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By

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بسم الله الرحمن الرحيم

اقْرَأْ بِاسْمِ رَبِّكَ الَّذِي خَلَقَ * خَلَقَ الْإِنسَانَ مِنْ عَلَقٍ * اقْرَأْ وَرَبُّكَ الْأَكْرَمُ * الَّذِي عَلَّمَ بِالْقَلَمِ * عَلَّمَ الْإِنسَانَ مَا لَمْ يَعْلَمْ

صدق الله العظيم

العلق – الايه (1-5)

Dedication

To My Loving Mother and Father,

Words cannot explain how deeply grateful I am for your innumerable sacrifices. You were my first professors, my staunchest supporters, and my refuge during every storm. Even when you were exhausted from long days, you had time to listen to my worries. When others doubted, you believed wholeheartedly. When I fell, you were there to help me up, not just with your hands, but with your heart. You spent sleepless nights worrying about my future, fought financially to pay for my education, and sobbed silently when I didn't achieve my full potential. And, despite everything, you never made me feel lonely. When I got lost, your love served as a compass to guide me back. And the light You spent sleepless nights worried about my future, struggled financially to pay for my education, and cried silently when I failed to reach my full potential. And, despite everything, you never made me feel alone. Your love served as a compass to direct me when I became disoriented, and a light to keep me going when the route was too dark. This thesis is as much yours as mine is. Every page bears the imprint of your patience, and every chapter echoes your encouragement. If these words could express even a fraction of love and respect, I bear you, they would still be insufficient.

To my supervisor, Prof.Dr. Nabeel Ezzulddin Arif for academic guidance and for creating an environment in which curiosity could Succeed. Words cannot explain how deeply grateful I am for your innumerable sacrifices.

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Above all, I thank Allah Almighty for His boundless blessings, power, and direction throughout my studies and in the completion of this thesis. I want to extend my appreciation to my supervisor for his valuable counsel, feedback, and motivation throughout this research. I also thank the department staff and faculty for their encouragement during my studies. My friends and colleagues are particularly valued for the valuable discussions and for all the encouragement they offered me whenever I required it during hard times. Lastly, I thank all those who, directly or indirectly, assisted in the successful completion of this work

Supervisor's Certification

I certify that the thesis entitled by **Computation of Some Topological Indices of Certain Chemical Structures** was prepared under my supervision at the Department of Mathematics, College of Computer Science and Mathematics, University of Tikrit, as a fulfilment of the requirement for the Degree of M.Sc in Mathematical Science.

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Report of Linguistic Evaluation

I certify that the linguistic evaluation of this thesis was carried out by me and its accepted linguistically and in expression.

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EXAMINATION COMMITTEE CERTIFICATION

We certify that we have read the thesis entitled "**Computation of Some Topological Indices of Certain Chemical Structures** ", and examining committee examined the student (**Maria Kawa Mahmood**) in its contents and what is related with it in / / , and that in our opinion it is adequate with ( ) standing as a thesis for the degree of M.Sc. of Mathematical Science.

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Symbols	**Meaning**
G	Graph
$V(G)$	The collection of G's vertices
$E(G)$	The collection of G's edges
$d_{(s)}$	Degree of vertex
$d_{(v)}$	Degree of edge
$\Delta(G)$	Maximum degree of G
$\delta(G)$	Minimum degree of G
P_n	Path Graph with n vertex
C_n	Cycle Graph with n vertex
S_n	Star Graph with n vertex
K_n	Complete Graph with n vertex
$K_{\|x\|,\|Y\|}$ or $K_{a,b}$	Complete bipartite graph
$AZP(G,x)$	Augmented Zagreb
$RM_1(G,x)$	1st Reformulated Zagreb
$RM_2(G,x)$	2nd Reformulated Zagreb
$IR(G,x)$	Edge Irregularity
$DS(G,x)$	Degree Edge Stability
$AZI(G)$	Augmented Zagreb Index
$AZP(G)$	Augmented Zagreb Polynomial

$RM_1(G)$	1st Reformulated Zagreb Index
$RM_2(G)$	2nd Reformulated Zagreb Index
$IR(G)$	Edge Irregularity Index
$DS(G)$	Degree Edge Stability Index
$(D_n, P_n[n])$	Porphyrin Dendrimer
$(PETIM[n])$	Dendrimer of Propyl (Ether Imine)
$(DPZ_n[n])$	Dendrimer of Zinc Porphyrin
$(PETAA[n])$	Dendrimer of Poly (Ethylene Amide Amine)
$(APD[n])$	Dendrimer of aminoisphthalate dister monomer
$(PD[n])$	Dendrimer of Poly(amidoamine)

ABSTRACT

This work focuses on computing and determining degree-based topological indices and its polynomial for various dendrimer including. The classical ones like the newer ones the Augmented Zagreb,1st and 2nd Reformulated Zagreb, Edge Irregularity, and Degree Edge Stability indices are taken into consideration. Dendrimers like porphyrin (D_n, P_n), Propyl Ether Imine dendrimers (PETIM), Zinc Porphyrin dendrimers (DPZ_n) Poly (Ethylene Amide Amine) (PETAA), aminoisophthalate diester monomer (APD[n]) and Poly (amid amine) (PD[n]) dendrimers. The study also illustrates the difference between the Augmented Zagreb and Edge Irregularity indices, obtaining new upper and lower bounds for them. Results verify the predictive behavior of topological indices for molecular structure and activity.

INTRODUCTION

Graph theory is a mathematical area dealing with structures composed of vertices (also called nodes) and edges that connect them. The structures, also called as graphs, are frequently used to represent linkages and interactions in a variety of domains, including biology, computer science, chemistry, and social networking. A chemist uses graph theory to represent molecular structures, with the atoms as vertices and the chemical bonds as edges. This approach makes it possible to calculate topological indices, which are numerical values derived from a graph that can be applied to estimate physical and chemical molecule properties. If a graph doesn't include any edges between the vertices, then it's called a null graph. [1].

The ordered pair (V(G), E(G)) can be used to represent the graph, where (V(G)) represents the set of vertices of G and each element inside (V(G)) is called a vertex or node. Likewise, the set of edges of G is represented by (E(G). Chemical graph theory has provided researchers in chemistry with a wide range of very potent analysis methods. In this situation, a molecular graph provides a graphical representation of a chemical structure using concepts from graph theory. In these models, the compound's elements are represented by nodes, while connections depict the interactions among them. This is the topological subfield of mathematical chemistry where graph theory is employed to describe and analyze chemical behaviors and structural properties mathematically. [2].

Alexandru Balaban, Ante Groovac, Ivan Gutman, Haruo Hosoya, Milan Randić, and Nenad Trinajstić, among others, are considered pioneers in the field of chemical graph theory. It was reported in 1988 that a large number of researchers were working in this area, producing approximately 500 articles per year. There have been several monographs that was published in this field, such as Triassic's two-volume work "Chemical Graph Theory," which provided a concise overview of the discipline up until the middle of the 1980s, [3-4].

In terms of mathematics, an undirected graph is called a molecular graph. G = (S, V), where S is a non-empty set of atom and V is a set of bound. Let s∈S is an element of the molecular structure of every vertex, and the vertex degree is the number of edges it has. Molecular graph structure and characteristics are studied based on the arrangement and degree of vertices to obtain various topological indices that represent the molecule's behavior and properties. A typical example of such indices was provided by Trinajstić et al. in their work, which discussed π-electron energy in relation to the branching of molecules. Two traditional indices were given by them as follows:

$$M_1 = \sum_{s \in S} d(s)^2 \qquad \text{and} \qquad M_1 = \sum_{sv \in E} d(s).d(v) .$$

Where d(s) is the degree of vertex s. These indices quantify the branching degree in molecular structures, the larger values tending to be associated with more complex molecular structures and smaller total π-electron energy.

Generalizing from graph theory, many other degree-based topological indices have been constructed to characterize other structural features of chemical graphs. These include the Augmented Zagreb Index (AZI), which gives more weight to molecular branching, the First and Second Reformulated Zagreb Indices (Re_1 and Re_2), which provide edge degree-based reformulations rather than vertex degree formulations, and the Edge Irregularity Index, which measures the imbalance in degrees of adjacent vertices. Additionally, the Degree-Based Stability Index is applied to assess structural stability of molecules according to the vertex degree distribution [5].

A topological indices of a graph, it's a quantitative parameter about G that represents its molecular topology by encoding necessary structural features of the graph. Indices are graph operations invariant, e.g., relabeling vertices, reordering edges, or isomorphism, in such a way that the numerical value describes intrinsic properties of the molecular structure and not arbitrary representations. Topological indices are thus very useful in drug design, material science, and molecular chemistry. We are concerned here to compute some important topological indices of some chemical structures so that we can know their structural features and potential chemical properties. [6].

Graph polynomials are algebraic polynomials on graphs that compactly embody important structural information. Graph polynomials, as studied in graph theory and discrete mathematics, are valuable tools for the study of the complexity, connectedness, and symmetry of molecular graphs. More specifically, in this thesis, graph polynomials are employed to study molecular graphs of compounds like porphyrin, propyl ether imine, zinc porphyrin, and ethylene amide amine dendrimers. These molecules have intricate architectures that are nicely modeled by graph polynomials, which enables us to calculate topological invariants to predict their chemical behavior, stability, and potential applications in materials science and medicine. [7].

In (2010) B. Furtula, A. Graovac, and D. Vukičević. In (2015) F. Zhan, Y. Qiao, and J. Cai. And in (2016) N. Idrees, A. Sadiq, M. J. Saif, and A. Rauf , [8-10], define Augmented Zagreb Index (AZI) as a means to improve the predictive power of classical Zagreb indices, particularly for molecular branching and thermodynamic properties. It employs a more sophisticated degree-based weighting function, which has made it particularly appealing for highly branched systems, such as dendrimers.For poly(propylene imine) (PPI) and poly(amidoamine) (PAMAM) dendrimers. In (2013) V. R. Kulli and I. Gutman . In (2017) N. De . In (2024) S. Anwar et.al . In (2014) S. Ji, X. Li, and Y. Qu, and in (2013) I. Gutman, B. Furtula, and V. R. Kulli. [11-15] introduced the result for the Reformulated Zagreb Indices, to generalize the traditional Zagreb indices considering the edge degrees instead of vertex egrees. They are more responsive to connectivity alterations in graphs and thus appropriately usable for complex ierarchical architectures like dendrimers. for the PAMAM dendrimer and the polyetherimide (PETIM) dendrimer.

In (2015) H. S. Abdo and D. M. Dimitrov, In (2024) M. Imran, and in (2018) I. Gutman and H. Abdo, [16-18], introduced the Edge Irregularity Index to quantify structural heterogeneity in terms of degree differences among neighboring vertices. The index has found broad use to characterize dendritic macromolecules, with irregular structures often occurring in higher generations.

In (2012) J. Chen, S. Li, and W. Wang, In (2017) N. De, et.al., In (2019) L. Yousefi-Azari, M. Saheli, and M. Azari. [19-21] introduced the Degree-Based Stability Index to measure molecular stability based on vertex degree distributions. It has been helpful for understanding thermodynamic stability in arborescent and hyperbranched dendrimers. In (2005) D.A. Tomalia and J.M. Jansen. developed, in the late 1980s, Polypropylenimine (PPI) dendrimers that possess a diaminobutane (DAB) core and tertiary amine branching units. PPI dendrimers are highly defined in their molecular architecture and are used extensively in gene delivery and nanomedicine because of their appropriate surface functionalities and biocompatibility, [22].In (2008) S. Kulhari, PETIM dendrimers were introduced in the early 2000s as a dendrimer family possessing ether and imine linkages. They are appealing due to their improved solubility in organic solvents and reduced cytotoxicity, making them suitable for use in biomedical and pharmaceutical applications. They are comparatively easy to synthesize compared to other dendrimer families. [23].

In (1998) G.R. Newkome, Zinc porphyrin dendrimers entrap porphyrin macrocycles with a zinc metal ion in the center, enabling them to have unique photochemical and electrochemical properties. The dendrimers that became popular during the 1990s are widely used in light-harvesting systems, photodynamic therapy, and solar energy conversion, [24]. In (1985) D.A. Tomalia, One of the most well studied and oldest dendrimers are PAMAM dendrimers, which were originally synthesized by Tomalia. they synthesized via a divergent growth strategy and are noted for their ethylenediamine core and iteratively repeated amide and amine branching. PAMAM dendrimers have extensive use in drug and gene delivery, diagnostics, and nanotechnology, [25]. In (1996) A. Harriman, Porphyrin-dendrimers are designed by placing porphyrin units at the periphery or core of the dendrimer system. Porphyrin-dendrimers are of interest for optoelectronics, photodynamic therapy, and catalysis due to the photo absorbing and redox activity of porphyrins. [26]. In (2016) Che, Z., & Chen, Z , define Lower and Upper Bounds of the Forgotten Topological Index, [27]. In (2020) Lin, W., Dimitrov, D., & Škrekovski, R. define the maximal of the Augmented Zagreb index. In (2013) N. E. Arif and R. Hasni, define the connectivity index of PAMAM dendrimers, [28].

In (2013) N. E. Arif, studied Graph Polynomials and Topological Indices of Some Dendrimers, [29]. In (2016) M. N. Husin, R. Hasni, N. E. Arif, and M. Imran, studied On topological indices of certain families of Nano star dendrimers, [30]. In (2023) A. S. Majeed and N. E. Arif, studied topological indices of certain neutrosophic graphs. [31]

This thesis is divided into five chapters, chapter one has presented preliminary definitions of graph theory, polynomials, a topological index of graph and dendrimer.

Chapter two comprises two sections, including the computation of

various polynomials, with their topological indices by taking it's derivative for a selected dendrimer. The first division entails the computation of the first kind of dendrimer, (D_n, P_n), which is also referred to as Porphyrin-dendrimers. The second section entails the computation of the second kind of dendrimer, $(PETIM)$, which is referred to as Propyl Ether Imine dendrimers.

Chapter three is divided into two section, including the computation of

various polynomials, with their topological indices by taking it's derivative for a selected dendrimer. The first division entails the computation of the first kind of dendrimer, Zinc porphyrin and ethylene amide amine $(PETIM)$ dendrimers respectively.

Chapter four is made up of two section. including the computation of various polynomials, with their topological indices by taking it's derivative for a selected Nano star dendrimer. aminoisophthalate diester monomer (APD[n]) And Poly(amidoamine) (PD[n]) in every detail.

Chapter five is made up of three section In the first section, the correlation between some topological indices is given. The second sections are devoted to figuring out the bottom and upper limits of the Augmented Zagreb index. The third sections are devoted to determining the lower and upper bounds of the Edge Irregularity Zagreb index.

Chapter One

Basic Concepts and Preliminaries

1.1 Preliminaries.

Definition 1.1.1: [6] **Graph (G):** The adjacency relation ($\aleph$:V ×V→ E) establishes the relationship between each edge and the vertex pairs of G.

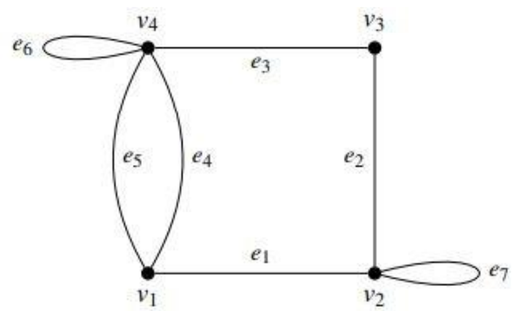


Figure 1.1 Graph Example

Definition1.1.2: [37] **Order of (G):** The order of a graph G, denoted by O(G), is the number of its vertices.

Definition1.1.3: [37] **Size of (G):** The size of graph G, denoted by e(G), is the number of its edges.

Definition 1.1.4: [35] **Graph polynomial**: is a way of turning the structure of a graph into a polynomial (an algebraic expression) that tells us useful information about the graph. It often includes variables related to the number of edges, vertices, or how they are connected.

Definition 1.1.5: [37] **Isolated vertex**: a vertex with degree zero in a graph is said to be isolated it has no edges connecting it to any other vertex.

Definition 1.1.6: [37] **Pendant vertex:** a pendant vertex, sometimes known as a leaf, is a vertex of degree one, which means that it has a single edge connecting it to precisely one other vertex.

Definition 1.1.7: [36] **Core vertex:** Is a vertex that is neither pendent nor isolated and also known as an intermediate vertex.

Definition 1.1.8: [37] 1) **Graph maximum:** $\Delta(G) = \max\{d_{(v)}: v \in V(G)\}$ is the definition of a graph G's greatest degree, denoted as $\Delta(G)$.

2) Graph minimum: $\min\{d_{(v)}: v \in V(G)\}$ is the definition of a graph G's least degree, represented by $\delta(G)$.

3) Keep in mind that $\delta(G) \leq d(v) \leq \Delta(G)$ for every vertex v in G.

Theorem 1.1.9: [37] In a graph G, the sum of the degrees of the vertices is equal to twice the number of edges. That is, $\sum_{v \in V(G)} d_{(v)} = 2\varepsilon$

Theorem 1.1.10: [37] For any graph G, $\delta(G) \leq \frac{2|E|}{|V|} \leq \Delta(G)$.

Theorem 1.1.11: [37] The number of vertices of odd degree in any given graph G is always even.

Definition 1.1.12: [37] **Loop:** Is an edge in a graph that connects a node to itself.

Definition 1.1.13: [37] **Parallel Edges:** edges that are parallel. Multiple or parallel edges are those that connect the same pair of vertices.

Definition 1.1.14: [37] **Simple Graph:** A graph G is said to as simple if it lacks parallel edges and loops.

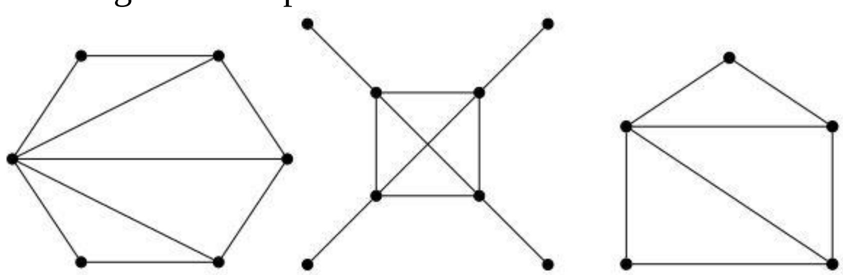


Figure1.2 Some examples of simple graph.

