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Dendrimers are highly defined hyperbranched artificial macromolecules, synthesised by convergent or divergent approach with specific applications in various fields. Dendrimers can be represented as graph models, from which a quantitative description can be drawn in relation with their structural properties. The distance-based and the degree-based descriptors have great importance and huge applications in structural chemistry. These indices together with entropy measures are found to be more effective and have found application in scientific fields. The idea of graph entropy is to characterise the complexity of graphs. The use of these graph invariants in quantitative structure property relationship and quantitative structure activity relationship studies has become of major interest in recent years. In this paper, the distance-based molecular descriptors of pyrene cored dendrimers are studied applying the technique of converting original graph into quotient graphs using $\Theta^*$-classes. It is to be noted that, since the pyrene cored dendrimer, $G_n$ is not a partial cube, usual cut method is not applicable. Further, various degree-based descriptors and their corresponding graph entropies of the pyrene cored dendrimers are also studied. Based on the obtained results, a comparative analysis as well as a regression analysis was carried out.

1. Introduction

Dendrimers are highly defined hyperbranched artificial macromolecules that represent a class of novel polymers. These molecules were discovered by Fritz Vogtle in 1978, Tomalia et al. [1] in the early 1980s and George R. Newkome during the same period but independently [1, 2]. They feature distinct 3D molecular architectures with well-defined structures that include three different units: the central core, dendrons, and terminal functional group. The core is surrounded by dendron layers known as generations or branches that extend outward and terminate with surface groups. Over the last few decades, a variety of dendrimers have been synthesised using either a convergent or divergent approach, with specialised uses in a variety of sectors [3]. Dendrimers have a compact and globular structure, a spherical shape, a regular architecture, and develop in a stepwise manner. These structures are non-crystalline and amorphous with lower glass temperatures. They also have high aqueous solubility, high nonpolar solubility and low compressibility. These qualities and properties distinguish dendrimer from linear or branching polymers [4]. Their high degree of molecular uniformity and low polydispersity make them attractive materials for the development of nanomedicines [5]. They also have applications in drug delivery [6, 7], material science and biology [8], magnetic resonance imaging [9], homogeneous catalysis, optical data storage, solar cells, science and engineering, organic light-emitting device, and so on [10, 11]. The dendrimer chemistry provides an effective tool for tuning the properties of the dendrimers by altering the core or tailoring the size, chemical, and topological structures of the dendrons [11]. The proper core selection and detailed design of dendrons are essential for the final attributes of a dendrimer.
Pyrene, a polycyclic aromatic hydrocarbon consisting of four fused benzene rings is a fascinating core for constructing light-emitting dendrimers. Carbazole is a luminescent compound with high hole-transporting ability arising from the lone pair electrons in nitrogen atom and have been incorporated as dendrons to construct dendrimer materials [12]. The combination of pyrene and carbazole is expected to provide improved thermal stability and good charge-transportation ability. Three generations of dendrimers G1, G2, and G3 with a pyrene core and 9-phenylcarbazole derivatives dendrons designed and synthesised by convergent approach were reported by You et al. [11, 12]. These dendrimers exhibit remarkable photophysical and redox properties [14].

A topological index is a numerical number associated with a graph that is related to the graph’s structural characteristics. Chemical structures can be represented as graph models and can be assigned with these numerical values, which are associated with the physical, chemical, and biological properties of the structure. Hence, the graph models may be utilised to investigate different aspects of the relevant chemical structure. In 1947, chemist Wiener [15] developed the Wiener index, the first molecular descriptor. Many additional molecular descriptors were added, each of which corresponds to a particular property of the chemical structure. The distance- and degree-based indices are generally recognised because of their numerous applications in structural chemistry. In recent years, there has been a lot of interest in using these graph invariants in quantitative structure–property relationships (QSPR) and quantitative structure–activity relationships (QSAR) research. They have also found application in various areas of chemistry, informatics, biology, etc. [15–22].

The concept of information entropy was first presented by Shannon [23] in order to analyse and quantify the complexity of data and information transmission. An important application of information entropy is to study the complexity and the quantum chemical electron densities of molecular structures [24]. Later Rasheysky introduced the idea of graph entropy in 1955 to characterise the complexity of graphs [25, 26]. The two categories of entropies are deterministic and probabilistic. The probabilistic method is applicable in characterising a chemical structure and it is classified into intrinsic and extrinsic, in which we determine the extrinsic measure. In intrinsic measures, a graph is partitioned into components sharing similar structures and a probability distribution is found over those components and in extrinsic measures, a probability function is assigned to elements of the graph, the vertices, or edges [27].

The topological indices of various dendrimers were studied in the past few years [28–33]. In this paper, the distance-based indices defined in Table 1 are studied for the pyrene cored dendrimers $Gn : n \geq 1$ and Py$Gn : n \geq 0$, where $n$ is the generation of the dendrimer. The various degree-based indices given in Table 2, and their corresponding graph entropies are also studied for the structures, see [46–50] for more recent papers in this field. The chemical applicability of these works is widely recognised by researchers and scientists. This motivated many researchers in studying the concept of topological indices of chemical structures, see [51–61] for applications of chemical graph theory in various fields. The structure of pyrene cored dendrimers $G2$ and Py$G2$ are given in Figure 1.

2. Mathematical Terminologies

Consider a simple, finite, connected graph $G$ with vertex set, $V(G)$ and edge set, $E(G)$. The number of edges connected to a vertex $p$ is the degree of vertex $p$, denoted by $d_p$. For more basic terminologies and definitions refer to [34, 62].

### Table 1: Distance-based indices of strength-weighted graph $G_{sw} = G$.

<table>
<thead>
<tr>
<th>Distance-based index</th>
<th>Mathematical formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wiener [34]</td>
<td>$W(G) = \sum_{p \neq q} w_p w_q d_{p,q}$</td>
</tr>
<tr>
<td>Szeged [34]</td>
<td>$S_z(G) = \sum_{p \neq q} a_{p,q}$</td>
</tr>
<tr>
<td>Edge Szeged [34]</td>
<td>$E_s(G) = \sum_{p \neq q} a_{p,q}$</td>
</tr>
<tr>
<td>Padmakar–Ivan [34]</td>
<td>$\sigma(G) = \sum_{p \neq q} a_{p,q}$</td>
</tr>
<tr>
<td>Mostar [35]</td>
<td>$M_o(G) = \sum_{p \neq q} a_{p,q}$</td>
</tr>
</tbody>
</table>

