The Topological Aspects of Phthalocyanines and Porphyrins Dendrimers

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ABSTRACT

Topological descriptors are the numerical quantities of a graph that characterize various structural properties of it. In environmental sciences, pharmacy and in mathematical chemistry such descriptors are used for the quantitative structure-activity and property relationships (QSAR/QSPR) studies in which physicochemical properties of compounds are correlated with their molecular structures. A large spectrum of topological descriptors is available, among which the distance-based and bond-additive indices are frequently used in QSPR/QSAR studies. In this paper, the different versions of Szeged, Padmakar-Iven (PI) and Mostar indices for the molecular graphs of two types of dendrimers having phthalocyanines and porphyrins as their cores are illustrated through the numerical way. We have obtained exact analytical expressions of these indices by using the cut method.

INDEX TERMS

Phthalocyanine dendrimers, porphyrins dendrimers, Mostar index, Szeged index, Padmakar-Iven (PI) index.

I. INTRODUCTION

Dendrimers are tree-like polymeric macromolecules with distinct and homogeneous sizes and shapes. The structure of dendrimers consists of three distinct parts, a central core, the interior structure having repeated branches, and the outer structure with functional groups. The increase in the number of repeated branching units identify the generation of the dendrimer and is answerable for the formation of a globular structure. Dendrimers attracted great attention in gene and drug delivery applications due to having highly controllable architecture [1]–[6]. By electrostatic or hydrophobic attraction, the drugs and oligonucleotides are either bound to the surface or encapsulated in their inner cavities. They can also be covalently linked by interacting with terminal functional groups.

In reticular chemistry, quantitative structure-property / quantitative structure-activity relationship (QSPR/QSAR) schemes are correlation/regression models used to associate with various biological and physicochemical activities. The Harold Wiener initiated this study; in 1947, he introduced a distance-based structure invariant to find out the boiling point of alkanes. In this process, the topologically invariant quantities change the chemical structure into a specific mathematical number named as topological descriptor or index. In chemical graph theory, the molecular structure descriptors establish, which models organic compounds into hydrogen-suppressed graphs with a relationship of vertices (resp. edges) to atoms (resp. bonds). The structure descriptors give efficient regression models, which correspond to different biological and physicochemical properties, including the critical temperature, critical volume, critical pressure, the boiling point, the heat of formation, enthalpy of vaporization of organic compounds. There are several classes of topological descriptors, including counting-based descriptors, valency-based descriptors, spectrum-based descriptors and distance-based descriptors. When distance-based descriptors correlate with physicochemical characteristics of organics structures, they provide the regression model with high prediction power. We refer to the books of Gutman and Furtula, and Todeschini and Consonni for readers for theory and applications of topological descriptors respectively.

A graph $S$ is an ordered pair $S(V(S), E(S))$, where $V(S)$ (resp. $E(S)$) is called the vertex (resp. edge) set of the graph.
A chemical graph is obtained from any given chemical structure in which atoms related to vertices whereas bonds related to edges. The degree of a vertex is the total number of edges attached with it. For example, the degree of a vertex is at most 4 in the chemical graph that is constructed from an organic compound. In this manuscript, every graph is assumed to be an undirected, simple and finite molecular graph.

A map from the set of simple connected graphs to the set of real numbers is called a topological descriptor which is topologically invariant under graph automorphisms. In literature till present, several different types of topological descriptors are introduced and studied. The distance-based topological descriptors are stated on degrees of vertices of any given graph such as the Randic connectivity index, the atom-the dd index, the (hyper) Wiener index. The degree-based additive/multiplicative Harary indices, the Gutman index, are introduced and studied. The distance-based topological descriptors are given in [43]–[41] for an introduction to this subject. We use the cut method, see [44].

Recently, Wang et al. [15] and Mogharrab et al. [16] examined the PI index for extremal cacti graphs and triangular-free graphs respectively. Motivated by the various productive indices such as PI [13], Szeged [8], Zagreb [17], irregularity [18], and revised-Szeged [19]–[21], recently, a novel bond-additive index introduced by Došlić et al. in [22] and it is famous as the Mostar index.

For any connected graph $S$, it was specified as:

$$M_{o_1}(S) = \sum_{e=uv \in E(S)} |n_u(e|S) - n_v(e|S)|.$$  \hspace{1cm} (7)

For further results related to different versions of Mostar index, the interested readers are referred to [24], [25], [27]–[31]. The evaluation and analysis of topological indices of molecular structures are modern trends of research, which are of the significant importance in nanotechnology and theoretical chemistry. We refer the interested reader to [28], [32]–[41] for an introduction to this subject. We use the cut method that was suggested in [42] and they used it to find the Wiener index of graphs. This method was extended for general graphs by setting up a correlation between the canonical metric representation of the graph and its Wiener index in [43]. The standard cut method was also established for other topological descriptors of chemical graphs. For a graph $S$, $e = uv$ and $f = u_1y_1$ edges of $S$ belong to the Djokovic-Winkler $\Theta$ relation if $d_S(u, u_1) + d_S(y_1, y'_1) \neq d_S(u, y'_1) + d_S(y', u_1)$ and it is always reflexive and symmetric, and transitive on partial cubes. The $\Theta$ relation will construct equivalence classes $F_1$, $F_2$, $\ldots$, $F_k$ of the edge set $E(S)$ of a partial cube $S$ and named as $\Theta$ cuts or classes. For a comprehensive study of the cut method, see [44].
II. THE TOPOLOGICAL ASPECTS OF CARBOXYLATE-TERMINATED ZINC PHTHALOCYANINE DENDRIMERS

The structural motif of phthalocyanines has invited important research works during the last couple of decades [45], [46]. This class of molecules has often been used as pigments and dyes in the early days, this interest has transferred in present-days for their usage as building blocks for the formation of new molecular materials for dye-sensitized solar cells [47]–[49], optoelectronics and electronics [45], [46]. Recently, Setaro et al. prepared highly water-soluble dendrimers consisting of a central zinc phthalocyanine moiety and dendritic wedges with terminal carboxylate groups. In this section, we present the results related to this dendrimer. Let $G_1(s)$ be the molecular graph of this dendrimer, where $s$ represents the generation stage of the dendrimer.

Now, we find the vertex PI, vertex Szeged and vertex Mostar indices of $G_1(s)$.

**Theorem 1:** For the molecular graph $G_1(s)$, we have

1) $PI(G_1(s)) = 1440 \times 2^{2s} + 720 \times 2^s + 104$.
2) $Sz(G_1(s)) = (992 + 9072s) \times 2^s + (23608 + 6804s) \times 2^s - 1160$.
3) $Mo_s(G_1(s)) = 1440 \times 2^{2s} + (360 - 252s) \times 2^s - 440$.

**Proof 1:** It is an easy exercise to observe that $|V(G_1(s))| = 9(2^{s+2} + 1)$ and $|E(G_1(s))| = 8(5 \times 2^s + 2)$. We define the pendant cuts $[P_i : 1 \leq i \leq 2^{s+2}]$, which take place on the boundaries of the dendrimer. The edges between two hexagons can be described in three sets $[T_i : 1 \leq s \leq l \leq s]$, $[T'_i : 1 \leq l \leq s]$ and $[T''_i : 1 \leq l \leq s]$. In the Table 1, we give the values of $n_{G_1(s)}(y)$ and $n_{G_1(s)}(w)$ in $P_i$, $T_i$, $T'_i$ and $T''_i$.

The cuts of a hexagon that is not in the core of $G_1(s)$ are shown in Figure 1 and represented by $[C_i : 1 \leq l \leq s]$,

![Figure 1. Cuts of $G_1(1)$.](image)

### Table 1. The values of $n_{G_1(s)}(y)$ and $n_{G_1(s)}(w)$ in $P_i$, $T_i$, $T'_i$ and $T''_i$.

| $yw$ | $E(G_1(s))$ | $n_{G_1(s)}(y)$ | $n_{G_1(s)}(w)$ | Frequency |
|------|-------------|-----------------|-----------------|-----------|
| $yw \in P_i$, $1 \leq l \leq 2^{s+2}$ | $9 \times 2^{l-2} + 8$ | $1$ | $2^{s+2}$ |
| $yw \in T_i$, $1 \leq l \leq s$ | $9 \times 2^l - 10$ | $9(2^{l+2} - 2^l) + 19$ | $2^{s+2}$ |
| $yw \in T'_i$, $1 \leq l \leq s$ | $9 \times 2^l - 9$ | $9(2^{l+2} - 2^l) + 18$ | $2^{s+2}$ |
| $yw \in T''_i$, $1 \leq l \leq s$ | $9 \times 2^l - 8$ | $9(2^{l+2} - 2^l) + 17$ | $2^{s+2}$ |

### Table 2. The values of $n_{G_1(s)}(y)$ and $n_{G_1(s)}(w)$ in $C_i$, $C_i'$, $C_i''$, $A_i$, $A_i'$ and $A_i''$.

| $yw$ | $E(G_1(s))$ | $n_{G_1(s)}(y)$ | $n_{G_1(s)}(w)$ | Frequency | Number of equidistant vertices from $w$ and $y$ |
|------|-------------|-----------------|-----------------|-----------|------------------------------------------|
| $yw \in C_i$, $1 \leq l \leq s$ | $\frac{9(2^l - 10)}{2}$ | $9(2^{l+2} - 2^l) + 14$ | $2^{s-l-2}$ | $0$ |
| $yw \in C_i'$, $1 \leq l \leq s$ | $\frac{9(2^l - 10)}{2}$ | $9(2^{l+2} - 2^l) + 14$ | $2^{s-l-2}$ | $0$ |
| $yw \in C_i''$, $1 \leq l \leq s$ | $9 \times 2^l - 13$ | $9(2^{l+2} - 2^l) + 22$ | $2^{s-l-2}$ | $0$ |
| $yw \in A_i$, $1 \leq l \leq 4$ | $9 \times 2^l - 5$ | $27 \times 2^l + 14$ | $2^{s-l-2}$ | $0$ |
| $yw \in A_i'$, $1 \leq l \leq 4$ | $9 \times 2^l - 5$ | $27 \times 2^l + 14$ | $2^{s-l-2}$ | $0$ |
| $yw \in A_i''$, $1 \leq l \leq 4$ | $9 \times 2^{l+4}$ | $2(9 \times 2^l - 2)$ | $2^{s-l-2}$ | $9(2^l + 1)$ |

