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Computing Generalized Zagreb Indices of Dendrimers for Drug Delivery Applications

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ABSTRACT

In the interdisciplinary fields of mathematical chemistry and chemical graph theory, molecular descriptors serve as graph invariants that project the physicochemical attributes of organic molecules. Within this framework, vertices and edges symbolize atoms and their connecting chemical bonds respectively. Dendrimers, a class of polymers widely recognized as fundamental building blocks in commercial nanotechnology, exhibit immense potential in drug delivery applications. The dynamic nature of their structural chemistry permits topological index manipulations, enabling the precise tailoring of dendrimers to meet the desired characteristics of target carrier vehicles. This study primarily focuses on the computation of the generalized Zagreb indices, a subset of degree:-based topological indices that are fundamentally defined considering the degrees of vertices and edges in a graph. The computed generalized Zagreb indices subsequently facilitate the determination of other degree-based topological indices. In addition, this paper provides a comprehensive graphical comparison of the topological indices of these dendrimers, thereby contributing to the broader understanding of their structural properties.

1. INTRODUCTION

1.1 Significance of topological indices

Topological indices, pivotal tools in chemical graph theory, find their extensive applications in chemical and pharmaceutical engineering to investigate the properties of substances and medications. Introduced initially by Wiener [1] in 1947 to compare the boiling points of select alkane isomers, topological indices have expanded, with over 3000 registered in chemical databases to date. The global populace, driven by concerns of health and well-being and the threats of detrimental lifestyle choices and dietary habits, exhibits a growing need for effective disease prevention and treatment strategies. As the proliferation of novel diseases necessitates innovative curative treatments, it becomes crucial to formulate medicines with the precise chemical composition that offers optimal therapeutic outcomes. Herein, topological indices of specific chemical compounds, derived in consideration of graph theory, assist in evaluating and producing effective medications.

Topological indices are utilized to construct quantitative structure-activity relationship (QSAR) models even in the absence of prior receptor knowledge. These models predict properties such as stability, vaporization, enthalpy, boiling point, toxicity, and a plethora of other physical, chemical, and biological characteristics. These indices serve as vital tools in correlating graph structure with physical and chemical properties and conducting QSAR/QSPR analyses, with their applications extensively documented in previous research [2-5]. Over time, numerous indices, based on underlying graph properties like degree, distance, and spectrum, have been developed and generalized. Topological indices find broad applications in multiple fields such as chemistry, drug delivery, toxicology, and complex network theory, where they characterize various network structural attributes [6]. The development of these indices proves instrumental in establishing quantitative structure-activity relationships for a variety of derivative chemical compounds.

1.2 Implications of dendrimers

Dendrimers, nanoscopic compounds characterized as monodisperse macromolecules, are generally perceived as homogenous [7]. Their discovery by Donald Tomalia and his team in the 1980s revolutionized the field of medicinal chemistry. These compounds, initially synthesized divergently by Fritz Vogtle in 1978, were known as "Cascade molecules" [8]. The connection or entrapment of pharmaceuticals and bioactive chemicals in the dendrimer structure can potentially enhance significant biological features like bioavailability, solubility, and selectivity. Owing to their capability to transport drugs by encapsulating them within the dendritic structure or carrying them on surfaces via electrostatic forces or covalent attachment, dendrimers hold a significant position in medicine.

Dendrimers find potential applications in numerous diagnostic and pharmacological areas, especially where drug

toxicity is high or solubility, bioavailability, and permeability are low [9, 10]. Their use can augment drug delivery, enhance bioavailability, and mitigate side effects in anticancer, antiretroviral, and gene therapy drug delivery systems. Dendrimers, characterized by monodispersity, nanoparticle size and shape, viscosity, high aqueous solubility, high non-planar solubility, and low compressibility, find extensive applications in drug discovery, drug delivery, and chemical toxicology. Dendrimers significantly contribute to applications such as anticancer drug delivery, solubility enhancement, cellular delivery, industrial processes, gene transfection, nanopowders, diagnostics, coating agents, dendritic catalysts and enzymes, contrast agents, and targeted drug delivery and controlled drug release [11].

Advancements in drug administration methodologies have significantly enhanced the safety and efficacy of therapeutic drug delivery. The burgeoning biopharmaceutical industry has fostered the development of novel therapeutic classes for prevalent diseases like oncology and diabetes, thereby paving the way for the creation of improved drug delivery systems. These systems are categorized based on their administration route, which can be oral, injectable, ocular, pulmonary, topical, implantable, nasal, or transmucosal. Over the past decade, dendrimers have emerged as potential nanocarriers for a wide spectrum of drugs, including anti-inflammatory, antibacterial, and anticancer medications, across various drug administration routes.

Employed as carriers or scaffolds in diagnostics and therapy, dendrimers offer several advantages. The notable properties of these nanotubes include cellular membrane penetration, an increased drug load, and a correlation between nanotubes and drug design, as discussed by Lakshmi and Parvathi [12]. These intriguing qualities have piqued the interest of drug discovery experts, particularly in studying the dendrimers' effects on prion diseases, Alzheimer's diseases, inflammation, human immunodeficiency virus (HIV), herpes simplex virus (HSV), bacteria, and cancer [13].

