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حساب بعض المؤشرات الطوبولوجية لمتفرعة بورفيرين الزنك (DPZ_n)

Computation of Some Topological Indices of zinc porphyrin Dendrimer (DPZ_n)

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الملخص:

تركز هذه الدراسة على حساب ودراسة بعض المؤشرات الطوبولوجية المعتمدة على الدرجات لهياكل المتفرعات (الديندريمرات). وقد شملت الدراسة المؤشرات التقليدية بالإضافة إلى بعض المؤشرات الحديثة، مثل مؤشر زغرب المعزز، ومؤشري زغرب المعاد صياغته الأول والثاني، ومؤشر عدم انتظام الحواف، ومؤشر استقرار درجة الحافة. وبشكل خاص، تم تطبيق هذه المؤشرات على متفرعة بورفيرين الزنك، وذلك لتحليل خصائصها البنائية والرياضية.

الكلمات المفتاحية:

(مؤشر زغرب المعزز- مؤشرا زغرب المعاد صياغته الأول والثاني- مؤشر عدم انتظام الحواف- مؤشر استقرار درجة الحافة- متفرعة بورفيرين الزنك (DPZ_n)).

Abstract. This study is focused on the computation and investigation of some degree-based topological indices of dendrimer skeletons. The traditional as well as recently introduced indices are considered, including the Augmented Zagreb Index, the First and Second Reformulated Zagreb Indices, the Edge Irregularity Index, and the Degree Edge Stability Index. Particularly, the study applies these indices to investigate the Zinc Porphyrin dendrimer, represented as DPZ_n, to analyze their structural as well as mathematical characteristics.

1. Introduction

Let G be connected and simple graph that can be represented by the ordered pair (V(G), E(G)), where (V(G)) is the set of vertices of G and each element inside (V(G)) is referred to as a vertex or node. Similarly, (E(G)) represents the set of edges of G, and each "edge" or "line" denotes an element in (E(G)). Chemistry researchers now have access to a variety of extremely powerful analysis techniques thanks to chemical graph theory. Among the most important are graph-based molecular polynomials, structural indices, and molecular topological characteristics. Numerous chemical compounds and materials can be represented by molecular graphs, allowing for the examination of key theoretical characteristics [1]. Dendrimers are widely applied in chemical and biomedical research due to their capability of being conjugated with an array of chemical species on the surface, including dye molecules, target agents, affinity ligands, imaging compounds, radio ligands, and drugs. The multivalence of their highly branched structure promotes multivalent interaction where more than one active agent can bind simultaneously. The hydrophobic core of dendrimers further enables photochemical reactions and targeted drug delivery under specific conditions. Carboxylic acid or phenol-terminated water-soluble dendrimers have proved to be highly successful in therapy, allowing for the drug and targeting molecule delivery with fewer side effects on non-drug molecules. Being capable of carrying out several tasks, dendrimers—such as the Zinc Porphyrin dendrimer—have been the focal point of intense scientific inquiry [2-8]. Graph theory offers a useful mathematical framework for researching

and analyzing such intricate chemical structures. In this case, a molecular graph is employed to represent atoms as vertices and bonds as edges to visualize and quantify structural properties. It is an application of the topological school of mathematical chemistry, through which topological indices can be calculated that identify important structural and chemical properties of dendrimers. In the following sections, we calculate such indices for the Zinc Porphyrin dendrimer as its shown in figure 1.1:

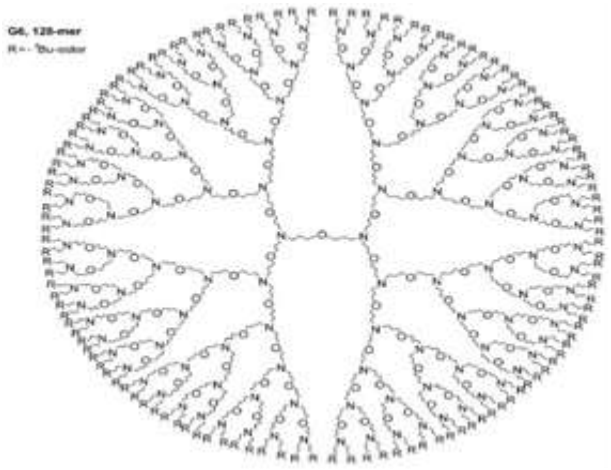

Figure 1: dendrimers (DPZn) is also known as Zinc Porphyrin.