### Table 3. The values of $n_{G_1(s)}(y)$ and $n_{G_1(s)}(w)$ in $O$, $Q$, $F$, and also the edges $w_1w_k$, $2 \leq k \leq 5$ in the core.

| $yw$ | $E(G_1(s))$ | $n_{G_1(s)}(y)$ | $n_{G_1(s)}(w)$ | Frequency | Number of equidistant vertices from $w$ and $y$ |
|------|-------------|-----------------|-----------------|-----------|------------------------------------------|
| $w_1w_k$, $2 \leq k \leq 5$ | $3(3 \times 2^{l+1} + 1)$ | $3(9 \times 2^l + 2)$ | $4$ | $0$ |
| $yw \in O$ | $3(3 \times 2^l + 1)$ | $3(9 \times 2^l + 2)$ | $8$ | $9 \times 2^{l-2}$ |
| $yw \in Q$ | $9 \times 2^l + 1$ | $9 \times 2^l + 10$ | $8$ | $9 \times 2^{l-2}$ |
| $yw \in F$ | $9 \times 2^l - 2$ | $9 \times 2^l + 13$ | $8$ | $9 \times 2^{l-2}$ |
index and vertex Mostar index.

\[ P_{I}(G_1(s)) = \sum_{l=1}^{2s+2} \left( \sum_{i \in \mathcal{P}_l} (9 \times 2^{s+2} + 8 + 1) + \sum_{l=1}^{s} \sum_{j \in \mathcal{T}_l} (9 \times 2^j) \right) - 10 + 9 \times 2^{s+2} - 9 \times 2^l + 19 + \sum_{l=1}^{s} \sum_{i \in \mathcal{C}_l} (9 \times 2^l) - 9 + 9 \times 2^{s+2} - 9 \times 2^l + 18 + \sum_{l=1}^{s} \sum_{i \in \mathcal{C}_l} (9 \times 2^l) - 8 + 9 \times 2^{s+2} - 9 \times 2^l + 17 + \sum_{l=1}^{s} \sum_{i \in \mathcal{C}_l} (9 \times 2^l) - 10 + 9 \times 2^{s+2} - 9 \times 2^l - 1 + 14 + \sum_{l=1}^{s} \sum_{i \in \mathcal{C}_l} (9 \times 2^l - 13) + 9 \times 2^{s+2} - 9 \times 2^l + 22 + \sum_{l=1}^{s} \sum_{i \in \mathcal{A}_l} (2(9 \times 2^l - 5 + 27 \times 2^l + 14) + 4 \sum_{l=1}^{s} \sum_{i \in \mathcal{A}_l} (2(9 \times 2^l - 5 + 27 \times 2^l + 14) + 4 \sum_{l=1}^{s} \sum_{i \in \mathcal{A}_l} (2(9 \times 2^l + 4 + 2(9 \times 2^l - 2)) + \sum_{k=2}^{5} \left( (3(9 \times 2^k + 1) + 3(9 \times 2^k + 2)) + \sum_{w \in \mathcal{O}} (3(3 \times 2^k + 1) + 3(9 \times 2^k + 2) + \sum_{w \in \mathcal{Q}} (9 \times 2^k + 1 + 9 \times 2^{k+1} + 10) + \sum_{w \in \mathcal{F}} (9 \times 2^{k+1} + 13) \right) \right) = 2^{s+2}(9 \times 2^{s+2} + 9) + \sum_{l=1}^{s} 2^{s-l+2}(9 \times 2^{s+2} + 9) + \sum_{l=1}^{s} 2^{s-l+2}(9 \times 2^{s+2} + 9) + \sum_{l=1}^{s} 2^{s-l+2}(9 \times 2^{s+2} + 9) + \sum_{l=1}^{s} 2^{s-l+2}(9 \times 2^{s+2} + 9) + \sum_{l=1}^{s} 2^{s-l+2}(9 \times 2^{s+2} + 9) + \sum_{l=1}^{s} 2^{s-l+2}(9 \times 2^{s+2} + 9) + 8(36 \times 2^l + 9) + 8(36 \times 2^l + 9) + 8 \times 27 \times 2^l + 2 \times 27 \times 2^l + 11) = 144 \times 2^{s+2} + 36 \times 2^l + 9 \times 4(2^l - 1)(9 \times 2^{s+l+2} + 9) + 288 \times 2^l + 72 + 288 \times 2^l + 72 + 216 \times 2^l + 144 \times 2^l + 36 + 288 \times 2^l + 72 + 216 \times 2^l + 88 + 216 \times 2^l + 88 = 1440 \times 2^{s+2} + 720 \times 2^l + 104 \]
\[2l^2 + 225 \times 2^l - 72 \times 2^{l+2} - 153) + 2 \sum_{l=1}^{s} 2r^{-l+2}(81 \times 2^{s+l+2} - 81 \times 2^{2l-1} + 171 \times 2^l - 90 \times 2^{s+l+2} - 190) + 2 \sum_{l=1}^{s} 2r^{-l+2}(81 \times 2^{s+l+2} - 81 \times 2^{2l-1} + 171 \times 2^l - 90 \times 2^{s+l+2} - 190) + 2 \sum_{l=1}^{s} 2r^{-l+2}(81 \times 2^{s+l+2} - 81 \times 2^{2l-1} + 171 \times 2^l - 90 \times 2^{s+l+2} - 190)
\]

\[-81 \times 2^l - 315 \times 2^l - 117 \times 2^{s+l+2} - 286) + 8(243 \times 2^{2s} - 9 \times 2^s - 70) + (243 \times 2^{2s} - 9 \times 2^s - 70) + 16(81 \times 2^{2s} + 8 \times 2^s - 8) + 36(27 \times 2^{2s} + 15 \times 2^s + 2) + 8(162 \times 2^{2s} + 99 \times 2^s + 26)
\]

\[= 144 \times 2^{s+2} + 32 \times 2^s + 2 \sum_{l=1}^{s} 2r^{-l+2}(567 \times 2^{s+l+2})
\]

\[-405 \times 2^l - 162 \times 2^{2l-1} + 1701 \times 2^l - 657 \times 2^{s+l+2} - 1457) + 21076 \times 2^{2s} + 3348 \times 2^l - 1160
\]

\[= 21220 \times 2^{2s} + 3380 \times 2^s - 1160 + 9072s
\]

\[\times 2^{2s} + 6804s \times 2^s - \sum_{l=1}^{s} (405 \times 2^{s+l+2} + 162 \times 2^{s+l+1} + 657 \times 2^{2s-l+4} + 1457 \times 2^{s-l+2})
\]

\[= (21220 + 9072s) \times 2^{2s} + (3380 + 6804s) \times 2^s - 1160 - 405 \times 2^l - 162 \times 2^{2l-1} + 1701 \times 2^l - 657 \times 2^{s+l+2} - 1457) + 21076 \times 2^{2s} + 3348 \times 2^l - 1160
\]

\[= (992 + 9072s) \times 2^{2s} + (23608 + 6804s) \times 2^s - 2^{s+2} + |2s^{s+2} + 8 - 1| + \sum_{l=1}^{s} \sum_{l \in T_j} |9 \times 2^{s+2} - 9 \times 2^l + 19 - 9 \times 2^l + 10|
\]

\[+ \sum_{l=1}^{s} \sum_{l \in T_j} |9 \times 2^{s+2} - 9 \times 2^l + 18 - 9 \times 2^l + 9|
\]

\[+ \sum_{l=1}^{s} \sum_{l \in T_j} |9 \times 2^{s+2} - 9 \times 2^l + 17|
\]

\[-9 \times 2^l + 8] + \sum_{l=1}^{s} \sum_{l \in C_i} |2|9 \times 2^{s+2} - 9 \times 2^l - 9 \times 2^{s-l+1} + 14 - 9 \times 2^{s-l+1} + 5|
\]

\[+ \sum_{l=1}^{s} \sum_{l \in C_i} |2|9 \times 2^{s+2} - 9 \times 2^l - 22 - 9 \times 2^l + 13|
\]

\[+ \sum_{l=1}^{s} \sum_{l \in C_i} |2|9 \times 2^{s+2} - 9 \times 2^l - 22 - 9 \times 2^l + 13|
\]

\[= 2^{s+2}(9 \times 2^s + 7) + \sum_{l=1}^{s} 2^{s-l+2}(9 \times 2^{s+2} - 18 \times 2^l + 29)
\]

\[+ \sum_{l=1}^{s} 2^{s-l+2}(9 \times 2^{s+2} - 18 \times 2^l + 27)
\]

\[+ \sum_{l=1}^{s} 2^{s-l+2}(9 \times 2^{s+2} - 18 \times 2^l + 25) + 4 \sum_{l=1}^{s} 2^{s-l+2}(9 \times 2^{s+2} - 18 \times 2^l + 19)
\]

\[+ \sum_{l=1}^{s} 2^{s-l+2}(9 \times 2^{s+2} - 18 \times 2^l + 19) + 16(18 \times 2^l + 19)
\]

\[+ 8(9 \times 2^l - 8) + 12(6 \times 2^s + 1) + 24(6 \times 2^s + 1)
\]

\[+ 8(9 \times 2^s + 9) + 8(9 \times 2^s + 15)
\]

\[= 144 \times 2^{2s} + 748 \times 2^s + 468 + \sum_{l=1}^{s} (81 \times 2^{2s-l+2} - 126 \times 2^{s-l+2} + 227 \times 2^{s-l+2})
\]

\[= 144 \times 2^{2s} + 748 \times 2^s + 468 - 126 \times 2^{s-l+2} + 227 \times 2^{s-l+2}
\]

\[= 144 \times 2^{2s} + 748 \times 2^s + 468 - 126 \times 2^{s-l+2} + 227 \times 2^{s-l+2}
\]

Now, we find the edge PI, edge Szeged and edge Mostar indices of \(G_1(s)\).