### Table 2: Degree-based indices of graph $G$.

<table>
<thead>
<tr>
<th>Degree-based index</th>
<th>Mathematical formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>First Zagreb [36]</td>
<td>$M_1(G) = \sum_{p \neq q} (d_p + d_q)$</td>
</tr>
<tr>
<td>Second Zagreb [36]</td>
<td>$M_2(G) = \sum_{p \neq q} (d_p \times d_q)$</td>
</tr>
<tr>
<td>Harmonic [37]</td>
<td>$H(G) = \frac{\sum_{p \neq q} (d_p + d_q)}{\sqrt{\sum_{p \neq q} d_p d_q}}$</td>
</tr>
<tr>
<td>Hyper Zagreb [38]</td>
<td>$HM(G) = \frac{\sum_{p \neq q} (d_p + d_q)^2}{\sum_{p \neq q} d_p d_q}$</td>
</tr>
<tr>
<td>Forgotten [39]</td>
<td>$F(G) = \sum_{p \neq q} ((d_p)^2 + (d_q)^2)$</td>
</tr>
<tr>
<td>Randić [20]</td>
<td>$R(G) = \frac{\sum_{p \neq q} (d_p + d_q)}{\sqrt{\sum_{p \neq q} d_p d_q}}$</td>
</tr>
<tr>
<td>Reciprocal Randić [40]</td>
<td>$RR(G) = \sum_{p \neq q} (\sqrt{d_p} \times \sqrt{d_q})$</td>
</tr>
<tr>
<td>Sum-connectivity [41]</td>
<td>$SC(G) = \frac{1}{\sum_{p \neq q} d_p d_q}$</td>
</tr>
<tr>
<td>Geometric arithmetic [42]</td>
<td>$GA(G) = \frac{1}{\sum_{p \neq q} \sqrt{d_p d_q}}$</td>
</tr>
<tr>
<td>Atom bond connectivity [43]</td>
<td>$ABC(G) = \frac{\sum_{p \neq q} (\sqrt{d_p} + \sqrt{d_q})^2}{\sum_{p \neq q} d_p d_q}$</td>
</tr>
<tr>
<td>Irregularity measure [44]</td>
<td>$irr(G) = \sum_{p \neq q}</td>
</tr>
<tr>
<td>Sigma [45]</td>
<td>$\sigma(G) = \sum_{p \neq q} (d_p - d_q)^2$</td>
</tr>
</tbody>
</table>
For an edge \( g = pq \in E(G) \),
\[
N_p(g|G) = \{ x \in V(G) : d_C(p, x) < d_C(q, x) \}, \quad \text{and}
\]
\[
M_p(g|G) = \{ y \in E(G) : d_C(p, y) < d_C(q, y) \}.
\]

The cardinality of the sets \( N_p(g|G) \) and \( M_p(g|G) \) are denoted as \( n_p(g|G) \) and \( m_p(g|G) \), respectively. The values of \( n_q(g|G) \) and \( m_q(g|G) \) are analogous. The strength weighted graph denoted by \( G_w = (G, [w_v, s_v], s_e) \), where \( w_v \) is the vertex weight, \( s_v \) is the vertex strength, and \( s_e \) is the edge strength was presented by Arockiaraj et al. [34]. And the sets \( N_p(G_w) = N_p(g|G) \) and \( M_p(g|G_w) = M_p(g|G) \) are described with cardinality:
\[
n_p(g|G_w) = \sum_{x \in N_p(g|G_w)} w_v(x) \quad \text{and} \quad m_p(g|G_w) = \sum_{x \in N_p(g|G_w)} s_v(x) + \sum_{y \in M_p(g|G_w)} s_e(y).
\] (1)

The values of \( n_q(g|G_w) \) and \( m_q(e|G_w) \) are analogous.

The Djoković–Winkler (\( \Theta \)) relation plays a major role in computing topological indices, which is defined as \( d_C(q, b) + d_C(p, a) \neq d_C(p, b) + d_C(q, a) \), for two edges \( g = pq \) and \( f = ab \) of \( G \). The relation \( \Theta \) is reflexive, symmetric, and transitive in the case of partial cubes. Its transitive closure \( \Theta^* \) forms an equivalence relation in general and partitions the edge set into convex components. Let \( F = \{ F_1, F_2, \ldots, F_j \} \) be the \( \Theta^* \) equivalence class. A partition \( \mathcal{E} = \{ E_1, E_2, \ldots, E_k \} \) of \( E(G) \) is said to be coarser than partition \( F \) if each set \( E_i \) is the union of one or more \( \Theta^* \)-classes of \( G \).

To determine the entropy measures, we have followed Shannons’s model. In communication and transmission of information, each element of the information are assigned with the probability functions in the form of symbols \( x_1, x_2, \ldots, x_n \). If \( N_i \) denotes the number of times \( x_i \) appear in the information and \( N \) denotes the total length of information, then the Shannon’s original information entropy measure, denoted by \( h \) is defined as follows [24]:
\[
h = - \sum_{i=1}^{n} p_i \log(p_i), \quad \text{where} \quad p_i = \frac{N_i}{N}.
\] (2)

In chemical graphs, the elements are the edges of the graph to which the probability function is assigned using the topological indices. If \( TI(G) \) denotes the topological index of \( G \), then in general:
\[
TI(G) = \sum_{g \in E(G)} t(g),
\] (3)

where \( t(g) \) is the functional characterisation of the topological index.

For example, if we consider the first Zagreb index, then the functional \( t(g) = d_p + d_q \).

The graph entropy measure is denoted by \( ENT_{TI}(G) \) and is defined as follows [24, 48, 63]:
\[
ENT_{TI}(G) = - \sum_{g \in E(G)} p_g \log(p_g),
\]

where \( p_g = \frac{t(g)}{\sum_{g \in E(G)} t(g)} \).

(4)
Therefore, \( \text{ENT}_{T}(G) = \log(T(G)) - \frac{1}{T(G)} \sum_{g \in T(G)} t(g) \log(t(g)) \).

\[
W(G, w) = m W(H) + m(m-1) \sum_{x \in V(H_1)} \sum_{y \in V(H_2)} w(x)w(y) + \sum_{x \in V(H_1)} w(x) \left\{ m w(e)d(e, x) + \frac{m(m-1)}{2} \sum_{y \in V(H_2)} w(y)(d(h_2, y) + d(x, h_1)) \right\},
\]

where \( e \in V(K_1) \).

**Theorem 2.** For \( n \geq 1 \):

\[
W(G_n) = (115,126 - 11.628n) \times 2^n + (51,984n - 84,246) \times 2^{2n} - 30,518,
\]

\[
S_a(G_n) = (214,786 - 19,304n) \times 2^n + (98,192n - 158,726) \times 2^{2n} - 55,052,
\]

\[
S_b(G_n) = (327,218 - 27,692n) \times 2^n + (143,888n - 241,638) \times 2^{2n} - 84,692,
\]

\[
P_l(G_n) = 8.096 \times 2^{2n} - 12.924 \times 2^n + 5,136,
\]

\[
M_0(G_n) = 6.688 \times 2^{2n} - (2.660n + 7.768) \times 2^n + 1,192,
\]

\[
M_0(G_n) = 8.096 \times 2^{2n} - (3.220n + 9,360) \times 2^n + 1,412.
\]

**Proof.** The molecular graph \( G_n \) has 76 \( \times 2^n - 60 \) vertices, 92 \( \times 2^n - 73 \) edges and 40 \( \times 2^n - 33 \) \( \theta^* \)-classes. Let us consider \( G_2 \). The sets \( E_i \), which is coarser than the \( \theta^* \)-classes chosen for \( G_2 \) are highlighted in Figure 2. We convert the original graph into quotient graphs \( G_n/E_i \) and we obtain \( 2n + 1 \) quotient graphs for \( G_n \). There are three types of quotient graphs \{ \( G_n/E_1 \), \( G_n/E_2 \), \( G_n/E_{2i+1} : 1 \leq i \leq n \) \} for \( G_n \).

**Theorem 1** (see [67]). Let \( G = K_o \circ H \) be a connected weighted graph, and let \( h_i \) be the root nodes of \( H_i \), where \( H_i \approx H_j, i \in [m]; m \geq 2 \). Then:

\[
fH \in V(H_1), y \in V(H_2),
\]

\[
\left\{ m w(e)d(e, x) + \frac{m(m-1)}{2} \sum_{y \in V(H_2)} w(y)(d(h_2, y) + d(x, h_1)) \right\}.
\]

The first type of quotient graph \( G_n/E_1 \) has 16 vertices and 19 edges, among which four vertices, \( a_i, 1 \leq j \leq 4 \) has \( \{w_r(a_j), s_r(a_j)\} = (19 \times 2^n - 18, 23 \times 2^n - 23) \). From the remaining vertices, vertex weight is 1 and vertex strength is 0, as given in Figure 3.

