A study of F-coindex for family of unicyclic graphs and dendrimers

by

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A thesis submitted to the

School of Natural Sciences (SNS),
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Dean/Principal

Dedicated

to my

Parents and Husband

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Abstract

Topological indices, sometimes also seen as graph-theoretic filters, maintain the order of molecular elements and provide mathematical language to predict features such as boiling points, radius of gyrations, viscosity, etc. These indices reflect topology and are usually mathematically holding fixed graph structures. There are certain important categories of topological indices relating to their specific topological features, such as degrees of vertices, distances between vertices, eccentricities of vertices, communication, etc. In this thesis, we study extremist graphs in relation to certain topological degree attackers. The graphs we emphasize include unicyclic graphs and dendrimers. Our main focus is on studying F-coindex. On smaller graphs the calculation of non-adjacent vertices is easily determined, however, on larger graphs, i.e., n vertices graphs, unicyclic graphs, chemical structures, etc., it is difficult to determine non-adjacent vertexes. First, we develop another F-coindex formula, which directly processes the non-adjacent vertices of large graphs, unicyclic networks, chemical structures, etc. The advantage of the changing formula is that it reduces calculation time and works effectively on almost every graph. Second, we determine the F-coindex of unicyclic networks, in addition, the minimum and maximum F-coindex of unicyclic networks are also estimated. Finally, we investigate the F-coindex of some dendrimers.

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Chapter 1

Fundamentals of Graph Theory

1.1 Introduction to Graph Theory

We start this dissertation with a brief and interesting historical note on the role of Euler in setting foundation of graph theory in this chapter. In Section 1.2, we will give a brief description of history of graph theory. In Section 1.3, we will utilize the vital terminologies, notions and definitions of modern graph theory. In Section 1.4, we will focus on different methods of graph operations. Section 1.5 is devoted to introduce the readers with trees and its related structures. In the last section, a short introduction on current research on extremal graphs is provided, whereas, all the notations defined in these sections will be followed throughout the thesis.

1.2 History of Graph Theory

Historically, most of the branches of mathematics come from basic problems of calculations and measurements. However, the ancestry of graph theory comes from mere puzzle like problems [1]. These problems caught the attention of mathematicians, as a result of which graph theory came into being. This subject has developed rapidly over the years. It has given many theoretical results of large variety, ranging from chemical structures to many

economic problems. In 1736, the city of Prussia named Königsberg was situated along the river which is familiar as Kaliningrad, Russia, in modern time. The river Pregelowed through the city was separated by a river into four land regions. These regions were joined by seven bridges. Residents of Königsberg are not sure about whether it was possible to walk from island to island by crossing seven bridges in one tour and come back to the initial point. This challenge is labeled by the Königsberg bridge problem. The mayor of Prussia Carl Gottlieb Ehler was concerned to this problem, and he wants to obtain the solution of it. Therefore, he discussed it with a Swiss mathematician Leonhard Euler in 1735. After which Euler studied the problem by eliminating the nonessential parts of the map as shown in the Figure 1.1. At that time, Euler concluded that the solution of

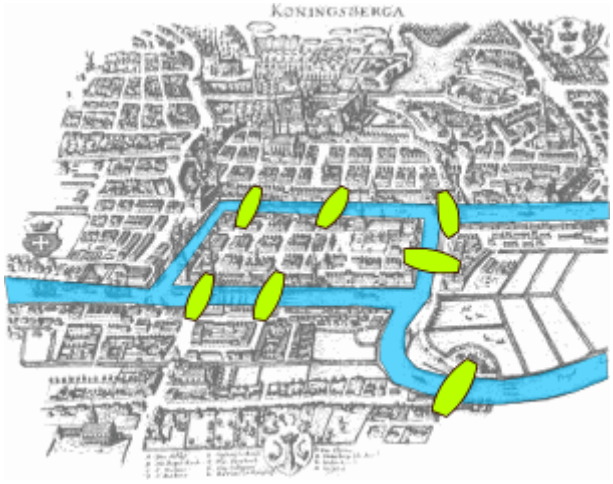

Figure 1.1: Königsberg bridge problem

the Königsberg bridge problem was impossible. Also, he wrote [2] on it and presented it in front of his teammates at the Academy of Sciences at St.Petersburg. Moreover, Euler gave the justification on it in [2] in 1736. It is noteworthy that Euler did not produce the type of graphs we use today. It was one century later that such graphs made an appearance. This kind of a solution in which a real life problem was converted into a mathematical phenomenon opened the gates to the solution of many other practical problems. Graph theory has solved many such problems by converting the elements

of certain problems into an abstract graph containing vertice, edges and preserving the relationship between vertices. Usually known that graph theory has implementations in combinatorics, but it has also beneficial applications in chemistry, optimization theory, biology, applied mathematics, electrical engineering, computer science, bioinformatics, network analysis, sociology, business administration, economics and other scientific and not-scientific areas.

1.3 Basics of Graph Theory

In this section, we will discuss some basic definitions and word phrases in relation to the concept of a graph. The graph, with the common notation $\tilde{G}$, can be defined as $\tilde{G} = (V(\tilde{G}), E(\tilde{G}))$, where the $v \in V$ item is defined as a vertex and the $e \in E$ item is called edge. Here each $e \in E$ item can be written as $\{u, v\}$ or simply uv for $u, v \in V$. The seamless graph, that is, $E = 0$ is called a null graph. V and E sets can also be represented by $V(\tilde{G})$ and $E(\tilde{G})$, respectively. In the graph, points indicate vertices and can represent anything, for example, people, cities, atoms, etc. The edges of the graph are indicated by lines or curves that connect the vertices and can represent acquaintances, roads, chemical bonds, etc. A graph with limited set of vertices and edges is called finite graph, otherwise, it is an endless (infinite) graph. Two or more edges that occur in one vertice are called multiple edges. A loop is an edge that joins the vertex itself. The e edge is said to be incident on v, only if v is the final vertex of e. The number of edges incident on a vertex v in $\tilde{G}$ represents its degree in the graph, denoted by d_u. Edges with a common end-vertex are called adjacent edges. Edges that do not have mutual end points are called separate edges or independent edges. Graphs that have multiple edges or loops are called multigraphs. Graphs that do not have many edges or loops are considered simple graphs. In a finite graph if their vertex is only one and there is no edge called a trivial graph. In a directed graph all the vertices are connected together, and all the edges are directed from one vertex to another. The null graph is a graph without

vertices. The total number of vertices and edges on the graph $|V(\tilde{G})| = \alpha$, $|E(\tilde{G})| = \beta$. Isolated vertex is that vertex which have no adjacent vertices and a pendent vertex have only adjacent vertex. Sequence of vertices $v_1, v_2, \ldots, v_\alpha$ in such a way that consecutive vertices are adjacent represent the walk. The first vertex in a row is called the first vertex, it says v_1, and the last vertex is called the last vertex, it says v_α. In a walk going through all the different edges is called a trail. If the walking vertices are different, then it becomes the path. The path in which the first and last vertex are the same is called the cycle. The order of the path or cycles is the number of vertices in it. Number of edges in path or cycle gives the length of the path and cycle. If no cycle is present in a connected graph then it is called a tree. An adjacency matrix of a graph $\tilde{G}$ is a square matrix used to represent a finite graph. Matrix entries indicate whether a pair of vertices are adjacent or not on the graph. The length of the short cycle contained in the graph is called the girth of the graph. If the graph does not have any cycles (that is, an acyclic graph), its magnitude is defined as infinite. For example, 4 -cycle (square) has girth 4.

1.4 Basic Operations

Basic operations are also known as graph editing functions. The graph editing function creates a new graph from the first with simple local changes, for example vertex additions, vertex or edges removal, vertices merging, vertices splitting, edge cutting, etc. We will describe some of the basic functions in graphs in this section, and these functions will be used to create new graphs with specific features. The basic graph in which these functions are used will significantly change the structure of the graph. First we describe some of the graph functions performed in a single graph. Let $\tilde{G}$ be a graph with vertex set $V(\tilde{G})$ and edge set $E(\tilde{G})$, after addition of a new vertex $u \notin V(\tilde{G})$ to $\tilde{G}$ then the resultant graph $\acute{\tilde{G}}$ will have $V(\acute{\tilde{G}}) = V(\tilde{G}) \cup \{u\}$ a new set of vertices. The edge set remains unchanged. This process is called vertex addition or a combination of graph and vertex. Similarly, when vertex v is removed from the $\tilde{G}$ graph, then vertex v and its incident edges are removed

to create a new graph, say Y. The vertex set and the edge of the new graph Y are offered by $V(Y) = V(\tilde{G}) \setminus \{v\}$ and $E(Y) = E(\tilde{G}) \setminus \{vw \in E(\tilde{G}) \mid w \in V(\tilde{G})\}$. This process is called vertex removal from the graph. When an edge $ab \notin E(\tilde{G})$, be added as a new edge to $\tilde{G}$ then the resultant graph Y' will have the new edge set $E(Y') = E(\tilde{G}) \cup \{ab\}$, this process is called edge addition and the vertex set remains unchanged. The deletion of an edge ab from $\tilde{G}$ involves removal of the edge $ab \in E(\tilde{G})$ such that the edge set of the new graph is given by $E(\tilde{G}) \setminus \{ab\}$ and vertex set remains unchanged. A vertex and an edge such that their removal transforms a connected graph into a graph having more than one components is called cut-vertex and cut-edge. Minimal edge set is the smallest possible set of edges required to keep the graph connected. There may exist more than one minimal edge sets.

Example 1.1. When we remove a vertex from a given graph of $\tilde{G}$, we must remove the entire edges incident on that vertex. Once we have removed the vertex then the adjacent matrix will not contain the row and column of the corresponding vertex. This function converts the vertex and edge family of the graph. Below the image helps to understand vertex removal.

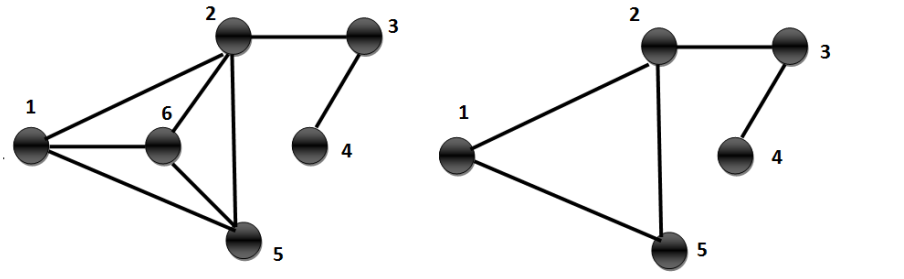

Figure 1.2: Vertex deletion

Example 1.2. Graph complement $\hat{G}$ is a graph that has the same vertices as $\tilde{G}$ but the edges defined by two vertices in the complement is adjacent only if they are not adjacent in $\tilde{G}$. The Complement of a graph is demonstrated in the below Figure 1.3.

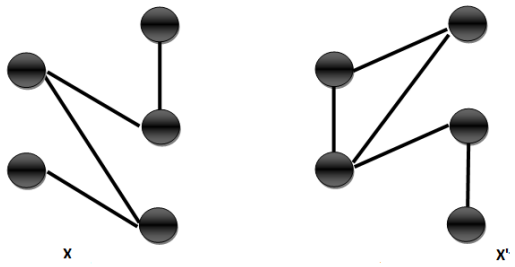

Figure 1.3: Complement

Several other operations on graphs can be found in Harary and Wilcox [3]. For advanced contents on graph operations, reader is referred to a handbook on product graphs [4].

1.5 Isomorphic Graphs

A graph can be constructed in miscellaneous ways in which the shape of edges are not significant. All such drawings of a graph refer to the same graph and are described as isomorphic graphs. These graphs fulfill some conditions. Consider two graphs, namely R and S such that $R = (V(R), E(R))$ and $S = (V(S), E(S))$. R and S are isomorphic if there exist functions r and s such that, $r : V(R) \rightarrow V(S)$ and $s : E(R) \rightarrow E(S)$ such that $s(uv) = s(u)k(v)$, where uv is an edge in graph R and $s(u)h(v)$ is an edge in graph S. In other words, both graphs should have the same number of vertices, edges, loops, components and parallel edges, etc. In isomorphism, both graphs must have the same properties, for example, layout, size, vertex degree sequence, equal number of cycle lengths, similar complements, etc. However, these scenarios are not enough to prove that the two graphs are isomorphic to each other for a large n.

1.6 Connectivity and Distances

In graph $\tilde{G}$, a subgraph that is not contained in any other connected subgraph of $\tilde{G}$ is called component. When $\tilde{G}$ has more than one components, it is called disconnected. In a connected graph $\tilde{G}$, a cut-vertex $v \in V(\tilde{G})$ has the property that $\tilde{G} - v$ is disconnected, and a cut-edge $e \in E(\tilde{G})$ is such that $\tilde{G} - e$ is disconnected. An edge (cut-edge) is a bridge if and only if it does not belong to a cycle. A connected subgraph of $\tilde{G}$ with no cut-vertex and is not contained in a larger connected subgraph of $\tilde{G}$ is known as a block. Distance $d_{\tilde{G}(k,l)}$ between k and l is defined as the length of a shortest path between them. Largest distance from a vertex k to any other vertex is called eccentricity $e_{\tilde{G}(k)}$ of k. A connected graph is that in which we find a path for every pair of vertices that connects them. If there exists vertices $k, l \in V$ in $\tilde{G}$ such that there exists no path between them then $\tilde{G}$ is called a disconnected graph. In acyclic graph there is not any cycle present. A connected and acyclic graph is known as a tree. There are some families of graphs which are called tree-like structures because they become a tree after deletion of a some edges.

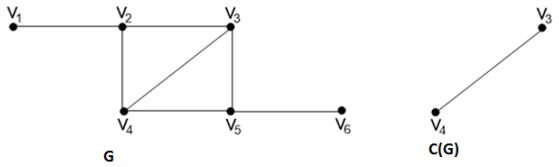

Figure 1.4: The center $C(\tilde{G})$ of a graph $\tilde{G}$.

1.7 Structure of Trees

Tree is a connected and acyclic graph and it is represented by T. In a tree T, a non-pendent vertex is said to be an internal vertex and every pair of distinct vertices of T are linked by a single path.Edges of the tree are called branches and the elements of trees are called their nodes. In the above figure. 1.7, all are trees with fewer than 6 vertices.

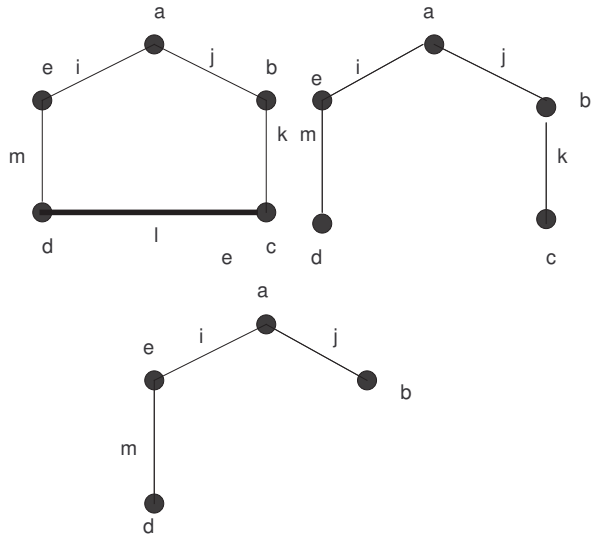

Figure 1.5: Deletion of an edge and vertex.

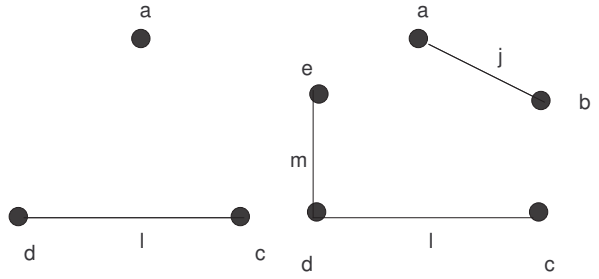

Figure 1.6: Edge-cut and vertex-cut.