**Theorem 2:** For the molecular graph \(G_1(s)\), we have

1. \(PI_1(G_1(s)) = 1600 \times 2^{2s} + 1008 \times 2^s + 144\)
2. \(Sz(G_1(s)) = (11200s - 53920) \times 2^{2s} + (10520s + 57224) \times 2^s + 6840\)
3. \(Mo_2(G_1(s)) = 3040 \times 2^{2s} - (560s + 568) \times 2^s - 496\)
Proof 2: We define the pendant cuts \( P_t : 1 \leq t \leq 2^{s+2} \), which take place on the boundaries of the dendrimer. The edges between two hexagons can be described in three sets such that \( \{T_1 : 1 \leq l \leq s \}, \{T'_1 : 1 \leq l \leq s \} \) and \( \{T''_1 : 1 \leq l \leq s \} \). In the Table 4, we give the values of \( m_{G_1(s)}(y) \) and \( m_{G_1(s)}(w) \) in \( P_t, T_1, T'_1 \) and \( T''_1 \).

The cuts of a hexagon that is not in the core of \( G_1(s) \) are shown in Figure 1 and represented by \( \{C_1 : 1 \leq l \leq s \}, \{C'_1 : 1 \leq l \leq s \} \) and \( \{C''_1 : 1 \leq l \leq s \} \) of the dendrimer. The cuts of a hexagon in the core are represented as \( \{A_1 : 1 \leq l \leq 4 \}, \{A'_1 : 1 \leq l \leq 4 \} \) and \( \{A''_1 : 1 \leq l \leq 4 \} \). In the Table 5, we give the values of \( m_{G_1(s)}(y) \) and \( m_{G_1(s)}(w) \) in \( C_1, C'_1, C''_1, A_1, A'_1 \) and \( A''_1 \).

Also, we represent the remaining vertices in the core of \( G_1(s) \) by \( w_{1k} \), \( 2 \leq k \leq 5 \), \( O = \{o_102, o_203, o_304, o_405, o_506, o_507, o_608, o_709, o_91011, o_11012 \}, Q = \{w_203, w_304, w_3012, w_406, w_407, w_509, w_5010 \} \) and \( F = \{o_3f_1, o_4f_2, o_6f_3, o_7f_4, o_8f_5, o_9f_6, o_12f_7, o_1f_8 \} \).

Therefore, by using the Tables 4-6, we get the following closed expressions for the edge PI index, edge Szeged index and edge Mostar index.

\[
\text{Pl}_e(G_1(s)) = \sum_{t=1}^{2^{s+2}} \sum_{y \in P_t} (40 \times 2^t + 15 + 0)
\]

| \( yw \) | \( E(G_1(s)) \) | \( m_{G_1(s)}(y) \) | \( m_{G_1(s)}(w) \) | Frequency | Number of equidistant vertices from \( w \) and \( y \) |
| --- | --- | --- | --- | --- | --- |
| \( yw \in P_t, 1 \leq l \leq 2^{s+2} \) | \( 40 \times 2^t + 15 \) | 0 | \( 2^{s+2} \) | 0 |
| \( yw \in T_1, 1 \leq l \leq s \) | \( 2(5 \times 2^2 - 6) \) | \( 40 \times 2^t - 10 \times 2^t + 27 \) | \( 2^{s+1-2} \) | 0 |
| \( yw \in T'_1, 1 \leq l \leq s \) | \( 5 \times 2^2 - 11 \) | \( 40 \times 2^t - 10 \times 2^t + 26 \) | \( 2^{s+1-2} \) | 0 |
| \( yw \in T''_1, 1 \leq l \leq s \) | \( 10(2^3 - 1) \) | \( 40 \times 2^t - 10 \times 2^t + 25 \) | \( 2^{s+1-2} \) | 0 |

| \( yw \) | \( E(G_1(s)) \) | \( m_{G_1(s)}(y) \) | \( m_{G_1(s)}(w) \) | Frequency | Number of equidistant vertices from \( w \) and \( y \) |
| --- | --- | --- | --- | --- | --- |
| \( yw \in C_1, 1 \leq l \leq s \) | \( 5 \times 2^t - 7 \) | \( 40 \times 2^t - 5 \times 2^t + 23 \) | \( 2^{s+1-2} \) | 0 |
| \( yw \in C'_1, 1 \leq l \leq s \) | \( 5 \times 2^t - 7 \) | \( 40 \times 2^t - 5 \times 2^t + 23 \) | \( 2^{s+1-2} \) | 0 |
| \( yw \in C''_1, 1 \leq l \leq s \) | \( 2(5 \times 2^2 - 8) \) | \( 40 \times 2^t - 10 \times 2^t + 30 \) | \( 2^{s+1-2} \) | 0 |
| \( yw \in A_1, 1 \leq l \leq 4 \) | \( 5 \times 2^2 - 7 \) | \( 35 \times 2^t + 23 \) | 4 | 0 |
| \( yw \in A'_1, 1 \leq l \leq 4 \) | \( 5 \times 2^2 - 7 \) | \( 35 \times 2^t + 23 \) | 4 | 0 |
| \( yw \in A''_1, 1 \leq l \leq 4 \) | \( 5(2^2+1 + 1) \) | \( 20 \times 2^t - 2 \) | \( 2^{s+1-2} \) | 0 |

\[
\begin{align*}
\text{TABLE 5. The values of } m_{G_1(s)}(y) & \text{ and } m_{G_1(s)}(w) \text{ in } C_1, C'_1, C''_1, A_1, A'_1 \text{ and } A''_1. \\
\text{TABLE 6. The values of } m_{G_1(s)}(y) & \text{ and } m_{G_1(s)}(w) \text{ in } O, Q \text{ and } F, \text{ and also the edges } w_{1k}, 2 \leq k \leq 5 \text{ in the core.}
\end{align*}
\]
\[ S_{G}^{2s+2}(G(s)) = \sum_{l=1}^{s} \sum_{yw} (40 \times 2^{s} + 15)(0) + \sum_{l=1}^{s} \sum_{yw} (2(5 \times 2^{l} - 6)) \times (40 \times 2^{s} - 10 \times 2^{l} + 27) + \sum_{l=1}^{s} \sum_{yw} (5 \times 2^{l+1} - 11)(40 \times 2^{s} - 10 \times 2^{l} + 26) + \sum_{l=1}^{s} \sum_{yw} (10(2^{l} - 1))(40 \times 2^{s} - 10 \times 2^{l} + 25) + \sum_{l=1}^{s} \sum_{yw} (2(5 \times 2^{l} - 7)(40 \times 2^{s} - 5 \times 2^{l} + 23) + \sum_{l=1}^{s} \sum_{yw} 2(5 \times 2^{l} - 7)(40 \times 2^{s} - 5 \times 2^{l} + 23) + \sum_{l=1}^{s} \sum_{yw} 2(5 \times 2^{l} - 8)(40 \times 2^{s} - 10 \times 2^{l} + 30) + \sum_{l=1}^{s} \sum_{yw} (5 \times 2^{s+1} - 2)(20 \times 2^{s} - 2) \times (5 \times 2^{s+1} + 3)(30 \times 2^{s} + 10) + \sum_{yw} (5 \times 2^{s+1} + 3)(20 \times 2^{s} + 16) + \sum_{yw} (5 \times 2^{s+1} - 3)(20(2^{s} + 1)) + \sum_{l=1}^{s} 2^{s-l+2}(400 \times 2^{s+l} + 390 \times 2^{l} - 100 \times 2^{2l} - 480 \times 2^{s} - 324) + \sum_{l=1}^{s} 2^{s-l+2}(400 \times 2^{s+l} + 370 \times 2^{l} - 100 \times 2^{2l} - 440) + \sum_{l=1}^{s} 2^{s-l+2}(400 \times 2^{s+l} + 160 \times 2^{2l} - 1900 \times 2^{s} + 692) + \sum_{l=1}^{s} 2^{s-l+2}(40 \times 2^{s+l} + 130 \times 2^{2l} + 19) + \sum_{l=1}^{s} 2^{s-l+2}(360 \times 2^{s+l} + 137) = 1600 \times 2^{2s} + 1008 \times 2^{s} + 144. \]
In the Table 7, we give the values of $t_{G_1}(y)$ and $t_{G_1}(w)$ in $P_t, T_t, T'_t$ and $T''_t$.

| $yw$ | $E(G_1(s))$ | $t_{G_1}(y)$ | $t_{G_1}(w)$ | Frequency |
|------|-------------|--------------|--------------|-----------|
| $yw \in P_t, 1 \leq t \leq 2^{l+2}$ | $76 \times 2^2 + 19$ | $76 \times 2^2 + 23 + 19$ | 24, 26 |
| $yw \in T_t, 1 \leq t \leq l \leq s$ | $76 \times 2^2 + 23 + 19$ | $76 \times 2^2 + 23 + 19$ | 18, 26 |
| $yw \in T'_t, 1 \leq t \leq l \leq s$ | $76 \times 2^2 + 23 + 19$ | $76 \times 2^2 + 23 + 19$ | 18, 26 |
| $yw \in T''_t, 1 \leq t \leq l \leq s$ | $76 \times 2^2 + 23 + 19$ | $76 \times 2^2 + 23 + 19$ | 18, 26 |

Now, we find the total PI, total Szeged and total Mostar indices of $G_1(s)$.