The second type of quotient graph \( G_n/E_2, 1 \leq j \leq n \) has a weighted core vertex, say \( c \) attached with \( m = 2i+1, 1 \leq i \leq n \) branches such that one vertex in each branch has same weighted values as given in Figure 4. Let us take those vertices to be \( b_k, 1 \leq k \leq m \). Then,

\[
\{w_r(c), s_r(c)\} = (38 \times 2^n - 60, 46 \times 2^n - 73),
\]

\[
\{w_r(b_k), s_r(b_k)\} = (19 \times 2^n - 24, 23 \times 2^n - 30).
\]

For the remaining vertices, vertex weight and vertex strength is 1 and 0, respectively.

The third type of quotient graph \( G_n/E_{2i+1}, 1 \leq i \leq n \) has a weighted core vertex, say \( f \) attached with \( m = 2i+1, 1 \leq i \leq n \) branches such that two vertices in each branch has same weighted values as given in Figure 5. Those vertices are \( d_r, 1 \leq r \leq 2m \). Then,

\[
\{w_r(f), s_r(f)\} = (50 \times 2^n - 60, 60 \times 2^n - 73),
\]

\[
\{w_r(d_r), s_r(d_r)\} = (19 \times 2^n - 18, 23 \times 2^n - 23).
\]
Also, $S_z(G/E_1) = 12 \left(4 + w_v(a_1)\right) \left(8 + 3 w_v(a_1)\right) + 4 \left(1 + 2 w_v(a_1)\right) \left(11 + 2 w_v(a_1)\right) + 3 \left(6 + 2 w_v(a_1)\right) \left(6 + 2 w_v(a_1)\right)$.

\[
S_z(G/E_1) = 23,104 \times 2^n - 36,024 \times 2^n + 13,928.
\]

$S_z(G/E_1) = 12 \left(s_v(a_1) + 4\right) \left(3s_v(a_1) + 12\right) + 4 \left(2 + 2s_v(a_1)\right) \left(15 + 2s_v(a_1)\right) + 3 \left(8 + 2s_v(a_1)\right) \left(8 + 2s_v(a_1)\right)$.

\[
S_z(G/E_1) = 3,3856 \times 2^n - 55,752 \times 2^n + 22,784.
\]

$PI(G/E_1) = 12 \left(\left(s_v(a_1) + 4\right) \left(3s_v(a_1) + 12\right)\right) + 4 \left(\left(2 + 2s_v(a_1)\right) \left(15 + 2s_v(a_1)\right)\right) + 3 \left(\left(8 + 2s_v(a_1)\right) \left(8 + 2s_v(a_1)\right)\right)$.

\[
PI(G/E_1) = 1,748 \times 2^n - 1,1440.
\]

\[
Mo(G/E_1) = 12 \left|4 + w_v(a_1)\right| - 8 + 3 w_v(a_1)\right)\left| + 4 \left(1 + 2 w_v(a_1)\right) - 11 + 2 w_v(a_1)\right)\left| + 3 \left|6 + 2 w_v(a_1)\right| - 6 + 2 w_v(a_1)\right)\left|
\]

\[
Mo(G/E_1) = 456 \times 2^n - 344.
\]

$Mo_v(G/E_1) = 12 \left|s_v(a_1) + 4\right| - 3s_v(a_1) + 12\left| \left| + 4 \left|2 + 2s_v(a_1)\right| - 15 + 2s_v(a_1)\right|\left| + 3 \left|8 + 2s_v(a_1)\right| - 8 + 2s_v(a_1)\right|\left|
\]

\[
Mo_v(G/E_1) = 552 \times 2^n - 404.
\]

Consider $G/E_2$ (Figure 4), with $w_v(c) = 38 \times 2^i - 60, s_v(c) = 46 \times 2^i - 73$.

For the remaining vertices, vertex weight is 1 and vertex strength is 0.

Consider the quotient graph $G/E_1$ (Figure 3). Using transmission index method [68], the Wiener index for graph $G$ is defined as, $W(G) = \frac{T(p)}{2}$, where $p \in V(G)$ and $T(p)$ is the transmission index of vertex $p$.

Therefore, $W(G/E_1) = \frac{T(p)}{2}, p \in V(G/E_1) = 24w_v(a_1)^2 + 152w_v(a_1) + 186$, where $(w_v(a_1), s_v(a_1)) = (19 \times 2^n - 18, 23 \times 2^n - 23)$.

Hence, $W(G/E_1) = 2,888 \times 2^n + 24(19 \times 2^n - 18)^2 - 2,550$.

(7)
Using Theorem 1:

\[
W(G_n/E_{2^i}) = 18m + 9mw_r(b_k) + 11mw_r(c) + 4mw_r(b_k)w_r(c) + 4m(m-1)(w_r(b_k))^2
+ 31m(m-1)w_r(b_k) + 55m(m-1),
= 38(173 \times 2^i - 304 \times 2^{2n-i} - 340 \times 2^{n+i} + 608 \times 2^{2n} - 140 \times 2^n).
\]

Hence, \( \sum_{i=1}^{n} W(G_n/E_{2^i}) = 50,540 \times 2^n - 37,392 \times 2^n + n(23,104 \times 2^{2n} - 5,320 \times 2^n) - 13,148. \)

Also, \( S_z(G_n/E_{2^i}) = 2^{i+1}(5 + w_r(b_k))(5(m-1) + w_r(b_k)(m-1) + w_r(c))
+ 6 \times 2^{i+1}(2 + w_r(b_k))(5(m-1) + w_r(b_k)(m-1) + w_r(c) + 3),
= 8(2,274 \times 2^i - 3,703 \times 2^{2n-i} - 4,416 \times 2^{n+i} + 7,406 \times 2^{2n} - 1,610 \times 2^n).
\]

\( \sum_{i=1}^{n} S_z(G_n/E_{2^i}) = 156,664 \times 2^n - 100,280 \times 2^n - 12,880n \times 2^n + 59,248n \times 2^n - 36,384. \)

\[
\Pi(G_n/E_{2^i}) = 2^{i+1}[(6 + s_r(b_k)) + (7(m-1) + s_r(b_k)(m-1) + s_r(c))]
+ 6 \times 2^{i+1}[(2 + s_r(b_k)) + (7(m-1) + s_r(b_k)(m-1) + s_r(c) + 3)],
= 8 \times 2^i(161 \times 2^n - 131).
\]

\( \sum_{i=1}^{n} \Pi(G_n/E_{2^i}) = 2,576 \times 2^{2n} - 4,672 \times 2^n + 2,096. \)

\[
\Mo(G_n/E_{2^i}) = 2^{i+1}[(5 + w_r(b_k)) - (5(m-1) + w_r(b_k)(m-1) + w_r(c))|
+ 6 \times 2^{i+1}[(2 + w_r(b_k)) - (5(m-1) + w_r(b_k)(m-1) + w_r(c) + 3)],
= 1,064 \times 2^{2n+i} - 1,064 \times 2^{n+i} - 236 \times 2^i.
\]

\( \sum_{i=1}^{n} \Mo(G_n/E_{2^i}) = 2,128 \times 2^{2n} - 1,064n \times 2^n - 2,600 \times 2^n + 472. \)

\[
\Mo_2(G_n/E_{2^i}) = 2^{i+1}[(6 + s_r(b_k)) - (7(m-1) + s_r(b_k)(m-1) + s_r(c))]
+ 6 \times 2^{i+1}[(2 + s_r(b_k)) - (7(m-1) + s_r(b_k)(m-1) + s_r(c) + 3)],
= 1,288 \times 2^{n+i} - 1,288 \times 2^i - 280 \times 2^i.
\]