In this research study, we calculate the generalized Zagreb indices for certain dendrimers, and derive some degree-based topological indices, including the First and Second Zagreb indices, the Forgotten Topological Index, the Redefined Zagreb Index, and the Symmetric Division Deg Index. For a connected graph H with a vertex set V(H) and an edge set E(H), if two vertices p and q are adjacent, the edge connecting them is denoted by pq. The generalized Zagreb index, introduced by Azari and colleagues in 2011, is based on well-known vertex degree-based topological indices and is defined as follows [14]:

$$Z_{a,b}(H) = d_H(p)^a d_H(q)^b + d_H(p)^b d_H(q)^a$$

The Zagreb index was developed in 1972 by Gutman and Trinajstic "to study the total π electron energy ($\in$) of carbon atoms" and is defined as [15]:

$$M_1(G) = \sum_{pq \in E(H)} [\deg(p) + \deg(q)]$$
$$M_2(G) = \sum_{pq \in E(H)} [\deg(p) . \deg(q)]$$

The Forgotten topological index was proposed by Gutman and Furtula in the year 2015 and is defined as [16]:

$$F(H) = \sum_{pq \in E(H)} [deg(p)^2 + deg(q)^2]$$

The Redefined third Zagreb index was proposed by Ranjini et al. in 2013 and is defined as [17]:

$$ReZM(H) = \sum_{pq \in E(H)} deg_H(p)\, deg_H(q)[deg_H(p) + deg_H(q)]$$

The Symmetric Division Deg index of a graph was proposed by Furtula et al. in the year 2018. It is one of discrete Adriatic indices that showed good predictive properties on the testing sets provided by International Academy of Mathematical Chemistry [18]:

$$SDD(H) = \sum_{pq \in E(H)} \left[\frac{d_H(p)}{d_H(q)} + \frac{d_H(q)}{d_H(p)}\right]$$

Table 1 shows that all the topological index values that we discussed above in this paper are derived from (a, b) Zagreb index for some specific values *a* and *b* [19].

Table 1. Topological indices corresponding to (a, b)-Zagreb index

Topological Index	Corresponding (a, b)-Zagreb Index
First Zagreb index $M_1(H)$	$Z_{1,0}(H)$
Second Zagreb index $M_2(H)$	$\frac{1}{2}Z_{1,1}(H)$
Forgotten topological index $F(H)$	$Z_{2,0}(H)$
Redefined Zagreb index $ReZM(H)$	$Z_{2,1}(H)$
Symmetric division deg index $SDD(H)$	$Z_{1,-1}(H)$

2. RESULTS AND DISCUSSION

In this section, generalized Zagreb index is derived and investigated for some dendrimers, namely, polyacetal dendrimer, polyester dendrimer, polyamidoamine dendrimer, and Propyl Ether Emine dendrimer. In this paper illustrates the explicit formula for the topological indices and values are computed with the family of dendrimers. Initially, we find vertex degree for each dendrimer then we proceed with the edge partition to obtain the required result.

2.1 Structure of polyacetal dendrimer

The polyacetal dendrimer was first reported by Tomalia and Fréchet [20] in 2002. The acidic condition of this polymer results in linear Poly ethylene oxide (PEO) chains with low molecular weight. Due to its high water solubility, many peripheral hydroxyl groups, and acid-dependent degradation, this dendrimer is a suitable option for the construction of dendrimer-drug conjugates.

In this structure, the edge set has divided into five partitions as shown in the Figure 1, where $V(H)$ is the vertex set, and $d_H(p)$, $d_H(q)$ is the degree of the vertex of p and q.

$$E_1(H) = \{e = pq \in V(H); d_H(p) = 1, d_H(q) = 2\}$$
$$E_2(H) = \{e = pq \in V(H); d_H(p) = 1, d_H(q) = 3\}$$
$$E_3(H) = \{e = pq \in V(H); d_H(p) = 2, d_H(q) = 2\}$$
$$E_4(H) = \{e = pq \in V(H); d_H(p) = 2, d_H(q) = 3\}$$
$$E_5(H) = \{e = pq \in V(H); d_H(p) = 2, d_H(q) = 4\}$$

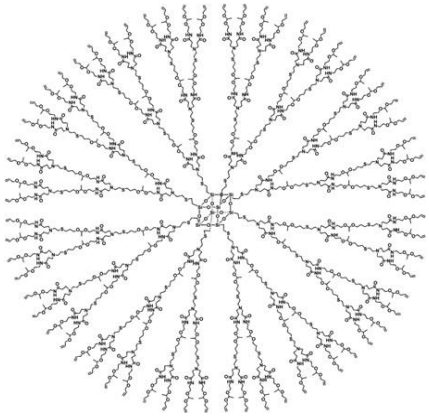

Figure 1. Structure of polyacetal dendrimer [20]

Note that the edge sets are given:

$$|E_1(H)| = 8 \cdot 2^n;$$
$$|E_2(H)| = 32 \cdot 2^n - 32;$$
$$|E_3(H)| = 128 \cdot 2^n - 128;$$
$$|E_4(H)| = 88 \cdot 2^n - 88;$$
$$|E_5(H)| = 32.$$

Theorem 2.1

The generalized Zagreb index of the polyacetal dendrimer is:

$$Z_{a,b}(H) = (8 \cdot 2^n)(2^a+2^b) + (32 \cdot 2^n - 32)(3^b + 3^a) + (128 \cdot 2^n - 128)(2^{a+b+1}) + (88 \cdot 2^n - 88)(2^a \cdot 3^b + 2^b \cdot 3^a) + 32(2^a \cdot 4^b + 2^b \cdot 4^a)$$

