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Extreme Star of Phenylenes for the Merrifield-Simmons Index

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Abstract: We identify extremal graphs concerning the number of independent sets for polyphenylene dendrimers. Specifically, we demonstrate that for a certain number of phenylenes, for example to k phenylenes, the compound formed as a star S_{pp}^k with a phenylene core achieves the maximum Merrifield-Simmons (M-S) index for a 1-connected component with an equal number of phenylenes. However, by relaxing the constraint of dendrimers to allow vertices with degrees greater than 3, it becomes possible to obtain topologies for compounds with a higher M-S index value. In this scenario, the starting point where every cut-edge is incident to the same vertex of the phenylene core emerges as the extremal topology concerning the M-S index for a 1-connected component with k phenylenes. These insights could facilitate the development of advanced molecular designs and contribute to enhanced performance in applications such as boiling points, drug delivery, molecular electronics and other nanotechnological innovations.

Keywords: counting independent sets, merrifield-simmons index, extremal topologies, dendrimer compounds, structural pattern recognition

MSC: 05C30, 05C35, 05C92

1. Introduction

Merrifield and Simmons demonstrated the relationship between the quantity of independent sets in G, denoted as $i(G)$, and the boiling points of the molecular graph represented by G [1]. This connection is a primary factor behind labeling the number of independent sets of a graph G in mathematical chemistry as the Merrifield-Simmons index (M-S) of G. However, within graph theory, $i(G)$ is referred to as the Fibonacci number of G.

A topological index refers to a mapping from the collection of chemical compounds, depicted as molecular graphs, to the set of real numbers. Numerous topological indices exhibit strong correlations with specific physicochemical properties of the compounds they represent. Among the most renowned topological indices in mathematical chemistry are the Merrifield-Simmons and the Hosoya indices [2, 3].

On the other hand, in the area of structural pattern recognition, it has been a relevant line of research to identify topologies on graphs matching the extreme values for certain topological indices [3]. Specifically, in graph theory, there is a wealth of research dedicated to characterizing extremal graphs concerning the Hosoya index and the Merrifield-Simmons index across various topological structures, including unicyclic graphs, trees, and configurations containing

pentagonal and hexagonal cycles [2–6]. For example, Haizhen and Zhang [6] determined the minimal M-S index for double hexagonal chains. In [7], Gutman et al. characterized the tree graph with the maximal M-S index among the trees with a given diameter.

Hexagonal array graphs have been extensively studied and are a significant area of focus in mathematical chemistry due to their utility in examining the intrinsic characteristics of molecular graphs. A notable subset of molecular graphs is comprised of phenylenes, which are defined as divalent aromatic radicals obtained from a benzene molecule through the removal of two hydrogen atoms. When the fundamental building block of a polymer is a phenylene, the resulting polymer is termed a polyphenylene (PP). Polyphenylenes constitute a significant group of benzene molecules that are used as precursors to various commercially and valuable materials, including polyphenylene oxide and polyphenylene sulfide. The fundamental representation of polyphenylene compounds involves a special class of graphs, wherein two hexagons are connected by an edge

The derivatives of polyphenylenes are commonly seen chemicals, which can be used in organic synthesis, drug synthesis, heat exchanger, etc [8]. Unbranched polyphenylenes are relevant in the realm of low-dimensional organic conductors, while their dendrimer-like equivalents (PPDs) have a relevant part in the synthesis of large graphene molecules [5]. Polyphenylenes exhibit numerous structural similarities with benzenoid compounds, which are depicted by hexagonal arrays. Consequently, closely related compound classes can be effectively modeled using both graph types. However, while the investigation of benzenoid compounds has often preceded or accompanied the exploration of benzenoid graphs, the graphs representing polyphenylene compounds have largely remained uncharted territory [9].

Polyphenylene dendrimers (PPDs) stand out as a distinctive category of macromolecules due to their backbone comprising twisted benzene repeat units, leading to a firm and shape-consistent structure [10]. PPDs are highly branched, monodisperse macromolecules that are shape-persistent because their backbone consists of substituted benzene rings. Thus, these dendrimers are extremely stable and can be modified in a site-specific manner since their dendrons cannot reorient due to the rigidity of the backbone [11, 12].