\( \sum_{i=1}^{n} \Mo_2(G_n/E_{2^i}) = 2,576 \times 2^{2n} - 1,288n \times 2^n - 3,136 \times 2^n + 560. \)

Consider \( G_n/E_{2^1} \) (Figure 5). Computing the indices likewise in quotient graph \( G_n/E_{2^1} \), we obtain the following equations:

\[
W(G_n/E_{2^1}) = 2(5,649 \times 2^n - 5,415 \times 2^{2n-i} - 11,172 \times 2^{i+n} + 14,440 \times 2^{2n+i} - 3,154 \times 2^n),
\]

\[
\sum_{i=1}^{n} W(G_n/E_{2^i+1}) = 78,114 \times 2^n - 55,518 \times 2^{2n} + n(28,880 \times 2^{2n} - 6,308 \times 2^n) - 22,596,
\]

\[
S_z(G_n/E_{2^1}) = 2(11,450 \times 2^n - 11,191 \times 2^{2n-i} - 23,332 \times 2^{i+n} + 28,880 \times 2^{2n} - 5,168 \times 2^n),
\]
$\sum_{i=1}^{n} \text{Sz}_v(Gn/E_{2i+1}) = 161,510 \times 2^n - 10,336n \times 2^n - 115,710 \times 2^{2n} + 57,760n \times 2^{2n} - 45,800$

$\text{Sz}_x(Gn/E_{2i+1}) = 2(17,773 \times 2^n - 16,399 \times 2^{2n} - 35,604 \times 2^{3n} + 42,320 \times 2^{4n} - 7,406 \times 2^{5n})$

$\sum_{i=1}^{n} \text{PI}(Gn/E_{2i+1}) = 246,306 \times 2^n - 14,812n \times 2^n - 175,214 \times 2^{2n} + 84,640n \times 2^{2n} - 71,092$

$W(Gn) = W(Gn/E_1) + \sum_{i=1}^{n} W(Gn/E_{2i}) + \sum_{i=1}^{n} W(Gn/E_{2i+1})$

$= (115,126 - 11,628n) \times 2^n + (51,984n - 84,246) \times 2^{2n} - 30,518$  \hspace{1cm} (16)

$\text{Sz}_v(Gn) = \text{Sz}_v(Gn/E_1) + \sum_{i=1}^{n} \text{Sz}_v(Gn/E_{2i}) + \sum_{i=1}^{n} \text{Sz}_v(Gn/E_{2i+1})$

$= (214,786 - 19,304n) \times 2^n + (98,192n - 158,726) \times 2^{2n} - 55,052$

$\text{Sz}_x(Gn) = \text{Sz}_x(Gn/E_1) + \sum_{i=1}^{n} \text{Sz}_x(Gn/E_{2i}) + \sum_{i=1}^{n} \text{Sz}_x(Gn/E_{2i+1})$

$= (327,218 - 27,692n) \times 2^n + (143,888n - 241,638) \times 2^{2n} - 84,692$

$\text{PI}(Gn) = \text{PI}(Gn/E_1) + \sum_{i=1}^{n} \text{PI}(Gn/E_{2i}) + \sum_{i=1}^{n} \text{PI}(Gn/E_{2i+1})$

$= 8,096 \times 2^{2n} - 12,924 \times 2^n + 5,136$  \hspace{1cm} (17)

$\text{Mo}(Gn) = \text{Mo}(Gn/E_1) + \sum_{i=1}^{n} \text{Mo}(Gn/E_{2i}) + \sum_{i=1}^{n} \text{Mo}(Gn/E_{2i+1})$

$= 6,688 \times 2^{2n} - (2,660n + 7,768) \times 2^n + 1,192$

$\text{Mo}_x(Gn) = \text{Mo}_x(Gn/E_1) + \sum_{i=1}^{n} \text{Mo}_x(Gn/E_{2i}) + \sum_{i=1}^{n} \text{Mo}_x(Gn/E_{2i+1})$

$= 8,096 \times 2^{2n} - (3,220n + 9,360) \times 2^n + 1,412$

\[ \square \]

**Theorem 3.** For \( n \geq 0 \):

$W(PyGn) = (720n + 10,996) \times 2^n + (14,400n - 2,340) \times 2^{2n} - 430$

$\text{Sz}_v(PyGn) = (1,080n + 14,428) \times 2^n + (21,600n + 2,280) \times 2^{2n} - 476$

$\text{Sz}_x(PyGn) = (2,040n + 21,032) \times 2^n + (27,744n - 3,400) \times 2^{2n} - 492$

$\text{PI}(PyGn) = 4.624 \times 2^{2n} - 1.884 \times 2^n + 172$

$\text{Mo}(PyGn) = 4.080 \times 2^{2n} - (720n + 2,272) \times 2^n - 96$

$\text{Mo}_x(PyGn) = 4.624 \times 2^{2n} - (816n + 2,464) \times 2^n - 140$

**Proof.** The graph \( PyGn \) has 60 \( 2^n \) - 12 vertices, 68 \( 2^n \) - 13 edges, and 44 \( 2^n \) - 13 \( \Theta^* \) - classes. Let us consider \( PyG2 \). The sets \( E_i \) which is coarser than the \( \Theta^* \)-classes chosen for \( PyG2 \) are highlighted in Figure 6. We convert the original graph into quoti- ent graphs and we obtain \((n + 2) \) quotient graphs for \( PyGn \). There are three types of weighted quotient graphs \( \{ PyGn/E_1, PyGn/E_2, PyGn/E_{n+2} : 2 \leq i \leq n+1, n \geq 0 \} \) for \( PyGn \).

The first type of quotient graph \( PyGn/E_1 \) has 16 vertices and 19 edges, among which four vertices, \( a_i : 1 \leq i \leq 4 \) has \( \{ w_v(a_i), s_v(a_i) \} = (15 \times 2^n \text{-} 6, 17 \times 2^n \text{-} 8 \) and for remaining vertices, vertex weight is 1 and vertex strength is 0, as given in Figure 7.

The second type of quotient graph \( PyGn/E_2 : 2 \leq i \leq n+1 \) has a weighted core vertex, say \( c \) attached with \( m = 2^i \). 2 \leq i \leq n + 1 branches such that two vertices in each branch have same weighted values, as given in Figure 8. Let us take those vertices to be \( b_k : 1 \leq k \leq 2m \). Then, \( \{ w_v(b_k), s_v(b_k) \} = (7 \times 2^n \text{-} 12, 8 \times 2^n \text{-} 13 \)

\( \{ w_v(b_k), s_v(b_k) \} = (15 \times 2^n+1-6, 17 \times 2^n+1-8) \).

For the remaining vertices, vertex weight and vertex strength is 1 and 0, respectively.

The third type of quotient graph \( PyGn/E_{n+2} \) has a weighted core vertex, say \( d \) attached with \( m = 2^n+2 \) branches, as given in Figure 9, where \( \{ w_v(d), s_v(d) \} = (28 \times 2^n \text{-} 12, 32 \times 2^n \text{-} 13 \) and all other vertices have vertex weight and vertex strength equal to 1 and 0, respectively.

Proceeding with the similar pattern applied in computing the indices of quotient graphs for \( Gn \), we obtain the following for \( PyGn \).