Proof

Using the definition of the generalized Zagreb index, then we have:

$$Z_{a,b}(H) = d_H(p)^a d_H(q)^b + d_H(p)^b d_H(q)^a = \sum_{pq \in E_1(H)} 1^a \cdot 2^b + 1^b \cdot 2^a + \sum_{pq \in E_2(H)} 1^a \cdot 3^b + 1^b \cdot 3^a + \sum_{pq \in E_3(H)} 2^a \cdot 2^b + 2^b \cdot 2^a + \sum_{pq \in E_4(H)} 2^a \cdot 3^b + 2^b \cdot 3^a + \sum_{pq \in E_5(H)} 2^a \cdot 4^b + 2^b \cdot 4^a$$

$$Z_{a,b}(H) = (8 \cdot 2^n)(1^a \cdot 2^b + 1^b \cdot 2^a) + (32 \cdot 2^n - 32)(1^a \cdot 3^b + 1^b \cdot 3^a) + (128 \cdot 2^n - 128)(2^a \cdot 2^b + 2^b \cdot 2^a) + (88 \cdot 2^n - 88)(2^a \cdot 3^b + 2^b \cdot 3^a) + 32(2^a \cdot 4^b + 2^b \cdot 4^a)$$

$$Z_{a,b}(H) = (8 \cdot 2^n)(2^a+2^b) + (32 \cdot 2^n - 32)(3^b + 3^a) + (128 \cdot 2^n - 128)(2^{a+b+1}) + (88 \cdot 2^n - 88)(2^a \cdot 3^b + 2^b \cdot 3^a) + 32(2^a \cdot 4^b + 2^b \cdot 4^a)$$

Hence the proof.

Corollary 2.2

Consider the generalized Zagreb index of polyacetal dendrimer, then we calculate the following indices are:

1. $M_1(H) = Z_{1,0}(H) = 1104 \cdot 2^n - 1272$
2. $M_2(H) = \frac{1}{2} Z_{1,1}(H) = 1152 \cdot 2^n - 880$
3. $F(H) = Z_{2,0}(H) = 2528 \cdot 2^n - 1848$
4. $ReZM(H) = Z_{2,1}(H) = 5120 \cdot 2^n - 3536$
5. $SDD(H) = \left(\frac{3440}{6}\right) 2^n - \left(\frac{2840}{6}\right)$

Proof

By theorem 2.1 using the result, and substituting the corresponding generalized Zagreb index, then we get the indices are following:

1. $M_1(H) = (8 \cdot 2^n)(2^a+2^b) + (32 \cdot 2^n - 32)(3^b + 3^a) + (128 \cdot 2^n - 128)(2^{a+b+1}) + (88 \cdot 2^n - 88)(2^a \cdot 3^b + 2^b \cdot 3^a) + 32(2^a \cdot 4^b + 2^b \cdot 4^a)$
$= (8 \cdot 2^n)(3) + (32 \cdot 2^n - 32)(4) + (128 \cdot 2^n - 128)(4) + (88 \cdot 2^n - 88)(5) + 32(6)$
$M_1(H) = Z_{1,0}(H) = 1104 \cdot 2^n - 1272$

2. $M_2(H) = \frac{1}{2} Z_{1,1}(H)$
$= (8 \cdot 2^n)(4) + (32 \cdot 2^n - 32)(6) + (128 \cdot 2^n - 128)(8) + (88 \cdot 2^n - 88)(12) + 32(16)$
$M_2(H) = \frac{1}{2} Z_{1,1}(H) = 1152 \cdot 2^n - 880$

3. $F(H) = Z_{2,0}(H)$
$= (8 \cdot 2^n)(5) + (32 \cdot 2^n - 32)(10) + (128 \cdot 2^n - 128)(8) + (88 \cdot 2^n - 88)(13) + 32(20)$
$F(H) = Z_{2,0}(H) = 2528 \cdot 2^n - 1848$

4. $ReZM(H) = Z_{2,1}(H)$
$= (8 \cdot 2^n)(6) + (32 \cdot 2^n - 32)(12) + (128 \cdot 2^n - 128)(16) + (88 \cdot 2^n - 88)(30) + 32(20)$
$ReZM(H) = Z_{2,1}(H) = 5120 \cdot 2^n - 3536$

5. $SDD(H) = Z_{1,-1}(H)$
$= (8 \cdot 2^n)\left(\frac{5}{2}\right) + (32 \cdot 2^n - 32)\left(\frac{10}{3}\right) + (128 \cdot 2^n - 128)(2) + (88 \cdot 2^n - 88)\left(\frac{13}{6}\right) + 32\left(\frac{5}{2}\right)$
$SDD(H) = Z_{1,-1}(H) = \left(\frac{3440}{6}\right) 2^n - \left(\frac{2840}{6}\right)$

Hence the proof.

2.2 Structure of polyester dendrimer

In 2009, Shen et al. reported [21, 22] the facile synthesis of alternating polyester dendrimers by sequential click-coupling of asymmetric monomers (2-[methacryloye)oxy]ethyl acrylate (MAEA) and cysteamine). Subsequently, they simplified the synthesis by using a β-cyclodextin core from which asymmetric alternating polyester dendrimers with high

molecular weight could be easily obtained without complicated purifications.

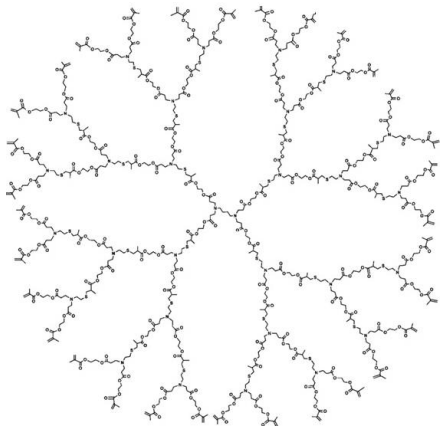

Figure 2. Structure of Polyester dendrimer [21, 22]

The edge sets are given below:

$$E_1(H) = \{e = pq \in V(H); d_H(p) = 1, d_H(q) = 2\}$$
$$E_2(H) = \{e = pq \in V(H); d_H(p) = 1, d_H(q) = 3\}$$
$$E_3(H) = \{e = pq \in V(H); d_H(p) = 2, d_H(q) = 2\}$$
$$E_4(H) = \{e = pq \in V(H); d_H(p) = 2, d_H(q) = 3\}$$
$$E_5(H) = \{e = pq \in V(H); d_H(p) = 3, d_H(q) = 3\}$$

The edge set $E_1(H)$ are given by:

$$|E_1(H)| = 2^{n+1},$$
$$|E_2(H)| = 12, 36, 84, and\ 12 \cdot 2^n - 12;$$
$$|E_3(H)| = 31, 87, 199, and\ 28 \cdot 2^n - 2;$$
$$|E_4(H)| = 22, 84, 166, and\ 22 \cdot 2^n - 22;$$
$$|E_5(H)| = 4, 12, 28, and\ 4 \cdot 2^n - 4.$$

where, *n* is the number of growth of generations.