PPDs can be synthetically tailored at their core, scaffold, and surface to introduce a wide range of chemical functionalities that influence their applications. The synergy between the unique macromolecular characteristics of polyphenylene dendrimers and remarkable synthetic creativity serves as a blueprint for the next wave of synthetic dendrimers, enabling the creation of intricate structures beyond the reach of other branches of chemistry [11]. This perspective delves into how advancements in synthetic chemistry have propelled polyphenylene dendrimers from their initial role as precursors for nanographene to the forefront of diverse applications, including next-generation dendrimers for organic electronic devices, sensors detecting volatile organic compounds (VOCs), nanocarriers for small molecules, and even their utilization in complexes with therapeutic drugs and viruses, among various other uses.

In this article, one of the main contributions is to show how general counting rules on independent sets can be applied to compute the M-S index on phenylenes compounds. In our analysis, we recognize extremal topologies for 1-connected components of phenylenes, under the restriction of considering a fixed number of phenylenes. This class of problems is relevant in the design of new chemical molecules, and they are a challenger in the structural pattern recognition area.

Our paper is structured as follows: Section 1 provides a general introduction. Section 2 introduces the preliminaries and the notation that will be employed. In Section 3, we present the initial extremal topologies for a connected component of a graph. Section 4 shows the extremal topologies for a single connected polyphenylene dendrimer. The final section offers conclusions drawn from this work.

2. Preliminaries

Let $G = (V, E)$ be an undirected simple graph, where V (or $V(G)$) denotes the set of vertices and E (or $E(G)$) denotes the set of edges. In this work, we consider that the graph does not have loops or parallel edges. The edge connecting the vertices u and v is denoted by uv, and sometimes $\{u, v\}$ is used to denote an edge uv.

The set $N(x) = \{y \in V : xy \in E\}$ denotes the neighborhood of $x \in V$. Meanwhile, $N[x] = N(x) \cup \{x\}$ denotes the closed neighborhood of x. We use $|A|$ to denote the cardinality of the set A. The degree of a vertex x in the graph G,

denoted by $\delta_G(x)$, is $|N(x)|$. The subindice G is omitted in the notation of the degree, if there is not doubt about what graph G is being considered. Meanwhile, $\Delta(G) = \max\{\delta_G(x) : x \in V\}$ is considered the degree of the graph G.

Given two distinct vertices v and w, we denote the path between both vertices (denoted by P_{vw} or simply as P_n), as the sequence of the edges: $v_0 v_1, v_1 v_2, \ldots, v_{n-1}v_n$ such that $v = v_0$, $v_n = w$, and $v_k v_{k+1} \in E$ for $0 \le k < n$, in this context, the size of the path is n. When in a path all the its vertices are distinct, it is called a simple path. But, if in a path only the first and last vertices are identical, then the path is a simple cycle.

For $u, v \in V(G)$, $d(u, v)$ denotes the distance between u and v, which is the length of the shortest path (number of edges) between u and v in G. The *vertex-connectivity* of a graph G is the minimum number of vertices whose deletion disconnects G. Any set of vertices whose deletion disconnects G is called a *separating set* or *vertex cut* of G. If G request at least k vertices to be disconnected, then G is a k-connected graph. Meanwhile, the *edge-connectivity* of G is the minimum number of edges whose deletion disconnects G. The set of edges whose deletion disconnects G is called *cutting edges*. We denote by P_{n-1}, C_n and S_n to a path, a simple cycle and a star graph, respectively, all of them containing n vertices. And we use kC_n or kP_{n-1} (with $k \in \mathcal{N}$) to denote k different disconnected cycles or paths, respectively.

A subset of vertices $S \subseteq V$ in a graph, G, is termed an "independent set" if for every pair of vertices u and v in S, the edge $\{u, v\}$ is not present in $E(G)$. $I(G)$ denotes the collection of all independent sets in the graph G. Meanwhile, the notation $I_v(G)$ is used to specifically denote the independent sets in G containing the vertex v, and conversely, $I_{-v}(G)$ represents the independent sets in G where the vertex v is absent.

