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Research Article

Keywords: Topological Descriptors, Chemical Graph Theory, Correlation, Decision Making

Posted Date: September 29th, 2026

DOI: <https://doi.org/10.21203/rs.3.rs-7510788/v1>

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Additional Declarations: No competing interests reported.

Machine Learning-Assisted Prediction of Szeged and Mostar Indices for Class of Dendrimers

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March 20, 2025

Abstract

Dendrimers are essential in drug design due to their effectiveness. Scientists are developing beneficial dendrimer molecules, leveraging mathematical chemistry tools like molecular descriptors to predict molecular properties. Topological descriptors help correlate chemical structures with physical, chemical, and biological activities. This study aims to determine distance-based molecular descriptors, particularly, Szeged (Sz), Edge Szeged (Sz_e), Total Szeged (Sz_t), Mostar (M), Edge Mostar (Mo_e), Total Mostar (Mo_t). The study also explores three types of dendrimers, Phosphorus-containing dendrimers, Perylenediimide-cored (PDI) dendrimers, and Aliphatic Polyamide dendrimers by calculating specific structural measures. These indices offer a mathematical framework to evaluate properties of chemicals, like boiling points, melting points, and radius of gyration. We determine growth of the dendrimers, also forecast various physicochemical and bioactive properties by integrating these descriptors into QSAR / QSPR modeling and developing regression models to predict their chemical properties, reducing the need for extensive laboratory experiments.

Keywords: Topological Descriptors; Chemical Graph Theory; Correlation; Decision Making.

1 Introduction

Dendrimers are a remarkable class of macromolecules distinguished by their unique, highly branched, and symmetric architecture [1,2]. These nanoscale structures, which consist of a central core surrounded by successive layers (generations) of branching units, exhibit unparalleled precision in their design [2]. Their well-defined size, shape, and surface functionality

make them highly versatile, finding applications in fields ranging from medicine and drug delivery [3] to material science and nanotechnology [4]. The precise control over their structure allows dendrimers to possess desirable properties such as chemical stability, low toxicity, high solubility, and the ability to form multivalent interactions, making them ideal candidates for diverse biological and chemical applications.

In the study of molecular structures like dendrimers [11], topological indices have emerged as powerful tools for translating structural information into numerical data. These indices, derived from the molecular graph representation of a compound, provide insights into various physicochemical, biological, and structural properties. Among these, bond-additive topological indices, such as Szeged and Mostar invariants, have gained significant attention due to their ability to reflect intricate details about molecular geometry, bonding, and connectivity. These indices are particularly valuable for quantifying the structural characteristics of dendrimers, including their peripheral shapes and symmetry, which are critical to their functionality.

This paper explores the intersection of dendrimer chemistry and bond-additive topological indices, focusing on the application and computation of advanced invariants for molecular graphs of dendrimers. By analyzing key dendrimer types such as Phosphorus Containing dendrimers, PDI Cored dendrimers, and Aliphatic Polyamide dendrimers.

Phosphorus-containing dendrimers are highly branched, tree-like macromolecules characterized by the incorporation of phosphorus atoms in their structure. These dendrimers are versatile due to their structural uniformity, high functionality, and tunable properties, making them suitable for applications in material science. Phosphorus-containing dendrimers have already been used as reusable and efficient catalysts, for the elaboration of nanomaterials, as fluorescent agents for bio-imaging, and as drugs by themselves, to name a few uses [6].

PDI-cored dendrimers feature a phthalocyanine diimide (PDI) core, known for its exceptional electronic, optical, and thermal properties. These dendrimers are particularly attractive for use in photonic devices, energy storage systems, and targeted drug delivery, owing to the synergistic interaction between the PDI core and the dendritic branches. In the past few years, PDI-cored dendrimers have been successfully prepared and applied in various fields. The advantages of water-soluble PDI-cored dendrimers include strong red fluorescence, excellent photostability, low cytotoxicity, high quantum yield, and versatile surface modification. The biological application of water-soluble PDI-cored dendrimers is broad, including fluorescence live-cell imaging, fluorescent labeling, and gene delivery, owing to the rapid development of these materials in the past decade [7]. On the other hand, Aliphatic polyamide dendrimers [8] are built from repeating aliphatic amide units, offering enhanced solubility, flexibility, and biocompatibility. These dendrimers are widely utilized in biomedical applications, including gene therapy, imaging, and as carriers for hydrophobic drugs. Aliphatic polyamide dendrimers are complex monodisperse, their core and branch multiplicities, as well as branch cell segment length, determine the generation number at which dendrimers become globular. The combination of phosphorus-containing frameworks with PDI or polyamide cores provides a unique platform for designing multifunctional materials tailored to specific scientific and industrial needs. This work aims to uncover deeper structural insights that can enhance our

understanding of their unique properties and expand their potential applications in science and industry.

Section (1), contains the introduction which provides ground to this research. Section (2), includes the basic theory of graph theory. The main results are included in Sections (3), (4) and (5), which comprise of Phosphorus-Containing Dendrimers, PDI-Cored Dendrimers and Aliphatic Polyamide Dendrimers, respectively. In sections (6) and (7), the relevance and Significance of Topological Descriptors as well as linear regression modeling is discussed. Conclusions and discussions are given in Section (8).

2 Graph theoretical concepts

A graph $G = (V, E)$ is an ordered pair, where V is called the vertex set and E is said to be the edge set. Graphs are constructed from a chemical structure in which the atoms (resp. bonds) correspond to vertices (resp. edges) in the chemical graph. The preliminary information regarding the various terminologies can be obtained from [40]. All the graphs $G = (V, E)$ considered in this paper are simple, undirected and connected graphs. The Szeged Index was studied by I. Gutman [9]. Later it became known as the Szeged index of G . In chemical graph theory this index gained popularity among researchers due to its non-trivial relationship to other topological invariants and intrinsic chemical interest. Afterward, Gutman and Ashrafi [18] introduced the new versions of the Szeged index known as Edge Szeged index. Mahmiani [19] introduced the total Szeged index. Došlić [20] established a new bond-additive index known as Mostar index. The new versions of the Mostar index are introduced by Arockiaraj known as edge Mostar and total Mostar indices. Table (1) provide the formula's of all the mentioned indices where $n_u(uv, G)$ represents the number of vertices

Topological descriptors	Computational expressions
Szeged	$Sz(G) = \sum_{uv \in E(G)} (n_u(uv, G) \times n_v(uv, G))$
Edge-szeged	$Sz_e(G) = \sum_{uv \in E(G)} (m_u(uv, G) \times m_v(uv, G))$
Total-szeged	$Sz_t(G) = \sum_{e=uv \in E(G)} (t_u(uv, G) \times t_v(uv, G))$
Mostar	$Mo(G) = \sum_{uv \in E(G)} n_u(uv, G) - n_v(uv, G) $
Edge Mostar	$Mo_e(G) = \sum_{e=uv \in E(G)} m_u(uv, G) - m_v(uv, G) $
Total Mostar	$Mo_t(G) = \sum_{e=uv \in E(G)} t_u(uv, G) - t_v(uv, G) $

Table 1: Topological descriptors and their computational expressions

of G closer to u than to v , $n_v(uv, G)$ can be defined in an analogous way, $m_u(uv, G)$ and $m_v(uv, G)$ are the number of edges of G lying closer to vertex u than to vertex v and the number of edges of G lying closer to vertex v than to vertex u , respectively. For notation write $n_u(uv, G)$, $n_v(uv, G)$, $m_u(uv, G)$ and $m_v(uv, G)$ as n_u , n_v , m_u and m_v respectively.

3 Phosphorus-Containing Dendrimers

Phosphorus containing dendrimers possess functionalities with pendant nitroxyl radicals, which exhibit strong attractive interactions [34]. Consider $D_1(n)$ as the molecular graph of phosphorus-containing dendrimers, where n indicates the generation stage of $D_1(n)$. The order and size of $D_1(n)$ are $6(33 \times 2^n - 12)$ and $6(35 \times 2^n - 13)$, respectively. In this study, we will calculate the Szeged and Mostar indices for the molecular graph of phosphorus containing dendrimer. The molecular graph of first generation of phosphorus containing dendrimer is shown in Figure (1).

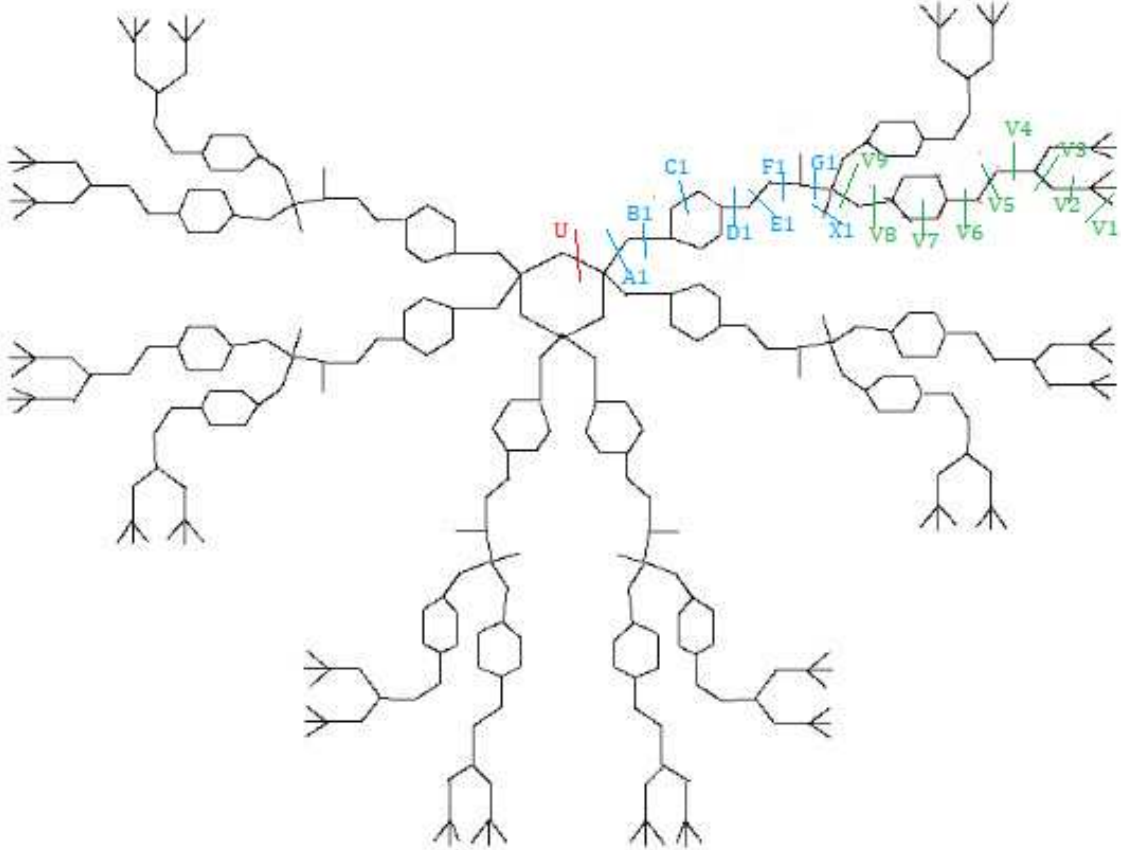


Figure 1: $D_1(n)$ for $n = 1$

Theorem 3.1. *The vertex Szeged index of graph of phosphorus containing dendrimers is given by:*

$$Sz_v(D_1(n)) = 2^{2n}[509652n - 168696] + 2^n[-90288n + 389202] - 68586. \quad (1)$$