Theorem 2.3

The generalized Zagreb index of the polyester dendrimer as shown in Figure 2 is given by:

$$\begin{aligned} Z_{a,b}(H) = {} & 2^{n+1}(2^b + 2^a) \\ & +(12 \cdot 2^n - 12)(3^b + 3^a) + \\ & (28 \cdot 2^n - 25)(2^{a+b+1}) + \\ & (22 \cdot 2^n - 22)(2^a \cdot 3^b + 2^b \cdot 3^a) + \\ & (4 \cdot 2^n - 4)(3^{a+b+1}) \end{aligned}$$

Proof

By using the definition of the generalized Zagreb index, we have:

$$\begin{aligned} Z_{a,b}(H) &= \sum_{pq \in E(H)} d_H(p)^a d_H(q)^b + d_H(p)^b d_H(q)^a \\ &= \sum_{pq \in E_1(H)} 1^a \cdot 2^b + 1^b \cdot 2^a + \\ & \sum_{pq \in E_2(H)} 1^a \cdot 3^b + 1^b \cdot 3^a + \\ & \sum_{pq \in E_3(H)} 2^a \cdot 2^b + 2^b \cdot 2^a + \\ & \sum_{pq \in E_4(H)} 2^a \cdot 3^b + 2^b \cdot 3^a + \\ & \sum_{pq \in E_5(H)} 3^a \cdot 3^b + 3^b \cdot 3^a \end{aligned}$$

$$\begin{aligned} Z_{a,b}(H) = {} & (2^{n+1})(1^a \cdot 2^b + 1^b \cdot 2^a) + \\ & (12 \cdot 2^n - 12)(1^a \cdot 3^b + 1^b \cdot 3^a) \\ & +(28 \cdot 2^n - 25)(2^a \cdot 2^b + 2^b \cdot 2^a) + \\ & (22 \cdot 2^n - 22)(2^a \cdot 3^b + 2^b \cdot 3^a) + \\ & 32\ (4 \cdot 2^n - 4)(3^a \cdot 3^b + 3^b \cdot 3^a) \end{aligned}$$

$$\begin{aligned} Z_{a,b}(H) = {} & 2^{n+1}(2^b + 2^a) + \\ & (12 \cdot 2^n - 12)(3^b + 3^a) + \\ & (28 \cdot 2^n - 25)(2^{a+b+1}) + \\ & (22 \cdot 2^n - 22)(2^a \cdot 3^b + 2^b \cdot 3^a) + \\ & (4 \cdot 2^n - 4)(3^{a+b+1}) \end{aligned}$$

Hence the proof.

Corollary 2.4

Consider the generalized Zagreb index of the polyester dendrimer, then we compute the indices:

$$1.\ M_1(H) = Z_{1,0}(H) = 312 \cdot 2^n - 294$$
$$2.\ M_2(H) = \frac{1}{2} Z_{1,1}(H) = 338 \cdot 2^n - 322$$
$$3.\ F(H) = Z_{2,0}(H) = 1146 \cdot 2^n - 1112$$
$$4.\ ReZM(H) = Z_{2,1}(H) = 1588 \cdot 2^n - 1528$$
$$5.\ SDD(H) = Z_{1,-1}(H) = \left(\frac{964}{6}\right) 2^n - \left(\frac{898}{6}\right)$$

Proof

By theorem 2.3 using the result then we get the indices as follows:

$$\begin{aligned} 1.\ M_1(H) = {} & 2^{n+1}(2^b + 2^a) + (12 \cdot 2^n - 12)(3^b + 3^a) \\ & + (28 \cdot 2^n - 25)(2^{a+b+1}) + \\ & (22 \cdot 2^n - 22)(2^a \cdot 3^b + 2^b \cdot 3^a) + \\ & (4 \cdot 2^n - 4)(3^{a+b+1}) \end{aligned}$$

$$\begin{aligned} M_1(H) = {} & Z_{1,0}(H) \\ & = 2^{n+1}(3) + (12 \cdot 2^n - 12)(4) + \\ & (28 \cdot 2^n - 25)(4) + (22 \cdot 2^n - 22)(5) + \\ & (4 \cdot 2^n - 4)(9) \end{aligned}$$

$$M_1(H) = Z_{1,0}(H) = 312 \cdot 2^n - 294$$

$$\begin{aligned} 2.\ M_2(H) = {} & 2^{n+1}(4) + (12 \cdot 2^n - 12)(6) + \\ & (28 \cdot 2^n - 25)(8) + (22 \cdot 2^n - 22)(12) + \\ & (4 \cdot 2^n - 4)(27) \end{aligned}$$

$$M_2(H) = \frac{1}{2} Z_{1,1}(H) = 338 \cdot 2^n - 322$$

$$\begin{aligned} 3.\ F(H) = {} & 2^{n+1}(5) + (12 \cdot 2^n - 12)(12) + \\ & (28 \cdot 2^n - 25)(8) + (22 \cdot 2^n - 22)(30) + \\ & (4 \cdot 2^n - 4)(27) \end{aligned}$$