Definition 1.1.15: [37] **Subgraph:** A graph $H(V_1, E_1)$ is considered to be a subgraph of a graph $G(V, E)$ if $V_1 \subseteq V \text{ and } E_1 \subseteq E$.

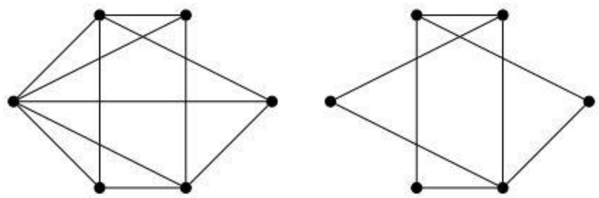


Figure1.3: Example of Subgraph

Definition 1.1.16: [37] **Spanning Subgraph:** A graph $H(V_1, E_1)$ considered a spanning subgraph of a graph when $G(V, E)$ if $V_1 = V$ and $E_1 \subseteq E$.

Definition 1.1.17: [37] **Complete Graph:** Is a simple undirected graph where each pair of distinct vertices is joined by a distinct edge.

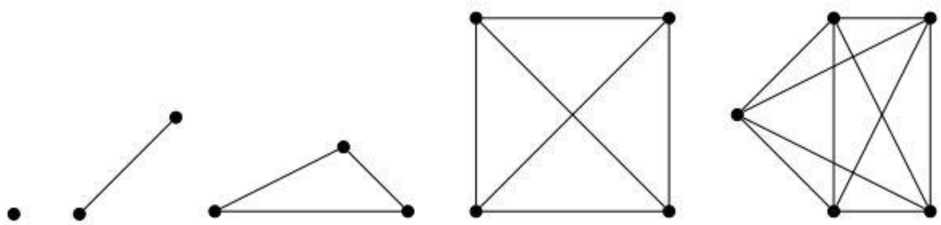


Figure1.4: First few complete graphs.

Definition 1.1.18: [37] **Bipartite Graph:** A graph G is said to be a bipartite graph if its vertex set V can be partitioned into two sets, say V_1 and V_2, such that no two vertices in the same partition can be adjacent.

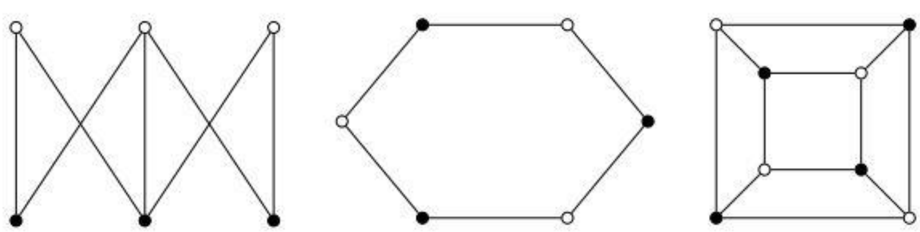


Figure 1.5: Example of Bipartite Graph.

Definition 1.1.19: [37] **Complete Bipartite Graph:** Is considered complete if every vertex in one partition is adjacent to every vertex. Complete bipartite graph with bipartition (x, Y) is denoted by $K_{|x|,|Y|}$ or $K_{a,b}$, where $a = |x|, b = |Y|$.

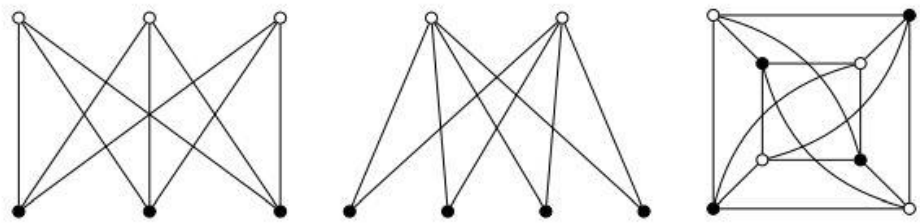


Figure 1.6: Example of Complete Bipartite Graphs.

Theorem 1.1.20: [37] The entire graph K_n can be expressed as the union of k bipartite graphs, If and only if $n \leq 2^K$.

Definition 1.1.21: [37] **Regular Graphs:** Graph G is regular when its vertices have the same degree. Graph G is said to be a $k-regular$ graph if $d_{(s)}= k \; \forall \; s \in S(G)$. Every complete graph is an $(n-1)$-regular graph.

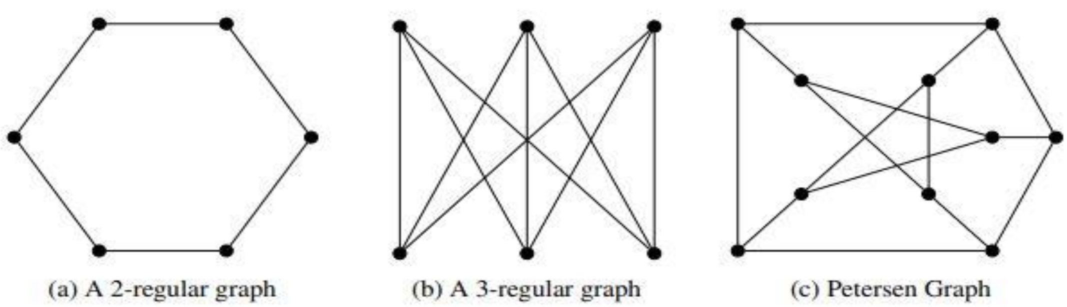


Figure 1.7: Examples of Regular Graphs

Definition 1.1.22: [37] **Walk:** Is any path through a graph that connects vertex to vertex via edges.

Definition 1.1.23: [37] **Trails:** A walk that doesn't cross the same edge over and over again.

Definition 1.1.24: [37] **Cycles:** Is possible exception of the start vertex being the same as the end.

Definition 1.1.25: [37] **1) Path:** Is a walk that does not involve any vertex twice. Path that begins and ends at the same vertex is called a cycle. Keep in mind that a path with n vertices has a length of n-1.

Definition 1.1.26: [37] **Geodesic distance:** The length (number of edges) of the shortest path (also called a graph geodesic) between two vertices s and v in a graph G.

Definition 1.1.27: [37] **Eccentricity of the vertex:** The longest geodesic distance between a vertex v and any other vertices is its eccentricity, which is denoted by the symbol d(s). It can be conceptualized as the separation between a vertex and the vertex in the graph that is most distant from it.

Definition 1.1.28: [37] **Graph's Radius:** The smallest eccentricity of any vertex in a graph G is its radius, denoted by rad(G), $rad(G) = \min_{s\in V(G)} d(s)$

Definition 1.1.29: [37] **Diameter of a graph:** The maximum eccentricity of any vertex in a graph G is its diameter, denoted as diam(G), $diam(G) = \max_{s\in V(G)} d(s)$.

Definition 1.1.30: [37] **Cut-Edge:** A cut edge (a bridge) is an edge in a graph whose removal increase the number of connected components in the graph.

Definition 1.1.31: [37] **Cut- Vertex:** In a connected graph, a cut vertex (also known as an articulation point) is a vertex whose removal increases the graph's connected components.

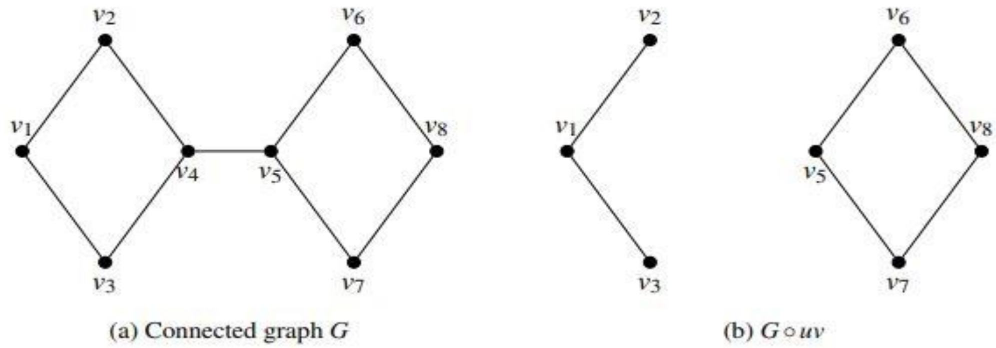


Figure 1.8: Disconnected graph $G - v_4$

Theorem 1.1.32: [37] A cut-edge of a graph G is one that is not contained in any of G's cycles.

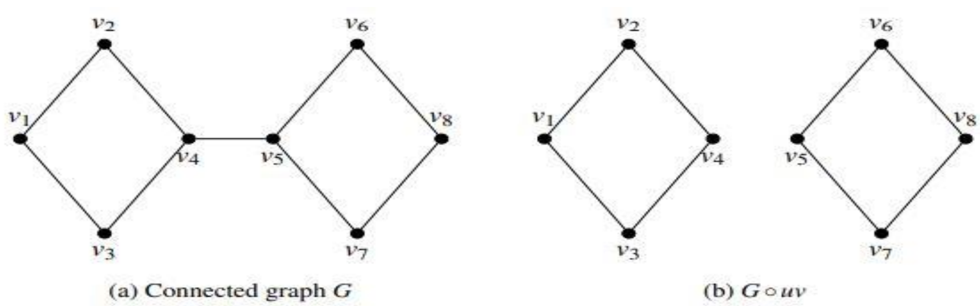


Figure 1.9: Disconnected graph $G - v_4v_5$.

1.2 Topological Index:

Introduction: A topological index is a quantity calculated from the molecular graph structure that characterizes the topology (connectivity) of the molecule. It is a graph-theoretical descriptor used very frequently in chemical graph theory for correlating molecular structure with chemical, physical, or biological activity. [36].

Definition 1.2.1: [30] The Augmented Zagreb Index of graph G define as:

$$\mathrm{AZI}(G) = \sum_{\mathrm{sv}\in \mathrm{E(G)}} \left(\frac{\mathrm{d}_{(\mathrm{S})} * \mathrm{d}_{(\mathrm{v})}}{\mathrm{d}_{(\mathrm{S})} + \mathrm{d}_{(\mathrm{v})} - 2}\right)^{3}$$

Definition 1.2.2: [15] The 1st Reformulated Zagreb Index of graph G define as:

$$RM_1(G) = \sum_{\mathrm{sv}\in \mathrm{E(G)}} (d_{(s)} + d_{(v)} - 2)^2$$

Definition 1.2.3: [15] The 2nd Reformulated Zagreb Index of graph G define as:

$$RM_2(G) = \sum_{\mathrm{sv}\in \mathrm{E(G)}} \big(d_{(s)} + d_{(v)} - 2\big)(d_{(s)} * d_{(v)})$$

Definition 1.2.4: [17] The Edge Irregularity Index of graph G define as:

$$IR\ (G) = \sum_{\mathrm{sv}\in \mathrm{E(G)}} |\, d_{(s)} - d_{(v)}|$$

Definition 1.2.5: [19] The Degree Edge Stability Index of graph G define as:

$$DS\ (G) = \sum_{\mathrm{sv}\in \mathrm{E(G)}} (d_{(s)} - d_{(v)})^2.$$

1.3 Graph Polynomials:

Introduction: Graph polynomial is a polynomial that represents information pertaining to the structure of a graph. It is built up from numbers or variables relating to the edges, vertices, or subgraphs of the graph. Graph polynomials are a means of expressing important properties like how a graph is connected, or how its components are paired. Graph polynomials are important both in pure mathematics as well as in applied fields like chemistry and physics. [35].

Definition 1.3.1: [8] The Augmented Zagreb polynomial of graph G define as:

$$\mathrm{AZP}\ (G,x) = \sum_{\mathrm{sv}\in \mathrm{E(G)}} x^{\left(\frac{\mathrm{d}_{(\mathrm{S})} * \mathrm{d}_{(\mathrm{v})}}{\mathrm{d}_{(\mathrm{S})} + \mathrm{d}_{(\mathrm{v})} - 2}\right)^{3}}$$

Definition 1.3.2: [14] The 1st Reformulated Zagreb polynomial of graph G define as:

$$RM_1(G,x) = \sum_{\mathrm{sv}\in \mathrm{E(G)}} x^{(d_{(s)}+d_{(v)}-2)^2}.$$

Definition 1.3.3: [14] The 2nd Reformulated Zagreb polynomial of graph G define as:

$$RM_2(G,x) = \sum_{\mathrm{sv}\in \mathrm{E(G)}} x^{\left(d_{(s)}+d_{(v)}-2\right)\left(d_{(s)}*d_{(v)}\right)}.$$

Definition 1.3.4: [16] The Edge Irregularity Polynomial of graph G define as:

$$IR\ (G,x) = \sum_{\mathrm{sv}\in \mathrm{E(G)}} x^{|\ d_{(s)}-\ d_{(v)}|}.$$

Definition 1.3.5: [19] The Degree Edge Stability Polynomial of graph G define as:

$$DS\ (G,x) = \sum_{\mathrm{sv}\in \mathrm{E(G)}} x^{(d_{(s)}-d_{(v)})^2}.$$

1.4 Dendrimers:

Dendrimers are artificially synthesized, highly branched, tree-like macromolecules with a core, uniform interior layers (generations), and terminal functional groups. Their extremely symmetrical, well-defined architecture provides them with a unique distinction from the traditional polymers and allows strict control of molecular size, shape, and functionality.

The concept of dendrimers was first mentioned in the late 1970s and early 1980s. The first synthesis of dendrimers, i.e., poly (amidoamine) (PAMAM) dendrimers, was performed by Donald A. Tomalia and colleagues at Dow Chemical Company in 1985. Around the same time, independently of one another, Fritz Vögtle in Germany and George Newkome in the USA also synthesized similar dendritic architectures. Various types of dendrimers have been prepared over the years to serve different chemical and biomedical purposes. Some of them are Propyl Ether Imine (PETIM) dendrimers, by virtue of their solubility and biocompatibility; Zinc Porphyrin and Porphyrin-based dendrimers, for use in photodynamic therapy and light-harvesting systems; Ethylene Amide Amine dendrimers, for drug delivery and molecular encapsulation; and Aminoisophthalate Diester Monomer-based dendrimers, as building blocks in the assembly of sophisticated dendritic systems. Due to their new structure and functional diversity, dendrimers have become of critical importance in fields such as drug delivery, diagnostics, nanotechnology, catalysis, and materials science. [39-42].

Chapter Two

Computation of Topological Indices and Polynomials of Porphyrin $(Dn\ Pn)$ and Propyl Ether Imine $(PETIM)$ Dendrimers

2.1 Computation of Topological Indices and Polynomials of Porphyrin Dendrimer $(D_n\,P_n)$.

Introduction: The topological indices are used to obtain the topological properties and steric structure of dendrimers or macromolecules. As has been said earlier throughout this chapter will deal with computing some polynomials for various different classes of dendrimers like porphyrin dendrimer $(D_n\,P_n)$ and Propyl Ether Imine dendrimer (PETIM).

Proposition 2.1.1: [41] It considered the first type of dendrimer $(D_n\,P_n)$ then:

1. **Order of** $(D_n\,P_n)$ is $84 \times 2^{n-1} - 51$
2. **The size of** $(D_n\,P_n)$ is $93 \times 2^{n-1} - 57$. See figure 2.1

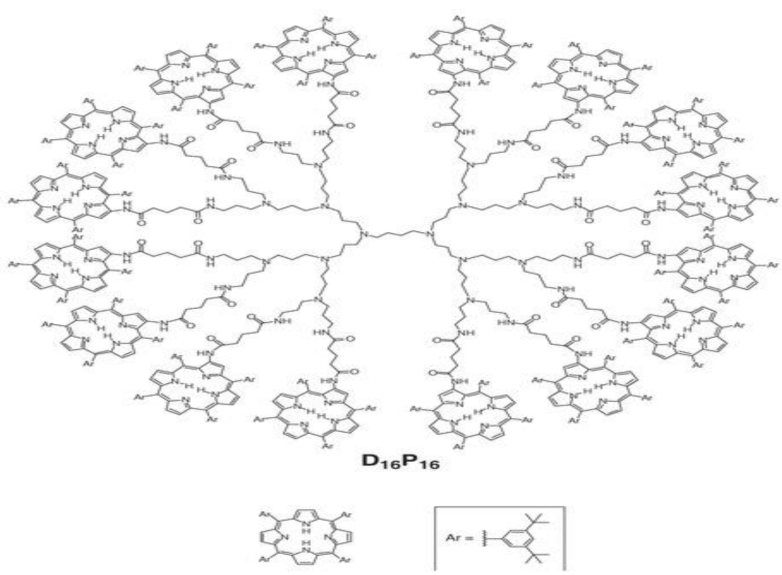


Figure 2.1: dendrimers $(D_n\,P_n)$ is also known as porphyrin.

($D_n P_n$) contain six types of edges based on degree of end vertices of each as given in table 2.1.

Table 2.1: Graph of the structures ($D_n P_n$)

(d_s, d_v)	(1,3)	(1,4)	(2,2)	(2,3)	(3,3)	(3,4)
No. of edges	$2n$	$24n$	$10n-5$	$48n-6$	$13n$	$8n$

First of all, we are going to calculate the Augmented Zagreb polynomial for the molecular ($D_n P_n$)

Theorem 2.1.1: Let n ∈ N, then the Augmented Zagreb polynomial of ($D_n P_n$) is given as **:**

$$AZP\ (D_n P_n, x) = (2n)\, x^{\frac{27}{8}} + (24n)x^{\frac{64}{27}} + (58n-11)x^{8} + (13\,n)x^{\frac{729}{64}} + (8\,n)x^{\frac{1728}{125}}.$$

Proof: The edge set of Porphyrin dendrimer ($D_n P_n$) is divided in to six sets E_1, E_2, E_3, E_4, $E_5$and E_6. Which are define as follow. See table 2.1.

$|E_1(D_n P_n)|$ Be composed of $2n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 3$, where $sv \in E\ (D_n P_n)$.

$|E_2(D_n P_n)|$ Be composed of $24\,n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 4$, where $sv \in E\ (D_n P_n)$.

$|E_3(D_n P_n)|$ Be composed of $10n-5$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where $sv \in E\ (D_n P_n)$.

$|E_4(D_n P_n)|$ Be composed of $48\,n-6$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv \in E\ (D_n P_n)$.

$|E_5(D_n P_n)|$ Be composed of $13n$ edges of type s, v s.t $d_{(s)} = 3$, $d_{(v)} = 3$, where $sv \in E(D_n P_n)$.