For \( PyGn/E_1 \) (Figure 7):

$W(PyGn/E_1) = 2,280 \times 2^n + 24(15 \times 2^n - 6) \times 2^n - 726$

$\text{Sz}_v(PyGn/E_1) = 14,400 \times 2^{2n} - 5,400 \times 2^n + 392$

$\text{Sz}_x(PyGn/E_1) = 18,496 \times 2^{2n} - 8,568 \times 2^n + 824$

$\text{PI}(PyGn/E_1) = 1,292 \times 2^{2n} - 300$

$\text{Mo}(PyGn/E_1) = 360 \times 2^n - 56$

$\text{Mo}_x(PyGn/E_1) = 408 \times 2^n - 44$

For \( PyGn/E_2 \) (Figure 8):

$W(PyGn/E_2) = 2(71 \times 2^{2n} - 6,300 \times 2^n - 1,020 \times 2^n - 720 \times 2^n \times 2^n)$

$\sum_{i=1}^{n} W(PyGn/E_1) = 15,028 \times 2^n - 14,460 \times 2^n + (n \times 2^{2n} + 720 \times 2^n) - 568$.
Figure 6: Illustration of sets $E_i$ of PyG2.

$\sum_{i=2}^{n+1} Sz_e(PyGn/E_i) = 217 \times 2^i - 18,000 \times 2^{2n-i} - 3,180 \times 2^{1+2n} + 21,600 \times 2^{2n} + 1,080 \times 2^n$,

$\sum_{i=2}^{n+1} SI_e(PyGn/E_i) = 22,588 \times 2^n - 21,720 \times 2^{2n} + n(21,600 \times 2^{2n} + 1,080 \times 2^n - 868)$,

$\sum_{i=2}^{n+1} Sz_s(PyGn/E_i) = 329 \times 2^n - 23,120 \times 2^{2n-i} - 4,828 \times 2^{1+2n} + 27,744 \times 2^{2n} + 2,040 \times 2^n$,

$\sum_{i=2}^{n+1} SI_s(PyGn/E_i) = 2,040n \times 2^n - 30,872 \times 2^n + 32,188 \times 2^n + 27,744n \times 2^n - 1,316$,

$W(PyGn) = W(PyGn/E_1) + \sum_{i=2}^{n+1} W(PyGn/E_i) + W(PyGn/E_{n+2})$,

$= (720n + 10,996) \times 2^n + (14,400n - 2,340) \times 2^{2n} - 430$.

$Sz_e(PyGn) = Sz_e(PyGn/E_1) + \sum_{i=2}^{n+1} Sz_e(PyGn/E_i) + Sz_e(PyGn/E_{n+2})$,

$= (1,080n + 14,428) \times 2^n + (21,600n + 2,280) \times 2^{2n} - 476$.

$Sz_s(PyGn) = Sz_s(PyGn/E_1) + \sum_{i=2}^{n+1} Sz_s(PyGn/E_i) + Sz_s(PyGn/E_{n+2})$,

$= (2,040n + 21,032) \times 2^n + (27,744n - 3,400) \times 2^{2n} - 492$.

$PI(PyGn) = PI(PyGn/E_1) + \sum_{i=2}^{n+1} PI(PyGn/E_i) + PI(PyGn/E_{n+2})$,

$= 4,624 \times 2^{2n} - 1,884 \times 2^n + 172$. 
Theorem 4. For \( n \geq 1 \):

\[
\begin{align*}
M_1(Gn) &= 464 \times 2^n - 370, \\
M_2(Gn) &= 588 \times 2^n - 467, \\
H(Gn) &= \frac{1}{3} (112 \times 2^n - 88), \\
HM(Gn) &= 2.392 \times 2^n - 1.908.
\end{align*}
\]

\( \square \)

4. Degree-Based Index and Graph Entropy

In this section, we compute the degree-based indices defined in Table 1 for the pyrene cored dendrimers \( G_n \) and \( PyGn \). Further, we have extended the work to the degree-based entropy measures of the dendrimers. We have used degree counting method and edge partition based on the vertices and edges of the dendrimer structure to compute the degree-based indices and further the graph entropies were determined using Equation (5) given in Section 2.

4.1. Theorems on Degree-Based Index and Entropy of \( G_n \)

**Theorem 4.** For degree-based index and entropy of \( G_n \)

\[
\begin{align*}
M_1(Gn) &= 464 \times 2^n - 370, \\
M_2(Gn) &= 588 \times 2^n - 467, \\
H(Gn) &= \frac{1}{3} (112 \times 2^n - 88), \\
HM(Gn) &= 2.392 \times 2^n - 1.908.
\end{align*}
\]

\( \square \)

\[
\begin{align*}
M_1(Gn) &= 4 \times (2^n - 14) + 5 \times (40 \times 2^n - 40) + 6 \times (28 \times 2^n - 19), \\
&= 464 \times 2^n - 370. \\
M_2(Gn) &= 4 \times (2^n - 14) + 6 \times (40 \times 2^n - 40) + 9 \times (28 \times 2^n - 19), \\
&= 588 \times 2^n - 467. \\
H(Gn) &= \frac{1}{2} (24 \times 2^n - 14) + \frac{2}{5} (40 \times 2^n - 40) + \frac{1}{3} (28 \times 2^n - 19), \\
&= \frac{1}{3} (112 \times 2^n - 88).
\end{align*}
\]

Proceeding likewise, the remaining degree-based indices are obtained.

**Theorem 5.** For \( n \geq 1 \):

\[
\begin{align*}
\text{ENT}_{M_1}(Gn) &= \log(464 \times 2^n - 370) - \frac{425583089622851948 \times 2^n - 33989828655842233}{112589906842624(232 \times 2^n - 185)}, \\
\text{ENT}_{M_2}(Gn) &= \log(588 \times 2^n - 467) - \frac{628706518870406948 \times 2^n - 497298819678705633}{562949953421312(588 \times 2^n - 467)}, \\
\text{ENT}_H(Gn) &= \log\left(\frac{1}{3} (112 \times 2^n - 88)\right) + \frac{4489926589657384 \times 2^n - 357638409783584073}{36028797018963968(14 \times 2^n - 11)}.
\end{align*}
\]
Table 3: Edge partition of the pyrene cored dendrimer $G_n$.

<table>
<thead>
<tr>
<th>Edge partition $(d_p, d_q)$</th>
<th>(2,2)</th>
<th>(2,3)</th>
<th>(3,3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of edges</td>
<td>$24 \times 2^n - 14$</td>
<td>$40 \times 2^n - 40$</td>
<td>$28 \times 2^n - 19$</td>
</tr>
</tbody>
</table>

\[
\text{ENT}_{HM}(G_n) = \log(2.392 \times 2^n - 1.908) - \frac{555613095933322220 \times 2^n - 442694178403221039}{28147976710656(598 \times 2^n - 477)},
\]

\[
\text{ENT}_G(G_n) = \log(1.216 \times 2^n - 974) - \frac{224460377070067932 \times 2^n - 179804685288579973}{140737488355328(608 \times 2^n - 487)},
\]

\[
\text{ENT}_R(G_n) = \log\left(\frac{\sqrt{6}}{6} (40 \times 2^n - 40) + \frac{1}{3} (64 \times 2^n - 40)\right) \quad \text{Proof. Using Equation (5):}
\]

\[
\text{ENT}_G(A) = \log\left(\frac{2\sqrt{6}}{5} (40 \times 2^n - 40) + 52 \times 2^n - 33\right) \quad \text{Therefore, using data from Theorem 4:}
\]

\[
\text{ENT}_M(G_n) = \log(464 \times 2^n - 370) - \frac{1}{(464 \times 2^n - 370)} \left\{ 4\log(4)(24 \times 2^n - 14) + 5\log(5)(40 \times 2^n - 40) + 6\log(6)(28 \times 2^n - 19) \right\},
\]

\[
= \log(464 \times 2^n - 370) - \frac{425583089622851948 \times 2^n - 339898286655842223}{112589906842624(232 \times 2^n - 185)}.
\]
For $n \geq 0$:

- $M_1(PyGn) = 328 \times 2^n - 58$,
- $M_2(PyGn) = 380 \times 2^n - 55$,
- $H(PyGn) = \frac{1}{5}(142 \times 2^n - 28)$,
- $HM(PyGn) = 1.592 \times 2^n - 244$,
- $F(PyGn) = 832 \times 2^n - 134$,
- $R(PyGn) = \sqrt{6}(56 \times 2^n - 24) + \frac{1}{4}(4\sqrt{3} \times 2^n) + 4 \times 2^n + 4$,
- $RR(PyGn) = \sqrt{6}(56 \times 2^n - 24) + 4\sqrt{3} \times 2^n + 16 \times 2^n + 31$,
- $SC(PyGn) = \frac{3}{4} + \frac{\sqrt{8}}{5}(56 \times 2^n - 24) + 6 \times 2^n + 1$,

PROOF. The graph $PyGn : n \geq 0$ has $68 \times 2^n - 13$ edges with four edge partitions, say $(1,3), (2,2), (2,3)$, and $(3,3)$. The number of edges in each partition is given in Table 4.