$$F(H) = Z_{2,0}(H) = 1146 \cdot 2^n - 1112$$

$$\begin{aligned} 4.\ ReZM(H) = {} & 2^{n+1}(6) + (12 \cdot 2^n - 12)(12) + \\ & (28 \cdot 2^n - 25)(16) + \\ & (22 \cdot 2^n - 22)(30) + (4 \cdot 2^n - 4)(81) \end{aligned}$$

$$ReZM(H) = Z_{2,1}(H) = 1588 \cdot 2^n - 1528$$

$$\begin{aligned} 5.\ SDD(H) = {} & 2^{n+1}\left(\frac{5}{2}\right) + (12 \cdot 2^n - 12)\left(\frac{10}{3}\right) + \\ & (28 \cdot 2^n - 25)(2) + (22 \cdot 2^n - 22)\left(\frac{13}{6}\right) + \\ & (4 \cdot 2^n - 4)(3) \end{aligned}$$

$$SDD(H) = Z_{1,-1}(H) = \left(\frac{964}{6}\right) 2^n - \left(\frac{898}{6}\right)$$

Hence the proof.

3. STRUCTURE OF POLYAMIDOAMINE DENDRIMER

The branching architecture of the poly-amidoamine dendrimer is considered for its characterization. Donald A. Tomalia invented PAMAM (polyamidoamine) in 1985 as a new family of polymers known as starburst polymers [23, 24]. Professor Tomalia's significant contribution paved the way for a new study field utilizing nanotechnological methods. Since then, PAMAM has been used by many researchers for various purposes, including biomedical applications.

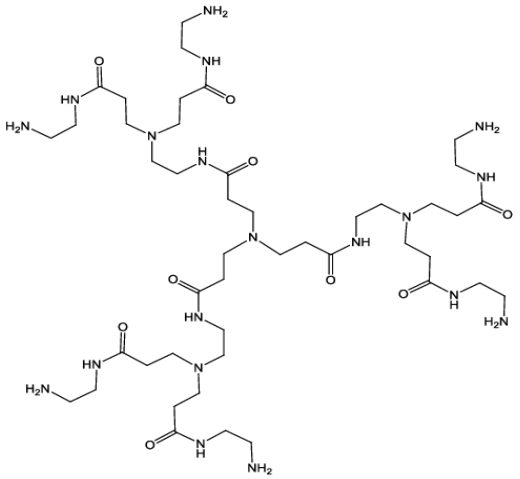

Figure 3. Structure of polyamidoamine dendrimer [23, 24]

The edge sets are given below:

$$E_1(H) = \{e = pq \in V(H); d_H(p) = 1, d_H(q) = 2\}$$
$$E_2(H) = \{e = pq \in V(H); d_H(p) = 1, d_H(q) = 3\}$$
$$E_3(H) = \{e = pq \in V(H); d_H(p) = 2, d_H(q) = 2\}$$
$$E_4(H) = \{e = pq \in V(H); d_H(p) = 2, d_H(q) = 3\}$$

Note that:

$$|E_1(H)| = \tfrac{3}{2} \cdot 2^{2n};$$
$$|E_2(H)| = 3 \cdot 2^{2n} - 3,$$
$$|E_3(H)| = 9 \cdot 2^{2n} - 9,$$
$$|E_4(H)| = 9 \cdot 2^{2n} - 6.$$

Theorem 2.5

The generalized Zagreb index of the polyamidoamine dendrimer as shown in Figure 3 is:

$$Z_{a,b}(H) = \frac{3}{2}(2^{2n})(2^b + 2^a) + (3 \cdot 2^{2n} - 3)(3^b + 3^a) + (9 \cdot 2^{2n} - 9)(2^{a+b+1}) + (9 \cdot 2^{2n} - 6)(2^a \cdot 3^b + 2^b \cdot 3^a)$$

Proof

By using the definition of (a, b)-Zagreb index, we have:

$$Z_{a,b}(H) = \sum_{pq \in E(H)} d_H(p)^a d_H(q)^b + d_H(p)^b d_H(q)^a$$
$$= \sum_{pq \in E_1(H)} 1^a \cdot 2^b + 1^b \cdot 2^a + \sum_{pq \in E_2(H)} 1^a \cdot 3^b + 1^b \cdot 3^a + \sum_{pq \in E_3(H)} 2^a \cdot 2^b + 2^b \cdot 2^a + \sum_{pq \in E_4(H)} 2^a \cdot 3^b + 2^b \cdot 3^a$$

$$Z_{a,b}(H) = \left(\frac{3}{2}\right)(2^{2n})(1^a \cdot 2^b + 1^b \cdot 2^a) + (3 \cdot 2^{2n} - 3)(1^a \cdot 3^b + 1^b \cdot 3^a) + (9 \cdot 2^{2n} - 9)(2^a \cdot 2^b + 2^b \cdot 2^a) + (9 \cdot 2^{2n} - 6)(2^a \cdot 3^b + 2^b \cdot 3^a)$$

$$Z_{a,b}(H) = \frac{3}{2}(2^{2n})(2^b + 2^a) + (3 \cdot 2^{2n} - 3)(3^b + 3^a) + (9 \cdot 2^{2n} - 9)(2^{a+b+1}) + (9 \cdot 2^{2n} - 6)(2^a \cdot 3^b + 2^b \cdot 3^a)$$

Hence the proof.