Proof. The definition of vertex Szeged index is used along with the values of Table (2), (3) are to prove the equation (1) in the following way:

$$Sz_v(D(n)) = \sum_{uv \in E(D(n))} (n_u(uv, D(n)) \times n_v(uv, D(n)))$$

Representation	n_u	n_v	Frequency
$uv \in u_1$	$2(66 \times 2^n) - 49$	$2(33 \times 2^n) - 23$	6
$uv \in v_1$	$6(33 \times 2^n) - 73$	1	$9 \times 2^{n+2}$
$uv \in v_2$	$6(33 \times 2^n) - 76$	4	$3 \times 2^{n+2}$
$uv \in v_3$	$6(33 \times 2^n) - 77$	5	$3 \times 2^{n+2}$
$uv \in v_4$	$6(33 \times 2^n) - 83$	11	$3 \times 2^{n+1}$
$uv \in v_5$	$6(33 \times 2^n) - 84$	12	$3 \times 2^{n+1}$
$uv \in v_6$	$6(33 \times 2^n) - 85$	13	$3 \times 2^{n+1}$
$uv \in v_7$	$6(33 \times 2^n) - 88$	16	$9 \times 2^{n+2}$
$uv \in v_8$	$6(33 \times 2^n) - 91$	19	$3 \times 2^{n+1}$
$uv \in v_9$	$6(33 \times 2^n) - 92$	20	$3 \times 2^{n+1}$

Table 2: Values of n_u and n_v of Phosphorus based dendrimers

Representation	n_u	n_v	Frequency
$uv \in A_i$	$6(33 \times 2^n) - 33 \times 2^i - 59$	$33 \times 2^i - 13$	$3 \times 2^{n-i+1}$
$uv \in B_i$	$6(33 \times 2^n) - 33 \times 2^i - 58$	$33 \times 2^i - 14$	$3 \times 2^{n-i+2}$
$uv \in C_i$	$6(33 \times 2^n) - 33 \times 2^i - 55$	$33 \times 2^i - 17$	$9 \times 2^{n-i+2}$
$uv \in D_i$	$6(33 \times 2^n) - 33 \times 2^i - 52$	$33 \times 2^i - 20$	$3 \times 2^{n-i+1}$
$uv \in E_i$	$6(33 \times 2^n) - 33 \times 2^i - 51$	$33 \times 2^i - 21$	$3 \times 2^{n-i+1}$
$uv \in F_i$	$6(33 \times 2^n) - 33 \times 2^i - 50$	$33 \times 2^i - 22$	$3 \times 2^{n-i+1}$
$uv \in G_i$	$6(33 \times 2^n) - 33 \times 2^i - 48$	$33 \times 2^i - 24$	$3 \times 2^{n-i+2}$
$uv \in X_i$	$6(33 \times 2^n) - 73$	1	$3 \times 2^{n-i+2}$

Table 3: Values of n_u and n_v of Phosphorus based dendrimers

$$\begin{aligned}
Sz_v(D_1(n)) = & 6 [(66 \times 2^n - 23)(132 \times 2^n - 49)] + 9 \times 2^{n+2} [198 \times 2^n - 73] \\
& + 3 \times 2^{n+2} [(198 \times 2^n - 76)(4)] + 3 \times 2^{n+2} [(198 \times 2^n - 77)(5)] \\
& + 3 \times 2^{n+1} [(198 \times 2^n - 83)(11)] + 3 \times 2^{n+1} [(198 \times 2^n - 84)(12)] \\
& + 3 \times 2^{n+1} [(198 \times 2^n - 85)(13)] + 3 \times 2^{n+2} [(198 \times 2^n - 88)(16)] \\
& + 3 \times 2^{n+1} [(198 \times 2^n - 91)(19)] + 3 \times 2^{n+2} [(198 \times 2^n - 92)(20)] \\
& + \sum_{i=1}^n \left[3 \times 2^{n-i+1} [(198 \times 2^n - 33 \times 2^i - 59)(33 \times 2^i - 13)] \right. \\
& + 3 \times 2^{n-i+1} [(198 \times 2^n - 33 \times 2^i - 58)(33 \times 2^i - 14)] \\
& + 3 \times 2^{n-i+1} [(198 \times 2^n - 33 \times 2^i - 52)(33 \times 2^i - 20)] \\
& + 3 \times 2^{n-i+1} [(198 \times 2^n - 33 \times 2^i - 51)(33 \times 2^i - 21)] \\
& + 3 \times 2^{n-i+1} [(198 \times 2^n - 33 \times 2^i - 50)(33 \times 2^i - 22)] \\
& + 9 \times 2^{n-i+2} [(198 \times 2^n - 33 \times 2^i - 55)(33 \times 2^i - 17)] \\
& + 3 \times 2^{n-i+2} [(198 \times 2^n - 33 \times 2^i - 48)(33 \times 2^i - 24)] \\
& \left. + 3 \times 2^{n-i+2} [(198 \times 2^n - 73)] \right]. \tag{2}
\end{aligned}$$

After further calculations, we get:

$$Sz_v(D_1(n)) = 2^{2n} \times [509652n - 168696] + 2^n \times [-90288n + 389202] - 68586. \tag{3}$$

□

Theorem 3.2. *For Phosphorus containing dendrimers the vertex Mostar Index is*

$$Mo(D_1(n)) = 2^{2n}(42768) - 2^n(5148n + 32460) + 3468. \tag{4}$$

Proof. Followed by values depicted in Tables (2), (3) and the expression of vertex Mostar

index, equation (4) can be calculated as follows:

$$\begin{aligned}
Mo(D_1(n)) &= 6 |(132 \times 2^n - 49) - (66 \times 2^n - 23)| + 9 \times 2^{n+2} |198 \times 2^n - 73 - 1| \\
&+ 3 \times 2^{n+2} |(198 \times 2^n - 76) - 4| + 3 \times 2^{n+2} |(198 \times 2^n - 77) - 5| \\
&+ 3 \times 2^{n+1} |(198 \times 2^n - 83) - 11| + 3 \times 2^{n+1} |(198 \times 2^n - 84) - 12| \\
&+ 3 \times 2^{n+1} |(198 \times 2^n - 85) - 13| + 3 \times 2^{n+2} |(198 \times 2^n - 88) - 16| \\
&+ 3 \times 2^{n+1} |(198 \times 2^n - 91) - 19| + 3 \times 2^{n+2} |(198 \times 2^n - 92) - 20| \\
&+ \sum_{i=1}^n \left[3 \times 2^{n-i+1} |(198 \times 2^n - 33 \times 2^i - 59) - 33 \times 2^i - 13| \right. \\
&+ 3 \times 2^{n-i+1} |(198 \times 2^n - 33 \times 2^i - 58) - 33 \times 2^i - 14| \\
&+ 3 \times 2^{n-i+1} |(198 \times 2^n - 33 \times 2^i - 52) - 33 \times 2^i - 20| \\
&+ 3 \times 2^{n-i+1} |(198 \times 2^n - 33 \times 2^i - 51) - 33 \times 2^i - 21| \\
&+ 3 \times 2^{n-i+1} |(198 \times 2^n - 33 \times 2^i - 50) - 33 \times 2^i - 22| \\
&+ 9 \times 2^{n-i+2} |(198 \times 2^n - 33 \times 2^i - 55) - 33 \times 2^i - 17| \\
&+ 3 \times 2^{n-i+2} |(198 \times 2^n - 33 \times 2^i - 48) - 33 \times 2^i - 24| \\
&\left. + 3 \times 2^{n-i+2} |(198 \times 2^n) - 73 - 1| \right] \tag{5}
\end{aligned}$$

Using simple calculations, we derive

$$Mo(D_1(n)) = 2^{2n}(42768) - 2^n(5148n + 32460) + 3468. \tag{6}$$

□

Theorem 3.3. *For Phosphorus containing dendrimers the Edge Szeged Index is calculated as:*

$$Sz_e(D_1(n)) = 2^{2n}[573300n - 259560] + 2^n[-1005590n + 492084] - 87180 \tag{7}$$

Proof. Edge Szeged index is defined as:

$$Sz_e(D(n)) = \sum_{uv \in E(D(n))} (q_u(uv, D(n))) \times q_v(uv, D(n)) \tag{8}$$

Representation	q_u	q_v	Frequency
$uv \in u$	$4 \times 35 \times 2^n - 54$	$2 \times 35 \times 2^n - 26$	6
$uv \in v_1$	$6 \times 35 \times 2^n - 79$	0	$9 \times 2^{n+2}$
$uv \in v_2$	$6 \times 35 \times 2^n - 82$	3	$3 \times 2^{n+2}$
$uv \in v_3$	$6 \times 35 \times 2^n - 83$	4	$3 \times 2^{n+2}$
$uv \in v_4$	$6 \times 35 \times 2^n - 89$	10	$3 \times 2^{n+1}$
$uv \in v_5$	$6 \times 35 \times 2^n - 90$	11	$3 \times 2^{n+1}$
$uv \in v_6$	$6 \times 35 \times 2^n - 91$	12	$3 \times 2^{n+1}$
$uv \in v_7$	$6 \times 35 \times 2^n - 95$	15	$9 \times 2^{n+2}$
$uv \in v_8$	$6 \times 35 \times 2^n - 98$	19	$3 \times 2^{n+1}$
$uv \in v_9$	$6 \times 35 \times 2^n - 99$	20	$3 \times 2^{n+1}$

Table 4: Values of q_u and q_v of Phosphorus based dendrimers

Representation	q_u	q_v	Frequency
$uv \in A_i$	$6 \times 35 \times 2^n - 35 \times 2^i - 64$	$35 \times 2^i - 15$	$3 \times 2^{n-i+1}$
$uv \in B_i$	$6 \times 35 \times 2^n - 35 \times 2^i - 63$	$35 \times 2^i - 16$	$3 \times 2^{n-i+1}$
$uv \in C_i$	$6 \times 35 \times 2^n - 35 \times 2^i - 60$	$35 \times 2^i - 20$	$9 \times 2^{n-i+2}$
$uv \in D_i$	$6 \times 35 \times 2^n - 35 \times 2^i - 56$	$35 \times 2^i - 23$	$3 \times 2^{n-i+1}$
$uv \in E_i$	$6 \times 35 \times 2^n - 35 \times 2^i - 55$	$35 \times 2^i - 24$	$3 \times 2^{n-i+1}$
$uv \in F_i$	$6 \times 35 \times 2^n - 35 \times 2^i - 54$	$35 \times 2^i - 25$	$3 \times 2^{n-i+1}$
$uv \in G_i$	$6 \times 35 \times 2^n - 35 \times 2^i - 52$	$35 \times 2^i - 27$	$3 \times 2^{n-i+2}$
$uv \in X_i$	$6 \times 35 \times 2^n - 79$	0	$3 \times 2^{n-i+2}$

Table 5: Values of q_u and q_v of Phosphorus based dendrimers

According to values in Tables (4), (5) and the definition of edge Szeged index the equation