The remaining proof is similar to Theorem 4. \(\square\)

**Table 4: Edge partition of the pyrene cored dendrimer PyGn.**

<table>
<thead>
<tr>
<th>Edge partition $(d_p, d_q)$</th>
<th>(1,3)</th>
<th>(2,2)</th>
<th>(2,3)</th>
<th>(3,3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of edges</td>
<td>$4 \times 2^n$</td>
<td>$8 \times 2^n + 2$</td>
<td>$56 \times 2^n - 24$</td>
<td>9</td>
</tr>
</tbody>
</table>

**Theorem 6.** For $n \geq 0$:

\[
\begin{align*}
\text{ENT}_{M_1}(PyGn) &= \log(328 \times 2^n - 58) - \frac{2911491280039878866 \times 2^n - 48012415846364161}{1125899906842624(164 \times 2^n - 29)}, \\
\text{ENT}_{M_2}(PyGn) &= \log(380 \times 2^n - 55) - \frac{371308249587494075 \times 2^n - 38814170884114593}{281479767105660(76 \times 2^n - 11)}, \\
\text{ENT}_H(PyGn) &= \log\left(\frac{142}{5} \times 2^n - \frac{28}{5}\right) + \frac{1111659321138413130 \times 2^n - 216506362811685245}{18014398509481984(71 \times 2^n - 14)}, \\
\text{ENT}_{HM}(PyGn) &= \log(1592 \times 2^n - 244) - \frac{(354571437852736794 \times 2^n - 47959291218450817)}{28147976710656(398 \times 2^n - 61)}, \\
\text{ENT}_F(PyGn) &= \log(832 \times 2^n - 134) - \frac{294489084091593460 \times 2^n - 42045734203777869}{28147976710656(416 \times 2^n - 67)}.
\end{align*}
\]
Table 5: Computed numerical values for initial generations of dendrimer $G_n$.

<table>
<thead>
<tr>
<th>Topological index</th>
<th>$n = 1$</th>
<th>$n = 2$</th>
<th>$n = 3$</th>
<th>$n = 4$</th>
<th>$n = 5$</th>
<th>$n = 6$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wiener</td>
<td>47,430</td>
<td>652,514</td>
<td>5,200,602</td>
<td>32,731,946</td>
<td>181,683,210</td>
<td>935,359,562</td>
</tr>
<tr>
<td>Szeged</td>
<td>93,776</td>
<td>1,252,188</td>
<td>9,894,340</td>
<td>62,060,820</td>
<td>343,937,076</td>
<td>1,769,303,412</td>
</tr>
<tr>
<td>Edge Szeged</td>
<td>123,360</td>
<td>1,740,852</td>
<td>14,030,108</td>
<td>88,860,492</td>
<td>495,224,812</td>
<td>2,556,665,772</td>
</tr>
<tr>
<td>Padmakar–Ivan</td>
<td>11,672</td>
<td>82,976</td>
<td>419,888</td>
<td>1,870,928</td>
<td>7,881,872</td>
<td>32,339,216</td>
</tr>
<tr>
<td>Mostar</td>
<td>7,088</td>
<td>55,848</td>
<td>303,240</td>
<td>1,418,792</td>
<td>6,175,528</td>
<td>25,876,648</td>
</tr>
<tr>
<td>Edge Mostar</td>
<td>8,636</td>
<td>67,748</td>
<td>367,396</td>
<td>1,718,148</td>
<td>7,476,996</td>
<td>31,327,108</td>
</tr>
</tbody>
</table>

\[
\text{ENT}_a(PyGn) = \log \left( \frac{\sqrt{6}}{6} (56 \times 2^n - 24) + \frac{4\sqrt{3}}{3} \times 2^n + 4 \times 2^n + 4 \right) + \frac{1104403639123091952\times 2^n}{4503599627370496} - \frac{43133755380997165}{9007199254740992}. \\
\text{ENT}_{RR}(PyGn) = \log \left( \frac{\sqrt{6} (56 \times 2^n - 24) + 4\sqrt{3} \times 2^n + 16 \times 2^n + 31}{\sqrt{6} (56 \times 2^n - 24) + 4\sqrt{3} \times 2^n + 16 \times 2^n + 31} \right). \\
\text{ENT}_{SC}(PyGn) = \log \left( \frac{3\sqrt{6}}{2} + \frac{5}{3} (56 \times 2^n - 24) + 6 \times 2^n + 1 \right) + \frac{109492655816804656\times 2^n}{4503599627370496} - \frac{4190464988099117}{9007199254740992}. \\
\text{ENT}_{AB}(PyGn) = \log \left( \frac{2\sqrt{6}}{5} (56 \times 2^n - 24) + 2\sqrt{3} \times 2^n + 8 \times 2^n + 11 \right) + \frac{291509393486320372\times 2^n}{18014398509481984} - \frac{1080788864645391}{2251799813685248}. \\
\text{ENT}_{ABC}(PyGn) = \log \left( 32\sqrt{2} \times 2^n - 11\sqrt{2} + \frac{4\sqrt{6}}{3} \times 2^n + 6 \right) + \frac{3\times 14723394923222034972\times 2^n}{9007199254740992} - \frac{1331110275350785}{1125899906842624}. \\
\text{ENT}_r(PyGn) = \log(64 \times 2^n - 24) - \frac{6243314768165359 \times 2^n}{1125899906842624(64 \times 2^n - 24)}. \\
\text{ENT}_e(PyGn) = \log(72 \times 2^n - 24) - \frac{6243314768165359 \times 2^n}{28147976710656(72 \times 2^n - 24)}. \\
\]

Proof. To determine the entropy measures of $PyGn$, the similar pattern used in Theorem 5 is followed. The data from Theorem 6 and Table 4 are applied in Equation (5) in order to obtain the required degree-based graph entropy measures. □

5. Comparative Analysis

The numerical values computed for the distance- and degree-based descriptors of $G_n$ up to the sixth generation and of $PyGn$ up to the fifth generation are presented in Tables 5–8. Further, the entropy measures computed for initial generations of the dendrimers are tabulated in Tables 9 and 10. A comparison between the descriptors and generations as well as between the entropies and generations of the dendrimers $G_n$ and $PyGn$ are represented graphically in Figures 10–12.