Corollary 2.6

Consider the generalized Zagreb index of the polyamidoamine dendrimer, then we compute the indices that are:

1. $M_1(H) = Z_{1,0}(H) = \left(\frac{125}{2}\right) \cdot 2^{2n} - 78$
2. $M_2(H) = \frac{1}{2} Z_{1,1}(H) = 204 \cdot 2^{2n} - 162$
3. $F(H) = Z_{2,0}(H) = 453 \cdot 2^{2n} - 180$
4. $ReZM(H) = Z_{2,1}(H) = 459 \cdot 2^{2n} - 360$
5. $SDD(H) = Z_{1,-1}(H) = \left(\frac{205}{4}\right) 2^{2n} - 41$

Proof

By theorem 2.3 using the result then we get the indices as follows:

1. $M_1(H) = \frac{3}{2}(2^{2n})(2^b + 2^a) + (3 \cdot 2^{2n} - 3)(3^b + 3^a) + (9 \cdot 2^{2n} - 9)(2^{a+b+1}) + (9 \cdot 2^{2n} - 6)(2^a \cdot 3^b + 2^b \cdot 3^a)$

$$M_1(H) = Z_{1,0}(H) = \left(\frac{3}{2} \cdot 2^{2n}\right)(3) + (3 \cdot 2^{2n} - 3)(4) + (9 \cdot 2^{2n} - 9)(4) + (9 \cdot 2^{2n} - 6)(5)$$
$$M_1(H) = Z_{1,0}(H) = \left(\frac{125}{2}\right) \cdot 2^{2n} - 78$$

2. $M_2(H) = \left(\frac{3}{2} \cdot 2^{2n}\right)(4) + (3 \cdot 2^{2n} - 3)(6) + (9 \cdot 2^{2n} - 9)(8) + (9 \cdot 2^{2n} - 6)(12)$

$$M_2(H) = \tfrac{1}{2} Z_{1,1}(H) = 204 \cdot 2^{2n} - 162$$

3. $F(H) = Z_{2,0}(H) = \left(\frac{3}{2} \cdot 2^{2n}\right)(5) + (3 \cdot 2^{2n} - 3)(10) + (9 \cdot 2^{2n} - 9)(8) + (9 \cdot 2^{2n} - 6)(13)$

$$F(H) = Z_{2,0}(H) = 453 \cdot 2^{2n} - 180$$

4. $ReZM(H) = \left(\frac{3}{2} \cdot 2^{2n}\right)(5) + (3 \cdot 2^{2n} - 3)(12) + (9 \cdot 2^{2n} - 9)(16) + (9 \cdot 2^{2n} - 6)(30)$

$$ReZM(H) = Z_{2,1}(H) = 459 \cdot 2^{2n} - 360$$

5. $SDD(H) = \left(\frac{3}{2} \cdot 2^{2n}\right)\left(\frac{5}{2}\right) + (3 \cdot 2^{2n} - 3)\left(\frac{10}{3}\right) + (9 \cdot 2^{2n} - 9)(2) + (9 \cdot 2^{2n} - 6)\left(\frac{13}{6}\right)$

$$SDD(H) = Z_{1,-1}(H) = \left(\frac{205}{4}\right)2^{2n} - 41$$

Hence the proof.

3.1 Structure of propyl ethine emine dendrimer

The propyl ether-amine dendrimer synthesized by iterative synthesis cycles with two reductions is considered to facilitate the synthesis and purification of higher-generation dendrimers. Propyl Ether Emine dendrimers help to mediate an effective gene delivery function. They exhibit significantly reduced toxicites, over a broad concentration range. The photophysical properties of these dendrimers are studied consist of either alcohols, amines, carboxylic acids, esters or nitriles at their peripheries. It is a series of dendrimers which are synthesized by iterative synthetic cycles of two reductions and Michael addition reactions [25].

$$E_1(H) = \{e = pq \in V(H); d_H(p) = 1, d_H(q) = 2\}$$
$$E_2(H) = \{e = pq \in V(H); d_H(p) = 2, d_H(q) = 2\}$$
$$E_3(H) = \{e = pq \in V(H); d_H(p) = 2, d_H(q) = 3\}$$

Note that the number of edge sets is

$$|E_1(H)| = 2 \cdot 2^n,$$
$$|E_2(H)| = 16 \cdot 2^n - 18,$$
$$|E_3(H)| = 6 \cdot 2^n - 6.$$

Here 'n' is the number of growth of generations.

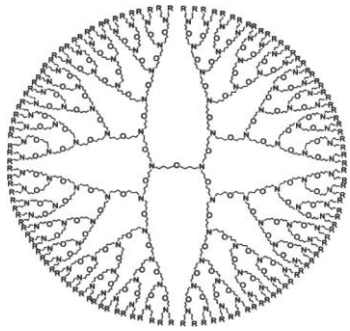

Figure 4. Structure of propylether emine dendrimer [25]

Theorem 2.7

The generalized Zagreb index of the propyl ether emine dendrimer as shown in Figure 4 is

$$Z_{a,b}(H) = (2 \cdot 2^n)(2^b + 2^a) + (16 \cdot 2^n - 18)(2^{a+b+1}) + (6 \cdot 2^n - 6)(2^a \cdot 3^b + 2^b \cdot 3^a)$$

Proof

$$Z_{a,b}(H) = \sum_{pq \in E(H)} d_H(p)^a d_H(q)^b + d_H(p)^b d_H(q)^a$$
$$= \sum_{pq \in E_1(H)} 1^a \cdot 2^b + 1^b \cdot 2^a + \sum_{pq \in E_2(H)} 2^a \cdot 2^b + 2^b \cdot 2^a + \sum_{pq \in E_3(H)} 2^a \cdot 3^b + 2^b \cdot 3^a$$
$$Z_{a,b}(H) = (2 \cdot 2^n)(1^a \cdot 2^b + 1^b \cdot 2^a) + (16 \cdot 2^n - 18)(2^a \cdot 2^b + 2^b \cdot 2^a) + (6 \cdot 2^n - 6)(2^a \cdot 3^b + 2^b \cdot 3^a)$$
$$Z_{a,b}(H) = (2 \cdot 2^n)(1^a \cdot 2^b + 1^b \cdot 2^a) + (16 \cdot 2^n - 18)(2^{a+b+1}) + (6 \cdot 2^n - 6)(2^a \cdot 3^b + 2^b \cdot 3^a)$$

Hence the proof.