$|E_6(D_n P_n)|$ Be composed of $8n$ edges of type s, v s.t $d_{(s)} = 3$, $d_{(v)} = 4$, where $sv \in E(D_n P_n)$.

$$\mathrm{AZP}(\mathrm{D_n P_n}, x) = \sum_{sv \in E(G)} x^{\left(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2}\right)^3}$$

$$= \sum_{sv \in E_1(G)} x^{\left(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2}\right)^3} + \sum_{sv \in E_2(G)} x^{\left(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2}\right)^3} +$$

$$\sum_{sv \in E_3(G)} x^{\left(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2}\right)^3} + \sum_{sv \in E_4(G)} x^{\left(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2}\right)^3} +$$

$$\sum_{sv \in E_5(G)} x^{\left(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2}\right)^3} + \sum_{sv \in E_6(G)} x^{\left(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2}\right)^3}$$

$$= (2n)\, x^{\left(\frac{1*3}{1+3-2}\right)^3} + (24n)\, x^{\left(\frac{1*4}{1+4-2}\right)^3} + (10n - 5)\, x^{\left(\frac{2*2}{2+2-2}\right)^3} + (48n -$$

$$6)\, x^{\left(\frac{2*3}{2+3-2}\right)^3} + (13n)\, x^{\left(\frac{3*3}{3+3-2}\right)^3} + (8n)\, x^{\left(\frac{3*4}{3+4-2}\right)^3}$$

$$\mathrm{AZP}(\mathrm{D_n P_n}, x) = (2n)x^{\frac{27}{8}} + (24n)x^{\frac{64}{27}} + (58n - 11)x^8 + (13n)x^{\frac{729}{64}}$$

$$+(8n)x^{\frac{1728}{125}}.$$

Corollary 2.1.1: [41] let n $\in$ N, then the Augmented Zagreb index of $(D_n P_n)$ is given as **:**

$$\mathrm{AZI}(D_n P_n) = \frac{38031}{100} n - 88$$

Proof: The edge set of Porphyrin dendrimer $(D_n P_n)$ is divided in to six sets E_1, E_2, E_3, E_4, $E_5$and E_6. Which are define in the theorem 2.1.1. By using definition of Augmented Zagreb topological index we will apply on Porphyrin dendrimer $(D_n P_n)$. By taken its derivative we will get the topological index.

AZI ($D_n\,P_n$) $= \sum_{sv \in E(G)} (\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2})^3$.

$\frac{d}{d(x)}[\,\text{AZP}(P_n, \text{x})]_{x=1} = (2n)\, x^{\frac{27}{8}} + (24n)\, x^{\frac{64}{27}} + (58n - 11)x^8 +$

$(13n)x^{\frac{729}{64}} + (8n)x^{\frac{1728}{125}}$

$\frac{d}{d(x)}[\,\text{AZP}(D_n\,P_n, x)]_{x=1} = \frac{27}{4}n + \frac{1536}{27}n + \frac{9477}{64}\,n + \frac{13824}{125}n + 58\,n - 88$

AZI($D_n\,P_n$) = $\frac{38031}{100}n - 88$.

Theorem 2.1.2: Let n ∈ N, then the 1st Reformulated Zagreb Polynomial of ($D_n\,P_n$) is define as **:**

$$RM_1(D_n\,P_n, x) = (60n - 11)x^4 + (26n)x^9 + (13n)x^{16} + (8n)x^{25}$$

Proof: The edge set of Porphyrin dendrimer ($D_n\,P_n$) is divided in to six sets E_1, E_2, E_3, E_4, $E_5$and E_6. Which are defined as follow. See table 2.1:

$|\,E_1(D_n\,P_n)|$ consist $2n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 3$, where

sv $\in E\ (D_n\,P_n)$.

$|\,E_2(D_n\,P_n)|$ consist $24n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 4$, where sv $\in E\ (D_n\,P_n)$.

$|\,E_3(D_n\,P_n)|$ consist $10n - 5$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where sv $\in E\ (D_n\,P_n)$.

$|\,E_4(D_n\,P_n)|$ consist $48n - 6$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv \in E\ (D_n\,P_n)$.

$|\,E_5(D_n\,P_n)|$ consist $13n$ edges of type s, v s.t $d_{(s)} = 3$, $d_{(v)} = 3$, where $sv \in E\ (D_n\,P_n)$.

$|E_6(D_n P_n)|$ consist $8n$ edges of type s, v s.t $d_{(s)} = 3$, $d_{(v)} = 4$, where $sv \in E\ (D_n P_n)$.

$RM_1(D_n P_n, x) = \sum_{sv \in E(G)} x^{(d_{(s)}+d_{(v)}-2)^2}$

$= \sum_{sv\in E_1(G)} x^{(d_{(s)}+d_{(v)}-2)^2} + \sum_{sv\in E_2(G)} x^{(d_{(s)}+d_{(v)}-2)^2} + \sum_{sv\in E_3(G)} x^{(d_{(s)}+d_{(v)}-2)^2} + \sum_{sv\in E_4(G)} x^{(d_{(s)}+d_{(v)}-2)^2} + \sum_{sv\in E_5(G)} x^{(d_{(s)}+d_{(v)}-2)^2} + \sum_{sv\in E_6(G)} x^{(d_{(s)}+d_{(v)}-2)^2}$

$= (2n)\ x^{(1+3-2)^2} + (24n)\ x^{(1+4-2)^2} + (10n-5)x^{(2+2-2)^2} + (48n - 6)\ x^{(1+3-2)^2} + (2n)\ x^{(2+3-2)^2} + (13n)\ x^{(3+3-2)^2} + (8n)\ x^{(3+4-2)^2}$

$RM_1(D_n P_n, x) = (60n-11)x^4 + (26n)x^9 + (13n)x^{16} + (8n)x^{25}$.

Corollary 2.1.2: Let n ∈ N, then the 1st Reformulated Zagreb index of $(D_n P_n)$ is given as **:**

$$RM_1(D_n P_n) = 1104n - 74.$$

Proof: By the same way of corollary 2.1.1, to compute the result of 1st Reformulated Zagreb Polynomial, which is denoted by $RM_1(D_n P_n, x)$, of the dendrimer $(D_n P_n)$, we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$\frac{d}{d(x)}[\ RM_1(D_n P_n, x)]\ |_{x=1} = (60n-11)x^4 + (26n)x^9 + (13n)x^{16} + (8n)x^{25}$.

$\frac{d}{d(x)}[\ RM_1(D_n P_n, x)|_{x=1} = 8n + 216n + 40n - 20 + 432n - 54 + 208n + 200n.$

Thus, the 1st Reformulated Zagreb Index of the porphyrin dendrimer is ($D_n P_n$) verified as:

$RM_1(D_n P_n) = 1104n - 74$.

Theorem 2.1.3: Let n ∈ N, then the 2nd Reformulated Zagreb Polynomial of ($D_n P_n$) is define as **:**

$$RM_2(D_n P_n) = (2n)x^6 + (10n-5)x^8 + (24n)x^{12} + (48n-6)x^{18} + (13n)x^{36} + (8n)x^{80}$$

Proof: The edge set of Porphyrin dendrimer ($D_n P_n$) is divided in to six sets E_1, E_2, E_3, E_4, $E_5$and E_6. Which are define as follow. See table (2.1).

$|E_1(D_n P_n)|$ include $2n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 3$, where $sv \in E(D_n P_n)$.

$|E_2(D_n P_n)|$ include $24n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 4$, where $sv \in E(D_n P_n)$.

$|E_3(D_n P_n)|$ include $10n - 5$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where $sv \in E(D_n P_n)$.

$|E_4(D_n P_n)|$ include $48n - 6$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv \in E(D_n P_n)$

$|E_5(D_n P_n)|$ include $13n$ edges of type s, v s.t $d_{(s)} = 3$, $d_{(v)} = 3$, where $sv \in E(D_n P_n)$.

$|E_6(D_n P_n)|$ include $8n$ edges of type s, v s.t $d_{(s)} = 3$, $d_{(v)} = 4$, where $sv \in E(D_n P_n)$.

$RM_2(D_n P_n, x) = \sum_{sv \in E(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})}$

$= \sum_{sv \in E_1(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv \in E_2(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} +$
$\sum_{sv \in E_3(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv \in E_4(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} +$
$\sum_{sv \in E_5(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv \in E_6(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})}$

$= (2n)\, x^{(1+3-2)(1*3)} + (24n)\, x^{(1+4-2)(1*4)} + (10n-5)x^{(2+2-2)(2*2)} +$
$(48n-6)x^{(2+3-2)(2*3)} + (13n)\, x^{(3+3-2)(3*3)} + (8n)\, x^{(3+4-2)(3*4)}$

$RM_2(D_n P_n, x) \quad = (2n)x^6 + (10n-5)x^8 + (24n)x^{12} + (48n-6)x^{18} +$
$(13n)x^{36} + (8n)x^{80}.$

Corollary 2.1.3: Let n ∈ N, then the 2nd Reformulated Zagreb index of ($D_n P_n$) is given as **:**

$$RM_2(D_n P_n) = 2288n - 148.$$

Proof: By way of corollary 2.1.1, confirm the result of 2nd Reformulated Zagreb Polynomial, which is denoted by $RM_2(D_n P_n, x)$, of the dendrimer ($D_n P_n$), we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$\frac{d}{d(x)}[\, RM_2(D_n P_n, x)]\ |_{x=1} = (2n)x^6 + (10n-5)x^8 + (24n)x^{12} + (48n-$
$6)x^{18} + (13n)x^{36} + (8n)x^{80}.$

$\frac{d}{d(x)}[\, RM_2(D_n P_n, x)|_{x=1} = 12n + 288\, n + 80n - 40 + 864n - 108$

$$+468\, n + 576n.$$

Thus, the 2nd Reformulated Zagreb Index of the porphyrin dendrimer is ($D_n P_n$) verified as:

$RM_2(D_n P_n) = 2352n - 148.$

Theorem2.1.4: Let n ∈ N, then the Edge Irregularity Polynomial of $(D_n\,P_n)$ is define as **:**

$$IR\ (D_n\,P_n, x) = (24n)x^3 + (2n)x^2 + (56n - 6)x + 23n - 5.$$

Proof*:* The edge set of Porphyrin dendrimer $(D_n\,P_n)$ is divided in to six sets E_1, E_2, E_3, E_4, $E_5$and E_6. Which are define as it's shown in the table (2.1).

$|\,E_1(D_n\,P_n)|$ consists $2n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 3$, where $sv\ \in E\ (D_n\,P_n)$.

$|\,E_2(D_n\,P_n)|$ consists $24\,n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 4$, where $sv\ \in E\ (D_n\,P_n)$.

$|\,E_3(D_n\,P_n)|$ consists $10n - 5$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where $sv\ \in E\ (D_n\,P_n)$.

$|\,E_4(D_n\,P_n)|$ consists $48\,n - 6$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv\ \in E\ (D_n\,P_n)$.

$|\,E_5(D_n\,P_n)|$ consists $13\,n$ edges of type s, v s.t $d_{(s)} = 3$, $d_{(v)} = 3$, where $sv\ \in E\ (D_n\,P_n)$.

$|\,E_6(D_n\,P_n)|$ consists $8\,n$ edges of type s, v s.t $d_{(s)} = 3$, $d_{(v)} = 4$, where $sv\ \in E\ (D_n\,P_n)$.

$IR\ (D_n\,P_n, x) = \sum_{sv\in E(G)} x^{|\,d_{(s)} - d_{(v)}|}$

$= \sum_{sv\in E_1(G)} x^{|\,d_{(s)} - d_{(v)}|} + \sum_{sv\in E_2(G)} x^{|\,d_{(s)} - d_{(v)}|} + \sum_{sv\in E_3(G)} x^{|\,d_{(s)} - d_{(v)}|} +$
$\sum_{sv\in E_4(G)} x^{|\,d_{(s)} - d_{(v)}|} + \sum_{sv\in E_5(G)} x^{|\,d_{(s)} - d_{(v)}|} + \sum_{sv\in E_6(G)} x^{|\,d_{(s)} - d_{(v)}|}$

= $(2n)x^{|1-3|} + (24n)\, x^{|1-4|} + (10n-5)x^{|2-2|} + (48n-6)\, x^{|2-3|} + (13n)\, x^{|3-3|} + (8n)x^{|3-4|}$.

$IR\,(D_n\,P_n, x) = (24n)x^3 + (2n)x^2 + (56n-6)x + 23n - 5.$

Corollary 2.1.4: Let n ∈ N, then the Edge Irregularity index of ($D_n\,P_n$) is given as **:**

$$IR\,(D_n\,P_n) = 132n - 6.$$

Proof: To demonstrate and evaluate the result of Edge Irregularity Polynomial, which is denoted by $IR\,(D_n\,P_n, x)$, of the dendrimer ($D_n\,P_n$), we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$\frac{d}{d(x)}[\,IR\,(D_n\,P_n, x)]\,|_{x=1} = (24n)x^3 + (2n)x^2 + (56\,n-6)x + 23n - 5$

$\frac{d}{d(x)}[\,IR\,(D_n\,P_n, x)|_{x=1} = 4n + 72n + 48n - 6 + 8n.$

Thus, the Edge Irregularity Index of the porphyrin dendrimer is ($D_n\,P_n$) verified as:

$IR\,(D_n\,P_n) = 132n - 6.$

Theorem2.1.5: Let n ∈ N, then the Degree Edge Stability Polynomial of ($D_n\,P_n$) is given as **:**

$$DS\,(D_n\,P_n, x) = (24n)x^9 + (56n-6)x^4 + (8n)x + 23n - 5$$

Proof: The edge set of Porphyrin dendrimer ($D_n\,P_n$) is divided in to six sets E_1, E_2, E_3, E_4, $E_5$and E_6. Which are define in the table (2.1).

$|\,E_1(D_n\,P_n)|$ contain $2n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 3$, where

$sv\ \in E\,(D_n\,P_n)$.

$|E_2(D_n P_n)|$ contain $24n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 4$, where $sv \in E\ (D_n P_n)$.

$|E_3(D_n P_n)|$ contain $10n - 5$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where $sv \in E\ (D_n P_n)$.

$|E_4(D_n P_n)|$ contain $48n - 6$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv \in E\ (D_n P_n)$.

$|E_5(D_n P_n)|$ contain $13n$ edges of type s, v s.t $d_{(s)} = 3$, $d_{(v)} = 3$, where $sv \in E\ (D_n P_n)$.

$|E_6(D_n P_n)|$ contain $8n$ edges of type s, v s.t $d_{(s)} = 3$, $d_{(v)} = 4$, where

$sv \in E\ (D_n P_n)$.

$DS\ (D_n P_n, x) = \sum_{sv \in E(G)} x^{(d_{(s)} - d_{(v)})^2}$

$= \sum_{sv \in E_1(G)} x^{(d_{(s)} - d_{(v)})^2} + \sum_{sv \in E_2(G)} x^{(d_{(s)} - d_{(v)})^2} + \sum_{sv \in E_3(G)} x^{(d_{(s)} - d_{(v)})^2} + \sum_{sv \in E_4(G)} x^{(d_{(s)} - d_{(v)})^2} + \sum_{sv \in E_5(G)} x^{(d_{(s)} - d_{(v)})^2} + \sum_{sv \in E_6(G)} x^{(d_{(s)} - d_{(v)})^2}$

$= (2n)\ x^{(1-3)^2} + (24n)\ x^{(1-4)^2} + (10n - 5)x^{(2-2)^2} + (48n - 6)x^{(1-3)^2} + (13n)\ x^{(3-3)^2} + (8n)\ x^{(3-4)^2}$

$DS\ (D_n P_n, x) = (24n)x^9 + (56n - 6)x^4 + (8n)x + 23n - 5.$

Corollary 2.1.5: Let n ∈ N, then the Degree Edge Stability index of ($D_n\, P_n$) is given as **:**

$$DS\ (D_n\, P_n) = 496n - 6.$$

Proof: To evaluate the result of Degree Edge Stability Polynomial by the same way of corollary 2.1.1, and denoted by $DS\ (D_n\, P_n, x)$, of the dendrimer ($D_n\, P_n$), we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$$\frac{d}{d(x)}[\ DS\ (D_n\, P_n, x)]\ |_{x=1} = (24n)x^9 + (56n - 6)x^4 + (8n)x + 23n - 5$$

$$\frac{d}{d(x)}[\ DS\ (D_n\, P_n, x)|_{x=1} = 8n + 432n + 40n + 48n - 6 + 8n.$$

Thus, the Degree Edge Stability Index of the porphyrin dendrimer is ($D_n\, P_n$) verified as:

$DS\ (D_n\, P_n) = 496n - 6.$

2.2 Computation of Topological Indices and Polynomials of Propyl Ether Imine Dendrimer (PETIM).

Proposition 2.2.2: [41] It considered the second type of dendrimer (PETIM) then:

1. **Order of** (PETIM) is $24 * 2^n - 23$
2. **Size of** (PETIM) is $24 * 2^n - 24$. See figure 2.2

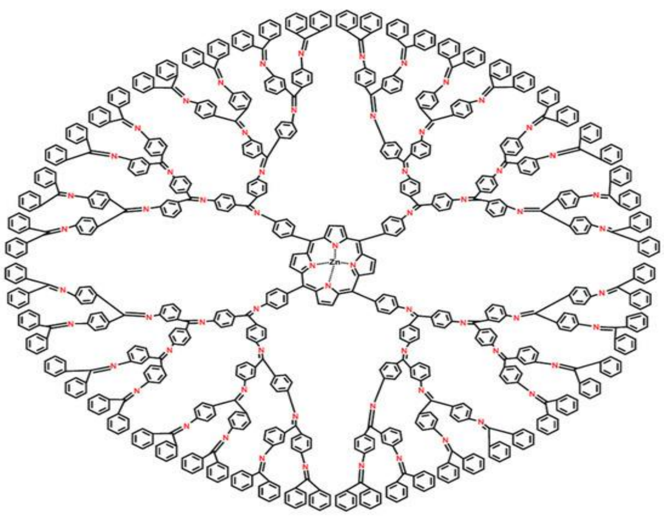


Figure 2.2: dendrimers (PETIM)is also known as Propyl Ether Imine.

(PETIM) contain three types of edges based on degree of end vertices of each as given in table 2.2.

Table 2.2: Graph of the structure (PETIM).

(d_s, d_v)	(1,2)	(2,2)	(2,3)
No. of edges	2^{n+1}	$2^{n+4} - 18$	$48n - 6$

Theorem 2.2.1: Let n ∈ N, then the Augmented Zagreb Polynomial of ($PETIM$) is given as**:**

$$\text{AZP}\ (PETIM, x) = 24 * x^{8}(2^{n} - 1)$$

Proof: The edge set of Propyl Ether Imine dendrimer ($PETIM$) is divided in to three sets E_1, E_2 and E_3. Which are define as follow. See table 2.2.