**Theorem 3:** For the molecular graph $G_1(s)$, we have

1) $P_{ft}(G_1(s)) = 3040 \times 2^{2s} + 1576 \times 2^s + 304$.
2) $S_{ZG}(G_1(s)) = (40432s - 138188) \times 2^{2s} + (34352s + 168116) \times 2^s + 22984$.
3) $M_{ot}(G_1(s)) = 11248 \times 2^{2s} + (1064s - 7060) \times 2^s - 992$.

**Proof:** We define the pendant cuts $[P_t : 1 \leq t \leq 2^{l+2}]$, which take place on the boundaries of the dendrimer. The edges between two hexagons can be described in three sets $[T_t : 1 \leq t \leq l], [T'_t : 1 \leq t \leq l]$, and $[T''_t : 1 \leq t \leq l]$. In the Table 7, we give the values of $t_{G_1}(y)$ and $t_{G_1}(w)$ in $P_t, T_t, T'_t$ and $T''_t$.

The cuts of a hexagon that is not in the core of $G_1(s)$ are shown in Figure 1 and represented by $[C_1 : 1 \leq l \leq s], [C'_1 : 1 \leq l \leq s]$ and $[C''_1 : 1 \leq l \leq s]$ and the cuts of a hexagon in the core are represented as $[A_1 : 1 \leq l \leq 4], [A'_1 : 1 \leq l \leq 4]$ and $[A''_1 : 1 \leq l \leq 4]$. In the Table 8, we give the values of $t_{G_1}(y)$ and $t_{G_1}(w)$ in $C_1, C'_1, C''_1, A_1, A'_1$ and $A''_1$.

Also, we represent the remaining vertices in the core of $G_1(s)$ by $w_i, w_k, 2 \leq k \leq 5$. In the Table 9, we give the values of $t_{G_1}(y)$ and $t_{G_1}(w)$ in $O, Q$ and $F$, and also the edges $w_i w_k, 2 \leq k \leq 5$ in the core.

| $yw$ | $E(G_1(s))$ | $t_{G_1}(y)$ | $t_{G_1}(w)$ | Frequency | Number of equidistant vertices from $w$ and $y$ |
|------|-------------|--------------|--------------|-----------|------------------------------------------|
| $yw \in C_1, 1 \leq i \leq s$ | $19 \times 2^i - 12$ | $19 \times 2^i - 12$ | 22, 26 | 0 |
| $yw \in C'_1, 1 \leq i \leq s$ | $19 \times 2^i - 12$ | $19 \times 2^i - 12$ | 22, 26 | 0 |
| $yw \in C''_1, 1 \leq i \leq s$ | $19 \times 2^i - 12$ | $19 \times 2^i - 12$ | 22, 26 | 0 |
| $yw \in A_1, 1 \leq i \leq 4$ | $19 \times 2^i - 12$ | $19 \times 2^i - 12$ | 22, 26 | 0 |
| $yw \in A'_1, 1 \leq i \leq 4$ | $19 \times 2^i - 12$ | $19 \times 2^i - 12$ | 22, 26 | 0 |
| $yw \in A''_1, 1 \leq i \leq 4$ | $19 \times 2^i - 12$ | $19 \times 2^i - 12$ | 22, 26 | 0 |
| $yw \in F, 2 \leq k \leq 5$ | $19 \times 2^k + 6$ | $19 \times 2^k + 6$ | 22, 26 | 0 |
| $yw \in O$ | $19 \times 2^k + 6$ | $19 \times 2^k + 6$ | 22, 26 | 0 |
| $yw \in Q$ | $19 \times 2^k + 6$ | $19 \times 2^k + 6$ | 22, 26 | 0 |

Q = \{w_2, w_3, w_4, w_5, w_6, w_7, w_8, w_9, w_{10}\} and $F = \{o_{1,1}, o_{1,2}, o_{1,3}, o_{1,4}, o_{1,5}, o_{1,6}, o_{1,7}, o_{1,8}\}$.

Therefore, by using the Tables 7-9, we get the following closed expressions for the total PI index, total Szeged index and total Mostar index.

$P_{ft}(G_1(s))$ = $\sum_{t=1}^{2^{l+2}} \sum_{i=1}^{s} (76 \times 2^i + 23 + 19) + \sum_{l=1}^{s} (19 \times 2^l)$

$-22 + 76 \times 2^l - 19 \times 2^l + 46 + \sum_{l=1}^{s} (19 \times 2^l)$

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\[-20 + 76 \times 2^s - 19 \times 2^l + 44 + \sum_{l=1}^{s} \sum_{yw \in T_i} (19 \times 2^l)\]
\[-18 + 76 \times 2^s - 19 \times 2^l + 42 + \sum_{l=1}^{s} \sum_{yw \in T_i} (19 \times 2^l)\]
\[-12 + 76 \times 2^s - \frac{19}{2} \times 2^l + 37 + \sum_{l=1}^{s} \sum_{yw \in C_i} (19 \times 2^l)\]
\[-12 + 76 \times 2^s - \frac{19}{2} \times 2^l + 37 + \sum_{l=1}^{s} \sum_{yw \in C_i} (19 \times 2^l)\]
\[-29 + 76 \times 2^s - 19 \times 2^l + 52 + \sum_{l=1}^{s} \sum_{yw \in A_l} (19 \times 2^l)\]
\[-12 + 62 \times 2^s + 37 + \sum_{l=1}^{s} \sum_{yw \in A_l} (19 \times 2^l)\]
\[+62 \times 2^s + 37 + \sum_{l=1}^{s} \sum_{yw \in A_l} (19 \times 2^l + 9 + 38 \times 2^s)\]
\[-6 + \sum_{k=2}^{s} (19 \times 2^s + 6 + 57 \times 2^s + 16) + \sum_{yw \in O} (19 \times 2^s + 4 + 38 \times 2^s + 29) + \sum_{yw \in Q} (19 \times 2^s - 5 + 38 \times 2^s + 33)\]
\[= 2^{s+2}(76 \times 2^s + 24) + \sum_{i=1}^{s} 2^{s-2}(684 \times 2^s + 218) + 3344 \times 2^s + 1176\]
\[= 304 \times 2^s + 96 \times 2^s + 3344 \times 2^s + 1176 + 4(2^s - 1) + 684 \times 2^s + 218\]
\[= 3040 \times 2^s + 1576 \times 2^s + 304.\]

\[S_{2l}(G_1(s))\]
\[= \sum_{l=1}^{s} \sum_{yw \in P_t} (76 \times 2^s + 23)(1) + \sum_{l=1}^{s} \sum_{yw \in T_i} (19 \times 2^l)\]
\[-22(76 \times 2^s - 19 \times 2^l + 46) + \sum_{l=1}^{s} \sum_{yw \in T_i} (19 \times 2^l)\]
\[-20(76 \times 2^s - 19 \times 2^l + 44) + \sum_{l=1}^{s} \sum_{yw \in T_i} (19 \times 2^l)\]
\[-18(76 \times 2^s - 19 \times 2^l + 42) + \sum_{l=1}^{s} \sum_{yw \in T_i} (19 \times 2^l)\]
\[-12(76 \times 2^s - \frac{19}{2} \times 2^l + 37) + \sum_{l=1}^{s} \sum_{yw \in C_i} (19 \times 2^l)\]
\[-12(76 \times 2^s - \frac{19}{2} \times 2^l + 37) + \sum_{l=1}^{s} \sum_{yw \in C_i} (19 \times 2^l)\]
\[-29(76 \times 2^s - 19 \times 2^l + 52) + \sum_{l=1}^{s} \sum_{yw \in A_l} (19 \times 2^l)\]
\[-12(62 \times 2^s + 37) + \sum_{l=1}^{s} \sum_{yw \in A_l} (19 \times 2^s - 12)\]
\[\times 2^s + 37 + \sum_{l=1}^{s} \sum_{yw \in A_l} (19 \times 2^s + 9)(38 \times 2^s - 6)\]
\[+ \sum_{k=2}^{s} (19 \times 2^s + 6)(57 \times 2^s + 16) + \sum_{yw \in O} (19 \times 2^s + 4)(38 \times 2^s + 29)\]
\[+ \sum_{yw \in F} (19 \times 2^s - 5)(38 \times 2^s + 33)\]
\[= 2^{s+2}(76 \times 2^s + 23) + \sum_{i=1}^{s} 2^{s-2}(10108 \times 2^{s-1} - \times 10336 \times 2^s - 2166 \times 2^{l} + 8588 \times 2^l - 7440)\]
\[+ 8(868 \times 2^{2s} - 226 \times 2^s - 444) + 8(868 \times 2^{2s} - 226 \times 2^s - 444) + 8(722 \times 2^{2s} + 228 \times 2^s - 54) + 4(1083 \times 2^{2s} + 646 \times 2^s + 96)\]
\[+ 8(1083 \times 2^{2s} + 646 \times 2^s + 96) + 8(722 \times 2^{2s} + 703 \times 2^s + 116) + 8(722 \times 2^{2s} + 437 \times 2^s - 165)\]
\[= 44516 \times 2^{2s} + 15172 \times 2^s - 6776 \times 40432s + 2^{2s} + 34352s \times 2^s - 10336 \times 2^{s+4}(2^s - 1) - 2166\]
\[\times 2^{s+3}(2^s - 1) - 7440 \times 4(2^s - 1)\]
\[= (40432s - 138188) \times 2^{2s} + (34352s + 168116) \times 2^s + 22984.\]