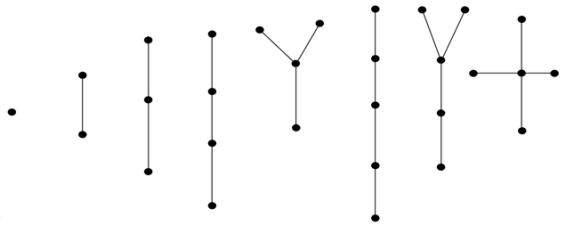

Figure 1.7: Trees with fewer than 6 vertices

1.8 Forest

In the context of graph theory, the undirected, disconnected and acyclic graph is called a forest. In other words, a disjoint collection of trees is known as forest. Each tree is

the part of a forest. Thus a forest is a graph such that all of its components are trees. There are no cycles in the given graph and it is a single disconnected graph therefore it

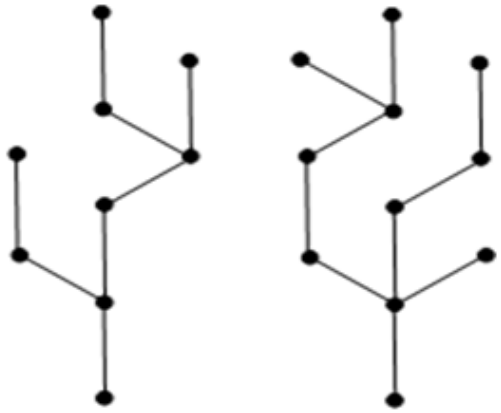

Figure 1.8: Forest

is a forest.

1.9 Star Graph

A star S_α is an α-vertex tree with $(\alpha - 1)$ pendent vertices. Star graph is a special type of graph where central vertex has $(\alpha - 1)$ degree and $(\alpha - 1)$ vertices have a degree 1. This looks likes $(\alpha - 1)$ vertices are connected to a one central vertex. A graph is said to be a caterpillar with a tree $\alpha \geq 3$ if the removal of its pendent vertices gives a path.

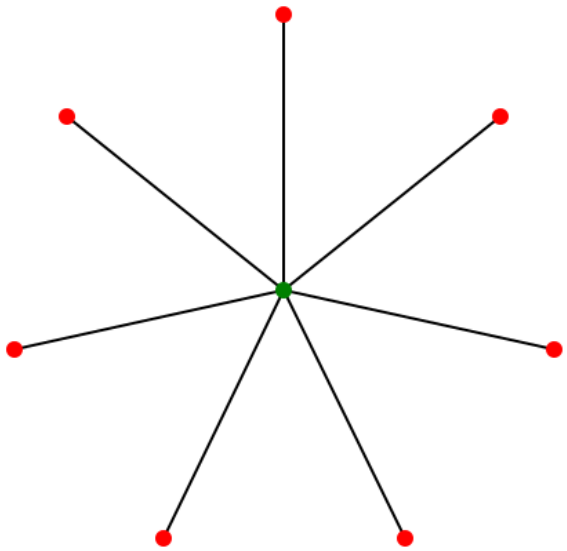

Figure 1.9: Star graph of order α

1.10 Extremal Graph Theory

In extremal graph theory, the researchers analyzed the effect of earth structures (order, size, analogy, independence number, etc.) of the graph on its local structures. To date, identifying extremal graphs (the smallest or largest) in a given category of graphs in relation to topological indices has become an important indicator in the concept of extremal graph. In line with these lines, excellent results have been obtained. We see that extremal graphs are proportional to certain given categories of graphs. In 1907, Mantel [5] provided an answer to the extremal problem of what is the largest size of the trianglae-free graph

$\tilde{G}$. At 1941, Turán [6] began work on advancing extremal graph theory when he decided to do a Mantel theorem.

Lemma 1.3. *(Turán [6]). For a given $r \in 3, 4 \ldots \alpha$, what is the maximal size graph that does not contain K_r.*

Other motivational work on extremal graphs can be found in [7], [8], [9].

Chapter 2

Chemical Graph Theory and Topological Invariants

Over the past two centuries, a lot of research work has been done in the implementations of chemistry and graph theory in different fields by investigators. In later 18^{th} century, chemical graphs were first used as the fundamental study of particles and matters. We mention some famous mathematicians who, in the past, have studied chemical problems. Cayley [10] used alkane trees to examine diferent categories of isomers. Sylvester [11] who observed the similarity between a chemical constitutional formula and a graph in 1878. In 1970, Read and Harary [12] studied the famous polyhex problem of enumerating polycyclic aromatic molecules.

A molecular graph $\tilde{G}$ is generally known as a chemical graph, where vertices and edges of $\tilde{G}$ correlate to atoms and chemical bonds, respectively. Topological indices are described as numerical parameters of molecular structures, and they perform a crucial part in the detection of the physical-chemical characterizations of molecules. For applications of topological indices in drug design, we refer to a book published by Kier and Hall [13]. This chapter comprises of basic definition of topological index which are provided in Section 2.1, whereas the details of oldest topological index and some important known results related to these index are included in Section 2.2.

2.1 Topological Invariants

Topological invariants have long been used in mathematical chemistry. These are the calculation based values, as the experimentation, availability of resources and manpower takes alot of time. These invariants provide the chemists and mathematicians with valuable information regarding structural, physical, organic and medicinal chemistry [14]. Many of the old indicies, to this date, which are conceptually simple and computationally straightforward offer satisfactory structure-property-activity relations. They are very useful in Quantitative structureactivity relationship models (QSAR models) and QSPR Quantitative Structure-Property Relationship (QSPRs) studies [15–21].To date, over 1000 research articles on the subject have appeared [22,23] and a book [24]. Topological indices may be classified into several categories depending upon the specific topological feature which they measure. Some basic topological features include degrees of vertices, distances between vertices, matching of different sizes in a graph, etc. These features categorize topological indices into degree-based, distance-based, counting-polynomials based indices and into some other types as well.

2.2 Some Old and New Topological Indices

Let $\tilde{G}$ be a connected and simple graph with vertex set $V(\tilde{G})$ and edge set $E(\tilde{G})$. Harold Wiener [25] in 1947 represented the first and the most notable indecator, the Wiener index $W(\tilde{G})$, in his study of the effect of pure diversity in the area where paraffin boils. He called it path number and is now known as Wiener index $W(\tilde{G})$ of graph $\tilde{G}$. Later on, Hosoya [26] in 1971, described the notion of Wiener index for $\tilde{G}$ as:

$$W(\tilde{G}) = \sum_{(u,v)\in V(\tilde{G})} d(u,v). \tag{2.1}$$

In study [25] he also introduced the concept of Wiener polarity index $W_p(\tilde{G})$. Physical-chemical interpretation of Winer polarity index $W_p(X)$ is found by Hosoya [26]. The

Winer polarity index [25] is defined by (2.2) for $u, v \in V$ as:

$$W_p(\tilde{G}) = \big|\{\{u, v\} \subseteq V(\tilde{G}) \mid d_X(u, v) = 3\}\big|. \tag{2.2}$$

To calculate paraffin boiling points a linear formula based on W and W_p was used. Some recent works of the Wiener polarity index for trees with different parameters are provided [27, 28]. It helped to calculate system robustness and also been used for lattice networks. Lukovits and Linert [29] introduced quantitative structural relationships in a series of hydrocarbons containing acyclic and cycles using the wiener polarity index. The Wiener polarity index for fullerenes and six-dimensional systems was read in [30]. Recently, Arockiaraj et al. [31], read the hyper-Wiener and Wiener polarity articles for silicate and oxide networks. The hyper Wiener $WW(\tilde{G})$ indicator is also an old indicator and a continuation of the Wiener index. Hyper Wiener index $WW(\tilde{G})$ of $\tilde{G}$, translated by Randiác [32], provided by:

$$WW(\tilde{G}) = \frac{1}{2} \sum_{u \in V(\tilde{G})} \sum_{v \in V(\tilde{G})} \left(d(u, v) + d(u, v)^2\right). \tag{2.3}$$

Relation between Wiener polarity index and Zagreb indices (M_1, M_2) was given by Muhuo Liu and Bolian Liu [33], which is given in following theorem:

Theorem 2.1. *For a graph $\tilde{G}$ with k vertices and l edges $W_p = M_2 - M_1 + k$, when $\tilde{G}$ is connected, $W_p = M_2 - M_1 + k$, if $\tilde{G}$ is a tree.*

In the most studied families of molecular graphs, Benzenoid systems and carbon nanotubes Niko Tratnik [34], in the year 2018, developed a method for computing the Wiener polarity index.

In this thesis, we emphasize on those topological indices which are defined in terms of degrees and distances in graph $\tilde{G}$. Now we discuss some degree and distance-based topological indices. A research on the structure-dependency of total π- electron energy E_π in 1972 proposed an approach to the branching of the carbon-atom skeleton by demonstrating that the sum of squares of the vertex degrees of the molecular graph can determine

E_π, that were described by Gutman and Trinajstic [35] and named it the Zagreb group indices. More details on total π-electron energy can be found in Gutman et al. [36–38], Angelina et al. [39], T$\ddot{u}$rker and Gutman [40], Jones et al. [41], Radenković and Gutman [42], Peric et al. [43], Morales [44], Markovic [45], and Morales [46]. Now a days, these invariants are titled with the Zagreb indices and are specified as follows:

$$M_1(\tilde{G}) = \sum_{v \in V(\tilde{G})} d_v^2 = \sum_{uv \in E(\tilde{G})} (d_u + d_v), \tag{2.4}$$

$$M_2(\tilde{G}) = \sum_{uv \in E(\tilde{G})} d_u d_v. \tag{2.5}$$

It was immediately recognized that these terms provide quantitative measures of molecular branching [47,51–56]. For properties of the two Zagreb indices [48–50]. New degreebased Zagreb index named hyper-Zagrebindex as:

$$HM(\tilde{G}) = \sum_{uv \in E(\tilde{G})} (d_u + d_v)^2. \tag{2.6}$$

are introduced by Shirdeletal. [58] in 2013. In 2012 Ghorbani and Azimi [59] determined the two new versions of Zagreb indices called first multiple Zagreb index $PM_1(\tilde{G})$ and second multiple Zagreb index $PM_2(\tilde{G})$ of graph $\tilde{G}$ are defined as:

$$PM_1(\tilde{G}) = \sum_{uv \in E(\tilde{G})} [d_u + d_v], \tag{2.7}$$

$$PM_2(\tilde{G}) = \sum_{uv \in E(\tilde{G})} [d_u \times d_v]. \tag{2.8}$$

The Zagreb polynomials $M_1(\tilde{G}, X)$, $M_2(\tilde{G}, X)$ are defined as:

$$M_1(\tilde{G}, X) = \sum_{uv \in E(\tilde{G})} X^{(d_u + d_v)}, \tag{2.9}$$

$$M_2(\tilde{G}, X) = \sum_{uv \in E(\tilde{G})} X^{(d_u \times d_v)}. \tag{2.10}$$

For some chemical structures the properties of $M_1(\tilde{G}, X)$, $M_2(\tilde{G}, X)$ polynomials have been studied in [60]. The redefined Zagreb index is defined by Ranjini et al. [61], named

as the redefined first, second and third Zagreb indices of graph G. These indices appear as:

$$ReZG_1(\tilde{G}) = \sum_{uv \in E(\tilde{G})} \frac{du + dv}{du.dv}, \tag{2.11}$$

$$ReZG_2(\tilde{G}) = \sum_{uv \in E(\tilde{G})} \frac{du.dv}{du + dv}, \tag{2.12}$$

$$ReZG_3(\tilde{G}) = \sum_{uv \in E(\tilde{G})} (du.dv)(du + dv). \tag{2.13}$$

For multiplicative Zagreb indices some upper bonds for different graph operations are derived by Das et al. [62]. Veylaki et al. [63], enmerate third hyper-Zagreb index and hyper-Zagreb coindices of some graph operations.

In 1975, Randić [64] investigated a novel topological invariant to judge the boundaries of branching of the carbon-atom skeleton of saturated hydrocarbons. Now a days, it is known as Randic index. The Randić index is the known and the most applied invariant among all topological invariants.it is described as follows:

$$R(\tilde{G}) = \sum_{(u,v) \in E(\tilde{G})} (d_u d_v)^{-\frac{1}{2}}. \tag{2.14}$$

It was designed to reflect the amount of branching present in a chemical species. Using this index, very good correlations were again obtained with a spacious range of physico-chemical properties, such as vapor pressure and chromatographic retention times. For drug designs randic index was immediately calculated. Later, in 1998, Bollobas and Erdós [65] presented the generalization of Randić index and called it general Randić index. It was specified as follows:

$$R_\gamma(\tilde{G}) = \sum_{(u,v) \in E(\tilde{G})} (d_u d_v)^{\gamma}, \tag{2.15}$$

where γ is a real number. Therefore the Randić connectivity index of graph G is $R^{-\frac{1}{2}}$. The general sum-connectivity index is a late topological invariant that was designed by Zhou and Trinajstić [66]. They replaced the product term $(d_u d_v)$ by $(d_u + d_v)$ in the

general Randić index and written as follows:

$$\chi_\gamma(\tilde{G}) = \sum_{(u,v)\in E(\tilde{G})} (d_u + d_v)^2, \tag{2.16}$$

where γ

is a real number. Therefore χ_γ is the classical sum-connectivity index, which was investigated by Zhou and Trinajstić [67]. Following zagreb first and second indices, Furtula and Gutman (2015) introduced forgotten topological index (also called F-index) which was defined as:

$$F(\tilde{G}) = \sum_{v\in V(\tilde{G})} d_v^3 = \sum_{uv\in E(\tilde{G})} (d_u^2 + d_v^2). \tag{2.17}$$

Where the degree of vertex v is denoted as d_v. In a contemporary research on the structure-dependency of the total π-electron energy, it was designate that another term on which this energy depends is F-index. Li and Zheng in [68], generalised the first Zagreb index and F-index as follows:

$$M^\gamma(\tilde{G}) = \sum_{(u)\in V(\tilde{G})} (d_u)^\gamma. \tag{2.18}$$

where, $\gamma \neq 0, 1$ clearly, when $\gamma = 2$ and $\gamma \in R$. According to the International Academy of Mathematical Chemistry, determining whether there is any topological index useful in predicting chemical properties, the coorelation between the values of that octane isomer formation and the parameter values associated with their specific physicochemical properties should be considered. Octane isomers are generally suitable for such studies, because the number of isomers of the octane structure is large enough to make the mathematical conclusion reliable. Fururtula and Gutman. [69] suggested that the predictive ability of the forgotten topological index is almost the same as that of the original Zagreb index with acentric factor and entropy, and both received coefficients greater than 0.95. On the other hand, in some physicochemical structures, either M_1 or F does not correspond satisfactorily. A simple linear model is devised for the improvement of the predictive ability of these indices:

$$M_1 + \lambda F \tag{2.19}$$

where λ is fitting parameter. Its value varied from -20 to 20 to achieve the best correlation. The above model has been applied to each physico-chemical properties provided in the octane database. Unfortunately, for all but one physico-chemical asset, the improvements achieved by the model (2.19) were not significant. Surprisingly, however, in the case of an octanol-water coefficient, significant improvements could be made. Although there have been a number of contributions to distance-based indices and degree based standardized cell structures, researchers have forgotten the F-index of specific specialized drug components. This fact explains why the forgotten index is useful in examining the chemical and pharmacological properties of drug molecules. F-index for different graph operations was read by the present authors in [70]. Recently, the forgotten topological index of certain drug molecular structures is demonstrated by, Gao et al. (2016a). Abdo et al. [71] manifested the extremal trees with respect to the F-index. As a result, great interest in education and industry has been drawn into researching the forgotten index of drug molecular structure from a mathematical perspective. With ongoing work on Gao et al. (2016a), we find a forgotten topological index of important chemical structures with high frequency in drug structures. Similar to other topological polynomials, the F-polynomial graph $\tilde{G}$ is also described as:

$$F(\tilde{G}, X) = \sum_{uv \in E(\tilde{G})} X^{(d_u^2 + d_v^2)}. \tag{2.20}$$

De at al. [72], study basic properties, some are prescribed in the following theorems:

Proposition 2.2. *(Furtula [69]) For a graph $\tilde{G}$ with β edges, and $M_1(\tilde{G})$ is first Zagreb index. Then*

$$F(\tilde{G}) \geq \frac{M_1(\tilde{G})^2}{2\beta}. \tag{2.21}$$

Proposition 2.3. *(Furtula [69]) Let $\tilde{G}$ be a graph with β edges, and $M_1(G)$, $M_2(\tilde{G})$ are first and second Zagreb indices respectively. Then*

$$F(\tilde{G}) \geq \frac{M_1(\tilde{G})^2}{\beta} - 2M_2(\tilde{G}). \tag{2.22}$$

Proposition 2.4. *(Furtula [69]) Let $\tilde{G}$ be a connected graph with α vertices and β edges, and $M_2(\tilde{G})$ is second Zagreb index. Then*

$$F(\tilde{G}) \geq 2M_2(\tilde{G}) + \beta(\alpha - 2). \tag{2.23}$$

Equality is accomplish if and only if $\tilde{G}$ is the star graph.