$|E_1(PETIM)|$ includes 2^{n+1} edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 2$ where $v \in E\ (PETIM)$

$|E_2(PETIM)|$ includes $2^{n+4} - 18$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$ where $sv \in E\ (PETIM)$

$|E_3(PETIM)|$ includes $6 * 2^{n} - 6$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$ where $sv \in E\ (PETIM)$.

$$\text{AZP}\ (PETIM, x) = \sum_{sv \in E(G)} x^{\left(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2}\right)^3}$$

$$= \sum_{sv \in E_1(G)} x^{\left(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2}\right)^3} + \sum_{sv \in E_2(G)} x^{\left(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2}\right)^3} + \sum_{sv \in E_3(G)} x^{\left(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2}\right)^3}.$$

$$= (2^{n+1}) x^{\left(\frac{1*2}{1+2-2}\right)^3} + (2^{n+4} - 18)\, x^{\left(\frac{2*2}{2+2-2}\right)^3} + (6 * 2^{n} - 6) x^{\left(\frac{2*3}{2+3-2}\right)^3}$$

$$= (2^{n+1}) x^{8} + (2^{n+4} - 18)\, x^{8} + (6 * 2^{n} - 6) x^{8}$$

$$\text{AZP}\ (PETIM, x) = 24 * x^{8}(2^{n} - 1).$$

Corollary 2.2.1: Let n ∈ N, then the Augmented Zagreb index of $(PETIM)$ is given as **:**

$$\text{AZI } (PETIM) = 2^{n+5} + 6 * 2^{n} - 192.$$

Proof: By demonstrating the result of Augmented Zagreb Polynomial, which is denoted by AZI $(PETIM, x)$, of the dendrimer $(PETIM)$, we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$$\frac{d}{d(x)}[\text{ AZP } (PETIM, x)]\ |_{x=1} = 24 * x^{8}(2^{n} - 1)$$

Thus, the Augmented Zagreb Index of the Propyl Ether Imine dendrimer is $(PETIM)$ verified as:

AZI $(PETIM) = 2^{n+5} + 6 * 2^{n} - 192$.

Theorem 2.2.2: Let n ∈ N, then the 1st Reformulated Zagreb Polynomial of $(PETIM)$ is given as **:**

$RM_1(PETIM) = (2 * 2^{n})x + (2^{n+3} - 9)x^{3} + 3 * x^{8}(2^{n} - 1)$

Proof: The edge set of Propyl Ether Imine dendrimer $(PETIM)$ is divided in to three sets E_1, E_2 and E_3. Which are define as follow.

$|E_1(PETIM)|$ consists 2^{n+1} edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 2$ where $sv \in E\ (PETIM)$.

$|E_2(PETIM)|$ consists $2^{n+4} - 18$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where $sv \in E\ (PETIM)$

$|E_3(PETIM)|$ consists $6 * 2^{n} - 6$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv \in E\ (PETIM)$.

$RM_1(PETIM, x) = \sum_{sv \in E(G)} x^{(d_{(s)}+d_{(v)}-2)^2}$

$= \sum_{sv \in E_1(G)} x^{(d_{(s)}+d_{(v)}-2)^2} + \sum_{sv \in E_2(G)} x^{(d_{(s)}+d_{(v)}-2)^2}$

$+\sum_{sv \in E_3(G)} x^{(d_{(s)}+d_{(v)}-2)^2}$

$= (2^{n+1})x^{(1+2-2)^2} + (2^{n+4} - 18)\, x^{(2+2-2)^2} + (6 * 2^n - 6)x^{(2+3-2)^2}$

$= x(2 * 2^n) + x^3(2^{n+3} - 9) + 3 * x^8(2^n - 1).$

Corollary 2.2.2: Let n $\in$ N, then the 1st Reformulated Zagreb index of $(PETIM)$ is given as **:**

$$RM_1(PETIM) = 120 * 2^n - 126.$$

Proof: Proving and calculating the result of 1st Reformulated Zagreb Polynomial, which is denoted by $RM_1(PETIM, x)$, of the dendrimer $(PETIM)$, we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$$\frac{d}{d(x)}[\, RM_1(PETIM, x)]\, |_{x=1} = (2 * 2^n)x + (2^{n+3} - 9)x^3$$

$$+(3 * 2^n - 3)x^8.$$

Thus, the 1st Reformulated Zagreb Index of the Propyl Ether Imine dendrimer is $(PETIM)$ verified as:

$RM_1(PETIM) = 120 * 2^n - 126.$

Theorem 2.2.3: Let n ∈ N, then the 2nd Reformulated Zagreb polynomial of $(PETIM)$ is given as **:**

$$RM_2(PETIM, x) = 2x^2 * 2^n + x^8(2^{n+3} - 9) + 3 * x^{18}(2^n - 1)$$

Proof: The edge set of Propyl Ether Imine dendrimer ($PETIM$) is divided in to three sets E_1, E_2 and E_3. Which are define as follow.

$|E_1(PETIM)|$ is composed of 2^{n+1} edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 2$,where $sv \in E\ (PETIM)$

$|E_2(PETIM)|$ is composed of $2^{n+4} - 18$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where $sv \in E\ (PETIM)$.

$|E_3(PETIM)|$ is composed of $6 * 2^n - 6$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv \in E\ (PETIM)$.

$RM_2(PETIM, x) = \sum_{sv \in E(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})}$

$= \sum_{sv \in E_1(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv \in E_2(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})}$

$+ \sum_{sv \in E_3(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})}$.

$= (2^{n+1})x^{(1+2-2)(1*2)} + (2^{n+4} - 18)\ x^{(2+2-2)(2*2)} + (6 *$
$2^n 6)\ x^{(2+3-2)(2*3)}$

$RM_2(PETIM, x) = (2 * 2^n)x + x^8(2^{n+3} - 9) + x^{18}(3 * 2^n - 3)$.

Corollary 2.2.3: Let n ∈ N, then the 2nd Reformulated Zagreb index of ($PETIM$) is given as **:**

$$RM_2(PETIM) = 240 * 2^n - 252.$$

Proof: To examine critically the result of 2nd Reformulated Zagreb polynomial, which is denoted by $RM_2(PETIM, x)$, of the dendrimer

($PETIM$), we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$$\frac{d}{d(x)}[\,RM_2(PETIM,x)]\,|_{x=1}=(2*\,2^n)x+\,x^8(2^{n+3}-9)$$

$$+x^{18}(3*2^n-3).$$

Thus, the 2nd Reformulated Zagreb Index of the Propyl Ether Imine dendrimer is $(PETIM)$ verified as:

$RM_2(PETIM)$ = 240$*$ $2^n\ -252$.

Theorem2.2.4: Let n ∈ N, then the Edge Irregularity polynomial of $(PETIM)$ is given as **:**

$$IR\ (PETIM,x) = 8*2^n*x+16*2^n-6*x-18.$$

Proof*:* The edge set of Propyl Ether Imine dendrimer $(PETIM)$ is divided in to three sets E_1, E_2 and E_3. Which are define as follow.

$|\,E_1(PETIM)|$ involve 2^{n+1} edges of type s,v s.t $d_{(s)}=1$, $d_{(v)}=2$, where $sv\ \in E\ (PETIM)$.

$|\,E_2(PETIM)|$ involve $2^{n+4}-18$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=2$, where $sv\ \in E\ (PETIM)$.

$|\,E_3(PETIM)|$ involve $6*2^n-6$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=3$, where $sv\ \in E\ (PETIM)$.

$IR\ (PETIM,x) = \sum_{sv\in E(G)} x^{|\,d_{(s)}-d_{(v)}|}$

$= \sum_{sv\in E_1(G)} x^{|\,d_{(s)}-d_{(v)}|}+\sum_{sv\in E_2(G)} x^{|\,d_{(s)}-d_{(v)}|}+\sum_{sv\in E_3(G)} x^{|\,d_{(s)}-d_{(v)}|}$.

$= (2^{n+1})x^{|1-2|}+(2^{n+4}-18)\ x^{|2-2|}+(6*2^n-6)\,x^{|2-3|}$

$IR\ (PETIM,x) = (8*2^n-6)x+(2^{n+4}-18)$.

Corollary 2.2.4: Let n ∈ N, then the Edge Irregularity index of ($PETIM$) is given as **:**

$$IR\ (PETIM) = 8 * 2^n\ - 6.$$

Proof: To prove critically the result of Edge Irregularity polynomial, which is denoted by $IR(PETIM, x)$, of the dendrimer ($PETIM$), we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$\frac{d}{d(x)} [\ IR(PETIM, x)]\ |_{x=1}$=$(8 * 2^n - 6)x + (2^{n+4} - 18)$.

$\frac{d}{d(x)} [\ IR(PETIM, x)]\ |_{x=1}$= $8 * 2^n\ - 6$

Thus, the Edge Irregularity Index of the Propyl Ether Imine dendrimer is ($PETIM$) verified as:

$IR\ (PETIM) = 8 * 2^n\ - 6$.

Theorem 2.2.5: Let n ∈ N, then the Degree Edge Stability Polynomial of ($PETIM$) is given as **:**

$$DS\ (PETIM, x) = \ (8 * 2^n - 6)x + (2^{n+4} - 18)$$

Proof*:* The edge set of Propyl Ether Imine dendrimer ($PETIM$) is divided in to three sets E_1, E_2 and E_3. Which are define as follow.

$|\ E_1(PETIM)|$ it has 2^{n+1} edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 2$, where $sv\ \in E\ (PETIM)$.

$|\ E_2(PETIM)|$ it has $2^{n+4} - 18$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where $sv\ \in E\ (PETIM)$.

$|E_3(PETIM)|$ it has $6 * 2^n - 6$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv \in E\ (PETIM)$.

$DS\ (PETIM, x) = \sum_{sv \in E(G)} x^{(d_{(s)} - d_{(v)})^2}$

$= \sum_{sv \in E_1(G)} x^{(d_{(s)} - d_{(v)})^2} + \sum_{sv \in E_2(G)} x^{(d_{(s)} - d_{(v)})^2} + \sum_{sv \in E_3(G)} x^{(d_{(s)} - d_{(v)})^2}$

$= (2^{n+1}) x^{(1-2)^2} + (2^{n+4} - 18)\ x^{(2-2)^2} + (6 * 2^n - 6)\, x^{(2-3)^2}$.

$DS\ (PETIM, x) = (8 * 2^n - 6)x + (2^{n+4} - 18)$.

Corollary 2.2.5: Let n $\in$ N, then the Degree Edge Stability index of $(PETIM)$ is given as **:**

$$DS\ (PETIM) = 8 * 2^n - 6.$$

Proof: To demonstrate and evaluate the result of Degree Edge Stability Polynomial, which is denoted by $DS(PETIM, x)$, of the dendrimer $(PETIM)$, we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$\frac{d}{d(x)}[\, DS(PETIM, x)]\ |_{x=1} = (8 * 2^n - 6)x + (2^{n+4} - 18)$.

$\frac{d}{d(x)}[\, DS(PETIM, x)]\ |_{x=1} = 8 * 2^n - 6$

Thus, the Degree Edge Stability Index of the Propyl Ether Imine dendrimer is $(PETIM)$ verified as:

$DS\ (PETIM) = 8 * 2^n - 6$

Chapter Three

Computation of Topological Indices and Polynomials of Zinc Porphyrin (DpZ_n) and Poly (Ethylene Amide Amine) (PETAA) Dendrimers.

3.1 Computation of Topological Indices and Polynomials of Zinc Porphyrin Dendrimer (DPZ_n).

Introduction: The topological indices are used to obtain the topological properties and steric structure of dendrimers or macromolecules. As has been said earlier throughout this chapter will deal with computing some polynomials for various different classes of dendrimers like p Zinc Porphyrin (DPZ_n). and Poly(Ethylene Amide Amine) dendrimers (PETAA).

Proposition 3.1.1: [41] It considered the first type of dendrimer (DPZ_n) then:

1. **Order of** (DPZ_n) is $96 * n - 10$

2. **Size of** (DPZ_n) is $105 * n - 11$. See figure.

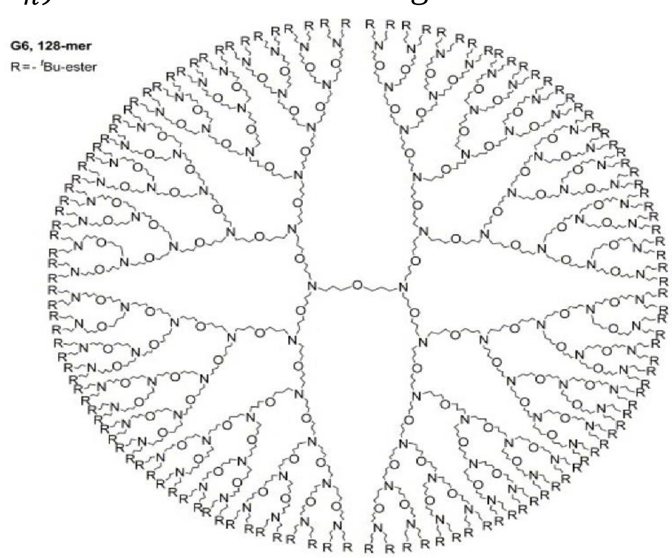


Figure 3.1: dendrimers (DPZ_n)is also known as Zinc Porphyrin.

($\mathrm{DP}Z_n$) strictures contain three types of edges based on degree of end vertices of each as given in table 3.1.

Table 3.1: Graph of the stretcher ($\mathrm{DP}Z_n$).

(d_s, d_v)	(2,2)	(2,3)	(3,3)	(3,4)
No. of edges	$16*2^n-4$	$40*2^n-16$	$8*2^n-16$	4

Theorem 3.1.1: Let n ∈ N, then the Augmented Zagreb Polynomial of ($\mathrm{DP}Z_n$)is given as **:**

$$\mathrm{AZP}(\mathrm{DP}Z_n, x) = 8*2^n*x^{\frac{729}{64}} + 56*\ 2^n*x^8 + 4*\ x^{\frac{1728}{125}} - 16*x^{\frac{726}{64}}$$

$$-20\,x^8$$

Proof*:* The edge set of Zinc Porphyrin dendrimer ($\mathrm{DP}Z_n$))is divided in to four sets E_1, E_2, $E_3$and E_4 . Which are done in the entirety of chapter two.

$|E_1(\mathrm{DP}Z_n)|$ contain $16*2^n-4$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=2$, where $sv \in E$ ($\mathrm{DP}Z_n$).

$|E_2(\mathrm{DP}Z_n)|$ contain $40*2^n-16$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=3$, where $sv \in E$ ($\mathrm{DP}Z_n$).

$|E_3(\mathrm{DP}Z_n)|$ contain $8*2^n-16$ edges of type s,v s.t $d_{(s)}=3$, $d_{(v)}=3$, where $sv \in E$ ($\mathrm{DP}Z_n$).

$|E_4(\mathrm{DP}Z_n)|$ contain 4 edges of type s,v s.t $d_{(s)}=3$, $d_{(v)}=4$, where

$sv \in E$ ($\mathrm{DP}Z_n$).

$$\mathrm{AZP}(\mathrm{DP}Z_n, x) = \sum_{sv\in E(G)} x^{\left(\frac{d_{(s)}*d_{(v)}}{d_{(s)}+d_{(v)}-2}\right)^3}.$$

$$= \sum_{sv \in E_1(G)} x^{(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2})^3} + \sum_{sv \in E_2(G)} x^{(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2})^3} +$$

$$\sum_{sv \in E_3(G)} x^{(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2})^3} + \sum_{sv \in E_4(G)} x^{(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2})^3}$$

$$= (16 * 2^n - 4)\, x^{(\frac{2*2}{2+2-2})^3} + (40 * 2^n - 16)\, x^{(\frac{2*3}{2+3-2})^3}$$

$$+ (8 * 2^n - 16)\, x^{(\frac{3*3}{3+3-2})^3} + (4)\, x^{(\frac{3*4}{3+4-2})^3}.$$

$$\text{AZP}(\text{DP}Z_n, x) = 8 * 2^n * x^{\frac{729}{64}} + 56 * 2^n * x^8 + 4 * x^{\frac{1728}{125}}$$

$$-16 * x^{\frac{726}{64}} - 20\, x^8.$$

Corollary 3.1.1: Let n ∈ N, then the Augmented Zagreb index of (DPZ_n) is given as **:**

$$\text{AZI } (\text{DP}Z_n) = 64 * 2^n - 231.95.$$

Proof: The edge set of Zinc Porphyrin dendrimer (DPZ_n)is divided in to four sets E_1, E_2, E_3 and E_4. Which are define in the theorem 3.1.1. By using definition of Augmented Zagreb topological index we will apply on Porphyrin dendrimer(DPZ_n). By taken its derivative we will get the topological index.

$$\text{AZI } (\text{DP}Z_n) = \sum_{\text{sv} \in \text{E(G)}} (\frac{\text{d}_{(\text{s})} * \text{d}_{(\text{v})}}{\text{d}_{(\text{s})} + \text{d}_{(\text{v})} - 2})^3.$$

$$\frac{d}{d(x)} [\, \text{AZP}(\text{DP}Z_n, x)]_{x=1} = 8 * 2^n * x^{\frac{729}{64}} + 56 * 2^n * x^8 + 4 * x^{\frac{1728}{125}}$$

$$-16 * x^{\frac{726}{64}} - 20\, x^8.$$

$$\frac{d}{d(x)} [\, \text{AZP}(\text{DP}Z_n, x)]_{x=1} = 64 * 2^n - 231.95.$$

AZP(DPZ_n, x) = 64∗ 2^n $-$ 231.95.

Theorem 3.1.2: let n ∈ N, then the 1st Reformulated Zagreb Polynomial of (DPZ_n) is given as **:**

$$RM_1(\text{DP}Z_n) = (16 * 2^n - 4)\, x^8 + (40 * 2^n - 16)x^{27}$$
$$+(8 * 2^n - 16)x^{64} + 4 * x^{125}.$$

Proof: The edge set of Zinc Porphyrin dendrimer (DPZ_n))is divided in to four sets E_1, E_2, $E_3$and E_4 . Which are done in the entirety of chapter three.

| E_1(DPZ_n)| includes$16 * 2^n - 4$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where sv ∈ E (DPZ_n).

| E_2(DPZ_n)| includes$40 * 2^n - 16$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where sv ∈ E (DPZ_n).

| E_3(DPZ_n)| includes$8 * 2^n - 16$ edges of type s, v s.t $d_{(s)} = 3$, $d_{(v)} = 3$, where sv ∈ E (DPZ_n).

| E_4(DPZ_n)| includes 4 edges of type s, v s.t $d_{(s)} = 3$, $d_{(v)} = 4$, where sv ∈ E (DPZ_n).