In chemical graph theory, topological indices are useful instruments that let researchers analyze and measure molecular graphs in a systematic and insightful manner. Without requiring any substantial quantum chemical computations, topological indices are commonly employed to forecast the physicochemical characteristics, bioactivities, and reactivity of chemical compounds [9].
In (2013) N. E. Arif, studied Graph Polynomials and Topological Indices of Some Dendrimers, [10]. In (2016) M. N. Husin, R. Hasni, N. E. Arif, and M. Imran, studied On topological indices of certain families of Nano star dendrimers, [11]. In (2023) A. S. Majeed and N. E. Arif, studied topological indices of certain neutrosophic graphs. [12]. 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. [13]. 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, [14].

2. Preliminaries

In mathematical chemistry, graph theory provides a vital structure for modeling and analyzing chemical compounds. Its most powerful application is possibly in the construction of molecular graphs. the symbolic forms allow researchers to apply mathematical tools to uncover chemical, physical, and biological properties of compounds. Among the numerous graph-based descriptors, topological indices and graph polynomials play a central role. They are quantitative parameters that encapsulate structural information and are used widely in Quantitative Structure-Activity Relationship (QSAR) and Quantitative Structure-Property Relationship (QSPR) studies. Dendrimers, and indeed Zinc Porphyrin Dendrimers (DPZn), as it mentions are a family of highly branched, tree-like macromolecules that have been applied in drug delivery, imaging, catalysis, and photodynamic therapy [15]. Their regular and periodic nature makes them ideal candidates for study with graph-theoretic methods. We focus in this thesis on the study of degree-based

topological polynomials of DPZn using tools such as the Augmented Zagreb polynomial, the 1st and 2nd Reformulated Zagreb polynomials, and the Edge Irregularity polynomial and Degree Edge Stability polynomial. These polynomials provide compact and clear formulas that express degree-based interaction of atoms in the molecular structure of the dendrimer. So in (2010) B. Furtula, A. Graovac, and D. Vukićević, define Augmented Zagreb Index [16] as:

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

Respectively.

Augmented Zagreb Index help us to define the Augmented Zagreb polynomial, In (2009) H. Fath‐Tabar, define Zagreb Polynomials and PI Indices of Some Nanostructures Digest J. Nanomater. Biostructures [17].

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

Also, First Reformulated Zagreb Index was defining in (2017) N. De, Computing Reformulated First Zagreb Index of Some Chemical Graphs [18] define as:

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

Respectively.

First Reformulated Zagreb Indices assist us in defining first reformulated Zagreb polynomial, in (2004) A. Miličević, S. Nikolić, N. Trinajstić, and G. Kovačević, work On reformulated Zagreb indices," Mol. Divers [19].

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

Second Reformulated Zagreb Index was defining in (2017) N. De, Computing Reformulated First Zagreb Index of Some Chemical Graphs [18] define as:

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

Than,

Second Reformulated Zagreb Index enable us to characterize in defining second reformulated Zagreb polynomial, in (2004) A. Miličević, S. Nikolić, N. Trinajstić, and G. Kovačević, work On reformulated Zagreb indices," Mol. Divers [19].

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

The Edge Irregularity Index of graph G was defining in (2015) by H. S. Abdo and D. M. Dimitrov, [20] as:

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

And,

The Edge Irregularity Polynomial of graph G was defining in (2016) by H. Abdo, N. Cohen & D. Dimitrov, "On the irregularity of some molecular structures" [21] as:

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

The Degree Edge Stability Index of graph G was defining in (2021) by J. Chen, S. Li, and W. Wang, [22] as:

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

Finally,

In (2022) by M. Imran and M. Riaz the degree edge stability polynomial of graph G [23], was defined as:

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

3. Augmented Zagreb, First and second Reformulated Zagreb, Edge Irregularity and Degree Edge Stability 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 section will deal with computing some polynomials for Zinc Porphyrin dendrimer (DPZ_n) [15].

Proposition 3.1: It considered the type of dendrimer (DPZ_n) then:

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

2. The size of (DPZ_n) is $105 * n - 11$. See figure.1:

(DPZ_n) strictures contain three types of edges based on degree of end vertices of each as given in table 3.1.

(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

Table 3.1: Graph of the stretcher (DPZ_n).