Wei.Gao. [73] studied the F-index of some chemical graphs some results are given as:

Theorem 2.5. *(Nilanjan [98]) Let $NS_1[k]$ be the nanostar dendrimer. Then*

$$F(NS_1[k]) = 5.2^k + 1 + 40(2^k - 1) + 8(12.2^k - 11). \tag{2.24}$$

Theorem 2.6. *(Nilanjan [98]) Let $NS_2[k]$ be the nanostar dendrimer. Then*

$$F(NS_2[k]) = 5.2^k + 1 + 8(8.2^k - 5) + 13(6.2^k - 6). \tag{2.25}$$

Theorem 2.7. *(Yasir [74]) Let $\tilde{G}$ be the molecular graph of $PETIM$ dendrimer. Then*

$$F(\tilde{G}) = 216 \times 2k - 222.$$

$$F(\tilde{G}, X) = 2^{k+1}x^5 + (16 \times 2^k - 18)x^8 + (6 \times 2^k - 6)x^13.$$

Y et.al [74] studied the F-index of some dendrimers sturcture some are given as:

Theorem 2.8. *(Yasir [74]) Let D_nP_n be a Porphyrin dendrimer. Then*

$$F(D_nP_n) = 1566k - 118.$$

$$F(D_nP_n, x) = 2kx^{10} + 24kx^{17} + (10k - 5)x^8 + (48k - 6)x^{13} + 13kx^{18} + 8kx^{25}.$$

Theorem 2.9. *(Yasir [74]) Let DPZ_n be a zincporphyrin dendrimer. Then*

$$F(DPZ_n) = 792 \times 2^k - 428.$$

Recently, Akther, et.al [75] manifested F-index of extremal graphs between the categories of unicyclic and bicyclic graphs. In the enumeration of weighted Wiener polynomial of certain composite graphs Doslic [76] introduced Zagreb coindices. Thus the Zagreb coindices of $\tilde{G}$ are termed as :

$$\bar{M_1} = \sum_{uv \notin E(\tilde{G})} [d_u + d_v], \tag{2.26}$$

and

$$\bar{M_2} = \sum_{uv \notin E(\tilde{G})} (d_u d_v). \tag{2.27}$$

Formal definitions of Zagreb coindices and basic properties were reported by Ashrafi, et. al. [77]. By the motivation of the work of Ashrafi, et al. [77], very recently, De, et. al. [72] have studied the coindex version of F-index. It is manifested as

$$\bar{F}(\tilde{G}) = \sum_{uv \notin E(\tilde{G})} \left(d_u^2 + d_v^2\right), \tag{2.28}$$

in which sum is taken over square of the degrees of every pair of non-adjacent vertices. The complement of graph $\tilde{G}$ is denoted by $\bar{\tilde{G}}$, is a simple graph in which two vertices u and v are non-adjacent on the same set of vertices $V(\tilde{G})$, if and only if they are adjacent in $\tilde{G}$. F-index and F-coindex research is an active research site now a days and we can find many good articles, for example D, at al. [72], analyze the performance of the newly launched F-coindex, basic mathematical properties and under various graph functions.Ruhul Amin [78] determines the extremal trees with the first minimum, second minimum and third minimum F-coindex. Using graph analysis and composition, Melaku Berhe [79] researches the F-coindex of other chemical molecular graphs that appear frequently in medical engineering. Nilanjan De. [80] study, explicit statements of F-index and coindex of extruded graphs such as line graph, division graph, vertex-semitotal graph, edge-semitotal graph, total graph, complete graph and paraline graph (line graph of subdivision graph) are obtained. In this thesis, we provide an alternative form of F-coindex. Then we use these properties to study extremal graphs for F-coindex for the

family of unicyclic graphs and also by using this alternative form we calculate F-coindex of some dendrimers. Now we have some results on F-coindex.

2.3 Basic Results

The basic calculation of the F-coindex can be performed for some special families of graphs as an introductory exercise. For an α-vertex graph X with $\alpha \geq 4$, a few such calculations are performed below. Let P_α, C_α, $K_{1,\alpha-1}$ and K_α be the path, cycle, star and complete graphs on n vertices. Then F-coindex for these graphs are as follows:

(i) $\bar{F}(P_\alpha) = 4\alpha^2 - 18\alpha + 20$

(ii) $\bar{F}(C_\alpha) = 4\alpha^2 - 12\alpha$

(iii) $\bar{F}(K(1, \alpha - 1)) = (\alpha - 1)(\alpha - 2)$

(iv) $\bar{F}(K_\alpha) = 0$

Ruhul Amin [78] determine the extremal trees with minimum, second minimum and third minimum F-coindex as given below:

Lemma 2.10. *(Rahul [78]) Let T_1 be a tree of order α. Assume that $P = u_{d1}u_d...u_\alpha$ is a longest path in T_1 with $d = d(u_d) \geq 2$, and $u_1, u_2, ..., u_{d2}$ are neighbours of u_d other than u_{d1}, u_{d+1}. T_2 is formed by deleting the edges $u_du_1, u_du_2, ..., u_du_{d2}$ and adding the edges $u_{d1}u_1, u_{d1}u_2, ..., u_{d1}u_{d2}$. Then*

$$\bar{F}(T_1) < \bar{F}(T_2),$$

if

$$d < \frac{[1 + 2\alpha]}{6} + 1.$$

Lemma 2.11. *(Rahul [78]) Let T_1 be a tree of order α. Assume that $P = u_{d1}u_d...u_\alpha$ is the longest path in T_1 with $d(u_d) = d(u_{\alpha 1}) = 2$, and $d = d(u_k) \geq 2$ for some $d + 1 \leq k \leq \alpha 2$.*

$u_1, u_2..., u_{d2}$ are the neighbors of u_k other than u_{k1}, u_{k+1}. T_2 is formed by deleting the edge $u_k u_1$ and adding a new edge $u_{d1}u_1$. Then

$$\bar{F}(T_1) > \bar{F}(T_2)$$

if

$$d < \frac{[2\alpha + 1]}{6} + 1$$

and

$$\bar{F}(T_1) < \bar{F}(T_2)$$

if

$$d > \frac{[2\alpha + 1]}{6} + 1.$$

Theorem 2.12. *(Rahul [78]) Among trees with α vertices The star S_α has minimum F-coindex when $\alpha > 3$. ,*

De at al. [72], study basic mathematical properties, some are given in the following theorems:

Proposition 2.13. *(Nilanjan [72]) Let $\tilde{G}$ be a simple graph with α vertices and β edges, then*

$$\bar{F}(\tilde{G}) = F(\bar{\tilde{G}}) - 2(\alpha - 1)M_1(\bar{\tilde{G}}) + 2\bar{\beta}(\alpha - 1)^2. \tag{2.29}$$

Proposition 2.14. *(Nilanjan [72]) Let $\tilde{G}$ be a simple graph with α vertices and β edges, then*

$$\bar{F}(\tilde{G}) = (\alpha - 1)M_1(\tilde{G}) - F(\tilde{G}). \tag{2.30}$$

Proposition 2.15. *(Nilanjan [72]) Let $\tilde{G}$ be a simple graph with α vertices and β edges, then*

$$\bar{F}(\tilde{G}) = 2\beta(\alpha - 1)^2 - (\alpha - 1)M_1(\tilde{G}) - \bar{F}(\tilde{G}). \tag{2.31}$$

Proposition 2.16. *(Nilanjan [72]) Let $\tilde{G}$ be a simple graph with α vertices and β edges, then*

$$\bar{F}(\tilde{G}_1 U \tilde{G}_2) = \bar{F}(\tilde{G}_1) + \bar{F}(\tilde{G}_2) + \alpha_2 M_1(\tilde{G}_1) + \alpha_1 M_1(\tilde{G}_2). \tag{2.32}$$

Proposition 2.17. *(Nilanjan [72]) Let $\tilde{G}$ be a simple graph with α vertices and β edges, then*

$$\bar{F}(\tilde{G}_1 + \tilde{G}_2) = \bar{F}(\tilde{G}_1) + \bar{F}(\tilde{G}_2) + 2\alpha_2\bar{M}_1(\tilde{G}_1) + 2\alpha_1\bar{M}_1(\tilde{G}_2) + 2\alpha_2^2\bar{\beta}_1 + 2\alpha_1^2\bar{\beta}_2. \quad (2.33)$$

Corollary 2.18. *(Nilanjan [72]) The F-coindex of suspension of $\tilde{G}$ is given by*

$$\bar{F}(\tilde{G} + K_1) = \bar{F}(\tilde{G}) + 2\bar{M}_1(\tilde{G}) + 2\bar{\beta}. \quad (2.34)$$

Nilanjan De. [80] study, the explicit expressions for F-index and coindex of derived graphs, some are given as:

Theorem 2.19. *(Nilanjan [72]) Let $\tilde{G}$ be the line graph of the subdivision graph of the cycle C_α with α vertices. Then F-coindex of $\tilde{G}$ is*

$$\bar{F}(\tilde{G}) = 16\alpha^2 - 16\alpha. \quad (2.35)$$

Theorem 2.20. *(Nilanjan [72]) Let $\tilde{G}$ be the line graph of the subdivision graph of the star S_α with α vertices. Then F-coindex of $\tilde{G}$ is*

$$\bar{F}(\tilde{G}) = (\alpha - 1)(\alpha - 2)(\alpha^2 - 2\alpha + 3). \quad (2.36)$$

Chapter 3

F-coindex of Extremal Graphs

In this chapter, we provide an alternative form of F-coindex. Then we use this to study different properties of unicyclic graphs. Then we use these properties to study extremal graphs for F-coindex for the family of unicyclic graphs. The subsequent part of this chapter is organized as; Section 3.1 covers basic definations and results, Section 3.2 provides main results on the unicyclic family of graphs having minimum and maximum F-coindex. Finally, we concluded our findings in the last section.

3.1 F-coindex an Alternative Formula

Let $\tilde{G}$ be a connected graph where $V(\tilde{G})$ and $E(\tilde{G})$ denote vertex and edge sets, respectively. Further note that the order and size of $\tilde{G}$ are given by $|V(\tilde{G})|$ and $|E(\tilde{G})|$, receptively. Note that an edge $e = uv \in E(\tilde{G})$ implies that u and v are adjacent. On the other hand $uw \notin E(\tilde{G})$ shows that vertices u and w are not adjacent. Moreover d_u denotes the degree of $u \in V(\tilde{G}) \left(or\ u \in \tilde{G}\right)$ and N_u denotes the number of vertices not adjacent to $u \in \tilde{G}$, Mathematically,

$$N_u = |\{w|uw \notin E(\tilde{G})\}|, \quad \text{for } u \in \tilde{G}. \tag{3.1}$$

The Forgotten topological index is defined by

$$F(\tilde{G}) = \sum_{v \in V(\tilde{G})} d_v^3. \tag{3.2}$$

The equation(3.2) can be written as

$$F(\tilde{G}) = \sum_{uv \in E(\tilde{G})} \left(d_u^2 + d_v^2\right). \tag{3.3}$$

It can be noted that first general Zagreb index is defined by $M_1^\alpha = \sum_{uv \in E(\tilde{G})} (d_u^{\alpha-1} + d_v^{\alpha-1})$, reduces to Forgotten index for $\alpha = 3$.

In the similar way, F-coindex is denoted and defined as follows

$$\bar{F}(\tilde{G}) = \sum_{uv \notin E(\tilde{G})} \left(d_u^2 + d_v^2\right). \tag{3.4}$$

The complement of $\tilde{G}$, denoted by $\bar{\tilde{G}}$, is a simple graph such that

$$V(\tilde{G}) = V(\bar{\tilde{G}}), \quad E(\bar{\tilde{G}}) = \{uv \mid uv \notin E(\tilde{G})\}.$$

Obviously, $E(\tilde{G}) \cup E(\bar{\tilde{G}}) = E(K_\alpha)$, where K_α, represents a complete graph of order α. So if v has degree d_v in $\tilde{G}$ then degree of the same vertex will be $\alpha - 1 - d_v$, in $\bar{\tilde{G}}$.

Lemma 3.1. *Let $\tilde{G}$ be any graph with n vertices and $u \in \tilde{G}$ such that degree of u is d_u. Then number of non-adjacent vertices to u is given by*

$$N_u = n - 1 - d_u. \tag{3.5}$$

Proof. There are $n-1$ vertices other than u and u is adjacent to d_u vertices. Thus there are $n - 1 - d_u$ vertices that are not adjacent to u.

Now we present a new form of F-coindex that makes computations of F-coindex simpler than $\sum_{uv \in E(\bar{\tilde{G}})}[d_u^2 + d_v^2]$. □

Theorem 3.2. *Let $\tilde{G}$ be any graph. Then F-coindex of $\tilde{G}$ may be written as*

$$\bar{F}(\tilde{G}) = \sum_{u \in \tilde{G}} d_u^2 \times N_u. \tag{3.6}$$

Proof. We know that for any graph $\tilde{G}$ we define F-coindex as follows

$$\bar{F}(\tilde{G}) = \sum_{uv \in E(\bar{\tilde{G}})} [d_u^2 + d_v^2], \quad \text{or} \quad \bar{F}(\tilde{G}) = \sum_{uv \notin E(\tilde{G})} [d_u^2 + d_v^2].$$

For any vertex u, the term d_u^2 appears in F-coindex for each pair of vertex that is not adjacent to u. This means that d_u^2 appears N_u times. The same is true for each vertex. Thus

$$\bar{F}(\tilde{G}) = \sum_{uv \notin E(\tilde{G})} [d_u^2 + d_v^2] = \sum_{u \in \tilde{G}} d_u^2 \times N_u.$$

Using expression of N_u from eq(3.5), in the last expression we obtain

$$\bar{F}(\tilde{G}) = \sum_{u \in \tilde{G}} \left[(n-1)\, d_u^2 - d_u^3 \right]. \tag{3.7}$$

□

3.2 Basic Results

Here we present some basic results by using alternative form of F-coindex. For an n-vertex graph $\tilde{G}$ with $n \geq 4$, a few such calculations are performed below. Let P_n, C_n, $K_{1,n-1}$ and K_n be the path, cycle, star and complete graphs on n vertices. Then F-coindex for these graphs are as follows:

Lemma 3.3. *(i)* $\bar{F}(P_n) = 4n^2 - 18n + 20$

(ii) $\bar{F}(S_n) = n^2 - 3n + 2$

(iii) $\bar{F}(C_n) = 4n^2 - 12n$

(iv) $\bar{F}(K1, n-1) = (n-1)(n-2)$

(v) $\bar{F}(K_n) = 0$

Proof. (i) Let we have an n-vertex path in which pendent vertices have degree 1 which are only two and remaning $n-2$ vertices have degree 2, now by using equation (3.6), we have

$$\overline{F}(P_n) = \sum_{u \in P_n} d_u^2 \times N_u = [(1)^2 \times (n-2) \times (2) + (2)^2 \times (n-3) \times (n-2)] = 4n^2 - 18n + 20.$$

(ii) Let we have an n-vertex star in which pendent vertices have degree 1 which are $n-1$ and remaning 1 vertix have degree $n-1$. Now by using equation (3.6), we have

$$\overline{F}(S_n) = \sum_{u \in S_n} d_u^2 \times N_u = [(1)^2 \times (n-2) \times (n-1) + (n-1)^2 \times (0) \times (1)] = n^2 - 3n + 2.$$