On the other hand, $i(G)$ is used to denote the number of independent sets in the graph G. Specifically, $i(G)$ corresponds to $|I(G)|$. The computation of $i(G)$ is a $\sharp$P-complete problem, even for graphs with $\Delta(G) \ge 3$, or when it is restricted to 3-regular graphs [13].

Consider a molecular graph $G = (V, E)$. Let $n(G, k)$ represent the count of ways to select k mutually independent vertices in G. By definition, $n(G, 0)$ equals 1 for all graphs, and $n(G, 1)$ equals $|V(G)|$. Additionally, define $i(G)$ as the Merrifield-Simmons index of G, which is the total number of independent sets in G, given by $\sum_{k \ge 0} n(G, k)$.

A polygon, also referred to as a polygonal graph, is fundamentally a simple cycle graph. Thus, a cycle graph C_n with n vertices represents an n-sided polygon or an n-gon. When two polygons share an edge, they are termed adjacent. The way in which two k-gons are connected, whether by a shared vertex or a shared edge, determines different categories of chemical compounds. A polygonal array, denoted as $P_{k, t}$, is a graph formed by combining a finite number of t congruent polygons, where each polygon in $P_{k, t}$ has exactly k sides.

3. Extremal basic topologies for the M-S index

There are three key principles that guide the enumeration of combinatorial objects on graphs, allowing us to decompose the graph either by choosing a vertex, or by selecting an edge, or considering the different connected components of a graph:

1. The counting rule based on a vertex-the vertex division: for $v \in V(G)$,

$$i(G) = i(G - v) + i(G - (N[v])) \tag{1}$$

2. The counting rule based on an edge-the edge division: for $e = \{x, y\} \in E(G)$,

$$i(G) = i(G - e) - i(G - (N[x] \cup N[y])) \tag{2}$$

3. The product rule for connected components. When a graph G is formed by a list $G_1, \ldots, G_k$ of connected components, then

$$i(G) = \prod_{j=1}^{k} i(G_j) \tag{3}$$

The Lemmas presented below will prove valuable information for our analysis. They demonstrate that in an initial graph $G = (V, E)$, adding new edges to $E(G)$ results in a decrease of $i(G)$. Conversely, adding new vertices to $V(G)$ leads to an increase in $i(G)$, even when these new vertices are connected to all the original vertices $v \in V(G)$.

Lemmas 1 Let x and y be two non-adjacent vertices of G, and let $e = \{x, y\}$ be an edge that is not in $E(G)$ originally, then $i(G) > i(G \cup e)$.

Proof. If we form $C_e = \{S \in I(G) : x, y \in S\}$ be the collection of independent sets containing the vertices $x, y \in V(G)$. $|C_e| > 0$ since at least the set $\{x, y\} \in C_e$, since $e \notin E(G)$. We have that $i(G \cup e) = i(G) - |C_e|$, consequently $i(G) > i(G \cup e)$. □

Lemmas 2 Let us consider a new vertex $x \notin V(G)$. Let $G_x = G \cup \{\{x, v\} : \text{for some } v \in V\}$, then $i(G_x) > i(G)$.

Proof. If x were adjacent with all vertex in G, then $I(G_x) = I(G) \cup \{\{x\}\}$, and then $i(G_x) = i(G) + 1$. If there are vertices do not adjacents to x in G_x then $i(G_x) > i(G) + 1$, in whatever case $i(G_x) > i(G)$. □

The sequence of Fibonacci numbers is obtained as $F_0 = 0$, $F_1 = 1$ and $F_n = F_{n-1} + F_{n-2}$. We denote the nth-Fibonacci number as F_n. The properties of Fibonacci numbers have proven valuable in the examination of structural compounds within the realm of mathematical chemistry.