(??) can be computed as

$$\begin{aligned}
Sz_e(D_1(n)) &= \sum_{uv \in E(D_1(n))} (q_u(uv, D_1(n))) \times q_v(uv, D_1(n)) \\
&= 6[(70 \times 2^n - 26)(140 \times 2^n - 54)] + 9 \times 2^{n+2}[(210 \times 2^n - 79)(0)] \\
&+ 3 \times 2^{n+2}[(210 \times 2^n - 82)(3)] + 3 \times 2^{n+2}[(210 \times 2^n - 83)(4)] \\
&+ 3 \times 2^{n+1}[(210 \times 2^n - 89)(10)] + 3 \times 2^{n+1}[(210 \times 2^n - 90)(11)] \\
&+ 3 \times 2^{n+1}[(210 \times 2^n - 91)(12)] + 9 \times 2^{n+2}[(210 \times 2^n - 95)(15)] \\
&+ 3 \times 2^{n+1}[(210 \times 2^n - 98)(19)] + 3 \times 2^{n+2}[(210 \times 2^n - 99)(20)] \\
&+ \sum_{i=1}^n \left[3 \times 2^{n-i+1} [(210 \times 2^n - 35 \times 2^i - 64)(35 \times 2^i - 15)] \right. \\
&+ 3 \times 2^{n-i+1} [(210 \times 2^n - 35 \times 2^i - 63)(35 \times 2^i - 16)] \\
&+ 9 \times 2^{n-i+2} [(210 \times 2^n - 35 \times 2^i - 60)(35 \times 2^i - 20)] \\
&+ 3 \times 2^{n-i+1} [(210 \times 2^n - 35 \times 2^i - 56)(35 \times 2^i - 23)] \\
&+ 3 \times 2^{n-i+1} [(210 \times 2^n - 35 \times 2^i - 55)(35 \times 2^i - 24)] \\
&+ 3 \times 2^{n-i+1} [(210 \times 2^n - 35 \times 2^i - 54)(35 \times 2^i - 25)] \\
&+ 3 \times 2^{n-i+2} [(210 \times 2^n - 35 \times 2^i - 52)(35 \times 2^i - 27)] \\
&\left. + 3 \times 2^{n-i+2} [(210 \times 2^n - 79)(0)] \right] \\
&= 2^{2n}[573300n - 259560] + 2^n[-1005590n + 492084] - 87180.
\end{aligned}$$

□

Theorem 3.4. *The edge Mostar index of phosphorus containing dendrimers is given by*

$$Mo_e(D_1(n)) = 2^{2n}(45360) - 2^n(5460n + 34404) + 3654. \quad (9)$$

Proof. By using Tables (4) and (5) in expression of edge Mostar index, we compute equation

(9) in the following way

$$\begin{aligned}
Mo_e(D_1(n)) &= 6 |(140 \times 2^n - 54) - (70 \times 2^n - 26)| + 9 \times 2^{n+2} |(210 \times 2^n - 79) - 0| \\
&+ 3 \times 2^{n+2} |(210 \times 2^n - 82) - 3| + 3 \times 2^{n+2} |(210 \times 2^n - 83) - 4| \\
&+ 3 \times 2^{n+1} |(210 \times 2^n - 89) - 10| + 3 \times 2^{n+1} |(210 \times 2^n - 90) - 11| \\
&+ 3 \times 2^{n+1} |(210 \times 2^n - 91) - 12| + 9 \times 2^{n+2} |(210 \times 2^n - 95) - 15| \\
&+ 3 \times 2^{n+1} |(210 \times 2^n - 98) - 19| + 3 \times 2^{n+2} |(210 \times 2^n - 99) - 20| \\
&+ \sum_{i=1}^n \left[3 \times 2^{n-i+1} |(210 \times 2^n - 35 \times 2^i - 64) - 35 \times 2^i - 15| \right. \\
&+ 3 \times 2^{n-i+1} |(210 \times 2^n - 35 \times 2^i - 63) - 35 \times 2^i - 16| \\
&+ 9 \times 2^{n-i+2} |(210 \times 2^n - 35 \times 2^i - 60) - 35 \times 2^i - 20| \\
&+ 3 \times 2^{n-i+1} |(210 \times 2^n - 35 \times 2^i - 56) - 35 \times 2^i - 23| \\
&+ 3 \times 2^{n-i+1} |(210 \times 2^n - 35 \times 2^i - 55) - 35 \times 2^i - 24| \\
&+ 3 \times 2^{n-i+1} |(210 \times 2^n - 35 \times 2^i - 54) - 35 \times 2^i - 25| \\
&+ 3 \times 2^{n-i+2} |(210 \times 2^n - 35 \times 2^i - 52) - 35 \times 2^i - 27| \\
&\left. + 3 \times 2^{n-i+2} |(210 \times 2^n - 79) - 0| \right] \tag{10}
\end{aligned}$$

After some simplifications, we obtain the following:

$$Mo_e(D_1(n)) = 2^{2n} (45360) - 2^n (5460n + 34404) + 3654. \tag{11}$$

□

Theorem 3.5. *The total Szeged index for phosphorus containing dendrimers is given by:*

$$Sz_t(D_1(n)) = 2^{2n} [2164032n - 851904] + 2^n [-381480n + 1757592] - 310530. \tag{12}$$

Proof. The total szeged index is defined as:

$$Sz_t(D(n)) = \sum_{uv \in E(D(n))} (t_u(uv, D(n)) \times t_v(uv, D(n)))$$

Representation	t_u	t_v	Frequency
$uv \in u$	$272 \times 2^n - 103$	$136 \times 2^n - 49$	6
$uv \in v_1$	$408 \times 2^n - 152$	1	$9 \times 2^{n+2}$
$uv \in v_2$	$408 \times 2^n - 158$	7	$3 \times 2^{n+2}$
$uv \in v_3$	$408 \times 2^n - 160$	9	$3 \times 2^{n+2}$
$uv \in v_4$	$408 \times 2^n - 172$	21	$3 \times 2^{n+1}$
$uv \in v_5$	$408 \times 2^n - 174$	23	$3 \times 2^{n+1}$
$uv \in v_6$	$408 \times 2^n - 176$	25	$3 \times 2^{n+1}$
$uv \in v_7$	$408 \times 2^n - 183$	31	$9 \times 2^{n+2}$
$uv \in v_8$	$408 \times 2^n - 189$	38	$3 \times 2^{n+1}$
$uv \in v_9$	$408 \times 2^n - 191$	40	$3 \times 2^{n+1}$

Table 6: Values of t_u and t_v of Phosphorus based dendrimers

Representation	t_u	t_v	Frequency
$uv \in A_i$	$408 \times 2^n - 68 \times 2^i - 123$	$68 \times 2^i - 28$	$3 \times 2^{n-i+1}$
$uv \in B_i$	$408 \times 2^n - 68 \times 2^i - 121$	$68 \times 2^i - 30$	$3 \times 2^{n-i+1}$
$uv \in C_i$	$408 \times 2^n - 68 \times 2^i - 115$	$68 \times 2^i - 37$	$9 \times 2^{n-i+2}$
$uv \in D_i$	$408 \times 2^n - 68 \times 2^i - 108$	$68 \times 2^i - 43$	$3 \times 2^{n-i+1}$
$uv \in E_i$	$408 \times 2^n - 68 \times 2^i - 106$	$68 \times 2^i - 45$	$3 \times 2^{n-i+1}$
$uv \in F_i$	$408 \times 2^n - 68 \times 2^i - 104$	$68 \times 2^i - 47$	$3 \times 2^{n-i+1}$
$uv \in G_i$	$408 \times 2^n - 68 \times 2^i - 100$	$68 \times 2^i - 51$	$3 \times 2^{n-i+2}$
$uv \in X_i$	$408 \times 2^n - 68 \times 2^i - 152$	1	$3 \times 2^{n-i+2}$

Table 7: Values of t_u and t_v of Phosphorus based dendrimers

According to values in Tables (6), (7) and the definition of total Mostar index the equation

(12) can be computed as:

$$\begin{aligned}
Sz_t(D_1(n)) &= 6[(136 \times 2^n - 49)(272 \times 2^n - 103)] + 9 \times 2^{n+2}[(408 \times 2^n - 152)(1)] \\
&+ 3 \times 2^{n+2}[(408 \times 2^n - 158)(7)] + 3 \times 2^{n+2}[(408 \times 2^n - 160)(9)] \\
&+ 3 \times 2^{n+1}[(408 \times 2^n - 172)(21)] \\
&+ 3 \times 2^{n+1}[(408 \times 2^n - 174)(23)] + 3 \times 2^{n+1}[(408 \times 2^n - 176)(25)] \\
&+ 9 \times 2^{n+2}[(408 \times 2^n - 183)(31)] + 3 \times 2^{n+1}[(408 \times 2^n - 189)(38)] \\
&+ 3 \times 2^{n+1}[(408 \times 2^n - 191)(40)] \\
&+ \sum_{i=1}^n \left[3 \times 2^{n-i+1}[(408 \times 2^n - 68 \times 2^i - 123)(68 \times 2^i - 28)] \right. \\
&+ 9 \times 2^{n-i+2}[(408 \times 2^n - 68 \times 2^i - 115)(68 \times 2^i - 37)] \\
&+ 3 \times 2^{n-i+1}[(408 \times 2^n - 68 \times 2^i - 121)(68 \times 2^i - 30)] \\
&+ 3 \times 2^{n-i+1}[(408 \times 2^n - 68 \times 2^i - 108)(68 \times 2^i - 43)] \\
&+ 3 \times 2^{n-i+1}[(408 \times 2^n - 68 \times 2^i - 106)(68 \times 2^i - 45)] \\
&+ 3 \times 2^{n-i+1}[(408 \times 2^n - 68 \times 2^i - 104)(68 \times 2^i - 47)] \\
&+ 3 \times 2^{n-i+2}[(408 \times 2^n - 68 \times 2^i - 100)(68 \times 2^i - 51)] \\
&\left. + 3 \times 2^{n-i+2}[(408 \times 2^n - 152)(1)] \right] \tag{13}
\end{aligned}$$

After some calculations, we obtain the following:

$$Sz_t(D_1(n)) = 2^{2n}[2164032n - 851904] + 2^n[-381480n + 1757592] - 310530. \tag{14}$$

□

Theorem 3.6. *The total Mostar index of phosphorus containing dendrimers is given by:*

$$Mo_t(D_1(n)) = 2^{2n}(88128) - 2^n(10608n + 66864) + 7122. \tag{15}$$

Proof. By using the values of Table 6, 7 and the definition of total Mostar index, we calculate

equation (15) in the following way:

$$\begin{aligned}
Mo_t(D_1(n)) &= 6 |(272 \times 2^n - 103) - (136 \times 2^n - 49)| + 9 \times 2^{n+2} |(408 \times 2^n - 152) - 1| \\
&+ 3 \times 2^{n+2} |(408 \times 2^n - 158) - 7| + 3 \times 2^{n+2} |(408 \times 2^n - 160) - 9| \\
&+ 3 \times 2^{n+1} |(408 \times 2^n - 172) - 21| \\
&+ 3 \times 2^{n+1} |(408 \times 2^n - 174) - 23| + 3 \times 2^{n+1} |(408 \times 2^n - 176) - 25| \\
&+ 9 \times 2^{n+2} |(408 \times 2^n - 183) - 31| + 3 \times 2^{n+1} |(408 \times 2^n - 189) - 38| \\
&+ 3 \times 2^{n+1} |(408 \times 2^n - 191) - 40| \\
&+ \sum_{i=1}^n \left[3 \times 2^{n-i+1} |(408 \times 2^n - 68 \times 2^i - 123) - 68 \times 2^i - 28| \right. \\
&+ 9 \times 2^{n-i+2} |(408 \times 2^n - 68 \times 2^i - 115) - 68 \times 2^i - 37| \\
&+ 3 \times 2^{n-i+1} |(408 \times 2^n - 68 \times 2^i - 121) - 68 \times 2^i - 30| \\
&+ 3 \times 2^{n-i+1} |(408 \times 2^n - 68 \times 2^i - 108) - 68 \times 2^i - 43| \\
&+ 3 \times 2^{n-i+1} |(408 \times 2^n - 68 \times 2^i - 106) - 68 \times 2^i - 45| \\
&+ 3 \times 2^{n-i+1} |(408 \times 2^n - 68 \times 2^i - 104) - 68 \times 2^i - 47| \\
&+ 3 \times 2^{n-i+2} |(408 \times 2^n - 68 \times 2^i - 100) - 68 \times 2^i - 51| \\
&\left. + 3 \times 2^{n-i+2} |(408 \times 2^n - 152) - 1| \right] \tag{16}
\end{aligned}$$

Employing simple calculations, we obtain the following relation

$$Mo_t(D_1(n)) = 2^{2n} (88128) - 2^n (10608n + 66864) + 7122. \tag{17}$$

□

4 PDI-Cored Dendrimers.

Water-soluble perylenediimide PDI-cored dendrimers hold a significant position among other dendrimers due to their broad range of potential applications [38]. They offer several advantages, including low cytotoxicity, excellent photostability, versatile surface modification, high quantum yield, strong red fluorescence, and various biological uses such as fluorescence live-cell imaging, gene delivery, and fluorescent labeling. In this study, we will calculate the Szeged and Mostar indices for the molecular graph of one type of water-soluble PDI-cored dendrimer. Let $D_2(n)$ represent the molecular graph of this dendrimer, where n indicates the generation stage of $D_2(n)$. The order and size of graph $D_2(n)$ are given by $20(2^n + 1)$ and $20 \times 2n + 26$, respectively [?].