(iii) Now we have an n-vertex cycle C_n in which all vertices have degree 2, now by using equation (3.6), we have

$$\overline{F}(C_n) = \sum_{u \in c_n} d_u^2 \times N_u = [(2)^2 \times (n-3) \times (n)] = 4n^2 - 12n.$$

same as for $(iv) - (v)$. □

3.3 F-coindex of Unicyclic Graphs

Unicyclic graphs are connected graphs with equal number of vertices and edges. Let U_n denotes the set of the unicyclic graphs with n vertices and U_n^k denotes the class of all unicyclic graphs with n vertices having a cycle of length k. Let $U_n^k(p_1, p_2, \cdots, p_k) \in U_n^k$ denotes a unicyclic graph with n vertices having cyclic of length k and each vertex i of cycle has p_i pendent vertices on it, here $1 \leq i \leq k$. For example $U_{12}^3(5, 4, 2)$ represents a unicyclic graph with 12 vertices having a cycle of length 3, where these 3 vertices of cycle has 5, 4 and 2 pendents, respectively. It is important to note that in

$$U_n^k(p_1, p_2, \cdots, p_k), \quad k + p_1 + p_2 + \cdots + p_k = n.$$

h

Theorem 3.4. *For $n \geq 4$, $U^3_\alpha(n-3,0,0) \in U^k_n$ has minimum F-coindex among the family of unicyclic graphs. The F-coindex for $U^3_n(n-3,0,0)$ is given by*

$$\bar{F}\left(U^3_n(n-3,0,0)\right) = (n-3)(n+6). \tag{3.8}$$

Proof. First we will calculate $U^3_n(n-3,0,0)$ and then show that it has minimum F-coindex among the family of unicyclic graphs. It is obvious from the structure of $U^3_n(n-3,0,0)$ that there would be two vertices of degree 2, one vertex of degree $n-1$ having $n-3$ pendents, as shown in Figure below. From the figure we can have the following table

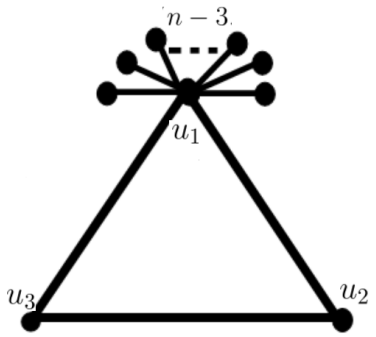

Figure 3.1: $U^3_n(n-3,0,0)$

d_u	N_u	Frequency
1	$n-2$	$n-3$
2	$n-3$	2
$n-1$	0	1

Using the formula given by eq(3.6), we get

$$\begin{aligned}\bar{F}\left(U^3_n(n-3,0,0)\right) &= (n-3)[(1)^2 \cdot (n-2)] + 2[(2)^2 \cdot (n-3)] \\ &= (n-3)(n-2) + 8(n-3) = (n-3)(n+6)\end{aligned}$$

Thus $\bar{F}\left(U^3_n(n-3,0,0)\right) = (n-3)(n+6)$.

Now we will show that $\bar{F}\left(U^3_n(n-3,0,0)\right) = (n-3)(n+6)$ is minimum value of F-coindex for the family of unicyclic graph. As we can see that in $U^3_n(n-3,0,0)$ the vertex

say u has degree $n-1$, that is maximum possible degree that any vertex can have in an unicyclic graph on n vertices. The contribution of u towards F-coindex is zero as it is connected to every other vertex of $U_n^3(n-3,0,0)$. This completes the proof. □

Theorem 3.5. *Let $\tilde{G} \in U_n$ and d_u be the degree of vertex $u \in V(\tilde{G})$. Let $u^* \in V(\tilde{G})$ be the vertex with maximum contribution towards $\bar{F}(\tilde{G})$ then degree of the vertex u^* is given by*

$$d_{u^*} = \begin{cases} \lceil \frac{2}{3}(n-1) \rceil & \text{if } n \equiv 2 \pmod 3, \\ \lfloor \frac{2}{3}(n-1) \rfloor & \text{otherwise.} \end{cases} \tag{3.9}$$

Proof. From equation (3.7) we know that F-coindex of a graph is given by

$$\bar{F}(\tilde{G}) = \sum_{u \in G} \left[(n-1)\, d_u^2 - d_u^3 \right].$$

Let u^* with degree d_{u^*} have maximum contribution towards $\bar{F}$. Then

$$\frac{\partial \bar{F}}{\partial d_{u^*}} = 2(n-1)d_{u^*} - 3\left(d_{u^*}\right)^2 = 0, \quad \text{this gives} \quad d_{u^*} = \frac{2(n-1)}{3}.$$

Also note that

$$\frac{\partial^2 \bar{F}}{\partial d_{u^*}^2} = -2(n-1) < 0.$$

This implies that the vertex with degree $d_{u^*} = \frac{2(n-1)}{3}$ will have maximum contribution towards $\bar{F}(\tilde{G})$. Note that d_{u^*} must be an integer value. To make d_{u^*} an integer value we round off $d_{u^*} = \frac{2(n-1)}{3}$ to nearest integer value to get

$$d_{u^*} = \begin{cases} \lceil \frac{2}{3}(n-1) \rceil & \text{if } n \equiv 2 \pmod 3, \\ \lfloor \frac{2}{3}(n-1) \rfloor & \text{otherwise.} \end{cases}$$

□

According to Theorem 3.5, it is evident that contribution of a vertex towards F-coindex in a unicyclic graph increase with an increase in degree of the vertex until degree of the vertex reaches a value given by equation(3.9).

Theorem 3.6. *Let $U_n^3(p_1,p_2,0) \in U_n$ with p_1, p_2 be the pendents on u_1 and u_2, respectively. Then*

(a) For $|p_1 - p_2| \leq 1$ the contribution of u_1 and u_2 towards $\bar{F}(\tilde{G})$ is given by

$$\tfrac{1}{4}(n+1)^2(n-3) \quad \text{if } n \text{ is odd}, \tag{3.10}$$

$$\tfrac{1}{4}(n^3 - n^2 - 6n - 8) \quad \text{if } n \text{ is even}, \tag{3.11}$$

(b) For $|p_1 - p_2| > 1$ contribution of u_1 and u_2 towards $\bar{F}(G)$ will be less than that of given by expressions (3.10) *and* (3.11).

Proof. (a) Let $U_n^3(p_1, p_2, 0) \in U_n$ and n be an odd number then we have $p_1 = p_2 = \frac{n-3}{2}$ be the pendents on u_1 and u_2, respectively. In this case, both of u_1 and u_2 will have degree $\frac{1}{2}(n+1)$ and both will be non-adjacent to $\frac{1}{2}(n-3)$. Thus contribution of both of u_1 and u_2 towards F-coindex given by

$$= 2.\left(\frac{1}{2}(n+1)\right)^2\left(\frac{n-3}{2}\right) = \frac{1}{4}(n+1)^2(n-3).$$

This proves the result when n is odd. Now let's assume that $U_n^3(p_1, p_2, 0) \in U_n$ and n be an even number. Here u_1 and u_2 have $p_1 = \frac{1}{2}(n-2)$ and $p_2 = \frac{1}{2}(n-4)$. In this case contribution of both of u_1 and u_2 towards F-coindex given by $\frac{1}{4}(n^3 - n^2 - 6n - 8)$.

(b) Let $m \geq 1$ be any positive integer and we assume that n is odd without loss of generality such that pendent at vertex u_1 are $p_1 = \frac{n-3}{2} + m$ and similarly for u_2, $p_2 = \frac{n-3}{2} - m$. It is easy to see that

$$d_{u_1} = \frac{n+1}{2} + m \quad \text{and} \quad d_{u_2} = \frac{n+1}{2} - m.$$

Note that

$$N_{u_1} = \frac{n+1}{2} - m \quad \text{and} \quad N_{u_2} = \frac{n+1}{2} + m.$$

So the contribution of u_1 and u_2 for $\bar{F}(\tilde{G})$ in this case, is given by

$$= \left(\frac{n+1}{2} + m\right)^2\left(\frac{n+1}{2} - m\right) + \left(\frac{n+1}{2} - m\right)^2\left(\frac{n+1}{2} + m\right)$$

$$= \frac{1}{4}(n+1)^2(n-3) - [nm^2 + n^2m + nm + 5m^2]$$

Using equation(3.10), it is obvious that if we have unequal degrees of two vertices that there contribution towards $\bar{F}(\tilde{G})$ reduces.

□

It is important to note here that if one vertex have degree d_{u^*} given by (3.9) then maximum possible degree of any other vertex, say u^{**} in a unicyclic graph would be $n-3-d_{u^*}$. Theorem 4.5 says that the contribution both of u^* and u^{**} towards $\bar{F}(\tilde{G})$ would be less than that if both vertices having degrees states in Theorem 4.5.

Theorem 3.7. *Let $U_n^k(p_1, p_2, \cdots, p_k) \in U_n^k$ such that $|p_i - p_j| \leq 1$, for $1 \leq i, j \leq k$, then $k = \frac{2n}{n-4}$ maximizes F-coindex of unicyclic graph.*

Proof. Without loss of generality we assume n such that each vertex has equal vertices that is $\frac{1}{k}(n-k)$. It is obvious from the structure of $U_n^k(p_1, p_2, \cdots, p_k)$ that there would be $(n-k)$ vertices of degree 1 and k vertices of degree $\frac{1}{k}(n+k)$ as shown in Figure 3.2.

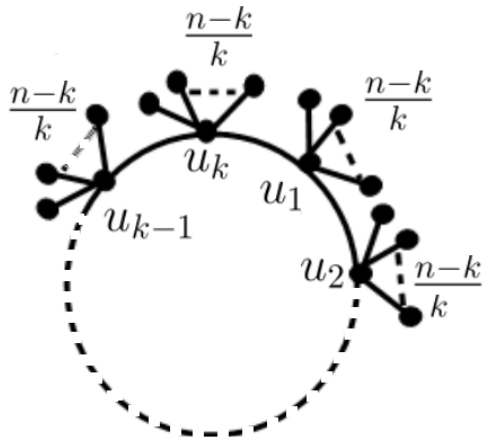

Figure 3.2: $U_n^k(p_1, p_2, \cdots, p_k)$ with $p_i = \frac{1}{k}(n-k)$, for $1 \leq i \leq k$.

From the Figure 3.2, we can have the following table Using the formula given by

d_u	N_u	Frequency
1	$n-2$	$n-k$
$\frac{n-k}{k}+2$	$\frac{n(k-1)-2k}{k}$	k

Table 3.1: For $U_n^k(p_1, p_2, \cdots, p_k)$ with $p_i = \frac{1}{k}(n-k)$, for $1 \leq i \leq k$.

equation(3.6), we get

$$\begin{aligned}\bar{F}\left(U_n^k(p_1, p_2, \cdots, p_k)\right) &= k\left[\frac{n-k}{k}+2\right]^2\left[\frac{n(k-1)-2k}{k}\right] + \left[(1)^2(n-k)(n-2)\right] \\ &= \frac{1}{k^2}\left[k^3(n-2)+k^2(2n^2-5n)+k(n^3-4n^2)-n^3\right] \\ &+ n^2 - kn - 2n + 2k \\ &= \frac{1}{k}\left(n^3-4n^2\right) - \frac{n^3}{k^2} + (3n^2-7n)\end{aligned}$$

In order to get the value of that maximizes $\bar{F}\left(U_n^k(p_1, p_2, \cdots, p_k)\right)$ we proceeds as follows.

$$\frac{d\bar{F}}{dk} = 0 \quad \text{implies that} \quad k = \frac{2n}{n-4}.$$

Also note that for $k = \frac{2n}{n-4}$, we have $\frac{d^2\bar{F}}{dk^2} < 0$. This means that $k = \frac{2n}{n-4}$ maximizes $\bar{F}\left(U_n^k(p_1, p_2, \cdots, p_k)\right)$. □

We know that k must be a positive integer. From the expression $k = \frac{2n}{n-4}$, it can be seen that for large value of n is close to 2 but for some values of n, k tends towards 3.

Theorem 3.8. *For $n \geq 28$, let $U_n^3(p_1, p_2, 0) \in U_n^k$, with $p_1, p_2 \in \left\{\lfloor\frac{n-3}{2}\rfloor, \lceil\frac{n-3}{2}\rceil\right\}$, such that $p_1 + p_2 = n-3$. In this case*

$$\bar{F}\left(U_n^3(p_1, p_2, 0)\right) = \begin{cases} \frac{1}{4}(n-3)(n^2+6n+9) & \text{if } n \text{ is odd,} \\ \frac{1}{4}(n^3+3n^2-10n-32) & \text{if } n \text{ is even.} \end{cases} \tag{3.12}$$

Furthermore, values given by equation(3.12) *are maximum F-coindex for family of unicyclic graph with $n \geq 28$.*

Proof. Let $U_n^3(p_1, p_2, 0) \in U_n^k$, with $p_1, p_2 \in \mathbb{N}$ such that $p_1 + p_2 = n-3$ and

$$|p_1 - p_2| = \begin{cases} 1 & \text{if } n \text{ is even,} \\ 0 & \text{if } n \text{ is odd,} \end{cases} \qquad \text{for } n \geq 28.$$

The structure of such graphs is shown in figure below.

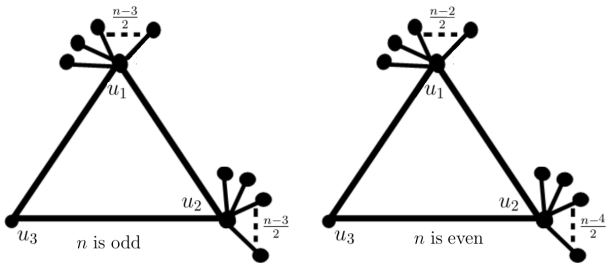

Figure 3.3: $U_n^3(p_1, p_2, 0)$, $n \geq 28$.

From Figure 3.3 we have the data in Table 3.2 and Table 3.3. In this case F-coindex is obtained by adding $(n-3)(n+2)$ the contribution of pendents and degree 2 vertices in equation(3.10) and equation(3.11), respectively for odd and even values of n. Thus Using

d_u	N_u	Frequency
1	$n-2$	$n-3$
2	$n-3$	1
$\frac{1}{2}(n+1)$	$\frac{1}{2}(n-3)$	2

Table 3.2: For $U_n^3(\frac{n-3}{2}, \frac{n-3}{2}, 0)$.

d_u	N_u	Frequency
1	$n-2$	$n-3$
2	$n-3$	1
$\frac{n}{2}$	$\frac{1}{2}(n-2)$	1
$\frac{1}{2}(n+2)$	$\frac{1}{2}(n-4)$	1

Table 3.3: For $U_n^3(\frac{n-2}{2}, \frac{n-4}{2}, 0)$.

the table given above we may write

$$\bar{F}\left(U_n^3(p_1, p_2, 0)\right) = \begin{cases} \frac{1}{4}(n-3)(n^2+6n+9) & \text{if } n \text{ is odd,} \\ \frac{1}{4}(n^3+3n^2-10n-32) & \text{if } n \text{ is even.} \end{cases} \tag{3.13}$$

It can easily be verified that $\bar{F}(U_n^3(p_1, p_2, 0))$ given by eq(3.13) is maximum by using Theorem 4.5 and Theorem 4.6. □

Theorem 3.9. *For* $11 \leq n \leq 27$, *let* $U_n^3(p_1, p_2, p_3) \in U_n^k$ *with* $p_i \in \left\{\lfloor \frac{n-3}{3} \rfloor, \lceil \frac{n-3}{3} \rceil\right\}$, *for* $i = 1, 2, 3$, *such that* $\sum_{i=1}^{3} p_i = n-3$ *then*

$$\bar{F}\left(U_n^3(p_1, p_2, p_3)\right) = \begin{cases} \frac{2n^3}{9} + \frac{5n^2}{3} - 7n & \text{if } n \equiv 0 \pmod 3, \\ \frac{6n^3}{27} + \frac{5n^2}{3} - \frac{53n}{9} - 4 & \text{if } n \equiv 1 \pmod 3, \\ \frac{2n^3}{9} + \frac{53n^2}{27} - 7n - \frac{22}{9} & \text{if } n \equiv 2 \pmod 3. \end{cases} \tag{3.14}$$

Proof. For $11 \leq n \leq 27$, let $U_n^3(p_1, p_2, p_3) \in U_n^k$ with $p_1, p_2, p_3 \in \mathbb{N}$ such that $p_1 + p_2 + p_3 = n - 3$ then we have following three possible cases for p_1, p_2 and p_3.

Case(I) When $n \equiv 0 \pmod 3$, then $p_1 = p_2 = p_3 = \frac{n-3}{3}$.

Case(II) When $n \equiv 1 \pmod 3$, then $p_1 = \lceil \frac{n-3}{3} \rceil$ and $p_2 = p_3 = \lfloor \frac{n-3}{3} \rfloor$.