With respect to extremal topologies associated to the M-S index of a graph G, if we consider G as just a 1-connected component with k vertices, and with a minimum number of edges that permit G to be connected, in this context, there exist two distinct topologies associated with the extremal values for the M-S index of G.
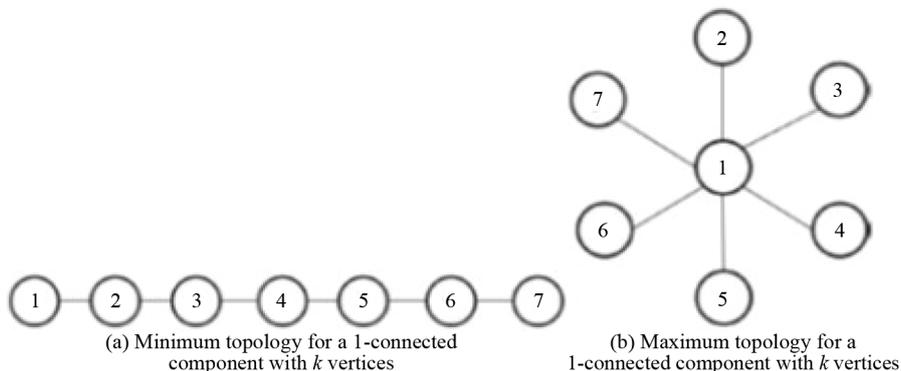

(a) Minimum topology for a 1-connected
component with k vertices

(b) Maximum topology for a
1-connected component with k vertices

Figure 1. Basic topology

It is known that the path P_{k-1} with k vertices and $k-1$ edges obtains a minimum value for $i(P_{k-1}) = F_{k+2}$ into all 1-connected component of k vertices. Meanwhile, the star S_k from k vertices and $k-1$ edges has the maximun value: $i(S_k) = 2^{k-1} + 1$ for any 1-connected component of k vertices [14]. In Figure 1, we show in 1(a) a path P_6, and in 1(b) we show a star S_6 that represent the extremal topologies for the M-S index for 1-connected graph of 7 vertices.
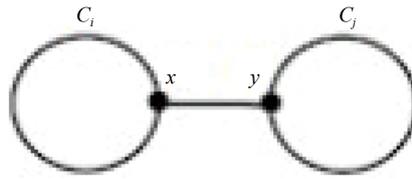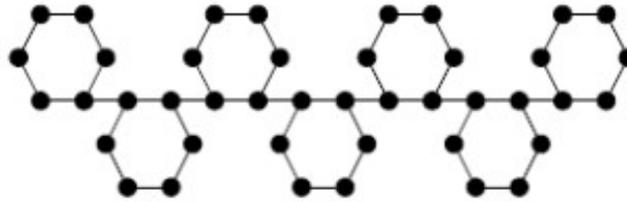
Figure 2. A Bipolygonal Graph

Figure 3. A zigzag polyphenylene chain

Let C_i and C_j represent two polygons with i and j vertices, respectively. A particular type of graph is created by connecting C_i and C_j through an edge $e = \{x, y\}$, where x is a vertex in C_i and y is a vertex in C_j (see Figure 3). This connected graph, formed via the edge cut $e = \{x, y\}$, is known as a bipolygonal graph and is denoted as $H_{i, j} = C_i \cup_e C_j$. Specifically, when C_i and C_j are hexagons, $H_{i, j}$ serves as the fundamental graph for constructing chains of bipolygonal graphs that model the structure of phenylenes dendrimers.

Now, let us delve into the edge division principle: suppose $e = \{x, y\} \in E(G)$, then $i(G) = i(G - e) - i(G - (N[x] \cup N[y]))$. We demonstrate how to apply this edge division technique to calculate the Merrifield-Simmons index for a single phenylene.

Proposition 1 Let $H_{i, j}$ be a bipolygonal graph, and let F_i be the notation for the ith-Fibonacci number. $i(H_{i, j}) = F_{i+1} \cdot F_{j+1} + F_{i+1} \cdot F_{j-1} + F_{i-1} \cdot F_{j+1}$.