Corollary 2.8

Consider the generalized Zagreb index of poly ether emine dendrimer, then we compute the indices are as follows:

1. $M_1(H) = Z_{1,0}(H) = 100 \cdot 2^n - 102$
2. $M_2(H) = \frac{1}{2}Z_{1,1}(H) = 104 \cdot 2^n - 108$
3. $F(H) = Z_{2,0}(H) = 216 \cdot 2^n - 222$
4. $ReZM(H) = Z_{2,1}(H) = 448 \cdot 2^n - 468$
5. $SDD(H) = Z_{1,-1}(H) = 50 \cdot 2^n - 49$

Proof

Using theorem 2.7 the result will apply, then we get the indices are as follows:

1. $M_1(H) = (2 \cdot 2^n)(1^a \cdot 2^b + 1^b \cdot 2^a) + (16 \cdot 2^n - 18)(2^{a+b+1}) + (6 \cdot 2^n - 6)(2^a \cdot 3^b + 2^b \cdot 3^a)$
$M_1(H) = (2 \cdot 2^n)(2) + (16 \cdot 2^n - 18)(4) + (6 \cdot 2^n - 6)(5)$
$M_1(H) = Z_{1,0}(H) = 100 \cdot 2^n - 102$

2. $M_2(H) = (2 \cdot 2^n)(4) + (16 \cdot 2^n - 18)(8) + (6 \cdot 2^n - 6)(12)$
$M_2(H) = \frac{1}{2}Z_{1,1}(H) = 104 \cdot 2^n - 108$

3. $F(H) = (2 \cdot 2^n)(4) + (16 \cdot 2^n - 18)(8) + (6 \cdot 2^n - 6)(13)$
$F(H) = Z_{2,0}(H) = 216 \cdot 2^n - 222$

4. $ReZM(H) = (2 \cdot 2^n)(6) + (16 \cdot 2^n - 18)(16) + (6 \cdot 2^n - 6)(30)$
$ReZM(H) = Z_{2,1}(H) = 448 \cdot 2^n - 468$

5. $SDD(H) = (2 \cdot 2^n)\left(\frac{5}{2}\right) + (16 \cdot 2^n - 18)(2) + (6 \cdot 2^n - 6)\left(\frac{13}{6}\right)$
$SDD(H) = Z_{1,-1}(H) = 50 \cdot 2^n - 49$

Hence the proof.

4. COMPARISON OF GRAPHICAL REPRESENTATION

The results gathered from the current study are of crucial importance for engineering applications. In this paper, several important chemical structures are considered, and using edge set partitioning and molecular graph structure analysis, the exact formulas of some important degree-based indices are computed for a few dendrimers such as polyacetal dendrimer, polyeser dendrimer, polyamidoamine dendrimer, and propyl ether emine dendrimer, as shown in the figure below. From Figure 5, it is observed that the values of all indices have increased but there is a decrease in the symmetric division deg index. Similar to Figure 6, it is noted that in Figure 7 and Figure 8 also there is an increase in the values of all indices while there is a decrease in the value of the symmetric division deg index.

The comparison of topological indices values of four dendrimers are tabulated in the below:

To get the topological index values for n=1 to 10, we first get the result of the generalized Zagreb Index of polyacetal dendrimer, Polyester dendrimer, Polyamidoamine dendrimer and Polyether Emine dendrimer by substituting these values. Then, we get the values from Table 2 to Table 5.