\[M_{2l}(G_1(s))\]
\[= \sum_{i=1}^{s} \sum_{yw \in P_t} |76 \times 2^s + 23 - 1| + \sum_{i=1}^{s} \sum_{yw \in T_i} |76 \times 2^s - 19 \times 2^l + 46| + \sum_{l=1}^{s} \sum_{yw \in T_i} (19 \times 2^l)\]
\[-19 \times 2^l + 46 - 19 \times 2^l + 22| + \sum_{l=1}^{s} \sum_{yw \in T_i} (19 \times 2^l)\]
\[-19 \times 2^l + 44 - 19 \times 2^l + 20| + \sum_{l=1}^{s} \sum_{yw \in T_i} (19 \times 2^l)\]
\[-19 \times 2^l + 42 - 19 \times 2^l + 18| + \sum_{l=1}^{s} \sum_{yw \in C_i} (19 \times 2^l)\]
\[-19 \times 2^l - \frac{19}{2} \times 2^l + 37 - \frac{19}{2} \times 2^l + 12| + \sum_{l=1}^{s} \sum_{yw \in C_i} (19 \times 2^l)\]
\[-19 \times 2^l - \frac{19}{2} \times 2^l + 37 - \frac{19}{2} \times 2^l + 12| + \sum_{l=1}^{s} \sum_{yw \in C_i} (19 \times 2^l)\]
ethylenediamine and methyl acrylate branching units, and have a full generation of amines and in half generations of the carboxyl terminated groups [50]–[53]. Raquel et al. synthesized the PAMAM dendrimers with a porphyrin core via the microwave method in [54]. In this section, we present the results related to this dendrimer. Let $G_2(s)$ be the molecular graph of this dendrimer, where $s$ represents the generation stage of the dendrimer. Now, we find the vertex PI, vertex Szeged and vertex Mostar indices of $G_2(s)$.

**Theorem 4:** For the molecular graph $G_2(s)$, we have

1) $P_I(G_2(s)) = 1024 \times 2^2s + 1024 \times 2^s + 296.$
2) $S_{Z}(G_2(s)) = (7168s - 3328)2^2s + (10126 + 8768s)2^s + 7468.$
3) $M_{o}(G_2(s)) = 1024 \times 2^ss + (816 - 448s)2^s - 672.$

**Proof 4:** It is an easy exercise to observe that $|V(G_2(s))| = 16(2^{s+1} + 1)$ and $|E(G_2(s))| = 8(2^{s+3} + 3)$. We define the pendant cuts $\{P_t : 1 \leq t \leq 2^{s+2}\}$, which take place on the boundaries of the dendrimer. The cuts of a hexagon of $G_2(s)$ are shown in Figure 2 and represented by $\{C_l : 1 \leq l \leq 4\}, \{C_l : 1 \leq l \leq 4\}$ and $\{C_l : 1 \leq l \leq 4\}$. Some cuts are denoted by $\{A_l : 1 \leq l \leq 4\}$. In the Table 10, 

III. THE TOPOLOGICAL ASPECTS OF PAMAM DENDRIMERS WITH PORPHYRIN CORE

Since the 1980s various types of dendrimers have been developed, but among all the one obtained from polyamidoamine (PAMAM) are apparently most useful in drug delivery, because they are biocompatible, hydrophilic and non-immunogenic systems. The PAMAM is mostly ethylenediamine, however the diaminobutane, diaminoxane and dianinododecane can also be practice. They comprise on
TABLE 10. The values of $n_{G_2(s)}(y)$ and $n_{G_2(s)}(w)$ in $P_t, C_l, C'_l, C''_l$ and $A_l$.

| $yw$ in $E(G_2(s))$ | $n_{G_2(s)}(y)$ | $n_{G_2(s)}(w)$ | Frequency |
|---------------------|-----------------|-----------------|-----------|
| $yw$ in $P_t$       | 16 $2^{s+1}$ + 15 | 1              | 2$(3 \times 2^s - 2)$ |
| $1 \leq t \leq 2(3 \times 2^s - 2)$ | 2$s+3$ - 5 | 24 $2^s + 21$ | 4 |
| $yw$ in $C_l$, $1 \leq l \leq 4$ | 2$s+3$ - 5 | 24 $2^s + 21$ | 4 |
| $yw$ in $C'_l$, $1 \leq l \leq 4$ | 2$s+3$ - 5 | 24 $2^s + 21$ | 4 |
| $yw$ in $A_l, 1 \leq l \leq 4$ | 2$(2^{s+2} - 1)$ | 24 $2^s + 18$ | 4 |

TABLE 11. The values of $n_{G_2(s)}(y)$ and $n_{G_2(s)}(w)$ in $T_l, U_l, W_l, X_l, Y_l, Z_l$ and $V_l$.

| $yw$ in $E(G_2(s))$ | $n_{G_2(s)}(y)$ | $n_{G_2(s)}(w)$ | Frequency |
|---------------------|-----------------|-----------------|-----------|
| $yw$ in $T_l$       | 2$(2^{s+2} - 7)$ | 32 $2^s - 8 \times 2^l$ + 30 | 2$s+1+2$ |
| $1 \leq l \leq s$   | 2$s+3$ - 13 | 32 $2^s - 8 \times 2^l$ + 29 | 2$s+1+2$ |
| $yw$ in $U_l$       | 4$(2^{s+2} - 3)$ | 32 $2^s - 8 \times 2^l$ + 28 | 2$s+1+2$ |
| $1 \leq l \leq s$   | 2$(2^{s+2} - 5)$ | 32 $2^s - 8 \times 2^l$ + 26 | 2$s+1+2$ |
| $yw$ in $W_l$       | 2$s+3$ - 9 | 32 $2^s - 8 \times 2^l$ + 25 | 2$s+1+2$ |
| $1 \leq l \leq s$   | 8$(2^l - 1)$ | 32 $2^s - 8 \times 2^l$ + 24 | 2$s+1+2$ |
| $yw$ in $X_l$       | 2$s+4$ - 15 | 32 $2^s - 2^{l+4}$ + 31 | 2$s+1+1$ |
| $1 \leq l \leq s$   | 8$(2^l + 1)$ | 8$(2^l + 1) + 8$ | 8 |

TABLE 12. The values of $n_{G_2(s)}(y)$ and $n_{G_2(s)}(w)$ in $O, Q$ and $F$.

| $yw$ in $E(G_2(s))$ | $n_{G_2(s)}(y)$ | $n_{G_2(s)}(w)$ | Frequency | Number of equidistant vertices from $w$ and $y$ |
|---------------------|-----------------|-----------------|-----------|-----------------------------------------------|
| $yw$ in $O$         | 8$2^{s+1} + 7$ | 8$2^{s+1} + 7$ | 4         | 2                                             |
| $yw$ in $Q$         | 8$(2^{s+1} + 8)$ | 8$(2^{s+1} + 6)$ | 8         | 0                                             |
| $yw$ in $F$         | 8$(2^{s+1} + 8)$ | 8$(2^{s+1} + 6)$ | 8         | 2                                             |

we give the values of $n_{G_2(s)}(y)$ and $n_{G_2(s)}(w)$ in $P_l, C_l, C'_l, C''_l$ and $A_l$.

The edges after the hexagons can be described in the following sets: $T_l = 1 \leq l \leq s$, $U_l = 1 \leq l \leq s$, $W_l = 1 \leq l \leq s$, $X_l = 1 \leq l \leq s$, $Y_l = 1 \leq l \leq s$, $Z_l = 1 \leq l \leq s$ and $V_l = 1 \leq l \leq s - 1$. In Table 11, we give the values of $n_{G_2(s)}(y)$ and $n_{G_2(s)}(w)$ in $T_l, U_l, W_l, X_l, Y_l, Z_l$ and $V_l$.

Also, we present the remaining vertices in the core of $G_2(s)$ by $w_{lwk}, 2 \leq k \leq 5, O = \{o_1 o_2, o_3 o_4, o_5 o_6, o_7 o_8\}, Q = \{q_1 q_2, q_3 q_4, q_5 q_6, q_7 q_8, q_9 q_{10}, q_{11} q_{12}, q_{13} q_{14}, q_{15} q_{16}\}$ and $F = \{q_1 q_3, q_4 q_6, q_7 q_9, q_{10} q_{11}, q_{12} q_{13}, q_{14} q_{15}, q_{16} q_{17}\}$.