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

$$\mathrm{AZP}(\mathrm{DPZ}_n) = 8 * 2^n * X^{\frac{729}{64}} + 56 * 2^n * X^8 + 4 * X^{\frac{1728}{125}} - 16 * X^{\frac{726}{64}} - 20\,X^8$$

Proof*:* The edge set of Zinc Porphyrin dendrimer (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.

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

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

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

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

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

$$= \sum_{sv\in E_1(G)} X^{(\frac{d(s)*d(v)}{d(s)+d(v)-2})^3} + \sum_{sv\in E_2(G)} X^{(\frac{d(s)*d(v)}{d(s)+d(v)-2})^3} + \sum_{sv\in E_3(G)} X^{(\frac{d(s)*d(v)}{d(s)+d(v)-2})^3}$$
$$+\sum_{sv\in E_4(G)} X^{(\frac{d(s)*d(v)}{d(s)+d(v)-2})^3}$$

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

$$AZP(DPZ_n, X) = 8*2^n*X^{\frac{729}{64}} + 56*2^n*X^8 + 4*X^{\frac{1728}{125}} - 16*X^{\frac{726}{64}} - 20X^8.$$

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

$$AZP(DPZ_n) = 64*2^n - 231.95.$$

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.

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

$$\frac{d}{d(x)}[AZP(DPZ_n, X)]_{x=1} =$$
$$8*2^n*X^{\frac{729}{64}} + 56*2^n*X^8 + 4*X^{\frac{1728}{125}} - 16*X^{\frac{726}{64}} - 20X^8.$$

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

$$AZI(DPZ_n, X) = 64*2^n - 231.95.$$

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

$$RM_1(DPZ_n) = (16*2^n-4)X^8 + (40*2^n-16)X^{27} + (8*2^n-16)X^{64} + 4*X^{125}.$$

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 $sv \in E\ (DPZ_n)$.

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

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

$|E_4(DPZ_n)|$ includes4 edges of type s, v s.t $d_{(s)} = 3$, $d_{(v)} = 4$, where $sv \in E\ (DPZ_n)$.

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

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

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

$$RM_1(DPZ_n, X) = (16 * 2^n - 4)\ X^8 + (40 * 2^n - 16)X^{27} + (8 * 2^n - 16)X^{64} + 4 * X^{125}.$$

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

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

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:

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

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 **:**

$RM_2(DPZ_n) =$
$(16 * 2^n - 4)X^8 + (40 * 2^n - 16)X^{18} + (8 * 2^n - 16)X^{36} + 4X^{60}.$

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.

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

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

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

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

$sv \in E(DPZ_n)$.

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

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

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

$RM_2(DPZ_n, X) =$
$(16 * 2^n - 4)X^8 + (40 * 2^n - 16)X^{18} + (8 * 2^n - 16)X^{36} + 4X^{60}).$

Corollary 3.1.3: Let n ∈ N, then the 2nd Reformulated Zagreb index of (DPZ_n) is given as **:**

$$RM_2(DPZ_n) = 1136 * 2^n - 656.$$

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 (DPZ_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 (DPZ_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 (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.

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

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

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

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

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

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

$= (16*2^n-4)X^{|\,2-2|}+(40*2^n-16)\,X^{|\,2-3|}+$
$(8*2^n-16)\,X^{|\,3-3|}+(4)X^{|\,3-4|}$
$IR\,(\mathrm{DPZ}_n, X) = (24*2^n-20)+(40*2^n-12)X.$

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

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

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:

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

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

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

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

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

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.

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

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

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

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

$$DS\ (\mathrm{DPZ}_n)| = \sum_{sv \in \mathrm{E(G)}} X^{(d_{(u)} - d_{(v)})^2}$$

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

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

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

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

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

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:

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

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

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

4. Conclusion

This study contributes to the growing intersection of mathematics and chemistry by exploring the topological properties of molecular structures through graph theoretical tools. By focusing on zinc porphyrins dendrimer we computed novel polynomial expressions and evaluated several prominent degree-based topological indices. These include the Augmented Zagreb Index (AZI), the First and Second Reformulated Zagreb Indices (RM_1 and RM_2), the Edge Irregularity Index, and the Degree-Based Stability Index. The derived polynomial forms for each index enabled more accurate modeling of molecular connectivity and branching shapes in different generations of dendrimers. In total, this work enriches the theoretical foundation for dendritic molecules research using graph polynomials and topological indices, and opens up new directions for future research in materials science and structural chemistry.

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