Case(III) When $n \equiv 2 \pmod 3$, then $p_1 = p_2 = \lceil \frac{n-3}{3} \rceil$ and $p_3 = \lfloor \frac{n-3}{3} \rfloor$.

Now we consider each case separately, to find the F-coindex of $U_n^3(p_1, p_2, p_3)$ for $11 \leq n \leq 27$. **Case(I):** When $n \equiv 0 \pmod 3$, then $p_1 = p_2 = p_3 = \frac{n-3}{3}$. In this class we discuss all

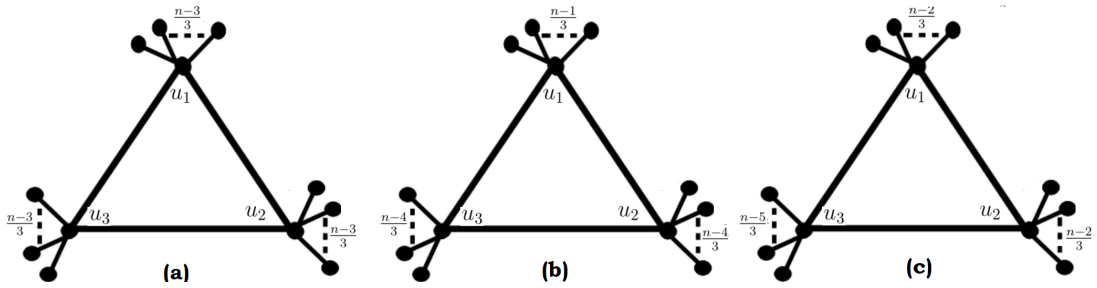

Figure 3.4: $U_n^3(p_1, p_2, p_3)$

that graphs for $11 \leq n \leq 27$ when n is divided by 3 with remainder is 0, that is, $n = 3k$, for $k = 4, 5, \cdots, 9$. For such graphs degree of each vertex of cycle is given by $\frac{n+3}{2}$ and there are $(n-3)$ are pendent vertices. From the figure we have the following table.

d_u	N_u	Frequency
$\frac{n+3}{3}$	$\frac{2}{3}(n-3)$	3
1	$n-2$	$n-3$

Table 3.4: For $U_n^3(p_1, p_2, p_3)$.

Using the formula given by eq(3.6), and the above table we get

$$\bar{F}(\tilde{G}) = 3.\left(\frac{n+3}{3}\right)^2\left(\frac{2}{3}(n-3)\right) + (n-2)(n-3)$$

d_u	N_u	Frequency
$\frac{1}{3}(n+2)$	$\frac{1}{3}(2n-5)$	2
$\frac{1}{3}(n+5)$	$\frac{2}{3}(n-4)$	1
1	$n-2$	$n-3$

Table 3.5: For $U_n^3(p_1, p_2, p_3)$.

Simplification of the above equation gives

$$\bar{F}(\tilde{G}) = \frac{2n^3}{9} + \frac{5n^2}{3} - 7n \tag{3.15}$$

Case(II): When $n \equiv 1 \pmod 3$, then $p_1 = \frac{n-1}{3}$ and $p_2 = p_3 = \frac{n-4}{3}$, for $n = 3k+1$ where $k = 4, 5, \cdots, 8$.

In this case we have following values of degrees, non-adjacent vertices and frequencies. Using the formula given by eq(3.6) and the above table we get

$$\bar{F}(\tilde{G}) = 2\left(\frac{n+2}{3}\right)^2\left(\frac{2n-5}{3}\right) + \left(\frac{n+5}{3}\right)^2\left(\frac{2n-8}{3}\right) + (n-3)(n-2)$$

After simplifying last equation we obtain

$$\bar{F}(\tilde{G}) = \frac{6n^3}{27} + \frac{5n^2}{3} - \frac{53n}{9} - 4 \tag{3.16}$$

Case(III): In the last case we consider the family of unicyclic graphs $U_n^3(p_1, p_2, p_3) \in U_n^k$ with $n \equiv 2(\pmod 3)$. Here $p_1 = p_2 = \frac{n-2}{3}$ and $p_3 = \frac{n-5}{3}$ where $n = 3k+2$ for $k = 4, 5, \cdots, 8$. It's easy to construct the following table.

d_u	N_u	Frequency
$\frac{1}{3}(n+4)$	$\frac{1}{3}(2n-7)$	2
$\frac{1}{3}(n+1)$	$\frac{2}{3}(n-2)$	1
1	$n-2$	$n-3$

Table 3.6: For $U_n^3(p_1, p_2, p_3)$.

Using the formula given by eq(3.6), and the above table we get

$$\bar{F}(\tilde{G}) = 2\left(\frac{n+4}{3}\right)^2\left(\frac{2n-7}{3}\right) + \left(\frac{n+1}{3}\right)^2\left(\frac{2n-4}{3}\right) + (n-3)(n-2)$$

Thus we obtain

$$\bar{F}(\tilde{G}) = \frac{2n^3}{9} + \frac{53n^2}{27} - 7n - \frac{22}{9} \tag{3.17}$$

□

Theorem 3.10. *Let $U_n^3(p_1, p_2, p_3) \in U_n^k$ with $p_i \in \left\{\lfloor \frac{n-3}{3} \rfloor, \lceil \frac{n-3}{3} \rceil\right\}$, for $i = 1, 2, 3$, such that $p_1 + p_2 + p_3 = n - 3$ then $\bar{F}\left(U_n^3(p_1, p_2, p_3)\right)$ has maximum F-coindex for the family of unicyclic graphs with $11 \leq n \leq 27$.*

Proof. By Theorem 4.6, we know that $k = \frac{2n}{n-4}$ maximizes F-coindex of unicyclic graph. This value must be integer as it represents number of vertices on which we should divide pendent vertices. The value 0f k given in Theorem 4.6 is close to 3 when $n = 11$ and it decreases as we increase n. Therefore, we can compare F-coindex of both values of k, that is, $k = 2$ and $k = 3$.

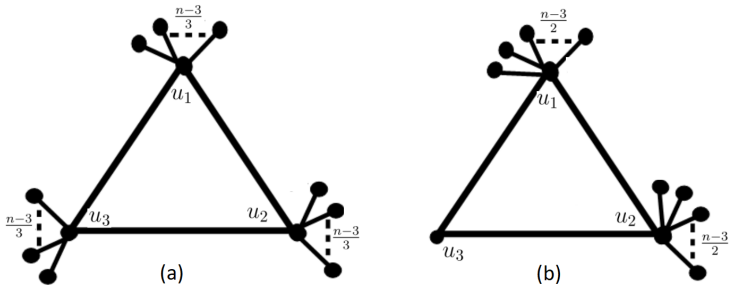

Figure 3.5: $U_n^3(p_1, p_2, p_3)$ and $U_n^3(p_1, p_2, 0)$

Without loss of generality we assume that $n - 3$ is even and divisible by 3 as well it is equivalent to say that n is odd and divisible by 3. As it is evident from the Figure or table below, that both $U_n^3(p_1, p_2, p_3)$ and $U_n^3(p_1, p_2, 0)$ have same pendent vertices with same number of non-adjacent vertices.

Therefore, contribution of pendent vertices would be same in both cases. It means that we should compare the contribution of other vertices for F-coindex of $U_n^3(p_1, p_2, p_3)$

d_u	N_u	Frequency
$\frac{n+3}{3}$	$\frac{2}{3}(n-3)$	3
1	$n-2$	$n-3$

Table 3.7: For $U_n^3(\frac{n-3}{3}, \frac{n-3}{3}, \frac{n-3}{3})$.

d_u	N_u	Frequency
1	$n-2$	$n-3$
2	$n-3$	1
$\frac{n+1}{2}$	$\frac{n-3}{2}$	2

Table 3.8: For $U_n^3(\frac{n-3}{2}, \frac{n-3}{2}, 0)$.

and $U_n^3(p_1, p_2, 0)$. As we can see that in $U_n^3(p_1, p_2, p_3)$ there are 3 vertices, say u_1, u_2 and u_3, with degree $\frac{n+3}{3}$ with non-adjacent vertices $\frac{2(n-3)}{3}$.

$$\bar{F}_{u_i} = \frac{2}{9}(n+3)^2(n-3), \quad \text{for} \quad i = 1, 2, 3, \tag{3.18}$$

here $\bar{F}_{u_i}$ for $i = 1, 2, 3$, represents contribution of u_1, u_2 and u_3 towards $\bar{F}\left(U_n^3(\frac{n-3}{3}, \frac{n-3}{3}, \frac{n-3}{3})\right)$.

Similarly, for $U_n^3(p_1, p_2, 0)$ contribution of v_1, v_2 and v_3 is given by

$$\bar{F}_{v_i} = \frac{1}{4}(n-3)\left(n^2+2n+17\right), \quad \text{for} \quad i = 1, 2, 3, \tag{3.19}$$

here $\bar{F}_{v_i}$ for $i = 1, 2, 3$, represents contribution of v_1, v_2 and $_3$ towards $\bar{F}\left(U_n^3(\frac{n-3}{2}, \frac{n-3}{2}, 0)\right)$. By analyzing eq(3.18) and eq(3.19), we have

$$\bar{F}_{u_i} = \bar{F}_{v_i} \quad \text{for} \quad n = 27, \quad \text{and} \quad \bar{F}_{u_i} > \bar{F}_{v_i} \quad \text{for} \quad 11 \leq n < 27. \tag{3.20}$$

In general we can write

$$\begin{cases} \bar{F}\left(U_n^3(p_1, p_2, p_3)\right) > \bar{F}\left(U_n^3(p_1, p_2, 0)\right) & \text{for } 11 \leq n < 27, \\ \bar{F}\left(U_n^3(p_1, p_2, p_3)\right) = \bar{F}\left(U_n^3(p_1, p_2, 0)\right) & \text{for } n = 27, \\ \bar{F}\left(U_n^3(p_1, p_2, p_3)\right) < \bar{F}\left(U_n^3(p_1, p_2, 0)\right) & \text{for } n > 27. \end{cases} \tag{3.21}$$

Therefore, for $11 \leq n \leq 27$, $\bar{F}\left(U_n^3(p_1, p_2, p_3)\right)$ has maximum F-coindex for the family of unicyclic graphs. □

Summary of the Results

In this chapter, we introduce an alternative form of F-coindex of graphs. We use this form to study different properties of unicyclic graphs. We also calculate maximum F-coindex of minimum F-coindex for the family of unicyclic graphs.

Chapter 4

F-coindex of Some Dendrimers Structure with Alternative Formula

Dendrimers are deeply expanded natural macromolecules with continuous layers of branch units covering the central context. These particles are essential to nanotechnology and can be widely used. Nanobiotechnology is a fast-growing region of rational and innovative use instruments and processes for nanofabrication to create gadgets for the testing of biological systems. In this emerging field of science dendrimers are crucial as well as fundamental elements. In fact, it is a molecule which is actually synthesized or produced from the expanded units which are known as monomers using nanoscale in the process of making. Now a days, dendrimers are recognized as one of the large scale commercially available nanoscale, complex and huge particles with large visible compound. Moreover, due to the magnificent three dimensional branched design the dendrimers are almost ideal for macromolecules. These macromolecules comprises of three main building blocks, one of them is core, the second one is branches and third is the end groups. New branches from the main center are inserted in the steps until a tree-like structure is formed. For some different applications regarding dendrimers, we refer to [81]. Y et. al read the F index of some dendrimers in [74]. To date, the study of the F-index of specialized chemicals and nano-structures has been severely limited. Therefore, we are interested in studying the

mathematical properties of F-coindex of some dendrimers. In this thesis, we determine F-coindex of poly (propyl) ether mines, porphyrin, and zinc-porphyrin dendrimers.

4.1 Some Families of Nanostar Dendrimers

The use of nanostar dendrimers is not limited to drug delivery or diagnosis, it is now expanded into genetic delivery, mixing, targeting other biological applications. Graovac et al. find the fifth geometric arithmetric index for nanostar dendrimers. To date, the study of the F-index of special chemical and structural components is very limited. Nilanjan De presented the direct F-index and F-polynomial presentations of the six unlimited classes of nanostar dendrimers. Thus, we are interested in studying the mathematical properties of F-coindex for some nanostar dendrimers.

4.2 F-coindex of type-I nanostar dendrimers $(D_1[k])$

The structures of Type-I nanostar dendrimer, for $k = 1$ and $k = 2$, are given in Figure 4.1. It can be seen that order and size of $D_1[1]$ are 24 and 27, respectively, where as of $D_1[2]$ its 60 and 67. Generally we can obtain order of $D_1[k]$ by $2^n(18) - 12$ and size of $D_1[k]$ is obtained by $27 + 42(n - 1)$. Following theorem gives us information about F-coindex of $D_1[k]$ nanostar dendrimers as shown in Figure (4.1).

Theorem 4.1. *The F-coindex of nanostar dendrimers $D_1[k]$ is denoted by $\overline{F}(D_1[k])$ and is given as follows:*

$$\overline{F}(D_1[k]) = 1836(4^k) - 2988(2^k) + 1224, \quad \text{for } k \geq 1. \tag{4.1}$$

Proof. As can be seen from Figure 4.1, growth of nanostar dendrimers $D_1[k]$ is symmetrical. We can use this symmetry to compute F-coindex of $D_1[k]$ just by labeling of single branch of $D_1[k]$. On the basis of frequency, non-adjacency and degree we select two representative vertices say u and v, for the central hexagon. Other representatives for the

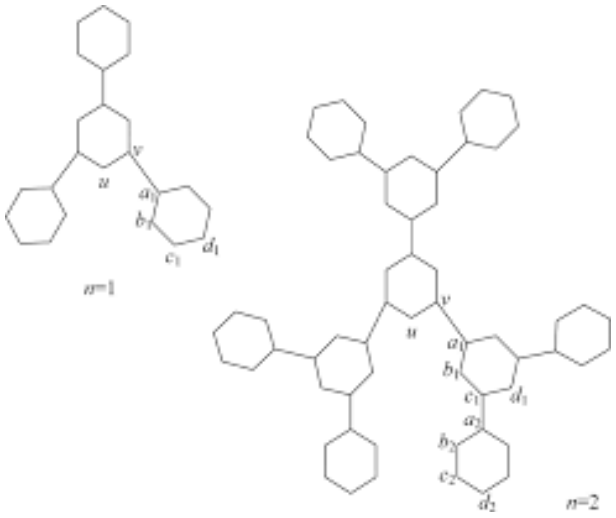

Figure 4.1: $D_1[k]$ with $k = 1$ and 2.

branch are labeled as: a_i, b_i, c_i, d_i where $1 \leq i \leq n$. Note that c_i for $1 \leq i \leq n-1$ and c_n would be different. The information required for computation of F-coindex for all these representatives are given in the Table 4.1 as follows: Now with the help of Table 4.1 and

Representative	Degree	Frequency	Non-adjacency
u	2	3	$2^k(18) - 15$
v	3	3	$2^k(18) - 16$
a_i	3	$3 \times 2^{i-1}$	$2^k(18) - 16$
b_i	2	$6 \times 2^{i-1}$	$2^k(18) - 15$
$c_i(i \neq k)$	3	$6 \times 2^{i-1}$	$2^k(18) - 16$
c_n	2	$6 \times 2^{k-1}$	$2^k(18) - 15$
d_i	2	$3 \times 2^{i-1}$	$2^k(18) - 15$

Table 4.1: Degrees, frequencies and non-adjacencies of the representative vertices of $D_1[k]$.

formula given by eq(3.6) we can write the F-coindex of $D_1[1]$ as follows.

$$\overline{F}\left(D_1[1]\right) = 2^2 \times 3 \times 21 + 3^2 \times 3 \times 20 + 3^2 \times 3 \times 20 + 2^2 \times 6 \times 21 + 2^2 \times 6 \times 21 + 2^2 \times 3 \times 21 = 2592$$

The F-coindex of $D_1[k]$ for $n \geq 2$ can be written as follows.

$$\begin{aligned}\overline{F}\left(D_1[k]\right) =& 4 \cdot \left(2^k(18) - 15\right) \cdot \left(3 + 6 \cdot \left(\sum_{i=1}^{k} 2^{i-1}\right) + 3 \cdot \left(\sum_{i=1}^{k} 2^{i-1}\right) + 6 \times 2^{k-1}\right) \\ &+ 9 \cdot \left(2^k(18) - 16\right) \left(3 + 3 \cdot \left(\sum_{i=1}^{k} 2^{i-1}\right) + 6 \cdot \left(\sum_{i=1}^{k-1} 2^{i-1}\right)\right)\end{aligned} \tag{4.2}$$

From well known formula for sum of geometric series we can write

$$\left(\sum_{i=1}^{k} 2^{i-1}\right) = 2^k - 1 \quad \text{and} \quad \left(\sum_{i=1}^{k-1} 2^{i-1}\right) = 2^{k-1} - 1. \tag{4.3}$$

Using eq(4.3) in eq(4.2) and simplifying we obtain

$$\begin{aligned}\overline{F}\left(D_1[k]\right) =& 4 \cdot \left(2^k(18) - 15\right) \cdot \left(3 + 9 \cdot \left(2^k - 1\right) + 3 \cdot 2^k\right) \\ &+ 9 \cdot \left(2^k(18) - 16\right) \left(3 + 3 \cdot \left(2^k - 1\right) + 6 \cdot \left(2^{k-1} - 1\right)\right)\end{aligned} \tag{4.4}$$

Eq(4.4) may be written as

$$\overline{F}\left(D_1[k]\right) = 24 \cdot \left(2^k(18) - 15\right) \left(2^{k+1} - 1\right) + 54 \cdot \left(2^k(18) - 16\right) \left(2^k - 1\right)$$

Further simplification of the above equation gives $\overline{F}\left(D_1[k]\right) = 1836(4^k) - 2988(2^k) + 1224$. □

4.3 F-coindex of type-II nanostar dendrimers $(D_2[k])$

The structure of $D_2[k]$ or type-II nanostar dendrimers is given in Figure 4.2. In case of $D_2[k]$, the order is given by $10(2^{k+1}) + 4(2^{k+2}) - 44$.