RM_1(DPZ_n) = $\sum_{sv \in E(G)} x^{(d_{(s)}+d_{(v)}-2)^2}$

= $\sum_{sv \in E_1(G)} x^{(d_{(s)}+d_{(v)}-2)^2}$ + $\sum_{sv \in E_2(G)} x^{(d_{(s)}+d_{(v)}-2)^2}$

+$\sum_{sv \in E_3(G)} x^{(d_{(s)}+d_{(v)}-2)^2}$ + $\sum_{sv \in E_4(G)} x^{(d_{(s)}+d_{(v)}-2)^2}$

= $(16 * 2^n - 4)x^{(2+2-2)^3}$ + $(40 * 2^n - 16)$ $x^{(2+3-2)^3}$ + $(8 * 2^n - 16)$ $x^{(3+3-2)^3}$ + (4) $x^{(3+4-2)^3}$.

$RM_1(\mathrm{DP}Z_n, x)= (16 * 2^n - 4)\ x^8 + (40 * 2^n - 16)x^{27} + (8 * 2^n - 16)x^{64} + 4 * x^{125}$.

Corollary 3.1.2: Let n ∈ N, then the 1st Reformulated Zagreb index of (DPZ_n) is given as **:**

$$RM_1\ (\mathrm{DP}Z_n)= 552 * 2^n - 411.75.$$

Proof: By the same way of corollary 3.1.1, to confirm and compute the result of 1st Reformulated Zagreb Polynomial, which is denoted by RM_1 (DPZ_n, x), of the dendrimer (DPZ_n), we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$\frac{d}{d(x)}[\ RM_1(\mathrm{DP}Z_n, x)]\ |_{x=1} = (16\ * 2^n - 4)\ x^8 + (40 * 2^n - 16)x^{27} + (8 * 2^n - 16)x^{64} + 4 * x^{125}$.

Thus, the 1st Reformulated Zagreb Index of the Zinc Porphyrin dendrimer is (DPZ_n) verified as:

RM_1 (DPZ_n)= $552 * 2^n - 411.75$.

Theorem 3.1.3: let n ∈ N, then the 2nd Reformulated Zagreb Polynomial of (DPZ_n) is given as **:**

$$RM_2(\mathrm{DP}Z_n) = (16 * 2^n - 4)x^8 + (40 * 2^n - 16)x^{18}$$
$$+(8 * 2^n - 16)x^{36} + 4x^{60}.$$

Proof: The edge set of Zinc Porphyrin dendrimer (DPZ_n))is divided in to four sets E_1, E_2, $E_3$and E_4 . Which are done in the entirety of chapter two.

$|E_1(\mathrm{DP}Z_n)|$ it has $16*2^n-4$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=2$, where $sv \in E$ $(\mathrm{DP}Z_n)$.

$|E_2(\mathrm{DP}Z_n)|$ it has $40*2^n-16$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=3$, where $sv \in E$ $(\mathrm{DP}Z_n)$.

$|E_3(\mathrm{DP}Z_n)|$ it has $8*2^n-16$ edges of type s,v s.t $d_{(s)}=3$, $d_{(v)}=3$, where $sv \in E$ $(\mathrm{DP}Z_n)$.

$|E_4(\mathrm{DP}Z_n)|$ it has 4 edges of type s,v s.t $d_{(s)}=3$, $d_{(v)}=4$, where

$sv \in E$ $(\mathrm{DP}Z_n)$.

$RM_2(\mathrm{DP}Z_n,x) = \sum_{sv\in E(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})}$

$= \sum_{sv\in E_1(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv\in E_2(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv\in E_3(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv\in E_4(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})}$

$= (16*2^n-4)\, x^{(2+2-2)(2*2)} + (40*2^n-16)\, x^{(2+3-2)(2*3)} + (8*2^n-16)\, x^{(3+3-2)(3*3)} + (4)\, x^{(3+4-2)(3*4)}$

$RM_2(\mathrm{DP}Z_n,x) = (16*2^n-4)x^8 + (40*2^n-16)x^{18} + (8*2^n-16)x^{36} + 4x^{60})$.

Corollary 3.1.3: Let n ∈ N, then the 2nd Reformulated Zagreb index of $(\mathrm{DP}Z_n)$ is given as **:**

$$RM_2\ (\mathrm{DP}Z_n) = 1136*2^n - 656.$$

Proof: By using a similar path used in the proof of corollary 3.1.1, we conclude the result by evaluating the polynomial at $x=1$, This yields:

$$\frac{d}{d(x)}[\, RM_2(\mathrm{DPZ}_n, x)] \,|_{x=1} = (16 * 2^n - 4)x^8 + (40 * 2^n - 16)x^{18}$$

$$+(8 * 2^n - 16)x^{36} + 4x^{60}).$$

Thus, the 2nd Reformulated Zagreb Index of the Zinc Porphyrin dendrimer is ($\mathrm{DP}Z_n$) verified as:

$$RM_2\ (\mathrm{DPZ}_n) = 1136 * 2^n - 656.$$

Theorem 3.1.4: Let n ∈ N, then the Edge Irregularity Polynomial of ($\mathrm{DP}Z_n$) is given as **:**

$$IR\ (\mathrm{DPZ}_n) = (24 * 2^n - 20) + (40 * 2^n - 12)x.$$

Proof: The edge set of Zinc Porphyrin dendrimer ($\mathrm{DP}Z_n$))is divided in to four sets E_1, E_2, $E_3$and E_4 . Which are done in the entirety of chapter three.

| $E_1(\mathrm{DPZ}_n)$| consists $16 * 2^n - 4$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where $sv \in E$ (DPZ_n).

| $E_2(\mathrm{DPZ}_n)$| consists $40 * 2^n - 16$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv \in E$ (DPZ_n).

| $E_3(\mathrm{DPZ}_n)$| consists $8 * 2^n - 16$ edges of type s, v s.t $d_{(s)} = 3$, $d_{(v)} = 3$, where $sv \in E$ (DPZ_n).

| $E_4(\mathrm{DPZ}_n)$| consists 4 edges of type s, v s.t $d_{(s)} = 3$, $d_{(v)} = 4$, where $sv \in E$ (DPZ_n).

$IR\ (\mathrm{DPZ}_n) = \sum_{sv \in E(G)} x^{|\, d_{(s)} - d_{(v)}|}$.

= $\sum_{sv\in E_1(G)} x^{|\, d_{(s)}-d_{(v)}|}$ + $\sum_{sv\in E_2(G)} x^{|\, d_{(s)}-d_{(v)}|} + \sum_{sv\in E_3(G)} x^{|\, d_{(s)}-d_{(v)}|}$ + $\sum_{sv\in E_4(G)} x^{|\, d_{(s)}-d_{(v)}|}$

= $(16 * 2^n - 4)x^{|\,2-2|}$+ $(40 * 2^n - 16\,)x^{|\,2-3|}$ + $(8 * 2^n - 16)\, x^{|\,3-3|}$

$$+(4)x^{|\,3-4|}$$

IR (DPZ_n, x) = $(24 * 2^n - 20) + (40 * 2^n - 12)x$.

Corollary 3.1.4: Let n ∈ N, then the Edge Irregularity index of (DPZ_n) is given as **:**

$$IR\ (\text{DP}Z_n) = 40 * 2^n\ - 12.$$

Proof: By using a similar path used in the proof of corollary 3.1.1, we conclude the result by evaluating the polynomial at $x = 1$, This yields:

$$\frac{d}{d(x)}[\, IR(\text{DP}Z_n, x)]\ |_{x=1} = (24 * 2^n - 20) + (40 * 2^n - 12)x.$$

Thus, the Edge Irregularity Index of the Zinc Porphyrin dendrimer is (DPZ_n) verified as:

IR (DPZ_n)= $40 * 2^n\ - 12$.

Theorem 3.1.5: Let n ∈ N, then the Degree – Edge Stability Polynomial of (DPZ_n) is given as **:**

$$DS\ (\text{DP}Z_n) = (24 * 2^n\ - 20) +\ (40 * 2^n - 12)x$$

Proof: The edge set of Zinc Porphyrin dendrimer (DPZ_n))is divided in to four sets E_1, E_2, $E_3$and E_4 . Which are done in the entirety of chapter two.

$|E_1(\mathrm{DP}Z_n)|$ is made up of $16*2^n-4$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=2$, where $sv\in E\ (\mathrm{DP}Z_n)$

$|E_2(\mathrm{DP}Z_n)|$ is made up of $40*2^n-16$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=3$, where $sv\in E\ (\mathrm{DP}Z_n)$.

$|E_3(\mathrm{DP}Z_n)|$ is made up of $8*2^n-16$ edges of type s,v s.t $d_{(s)}=3$, $d_{(v)}=3$, where $sv\in E\ (\mathrm{DP}Z_n)$.

$|E_4(\mathrm{DP}Z_n)|$ is made up of 4 edges of type s,v s.t $d_{(s)}=3$, $d_{(v)}=4$, where $sv\in E\ (\mathrm{DP}Z_n)$.

$DS\ (\mathrm{DP}Z_n)| = \sum_{sv\in E(G)} x^{(d_{(u)}-d_{(v)})^2}$

$= \sum_{sv\in E_1(G)} x^{(d_{(s)}-d_{(v)})^2} + \sum_{sv\in E_2(G)} x^{(d_{(s)}-d_{(v)})^2} + \sum_{sv\in E_3(G)} x^{(d_{(s)}-d_{(v)})^2} + \sum_{sv\in E_4(G)} x^{(d_{(s)}-d_{(v)})^2}.$

$= (16*2^n-4)\ x^{(2-2)^2} + (40*2^n-16)\ x^{(2-3)^2} + (8*2^n-16)\ x^{(3-3)^2} + (4)\ x^{(3-4)^2}$

$DS\ (\mathrm{DP}Z_n, x) = (24*2^n-20) + (40*2^n-12)x.$

Corollary 3.1.5: Let n ∈ N, then the Degree Edge Stability index of $(\mathrm{DP}Z_n)$ is given as **:**

$$DS(\mathrm{DP}Z_n) = 40*2^n - 12.$$

Proof: By using a similar approach used in the proof of corollary 3.1.1, we conclude the result by evaluating the polynomial at $x=1$, This yields:

$\frac{d}{d(x)}[\, DS(\mathrm{DP}Z_n, x)] \,|_{x=1} = (24 * 2^n - 20) + (40 * 2^n - 12)x.$

Thus, the Degree Edge Stability Index of the Zinc Porphyrin dendrimer is $(\mathrm{DP}Z_n)$ verified as:

$DS(\mathrm{DP}Z_n) = 40 * 2^n - 12.$

3.2: Computation of Topological Indices and Polynomials of Poly (Ethylene Amide Amine) (PETAA) Dendrimer.

Proposition 3.2.1: [41] It considered the second type of dendrimer (PETAA) then:

1. **Order of** (PETAA) is $44 * 2^n - 18$

2. **Size of** (PETAA) is $44 * 2^n - 19$. See figure 3.2

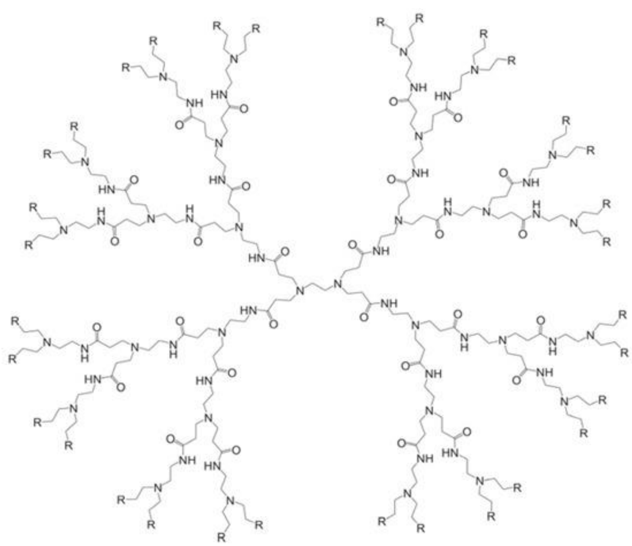


Figure 3.2: dendrimers (PETAA) is also known as Poly(Ethylene Amide Amine).

(PETAA) stricture have four types of edges based on degree of end vertices of each as given in table 3.2.

Table 3.2: Graph of the stricture (PETAA).

(d_s, d_v)	(1,2)	(1,3)	(2,2)	(2,3)
No. of edges	$4 * 2^n$	$4 * 2^n - 2$	$16 * 2^n - 8$	$20 * 2^n - 9$

Theorem 3.2.1: Let n ∈ N, then the Augmented Zagreb Polynomial of (PETAA)is given as **:**

AZP (PETAA, x)= $(40 * 2^n - 17)x^8 + (4 * 2^n - 2)x^{\frac{27}{8}}$

Proof: The edge set of Poly(Ethylene Amide Amine) dendrimer (PETAA))is divided in to four sets E_1, E_2, $E_3$and E_4 . Which are define as follow

| E_1(PETAA) | consists $4 * 2^n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 2$, where sv ∈ E (PETAA).

| E_2(PETAA)| consists $4 * 2^n - 2$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 3$, where sv ∈ E (PETAA).

| E_3(PETAA)|consists $16 * 2^n - 8$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where sv ∈ E (PETAA).

| E_4(PETAA)| consists$20 * 2^n - 9$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where sv ∈ E (PETAA).

AZP (PETAA, x)= $\sum_{sv \in E(G)} x^{(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2})^3}$.

$= \sum_{sv\in E_1(G)} x^{(\frac{d_{(s)} * d_{(v)}}{d_{(s)}+ d_{(v)}-2})^3} + \sum_{sv\in E_2(G)} x^{(\frac{d_{(s)} * d_{(v)}}{d_{(s)}+ d_{(v)}-2})^3} +$

$\sum_{sv\in E_3(G)} x^{(\frac{d_{(s)} * d_{(v)}}{d_{(s)}+ d_{(v)}-2})^3} + \sum_{sv\in E_4(G)} x^{(\frac{d_{(s)} * d_{(v)}}{d_{(s)}+ d_{(v)}-2})^3}$

$= (4 * 2^n) x^{(\frac{1*2}{1+2-2})^3} + (4 * 2^n - 2)\ x^{(\frac{1*3}{1+3-2})^3} + (16 * 2^n - 8)\ x^{(\frac{2*2}{2+2-2})^3} +$

$(20 * 2^n - 9)\ x^{(\frac{2*3}{2+3-2})^3}$

AZP (PETAA, x)= $(40 * 2^n - 17)x^8 + (4 * 2^n - 2)x^{\frac{27}{8}}$.

Corollary 3.2.1: Let n ∈ N, then the Augmented Zagreb index of (PETAA) is given as **:**

$$\text{AZI (PETAA)} = 333.5 * 2^n - 142.7$$

Proof: By using a similar approach used in the proof of corollary 3.1.1, we conclude the result by evaluating the polynomial at $x = 1$, This yields:

$\frac{d}{d(x)}$[AZP (PETAA, x)] $|_{x=1}$= $(40 * 2^n - 17)x^8 + (4 * 2^n - 2)x^{\frac{27}{8}}$.

Thus, the Augmented Zagreb Index of the Poly(Ethylene Amide Amine) dendrimer is (PETAA) verified as:

AZI (PETAA) = $333.5 * 2^n - 142.7$

Theorem 3.2.2: let n ∈ N, then the 1st Reformulated Zagreb Polynomial of (PETAA) is given as **:**

$$RM_1(PETAA) = (4*2^n)x + (20*2^n - 10)x^8 + (20*2^n - 9)x^{27}$$

Proof*:* The edge set of Poly(Ethylene Amide Amine) dendrimer (PETAA))is divided in to four sets E_1, E_2, $E_3$and E_4 . Which are define as follow.

| E_1(PETAA)| is made up of $4*2^n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 2$, where $sv \in E$ (PETAA).

| E_2(PETAA)| is made up of $4*2^n - 2$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 3$, where $sv \in E$ (PETAA).

| E_3(PETAA)|is made up of $16*2^n - 8$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where $sv \in E$ (PETAA).

| E_4(PETAA)| is made up of $20*2^n - 9$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv \in E$ (PETAA).

$RM_1(\text{PETAA}, x) = \sum_{sv\in E(G)} x^{(d_{(s)}+d_{(v)}-2)^2}$

$=\sum_{sv\in E_1(G)} x^{(d_{(s)}+d_{(v)}-2)^2} + \sum_{sv\in E_2(G)} x^{(d_{(s)}+d_{(v)}-2)^2}$

$+\sum_{sv\in E_3(G)} x^{(d_{(s)}+d_{(v)}-2)^2} + \sum_{sv\in E_4(G)} x^{(d_{(s)}+d_{(v)}-2)^2}$

$=(4*2^n)x^{(1+2-2)^3} + (4*2^n - 2)\ x^{(1+3-2)^3} + (16*2^n - 8)\ x^{(2+2-2)^3} + (20*2^n - 9)\ x^{(2+3-2)^3}$.

$RM_1(\text{PETAA}, x) = (4*2^n)x + (20*2^n - 10)x^8 + (20*2^n - 9)x^{27}$

Corollary 3.2.2: Let n ∈ N, then the 1st Reformulated Zagreb index of (PETAA) is given as **:**

$$RM_1(\text{PETAA}) = 520 * 2^n - 238.$$

Proof: By using a similar approach we conclude the result by evaluating the polynomial at $x = 1$, This yields:

$$\frac{d}{d(x)}[RM_1(\text{PETAA}, \text{x})]\,|_{x=1} = (4 * 2^n)x + (20 * 2^n - 10)x^8$$

$$+(20 * 2^n - 9)x^{27}$$

Thus, the 1st Reformulated Zagreb Index of the Poly(Ethylene Amide Amine) dendrimer is (PETAA) verified as:

$RM_1(\text{PETAA}) = 520 * 2^n - 238.$

Theorem 3.2.3: Let n ∈ N, then the 2nd Reformulated Zagreb Polynomial of (PETAA)is given as **:**

$$RM_2(\text{PETAA}) = (4 * 2^n)x^2 + (20 * 2^n - 10)x^8 + (20 * 2^n - 9)x^{27}$$

Proof: The edge set of Poly(Ethylene Amide Amine) dendrimer (PETAA))is divided in to four sets E_1, E_2, $E_3$and E_4 . Which are as follow.

| E_1(PETAA)| include $4 * 2^n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 2$, where $sv \in E$ (PETAA).

| E_2(PETAA)| include $4 * 2^n - 2$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 3$, where $sv \in E$ (PETAA).

| E_3(PETAA)|include $16 * 2^n - 8$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where $sv \in E$ (PETAA).

| E_4(PETAA)| include $20 * 2^n - 9$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv \in E$ (PETAA).