Proof. According to the edge division rule applied on the edge cut:

$$i(H_{i, j}) = i(C_i) \cdot i(C_j) - i(P_{i-3} \cdot P_{j-3}) = (F_{i+1} + F_{i-1}) \cdot (F_{j+1} + F_{j-1}) - F_{i-1} \cdot F_{j-1}$$

$$= F_{i+1}F_{j+1} + F_{i+1}F_{j-1} + F_{i-1}F_{j+1} + F_{i-1}F_{j-1} - F_{i-1}F_{j-1}$$

$$= F_{i+1}F_{j+1} + F_{i+1}F_{j-1} + F_{i-1}F_{j+1}.$$

This result can be seen as $F_{i+1} \cdot (F_{j+1} + F_{j-1}) + F_{i-1} \cdot F_{j+1}$ where $(F_{j+1} + F_{j-1})$ represents the j-th Lucas Number. $\square$

In [15], an analysis was conducted to identify extremal topologies for the M-S index on bipolygonal graphs. Specifically, in the case of a phenylene (a bihexagonal graph), it was found that its M-S index does not represent an extremal value within the set of bipolygonal graphs composed of 12 vertices.

Parallel studies to the previous result have been done in the analysis to recognize extremal topologies for the average size of independent sets, instead of the exact value of $i(G)$ (see for example [16] for the case of unicyclic graphs), and considering basic topologies such as trees, stars, and unicyclic bipartite graphs.

In this article, we will analyze the M-S index for a polygonal chain H_n formed by a sequence of n polygons h_i, $i = 1, \ldots, n$, where each consecutive pair of polygons $h_i \cdot h_{i+1}$ are joined by a cutting edge $e_i = \{x_i, y_i\}$, $i = 1, \ldots, n-1$ where

$x_i \in V(h_i)$, $y_i \in V(h_{i+1})$. This means that $H_n = h_1 \cup_{e_1} h_2 \cup_{e_2} \ldots \cup_{e_{n-2}} h_{n-1} \cup_{e_{n-1}} h_n$. Note that in this case, $(V(h_i) \cap V(h_j)) = \emptyset$ for $i \neq j$, i, $j = 1, \ldots, n$. Also, that $\delta(x_i) = \delta(y_i) = 3$, $i = 1, \ldots, n-1$, while the remaining vertices have degree 2. We call this type of graph a polygonal chain joined by cutting edges. When each polygon in the chain H_n of n polygons is a k-gons, then we say that H_n is a regular polygonal chain, or simply, a polygonal chain denoted as $H_{k, n}$.

Notice that a single phenylene is a 1-connected graph, where there exist two cut vertices and one cutting edge (see Figure 3). Meanwhile, a polyphenylene chain (A chain of hexagons joined by cutting edges) comprises two distinctive hexagons, each one with only one cut-vertex. These hexagons are referred to as terminals, while all other hexagons are considered internal (see Figure 4). The count of hexagons in a specific polyphenylene chain directly relates to its length.

An internal hexagon is called ortho-hexagon, meta-hexagon, or para-hexagon if its respective cut-vertices are at distance 1, 2, or 3, respectively. If all internal hexagons in a polyphenylene chain are of the same type, say ortho (or meta-chain, or para-chain), the chain is an ortho-chain (or meta-chain, or para-chain). For example, in Figure 4 we show an ortho-chain, also called a zigzag polyphenylene chain.
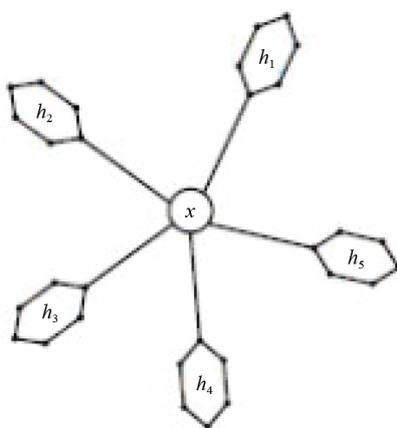