Theorem 4.2. *The F-coindex of nanostar dendrimers $D_2[k]$ is denoted by $\overline{F}(D_2[k])$ and is given as follows:*

$$\overline{F}(D_2[k]) = -7344 \cdot 4^k - 18680 \cdot 2^k + 11812, \quad \textit{for } k \geq 1. \tag{4.5}$$

Proof. From Figure 4.2 we can analyze that expansion of $D_2[k]$ follows a symmetrical pattern. Therefore, for the computation of F-coindex for $D_2[k]$, labeling of a single branch

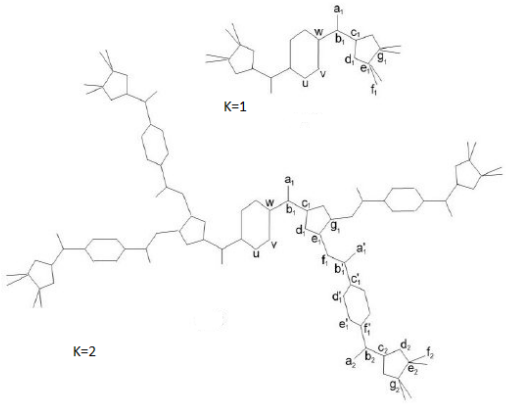

Figure 4.2: $D_2[k]$ with $k = 1$ and 2.

of $D_2[k]$ may be used. Following the symmetry of the structure three representatives namely u, v and w, are needed for central hexagon. The remaining representatives are divided into two groups. Representatives of first group are labeled as a_i, b_i, c_i, d_i, e_i and f_i for $1 \leq i \leq k$. The second group of representatives for $1 \leq i'_i \leq k-1$ are denoted with the symbols $\grave{a}_i, \grave{b}_i, \grave{c}_i, \grave{d}_i, \grave{e}_i, \grave{f}_i$. The information required for computation of F-coindex is given in the Table 4.2 and Table 4.3. Note that the order of $D_2[1]$ is 28 and

$$N_u = 27 - d_u \quad \text{for} \quad u \in D_2[1].$$

Now with the help of Table 4.2 and formula given by eq(3.6) we can write the F-coindex of $D_2[1]$ as follows.

$$\overline{F}(D_2[1]) = 1^2 \cdot 26\,(2+8) + 2^2 \cdot 25\,(2+2+4) + 3^2 \cdot 24\,(2+2+2) + 4^2 \cdot 23\,(4) = 3828$$

In order to calculate $\overline{F}\,(D_2[k])$ for $k \geq 2$, we have

$$N_u = 10(2^{k+1}) + 4(2^{k+2}) - 45 - d_u = 36 \cdot 2^k - 45 - d_u \quad \text{for} \quad u \in D_2[k].$$

We have to use the data of both the tables, that is, Table 4.2 and Table 4.3. Hence

Representative	Degree	Frequency	Non-adjacency
u	2	2	$36 \cdot 2^k - 47$
v	2	2	$36 \cdot 2^k - 47$
w	3	2	$36 \cdot 2^k - 48$
a_i	1	2^i	$36 \cdot 2^k - 46$
b_i	3	2^i	$36 \cdot 2^k - 48$
c_i	3	2^i	$36 \cdot 2^k - 48$
d_i	2	2^{i+1}	$36 \cdot 2^k - 47$
$e_i (i \neq k)$	3	2^{i+1}	$36 \cdot 2^k - 48$
e_k	4	2^{k+1}	$36 \cdot 2^k - 49$
$f_i (i \neq k)$	2	2^{i+1}	$36 \cdot 2^k - 47$
f_k	1	2^{k+2}	$36 \cdot 2^k - 46$

Table 4.2: Degrees, frequencies and non-adjacencies of the representative vertices of $D_2[k]$, for $1 \leq i \leq k$

Representative	Degree	Frequency	Non-adjacency
$\acute{a}_i$	1	2^{i+1}	$36 \cdot 2^k - 46$
$\acute{b}_i$	3	2^{i+1}	$36 \cdot 2^k - 48$
$\acute{c}_i$	3	2^{i+1}	$36 \cdot 2^k - 48$
$\acute{d}_i$	2	2^{i+2}	$36 \cdot 2^k - 47$
$\acute{e}_i$	2	2^{i+2}	$36 \cdot 2^k - 47$
$\acute{f}_i$	3	2^{i+1}	$36 \cdot 2^k - 48$

Table 4.3: Degrees, frequencies and non-adjacencies of the representative vertices of $D_2[k]$, $\quad 1 \leq i \leq k-1$ and $k \geq 2$

the F-coindex of $D_2[k]$ for $k \geq 2$ can be written as :

$$\begin{aligned}\overline{F}(D_2[k]) = 1^2 \cdot \left(36 \cdot 2^k - 46\right) &\left(\sum_{i=1}^{k} 2^i + 2^{k+2} + \sum_{i=1}^{k-1} 2^{i+1}\right) \\ + 2^2 \cdot \left(36 \cdot 2^k - 47\right) &\left(4 + \sum_{i=1}^{k} 2^{i+1} + \sum_{i=1}^{k-1} 2^{i+1} + 2\sum_{i=1}^{k-1} 2^{i+2}\right) \\ + 3^2 \cdot \left(36 \cdot 2^k - 48\right) &\left(2 + 2\sum_{i=1}^{k} 2^i + 4\sum_{i=1}^{k-1} 2^{i+1}\right) + 4^2 \cdot \left(36 \cdot 2^k - 49\right)\left(2^{k+1}\right).\end{aligned}$$

Using following geometric series sum

$$\sum_{i=1}^{k} 2^{i+p} = 2^{p+1}\left(2^k - 1\right), \quad \text{for any poitive integer } p,$$

in eq(4.6) and simplifying we obtain

$$\begin{aligned}\overline{F}(D_2[k]) &= \left(36\cdot 2^k - 46\right)\left(8\cdot 2^k - 6\right) + 4\cdot\left(36\cdot 2^k - 47\right)\left(14\cdot 2^k - 20\right) \\ &\quad + 9\cdot\left(36\cdot 2^k - 48\right)\left(12\cdot 2^k - 18\right) + 32\cdot\left(36\cdot 2^k - 49\right)\left(2^k\right) \\ &= 36\cdot 4^k\,(204) - 36\cdot 2^k\,(248) - 2^k\,(9752) + 11812\end{aligned} \tag{4.7}$$

after further simplification of above equation, we obtain the F-coindex of $D_2[k]$ in the following form $\overline{F}\,(D_2[k]) = 7344\cdot 4^k - 18680\cdot 2^k + 11812$. □

4.4 Hetrofunctional Dendrimers

In this section, we study the molecular graph of a class of hetrofunctional dendimers (HFD).In this thesis we select a HFD(ei)-G3-e(allyl)16-i-(hydroxyl)28 denoted by $D[k]$ indicated in Fig 4.3.Graphs for different growth stages are shown in Fig. 4.3-4.8. It is evident that order and size of $D[k]$ are equal i.e.

$$|V(D[k])| = |E(D[k])|.$$

The order and size of $D[k]$ is given as:.

$$|V(D[k])| = \begin{cases} 16\times 2^{t+1} + 8\times 2^t - 38 & if k = 2t, t \geq 1, \\ 24\times 2^{t+1} - 38 & if k = 2t+1, t \geq 0. \end{cases}$$

4.5 The F-coindex of Hetrofunctional Dendimers

In this section we compute the F-coindex of hetrofunctional dendimers $D[k]$ as shown in Fig. 4.3.

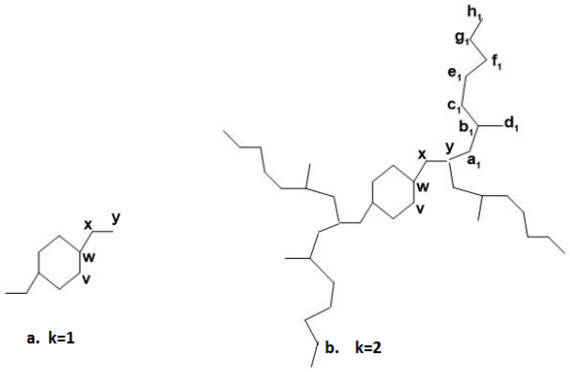

Figure 4.3: $D_1[k]$ with $k = 1$ and 2.

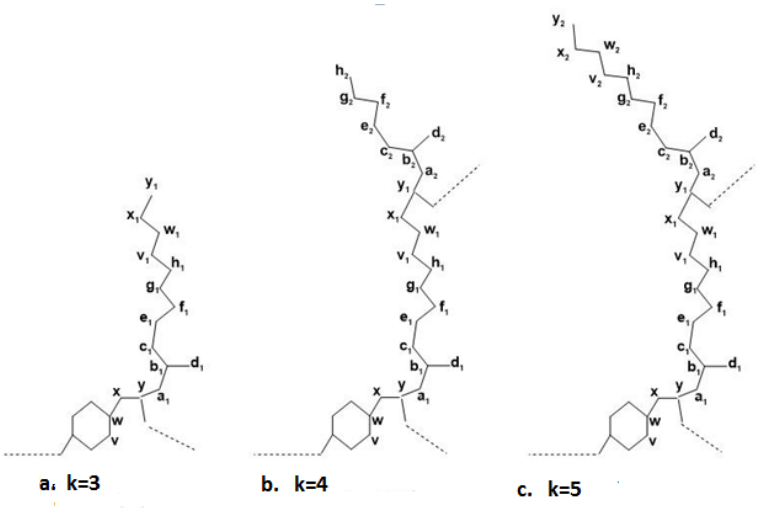

Figure 4.4: $D_2[k]$ with $k = 1$ and 2.

Theorem 4.3. *The F-coindex of $D[k]$ for $k = 2t + 1$ where $t \geq 0$ is given by*

$$\bar{F}(D[k]) = 9792(2^{2t}) - 16092(2^t) + 6592.$$

Proof. As can be seen from the Fig 4.3-4.8 growth of hetrofunctional dendimers $D[k]$ is symmetrical. We can use this symmetry to compute F-coindex of $D[k]$ just by labeling of single branch of $D[k]$. On the basis of frequency, non-adjacency and degree we select representative vertices from set of vertices these are labelled as $v, w, x, y, a_i, b_i, c_i, d_i, e_i, f_i, g_i, h_i, v_i, w_i, x_i, y_i$. Here $1 \leq i \leq \frac{k-1}{2}$ when $k \geq 3$. The information required for computation of F-coindex

for all these representatives are given in the Table 4.4 as follows:

Representative	Degree	Frequency	Non-adjacency
v	2	4	$24(2^{t+1}) - 41$
w	3	2	$24(2^{t+1}) - 42$
x	2	2	$24(2^{t+1}) - 41$
$y(k = 1)$	1	2	$24(2^{t+1}) - 40$
$y(k \neq 1)$	3	2	$24(2^{t+1}) - 42$

Table 4.4: The vertices introduced at core (first generation) with their degrees, frequencies and non adjacencies for $k \geq 1$, where k is odd.

when $k = 1$ then $t = 0$. using table 4.4 the F-coindex for $D[k]$ can be written as follows:

$$\bar{F}(D[1]) = (2^2 \times 7 \times 4) + (3^2 \times 6 \times 2) + (2^2 \times 7 \times 2) + (1 \times 8 \times 2) = 292, \tag{4.8}$$

Representative	Degree	Frequency	Non-adjacency
a_i	2	2^{i+1}	$24(2^{t+1}) - 41$
b_i	3	2^{i+1}	$24(2^{t+1}) - 42$
c_i	2	2^{i+1}	$24(2^{t+1}) - 41$
d_i	1	2^{i+1}	$24(2^{t+1}) - 40$
e_i	2	2^{i+1}	$24(2^{t+1}) - 41$
f_i	2	2^{i+1}	$24(2^{t+1}) - 41$
g_i	2	2^{i+1}	$24(2^{t+1}) - 41$
h_i	2	2^{i+1}	$24(2^{t+1}) - 41$

Table 4.5: The verties introduced at 2^{nd} generation with their degrees, frequencies and non-adjacencies for $k \geq 3$, where k is odd.

Representative	Degree	Frequency	Non-adjacency
v_i	2	2^{i+1}	$424(2^{t+1}) - 41$
w_i	2	2^{i+1}	$24(2^{t+1}) - 41$
x_i	2	2^{i+1}	$24(2^{t+1}) - 41$
$y_i(i = t)$	1	2^{i+1}	$24(2^{t+1}) - 40$
$y_i(i \neq t)$	3	2^{i+1}	$24(2^{t+1}) - 42$

Table 4.6: The vertices introduced at third generation with their degrees, frquencies and non-adjacencies for $k \geq 3$, where k is odd.

when $k \geq 3$ then using table 4.4-4.6 the F-coindex of $D[k]$ is written as follows:
$\bar{F}(D[k]) = (2^2 \times 4 \times (24(2^{t+1}) - 41)) + (3^2 \times 2 \times (24(2^{t+1}) - 42)) + (2^2 \times 4 \times (24(2^{t+1}) - 41)) + (3^2 \times 2 \times (24(2^{t+1}) - 42)) + \sum_{i=1}^{t}[(2^2 \times 2^{i+1} \times (24(2^{t+1}) - 41)) + (3^2 \times 2^{i+1} \times (24(2^{t+1}) - 42)) + (2^2 \times 2^{i+1} \times (24(2^{t+1}) - 41)) + (1 \times 2^{i+1} \times (24(2^{t+1}) - 40)) + (2^2 \times 2^{i+1} \times (24(2^{t+1}) - 41)) + (2^2 \times 2^{i+1} \times (24(2^{t+1}) - 41)) + (2^2 \times 2^{i+1} \times (24(2^{t+1}) - 41))] + \sum_{i=1}^{t}[(2^2 \times 2^{i+1} \times (24(2^{t+1}) - 41)) + (2^2 \times 2^{i+1} \times (24(2^{t+1}) - 41)) + (2^2 \times 2^{i+1} \times (24(2^{t+1}) - 41))] + \sum_{i=1}^{t-1}[(3^2 \times 2^{i+1} \times (24(2^{t+1}) - 42))] + (1 \times 2^{t+1} \times (24(2^{t+1}) - 40))$,
after simplification we get the following result.

$$\bar{F}(D[k]) = 9792(2^{2t}) - 16092(2^t) + 6592$$

this completes the proof. □

Theorem 4.4. *The F-coindex of $D[k]$ for $k = 2t$, where $t \geq 1$ is given by*

$$\bar{F}(D[k]) = 6880(2^{2t}) - 13500(2^t) + 6592.$$

Proof. As can be seen from the Fig 4.3-4.8 growth of hetrofunctional dendimers $D[k]$ is symmetrical. We can use this symmetry to compute F-coindex of $D[k]$ just by labeling of single branch of $D[k]$. On the basis of frequency, non-adjacency and degree we select representative vertices from set of vertices these are labelled as $v, w, x, y, a_i, b_i, c_i, d_i, e_i, f_i, g_i, h_i, v_i, w_i, x_i, y_i$. Here $1 \leq i \leq \frac{k}{2}$.

