}(2^{i+1}\times 4)\Big) \\ &\quad \times\big(2\times 2\big)^{-\frac{1}{2}} + \Big(\sum_{i=1}^{t} 2^{i+1}\Big)\times\big(1\times 3\big)^{-\frac{1}{2}} + 2^{t+1}\times\big(1\times 2\big)^{-\frac{1}{2}} \\ &= 2^{\frac{2t+1}{2}}\times\big(1+\frac{7}{\sqrt{3}}\big)+2^t\times\big(14+\frac{4}{\sqrt{3}}\big)-\frac{4}{3}\sqrt{6}-\frac{4}{3}\sqrt{3}-13. \end{aligned}$$

This completes the proof. □

Theorem 4.6.2. *The Randić index of $D[n]$ for $n=2t$, where $t\geq 1$, can be defined as*

$$R_\alpha(D[n]) = \begin{cases} 90\times 2^{t+1}-164 & \text{if } \alpha=1, \\ 2^{\frac{2t+1}{2}}\times\big(14\sqrt{3}+\sqrt{2}\big)+2^t\times\big(4\sqrt{3}+40\big)-8\sqrt{6}-4\sqrt{3}-52 & \text{if } \alpha=\frac{1}{2}, \\ 2^{2t+1}\times\frac{29}{6}-\frac{55}{6} & \text{if } \alpha=-1, \\ 2^{\frac{2t+1}{2}}\times\big(1+\frac{7}{\sqrt{3}}\big)+2^t\times\big(10+\frac{4}{\sqrt{3}}\big)-\frac{4}{3}\sqrt{6}-\frac{4}{3}\sqrt{3}-13 & \text{if } \alpha=-\frac{1}{2}. \end{cases}$$

Proof. We use the Table 4.1 to prove the results.

When $\alpha = 1$:

By using the edge partition in Table 4.1 and formula (4.11), we get:

$$\begin{aligned} R_1(D[n]) &= \sum_{uv\in E(D[n])} \big(d_u d_v\big)^1 \\ &= \Big(\sum_{i=1}^{t} 2^i + \sum_{i=0}^{t}(2^i\times 6)\Big)\times\big(2\times 3\big)^1 + \Big(2+\sum_{i=2}^{t+1}(2^i\times 3)+\sum_{i=2}^{t}(2^i\times 4)\Big) \\ &\quad \times\big(2\times 2\big)^1 + \Big(\sum_{i=1}^{t} 2^{i+1}\Big)\times\big(1\times 3\big)^1 + 2^{t+1}\times\big(1\times 2\big)^1 \\ &= 90\times 2^{t+1} - 164. \end{aligned}$$

When $\alpha = \frac{1}{2}$:

By using the edge partition in Table 4.1 and formula (4.11), we get:

$$\begin{aligned} R_{\frac{1}{2}}(D[n]) &= \sum_{uv\in E(D[n])} \big(d_u d_v\big)^{\frac{1}{2}} \\ &= \Big(\sum_{i=1}^{t} 2^i + \sum_{i=0}^{t}(2^i\times 6)\Big)\times\big(2\times 3\big)^{\frac{1}{2}} + \Big(2+\sum_{i=2}^{t+1}(2^i\times 3)+\sum_{i=2}^{t}(2^i\times 4)\Big) \\ &\quad \times\big(2\times 2\big)^{\frac{1}{2}} + \Big(\sum_{i=1}^{t} 2^{i+1}\Big)\times\big(1\times 3\big)^{\frac{1}{2}} + 2^{t+1}\times\big(1\times 2\big)^{\frac{1}{2}} \\ &= 2^{\frac{2t+1}{2}}\times\big(14\sqrt{3}+2\big) + 2^t\times\big(4\sqrt{3}+40\big) - 8\sqrt{6} - 4\sqrt{3} - 52. \end{aligned}$$

When $\alpha = -1$:

By using the edge partition in Table 4.1 and formula (4.11), we get:

$$\begin{aligned} R_{-1}(D[n]) &= \sum_{uv\in E(D[n])} \big(d_u d_v\big)^{-1} \\ &= \Big(\sum_{i=1}^{t} 2^i + \sum_{i=0}^{t}(2^i\times 6)\Big)\times\big(2\times 3\big)^{-1} + \Big(2+\sum_{i=2}^{t+1}(2^i\times 3)+\sum_{i=2}^{t}(2^i\times 4)\Big) \\ &\quad \times\big(2\times 2\big)^{-1} + \Big(\sum_{i=1}^{t} 2^{i+1}\Big)\times\big(1\times 3\big)^{-1} + 2^{t+1}\times\big(1\times 2\big)^{-1} \\ &= 2^{t+1}\times\frac{29}{6} - \frac{55}{6}. \end{aligned}$$

When $\alpha = -\frac{1}{2}$:
By using the edge partition in Table 4.1 and formula (4.11), we get:

$$\begin{aligned} R_{-\frac{1}{2}}(D[n]) &= \sum_{uv\in E(D[n])} \big(d_u d_v\big)^{-\frac{1}{2}} \\ &= \Big(\sum_{i=1}^{t} 2^i + \sum_{i=0}^{t}(2^i\times 6)\Big)\times\big(2\times 3\big)^{-\frac{1}{2}} + \Big(2+\sum_{i=2}^{t+1}(2^i\times 3)+\sum_{i=2}^{t}(2^i\times 4)\Big) \\ &\quad \times\big(2\times 2\big)^{-\frac{1}{2}} + \Big(\sum_{i=1}^{t} 2^{i+1}\Big)\times\big(1\times 3\big)^{-\frac{1}{2}} + 2^{t+1}\times\big(1\times 2\big)^{-\frac{1}{2}} \\ &= 2^{\frac{2t+1}{2}}\times\big(1+\frac{7}{\sqrt{3}}\big) + 2^t\times\big(10+\frac{4}{\sqrt{3}}\big) - \frac{4}{3}\sqrt{6} - \frac{4}{3}\sqrt{3} - 13. \end{aligned}$$

This completes the proof. □

4.7 Conclusion

Topological indices are the numeric numbers which represent the whole structure of the graph. Topological indices developed for the purpose of obtaining correlations with physicochemical properties and biological activity of chemical substances have been applied for a very extensive rang.

In this thesis, first we introduce the graph theory and chemical graph theory. Further we discuss topological indices and give a brief introduction of different types of topological indices. After that, we consider a calss of hetrofunctional dendrimer and compute their eccentricity based topological indices, that is, eccentric connectivity indices. We also compute some eccentricity based Zagreb indices for this family of dendrimers.

Furthermore, for the matching based topological indices, we study number of perfect matchings and anti-Kekulé number of the dendrimer, when there is no perfect matching then we find size of maximum matching . For spectrum based topological indices, we computed nullity of the molecular these dendrimer. In the case of degree based topological indices, first we calculate the exact formula for the first and fourth of atom-bond connectivity index, first and fifth version of geometric-arithmatic index and Randić index for the hetrofunctional dendrimer.

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