Figure 4. A zigzag polyphenylene chain

4. A note on polyphenylene dendrimers

In this section, we identify the extremal topologies that maximize the Merrifield-Simmons index for a polyphenylene dendrimer with a bound number of phenylenes. Polyphenylene dendrimers (PPDs) are highly branched, rigid, monodisperse macromolecules consisting of substituted benzene rings. They represent a unique class of dendrimers based on their rigid, shape persistent chemical structure [10].
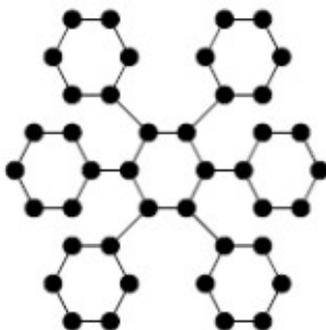

Figure 5. A star of polyphenylenes (S_{pp}^5) with a vertex core

We analyze a star formed of polyphenylenes (PP), considering a single vertex x as the center of the PPDs. Each polyphenylene is linked to x by a cutting edge. The vertex x is called the core of the PPDs, and we call this PPDs a star (denoted by S_{pp}^k), where $k = \delta(x)$. A PPDs star S_{pp}^5 is illustrated in Figure 5.

According to the vertex reduction rule, when a single vertex x is eliminated, in order to maximize the independence of the components of the graph, x must be incident to the highest number of cutting edges. And due to Lemma 1, the number of independent sets is increased according to the number of removed edges. In addition, due to the fact that the set of PP was linked by this single vertex x, when x is removed by the application of the vertex reduction rule, then the independence between the substructures involved in the polyphenylene dendrimer is maximized.

Let us calculate $i(S_{pp}^k)$ based on the vertex reduction rule applied to the core x of the star.

$$i(S_{pp}^k) = i(S_{pp}^k - \{x\}) + i(S_{pp}^k - N[x]) = \prod_{j=1}^{k} i(h_j) + \prod_{j=1}^{k} i(P_{6-1})$$

$$= \prod_{j=1}^{k}(F_{6+2} - F_{6-2}) + \prod_{j=1}^{k} F_{5+2} = \prod_{j=1}^{k}(F_8 + F_7 - F_4) = (F_9)^k - (F_4)^k \tag{4}$$

Since we are regarding polyphenylenes as the basic polygon of the star, the base index of the Fibonacci number is 6 (corresponding to each hexagon h_j, $j = 1, \ldots, k$). However, in previous equation (4), the final term can be replaced by $i(S_r^k) = (F_{r+3})^k - (F_{r-2})^k$, when polygons of size r are considered instead of hexagonal phenylenes.

On the other hand, using the relation $i(C_r) = F_{r+1} + F_{r-1}$ for cycles of size r, then eq. (4) can be rewritten as:

$$i(S_{pp}^k) = \prod_{j=1}^{k} i(C_r) + \prod_{j=1}^{k} i(P_5) = \prod_{j=1}^{k}(F_7 + F_5 + F_7) = 2^k(F_7)^k + (F_5)^k$$

This final expression demonstrates the exponential growth pattern of the Merrifield-Simmons index value for the star $i(S_{pp}^k)$, as determined by the number k of PP's composing it.

The selection of the core molecule in a polyphenylene dendrimer (PPDs) plays a crucial role in determining the macromolecule's geometry, which in turn significantly impacts the resulting material properties. For instance, substituting the core x in Figure 5 with a phenylene leads to the formation of Star Polyphenylene Dendrimers (SPDs), as illustrated in Figure 5.

If we expand the extremal topologies introduced in Figure 1 for a 1-connected component in the case of phenylenes, replacing each vertex of the path and the star with one phenylene, we find that in the case of the minimum topology, corresponding to a path P_n, this topology results in a chain of phenylenes. When forming the bonds of the links of the phenylenes chain, there are three possibilities for the links, depending on where the cutting edge of the phenylenes is placed, as it was described at the end of previous section.

In the realm of polyphenylene chains, it is recognized that an ortho-chain, where each cutting edge is positioned at a distance of 1 from its predecessor, represents the minimal topology in terms of the Merrifield-Simmons (M-S) index [9]. Figure 4 depicts an ortho-chain of size 7, commonly referred to as the zigzag polyphenylene chain.