$RM_2(\text{PETAA}, x) = \sum_{sv\in E(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})}$

$= \sum_{sv\in E_1(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv\in E_2(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv\in E_3(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv\in E_4(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})}$

$= (4 * 2^n)x^{(1+2-2)(1*2)} + (4 * 2^n - 2)\ x^{(1+3-2)(1*3)} + (16 * 2^n - 8)\ x^{(2+2-2)(2*2)} + (20 * 2^n - 9)\ x^{(2+3-2)(2*3)}$

$RM_2(\text{PETAA}, x) = (4 * 2^n)x + (20 * 2^n - 10)x^8 + (20 * 2^n - 9)x^{27}$.

Corollary 3.2.3: Let n ∈ N, then the 2nd Reformulated Zagreb index of (PETAA) is given as **:**

$$RM_2(\text{PETAA}) = 704 * 2^n - 323.$$

Proof: By using a similar approach used in the proof of corollary 3.1.1, we conclude the result by evaluating the polynomial at $x = 1$, This yields:

$$\frac{d}{d(x)}[\ RM_2(\text{PETAA}, \mathrm{x})]\ |_{x=1} = (4 * 2^n)x + (20 * 2^n - 10)x^8$$

$$+(20 * 2^n - 9)x^{27}.$$

Thus, the 2nd Reformulated Zagreb Index of the Poly(Ethylene Amide Amine) dendrimer is (PETAA) verified as:

$RM_2(\text{PETAA}) = 704 * 2^n - 323$.

Theorem 3.2.4: let n ∈ N, then the Edge Irregularity Polynomial of (PETAA) is given as **:**

$$IR\ (\text{PETAA}, x) = (16 * 2^n - 8) + (24 * 2^n - 9)x + (4 * 2^n - 2)x^2.$$

Proof*:* The edge set of Poly(Ethylene Amide Amine) dendrimer (PETAA))is divided in to four sets E_1, E_2, $E_3$and E_4 . Which are define as follow.

$|E_1(\text{PETAA})|$ have $4 * 2^n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 2$, where $sv \in E$ (PETAA).

$|E_2(\text{PETAA})|$ have $4 * 2^n - 2$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 3$, where $sv \in E$ (PETAA).

$|E_3(\text{PETAA})|$ have $16 * 2^n - 8$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where $sv \in E$ (PETAA).

$|E_4(\text{PETAA})|$ have $20 * 2^n - 9$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv \in E$ (PETAA).

$IR\ (\text{PETAA}, \text{x}) = \sum_{sv \in \text{E(G)}} x^{|d_{(s)} - d_{(v)}|}$

$= \sum_{sv \in E_1(\text{G})} x^{|d_{(s)} - d_{(v)}|} + \sum_{sv \in E_2(\text{G})} x^{|d_{(s)} - d_{(v)}|} + \sum_{sv \in E_3(\text{G})} x^{|d_{(s)} - d_{(v)}|} + \sum_{sv \in E_4(\text{G})} x^{|d_{(s)} - d_{(v)}|}.$

$= (4 * 2^n) x^{|1-2|} + (4 * 2^n - 2)\ x^{|1-3|} + (16 * 2^n - 8)\ x^{|2-2|} + (20 * 2^n - 9)\ x^{|2-3|}$

$IR\ (\text{PETAA}, \text{X}) = (16 * 2^n - 8) + (24 * 2^n - 9)x + (4 * 2^n - 2)x^2.$

Corollary 3.2.4: Let n ∈ N, then the Edge Irregularity index of (PETAA) is given as **:**

$$IR\text{ (PETAA)} = 32 * 2^n - 13$$

Proof: By using a similar approach used in the proof of corollary 3.1.1, we conclude the result by evaluating the polynomial at $x = 1$, This yields:

$$\frac{d}{d(x)}[\, IR\text{ (PETAA, x)}]\,|_{x=1} = (16 * 2^n - 8) + (24 * 2^n - 9)x$$

$$+(4 * 2^n - 2)x^2.$$

Thus, the Edge Irregularity Index of the Poly(Ethylene Amide Amine) dendrimer is (PETAA) verified as:

IR (PETAA) $= 32 * 2^n - 13$.

Theorem 3.2.5: let n ∈ N, then the Degree Edge Stability Polynomial of (PETAA)is given as**:**

$$DS\text{ (PETAA, x)} = (16 * 2^n - 8) + (24 * 2^n - 9)x + (4 * 2^n - 2)x^4$$

Proof: The edge set of Poly(Ethylene Amide Amine) dendrimer (PETAA))is divided in to four sets E_1, E_2, $E_3$and E_4 . Which are define as follow

| E_1(PETAA)| contain $4 * 2^n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 2$, where $sv \in E$ (PETAA).

| E_2(PETAA)| contain $4 * 2^n - 2$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 3$, where $sv \in E$ (PETAA).

| E_3(PETAA)|contain $16*2^n-8$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=2$, where $sv \in E$ (PETAA).

| E_4(PETAA)| contain $20*2^n-9$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=3$, where $sv \in E$ (PETAA).

DS (PETAA, x)= $\sum_{sv\in \mathrm{E(G)}} x^{(d_{(u)}-d_{(v)})^2}$

$= \sum_{sv\in E_1(\mathrm{G})} x^{(d_{(s)}-d_{(v)})^2} + \sum_{sv\in E_2(\mathrm{G})} x^{(d_{(s)}-d_{(v)})^2} + \sum_{sv\in E_3(\mathrm{G})} x^{(d_{(s)}-d_{(v)})^2}$
$+\sum_{sv\in E_4(\mathrm{G})} x^{(d_{(s)}-d_{(v)})^2}$.

$= (4*2^n)x^{(1-2)^2} + (4*2^n-2)\ x^{(1-3)^2} + (16*2^n-8)\,x^{(2-2)^2} + (20*2^n-9)\,x^{(2-3)^2}$

DS (PETAA, x) $=(16*2^n-8)+(24*2^n-9)x+(4*2^n-2)x^4$.

Corollary 3.2.5: Let n ∈ N, then the Degree Edge Stability index of (PETAA) is given as**:**

$$DS\text{ (PETAA)} = 40*2^n-17$$

Proof: By using a similar approach used in the proof of corollary 3.1.1, we conclude the result by evaluating the polynomial at $x=1$, This yields:

$$\frac{d}{d(x)}[\,DS\text{ (PETAA, x)}\,]\,|_{x=1}=(16*2^n-8)+(24*2^n-9)x$$
$$+(4*2^n-2)x^4.$$

Thus, the Degree Edge Stability Index of the Poly(Ethylene Amide Amine) dendrimer is (PETAA) verified as:

DS (PETAA) $= 40*2^n-17$

Chapter Four

Computation of Topological Indices and Polynomials of Aminoisophthalate Dister Monomer ($APD[n]$) and Poly (Amid Amine) ($PD[n]$) Dendrimers

4.1 Computation of Topological Indices and Polynomials of Aminoisophthalate Dister Monomer Dendrimer ($APD[n]$).

Introduction: The topological indices are used to obtain the topological properties and steric structure of dendrimers or macromolecules. As has been said earlier throughout this chapter will deal with computing some polynomials for various different classes of dendrimers like aminoisophthalate dister monomer ($APD[n]$) and poly (amidoamine) dendrimer ($PD[n]$).

Proposition 4.1: [41] It considered the first type of dendrimer ($APD[n]$) then:

1. **Order of** ($APD[n]$) is $30 * 2^{n+1} - 48$
2. **Size of** ($APD[n]$) is $33 * 2^{n+1} - 54$. See figure 4.1

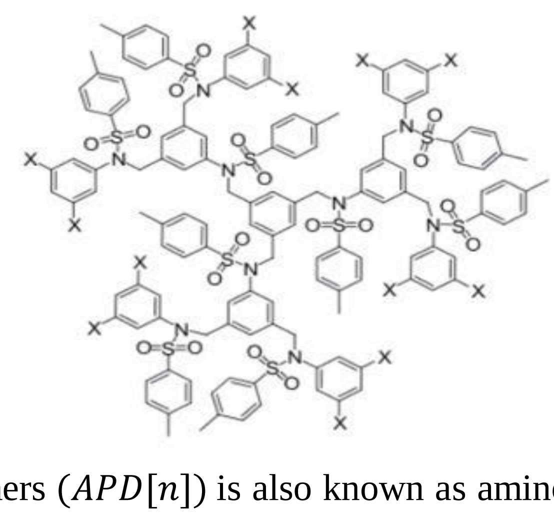


Figure 4.1: dendrimers ($APD[n]$) is also known as aminoisophthalate dister monomer .

($APD[n]$)structures consist six types of edges based on degree of end vertices of each as given in table 4.1.

Table 4.1: Graph of the structures ($APD[n]$)

(d_s, d_v)	(1,2)	(1,3)	(1,4)	(2,2)	(2,3)	(3,4)
No. of edges	$3 * 2^n$	$3 * 2^n - 3$	$6 * 2^n - 6$	$6 * 2^n - 6$	$42 * 2^n - 33$	$6 * 2^n - 6$

First of all, we are going to calculate the Augmented Zagreb polynomial for the molecular ($APD[n]$)

Theorem 4.1.1: Let n ∈ N, then the Augmented Zagreb polynomial of ($APD[n]$) is given as **:**

AZP $(APD[n]), x) = (6 * 2^n - 6)\, x^{\frac{1728}{125}} + (6 * 2^n - 6)x^{\frac{64}{27}} + (3 * 2^n - 3)x^{\frac{27}{8}} + (51 * 2^n - 39)x^8$.

Proof: The edge set of aminoisophthalate dister monomer dendrimer ($APD[n]$) is divided in to six sets E_1, E_2, E_3, E_4, $E_5$and E_6. Which are define as follow. See table 4.1.

$|E_1(APD[n])|$ Comprise $3 * 2^n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 2$, where $sv \in E\ (APD[n])$.

$|E_2(APD[n])|$ Comprise $3 * 2^n - 3$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 3$, where $sv \in E\ (APD[n])$ **.**

$|E_3(APD[n])|$ Comprise $6 * 2^n - 6$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 4$, where $sv \in E\ (APD[n])$.

$|E_4(APD[n])|$ Comprise $6*2^n-6$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=2$, where $sv \in E\ (APD[n])$.

$|E_5(APD[n])|$ Comprise $42*2^n-33$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=3$, where $sv \in E\ (APD[n])$.

$|E_6(APD[n])|$ Comprise $6*2^n-6$edges of type s,v s.t $d_{(s)}=3$, $d_{(v)}=4$, where $sv \in E\ (APD[n])$.

$$\text{AZP}\ (APD[n],x)\ =\sum_{sv\in \mathrm{E(G)}} x^{\left(\frac{\mathrm{d}_{(s)}*\mathrm{d}_{(v)}}{\mathrm{d}_{(s)}+\mathrm{d}_{(v)}-2}\right)^3}$$

$$=\sum_{sv\in E_1(\mathrm{G})} x^{\left(\frac{\mathrm{d}_{(s)}*\mathrm{d}_{(v)}}{\mathrm{d}_{(s)}+\mathrm{d}_{(v)}-2}\right)^3}+\sum_{sv\in E_2(\mathrm{G})} x^{\left(\frac{\mathrm{d}_{(s)}*\mathrm{d}_{(v)}}{\mathrm{d}_{(s)}+\mathrm{d}_{(v)}-2}\right)^3}+$$
$$\sum_{sv\in E_3(\mathrm{G})} x^{\left(\frac{\mathrm{d}_{(s)}*\mathrm{d}_{(v)}}{\mathrm{d}_{(s)}+\mathrm{d}_{(v)}-2}\right)^3}+\sum_{sv\in E_4(\mathrm{G})} x^{\left(\frac{\mathrm{d}_{(s)}*\mathrm{d}_{(v)}}{\mathrm{d}_{(s)}+\mathrm{d}_{(v)}-2}\right)^3}+$$
$$\sum_{sv\in E_5(\mathrm{G})} x^{\left(\frac{\mathrm{d}_{(s)}*\mathrm{d}_{(v)}}{\mathrm{d}_{(s)}+\mathrm{d}_{(v)}-2}\right)^3}+\sum_{sv\in E_6(\mathrm{G})} x^{\left(\frac{\mathrm{d}_{(s)}*\mathrm{d}_{(v)}}{\mathrm{d}_{(s)}+\mathrm{d}_{(v)}-2}\right)^3}$$

$$=(3*2^n)\ x^{\left(\frac{1*2}{1+2-2}\right)^3}+(3*2^n-3\ )\ x^{\left(\frac{1*3}{1+3-2}\right)^3}+(6*2^n-6)\ x^{\left(\frac{1*4}{1+4-2}\right)^3}+$$
$$(6*2^n-6)\ x^{\left(\frac{2*2}{2+2-2}\right)^3}+(42*2^n-33)\ x^{\left(\frac{2*3}{2+3-2}\right)^3}+(6*2^n-6)\ x^{\left(\frac{3*4}{3+4-2}\right)^3}$$

$$\text{AZP}(APD[n],x)=\ (6*2^n-6)x^{\frac{1728}{125}}+\ (6*2^n-6)x^{\frac{64}{27}}$$
$$+(3*2^n-3)x^{\frac{27}{8}}+(51*2^n-39)x^8.$$

Corollary 4.1.1: Let n ∈ N, then the Augmented Zagreb index of ($APD[n]$) is given as **:**

$$\text{AZI } (APD[n]) = 515.291 * 2^n - 419.291$$

Proof: By using a similar path we conclude the result by evaluating the polynomial at $x = 1$, This yields:

$$\frac{d}{d(x)}[\text{ AZP } (APD[n], x)]_{x=1} = (6 * 2^n - 6)x^{\frac{1728}{125}} + (6 * 2^n - 6)x^{\frac{64}{27}}$$

$$+(3 * 2^n - 3)x^{\frac{27}{8}} + (51 * 2^n - 39)x^8.$$

Thus, the Augmented Zagreb Index of the aminoisophthalate dister monomer dendrimer is ($APD[n]$) verified as:

$\text{AZI } (APD[n]) = 515.291 * 2^n - 419.291$

Theorem 4.1.2: Let n ∈ N, then the 1st Reformulated Zagreb Polynomial of ($APD[n]$) is define as **:**

$$RM_1(APD[n], x) = (3 * 2^n)x + (9 * 2^n - 9)x^4 + (48 * 2^n - 39)x^9$$

$$+(6 * 2^n - 6)x^{25}.$$

Proof: The edge set of aminoisophthalate dister monomer dendrimer ($APD[n]$) is divided in to six sets E_1, E_2, E_3, E_4, $E_5$and E_6. Which are define as follow. See table 4.1.

$| E_1(APD[n]) |$ consists $3 * 2^n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 2$, where $sv \in E\ (APD[n])$.

$|E_2(APD[n])|$ consists $3*2^n-3$ edges of type s,v s.t $d_{(s)}=1$, $d_{(v)}=3$, where $sv \in E\ (APD[n])$.

$|E_3(APD[n])|$ consists $6*2^n-6$ edges of type s,v s.t $d_{(s)}=1$, $d_{(v)}=4$, where $sv \in E\ (APD[n])$.

$|E_4(APD[n])|$ consists $6*2^n-6$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=2$, where $sv \in E\ (APD[n])$.

$|E_5(APD[n])|$ consists $42*2^n-33$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=3$, where $sv \in E\ (APD[n])$.

$|E_6(APD[n])|$ consists $6*2^n-6$ edges of type s,v s.t $d_{(s)}=3$, $d_{(v)}=4$, where $sv \in E\ (APD[n])$.

$RM_1(APD[n],x) = \sum_{sv\in E(G)} x^{(d_{(s)}+d_{(v)}-2)^2}$

$=\sum_{sv\in E_1(G)} x^{(d_{(s)}+d_{(v)}-2)^2} + \sum_{sv\in E_2(G)} x^{(d_{(s)}+d_{(v)}-2)^2} +$
$\sum_{sv\in E_3(G)} x^{(d_{(s)}+d_{(v)}-2)^2} + \sum_{sv\in E_4(G)} x^{(d_{(s)}+d_{(v)}-2)^2} +$
$\sum_{sv\in E_5(G)} x^{(d_{(s)}+d_{(v)}-2)^2} + \sum_{sv\in E_6(G)} x^{(d_{(s)}+d_{(v)}-2)^2}$

$= \quad (3*2^n)\, x^{(1+2-2)^2} + (3*2^n-3)\, x^{(1+3-2)^2} + (6*2^n-6)x^{(1+4-2)^2} + (6*2^n-6)\, x^{(2+2-2)^2} + (42*2^n-33\ )\, x^{(2+3-2)^2} + (6*2^n-6)\, x^{(3+4-2)^2}$

$RM_1(APD[n],x) \ = (3*2^n)x + (9*2^n-9)x^4 + (48*2^n-39)x^9 + (6*2^n-6)x^{25}$.

Corollary 4.1.2: Let n ∈ N, then the 1st Reformulated Zagreb index of ($APD[n]$) is given as **:**

$$RM_1(APD[n]) = 621 * 2^n - 537.$$

Proof: To confirm and compute the result of 1st Reformulated Zagreb Polynomial, which is denoted by $RM_1(APD[n], x)$, of the dendrimer ($APD[n]$), we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$$\frac{d}{d(x)}[\, RM_1(APD[n], x)] \,|_{x=1} = (3 * 2^n)x + (9 * 2^n - 9)x^4$$

$$+(48 * 2^n - 39)x^9 + (6 * 2^n - 6)x^{25}.$$

Thus, the 1st Reformulated Zagreb Index of the porphyrin dendrimer is ($APD[n]$) verified as:

$RM_1(APD[n]) = 621 * 2^n - 537.$

Theorem 4.1.3: Let n ∈ N, then the 2nd Reformulated Zagreb Polynomial of ($APD[n]$) is define as **:**

$RM_2(APD[n], x) = (3 * 2^n)\, x^2 + (3 * 2^n - 3)\, x^6 + (6 * 2^n - 6)x^8 + (6 * 2^n - 6)x^{12} + (42 * 2^n - 33)\, x^{18} + (6 * 2^n - 6)\, x^{60}$

Proof: The edge set of aminoisophthalate dister monomer dendrimer ($APD[n]$) is divided in to six sets E_1, E_2, E_3, E_4, $E_5$and E_6. Which are define as follow. See table 4.1.