Therefore, by using the Tables 10-12, we get the following closed expressions for the vertex PI index, vertex Szeged index and vertex Mostar index.

$$PI_v(G_2(s)) = \sum_{t=1}^{2(3 \times 2^l - 2)} \sum_{y \in P_t} (16 \times 2^{s+1} + 15 + 1)$$

$$+ \sum_{l=1}^{8} \sum_{yw \in U_l} 2(s+3) - 5 + 24 \times 2^s + 21$$

$$+ \sum_{l=1}^{8} \sum_{yw \in W_l} 2(s+3) - 5 + 24 \times 2^s + 21$$

$$+ \sum_{l=1}^{8} \sum_{yw \in X_l} 2(s+3) - 5 + 24 \times 2^s + 21$$

$$+ \sum_{l=1}^{8} \sum_{yw \in Y_l} 2(s+3) - 5 + 24 \times 2^s + 21$$

$$+ \sum_{l=1}^{8} \sum_{yw \in Z_l} 2(s+3) - 5 + 24 \times 2^s + 21$$

$$+ \sum_{l=1}^{8} \sum_{yw \in V_l} 2(s+3) - 5 + 24 \times 2^s + 21$$

$$= (6 \times 2^s - 4)(32 \times 2^s + 16) + 24(32 \times 2^s + 16) + 4(32 \times 2^s + 16) + 4(32 \times 2^s + 14) + 8(32 \times 2^s + 16)$$

$$+ 8(32 \times 2^s + 14) + 6 \sum_{l=1}^{s-1} 2s-l+2 \times 2^s + 16$$

$$+ \sum_{l=1}^{s-1} 2s-l+2 \times 2^s + 16$$

$$= 192 \times 2^s - 32 \times 2^s - 64 + 1536 \times 2^s + 744 + 6 \times 4(2^s - 1)(32 \times 2^s + 16) + 2(2^s - 2)(32 \times 2^s + 16)$$
\[ S_{v}(G_2(s)) = \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in P_i} (16 \times 2^{s+1} + 15)(1) \]

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in P_i} 2(2^{i+3} - 5)(24 \times 2^i + 21)

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in C_i'} 2(2^{i+3} - 5)(24 \times 2^i + 21)

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in C_i'} 2(2^{i+3} - 5)(24 \times 2^i + 21)

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in A_i} (2(2^{i+2} - 1))(24 \times 2^s + 18)

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in O} (8 \times 2^{s+1} + 7)(8 \times 2^{s+1} + 7)

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in Q} (8(2^{i+1} + 1))(8(2^{i+1} + 1))

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in F} (8 \times 2^{s+1} + 8)(8 \times 2^{s+1} + 6)

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in T_i} (2(2^{i+2} - 7))(32 \times 2^s - 8 \times 2^i) + 30

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in U_i} (2(2^{i+3} - 13)(32 \times 2^s - 8 \times 2^i) + 29)

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in W_i} (4(2^{i+2} - 3))(32 \times 2^s - 8 \times 2^i) + 28

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in X_i} (2(2^{i+2} - 5))(32 \times 2^s - 8 \times 2^i) + 26

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in Y_i} (2^{i+3} - 9)(32 \times 2^s - 8 \times 2^i) + 25

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in Z_i} (8(2^i - 1))(32 \times 2^s - 8 \times 2^i) + 24

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in V_i} (2^{i+4} - 15)(32 \times 2^s - 2^{i+4}) + 31

= (6 \times 2^s - 4)(32 \times 2^i + 15) + 24(192 \times 2^{2i} + 48 \times 2^s - 105) + 4(192 \times 2^{2i} + 96 \times 2^s - 36) + 4(256 \times 2^{2i} + 224 \times 2^i + 49) + 512(4 \times 2^{2i} + 4 \times 2^s + 1) + 8(256 \times 2^{2i} + 224 \times 2^i + 48) + \sum_{i=1}^{s} 2^{s-2l+2}(256 \times 2^{s+l} - 64 \times 2^l + 320 \times 2^l)

+ \sum_{i=1}^{s} 2^{s-l+2}(256 \times 2^{s+l} - 64 \times 2^l + 320 \times 2^l)

+ 384 \times 2^s - 336) + \sum_{i=1}^{s} 2^{s-l+2}(256 \times 2^{s+l} - 64 \times 2^l + 320 \times 2^l)

+ 288 \times 2^l - 320 \times 2^2(256 \times 2^{s+l} - 64 \times 2^l + 320 \times 2^l)

+ \sum_{i=1}^{s} 2^{s-l+2}(256 \times 2^{s+l} - 64 \times 2^l + 320 \times 2^l)

+ 2^{s-l+2}(256 \times 2^{s+l} - 64 \times 2^l + 320 \times 2^l)

+ 512 \times 2^{s+l} - 256 \times 2^2(256 \times 2^{s+l} - 64 \times 2^l + 320 \times 2^l)

= (7168s - 3328)2^{2s} + (10126 + 87668s)2^s + 7468.

\[ M_{v}(G_2(s)) = \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in P_i} [16 \times 2^{s+1} + 15 - 1] \]

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in P_i} 2(2^{i+3} + 21 - 2^{s+3} + 5)

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in C_i'} 2(2^{i+3} + 21 - 2^{s+3} + 5)

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in C_i'} 2(2^{i+3} + 21 - 2^{s+3} + 5)

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in A_i} (2(2^{i+2} + 18 - 2(2^{s+2} - 1))| \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in O} (8(2^{i+1} + 7) - 8 \times 2^{s+1} + 7)\]

+ \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in Q} (8(2^{i+1} + 1) - 8(2^{s+1} + 1)| \sum_{i=1}^{2^{(3\times 2^i-2)}} \sum_{y \in Q} (8(2^{i+1} + 1) - 8(2^{s+1} + 1) |
\[\sum_{y \in T_I} g_G(y) = \sum_{l=1}^{s} \sum_{y \in U_I} |2s^2 - 8 + 2^l + 1| + 2(2^l + 2 - 7)| + \sum_{l=1}^{s} \sum_{y \in W_I} |2s^2 - 8 + 2^l + 1| + 2(2^l + 2 - 3)| + \sum_{l=1}^{s} \sum_{y \in X_I} |2s^2 - 8 + 2^l + 1| + 2(2^l + 2 - 5)| + \sum_{l=1}^{s} \sum_{y \in Y_I} |2s^2 - 8 + 2^l + 1| + 2(2^l + 2 - 9)| + \sum_{l=1}^{s} \sum_{y \in Z_I} |2s^2 - 8 + 2^l + 1| + 2(2^l + 1)| = (6 \times 2^l - 4)(32 \times 2^l + 14) + 24(16 \times 2^l + 26) + 4(16 \times 2^l + 20) + 16 + \sum_{l=1}^{s} 2^{l+2} \left(192 \times 2^l - 96 \times 2^l + 228 \right) + \sum_{l=1}^{s} 2^{l+1} \left(32 \times 2^l - 32 \times 2^l + 46 \right) = 192 \times 2^s + 404 \times 2^l + 664 - 384s \times 2^l - 64(s - 1)2^l + 4(2^l - 1)(192 \times 2^l + 228) + 2(2^l - 2)(32 \times 2^l + 46) = 1004 \times 2^s + 816 - 448s \times 2^s - 672.

Now, we find the edge PI, edge Szeged and edge Mostar indices of \(G_2(s)\).

**Theorem 5:** For the molecular graph \(G_2(s)\), we have
1. \(PL_{s}(G_2(s)) = 1024 \times 2^s + 1248 \times 2^s + 324.
2. \(S_{g}(G_2(s)) = \left(71680 - 4352s\right)2^{2s} + (20944 + 10784s)2^s + 310868.
3. \(M_{s}(G_2(s)) = 1024 \times 2^s + (864 - 448s)2^s - 349.

**Proof:** To find the pendant cuts \(P_I : 1 \leq l \leq 2^{l+2}\), which take place on the boundaries of the dendrimer. The cuts of a hexagon of \(G_2(s)\) are shown in Figure 2 and represented by \(|C_I| : 1 \leq l \leq 4\), \(|C^l_I| : 1 \leq l \leq 4\) and \(|C^l_J| : 1 \leq l \leq 4\) and some cuts are represented by \(|A_l| : 1 \leq l \leq 4\). In the Table 13, we give the values of \(m_{g}(G_2(s))\) and \(m_{g}(G_2(s))\) in \(P_I, C_I, C^l_I, C^l_J, A_l\) and \(A_l\).

The edges after the hexagons can be described in the sets \(\{T_I : 1 \leq l \leq s\}, \{U_I : 1 \leq l \leq s\}, \{W_I : 1 \leq l \leq s\}, \{X_I : 1 \leq l \leq s\}, \{Y_I : 1 \leq l \leq s\}, \{Z_I : 1 \leq l \leq s\}\) and \(\{V_I : 1 \leq l \leq s - 1\}\). In the Table 14, we give the values of \(m_{g_2}(G_2(s))\) and \(m_{g_2}(G_2(s))\) in \(T_I, U_I, W_I, X_I, Y_I, Z_I\) and \(V_I\).

Also we present the remaining vertices in the core of \(G_2(s)\) by \(w_{1}w_{2}, 2 \leq k \leq 5, O = \{o_1o_2, o_3o_4, o_5o_6, o_7o_8\}\), \(Q = \{q_1q_2, q_3q_4, q_5q_6, q_7q_8, q_9q_{10}, q_{12}q_{13}, q_{13}q_{14}, q_{16}q_{15}\}\) and \(F = \{q_2q_3, q_4q_5, q_6q_7, q_8q_9, q_{10}q_{11}, q_{12}q_{13}, q_{14}q_{15}, q_{15}q_{16}\}\).