Representative	Degree	Frequency	Non-adjacency
v	2	4	$16(2^{t+1}) + 8(2^t) - 41$
w	3	2	$16(2^{t+1}) + 8(2^t) - 42$
x	2	2	$16(2^{t+1}) + 8(2^t) - 41$
y	3	2	$16(2^{t+1}) + 8(2^t) - 42$

Table 4.7: The vertices introduced at core (first generation) with their degrees, frequencies and non-adjacencies for $k \geq 2$, where k is even.

Representative	Degree	Frequency	Non-adjacency
a_i	2	2^{i+1}	$16(2^{t+1}) + 8(2^t) - 41$
b_i	3	2^{i+1}	$16(2^{t+1}) + 8(2^t) - 42$
c_i	2	2^{i+1}	$16(2^{t+1}) + 8(2^t) - 41$
d_i	1	2^{i+1}	$16(2^{t+1}) + 8(2^t) - 40$
e_i	2	2^{i+1}	$16(2^{t+1}) + 8(2^t) - 41$

Table 4.8: The vertices introduced at 2nd generation with their degrees, frequencies and non-adjacencies for $k \geq 2$, where k is even.

Representative	Degree	Frequency	Non-adjacency
f_i	2	2^{i+1}	$16(2^{t+1}) + 8(2^t) - 41$
g_i	2	2^{i+1}	$16(2^{t+1}) + 8(2^t) - 41$
$h_i(i = t)$	1	2^{i+1}	$16(2^{t+1}) + 8(2^t) - 40$
$h_i(i \neq t)$	2	2^{i+1}	$16(2^{t+1}) + 8(2^t) - 41$

Representatie	Degree	Frequency	Non-adjacency
v_i	2	2^{i+1}	$16(2^{t+1})+8(2^t)-41$
w_i	2	2^{i+1}	$16(2^{t+1})+8(2^t)-41$
x_i	2	2^{i+1}	$16(2^{t+1})+8(2^t)-41$
y_i	2	2^{i+1}	$16(2^{t+1})+8(2^t)-41$

Table 4.9: The vertices introduced at third generation with their degrees, frequencies and non-adjacency for $k \geq 4$, where k is even.

Now we take representative from set of vertices which are introduced at $k = 3$ and have same degree and non-adjacency. These representatives are labelled as v_i, w_i, x_i, y_i. Here $1 \leq i \leq t-1$ and $t = \frac{k}{2}$. when $k = 2$ then $t = 1$, using table 4.9 we get;
$\bar{F}(D[2]) = 2^2\times4\times39)+(3^2\times2\times38)+(2^2\times2\times39)+(3^2\times2\times38)+(2^2\times4\times39)+(3^2\times4\times38)+(2^2\times4\times39)+(1\times4\times40)+(2^2\times4\times39)+(2^2\times4\times39)+(2^2\times4\times39)+(2^2\times4\times39)+(1\times4\times40) = 7736.$

when $k \geq 4$ then using Table 4.7-4.8-4.9 , the F-coindex of $D[k]$ can be written as follows;
$\bar{F}(D[k]) = (2^2 \times 4 \times (16(2^{t+1})+8(2^t)-41))+(3^2 \times 2 \times (16(2^{t+1})+8(2^t)-42))+(2^2 \times 4 \times (16(2^{t+1})+8(2^t)-41))+(3^2 \times 2 \times (16(2^{t+1})+8(2^t)-42))+\sum_{i=1}^{t}[(2^2 \times 2^{i+1} \times (16(2^{t+1})+8(2^t)-41))+(3^2 \times 2^{i+1} \times (16(2^{t+1})+8(2^t)-42))+(2^2 \times 2^{i+1} \times (16(2^{t+1})+8(2^t)-41))+(1 \times 2^{i+1} \times (16(2^{t+1})+8(2^t)-40))+(2^2 \times 2^{i+1} \times (16(2^{t+1})+8(2^t)-41))+(2^2 \times 2^{i+1} \times (16(2^{t+1})+8(2^t)-41))+(2^2 \times 2^{i+1} \times (16(2^{t+1})+8(2^t)-41))]+\sum_{i=1}^{t-1}[(2^2 \times 2^{i+1} \times (16(2^{t+1})+8(2^t)-41))]+(1 \times 2^{t+1} \times (16(2^{t+1})+8 \times 2^t-40)+\sum_{i=1}^{t-1}[(2^2 \times 2^{i+1} \times (16(2^{t+1})+8(2^t)-41))+(2^2 \times 2^{i+1} \times (16(2^{t+1})+8(2^t)-41))+(2^2 \times 2^{i+1} \times (16(2^{t+1})+8(2^t)-41))+(3^2 \times 2^{i+1} \times (16(2^{t+1})+8(2^t)-42))]$,
after simplification we get the following result.

$$\bar{F}(D[k]) = 6880(2^{2t}) - 13500(2^t) + 6592,$$

which completes the proof. □

4.6 F-coindex of Poly(Propyl) Ether Imine (PETIM) Dendrimer

We now compute the F-coindex of Polynomial of Poly(Propyl) Ether Imine (PETIM) dendrimer in this section. We denote PETIM dendrimer by $\mathbb{G}[k]$ where k represents the k^{th} growth stages of $\mathbb{G}[k]$. The structure of $\mathbb{G}[k]$ for $k \geq 1$ is shown in Figure 4.5. It is a tree with order and size given by $24 \times 2^k - 23$ and $24 \times 2^k - 24$, respectively.

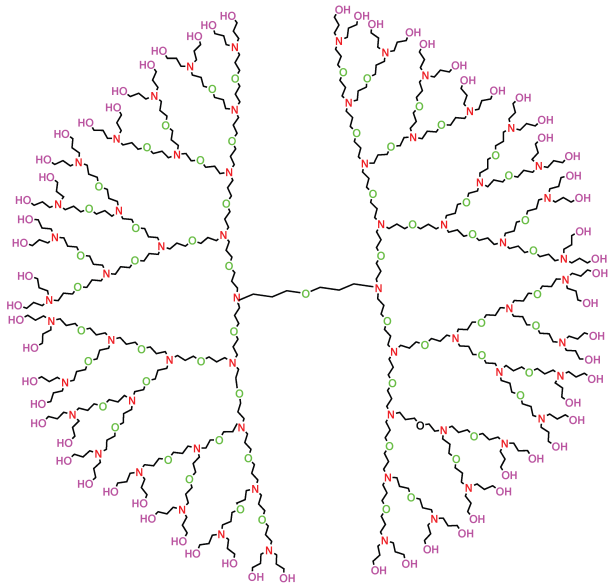

Figure 4.5: Growth of of poly(propyl) ether imine (PETIM) dendrimer at k = 5.

To compute F-coindex for the $\mathbb{G}[k]$ shown in Figure 4.5, we have to use Table 4.10 that contains information about degree, frequency and non-adjacency of the vertices of $\mathbb{G}[k]$.

Representative	Degree	Frequency	Non-adjacency
a	1	2^{k+1}	$24(2^k) - 25$
b	2	$20(2^k) - 21$	$24(2^k) - 26$
c	3	$2^{k+1} - 2$	$24(2^k) - 27$

Table 4.10: Degrees, frequencies and non-adjacencies of $\mathbb{G}[k]$ for $k \geq 1$

Theorem 4.5. *Let $\tilde{\mathbb{G}}[k]$ be the molecular structure of PETIM dendrimer. Then F-coindex of $\mathbb{G}[k]$ denoted by $\overline{F}(\tilde{\mathbb{G}}[k])$ and is given by*

$$\overline{F}(\tilde{\mathbb{G}}[k]) = 2400 \cdot 4^k - 5064 \cdot 2^k + 2670. \tag{4.9}$$

Proof. Let $\tilde{\mathbb{G}}[k]$ be the molecular structure of PETIM dendrimer. Depending upon the structure of $\tilde{\mathbb{G}}[k]$, edge set $V(\tilde{\mathbb{G}}[k])$ may be explained with the help of three representatives, namely a, b and c. This division is done on the basis of degree of vertices. The degrees of a, b and c are 1, 2 and 3, respectively. Note that,

$$N_u = 24(2^k) - 24 - d_u, \quad \text{for} \quad u \in \tilde{\mathbb{G}}[k],$$

By using the formula given in eq(**??**) and data given in Table 4.10, F-coindex of $\tilde{\mathbb{G}}[k]$ is obtained as follows:

$$\overline{F}(\tilde{\mathbb{G}}[k]) = 1^2 \cdot \left(24 \cdot 2^k - 25\right) \cdot 2^{k+1} + 2^2 \cdot \left(24 \cdot 2^k - 26\right) \cdot \left(20 \cdot 2^k - 21\right) + 3^2 \cdot \left(24 \cdot 2^k - 27\right) \cdot \left(2^{k+1} - 2\right)$$

Simplifying the above equation gives $\overline{F}(\tilde{\mathbb{G}}[k]) = 2400 \cdot 4^k - 5064 \cdot 2^k + 2670$, which is required. □

4.7 The F-coindex of Porphyrin Dendrimers

The class of porphyrin dendrimers is shown in Figure 4.6 and Figure 4.7, for growth stages 4 and 16, respectively. It is important to note that porphyrin dendrimers are mathematically represented by D_kP_k, where $k = 2^m$ for $m \geq 2$. Here we present the F-coindex for Porphyrin dendrimers. The order of D_kP_k is given by $96k - 10$, where as its size is $105k - 11$. Based upon the structure of D_kP_k we need four representatives. These four representatives and required information for the computation of F-coindex of D_kP_k are given in the Table 4.11.

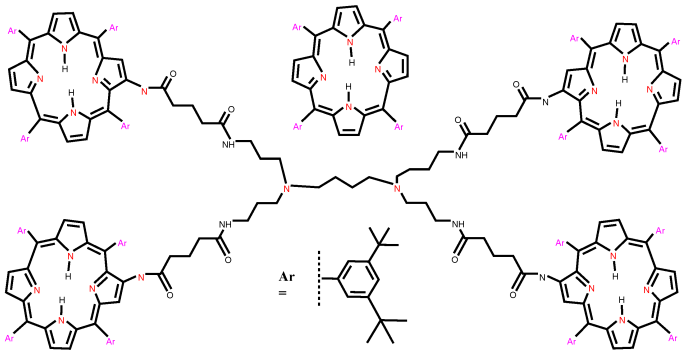

Figure 4.6: Molecular structure of porphyrin dendrimer D_4P_4.

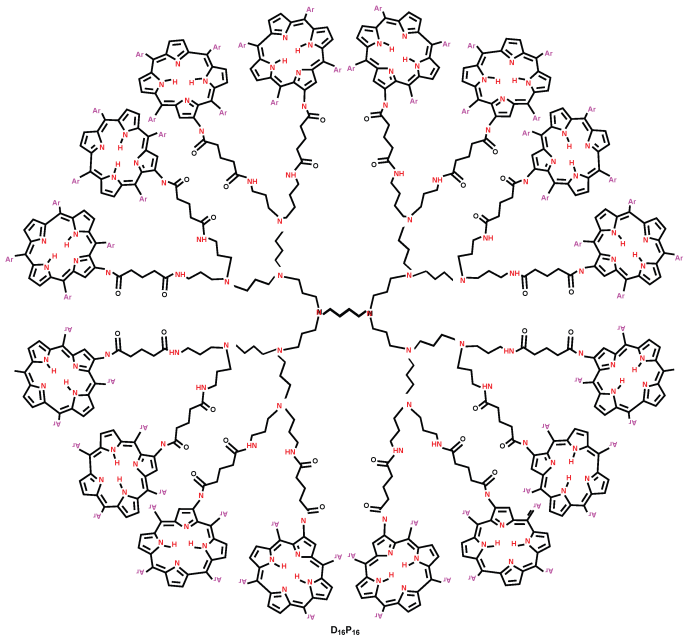

Figure 4.7: Molecular structure of porphyrin dendrimer $D_{16}P_{16}$.

Theorem 4.6. *Let D_kP_k be a Porphyrin dendrimer, then F-coindex of D_kP_k denoted by $\overline{F}(D_kP_k)$ and is given by*

$$\overline{F}(D_kP_k) = 52032k^2 - 12328k + 668$$

Proof. Let D_kP_k be a Porphyrin dendrimer, four representatives v, w, x and y of D_kP_k and their degrees, frequencies and non-adjacencies are given in the Table 4.11. Using eq(3.6) and Table 4.11 we have

Representative	Degree	Frequency	Non-adjacency
v	1	$26k$	$96k-12$
w	2	$34k-8$	$96k-13$
x	3	$28k-2$	$96k-14$
y	4	$8k$	$96k-15$

Table 4.11: Degrees, frequencies and non-adjacencies for the representatives in D_kP_k

$$\overline{F}((D_kP_k) = \big(1^2 \cdot (96k-12) \cdot 26k\big) + \big(2^2 \cdot (34k-8) \cdot (96k-13)\big) + \big(3^2 \cdot (28k-2) \cdot (96k-14)\big) + \big(4^2 \cdot (96k-14) \cdot 8k\big)$$

On simplifying the above equation we obtain the required result, that is, $\overline{F}(D_kP_k) = 52032k^2 - 12328k + 668$. □

4.8 The F-coindex of ZincPorphyrin Dendrimer

The class of dendrimer zinc-porphyrin is denoted by DPZ_k and is shown in Figure 4.8. Representative vertices and their degrees, frequencies and non-adjacencies are given in the Table 4.12.

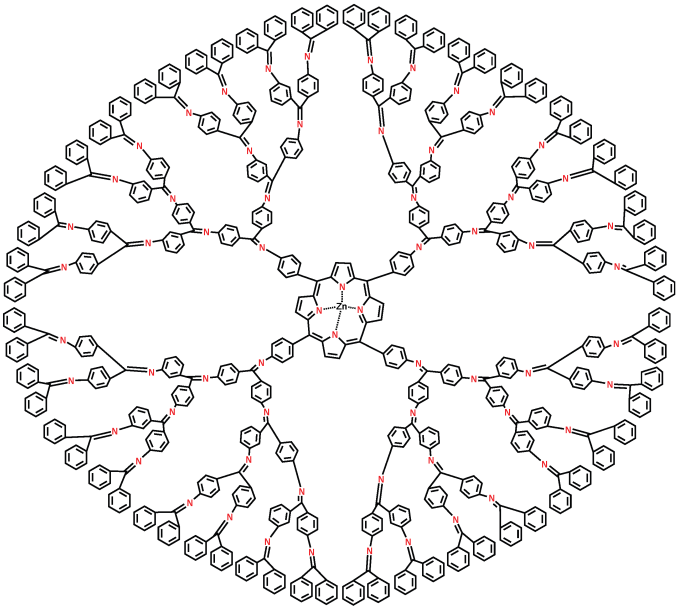

Figure 4.8: Molecular structure of dendrimer zinc porphyrin DPZ_4.

Representative	Degree	Frequency	Non-adjacency
e	2	$44 \times 2^n - 12$	$56(2^n) - 10$
f	3	$12 \times 2^n + 4$	$56(2^n) - 11$
g	4	1	$56(2^n) - 12$

Table 4.12: Degrees, frequencies and non-adjacencies for the representatives in DPZ_k for $k \geq 1$.