$|E_1(APD[n])|$ it has $3*2^n$ edges of type s,v s.t $d_{(s)}=1$, $d_{(v)}=2$, where $sv \in E\ (APD[n])$.

$|E_2(APD[n])|$ it has $3*2^n-3$ edges of type s,v s.t $d_{(s)}=1$, $d_{(v)}=3$, where $sv \in E\ (APD[n])$.

$|E_3(APD[n])|$ it has $6*2^n-6$ edges of type s,v s.t $d_{(s)}=1$, $d_{(v)}=4$, where $sv \in E\ (APD[n])$.

$|E_4(APD[n])|$ it has $6*2^n-6$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=2$, where $sv \in E\ (APD[n])$.

$|E_5(APD[n])|$ it has $42*2^n-33$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=3$, where $sv \in E\ (APD[n])$.

$|E_6(APD[n])|$ it has $6*2^n-6$ edges of type s,v s.t $d_{(s)}=3$, $d_{(v)}=4$, where $sv \in E\ (APD[n])$.

$RM_2(APD[n],x) = \sum_{sv\in \mathrm{E(G)}} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})}$

$= \sum_{sv\in E_1(\mathrm{G})} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv\in E_2(\mathrm{G})} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv\in E_3(\mathrm{G})} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv\in E_4(\mathrm{G})} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv\in E_5(\mathrm{G})} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv\in E_6(\mathrm{G})} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})}$

$= (3*2^n)\, x^{(1+2-2)(1*2)} + (3*2^n-3)\, x^{(1+3-2)(1*3)} + (6*2^n-6)x^{(1+4-2)(1*4)} + (6*2^n-6)x^{(2+2-2)(2*2)} + (42*2^n-33)\, x^{(2+3-2)(2*3)} + (6*2^n-6)\, x^{(3+4-2)(3*4)}$.

$RM_2(APD[n],x) = (3*2^n)\, x^2 + (3*2^n-3)\, x^6 + (6*2^n-6)x^8 + (6*2^n-6)x^{12} + (42*2^n-33)\, x^{18} + (6*2^n-6)\, x^{60}$

Corollary 4.1.3: Let n ∈ N, then the 2nd Reformulated Zagreb index of ($APD[n]$) is given as **:**

$$RM_2(APD[n]) = 1260 * 2^n - 1092.$$

Proof: To confirm and compute the result of 2nd Reformulated Zagreb Polynomial, which is denoted by $RM_2(APD[n], x)$, of the dendrimer ($APD[n]$), we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$\frac{d}{d(x)}[RM_2(APD[n], x)] |_{x=1} = (3 * 2^n) x^2 + (3 * 2^n - 3) x^6 + (6 * 2^n - 6)x^8 + (6 * 2^n - 6)x^{12} + (42 * 2^n - 33) x^{18} + (6 * 2^n - 6) x^{60}.$

Thus, the 2nd Reformulated Zagreb Index of the porphyrin dendrimer is ($APD[n]$) verified as:

$RM_2(APD[n]) = 1260 * 2^n - 1092.$

Theorem4.1.4: Let n ∈ N, then the Edge Irregularity Polynomial of ($APD[n]$) is define as **:**

$IR(APD[n], x) = (6 * 2^n - 6) + (51 * 2^n - 39)x + (3 * 2^n - 3)x^2 + (6 * 2^n - 6)x^3.$

Proof*:* The edge set of aminoisophthalate dister monomer dendrimer ($APD[n]$) is divided in to six sets E_1, E_2, E_3, E_4, $E_5$and E_6. Which are define as follow. See table 4.1.

$| E_1(APD[n]) |$ include $3 * 2^n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 2$, where $sv \in E (APD[n])$.

$|E_2(APD[n])|$ include $3*2^n-3$ edges of type s,v s.t $d_{(s)}=1$, $d_{(v)}=3$, where $sv\in E\ (APD[n])$.

$|E_3(APD[n])|$ include $6*2^n-6$ edges of type s,v s.t $d_{(s)}=1$, $d_{(v)}=4$, where $sv\in E\ (APD[n])$.

$|E_4(APD[n])|$ include $6*2^n-6$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=2$, where $sv\in E\ (APD[n])$.

$|E_5(APD[n])|$ include $42*2^n-33$ edges of type s,v s.t $d_{(s)}=2$, $d_{(v)}=3$, where $sv\in E\ (APD[n])$.

$|E_6(APD[n])|$ include $6*2^n-6$ edges of type s,v s.t $d_{(s)}=3$, $d_{(v)}=4$, where $sv\in E\ (APD[n])$.

$IR\ (APD[n],x)=\sum_{sv\in E(G)} x^{|d_{(s)}-d_{(v)}|}$

$=\sum_{sv\in E_1(G)} x^{|d_{(s)}-d_{(v)}|}+\sum_{sv\in E_2(G)} x^{|d_{(s)}-d_{(v)}|}+\sum_{sv\in E_3(G)} x^{|d_{(s)}-d_{(v)}|}+$
$\sum_{sv\in E_4(G)} x^{|d_{(s)}-d_{(v)}|}+\sum_{sv\in E_5(G)} x^{|d_{(s)}-d_{(v)}|}+\sum_{sv\in E_6(G)} x^{|d_{(s)}-d_{(v)}|}$

$=(3*2^n)x^{|1-2|}+(3*2^n-3)\,x^{|1-3|}+(6*2^n-6)x^{|1-4|}+(6*2^n-6)\,x^{|2-2|}+(42*2^n-33)\,x^{|2-3|}+(6*2^n-6)x^{|3-4|}$.

$$IR\ (APD[n],x)=(6*2^n-6)+(51*2^n-39)x+(3*2^n-3)x^2$$
$$+(6*2^n-6)x^3.$$

Corollary 4.1.4: Let n ∈ N, then the Edge Irregularity index of ($APD[n]$) is given as **:**

$$IR\ (APD[n]) = 75 * 2^n - 63.$$

Proof: To demonstrate the result of Edge Irregularity Polynomial, which is denoted by $IR\ (APD[n], x)$, of the dendrimer ($APD[n]$), we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$\frac{d}{d(x)}[\ IR\ (APD[n], x)]\ |_{x=1} = (6 * 2^n - 6) + (51 * 2^n - 39)x + (3 * 2^n - 3)x^2 + (6 * 2^n - 6)x^3.$

Thus, the Edge Irregularity Index of the porphyrin dendrimer is ($APD[n]$) verified as:

$IR\ (APD[n]) = 75 * 2^n - 63.$

Theorem4.1.5: Let n ∈ N, then the Degree Edge Stability Polynomial of ($APD[n]$)is given as **:**

$DS\ (APD[n], x) = (6 * 2^n - 6) + (51 * 2^n - 39)x + (3 * 2^n - 3)x^4 + (6 * 2^n - 6)x^9$

Proof: The edge set of aminoisophthalate dister monomer dendrimer ($APD[n]$) is divided in to six sets E_1, E_2, E_3, E_4, $E_5$and E_6. Which are define as follow. See table 4.1.

$|\ E_1(APD[n])\ |$ consists $3 * 2^n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 2$, where $sv \in E\ (APD[n])$.

$|E_2(APD[n])|$ consists $3 * 2^n - 3$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 3$, where $sv \in E\ (APD[n])$.

$|E_3(APD[n])|$ consists $6 * 2^n - 6$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 4$, where $sv \in E\ (APD[n])$.

$|E_4(APD[n])|$ consists $6 * 2^n - 6$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where $sv \in E\ (APD[n])$.

$|E_5(APD[n])|$ consists $42 * 2^n - 33$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv \in E\ (APD[n])$.

$|E_6(APD[n])|$ consists $6 * 2^n - 6$ edges of type s, v s.t $d_{(s)} = 3$, $d_{(v)} = 4$, where $sv \in E\ (APD[n])$.

$DS\ (APD[n], x) = \sum_{sv\in E(G)} x^{(d_{(s)}-d_{(v)})^2}$.

$= \sum_{sv\in E_1(G)} x^{(d_{(s)}-d_{(v)})^2} + \sum_{sv\in E_2(G)} x^{(d_{(s)}-d_{(v)})^2} + \sum_{sv\in E_3(G)} x^{(d_{(s)}-d_{(v)})^2} + \sum_{sv\in E_4(G)} x^{(d_{(s)}-d_{(v)})^2} + \sum_{sv\in E_5(G)} x^{(d_{(s)}-d_{(v)})^2} + \sum_{sv\in E_6(G)} x^{(d_{(s)}-d_{(v)})^2}$

$= (3 * 2^n)\ x^{(1-2)^2} + (3 * 2^n - 3)\ x^{(1-3)^2} + (6 * 2^n - 6)x^{(1-4)^2} + (6 * 2^n - 6)x^{(2-2)^2} + (42 * 2^n - 33)\ x^{(2-3)^2} + (6 * 2^n - 6)\ x^{(3-4)^2}$

$DS\ (APD[n], x) = (6 * 2^n - 6) + (51 * 2^n - 39)x + (3 * 2^n - 3)x^4 + (6 * 2^n - 6)x^9$.

Corollary 4.1.5: Let n ∈ N, then the Degree Edge Stability index of ($APD[n]$) is given as **:**

$$DS\ (APD[n]) = 117 * 2^n - 105.$$

Proof: To evaluate the result of Degree Edge Stability Polynomial, which is denoted by $DS\ (APD[n], x)$, of the dendrimer ($APD[n]$), we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$\frac{d}{d(x)}[\ DS\ (APD[n], x)]\ |_{x=1} = (6 * 2^n - 6) + (51 * 2^n - 39)x + (3 * 2^n - 3)x^4 + (6 * 2^n - 6)x^9$

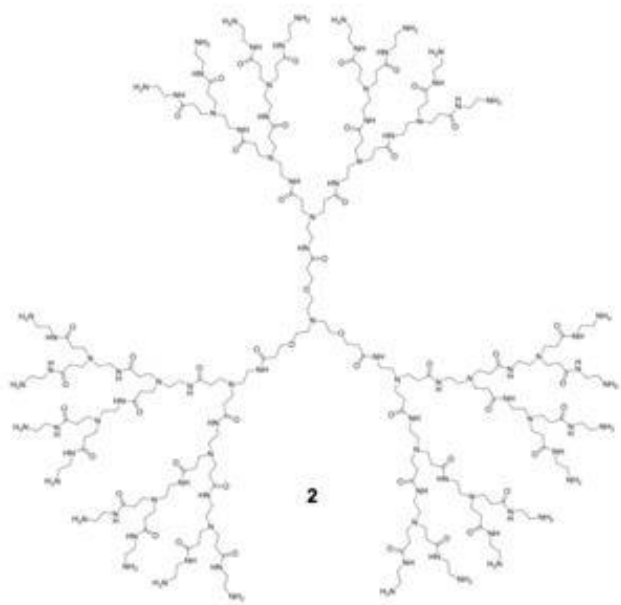
Thus, the Edge Irregularity Index of the porphyrin dendrimer is ($APD[n]$) verified as:

$DS\ (APD[n]) = 117 * 2^n - 105.$

4.2 Computation of Topological Indices and Polynomials of Poly (Amidoamine) Dendrimer ($PD[n]$).

Proposition 4.2:[41] It considered the first type of dendrimer ($PD[n]$)then:

1. **Order of** ($PD[n]$) is $12 * 2^{n+2} - 14$
2. **Size of** ($PD[n]$) is $12 * 2^{n+2} - 15$. See figure 4.2



2

Figure 4.2: dendrimers ($PD[n]$) is also known as poly (amidoamine).

($PD[n]$) stretcher made up of four types of edges based on degree of end vertices of each as given in table 4.2.

Table 4.2: Graph of the stretcher ($PD[n]$).

(d_s, d_v)	(1,2)	(1,3)	(2,2)	(2,3)
No. of edges	$3 * 2^n$	$6 * 2^n - 3$	$18 * 2^n$	$21 * 2^n - 12$

First of all, we are going to calculate the Augmented Zagreb polynomial for the molecular ($PD[n]$).

Theorem 4.2.1: Let n ∈ N, then the Augmented Zagreb polynomial of ($PD[n]$) is given as **:**

AZP($PD[n], x$) = $(42 * 2^n - 12)x^8 + (6 * 2^n - 3)\, x^{\frac{27}{8}}$

Proof: The edge set of poly (amidoamine) dendrimer ($PD[n]$) is divided in to four sets $E_1, E_2, E_3, and\ E_4$. Which are define as follow. See table 4.2.

$|E_1(PD[n])|$ contain $3 * 2^n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 2$, where $sv \in E\ (PD[n])$.

$|E_2(PD[n])|$ contain $6 * 2^n - 3$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 3$, where $sv \in E\ (PD[n])$.

$|E_3(PD[n])|$ contain $18 * 2^n$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where $sv \in E\ (PD[n])$.

$|E_4(PD[n])|$ contain $21 * 2^n - 12$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv \in E\ (PD[n])$.

AZP ($PD[n], x$) $= \sum_{sv \in E(G)} x^{\left(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2}\right)^3}$

$= \sum_{sv \in E_1(G)} x^{(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2})^3} + \sum_{sv \in E_2(G)} x^{(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2})^3} +$

$\sum_{sv \in E_3(G)} x^{(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2})^3} + \sum_{sv \in E_4(G)} x^{(\frac{d_{(s)} * d_{(v)}}{d_{(s)} + d_{(v)} - 2})^3}$

$= (3 * 2^n)\, x^{(\frac{1*2}{1+2-2})^3} + (6 * 2^n - 3)\, x^{(\frac{1*3}{1+3-2})^3} + (18 * 2^n)\, x^{(\frac{2*2}{2+2-2})^3} + (21 * 2^n - 12)\, x^{(\frac{2*3}{2+3-2})^3}$.

AZI$(PD[n], x)$ = $(42 * 2^n - 12)x^8 + (6 * 2^n - 3)\, x^{\frac{27}{8}}$.

Corollary 4.2.1: Let n ∈ N, then the Augmented Zagreb index of ($PD[n]$) is given as **:**

$$\text{AZI}\ (PD[n]) = 356.25 * 2^n - 106.125$$

Proof: By using a similar approach we conclude the result by evaluating the polynomial at $x = 1$, This yields:

$\frac{d}{d(x)}[\ \text{AZP}(PD[n], x)\ ]_{x=1} = (42 * 2^n - 12)x^8 + (6 * 2^n - 3)\, x^{\frac{27}{8}}$

Thus, the Augmented Zagreb Index of the poly (amidoamine) dendrimer is ($PD[n]$) verified as:

AZI ($PD[n]$) $= 356.25 * 2^n - 106.125$.

Theorem 4.2.2: Let n ∈ N, then the 1st Reformulated Zagreb Polynomial of ($PD[n]$)is define as **:**

$RM_1(PD[n], x)$= $(3 * 2^n)x + (24 * 2^n - 3)x^4 + (21 * 2^n - 12)x^9$.

Proof: The edge set of poly (amidoamine) dendrimer ($PD[n]$) is divided in to four sets E_1, E_2, E_3, $and\ E_4$. Which are define as follow. See table 4.2.

$|E_1(PD[n])|$ have $3 * 2^n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 2$, where $sv \in E(PD[n])$.

$|E_2(PD[n])|$ have $6 * 2^n - 3$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 3$, where $sv \in E(PD[n])$.

$|E_3(PD[n])|$ have $18 * 2^n$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where $sv \in E(PD[n])$.

$|E_4(PD[n])|$ have $21 * 2^n - 12$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv \in E(PD[n])$.

$RM_1(PD[n]), x) = \sum_{sv\in E(G)} x^{(d_{(s)}+d_{(v)}-2)^2}$

$= \sum_{sv\in E_1(G)} x^{(d_{(s)}+d_{(v)}-2)^2} + \sum_{sv\in E_2(G)} x^{(d_{(s)}+d_{(v)}-2)^2} +$
$\sum_{sv\in E_3(G)} x^{(d_{(s)}+d_{(v)}-2)^2} + \sum_{sv\in E_4(G)} x^{(d_{(s)}+d_{(v)}-2)^2} +$

$= (3 * 2^n)\, x^{(1+2-2)^2} + (6 * 2^n - 3)\, x^{(1+3-2)^2} + (18 * 2^n)\, x^{(2+2-2)^2} +$
$(21 * 2^n - 12)\, x^{(2+3-2)^2}$.

$RM_1(PD[n], x) = (3 * 2^n)x + (24 * 2^n - 3)x^4 + (21 * 2^n - 12)x^9$.

Corollary 4.2.2: Let n ∈ N, then the 1st Reformulated Zagreb index of ($PD[n]$) is given as **:**

$$RM_1(PD[n]) = 288 * 2^n - 120.$$

Proof: To confirm the result of 1st Reformulated Zagreb Polynomial, which is denoted by $RM_1(PD[n], x)$, of the dendrimer ($PD[n]$), we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$\frac{d}{d(x)}[\ RM_1(PD[n],x)]\ |_{x=1}= (3*2^n)x + (24*2^n - 3)x^4$

$$+(21*2^n - 12)x^9$$

Thus, the 1st Reformulated Zagreb Index of the poly (amidoamine) dendrimer is ($PD[n]$) verified as:

$RM_1(PD[n]) = 288*2^n - 120.$

Theorem 4.2.3: Let n ∈ N, then the 2nd Reformulated Zagreb Polynomial of ($PD[n]$)is define as **:**

$RM_2(PD[n],x)$=$(3*2^n)x^2 + (6*2^n - 3)x^6 + (18*2^n)x^8 + (21*2^n - 12)x^{18}$

Proof: The edge set of poly (amidoamine) dendrimer ($PD[n]$) is divided in to four sets $E_1, E_2, E_3, and\ E_4$. Which are define as follow. See table 4.2.

$|E_1(PD[n])|$ Be composed of $3*2^n$ edges of type s,v s.t $d_{(s)} = 1$

$d_{(v)} = 2$, where $sv \in E\ (PD[n])$.

$|E_2(PD[n])|$ Be composed of $6*2^n - 3$ edges of type s,v s.t $d_{(s)} = 1$, $d_{(v)} = 3$, where $sv \in E\ (PD[n])$ **.**

$|E_3(PD[n])|$ Be composed of $18*2^n$ edges of type s,v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where $sv \in E\ (PD[n])$.