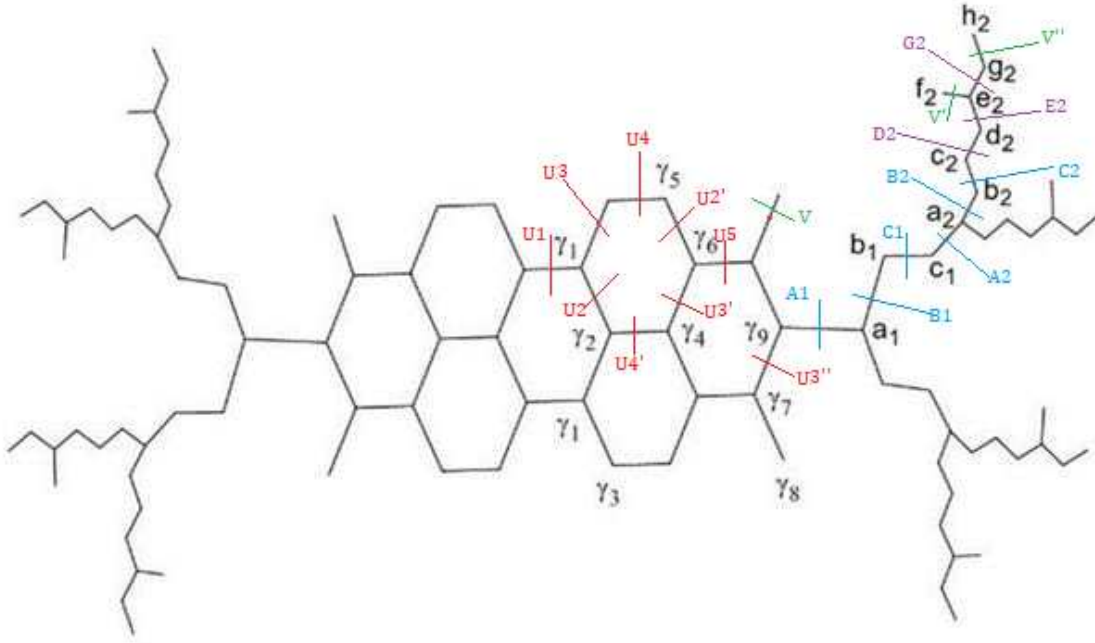


Figure 2: $D_1(n)$ for $n = 1$

Theorem 4.1. *The vertex Szeged index of PDI-cored dendrimer is as follows:*

$$Sz(D_2(n)) = (1200n + 2160) \times 2^{2n} + (1680n + 7556) \times (2^n) + 2664, \quad n \geq 1 \quad (18)$$

Proof. By using the values of Table 8 and the definition of vertex Szeged Index, we calculate (18) in the following way:

Representative	n_u	n_v	Frequencies
$uv \in F_n$	$20 \times 2^n + 19$	1	$2^{n+2} + 4$
$uv \in U_1$	$10(2^n + 1)$	$10(2^n + 1)$	2
$uv \in U_2$	$10(2^n + 1)$	$10(2^n + 1)$	8
$uv \in U_3$	$10 \times 2^n + 1$	$10 \times 2^n + 19$	12
$uv \in U_4$	$10 \times 2^n + 5$	$10 \times 2^n + 15$	6
$uv \in U_5$	10×2^n	$10 \times 2^n + 20$	4
$uv \in A_i$	$5 \times 2^{i+1} - 5$	$20 \times 2^n - 5 \times 2^{i+1} + 25$	2^{n-i+1}
$uv \in B_i$	$5 \times 2^i - 3$	$20 \times 2^n - 5 \times 2^i + 23$	2^{n-i+2}
$uv \in C_i$	$5 \times 2^i - 4$	$20 \times 2^n - 5 \times 2^i + 24$	2^{n-i+2}
$uv \in D_n$	5	$20 \times 2^n + 15$	2^{n+1}
$uv \in E_n$	4	$20 \times 2^n + 16$	2^{n+1}
$uv \in G_n$	2	$20 \times 2^n + 18$	2^{n+1}

Table 8: The values of n_u and n_v of graph PDI-cored dendrimers

$$\begin{aligned}
Sz(D_2) = & (2^{n+2} + 4)(20 \times 2^n + 19)(1) + 2(10(2^n + 1))^2 + 8(10(2^n + 1))^2 \\
& + 12(10 \times 2^n + 1)(10 \times 2^n + 19) + 6(10 \times 2^n + 5)(10 \times 2^n + 15) \\
& + 4(10 \times 2^n) + (10 \times 2^n + 20) \\
& + \sum_{i=1}^n 2^{n-i+1}(10 \times 2^{i+1} - 5)(20 \times 2^n - 5 \times 2^{i+1} + 25) \\
& + \sum_{i=1}^n 2^{n-i+2}(10 \times 2^i - 3)(20 \times 2^n - 5 \times 2^i + 23) \\
& + \sum_{i=1}^n 2^{n-i+2}(10 \times 2^i - 4)(20 \times 2^n - 5 \times 2^i + 24) \\
& + 2^{n+1}(20 \times 2^n + 15)(5) + 2^{n+1}(20 \times 2^n + 16)(4) \\
& + 2^{n+1}(20 \times 2^n + 18)(2)
\end{aligned} \tag{19}$$

After some calculations, we obtain the following:

$$Sz(D_2(n)) = (1200n + 2160) \times 2^{2n} + (1680n + 7556) \times 2^n + 2664, \quad n \geq 1$$

□

Theorem 4.2. *The vertex Mostar index of PDI cored dendrimer is given by*

$$Mo(D_2(n)) = 400 \times 2^{2n} - (120n - 304)(2^n) + 152, \quad n \geq 1 \tag{20}$$

Proof. Followed by values depicted in Tables 8 and the expression of ertex Mostar index, equation (20) can be calculated as follows:

$$\begin{aligned} Mo(D_2(n)) = & (2^{n+2} + 4)|20 \times 2^n + 19 - 1| + 12|10 \times 2^n + 19 - 10 \times 2^n - 1| + 2|10(2^{n+1} + 1) - 10(2^{n+1} + 1)| + \\ & 8[10(2^{n+1} + 1) - 10(2^{n+1} + 1)] + 6[10 \times 2^n + 15 - 10 \times 2^n - 5] + 4[10 \times 2^n + 20 - 10 \times 2^n] + \sum_{i=1}^n 2^{n-i+1}[20 \times 2^n \\ & - 5 \times 2^{i+1} + 25 - 5 \times 2^{i+1} + 5] + \sum_{i=1}^n 2^{n-i+2}[20 \times 2^n - 5 \times 2^i + 23 - 5 \times 2^i + 3] + \sum_{i=1}^n 2^{n-i+2}[20 \times 2^n - 5 \times 2^i + 24] \end{aligned} \quad (21)$$

After further calculations we get

$$Mo(D_2(n)) = 400 \times 2^{2n} - (120n - 304)(2^n) + 152, \quad n \geq 1$$

□

Theorem 4.3. *The edge Szeged index for PDI-cored dendrimer is given by:*

$$Sz_e(D_2(n)) = (1200n + 1760) \times 2^{2n} + (2100n + 8012) \times (2^n) + 3132, \quad n \geq 1 \quad (22)$$

Proof. According to values in Table 9, and the definition of edge Szeged index the equation (22) can be computed as: Then using table 9, we have edge Szeged Index Computation for PDI :

$$\begin{aligned} Sz_e(D_2) = & (2^{n+2} + 4)(20 \times 2^n + 25)(0) + 2(10(2^n + 12))^2 + 8(10(2^n + 11))^2 \\ & + 12(10 \times 2^n + 12)(10 \times 2^n + 23) + 6(10 \times 2^n + 5)(10 \times 2^n + 18) + 4(10 \times 2^n - 1) \\ & + (10 \times 2^n + 25) + \sum_{i=1}^n 2^{n-i+1}(5 \times 2^{i+1} - 6)(20 \times 2^n - 5 \times 2^{i+1} + 31) \\ & + \sum_{i=1}^n 2^{n-i+2}(5 \times 2^i - 4)(20 \times 2^n - 5 \times 2^i + 29) + \sum_{i=1}^n 2^{n-i+2}(5 \times 2^i - 5) \\ & + (20 \times 2^n - 5 \times 2^i + 30) + 2^{n+1}(20 \times 2^n + 22)(3) + 2^{n+1}(20 \times 2^n + 24)(1) \\ & + 2^{n+1}(20 \times 2^n + 25)(0) \end{aligned} \quad (23)$$

After further calculations, we get

$$Sz_e(D_2(n)) = (1200n + 1760) \times 2^{2n} + (2100n + 8012) \times (2^n) + 3132, \quad n \geq 1 \quad (24)$$

□

Theorem 4.4. *The edge Mostar index of PDI-cored dendrimer is given by:*

$$Mo_e(D_2(n)) = 400 \times 2^{2n} - (2^n)(120n - 444) + 212, \quad n \geq 1 \quad (25)$$

Representation	q_u	q_v	Frequencies
$uv \in F_n$	$20 \times 2^n + 25$	0	$2^{n+2} + 4$
$uv \in U_1$	$10 \times 2^n + 12$	$10 \times 2^n + 12$	2
$uv \in U_2$	$10 \times 2^n + 11$	$10 \times 2^n + 11$	8
$uv \in U_3$	10×2^n	$10 \times 2^n + 23$	12
$uv \in U_4$	$10 \times 2^n + 5$	$10 \times 2^n + 18$	6
$uv \in U_5$	$10 \times 2^n - 1$	$10 \times 2^n + 25$	4
$uv \in A_i$	$5 \times 2^{i+1} - 6$	$20 \times 2^n - 5 \times 2^{i+1} + 31$	2^{n-i+1}
$uv \in B_i$	$5 \times 2^i - 4$	$20 \times 2^n - 5 \times 2^i + 29$	2^{n-i+2}
$uv \in C_i$	$5 \times 2^i - 5$	$20 \times 2^n - 5 \times 2^i + 30$	2^{n-i+2}
$uv \in D_n$	4	$20 \times 2^n + 21$	2^{n+1}
$uv \in E_n$	3	$20 \times 2^n + 22$	2^{n+1}
$uv \in G_n$	1	$20 \times 2^n + 24$	2^{n+1}