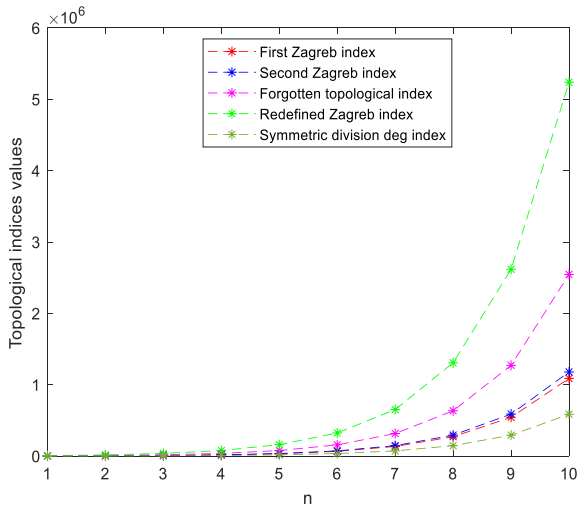

Figure 5. Graphical representation of polyacetal dendrimer

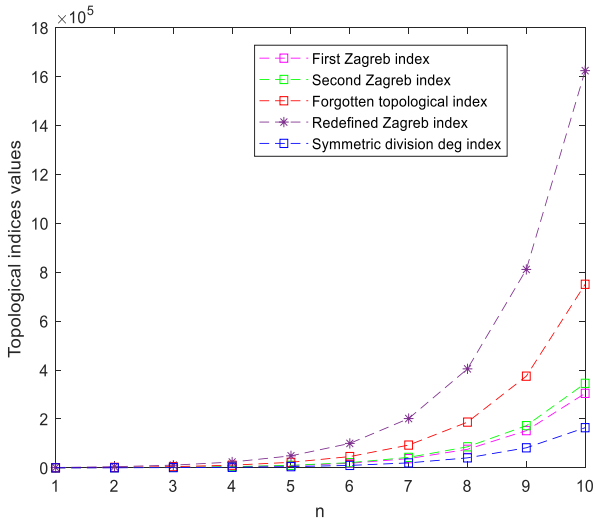

Figure 6. Graphical representation of polyester dendrimer

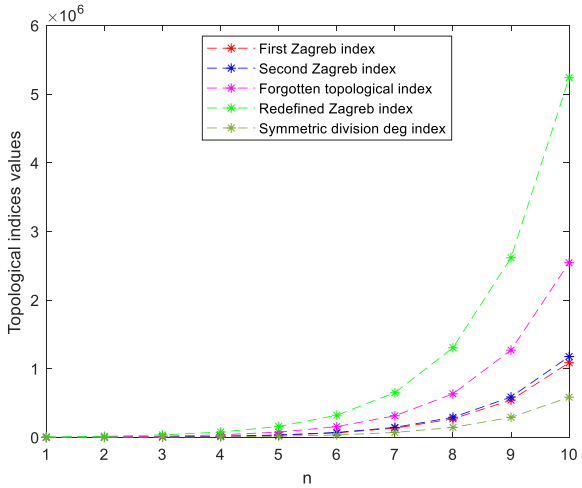

Figure 7. Graphical representation of polyamidoamine dendrimer

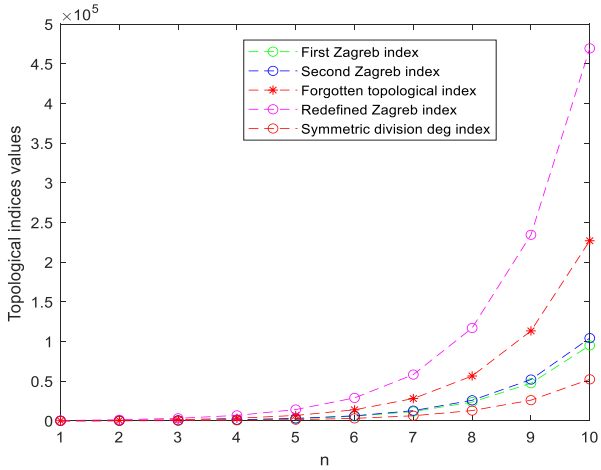

Figure 8. Graphical representation of propyl ether emine dendrimer

Table 2. Comparison of topological indices of polyacetal dendrimer

N	$M_1(H)$	$M_2(H)$	F (H)	ReZM (H)	SDD (H)
1	1272	1424	3060	6704	673.3
2	3400	3728	7936	16944	1820
3	7656	8336	17688	37424	4113.3
4	16168	17552	37192	78384	8700
5	33192	35984	76200	160304	17873.3
6	67240	72848	154216	324144	36220
7	135336	146576	310248	651824	72913.3
8	271528	294032	622312	1307184	146300
9	543912	588944	1246440	2617904	293073.3
10	1088680	1178768	2494696	5239344	586620

Table 3. Comparison of topological indices of polyester dendrimer

N	$M_1(H)$	$M_2(H)$	F (H)	ReZM (H)	SDD (H)
1	314	354	766	1648	171.3
2	910	1030	2234	4824	493
3	2102	2382	5170	11176	1135.7
4	4486	5086	11042	23880	2421
5	9254	10494	22786	49288	4991.7
6	18790	21310	46274	100104	10133
7	37862	42942	93250	201736	20415.7
8	76006	86206	187202	405000	40981
9	152294	172734	375106	811528	82111.7
10	304870	345790	750914	1624584	164373

Table 4. Comparison of topological indices of polyamidoamine dendrimer

N	$M_1(H)$	$M_2(H)$	F (H)	ReZM (H)	SDD (H)
1	111	246	267	558	61.5
2	297	654	711	1476	164
3	669	1470	1599	3312	369
4	1413	3102	3375	6984	779
5	2901	6366	6927	14328	1599
6	5877	12894	14031	29016	3239
7	11829	25950	28239	58392	6519
8	23733	52062	56655	117144	13079
9	47541	104286	113487	234648	26199
10	95157	208734	227151	469656	52439

Table 5. Comparison of topological indices of propyl ether emine dendrimer

N	M_1(H)	M_2(H)	F (H)	ReZM (H)	SDD (H)
1	94	100	206	428	51
2	290	308	634	1324	151
3	682	724	1490	3116	351
4	1466	1556	3202	6700	751
5	3034	3220	6626	13868	1551
6	6170	6548	13474	28204	3151
7	12442	13204	27170	56876	6351
8	24986	26516	54562	114220	12751
9	50074	53140	109346	228908	25551
10	100250	106388	218914	458284	51151

5. CONCLUSIONS

The description of the structure or shape of a molecule is extremely useful in predicting the activity and properties of molecules in complex studies. Molecular descriptors are used for the important purpose of mathematical representation, as mathematical values play an important role, particularly in topological indices. Topological indices specified on chemical structures can assist researchers in recognizing the biological activity, chemical reactivity and physical features. Through topological indices, researchers can predict the distinct physicochemical properties of the molecular descriptors. The results obtained investigations on dendrimers show that they have an important function in the delivery of drugs such as anti-inflammatory, antibacterial and anticancer agents. The actual application of topological indices in drug design and discovery covers a large part of the field, including lead discovery and optimization. These fields mainly cover virtual screening, drug delivery, QSAR structure-toxicity relationships, and so forth. In this work, some topological indices are calculated for some well-known bio-degradable dendrimers, and for dendrimers based on glycerol and succinic acid which are used for cancer therapy.

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NOMENCLATURE

QSPR	Quantitative Structure-Property Relationship
QSAR	Quantitative Structure-Activity Relationship
HSV	Herpes Simplex Virus