$|E_4(PD[n])|$ Be composed of $21*2^n - 12$ edges of type s,v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv \in E\ (PD[n])$.

$RM_2(PD[n],x) = \sum_{sv\in E(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})}$.

$= \sum_{sv \in E_1(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv \in E_2(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv \in E_3(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} + \sum_{sv \in E_4(G)} x^{(d_{(s)}+d_{(v)}-2)(d_{(s)}*d_{(v)})} +$

$= (3 * 2^n)x^{(1+2-2)(1*2)} + (6 * 2^n - 3)x^{(1+3-2)(1*3)} + (18 * 2^n)x^{(2+2-2)(2*2)} + (21 * 2^n - 12)x^{(2+3-2)(2*3)}.$

$RM_2(PD[n], x) = (3 * 2^n)x^2 + (6 * 2^n - 3)x^6 + (18 * 2^n)x^8 + (21 * 2^n - 12)x^{18}.$

Corollary 4.2.3: Let n ∈ N, then the 2nd Reformulated Zagreb index of ($PD[n]$) is given as **:**

$$RM_2(PD[n]) = 564 * 2^n - 234.$$

Proof: To compute the result of 2nd Reformulated Zagreb Polynomial, which is denoted by $RM_2(PD[n], x)$, of the dendrimer ($PD[n]$), we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$\frac{d}{d(x)}[RM_2(PD[n], x)]|_{x=1} = (3 * 2^n)x^2 + (6 * 2^n - 3)x^6 + (18 * 2^n)x^8 + (21 * 2^n - 12)x^{18}$

Thus, the 2nd Reformulated Zagreb Index of the poly (amidoamine) dendrimer is ($PD[n]$) verified as:

$RM_2(PD[n]) = 564 * 2^n - 234.$

Theorem4.2.4: Let n ∈ N, then the Edge Irregularity Polynomial of ($PD[n]$)is define as **:**

$$IR\ (PD[n], x) = (18 * 2^n) + (24 * 2^n - 12)x + (6 * 2^n - 3)x^2.$$

Proof*:* The edge set of poly (amidoamine) dendrimer ($PD[n]$) is divided in to four sets $E_1, E_2, E_3, and\ E_4$. Which are define as follow. See table 4.2.

$|E_1(PD[n])|$ consists $3 * 2^n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 2$, where $sv \in E\ (PD[n])$.

$|E_2(PD[n])|$ consists $6 * 2^n - 3$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 3$, where $sv \in E\ (PD[n])$ **.**

$|E_3(PD[n])|$ consists $18 * 2^n$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where $sv \in E\ (PD[n])$.

$|E_4(PD[n])|$ consists $21 * 2^n - 12$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv \in E\ (PD[n])$.

$IR\ (PD[n], x) = \sum_{sv \in E(G)} x^{|d_{(s)} - d_{(v)}|}$

$= \sum_{sv \in E_1(G)} x^{|d_{(s)} - d_{(v)}|} + \sum_{sv \in E_2(G)} x^{|d_{(s)} - d_{(v)}|} + \sum_{sv \in E_3(G)} x^{|d_{(s)} - d_{(v)}|} + \sum_{sv \in E_4(G)} x^{|d_{(s)} - d_{(v)}|}$.

$= (3 * 2^n)x^{|1-2|} + (6 * 2^n - 3)x^{|1-3|} + (18 * 2^n)x^{|2-2|} + (21 * 2^n - 12)x^{|2-3|}$.

$IR\ (PD[n], x) = (18 * 2^n) + (24 * 2^n - 12)x + (6 * 2^n - 3)x^2$.

Corollary 4.2.4: Let n ∈ N, then the Edge Irregularity index of ($PD[n]$) is given as **:**

$$IR\ (PD[n]) = 36 * 2^n - 18.$$

Proof: To demonstrate the result of Edge Irregularity Polynomial, which is denoted by $IR\ (PD[n], x)$, of the dendrimer ($PD[n]$), we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$\frac{d}{d(x)}[\ IR\ (PD[n], x)]\ |_{x=1} = (18 * 2^n) + (24 * 2^n - 12)x + (6 * 2^n - 3)x^2$.

Thus, the Edge Irregularity Index of the poly (amidoamine) dendrimer is ($PD[n]$) verified as:

$IR\ (PD[n]) = 36 * 2^n - 18.$

Theorem4.2.5: Let n ∈ N, then the Degree Edge Stability Polynomial of ($PD[n]$) is given as **:**

$DS\ (PD[n], x) = (18 * 2^n) + (24 * 2^n - 12)x + (6 * 2^n - 3)x^4.$

Proof: The edge set of poly (amidoamine) dendrimer ($PD[n]$) is divided in to four sets E_1, E_2, E_3, and E_4. Which are define as follow. See table 4.2.

$|\ E_1(PD[n])\ |$ include $3 * 2^n$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 2$, where $sv \in E\ (PD[n])$.

$|\ E_2(PD[n])|$ include $6 * 2^n - 3$ edges of type s, v s.t $d_{(s)} = 1$, $d_{(v)} = 3$, where $sv \in E\ (PD[n])$ **.**

$|E_3(PD[n])|$ include $18 * 2^n$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 2$, where $sv \in E\ (PD[n])$.

$|E_4(PD[n])|$ include $21 * 2^n - 12$ edges of type s, v s.t $d_{(s)} = 2$, $d_{(v)} = 3$, where $sv \in E\ (PD[n])$.

$DS\ (PD[n], x) = \sum_{sv\in E(G)} x^{(d_{(s)}-d_{(v)})^2}$

$= \sum_{sv\in E_1(G)} x^{(d_{(s)}-d_{(v)})^2} + \sum_{sv\in E_2(G)} x^{(d_{(s)}-d_{(v)})^2} + \sum_{sv\in E_3(G)} x^{(d_{(s)}-d_{(v)})^2} + \sum_{sv\in E_4(G)} x^{(d_{(s)}-d_{(v)})^2}$.

$= (3 * 2^n)x^{(1-2)^2} + (6 * 2^n - 3)x^{(1-3)^2} + (18 * 2^n)x^{(2-2)^2}$

$$+(21 * 2^n - 12)x^{(2-3)^2}.$$

$DS\ (PD[n], x) = (18 * 2^n) + (24 * 2^n - 12)x + (6 * 2^n - 3)x^4$

Corollary 4.2.5: Let n ∈ N, then the Degree Edge Stability index of ($PD[n]$) is given as **:**

$$DS\ (PD[n]) = 48 * 2^n - 24.$$

Proof: To calculate the result of Degree Edge Stability Polynomial, which is denoted by $DS\ (PD[n], x)$, of the dendrimer ($PD[n]$), we differentiate it with respect to x, evaluating at $x = 1$, This yields:

$\frac{d}{d(x)}[\ DS\ (PD[n], x)]\ |_{x=1} = (18 * 2^n) + (24 * 2^n - 12)x$

$$+(6 * 2^n - 3)x^4.$$

Thus, the Edge Irregularity Index of the poly (amidoamine) dendrimer is ($PD[n]$) verified as:

$DS\ (PD[n]) = 48 * 2^n - 24.$

Chapter Five

Differences Between Augmented Zagreb Index and Edges Irregularity Index.

Introduction: we examine new mathematical relationships between two significant degree-based topological indices. the Augmented Zagreb Index (AZI) and the Edge Irregular Stability Index (EIS). Using the classical inequalities Cauchy-Schwarz and Jensen's inequalities, we derive new upper and lower bounds for these indices. These bounds enhance our understanding of the structural behavior of graphs and provide useful tools in chemical graph theory. Prior to declaring the main results, we recall basic inequalities that are at the heart of our derivations.

1. Cauchy- Schwarz inequality: [34,42] if $a_1, \dots , a_n$ and $b_1, \dots , b_n$ are real number

Than

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \left(\sum_{i=1}^{n} {a_i}^2\right)\left(\sum_{i=1}^{n} {b_i}^2\right)$$

Or

$$\left|\sum_{i=1}^{n} a_i b_i\right| \leq \sqrt{\sum_{i=1}^{n} {a_i}^2}\,\sqrt{\sum_{i=1}^{n} {b_i}^2}$$

2. Jensen’s inequality: [35] let $f(x)$ be a convex function defined on interval I if $x_i, \dots , x_n \in I$ and $\lambda_1, \dots , \lambda_n \geq 0$ with $\sum_{i=1}^{n} \lambda_i$ then

$$f\left(\sum_{i=1}^{n} \lambda_i \; x_1\right) \leq \sum_{i=1}^{n} \lambda_i \; \mathrm{f}(x_i)$$

5.1: Relation between Augmented Zagreb index and Edge Irregularity Stability index.

In this section we introduce a link with the Augmented Zagreb Index and the Edge Irregular Stability Index. Such indices have different degree values on which they depend, but can be linked via inequalities and structural graph properties.

Proposition 5.1: [32,33] Let G be connected graph with m edges. Then

$AZI(G) = \sum_{sv\in E(G)}(\frac{d_s*d_v}{d_s+d_v-2})^3$. Using Jensen's Inequality with the convex function $f(x) = x^3$ so, we will have

$$AZI(G) \geq m\,(\frac{1}{m}\sum_{sv\in E(G)}(\frac{d_s*d_v}{d_s+d_v-2})^3).$$

Let us denoted this average value by A = $\frac{1}{m}\sum_{sv\in E(G)}(\frac{d_s*d_v}{d_s+d_v-2})^3)$. So,

$$AZI(G) \geq m\,(A)^3$$

To bound A, note that the denominator: $d_s + d_v - 2 \geq |d_s - d_v|$, thus

$\frac{d_s*d_v}{d_s+d_v-2} \geq \frac{d_s*d_v}{|d_s-d_v|+2}$. By using Cauchy – Schwarz inequality:

$(\sum_{sv\in E(G)} d_s d_v)^2 \leq m\sum_{sv\in E(G)}(d_s * d_v)^2$. If we combine both side, we get that.

$AZI(G) \geq \frac{1}{m^2}\quad (\sum_{sv\in E(G)} d_s d_v)^3 \Big/ (\sum_{sv\in E(G)}|d_s - d_v|)^3$. It was proved $EIS\,(G) \neq 0$

If we let:

$$S_1 = (\sum_{sv\in E(G)} d_s d_v)^3 \text{ and } S_2 = (\sum_{sv\in E(G)}|d_s - d_v|)^3.$$

Then by Holder's inequality (in a generalized form), we approximate

$$AZI(G) \geq \frac{S_1}{m^2(S_2)}$$

This connects the AZI to the irregularity measured by EIS.

Example: 5.1.1: Consider the star graph S_n it has one central vertex of degree $n-1$ *and* $n-1$ leaves of degree 1. Than,

$EIS(S_n) = (n-1)(n-2),$ and $AZI\ (S_n) = (n-1)(\frac{n-1}{n-2})$

Now let us to compute:

$S_1 = (n-1)(n-1),$ and $S_2 = (n-1)(n-2)$

Thus;

$$AZI\ (S_n) \geq \frac{(n-1)^3}{(n-1)^2(n-2)^3} \quad ; \quad \text{Simplify}$$

$$AZI\ (S_n) \geq \frac{n-1}{(n-2)^3}$$

$$AZI\ (S_n) = (\frac{1}{n-2})^3$$

Let $m = n-1$ and we will multiply by m we recover .

$$AZI\ (S_n) \geq (n-1)(\frac{1}{n-2})^3$$

Matching the earlier exact formula.

Example 5.1.2: consider the complete graph K_n, has all vertex degrees are equal $(d = n - 1)$. So,

$EIS\ (K_n) = 0$ and $AZI\ (K_n) = \binom{n}{2}\ (\frac{(n-1)^2}{2(n-1)-2})^3$

This shows that whenever the graph is regular $(d_u = d_v)$, the n AZI is maximal in uniform degree graphs while EIS vanishes.

Example 5.1.3: Let G be a path graph P_4 with vertices of degrees $(1,2,2,1)$. Than;

$EIS\ (P_n) = |1 - 2| + |2 - 2| + |2 - 1| = 2$. When edges are $(1,2), (2,2), (2,1)$. And;

$$AZI(P_n) = (\frac{1 * 2}{1 + 2 - 2})^3 + (\frac{2 * 2}{2 + 2 - 2})^3 + (\frac{2 * 1}{2 + 1 - 2})^3$$

$$AZI(P_n) = 20$$

Now, compute

$$S_1 = 1.2 + 2.2 + 2.1$$

$$S_1 = 8$$

$$S_2 = 1 + 0 + 1$$

$$S_2 = 2 \text{ , Let } m = 3;$$

$$AZI(P_n) \geq \left(\frac{8}{3^2\ * 2}\right) = \frac{512}{72} \approx 7.11$$

5.2: New upper and lower bounds of Augmented Zagreb index AZI(G)

Theorem 5.2.1: Let G be a graph with minimum degree δ , maximum degree Δ , and m edges. Then,

$$AZI(G) \geq m\left(\frac{\delta^2}{2\Delta - 2}\right)^3$$

Proof: Since $d_s \geq \delta$ and $d_v \geq \delta$ if follows that the numerator $d_s d_v \geq \delta^2$. Meanwhile, the maximum possible denominator is $d_s + d_v - 2 \leq 2\Delta - 2$ therefor for every edge $sv \in E(G)$.

$$(\frac{d_s d_v}{d_s + d_v - 2})^3 \geq \left(\frac{\delta^2}{2\Delta - 2}\right)^3$$

Now summing over all m edges we get.

$$AZI(G) \geq m\left(\frac{\delta^2}{2\Delta - 2}\right)^3$$

Equality holds if and only if all vertex degrees equal δ and $d_s + d_v - 2 = 2\Delta - 2$, i.e. the graph is regular.

Theorem 5.2.2: Under the same conditions we have the upper bound

$$AZI(G) \leq m \left(\frac{\Delta^2}{2\delta - 2}\right)^3$$

Proof: Here, $d_s \leq \Delta$ and $d_v \leq \Delta$ if follows that the numerator $d_s d_v \leq \Delta^2$. Meanwhile, the minimum possible denominator is $d_s + d_v - 2 \geq 2\delta - 2$ therefor for every edge $uv \in E(G)$.

$$AZI(G) \leq m \left(\frac{\Delta^2}{2\delta - 2}\right)^3$$

The equality is attained when all degrees are equal to Δ.

5.3: New Upper and Lower Bounds of Edges Irregularity Stability Index EIS (G)

Theorem: 5.3.1: [16,17] For a graph G with m edges and degree range $\delta\ to\ \Delta$.

$$\mathrm{EIS}\ (\mathrm{G}) \geq |\Delta - \delta|$$

Proof: at minimum if only one edge in the graph connects vertices of degrees $\delta\ and\ \Delta$ than the sum is at least $|\Delta - \delta|$ therefor

$$\mathrm{EIS}\ (\mathrm{G}) \geq |\Delta - \delta|$$

Equality holds if and only if all other edges contributes zero (i.e., they connect verities of equal degrees).

Theorem: 5.3.2: [9,32] Under the same condition

$$\mathrm{EIS}\ (\mathrm{G}) \leq m\ |\Delta - \delta|$$

Proof: since the maximum absolute difference for any edges $uv\ \in E(G)$ is $\Delta - \delta$ the sum over all m edges is bounded above by .

$$\mathrm{EIS}\ (\mathrm{G}) \leq m\ (\Delta - \delta)$$

Equality holds in highly irregular graphs like star graphs.

Example 5.3.1: consider the star graph S_n where one vertex has degrees $n - 1$ and $n - 1$others have degree 1

Than,

$$EIS\ (S_n) = \sum_{i=1}^{n-1} |(n-1) - 1| = (n-1)(n-2)$$

This is the case of maximum irregularity.

Example 5.3.2: for a complete graph K_n all degrees are equal, So;

$$EIS\ (K_n) = 0$$

This is illustrating the equality case for regular graphs

Chapter Six

Conclusion and Future Studies

6.1 Conclusion:

This study applies graph-theoretical tools to investigate the topological properties of key dendrimer families such as PETIM, PAMAM, poly propylenimine octaamin, zinc porphyrins, and porphyrins. Polynomial expressions were derived for several degree-based indices, including the Augmented Zagreb Index (AZI), Reformulated Zagreb Indices (RM_1, RM_2), the Edge Irregularity Index, and the Degree-Based Stability Index. These polynomials provide improved modeling of molecular branching across dendrimer generations. Analytical relationships and bounds between AZI and the Edge Irregularity Index were also established, offering new mathematical insight into molecular irregularity and stability. Overall, this work strengthens the theoretical foundation for dendrimer research and suggests new applications in chemistry, nanotechnology, and materials science.

6.2 Recommendations and Future Studies.

Future research is suggested by this study, as explained below:

1. The computation of topological indices and new graph polynomials for dendrimers that are discussed in the paper.

2. The investigation of novel dendrimers for the same topological indices and graph polynomials that are calculated in this work.

3. Determining updated upper and lower bounds for the stability Zagreb indices based on degree.

4. Determining the first and second reformulated Zagreb index's new upper and lower bounds.

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المستخلص

تركّز هذه الدراسة على حساب وتحليل المؤشرات الطوبولوجية المعتمدة على درجات الرؤوس لعدد من تراكيب الديندريمرات. تم تناول مؤشرات كلاسيكية أحدث مثل مؤشر زغرب المعزز، مؤشري زغرب المعاد صياغتهما، مؤشر عدم انتظام الحواف، ومؤشر ثبات درجة الحافة. تم اشتقاق صيغ عامة لهذه المؤشرات اعتمادًا على معلمات الرسم البياني مثل عدد الرؤوس، الحواف، والدرجات، وذلك لتراكيب ديندريمر مختلفة تشمل PD[n] And APD[n]، وPETAA، DPZ_n، PETIM، (D_n, P_n). كما تسلط الدراسة الضوء على الفروقات بين مؤشري زغرب المعزز وعدم انتظام الحواف، من خلال تحديد حدود علوية وسفلية جديدة لكليهما. وتدعم النتائج قوة المؤشرات الطوبولوجية في التنبؤ بالبنية الجزيئية وسلوكها

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رسالة ماجستير مقدمة الى

مجلس كلية علوم الحاسوب والرياضيات في جامعة تكريت

وهي جزء من متطلبات نيل شهادة ماجستير في علوم الرياضيات

من قبل الطالبة

ماريه كاوه محمود

بإشراف

أ.د.نبيل عزالدين عارف

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