Table 9: Values of q_u and q_v of PDI cored dendrimers

Proof. By using the values of Table (9) and the definition of edge Mostar index, we calculate (25) in the following way:

$$\begin{aligned}
Mo_e(D_3) &= (2^{n+2} + 4)|20 \times 2^n + 25 - 0| + 2|10(2^n + 12) - 10(2^n + 12)| \\
&+ 8|10(2^n + 11) - 10(2^n + 11)| + 12|10 \times 2^n + 12 - 10 \times 2^n + 23| \\
&+ 6|10 \times 2^n + 5 - 10 \times 2^n + 18| + 4|10 \times 2^n - 1 - 10 \times 2^n + 25| \\
&+ \sum_{i=1}^n 2^{n-i+1} |5 \times 2^{i+1} - 6 - 20 \times 2^n - 5 \times 2^{i+1} + 31| \\
&+ \sum_{i=1}^n 2^{n-i+2} |5 \times 2^i - 4 - 20 \times 2^n - 5 \times 2^i + 29| \\
&+ \sum_{i=1}^n 2^{n-i+2} |5 \times 2^i - 5 - 20 \times 2^n - 5 \times 2^i + 30| \\
&+ 2^{n+1}|20 \times 2^n + 22 - 3| + 2^{n+1}|20 \times 2^n + 24 - 1| \\
&+ 2^{n+1}(20 \times 2^n + 25)(0)
\end{aligned} \tag{26}$$

After some simplifications, we obtain the following:

$$Mo_e(D_3(n)) = 400 \times 2^{2n} - 2^n \times (120n - 444) + 212, \quad n \geq 1. \tag{27}$$

□

Theorem 4.5. *The total Szeged index for PDI-cored dendrimer is given by:*

$$Sz_t(D_2(n)) = (4800n + 7840) \times 2^{2n} + (7560n + 31256) \times (2^n) + 11608, \quad n \geq 1 \quad (28)$$

Proof. Followed by values depicted in Table (10) and the expression of total Szeged index, equation (28) can be calculated as follows:

Representation	t_u	t_v	Frequencies
$uv \in F_n$	$40 \times 2^n + 44$	1	$2^{n+2} + 4$
$uv \in U_1$	$20 \times 2^n + 22$	$20 \times 2^n + 22$	2
$uv \in U_2$	$20 \times 2^n + 21$	$20 \times 2^n + 21$	8
$uv \in U_3$	$20 \times 2^n + 1$	$20 \times 2^n + 42$	12
$uv \in U_4$	$20 \times 2^n + 10$	$20 \times 2^n + 33$	6
$uv \in U_5$	$20 \times 2^n - 1$	$20 \times 2^n + 45$	4
$uv \in A_i$	$10 \times 2^{i+1} - 11$	$40 \times 2^n - 10 \times 2^{i+1} + 56$	2^{n-i+1}
$uv \in B_i$	$10 \times 2^i - 7$	$40 \times 2^n - 1 \times 2^i + 52$	2^{n-i+2}
$uv \in C_i$	$10 \times 2^i - 9$	$40 \times 2^n - 5 \times 2^i + 54$	2^{n-i+2}
$uv \in D_n$	9	$40 \times 2^n + 36$	2^{n+1}
$uv \in E_n$	7	$40 \times 2^n + 38$	2^{n+1}
$uv \in G_n$	3	$40 \times 2^n + 42$	2^{n+1}

Table 10: Values of t_u and t_v of PDI cored dendrimers

By using table 10 we have total Szeged Index Computation for PDI :

$$\begin{aligned}
Sz_t(D_2(n)) &= (2^{n+2} + 4)(40 \times 2^n + 44)(1) + (20 \times 2^n + 22)^2 \times 2 \\
&+ (20 \times 2^n + 21)^2 \times 8 + (20 \times 2^n + 10) \times (20 \times 2^n + 33) \times 6 \\
&+ (20 \times 2^n - 1) \times (20 \times 2^n + 45) \times 4 + (20 \times 2^n - 1) \times (20 \times 2^n + 45) \times 4 \\
&+ \sum_{i=1}^n 2^{n-i+1} (40 \times 2^n - 10 \times 2^{i+1} + 56) (10 \times 2^{i+1} - 11) \\
&+ \sum_{i=1}^n 2^{n-i+2} (40 \times 2^n - 10 \times 2^{i+1} + 52) \times (10 \times 2^{i+1} - 7) \\
&+ \sum_{i=1}^n 2^{n-i+2} (40 \times 2^n - 10 \times 2^{i+1} + 54) (10 \times 2^{i+1} - 9) \\
&+ (9 \times (40 \times 2^n + 36) \times 2^{n+1}) \\
&+ (7 \times (40 \times 2^2 + 38) \times 2^{n+1}) \\
&+ (3 \times (40 \times 2^n + 42) \times 2^{n+1}).
\end{aligned} \tag{29}$$

we obtain the following expression is obtained after simplification

$$Sz_t(D_2(n)) = (4800n + 7840) \times 2^{2n} + (7560n + 31256) \times 2^n + 11608, \quad n \geq 1. \tag{30}$$

□

Theorem 4.6. *The total Mostar Index for PDI-cored dendrimer is given by:*

$$Mo_t(D_3(n)) = 800 \times 2^{2n} - (240n - 748) \times (2^n) + 364, \quad n \geq 1. \tag{31}$$

Proof. By using values of Table 10 and definition of total Mostar index, we calculate (31) in the following way:

$$\begin{aligned}
Mo_t(D_2(n)) &= (2^{n+2} + 4) \left| 40 \times 2^n + 44 - 1 \right| + 2 \left| 20 \times 2^n + 22 - 20 \times 2^n + 22 \right| \\
&+ 8 \left| 20 \times 2^n + 21 - 20 \times 2^n - 21 \right| + 6 \left| 20 \times 2^n + 10 - 20 \times 2^n + 33 \right| \\
&+ 4 \left| 20 \times 2^n - 1 \right| - (20 \times 2^n + 45) + \sum_{i=1}^n 2^{n-i+1} \left[(40 \times 2^n - 10 \times 2^{i+1} + 56) \right. \\
&- (10 \times 2^{i+1} - 11) \left. \right] + \sum_{i=1}^n 2^{n-i+2} \left[(40 \times 2^n - 10 \times 2^{i+1} + 52) \right. \\
&- (10 \times 2^{i+1} - 7) \left. \right] + \sum_{i=1}^n 2^{n-i+2} \left[(40 \times 2^n - 10 \times 2^{i+1} + 54) \right. \\
&- (10 \times 2^{i+1} - 9) \left. \right] + 2^{n+1} \left[(40 \times 2^n + 36) - 9 \right] \\
&+ 2^{n+1} \left[(40 \times 2^n + 38) - 7 \right] + 2^{n+1} \left[(40 \times 2^n + 42) - 9 \right].
\end{aligned} \tag{32}$$

After further calculations, we get:

$$Mo_t(D_2(n)) = 800 \times 2^{2n} - (240n - 748) \times 2^n + 364, \quad n \geq 1. \quad (33)$$

□

5 Aliphatic Polyamide Dendrimers

Jishkariani [8], conducted the recent study on Aliphatic polyamide dendrimers containing Ethylenediamine and Piperazine. These dendrimers demonstrate stability both enzymatically and hydrolytically. Let $D_5(n)$ represent the molecular graph of these aliphatic polyamide-based dendrimers, which consists of a core with reactive proups, layers with repetitive branching units, and terminal functional groups that form surface of the dendrimers. The order and size of graph $D_2(n)$ same [?], which is given by $2(2^{n+3} - 5)$. High (6392) percent yields were achieved for the first four generations using both methods. Piperazine generated five generations for dendrimers, whereas ethylenediamine core allow synthesis for only four generation. Figure (3) shows the molecular graph of $D_3(n)$.

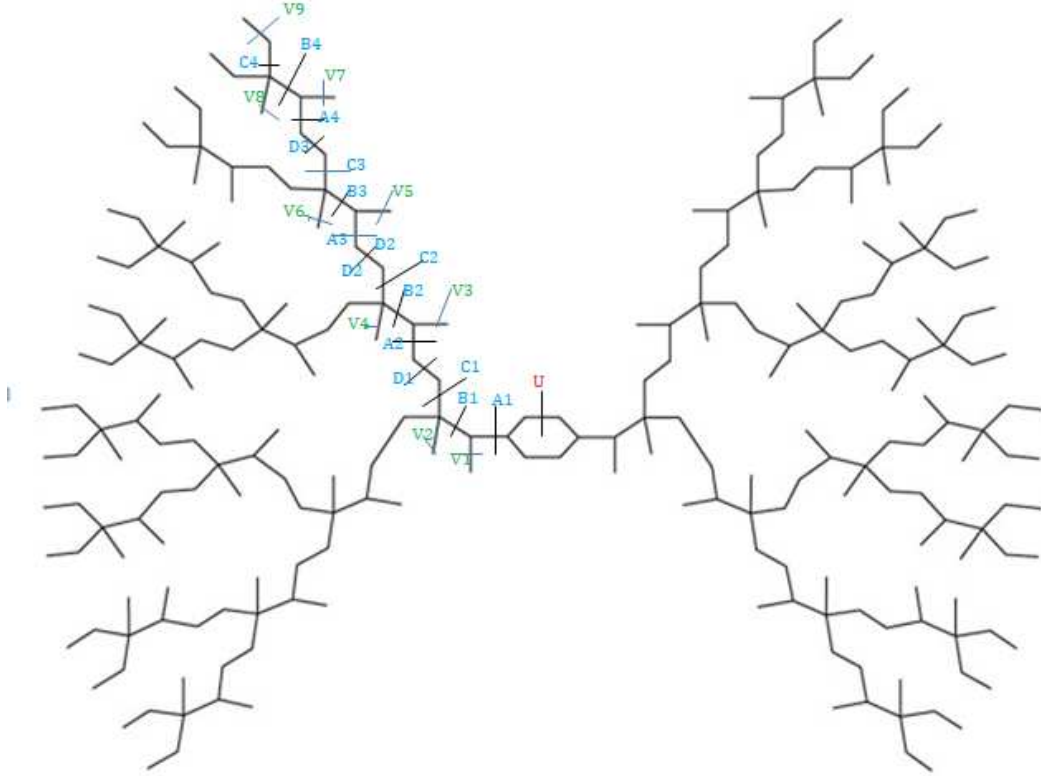


Figure 3: Aliphatic polyamide dendrimer

Theorem 5.1. *The vertex Szeged index for Aliphatic Polyamide dendrimers is given as:*

$$Sz(D_3(n)) = 2^{2n}[1024n - 1728] + 2^n[1800 - 352n] - 18 \quad (34)$$

Proof. Followed by values depicted in Table (11) and the expression of vertex Szeged index, we calculated equation (34) in the following way:

Representation	n_u	n_v	Frequency
$uv \in V_m, 1 \leq m \leq 2(3 \times 2^n - 2)$	$2^{n+4} - 11$	1	$3 \times 2^{n+1} - 4$
$uv \in U_m, 1 \leq m \leq n$	$2^{n+3} - 5$	$2^{n+3} - 5$	6
$uv \in A_i, 1 \leq i \leq n$	$2^{n+4} - 2^{i+3} - 2$	$2 \times (2^{i+2} - 4)$	2^{n-i+1}
$uv \in B_i, 1 \leq i \leq n$	$2^{n+4} - 2^{i+3}$	$2 \times (2^{i+2} - 5)$	2^{n-i+1}
$uv \in C_i, 1 \leq i \leq n$	$2^{n+4} - 2^{i+2} - 4$	$2^{i+2} - 6$	2^{n-i+2}
$uv \in D_i, 1 \leq i \leq n - 1$	$2^{n+4} - 2^{i+3} - 3$	$2^{i+3} - 7$	2^{n-i+1}