In the context of the maximum topology of a 1-connected polyphenylene dendrimer, two types of stars emerge: the phenylenes star, where each cutting edge originates from a different vertex of the hexagonal core, denoted as S_{pp}^6 (see Figure 5), and the star depicted on the right and top side of Figure 6, where all cutting edges stem from the same vertex of the central hexagon, labeled as S_x^6 to signify that x is the cut-vertex joining a total of 7 phenylenes.

It is known to exact formulas for computing the number of independent sets on basic graph topologies. For example, $i(P_n) = F_{n+3}$, and $i(C_n) = F_{n+2} - F_{n-2}$, where P_n, C_n, F_{n+2} represent paths and cycles of size n and F_{n+2} is the $n+2$-th

Fibonacci number, respectively. In our case, as a phenylene is a cycle of size 6, then $i(C_6) = F_8 - F_4 = 21 - 3 = 18$, and for paths of size 4, $i(P_4) = 13$.

Let $x \in V(S_{pp}^6)$ be one of the vertices of the hexagon core, applying the vertex reduction rule on x for computing $i(S_{pp}^6)$, and according to equation (1), we have that $i(S_{pp}^6) = i(S_{pp}^6 - \{x\}) + i(S_{pp}^6 - N[x])$, whose connected components are drawn in the left-down part in Figure 6.

Applying the product rule for connected components (eq. 3), we obtain $i(S_{pp}^6) = i(C_6) * i(P_4 || 5C_6) + i(C_6)^2 * i(P_4) * i(P_2 || 3C_6) = 18 * 15,338,484 + 4,212 * 21,510 = 276,092,712 + 90,600,120 = 366,692,832$.

On the other hand, let x be the cut-vertex of the hexagon core in the star S_x^6, we obtain for the application of the vertex reduction rule on x, $i(S_x^6) = i(S_x^6 - \{x\}) + i(S_x^6 - N[x])$, whose connected components correspond with the graphs drawn in the right-down part in Figure 6. And by the application of the product rule for connected components (eq. 3), $i(S_x^6) = i(C_6)^6 * i(P_4) + i(P_4)^6 * i(P_2) = (18)^6 * 13 + (13)^6 * 5 = 442,158,912 + 24,134,045 = 466,292,957$.

Thus, the product rule for connected components justifies the fact that $i(S_x^6) > i(S_{pp}^6)$. Both graphs, S_{pp}^6 and S_x^6, are 1-connected graphs, featuring precisely 6 distinct sets of cutting edges. However, in S_x^6, the cut-vertex x serves to connect 7 different hexagons. Consequently, its removal disconnects S_x^6 into 7 connected component subgraphs. According to the product rule for connected components, this maximizes the M-S index of the original graph due to the exponential nature of the product rule among a series of connected components.

Thus, it is not difficult to recognize that the star topology S_x^6 is extremal and corresponds to the topology that maximizes the M-S index for k phenylenes. However, it is the phenylene star (S_{pp}^6) that maintains a topology akin to phenylene dendrimers. This dendrimer (see the star in Figure 5) corresponds to the extremal topology that maximizes the M-S index for phenylene dendrimers. This latter topology also ensures that the degree for any vertex in the compound is either 2 or 3.

The selected dendrimer core can be used to establish the number of arms and geometry of the macromolecule, while it can also influence the overall characteristics of the system such as photophysical properties, ion dissociation, or conductivity. In general, substituting the core of a dendrimer for different molecules to form asymmetric PPDs is extremely useful for applications such as interfacial or surface bound chemistries, or for the synthesis of Janus type particles [10].