6. QSPR/QSAR Modelling of Structural Descriptors

Theoretical structural descriptors are the numerical representation of chemical compounds, which encodes the structures topology and chemical information. There have been a number of molecular descriptors such as physicochemical, constitutional and geometrical, electrostatic, topological, and quantum chemical indices which are widely used in
quantitative structure–activity–property research for predicting biological activities and properties of chemicals. Quantitative structure–property relationships (QSPRs)/quantitative structure–activity relationships (QSARs) are the final results of a process that starts with a suitable descriptor of a molecular structure and ends with some inference, hypothesis and prediction on the behaviour, properties, and characteristics of the molecule. As an initial step, it is assumed that the molecule’s structure has features responsible for some physical, chemical, and biological properties and the ability to capture these features into numerical descriptors, followed by gathering data regarding the molecules, which can be produced experimentally or retrieved from literature. A limiting factor at this step is the availability of high-quality experimental data and its accuracy. Another important phase of the QSPR/QSAR process is the selection of best structural descriptor for modelling in analysis. Since there is no awareness about the best among the molecular descriptors, all possible descriptors are determined.

A major application of QSPR/QSAR models is that the properties, activities, behaviour, etc., of a newly designed or untested chemical compound can be inferred from the

| Table 6: Computed numerical values of indices for initial generations of dendrimer PyGn. |
|---------------------------------|----------------|----------------|----------------|----------------|----------------|----------------|
| Topological index | $n = 0$ | $n = 1$ | $n = 2$ | $n = 3$ | $n = 4$ | $n = 5$ |
| Wiener | 8,226 | 71,242 | 472,674 | 2,719,858 | 14,368,146 | 71,798,482 |
| Szeged | 16,232 | 126,060 | 793,556 | 4,433,988 | 23,001,572 | 113,560,740 |
| Edge Szeged | 17,140 | 143,028 | 933,364 | 5,325,972 | 28,006,036 | 139,566,612 |
| Padmakar–Ivan | 2,912 | 14,900 | 66,620 | 281,036 | 1,153,772 | 4,674,860 |
| Mostar | 1,712 | 10,240 | 50,336 | 225,568 | 961,952 | 3,989,920 |
| Edge Mostar | 2,020 | 11,796 | 57,460 | 256,500 | 1,091,956 | 4,525,428 |

| Table 7: Degree-based indices of Gn upto $n = 6$. |
|---------------------------------|----------------|----------------|----------------|----------------|----------------|----------------|
| Degree-based index | $n = 1$ | $n = 2$ | $n = 3$ | $n = 4$ | $n = 5$ | $n = 6$ |
| First Zagreb | 558 | 1,486 | 3,342 | 7,054 | 14,478 | 29,326 |
| Second Zagreb | 709 | 1,885 | 4,237 | 8,941 | 18,349 | 37,165 |
| Harmonic | 45,333 | 120 | 269,333 | 568 | 1,165,333 | 2,360 |
| Hyper Zagreb | 2,876 | 7,660 | 17,228 | 36,364 | 74,636 | 151,180 |
| Forgotten | 1,458 | 3,890 | 8,754 | 18,482 | 37,938 | 76,850 |
| Randić | 45.6633 | 120.9897 | 271.6428 | 572.9490 | 1,175.5612 | 2,380.7857 |
| Reciprocal Randić | 276.7976 | 736.9388 | 1,656.8571 | 3,496.6938 | 7,176.3673 | 14,535.7142 |
| Sum-connectivity | 49.9937 | 132.6327 | 297.9107 | 628.4667 | 1,289.5786 | 2,611.8025 |
| Geometric arithmetic | 110.1918 | 292.5755 | 657.3429 | 1,386.8775 | 2,845.9469 | 5,764.0857 |
| Atom bond connectivity | 76.9926 | 204.8356 | 460.5216 | 971.8936 | 1,994.6376 | 4,040.1256 |
| Irregularity and sigma | 40 | 120 | 280 | 600 | 1,240 | 2,520 |

| Table 8: Degree-based indices of PyGn upto $n = 5$. |
|---------------------------------|----------------|----------------|----------------|----------------|----------------|----------------|
| Degree-based index | $n = 0$ | $n = 1$ | $n = 2$ | $n = 3$ | $n = 4$ | $n = 5$ |
| First Zagreb | 270 | 598 | 1,254 | 2,566 | 5,190 | 10,438 |
| Second Zagreb | 325 | 705 | 1,465 | 2,985 | 6,025 | 12,105 |
| Harmonic | 22.8 | 51.2 | 108 | 221.6 | 448.8 | 903.2 |
| Hyper Zagreb | 1,348 | 2,940 | 6,124 | 12,492 | 25,228 | 50,700 |
| Forgotten | 698 | 1,530 | 3,194 | 6,522 | 13,178 | 26,490 |
| Randić | 23.3733 | 52.5447 | 110.8873 | 227.5725 | 460.9429 | 927.6838 |
| Reciprocal Randić | 132.3119 | 292.4115 | 612.6108 | 1,253.0093 | 2,533.8063 | 5,095.4004 |
| Sum-connectivity | 24.9851 | 56.0290 | 118.1170 | 242.2928 | 490.6445 | 987.3479 |
| Geometric arithmetic | 53.8176 | 120.1502 | 252.8156 | 518.1463 | 1,048.8076 | 2,110.1304 |
| Atom bond connectivity | 38.9645 | 87.4853 | 184.5269 | 378.6102 | 766.7768 | 1,543.1099 |
| Irregularity measure | 40 | 104 | 232 | 488 | 1,000 | 2,024 |
| Sigma | 48 | 120 | 264 | 552 | 1,128 | 2,280 |
molecular structure of similar compounds whose properties, activities, characteristics, etc., have already been assessed. Researchers have done the analysis and they have highlighted their outcomes in [69–71].

A flowchart diagram is drawn based on the QSPR/QSAR modelling with respect to structural descriptors of chemical structures, especially with respect to dendrimers. The same is presented in Figure 13.

<table>
<thead>
<tr>
<th>Table 9: Degree-based entropies of ( G_n ) upto ( n = 6 ).</th>
</tr>
</thead>
<tbody>
<tr>
<td>Degree-based entropy</td>
</tr>
<tr>
<td>First Zagreb</td>
</tr>
<tr>
<td>Harmonic</td>
</tr>
<tr>
<td>Randić</td>
</tr>
<tr>
<td>Reciprocal Randić</td>
</tr>
<tr>
<td>Sum-connectivity</td>
</tr>
<tr>
<td>Geometric arithmetic</td>
</tr>
<tr>
<td>Atom bond connectivity</td>
</tr>
<tr>
<td>Irregularity and sigma</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 10: Degree-based entropies of ( PyG_n ) upto ( n = 5 ).</th>
</tr>
</thead>
<tbody>
<tr>
<td>Entropy</td>
</tr>
<tr>
<td>First Zagreb</td>
</tr>
<tr>
<td>Second Zagreb</td>
</tr>
<tr>
<td>Harmonic</td>
</tr>
<tr>
<td>Forgotten</td>
</tr>
<tr>
<td>Randić</td>
</tr>
<tr>
<td>Reciprocal Randić</td>
</tr>
<tr>
<td>Sum-connectivity</td>
</tr>
<tr>
<td>Geometric arithmetic</td>
</tr>
<tr>
<td>Sigma</td>
</tr>
</tbody>
</table>

Figure 10: Comparison graph based on distance-based indices.
FIGURE 11: Comparison graph based on degree-based indices.

FIGURE 12: Comparison graph based on graph entropy measures.

FIGURE 13: QSAR/QSPR flowchart model.
Tables 5 and 7, the correlation coefficient (\( R \)) between band gap energy of G\( n \) and its descriptors.