Table 11: The values of n_u and n_v of graph Aliphatic polyamide dendrimers

$$\begin{aligned}
Sz(D_3(n)) &= (2^{n+4} - 11) \times (1) \times (3 \times 2^{n+1} - 4) + (6 \times (2^{n+3} - 5)^2) \\
&+ \sum_{i=1}^n 2^{n-i+1} \times (2^{n+4} - 2^{i+3} - 2) \times (2 \times 2^{i+2} - 4) \\
&+ \sum_{i=1}^n 2^{n-i+1} \times (2 \times 2^{i+2} - 5) \times (2^{n+4} - 2^{i+3}) \\
&+ \sum_{i=1}^n 2^{n-i+2} \times (2^{n+4} - 2^{i+2} - 4) \times (2^{i+2} - 6) \\
&+ \sum_{i=1}^{n-1} 2^{n-i+2} \times (2^{n+4} - 2^{i+3} - 3) \times (2^{i+3} - 7)
\end{aligned} \quad (35)$$

After further calculations, we get:

$$Sz(D_3(n)) = 2^{2n}[1024n - 1728] + 2^n[1800 - 352n] - 18. \quad (36)$$

□

Theorem 5.2. *The vertex Mostar index of Aliphatic polyamide dendrimers given by:*

$$Mo(D_3(n)) = 2^{2n}[256n - 1728] + 2^n[128n + 248]. \quad (37)$$

Proof. By using the values of Table (11) and the definition of vertex Mostar index, we calculate (37) in the following way:

$$\begin{aligned}
MoD_5(n) &= |2^{n+4} - 11 - 1| \times (3 \times 2^{n+1} - 4) + (6 \times |(2^{n+3} - 5) - (2^{n+3} - 5)|) \\
&+ \sum_{i=1}^n 2^{n-i+1} |(2^{n+4} - 2^{i+3} - 2) - (2 \times 2^{i+2} - 4)| \\
&+ \sum_{i=1}^n 2^{n-i+1} |(2 \times 2^{i+2} - 5) - (2^{n+4} - 2^{i+3})| \\
&+ \sum_{i=1}^n 2^{n-i+2} |(2^{n+4} - 2^{i+2} - 4) - (2^{i+2} - 6)| \\
&+ \sum_{i=1}^{n-1} 2^{n-i+2} |(2^{n+4} - 2^{i+3} - 3) - (2^{i+3} - 7)|
\end{aligned} \tag{38}$$

Simplification is performed and the following results are obtained

$$Mo(D_3(n)) = 2^{2n}[256] + 2^n[128n + 248]. \tag{39}$$

□

Theorem 5.3. *The edge Szeged Index of aliphatic polyamide dendrimers is given by:*

$$Sz_e(D_3(n)) = 2^{2n}[1024n - 1984] + 2^n[2036 - 416n] - 28. \tag{40}$$

Proof. According to values in Table 12 and the definition of edge Szeged index the equation (40) can be computed as:

Representation	n_u	n_v	Frequency
$uv \in V_m, 1 \leq m \leq 2(3 \times 2^n - 2)$	$2^{n+4} - 11$	0	$2(3 \times 2^n - 2)$
$uv \in U_i, 1 \leq i \leq n$	$2^{n+3} - 6$	$2^{n+3} - 6$	6
$uv \in A_i, 1 \leq i \leq n$	$2^{i+3} - 9$	$2^{n+4} - 2^{i+3} - 2$	2^{n-i+1}
$uv \in B_i, 1 \leq i \leq n$	$2^{i+3} - 11$	$2^{n+4} - 2^{i+3}$	2^{n-i+1}
$uv \in C_i, 1 \leq i \leq n$	$2^{i+2} - 7$	$2^{n+4} - 2^{i+2} - 4$	2^{n-i+2}
$uv \in D_i, 1 \leq i \leq n - 1$	$2^{i+3} - 8$	$2^{n+4} - 2^{i+3} - 3$	2^{n-i+1}

Table 12: The values of q_u and q_v of graph Aliphatic polyamide dendrimers

$$\begin{aligned}
Sz_e(D_3(n)) &= (2^{n+4} - 11) \times (0) \times (2 \times (3 \times 2^n - 2)) + (6 \times (2^{n+3} - 6)^2) \\
&+ \sum_{i=1}^n 2^{n-i+1} (2^{n+4} - 2^{i+3} - 2) (2^{i+3} - 9) \\
&+ \sum_{i=1}^n 2^{n-i+1} (2^{i+3} - 11) (2^{n+4} - 2^{i+3}) \\
&+ \sum_{i=1}^n 2^{n-i+2} (2^{n+4} - 2^{i+2} - 4) (2^{i+2} - 7) \\
&+ \sum_{i=1}^{n-1} 2^{n-i+2} (2^{n+4} - 2^{i+3} - 3) (2^{i+3} - 8)
\end{aligned} \tag{41}$$

After some simplifications, we obtain the following:

$$Sz_e(D_3(n)) = 2^{2n}[1024n - 1984] + 2^n[2036 - 416n] - 28. \tag{42}$$

□

Theorem 5.4. *The edge Mostar index of aliphatic polyamide dendrimers is given by:*

$$Mo_e(D_3(n)) = 2^{2n}[256n] + 2^n[128n + 232] - 24 \tag{43}$$

Proof. The table 12 illustrates the computations for edge Mostar index of aliphatic polyamide dendrimers(43):

$$\begin{aligned}
Mo_e(D_3(n)) &= |(2^{n+4} - 11) - (0)| \times (2 \times (3 \times 2^n - 2)) \\
&+ 6 \times |(2^{n+3} - 6) - (2^{n+3} - 6)| \\
&+ \sum_{i=1}^n 2^{n-i+1} \times |(2^{n+4} - 2^{i+3} - 2) - (2^{i+3} - 9)| \\
&+ \sum_{i=1}^n 2^{n-i+1} \times |(2^{i+3} - 11) - (2^{n+4} - 2^{i+3})| \\
&+ \sum_{i=1}^n 2^{n-i+2} \times |(2^{n+4} - 2^{i+2} - 4) - (2^{i+2} - 7)| \\
&+ \sum_{i=1}^{n-1} 2^{n-i+2} \times |(2^{n+4} - 2^{i+3} - 3) - (2^{i+3} - 8)|
\end{aligned} \tag{44}$$

After some calculations, we obtain the following:

$$Mo_e(D_3(n)) = 2^{2n}[256n] - 2^n[128n + 232] - 24. \tag{45}$$

□

Theorem 5.5. *The total Szeged index of aliphatic polyamide dendrimers is given by:*

$$Sz_t(D_3(n)) = 2^{2n}[4096n - 7424] + 2^n[1536n + 7672] + 98 \quad (46)$$

Proof. By using the values of Table 13 and the definition of total Szeged index, we calculate equation (46) in the following way:

Representation	t_u	t_v	Frequency
$uv \in V_m, 1 \leq m \leq 2(3 \times 2^n - 2)$	$2^{n+5} - 22$	1	$3 \times 2^{n+1} - 4$
$uv \in U_m, 1 \leq m \leq 6$	$2^{n+4} - 11$	$2^{n+4} - 11$	6
$uv \in A_i, 1 \leq i \leq n$	$2^{n+5} - 2^{i+4} - 4$	$2^{i+4} - 17$	2^{n-i+1}
$uv \in B_i, 1 \leq i \leq n$	$2^{n+5} - 2^{i+4}$	$2^{i+4} - 21$	2^{n-i+1}
$uv \in C_i, 1 \leq i \leq n$	$2^{n+5} - 2^{i+3} - 8$	$2^{i+3} - 13$	2^{n-i+2}
$uv \in D_i, 1 \leq i \leq n - 1$	$2^{n+5} - 2^{i+4} - 6$	$2^{i+4} - 15$	2^{n-i+1}

Table 13: The values of t_u and t_v of garph Aliphatic polyamide dendrimers

$$\begin{aligned}
Sz_t(D_3(n)) &= (2^{n+4} - 22)(1)(3 \times 2^{n+1} - 4) + 6(2 \times 2^{n+3} - 11)^2 \\
&+ \sum_{i=1}^n 2^{n-i+1}(2 \times 2^{n+4} - 2 \times 2^{i+3} - 4)(2 \times 2^{i+2} - 13) \\
&+ \sum_{i=1}^n 2^{n-i+1}(2 \times 2^{i+3} - 16)(2 \times 2^{n+4} - 2 \times 2^{i+3}) \\
&+ \sum_{i=1}^n 2^{n-i+2}(2 \times 2^{n+4} - 2 \times 2^{i+2} - 8)(2 \times 2^{i+2} - 13) \\
&+ \sum_{i=1}^{n-1} 2^{n-i+1}(2 \times 2^{n+4} - 2 \times 2^{i+3} - 6)(2 \times 2^{i+3} - 15) \quad (47)
\end{aligned}$$

Using simple calculations, we derive:

$$Sz(D_3(n)) = 2^{2n}[4096n - 7424] + 2^n[1536n + 7672] + 98. \quad (48)$$

□

Theorem 5.6. *The total Mostar index of aliphatic polyamide dendrimers is given by:*

$$Mot(D_3(n)) = 2^{2n}[512] - 2^n[256n + 480] - 32 \quad (49)$$

Proof. Followed by values depicted in Table 13 and the expression of total Mostar index, we calculated equation (49) in the following way:

$$\begin{aligned}
Mo_t(D_3(n)) &= (3 \times 2^{n+1} - 4) \times |2^{n+4} - 22 - 1| \\
&+ (6 \times |(2 \times 2^{n+3} - 11) - (2 \times 2^{n+3} - 11)|) \\
&+ \sum_{i=1}^n 2^{n-i+1} |(2 \times 2^{n+4} - 2 \times 2^{i+3} - 4) - (2 \times 2^{i+2} - 13)| \\
&+ \sum_{i=1}^n 2^{n-i+1} |(2 \times 2^{i+3} - 16) - (2 \times 2^{n+4} - 2 \times 2^{i+3})| \\
&+ \sum_{i=1}^n 2^{n-i+2} |(2 \times 2^{n+4} - 2 \times 2^{i+2} - 8) - (2 \times 2^{i+2} - 13)| \\
&+ \sum_{i=1}^{n-1} 2^{n-i+1} |(2 \times 2^{n+4} - 2 \times 2^{i+3} - 6) - (2 \times 2^{i+3} - 15)| \quad (50)
\end{aligned}$$

After further calculations, we get:

$$Mo_t(D_3(n)) = 2^{2n}[512] - 2^n[256n + 480] - 32. \quad (51)$$

□

6 Significance of Topological Descriptors in Property Prediction

Molecular descriptors are crucial in QSAR/QSPR modeling, as they provide a computational approach to predict the characteristics of dendrimers. This minimizes the need for costly and time-consuming experimental procedures. By analyzing molecular properties through descriptors, researchers can make informed predictions about chemical behavior. The systematic study of molecular descriptors, which began in the 1960s, has its roots in graph theory. This mathematical approach has facilitated the development of numerous descriptors that provide valuable insights into molecular behavior [21–26, 32]. Essential for predicting dendrimer characteristics, reducing the need for experimental procedures. Researchers have focused on topological analysis across various chemical disciplines, recognizing its predictive power.

Generation	Molecular weight	IR absorption <i>band – CO</i>	Glass transition temperature
$D_1(1)$	1423.4	1700	74.75
$D_1(2)$	3417.3	1703	97.6
$D_1(3)$	7405	1704	116.45

Table 14: Tabular values obtained for three generations of Phosphorus containing dendrimer ([34–37])

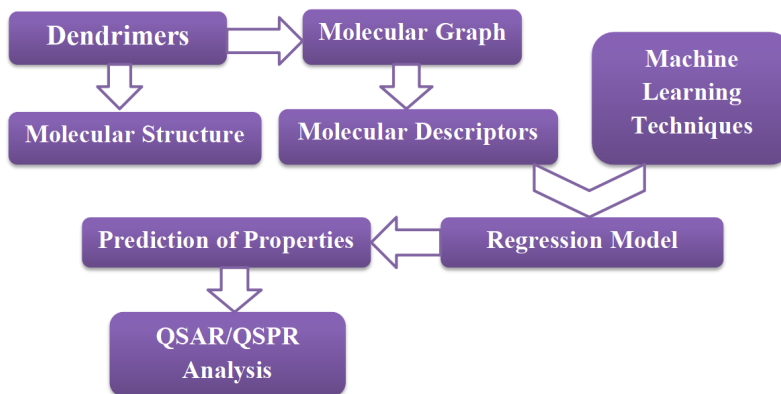


Figure 4: Flow chart represents significance of topological descriptors.