Therefore, by using the Tables 13-15, we get the following closed expressions for the edge PI index, edge Szeged index and edge Mostar index.

\[\sum_{r=1}^{s} \sum_{y \in P_I} (32 \times 2^l + 23 + 0)\]
\[ + \sum_{l=1}^{s} \sum_{y \in C_l} 2(2^{l+3} - 6 + 24 \times 2^s + 28) \\
+ \sum_{l=1}^{s} \sum_{y \in C'_l} 2(2^{l+3} - 6 + 24 \times 2^s + 28) \\
+ \sum_{l=1}^{s} \sum_{y \in C''_l} 2(2^{l+3} - 6 + 24 \times 2^s + 28) \\
+ \sum_{l=1}^{s} \sum_{y \in A_l} (2^{l+2} - 1) + 24 \times 2^s + 25) \\
+ \sum_{y \in O} (4 \times 2^{s+2} + 11 + 4 \times 2^{s+2} + 11) \\
+ \sum_{y \in Q} (4 \times 2^{s+2} + 11 + 4 \times 2^{s+2} + 11) \\
+ \sum_{y \in F} (4(2^{s+2} + 3) + 16 \times 2^s + 10) \\
+ \sum_{l=1}^{s} \sum_{y \in T_l} (2^{l+3} - 15 + 32 \times 2^s - 8 \times 2^l) + 38) \\
+ \sum_{l=1}^{s} \sum_{y \in U_l} (2^{l+3} - 14 + 32 \times 2^s - 8 \times 2^l) + 37) \\
+ \sum_{l=1}^{s} \sum_{y \in W_l} (2^{l+3} - 13 + 32 \times 2^s - 8 \times 2^l) + 36) \\
+ \sum_{l=1}^{s} \sum_{y \in X_l} (2^{l+3} - 11 + 32 \times 2^s - 8 \times 2^l) + 34) \\
+ \sum_{l=1}^{s} \sum_{y \in Y_l} (2^{l+3} - 10 + 32 \times 2^s - 8 \times 2^l) + 33) \\
+ \sum_{l=1}^{s} \sum_{y \in Z_l} (2^{l+3} - 9 + 32 \times 2^s - 8 \times 2^l) + 32) \\
+ \sum_{l=1}^{s-1} \sum_{y \in V_l} (2^{l+4} - 16 + 32 \times 2^s - 2^{l+4}) + 39) \\
= (6 \times 2^4 - 4)(32 \times 2^4 + 23) + 24(32 \times 2^4 + 22) \\
+4(32 \times 2^4 + 23) + 4(32 \times 2^4 + 22) \\
+8(32 \times 2^4 + 22) + 8(32 \times 2^4 + 22) \\
+ \sum_{l=1}^{s} 2^{s-l+2}(192 \times 2^2 + 138) \\
+ \sum_{l=1}^{s-1} 2^{s-l+1}(32 \times 2^2 + 23) \\
= 192 \times 2^2 + 10 \times 2^4 - 92 + 1536 \times 2^4 + 1060 \\
+4(2^4 - 1) \times (192 \times 2^2 + 138) + 2(2^4 - 2) \\
\times(32 \times 2^2 + 23) \\
= 1024 \times 2^2 + 1248 \times 2^4 + 324.
\]

\[ \text{Sz}_a(G_2(s)) = \frac{1}{2(3 \times 2^s - 2)} \sum_{t=1}^{s} \sum_{y \in P_t} (32 \times 2^t + 23)(0) \\
+ \sum_{l=1}^{s} \sum_{y \in C_l} 2(2^{s+3} - 6)(24 \times 2^s + 28) \\
+ \sum_{l=1}^{s} \sum_{y \in C'_l} 2(2^{s+3} - 6)(24 \times 2^s + 28) \\
+ \sum_{l=1}^{s} \sum_{y \in C''_l} 2(2^{s+3} - 6)(24 \times 2^s + 28) \\
+ \sum_{l=1}^{s} \sum_{y \in A_l} (2^{s+2} - 1)(24 \times 2^s + 25) \\
+ \sum_{y \in O} (4 \times 2^{s+2} + 11)(4 \times 2^{s+2} + 11) \\
+ \sum_{y \in Q} (4 \times 2^{s+2} + 11)(4 \times 2^{s+2} + 11) \\
+ \sum_{y \in F} (4(2^{s+2} + 3))(16 \times 2^s + 10) \\
+ \sum_{l=1}^{s} \sum_{y \in T_l} (2^{s+3} - 15)(32 \times 2^s - 8 \times 2^t + 38) \\
+ \sum_{l=1}^{s} \sum_{y \in U_l} (2^{s+3} - 14)(32 \times 2^s - 8 \times 2^t + 37) \\
+ \sum_{l=1}^{s} \sum_{y \in W_l} (2^{s+3} - 13)(32 \times 2^s - 8 \times 2^t + 36) \\
+ \sum_{l=1}^{s} \sum_{y \in X_l} (2^{s+3} - 12)(32 \times 2^s - 8 \times 2^t + 34) \\
+ \sum_{l=1}^{s} \sum_{y \in Y_l} (2^{s+3} - 11)(32 \times 2^s - 8 \times 2^t + 33) \\
+ \sum_{l=1}^{s} \sum_{y \in Z_l} (2^{s+3} - 10)(32 \times 2^s - 8 \times 2^t + 32) \\
+ \sum_{l=1}^{s-1} \sum_{y \in V_l} (2^{s+4} - 16)(32 \times 2^s - 2^{t+4} + 39) \\
= 0 + 24(16 \times 2^s + 34) + 4(192 \times 2^{2s} + 80 \times 2^s \\
- 168) + 4(192 \times 2^{2s} + 152 \times 2^s - 50) + 4(256 \times 2^{2s} \\
+ 352 \times 2^s + 121) + 8(256 \times 2^s + 352 \times 2^s + 121) \\
+ 8(256 \times 2^{2s} + 352 \times 2^s + 120) + \sum_{l=1}^{s} 2^{s-l+2}(256 \\
\times 6 \times 2^{s+l} - 64 \times 6 \times 2^{2l} + 2256 \times 2^s - 2304 \times 2^s \\
- 2548) + \sum_{l=1}^{s} 2^{s-l+1}(512 \times 2^{s+l} - 256 \times 2l + 880 \\
\times 2^l - 512 \times 2^s - 624).\]
\[= 10496 \times 2^{2s} + 9568 \times 2^s - 1820 + 6144s \times 2^{2s} + 9024s \times 2^t + 1024(s-1)2^s2s + 1760(s-1)2^s - 384 \times 2^{t+3}(2^s - 1) - 2304 \times 2^{2t+2}(2^s - 1) - 2548 \times 4(2^s - 1) - 256 \times 2^{t+1}(2^s - 2) - 512 \times 2^{t+1} \times (2^s - 2) - 624 \times 2(2^s - 2) \]
\[= (71680 - 4352s)2^s + (20944 + 10784s)2^s + 310868. \]

We now find the total PI, total Szeged and total Mostar indices of \(G_2(s)\).

**Theorem 6:** For the molecular graph \(G_2(s)\), we have

1. \(P_t(G_2(s)) = 2048 \times 2^{2s} + 2266 \times 2^{s+3} + 3058.\)
2. \(S_2(G_2(s)) = 2(2672s - 15360)2^s + (468163,8112s)2^s + 36320.\)
3. \(M_D(G_2(s)) = 2048 \times 2^{2s} + (8940 - 896)s2^t - 8432.\)

**Proof 6:** We define the pendant cuts \(\{P_t : 1 \leq t \leq 2^{s+2}\}\), which take place on the boundaries of the dendrimer. The cuts of a hexagon of \(G_2(s)\) are shown in Figure 2 and represented by \(|C_1 : 1 \leq l \leq 4|, |C_2 : 1 \leq l \leq 4|\) and \(|C_2' : 1 \leq l \leq 4|\) and some cuts are denoted by \(|A_1 : 1 \leq l \leq 4|\). In the Table 16, we give the values of \(t_G(\delta(y))\) and \(t_G(\delta(w))\) in \(P_t, C_1, C_2, C_2', A_1\).

**Table 16. The values of \(t_G(\delta(y))\) and \(t_G(\delta(w))\) in \(P_t, C_1, C_2, C_2', A_1\).**

| \(yw\) | \(E(G_2(s))\) | \(t_G(\delta(y))\) | \(t_G(\delta(w))\) | Frequency |
|-------|----------------|-----------------|-----------------|-----------|
| \(yw \in P_t, 1 \leq t \leq 2^{3s-2}\) | 64 \times 2^t + 38 | 1 | \(2(3 \times 2^{s-1})\) |
| \(yw \in C_1, 1 \leq l \leq 4\) | 16 \times 2^t - 11 | 48 \times 2^t + 49 | 4 |
| \(yw \in C_2, 1 \leq l \leq 4\) | 16 \times 2^t - 11 | 48 \times 2^t + 49 | 4 |
| \(yw \in C_2', 1 \leq l \leq 4\) | 16 \times 2^t - 11 | 48 \times 2^t + 49 | 4 |
| \(yw \in A_1, 1 \leq l \leq 4\) | 4(2^{t+2} - 1) | 48 \times 2^t + 43 | 4 |

The edges after the hexagons can be described in the following sets such that \(\{T_l : 1 \leq l \leq s\}, \{U_l : 1 \leq l \leq s\}, \{W_l : 1 \leq l \leq s\}, \{X_l : 1 \leq l \leq s\}, \{Y_l : 1 \leq l \leq s\}, \{Z_l : 1 \leq l \leq s\}\) and \(\{V_l : 1 \leq l \leq s - 1\}\). In the Table 17, we give the values of \(t_G(\delta(y))\) and \(t_G(\delta(w))\) in \(T_l, U_l, W_l, X_l, Y_l, Z_l, V_l\).

**Also, we present the remaining vertices in the core of**

\(G_2(s)\) by \(w_{1+w}k, 2 \leq k \leq 5, O = \{o_1o_2, o_2o_4, o_5o_6, o_7o_8\}, Q = \{q_1q_2, q_2q_3, q_3q_4, q_4q_5, q_5q_6, q_6q_7, q_7q_8, q_8q_9, q_9q_{10}, q_{10}q_{11}, q_{11}q_{12}, q_{12}q_{13}, q_{13}q_{14}, q_{14}q_{15}, q_{15}q_{16}\} \) and \(F = \{q_1q_2, q_2q_3, q_3q_4, q_4q_5, q_5q_6, q_6q_7, q_7q_8, q_8q_9, q_9q_{10}, q_{10}q_{11}, q_{11}q_{12}, q_{12}q_{13}, q_{13}q_{14}, q_{14}q_{15}, q_{15}q_{16}\} \).