Theorem 4.7. *Let DPZ_k be a zinc-porphyrin dendrimer,then F-coindex of DPZ_k denoted by $\overline{F}(DPZ_k)$ and is given by*

$$\overline{F}(DPZ_k) = 15904(2^{2k}) - 348(2^k) - 108$$

Proof. Let DPZ_k be a zinc-porphyrin dendrimer, representative vertices e, f, g depending upon degrees are given in the Table 4.12. With the help of eq(3.6) and the Table 4.12 we have

$$\overline{F}(DPZ_k) = 2^2 \cdot \big(44 \cdot 2^k - 12\big) \cdot \big(56 \cdot 2^k - 10\big) + 3^2 \cdot \big(12 \cdot 2^k + 4\big) \cdot \big(56 \cdot 2^k - 11\big) + 4^2 \cdot \big(56 \cdot 2^k - 12\big)$$

simplification gives us following expression $\overline{F}(DPZ_k) = 15904(2^{2k}) - 348(2^k) - 108.$ □

4.9 Conclusions

To deal with novel diseases, due to continuous growth of viruses, the development of new drugs is of prime significance. To test and predict chemical properties of these new drugs concept of topological indices is very useful especially for developing countries. In this paper, we achieved the forgotten coindex of dendrimers that are very vital for targeted delivery for cancer therapy. These results may be used in material engineering, pharmaceutical and chemical industries.

References

[1] E, Kieth., L, Norman., j, Robin. (1976). 1-Graph theory $1736 - 1936$. Clarendon press, oxford, $1 - 4$.

[2] L, Gerald. (2006). Euler And Konigsberg's Bridges. Bullet. (New Series) of the Amer. Math. Soci. 43(4), $567 - 573$.

[3] F, Harary., G, Wilcox. (1967). Boolean operations on graphs. Math. Stand, $20, 41-51$.

[4] R, Hammack., W, Imrich., S, Klavzar. (2011). Handbook of product graphs. CRC, Press.

[5] W, Mantel. (1907). Problem 28 Solution. Wiskundige Opgaven,10, $60 - 61$.

[6] P, Turán. (1941). Eine extremalaufgabe aus der graphentheorie. Mat. Fiz. Lapok, 48, $435 - 452$.

[7] P, Erdös. (1962). On the number of complete subgraphs contained in certain graphs. Publ. Math. Inst. Hung. Acad. Sci., VII, Ser, $A3$, $459 - 464$.

[8] P, Erdös., A, Goodman., L, Pósa. (1966). The representation of a graph by set intersections. Canad. J .Math, $18, 106 - 112$..

[9] F, Harary. (1967). A seminar on graph theory: Chapter 8 - Extremal problems in graph theory (P. Erdös). Holt, Rinehart and Winston, New York.

[10] A, Cayley. (1874). On the mathematical theory of isomers. Philos. Mag, 10, $444-446$.

[11] J,J. Sylvester. (1878). Chemistry and algebra. Nature, 17, 284

[12] R, C. Read., F, Harary. (1970). The enumeration of tree-like polyhexes. Proc. Edinburgh Math. Soc, $17, 1 - 13$.

[13] L,B. Kier., L,H. Hall. (1976). Molecular connectivity in chemistry and drug research. Academic Press, New York and London.

[14] Pisanski,T., Randič, M. (2010). Use of the Szeged index and the revised Szeged index for measuring network. Dis. Appl. Math. 158 ,$1936 - 1944$.

[15] S, Bajaj., S,S. Sambi., S, Gupta., A, K. Madan. (2006). Model for prediction of anti-HIV activity of 2-pyridinone derivatives using novel topological descriptor. QSAR Comb. Sci. $25813 - 823$.

[16] J, Devillers., A. T. Balaban. (1999). Topological indices and related descriptors in QSAR and QSPR. Gordon & Breach, Amsterdam.

[17] S, Gupta., M. Singh., A.K. Madan. (2002). Application of graph theory: Relationship of eccentric connectivity index and Wiener's index with anti-inflammatory activity. J. Math. Anal. Appl, 266, $259 - 268$.

[18] C, Hansch., L. Leo. (1996). Exploring QSAR fundamentals and applicability in chemistry and biology. Amer. Chem. Soc., Washington DC.

[19] S, Sardana., A, K. Madan. (2001). Application of graph theory: Relationship of molecular connectivity index, Wieners index and eccentric connectivity index with diuretic activity. match Commun. Math. Comput. Chem., $43, 85 - 98$.

[20] S, Sardana., A. K, Madan. (2002). Application of graph theory: Relationship of antimycobacterial activity of quinolone derivatives with eccentric connectivity index and Zagreb group parameters. match Commun. Math. Comput. Chem, $45, 35 - 53$.

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

[22] A,T. Balaban. (1975). Some chemical applications of graph theory. MATCH Commun. Math.Comput. Chem., 1 : 3360.

[23] D, H. Rouvray. (1974). Uses of graph theory. Chem. Brit., 10, 11 − 18.

[24] A, T. Balaban. Chemical applications of graph theory. 1976. Academic Press, London and New York.

[25] H, Wiener. (1947). Structural determination of the paraffin boiling points. J. Am. Chem. Soc, 69, 17 − 20.

[26] H, Hosoya. (1971). Newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons. Bull. Chem. Soc. Jpn., 44(9), 2332 − 2339.

[27] J, Ma., Y, Shi., J, Yue. (2014). On the extremal wiener polarity index of unicyclic graphs with a given diameter. Math. Chem. Mono,177 − 192.

[28] J, Ma., Y, Shi., J, Yue. (2014) The wiener polarity index of graph products. Ars Combin, 116, 235 − 244.

[29] I, Lukovits., W, Linert. (1998). Polarity-numbers of cycle-containing structures. J Chem Inf Comput Sci 38, 715 − 719.

[30] A, Behmaram., H,Y. Azaria., A,R. Ashrafi. (2012). Wiener polarity index of fullerenes and hexagonal systems. Appl. Math. Lett. 25(10).

[31] M, Arockiaraj., S,R. Kavitha., K, Balasubramanian., I, Gutman. (2018). Hyper-Wiener and Wiener polarity indices of silicate and oxide frameworks. J. Math. Chem. 56, 1493 − 1510.

[32] M, Randiác. (1993). Novel molecular descriptor for structure-property studies, Chem. Phys. Lett, $211(4-5), 478-483$.

[33] M, Liu., B, Liu. (2011). On the Wiener Polarity Index, match Commun. Math. Comput. Chem, 66, $293-304$.

[34] N, Trank. (2018). The Wiener Polarity Index of Benzenoid Systems and Nanotubes, Croat. Chem. Acta, 91(3), $309-315$.

[35] I, Gutman., N, Trinajstić. (1972). Graph theory and molecular orbitals. III. Total π-electron energy of alternant hydrocarbons, Chem. Phys. Lett. 17 , $535-538$.

[36] I, Gutman. (2016). Total π-electron energy of conjugated molecules with non-bonding molecular orbitals. Journ. Phys. Scien. $71, 161-164$.

[37] I, Gutman., G, Indulal., R. Todeschini. (2008). Generalizing the Mcclelland bounds for total π-electron energy. $63, 280-282$.

[38] I, Gutman., S, Gojak., B. Furtula., S. Radenković., and A. Vodopivec. (2006). Relating total π-electron energy and resonance energy of benzenoid molecules with Kekulè- and Clarstructure-based parameters. Monatshefte fur Chemie, $137, 1127-1138$.

[39] E, L. Angelina., D, J. R. Duarte., and N. M. Peruchena. (2013). Is the decrease of the total electron energy density a covalence indicator in hydrogen and halogen bonds. Journ. Mol. Mod, $19, 2097-2106$.

[40] L, Tür̈ker., I,Gutman. 2005. Iterative estimation of total π-electron energy. Journ. Serb. Chemi. Soci, $70, 1193-1197$.

[41] N, C. Jones., D, Field., and J,P. Ziesel. (2008). Low-energy total electron scattering in the methyl halides CH3Cl, CH3Br and CH3I. Inter. Jour. Mas. Spectro, 277, $1-3$, $91-95$.

[42] S, Radenković., I, Gutman. (2007). Total π-electron energy and Laplacian energy: how far the analogy goes. Journ. Serbi. Chemi. Soci, $72, 1343 - 1350$.

[43] M, Peric., I, Gutman., and J, Radic-Peric. (2006). The Hückel totaL π-electron energy puzzle, Journ. Serbi. Chemi. Soci, $71, 771 - 783$.

[44] D, A. Morales. (2005). The total π-electron energy as a problem of moments: application of the Backus-Gilbert method. Journ. Math. Chemi, $38, 389 - 397$.

[45] S, Markovic. (2003). Approximating total π-electron energy of phenylenes in terms of spectral moments. Indi. Journ. Chemi. $42, 1304 - 1308$.

[46] D, A. Morales. (2003). Systematic search of bounds for total π-lectron energy. Inter. Journ. Quant. Chemi, $93, 20 - 31$.

[47] I, Gutman. (2013). Degree-based topological indices. Croat. Chem. Acta, $86, 351 - 361$.

[48] B, Borovicanin., K.C. Das., B. Furtula., and I, Gutman. (2017). Bounds for zagreb indices, match Commun. Math. Comput. Chem , $78, 17 - 100$.

[49] K,C. Das and I, Gutman. 52(2004). Some properties of the second zagreb index, match Commun. Math. Comput. Chem , $1, 103 - 112$.

[50] I, Gutman and K.C. Das. (2004). The first zagreb index 30 years after, match Commun. Math. Comput. Chem $50, 83 - 92$.

[51] B, Liu., Z, You. (2011). A survey on comparing Zagreb indices. match Commun. Math. Comput. Chem, 65, 581593.

[52] A, Behtoei., M, Jannesari., B, Taeri. (2009). Maximum Zagreb index, minimum hyper-Wiener index and graph connectivity. Appl. Math. Lett. 22, 15711576.

[53] K,C. Das. (2004). Maximizing the sum of the squares of degrees of a graph, Disc. Math, 257, 5766.

[54] H,Y. Deng. (2007). A unified approach to the extremal Zagreb indices for trees, unicyclic graphs and bicyclic graphs. match Commun. Math. Comput. Chem, 57, 597616.

[55] S, Li., H, Zhou. (2010). On the maximum and minimum Zagreb indices of graphs with connectivity at most k. Appl. Math. Lett, 23, 128132.

[56] B, Zhou. (2004). Zagreb indices. match Commun. Math. Comput. Chem. 52, 113118.

[57] M, Khalifeh., H, Yousefi-Azari., A, Ashrafi. (2009). The first and second Zagreb indices of some graph operations. Discret Appl Math $157(4), 804 - 811$

[58] G, Shirdel., H. H, Rezapour., A.M, Sayadi. (2013). The Hyper-Zagreb index of graph operations. Irani. Journ. Math. Chem, $4(2), 213 - 220$.

[59] M, Ghorbani., N, Azimi. (2013). Note on multiple Zagreb indices. Irani. Journ. Math. Chem, $3, 137 - 143$

[60] G.H, Fath-Tabar. (2009). Zagreb Polynomial and Pi Indices of some Nano Structures. Digest J. Nanomat. Biostr, $4(1), 189 - 191$.

[61] A.R, Bindusree., I.N, Cangul., V, Lokesha., A.S, Cevik. (2016). Zagreb polynomials of three graph operators. Filomat., $30(7), 1979 - 1986$.

[62] K,Das., A, Yurttas, M, Togan., A, Cevik., Cangul. (2013). The multiplicative Zagreb indices of graph operations. J Inequal Appl.

[63] M, Veylaki., MJ,Nikmehr., HA, Tavallaee. (2015). The third and hyper-Zagreb coindices of some graph operations. J Appl Math Comput.

[64] M, Randić*c*. 97(1975). On characterization of molecular branching. J. Amer. Chem. Soc., $6609 - 6615$.

[65] B, Bollob*á*s., P, Erd*ó*s. (1998). Graphs of extremal weights. Ars Comb, 50, $225 - 233$.

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

[67] B, Zhou., N, TrinajstiĆ. (2009). On a novel connectivity index. J. Math. Chem. $46(4), 1252 - 1270$.

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

[69] B, Furtula., I, Gutman. (2015). A forgotten topological index. J Math Chem $53(4), 1184 - 1190$

[70] N, Nayeem, S.M.A., A,Pal. (2016). F-index of some graph operations. Discret. Math. Algorithms Appl. 8.

[71] H, Abdo., D, Dimitrov., I, Gutman. (2015). On extremal trees with respect to the F-index.

[72] De, N. A, Nayeem., S, M., A, Pal. (2016). The F-coindex of some graph operations.Springer Plus 5.

[73] W,Gao., M, Farahani., R, Shi. L. (2016). Forgotten topological index of some drug structures. Acta Med. Medit, 32(1), $579 - 585$.

[74] Y, Bashir., A, Aslam., M, Kamran Qureshi., M. I, Jahangir. A, Rafiq., N, Bibi., M, Muhammad. (2017). On Forgotten Topological Indices of Some Dendrimers Structure. Molecules MDPI, 22(6), 867.

[75] S, Akhter., M, Imran., Farahani., M.R. (2017). Extremal unicyclic and bicyclic graphs with respect to the F-index. AKCE International Journal of Graphs and Combinatorics. $14, 80 - 91$.

[76] T, Doslic. (2008). Vertex-weighted Wiener polynomials for composite graphs. Ars Math Contemp, $1, 66 - 80$.

[77] A. R, Ashrafi., T, Doslic., A, Hamzeh. 2010. The Zagreb coindices of graph operations. Discreet Appl. Math. 158, 1571 − 1578.

[78] R, Amin., A, Nayeem., S, M. (2017). Trees with minimum F-coindex. Elect. Not. Disc. Math, 63, 303 − 310.

[79] M, Berhe., C, Wang. (2019). Computation of certain topological coindices of graphene sheet and C4C8(S) nanotubes and nanotorus. Appl. Math. Nonlinear Scien, 4(2), 455468.

[80] N, De. 8(2018). F-index and co-index of some derived graphs. bullet. inter. math. virtual institute. 81 − 88.

[81] M.V, Diudea., A.E, Vizitiu., M, Mirzagar., A.R, Ashrafi. (2010). Sadhana polynomial in nano-dendrimers. Carpathian Journ. Math,26(1), 59 − 66.

[82] S, Iijima. (1991). Nature. 354, 56 .

[83] O, Adisa., B.J, Cox., J. M, Hill. (2011). Carbon 49, 3212.

[84] J, Zhao., A, Buldum., J, Han., J. P, Lu. (2002). Nanotechnology, 13 195 .

[85] A. R, Ashrafi., T, Doslic., A, Hamzeh. (2010). The Zagreb conindncies of graph operation. Discreet Appl. Math, 158, 1571 − 1578.

[86] M. V, Diudea., A. E, Vizitiu., M, Mirzagar., A.R, Ashrafi. (2010). Carpathian J. Math. 26, 59 .

[87] E, Bhuleier., W, Wehner., F, VOgtle. (1978). Synthesis, 2, 155 .

[88] B. K, Nanjwade., H.M, Bechara., G.K, Derkar., F.V, Manvi., V. K, Nanjwade. (2009). European journ. pharma, 38, (3), 185.

[89] A, Graovac., M, Ghorbani., M.A, Hosseinzadeh. (2011). Computing fifth geometric-arithmetic index for nanostar dendrimers. J. Math. Nanosci, 1(1) , 33 − 42.

[90] M. V, Walter., M, Malkoch. (2012). Chem. Soc. Rev., 41, 4593.

[91] A, Thackray. (1970). Atoms and Powers: an essay on Newtonian matter-theory and the development of chemistry, Harvard University Press, Cambridge, Massachusetts.

[92] L, Euler. (1736). Solutio problematis ad geometriam situs pertinentiss, Commentarii academiae scientiarum Petropolitanae, 8, $128-140$.

[93] F, Harary., G, Wilcox. (1967). Boolean operations on graphs. Math. Stand, $20, 41-51$.

[94] R, Hammack., W, Imrich., and S, Klavzar. (2011). Handbook of product graphs. Taylor and Francis Group, LLC, Chapman and Hall, Boca Raton. W, Mantel. (1907). Problem 28. Wiskundige Opgaven, 10, $60-61$. P, Turáan. (1941). Eine extremalaufgabe aus der graphentheorie. Mat. Fiz. Lapok, 48, $435-4524$.

[95] R. C, Entringer., D. E, Jackson., D. A, Snyder. (1976). Distance in graphs. Czech. Math. J, $26(2), 283-296$.

[96] I, Gutman. 1997. A property of the Wiener number and its modifications. Indian J. Chem, $36A, 128-132$.

[97] K, Xua., M, Liu., K.Ch. Das., I, Gutman., B, Furtula. (2014). A survey on graphs extremal with respect to distance-based topological indices. match Commun. Math. Comput. Chem,$71, 461-508$.

[98] De,N., S.K.A,N. (2016). Computing the F-index of nanostar dendrimers. Natural Scien. Engin, $18, 14-21$.

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