Generation	Molecular weight	IR absorption <i>band – CO</i>	Glass transition temperature
$D_3(1)$	834.82	1690	75
$D_3(2)$	1427.45	1685	80
$D_3(3)$	2612.7	1680	85

Table 15: Tabular values obtained for three generations of PDI cored dendrimer ([38], ChemDraw.)

Generation	Molecular weight	IR absorption <i>band – CO</i>	Glass transition temperature
$D_5(1)$	314	1629	–29.4
$D_5(2)$	771	1632	–26.6
$D_5(3)$	1684	1632	–21.6

Table 16: Tabular values obtained for three generations of Aliphatic polyamide dendrimer ([8])

Notable contributions from Kier [27], Randic [28], and Balaban [29, 30] significantly enhanced QSAR methodologies based on topological indices. The flow chart in Figure (4) presents the connection between molecular descriptors, QSAR/QSPR studies and considerable techniques. The continued evolution of topological and graph-theoretical approaches will likely lead to even more precise predictive models, reinforcing the importance of computational chemistry in modern research.

Descriptors	Molecular weight	IR absorption <i>band</i> – <i>CO</i>	Glass transition temperature
S_v	0.9802977	0.7838295	0.9083464
S_e	0.9799478	0.7827328	0.9076072
S_t	0.9801212	0.7832753	0.9079730
M_v	0.9874042	0.8080040	0.9243240
M_e	0.9874056	0.8080092	0.9243274
M_t	0.9874049	0.8080066	0.9243258

Table 17: Correlation of indices for Phosphorus containing dendrimer

Descriptors	Molecular weight	IR absorption <i>band</i> – <i>CO</i>	Glass transition temperature
S_v	0.9887856	−0.9427459	0.9427459
S_e	0.9891291	−0.9435164	0.9435164
S_t	0.9886226	−0.9423826	0.9423826
M_v	0.9900660	−0.9456546	0.9456546
M_e	0.9902872	−0.9461680	0.9461680
M_t	0.9904021	−0.9464359	0.9464359

Table 18: Correlation of indices of PDI cored dendrimer

Descriptors	Molecular weight	IR absorption <i>band</i> – <i>CO</i>	Glass transition temperature
S_v	0.9766048	0.5976831	0.9700975
S_e	0.9752136	0.5925582	0.9685300
S_t	0.9759563	0.5952790	0.9693662
M_v	0.9837151	0.6261659	0.9782086
M_e	0.9839778	0.6273093	0.9785122
M_t	0.9838472	0.6267401	0.9783612

Table 19: Correlation of indices of Aliphatic polyamide dendrimer

7 Linear Modeling and Comparative Analysis Pathway to Decision Making

The use of mathematical, statistical techniques and machine learning techniques, such as correlation theory, linear regression analysis, enhances the reliability of molecular descriptors.

These methods allow for the identification of meaningful relationships between molecular structures and their physico-chemical properties. Researchers have focused on topological analysis across various chemical disciplines, recognizing its predictive power. Linear regression or least square method are used to analyze the correlation values and identifies the most suitable fit straight line. The index with the highest correlation is considered the best fit for the given molecular characteristics [31]. A correlation coefficient values ranging from -1 to 1 [33]. The strongest correlation occurs when the coefficient is close to either +1 or -1. The regression model used for this analysis is linear

$$Y = A + BX, \quad (52)$$

where Y , A , B and X represents, y -axis, intercept, slope of the line, property, molecular descriptor. The properties of these dendrimers taken for the study are molecular weight, IR absorption band-CO and glass transition temperature. The property values are provided in Tables (14), (15), (16) [34]- [39]. The correlation value of related to Phosphorus, PDI and Alaphatic dendrimers related to Szeged indices (vertex, edge and total) and Mostar indices(vertex, edge and total) for generation values varying from $n = 1 \dots 7$ are provided in Table (17), (18) and (19).

The analysis reveals that among the considered topological indices, the Edge Mostar index Edge Mostar index (Mo_e) exhibits the highest correlation value for phosphorus-containing dendrimers. Notably, Mo_e index demonstrates a strong correlation with all three investigated properties: Molecular Weight, IR absorption- Co, and Glass Transition Temperature. This suggests that Mo_e serves as a more comprehensive descriptor of these properties compared to other indices. Furthermore, the best-fit linear regression equations for Molecular Weight, IR absorption (Co), and Glass Transition Temperature have been determined and are presented in Table (20). The regression line for first three stages $D_1(1)$, $D_1(2)$ and $D_1(3)$ of phosphorous containg dendrimer is represented in Figure (5).

Property	Descriptors	Regression Line	R^2
Molecular weight	Edge Mostar	$y = 1601 + 0.00236x$	0.975
IR absorption <i>band – CO</i>	Edge Mostar	$y = 1071 + 0.00000132x$	0.6529
Glass transition temperature	Edge Mostar	$y = 81.07 + 0.00001477x$	0.8544

Table 20: Values for each of the properties for three generation of Phosphorus containing dendrimer

For PDI-cored structures, the total Mostar index (Mo_t) exhibits the highest correlation with key physicochemical properties, including Molecular Weight, IR absorption- Co, and glass transition Temperature. Among these, the coefficient of coorelations R^2 for Molecular Weight demonstrates the highest value, indicating a strong and best-fit relationship. Additionally, glass transition temperature also shows a significant correlation with Mo_t , further reinforcing its predictive capability for structural-property relationships. It has been observed

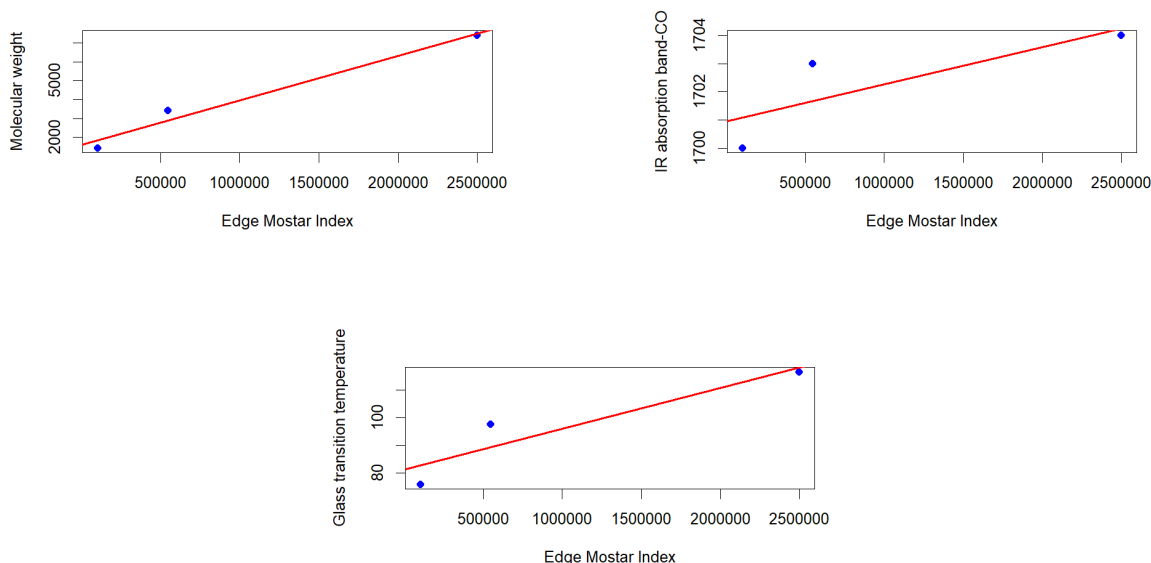


Figure 5: Scatter diagrams of Phosphorus containing dendrimer (PDI) for the best fit of attributes

that IR absorption-Co reflect inverse relation with the Mo_t . The equations presented in Table (21) represent the best-fit linear regression models, while their graphical illustrations are provided in Figure (6). We observed that Total Mostar index as a key topological descriptor for predicting essential molecular properties in PDI-cored dendrimers.

Property	Descriptors	Regression Line	R^2
Molecular weight	Total Mostar	$y = 778.9 + 0.03595x$	0.9809
IR absorption <i>band - CO</i>	Total Mostar	$y = 1689 - 0.0001897x$	0.8957
Glass transition temperature	Total Mostar	$y = 75.53 + 0.0001897x$	0.8957

Table 21: Values for each of the properties for three generation of PDI cored dendrimer

The correlation analysis of Aliphatic dendrimers (Table (19)) reveals a varied relationship with the considered indices. The high R^2 value of the Total Mostar index indicates a strong correlation with Glass Transition Temperature, while the Edge Mostar index serves as the best predictor for Molecular Weight, with a value close to 1. The best-fit linear regression equations are provided in Table (22). The scatter diagram for Aliphatic dendrimers is presented in Figure (7). In chemical processes, molecular weight is crucial for calculating stoichiometry, enabling chemists to determine reactant and product proportions, measure precise amounts, balance equations, and predict yields. Similarly, an absorption band repre-

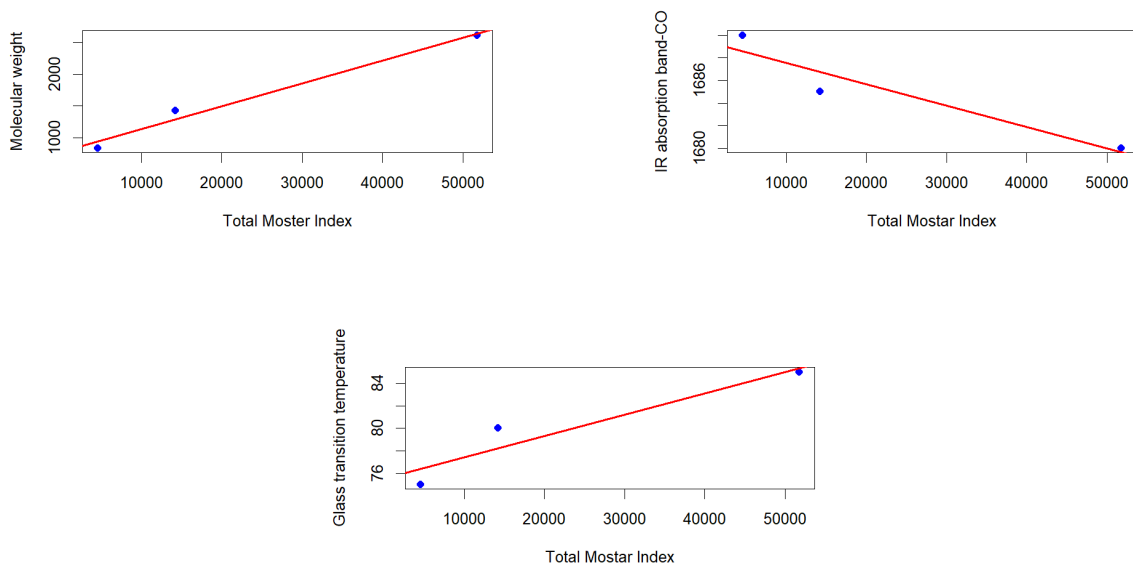


Figure 6: Scatter diagrams of Phosphorus containing dendrimer (PDI) for the best fit of attributes