<table>
<thead>
<tr>
<th>Descriptor</th>
<th>( R )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wiener</td>
<td>-0.94484</td>
</tr>
<tr>
<td>Szeged</td>
<td>-0.94508</td>
</tr>
<tr>
<td>Edge Szeged</td>
<td>-0.94449</td>
</tr>
<tr>
<td>Padmakar–Ivan</td>
<td>-0.96186</td>
</tr>
<tr>
<td>Mostar</td>
<td>-0.95905</td>
</tr>
<tr>
<td>Edge Mostar</td>
<td>-0.95909</td>
</tr>
<tr>
<td>First Zagreb</td>
<td>-0.994191626</td>
</tr>
<tr>
<td>Second Zagreb</td>
<td>-0.994191626</td>
</tr>
<tr>
<td>Harmonic</td>
<td>-0.994191804</td>
</tr>
<tr>
<td>Hyper Zagreb</td>
<td>-0.994191626</td>
</tr>
<tr>
<td>Forgotten</td>
<td>-0.994191626</td>
</tr>
<tr>
<td>Reciprocal Randić</td>
<td>-0.994191628</td>
</tr>
<tr>
<td>Sum-connectivity</td>
<td>-0.994191626</td>
</tr>
<tr>
<td>Geometric arithmetic</td>
<td>-0.994191626</td>
</tr>
<tr>
<td>Atom bond connectivity</td>
<td>-0.994191626</td>
</tr>
<tr>
<td>Irregularity</td>
<td>-0.994191626</td>
</tr>
<tr>
<td>Sigma</td>
<td>-0.994191626</td>
</tr>
</tbody>
</table>

6.1. Linear Regression Model for Descriptors of Pyrene Cored Dendrimers. In this section, the linear regression models for few properties of the pyrene cored dendrimers with their distance- and degree-based descriptors are obtained using least square procedure. The following regression model is considered for the analysis:

\[
P = x(\text{SD}) + y,
\]

where \( P \) and \( \text{SD} \) stand for property and structural descriptor, respectively.

6.1.1. Linear Regression Model for the Structural Descriptors of G\( n \). The linear regression model for band gap energy of G\( n \) with their distance- and degree-based descriptors is determined in this section. A band gap is defined as the energy difference between the upper edge of the valence band and the lower edge of the conduction band of a solid. The respective energy difference is called band gap energy (\( E_g \)). The band gap energy for G1, G2, and G3 are 2.92, 2.86, and 2.78, respectively, as given in You et al.’s [11] study. Analysing these data with respect to the corresponding descriptor value given in Tables 5 and 7, the correlation coefficients (\( R \)) are determined and the same are presented in Table 11.

Based on the correlation coefficient (\( R \)), the regression model for Padmakar–Ivan index, PI is found to be best fitted among the distance-based descriptors, which can be as follows:

\[
P = -0.00003097(\text{PI}) + 2.9065.
\]

The regression model for Harmonic index, \( H \) is found to be best fitted among the degree-based descriptors and can be as follows:

\[
P = -0.0006(H) + 2.942.
\]

Table 11: Correlation coefficient (\( R \)) between band gap energy of G\( n \) and its descriptors.

The scatter diagrams to show relation between property and descriptors are given in Figure 14.

6.1.2. Linear Regression Model for the Structural Descriptors of PyG\( n \). The linear regression model for band emission of PyG\( n \) with their distance- and degree-based descriptors is determined in this section. Band emission is the fraction of the total emission from a blackbody that is in a certain wavelength interval or band. The emission bands for first three dendrimer generations in CHCl\(_3\) solutions strongly red-shifted with maximum at 448 nm for PyG0, 452 nm for PyG1, and 457 nm for PyG2 [72]. Analysing these data with respect to its corresponding descriptor value given in Tables 6 and 8, the correlation coefficients are determined and presented in Table 12.

Based on the correlation coefficient (\( R \)), the regression model for Padmakar–Ivan index, PI is found to be best fitted among the distance-based descriptors and can be as follows:

\[
P = 0.0001(\text{PI}) + 448.73.
\]

The regression model for Randić index, \( R \) is found to be best fitted among the degree-based descriptors and can be as follows:

\[
P = 0.1004(R) + 446.08.
\]

The scatter diagrams to show relation between property and descriptors are given in Figure 15.

Thus, it can be concluded that the abovementioned properties of the pyrene cored dendrimers can be predicted with the help of regression equations using the computed structural descriptors.

7. Discussion

We have computed the numerical values of the distance- and degree-based descriptors for the initial generation dendrimer structures. Also, the entropy for G\( n \) and PyG\( n \) was also computed using the determined expressions. Based on the obtained values, a comparison between the descriptors and generations as well as between the entropies and generations of the dendrimers G\( n \) and PyG\( n \) are presented graphically in Section 5. The numerical computations and plotting of the comparison graphs were prepared with the help of MATLAB software. A regression analysis was also performed based on a few dendrimer structure properties, and the best fit regression models were identified and are presented in Section 6. Microsoft Excel analysis tools were used for the regression analysis.
\[ P = 0.1004 (R) + 446.08 \]

\[ P = -0.0001 (PI) + 448.73 \]

**FIGURE 14:** Scatter diagram for band energy gap with descriptors of pyrene cored dendrimer, G\(_n\).

**TABLE 12:** Correlation coefficient (\(R\)) between band emission of PyG\(_n\) and its descriptors.

<table>
<thead>
<tr>
<th>Descriptor</th>
<th>(R)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wiener</td>
<td>0.94469</td>
</tr>
<tr>
<td>Szeged</td>
<td>0.94649</td>
</tr>
<tr>
<td>Edge Szeged</td>
<td>0.94524</td>
</tr>
<tr>
<td>Padmakar–Ivan</td>
<td>0.96062</td>
</tr>
<tr>
<td>Mostar</td>
<td>0.95693</td>
</tr>
<tr>
<td>Edge Mostar</td>
<td>0.95721</td>
</tr>
<tr>
<td>First Zagreb</td>
<td>0.992064533</td>
</tr>
<tr>
<td>Second Zagreb</td>
<td>0.992064533</td>
</tr>
<tr>
<td>Harmonic</td>
<td>0.992064533</td>
</tr>
<tr>
<td>Hyper Zagreb</td>
<td>0.992064533</td>
</tr>
<tr>
<td>Forgotten</td>
<td>0.992064533</td>
</tr>
<tr>
<td>Randić</td>
<td>0.99206464</td>
</tr>
<tr>
<td>Reciprocal Randić</td>
<td>0.992064533</td>
</tr>
<tr>
<td>Sum-connectivity</td>
<td>0.992064433</td>
</tr>
<tr>
<td>Geometric arithmetic</td>
<td>0.992064486</td>
</tr>
<tr>
<td>Atom bond connectivity</td>
<td>0.970998101</td>
</tr>
<tr>
<td>Irregularity</td>
<td>0.992064533</td>
</tr>
<tr>
<td>Sigma</td>
<td>0.992064533</td>
</tr>
</tbody>
</table>

**FIGURE 15:** Scatter diagram for band emission with descriptors of pyrene cored dendrimer, PyG\(_n\).
8. Conclusion

The distance-based descriptors of pyrene cored dendrimers \( G_n : n \geq 1 \) and \( PyG_n : n \geq 0 \) are computed by transforming the original graph into quotient graphs. The degree-based descriptors for the pyrene cored dendrimers \( G_n \) and \( PyG_n \) are also discussed, for which the degree counting method and edge partition based on the vertices and edges are used. Further, the degree-based entropy measures were determined for the dendrimer structures using Shannon’s method. These values are related to different physical, chemical, and biological properties of the dendrimers, which has wide range of application in disparate fields. The determined topological descriptors and the entropy values can be used to predict the physicochemical, thermochemical, electrical, mechanical, and optical properties of the structures. Also, this work would be useful in QSPR and QSAR analysis of these hyperbranched nanomaterials. Further, it may help in developments and recognitions in the field of macromolecules and in deriving its properties and applications.

Data Availability

All the data and material used in this research are included in the paper.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

References