In this context, the SPD retains the property of having a maximum Merrifield-Simmons index for compounds consisting of exactly 7 phenylenes. This is due to its preservation of the topology of a star tree, where each vertex of the core is associated with a single cutting edge.
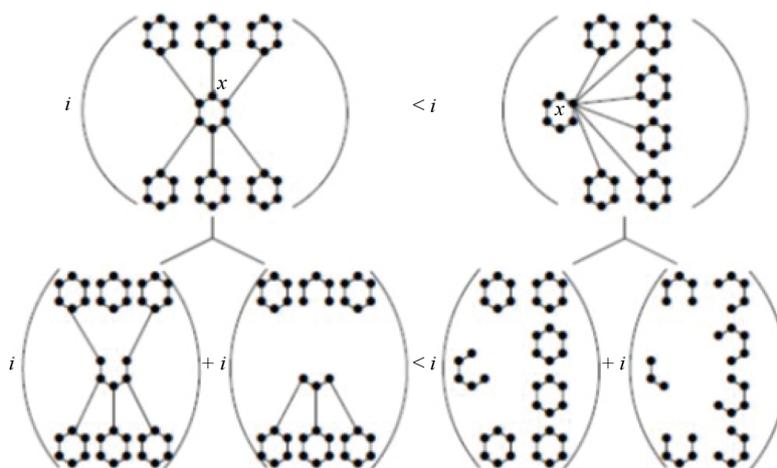

Figure 6. Comparing the M-S index for two polyphenylene starts

These kind of dendrimers can undergo synthetic modifications at their central structure, supporting framework, and outer layer to incorporate various chemical functionalities, affecting their potential uses. Typically categorized as 'core dense', dendrimers feature flexible arms composed of molecules that assume a random coil configuration, often causing them to collapse around the central core [17]. This viewpoint aims to give an insight into the intricate syntheses of diverse PPDs, focusing on their central structure, supporting framework, and external features, while exploring how these alterations impact their overall characteristics. It seeks to establish a narrative linking cutting-edge dendrimer syntheses with groundbreaking applications such as organic electronic layers, functional nanographenes, biomimetic polymers, nanocarriers for medications, and beyond [11].

Summarizing: if we fix the number of phenylenes, for example to k phenylenes, the compound that provides the minimum value for the M-S index is achieved for the zig-zag polyphenylene chain (the ortho-chain), in Figure 4 we have shown a zig-zag polyphenylene chain with 7 phenylenes. Meanwhile, the compound formed as a star S_{pp}^k with a phenylene core achieves the maximum M-S index for one connected component with a same number of phenylenes, as it was illustrated in Figure 5. However, breaking the constraint of dendrimers with vertices of maximum degree 3, it is possible to get topologies for polyphenylene with a bigger value for its M-S index. In this instance, the star depicted on the right and top side of Figure 6, where all cut-edges converge at a single vertex of the phenylene core, represents the extremal topology in terms of the Merrifield-Simmons index for a connected component containing 7 phenylenes.

5. Conclusions

It is known that the path P_{k-1} with k vertices and $k-1$ edges obtains a minimum value for $i(P_{k-1}) = F_{k+2}$ into all 1-connected component of k vertices. Meanwhile, the star S_k from k vertices and $k-1$ edges has the maximum value: $i(S_k) = 2^{k-1} + 1$ for any 1-connected component of k vertices.

We expand upon the previous topologies to include considerations for polyphenylene dendrimers. We acknowledge that the zig-zag polyphenylene chain represents the extremal minimum value for the Merrifield-Simmons index for any 1-connected polyphenylene chain.

Furthermore, for any given number of phenylenes, such as k phenylenes (where $k \leq 7$), the structure formed as a star S_{pp}^k with a phenylene core achieves the maximum M-S index for a 1-connected component containing the same number of phenylenes. However, by relaxing the constraint of dendrimers with vertices of maximum degree 3, it becomes possible to obtain topologies for polyphenylenes with a higher M-S index value. In this scenario, the structure where all cut-edges converge at a single vertex of the phenylene core represents the extremal maximum topology concerning the M-S index for a connected component containing any given number of phenylenes.

In this article, we have explored extremal topologies for an initial layer originating from the core of a dendrimer. Nevertheless, a deep analysis will be required to identify extremal topologies for dendrimer compounds with multiple layers in their structural configurations.

Conflict of interest

The authors declare no conflicts of interest.

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