Property	Descriptors	Regression Line	R^2
Molecular weight	Edge Mostar	$y = 393.6896 + 0.1148x$	0.9682
IR absorption <i>band - CO</i>	Edge Mostar	$y = 1630 + 0.0001817x$	0.3935
Glass transition temperature	Total Mostar	$y = -28.85 + 0.0006467x$	0.9575

Table 22: Values obtained for each of the properties of three generation of Aliphatic containing dendrimer

sents a specific range of wavelengths, frequencies, or energies in the electromagnetic spectrum where a material absorbs radiation due to electronic, vibrational, or rotational transitions of molecules. The glass transition temperature is the point at which an amorphous material, such as polymers or glasses, transitions from a hard and brittle state to a soft and rubbery state. Unlike the sharp melting point of crystalline solids, this transition is gradual and reversible. Overall, the correlation data suggest that all indices exhibit a significant relationship with the studied properties. Among them, the best fit is obtained is edge Mostar for Phosphorus, total Mostar for PDI and Edge and Total Mostar for Aliphatic dendrimer. The

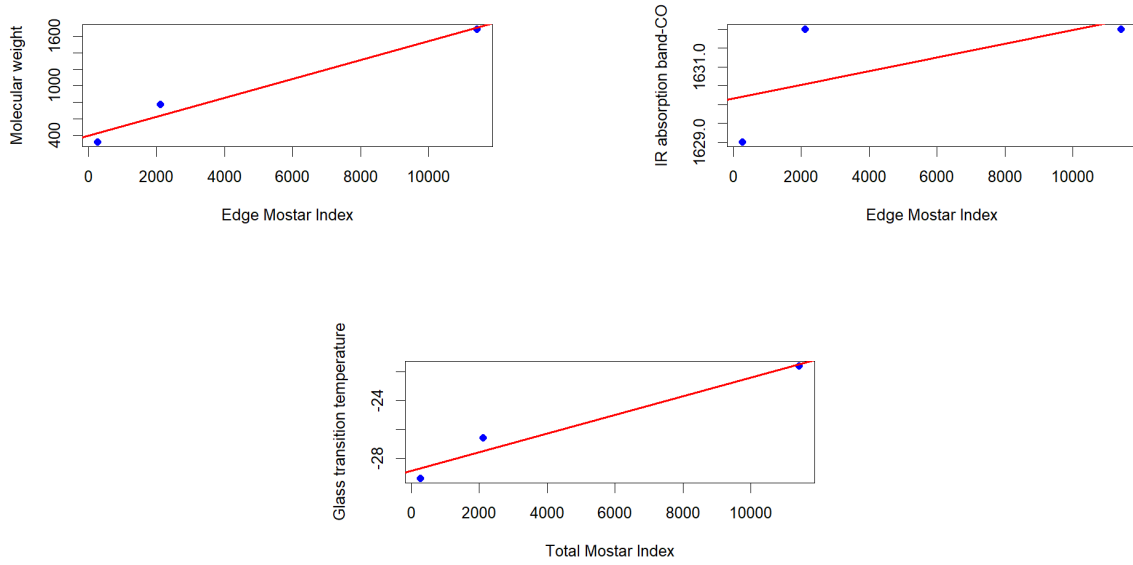


Figure 7: Scatter diagrams of Phosphorus containing dendrimer (PDI) for the best fit of attributes

linear regression of PDI dendrimer obtained is as follows:

$$\begin{aligned}
 MW &= 1601 + 0.00236Mo_e, \\
 IR - Co &= 1701 + 0.00000132Mo_e, \\
 Tg &= 81.07 + 0.00001477Mo_e.
 \end{aligned} \tag{53}$$

$$\begin{aligned}
 MW &= 778.9 + 0.03595Mo_e, \\
 IR - Co &= 1689 - 0.0001897Mo_e, \\
 Tg &= 75.53 + 0.0001897Mo_e.
 \end{aligned} \tag{54}$$

Linear regression of Alaphatic dendrimer

$$\begin{aligned}
 MW &= 75.53 + 0.0001897Mo_e, \\
 IR - Co &= 1630 + 0.0001817Mo_e, \\
 Tg &= -28.85 + 0.0006467Mo_e.
 \end{aligned} \tag{55}$$

where MW , $IR - Co$, Tg represents Molecular weight, IR Absorption band, Glass transition temperature. The graphs are plotted with the help of R Studio.

n	Sz	Sze	Szt	Mo	Moe	Mot
1	1893066	1950768	7690206	99324	105366	204690
2	14375646	15269076	59286558	516732	548118	1064850
3	87934758	94897092	365566974	2357388	2500422	4857810
4	479077686	521960240	2001275666	10103244	10715910	20819154
5	2484613334	2669076688	1.020238×10^{10}	4193500	44477766	86413266
6	11824398486	1.301904×10^{10}	4.965953×10^{10}	171126924	181499718	352626642
7	5.565559×10^{10}	6.14707×10^{10}	2.341×10^{11}	691946882	733886022	1.425832914×10^9

Table 23: Data representation of descriptors of Phosphorus Containing dendrimer

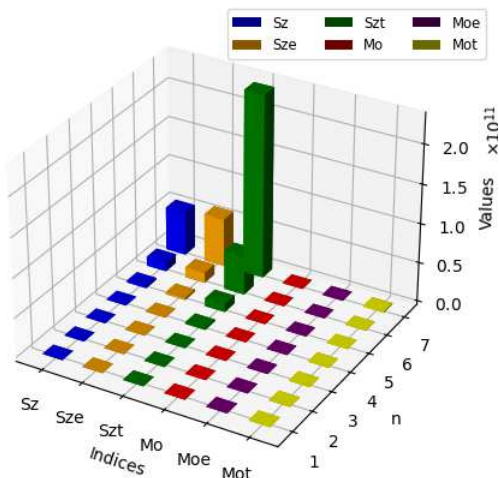
n	Sz	Sze	Szt	Mo	Moe	Mot
1	34576	35196	139800	2120	2460	4580
2	119288	118540	476152	6808	7428	14236
3	472072	460668	1886456	25304	26844	51788
4	2012840	1945084	7917784	99736	102036	201772
5	8869096	8541756	34825560	400280	404820	805100
6	39469288	38022460	154992472	1611928	1620948	3222876
7	175490152	169371708	689739096	6485144	6503124	12988268

Table 24: Data representation of descriptors of PDI Cored Dendrimer

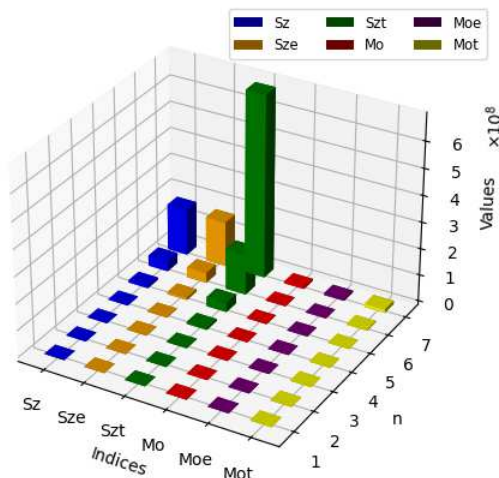
n	Sz	Sze	Szt	Ao	Moe	Mot
1	1470	1036	5006	272	280	544
2	15118	12468	55166	2080	2120	4192
3	108846	95876	409438	11328	11432	22752
4	657518	599844	2514718	53876	53608	106976
5	3587310	3429480	13860510	233728	234216	467936
6	18338286	17329380	71355326	983552	984552	1968096
7	89674734	85567972	350485406	4047872	4649896	8097760

Table 25: Data representation of descriptors of Aliphatic Polyamide dendrimer

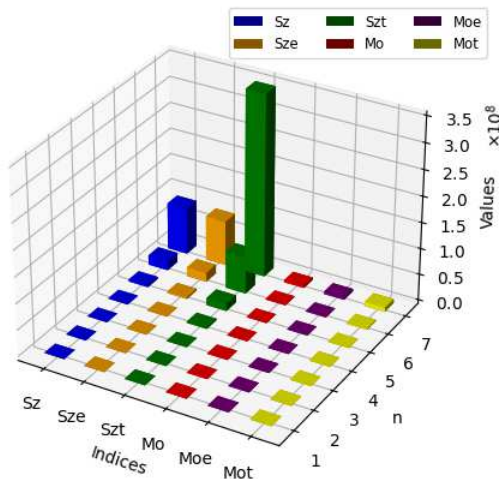
The mathematical analysis and comparison of distance-based molecular descriptors for Phosphorus-containing, PDI-cored and Aliphatic dendrimers is presented in Table (25, 24,



(a) Growth of Phosphorus Cotaining Dendrimers with respect to descriptors



(b) Growth of PDI Cored Dendrimers with respect to descriptors



(c) Growth of Aliphatic Polyamide Dendrimers with respect to descriptors

Figure 8: A comparison graphs of the topological indices

23). Graphical and numerical representations (Figures (8) , Tables 23-25) illustrate variations in topological indices across generations 1 to 7. The Total Szeged index exhibits exponential growth in phosphorus-containing dendrimers, while the Mostar index grows slowly. Similarly, in PDI-cored and aliphatic dendrimers, the Total Szeged index reaches its highest value in the 7th generation, whereas the Total Mostar index remains the lowest. Overall, the Total Szeged index shows the most significant growth trend. A significant research gap remains in the study of this dendrimer group, particularly in areas such as the neighborhood method, M-polynomial technique, reverse degree approach, and multiplicative degree approach, among others. Evaluating and comparing topological descriptors can help identify the most effec-

tive descriptor for feature correlation, ultimately reducing the reliance on time-consuming laboratory experiments.

8 Conclusions

Dendrimers exhibit a unique structural composition that makes them highly valuable in various scientific and industrial applications, particularly in drug delivery and molecular engineering. This study has successfully established a distance-based characterization of these dendrimers through topological descriptors, enabling a deeper understanding of their molecular properties. By deriving numerical expressions for key descriptors such as the Szeged, Edge Szeged, total Szeged, Mostar, edge Mostar and total Mostar indices, we have provided a framework for predicting the physicochemical properties of successive dendrimer generations.

Moreover, the application of QSAR/QSPR modeling has demonstrated the strong correlation between these descriptors and key molecular attributes, facilitating property prediction without the need for extensive experimental trials. The regression models developed in this work further support the potential of mathematical chemistry in streamlining molecular characterization, saving time and resources in laboratory settings.

The phosphorus containing dendrimer has the highest Szeged indices, meaning it has a highly branched structure that can hold a large amount of drug molecules. However, its high Mostar indices indicate significant structural asymmetry, which could make it less soluble and harder for the drug to diffuse properly in the body.

The PDI cored dendrimer has a more balanced structure, with moderate Szeged and Mostar indices. This suggests that it can efficiently load drugs while still maintaining good stability and uniformity, making it a strong candidate for controlled drug release. The aliphatic polyamide dendrimer has the simplest structure, with the lowest Szeged indices (fewer branches) and the lowest Mostar indices (more symmetrical). This makes it highly biocompatible and soluble, which is important for predictable drug diffusion in the bloodstream.

By integrating mathematical models with experimental validation, the field of dendrimer research can progress towards more precise and efficient molecular design, ultimately enhancing their applicability in real-world scenarios. This interdisciplinary approach minimizes the reliance on vast laboratory experiments, property evaluation becoming more productive and time-saving.

Data Availability Statement: The data that support the findings of this study are available from the corresponding author.

Acknowledgements: We would like to express our sincere gratitude to Dr. Isra at National University of Modern Languages, Islamabad, for her invaluable assistance with the statistical data analysis in this study.

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