Therefore, by using the Tables 16-18, we get the following closed expressions for the total PI index, total Szeged index.
and total Mostar index.

$$P_{\text{f}}(G_2(s)) = \sum_{l=1}^{s} \sum_{yw \in P_l} (2 \times 2^l + 1)$$

+ \sum_{l=1}^{s} \sum_{yw \in C_l} (4 \times 2^l + 1) + 2(16 	imes 2^l + 11 + 48 	imes 2^l + 49)

+ \sum_{l=1}^{s} \sum_{yw \in C\text{'}_l} (4 \times 2^l + 1) + 2(16 	imes 2^l + 11 + 48 	imes 2^l + 49)

+ \sum_{l=1}^{s} \sum_{yw \in A_l} (2 \times 2^l + 11 + 48 	imes 2^l + 49)

+ \sum_{l=1}^{s} \sum_{yw \in O} \sum_{l=1}^{s} (2 \times 2^l + 11 + 48 	imes 2^l + 49)

+ \sum_{l=1}^{s} \sum_{yw \in Q} \sum_{l=1}^{s} (2 \times 2^l + 11 + 48 	imes 2^l + 49)

+ \sum_{l=1}^{s} \sum_{yw \in F} \sum_{l=1}^{s} (2 \times 2^l + 11 + 48 	imes 2^l + 49)

+ \sum_{l=1}^{s} \sum_{yw \in C\text{'}_l} (4 \times 2^l + 1) + 2(16 	imes 2^l + 11 + 48 	imes 2^l + 49)

+ \sum_{l=1}^{s} \sum_{yw \in A_l} (2 \times 2^l + 11 + 48 	imes 2^l + 49)

+ \sum_{l=1}^{s} \sum_{yw \in O} \sum_{l=1}^{s} (2 \times 2^l + 11 + 48 	imes 2^l + 49)

+ \sum_{l=1}^{s} \sum_{yw \in Q} \sum_{l=1}^{s} (2 \times 2^l + 11 + 48 	imes 2^l + 49)

+ \sum_{l=1}^{s} \sum_{yw \in F} \sum_{l=1}^{s} (2 \times 2^l + 11 + 48 	imes 2^l + 49)

= 2048 \times 2^{2s} + 2266 \times 2^s + 3058.

$S_{\text{f}}(G_2(s))$

$$= \sum_{l=1}^{s} \sum_{yw \in P_l} (6 \times 2^l + 11 + 48 \times 2^l + 49) + \sum_{l=1}^{s} \sum_{yw \in C_l} (4 \times 2^l + 1) + 2(16 	imes 2^l + 11 + 48 \times 2^l + 49)$$

+ \sum_{l=1}^{s} \sum_{yw \in C\text{'}_l} (4 \times 2^l + 1) + 2(16 	imes 2^l + 11 + 48 \times 2^l + 49)

+ \sum_{l=1}^{s} \sum_{yw \in A_l} (2 \times 2^l + 11 + 48 \times 2^l + 49)

+ \sum_{l=1}^{s} \sum_{yw \in O} \sum_{l=1}^{s} (2 \times 2^l + 11 + 48 \times 2^l + 49)

+ \sum_{l=1}^{s} \sum_{yw \in Q} \sum_{l=1}^{s} (2 \times 2^l + 11 + 48 \times 2^l + 49)

+ \sum_{l=1}^{s} \sum_{yw \in F} \sum_{l=1}^{s} (2 \times 2^l + 11 + 48 \times 2^l + 49)

= 168646.$$
of chemicals, molecular design and novel drug discovery. In QSAR/QSPR studies appropriate for hazard assessment.

\[ \sum_{y \in F} (32 \times 2^i + 20 + 32 \times 2^i + 16) + \sum_{l=1}^{s} \sum_{y \in T_l} (2 \times 2^{i+3} - 29)(64 \times 2^i - 16 \times 2^i) + 68 \]

\[ + \sum_{l=1}^{s} \sum_{y \in U_l} (2 \times 2^{i+3} - 27)(64 \times 2^i - 16 \times 2^i) + 66 \]

\[ + \sum_{l=1}^{s} \sum_{y \in W_l} (2 \times 2^{i+3} - 25)(64 \times 2^i - 16 \times 2^i) + 64 \]

\[ + \sum_{l=1}^{s} \sum_{y \in X_l} (2 \times 2^{i+3} - 21)(64 \times 2^i - 16 \times 2^i) + 60 \]

\[ + \sum_{l=1}^{s} \sum_{y \in Y_l} (2 \times 2^{i+3} - 19)(64 \times 2^i - 16 \times 2^i) + 58 \]

\[ + \sum_{l=1}^{s} \sum_{y \in Z_l} (2 \times 2^{i+3} - 17)(64 \times 2^i - 16 \times 2^i) + 56 \]

\[ + \sum_{l=1}^{s-1} \sum_{y \in V_l} (2 \times 2^{i+4} - 31)(64 \times 2^i - 2 \times 2^{i+4}) + 70 \]

\[ = (6 \times 2^4 - 4)(64 \times 2^i + 38) + 24(768 \times 2^{2i} + 256 \times 2^i - 539) + 4(768 \times 2^{2i} + 496 \times 2^i - 172) + 4(1024 \times 2^{2i} + 1152 \times 2^i + 324) + 8(1024 \times 2^{2i} + 1216 \times 2^i + 361) + 8(1024 \times 2^{2i} + 1152 \times 2^i + 320) + \sum_{l=1}^{s} 2^{i-l+2}(6144 \times 2^{2i+l} - 1536 \times 2^{2i} + 8160 \times 2^i - 8832 \times 2^i - 8668) + \sum_{l=1}^{s} 2^{i-l+1}(2048 \times 2^{i+l} - 1024 \times 2^{2i} + 2736 \times 2^i - 1984 \times 2^i - 2170) = 42368 \times 2^{2s} + 3165 \times 2^s - 7032 + 24576s \times 2^{2s} + 32640s \times 2^s + 4096(s - 1)^2 \times 5472(s - 1)^2 - 1536 \times 2^{i+3}(2^s - 1) - 8832 \times 2^{i+2}(2^s - 1) - 1024 \times 2^{i+3}(2^s - 2) - 8668 \times 2^s - 2^s - 1984 \times 2^{i+1} \times 2^s - 2170 \times 2^{2s} - 2 = (28672s - 15360)2^{2s} + (46816s3112s)2^s + 36320. \]

\[ \text{Mo}_{y}(G_2(s)) = \sum_{l=1}^{s} \sum_{y \in F_l} |64 \times 2^s + 38 - 1| + \sum_{l=1}^{s} \sum_{y \in C_l} 2|48 \times 2^i + 49 - 16 \times 2^i + 11| + \sum_{l=1}^{s} \sum_{y \in C_l} 2|48 \times 2^i + 49 - 16 \times 2^i + 11| + \sum_{l=1}^{s} \sum_{y \in C_l} 2|48 \times 2^i + 49 - 16 \times 2^i + 11| + \sum_{l=1}^{s} \sum_{y \in C_l} |48 \times 2^i + 43 - 4(2^{s+2} - 1)| + \sum_{y \in O} [48 \times 2^i + 18 - 32 \times 2^i - 18] + \sum_{y \in Q} [48 \times 2^i + 18 - 32 \times 2^i - 18] + \sum_{y \in F} [48 \times 2^i + 20 - 32 \times 2^i - 16] + \sum_{l=1}^{s} \sum_{y \in F_l} |64 \times 2^s - 68 - 2 \times 2^{i+3} + 29| + \sum_{l=1}^{s} \sum_{y \in Y_l} |64 \times 2^s - 68 - 2 \times 2^{i+3} + 21| + \sum_{l=1}^{s} \sum_{y \in Z_l} |64 \times 2^s - 68 - 2 \times 2^{i+3} + 19| + \sum_{l=1}^{s} \sum_{y \in V_l} |64 \times 2^s - 68 - 2 \times 2^{i+3} + 17| + \sum_{l=1}^{s} \sum_{y \in V_l} |64 \times 2^s - 68 - 2 \times 2^{i+3} + 31| = (6 \times 2^4 - 4)(64 \times 2^i + 37) + 24(32 \times 2^i + 60) + 4(32 \times 2^i + 47) + 4(0) + 8(0) + 8(4) + \sum_{l=1}^{s} 2^{s-l+2} \times (64 \times 6 \times 2^s + 32 \times 6 \times 2^i + 2385) + \sum_{l=1}^{s} 2^{s-l+1}(64 \times 2^s - 64 \times 2^i + 101) = 384 \times 2^{2s} - 34 \times 2^i - 148 + 896 \times 2^i + 1660 - 768s \times 2^s - 128(s - 1)2^s + 4(2^s - 1)(384 \times 2^s + 2385) + 2(2^s - 2) \times (64 \times 2^i + 101) = 2048 \times 2^{2s} + (8940 - 896s)2^s - 8432. \]

IV. CONCLUSION

An ongoing direction in mathematical and computational chemistry is the characterization of molecular structures with the help of graphical descriptors. These invariants have been established as a better alternative for hazard assessment of chemicals, molecular design and novel drug discovery. Dendrimers have an eye-catching place in the research
considering that of their remarkable physical and chemical properties and the comprehensive range of promising applications in various areas such as physics, chemistry, biology, medicine, and engineering. The Szeged indices have been proven that they can associate highly with various physicochemical and biological properties, for instance, see [9]. Different chemical applications of the PI indices were yielded, and it has proven that the PI indices associates well with the various indices as well as with the biological activities and physico-chemical properties of the underline structure, for instance, see [13]. Mostar index is a new suggested quantity; it has not been so far applied and suggested to be used in its physicochemical or biological researches. Recently, one such work has been performed in this direction for the acentric factor of some octane isomers, and it is confirmed that there is a linear relation between Mostar index and acentic factors of these isomers. In this paper, we have obtained exact analytical expressions of different versions of Szeged, PI and Mostar indices for the molecular graphs of two types of dendrimers by using the cut method. Our results could be beneficial in the models of QSRR/QSAR relationships for these molecular structures for assessing their properties.

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