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# THE MERRIFIELD-SIMMONS INDEX OF AN INFINITE CLASS OF DENDRIMERS

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A dendrimer is a tree-like highly branched polymer molecule. Dendrimers are synthesized from monomers with new branches added in discrete steps to form a tree-like architecture. They have some proven applications, and numerous potential applications. The Merrifield-Simmons index of a graph is defined as the total number of the independent sets of the graph. In this paper, we give a relation for computing Merrifield-Simmons index of an infinite family of dendrimers.

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## 1. Introduction

Dendrimers are nanostructures that can be precisely designed and manufactured for a wide variety of applications. Dendrimers are the first large, man-made molecules with precise, nano-sized composition and well-defined three-dimensional shapes. The first dendrimers were synthesized divergently by Vögtle in 1978 [1]. Dendrimers then experienced an explosion of scientific interest because of their unique molecular architecture.

Let $G = (V, E)$ be a simple molecular graph (i.e. an undirected graph containing no graph loops or multiple edges) whose vertex and edge-shapes are represented by $V(G)$ and $E(G)$, respectively. The elements of $E$ are 2-element subset of $V$. Two vertices of $G$ are said to be independent if there are not any edges between them. For any $v \in V(G)$, $N_G(v) = \{u \mid uv \in E(G)\}$ denotes the neighbors of $v$. Let $W \subseteq V(G)$, $G - W$ denotes the subgraph of $G$ obtained by deleting the vertices of $W$ and the edges incident with them.

A topological index is a real number related to a molecular graph. It must be a structural invariant, i.e. it does not depend on the labeling or the pictorial representation of a graph. The Merrifield-Simmons index [2- 4] is one of the topological indices whose mathematical properties were studied in some detail [5- 9]. In [3] it was shown that this index is correlated with the boiling points.

Let $G(V, E)$ be a simple graph on *n* vertices. A $k$-independent set of $G$ is a set of $k$ mutually independent vertices. Denote by $i(G, k)$ the number of the $k$-independent sets of $G$. By definition, the empty vertex set is an independent set. Then $i(G,0) = 1$ for any graph $G$. The Merrifield-Simmons index of $G$, denoted by $i(G)$, is defined as

$$i(G) = \sum_{k=0}^{n} i(G, k) .$$

So $i(G)$ is equal to the total number of the independent sets of $G$.

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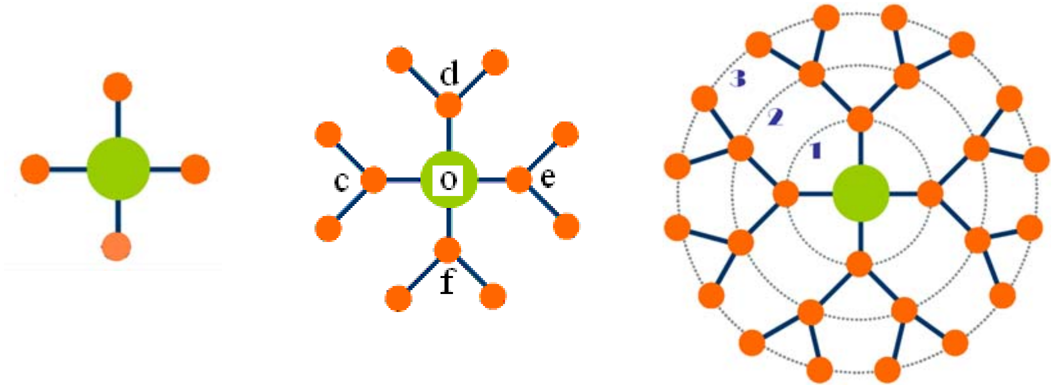
In this paper we investigate the Merrifield-Simmons index for an infinite family of dendrimers.

Structure of denrimer, $D[n]$, which is used in this study is as depicted in figure 1. Here $n$ is the step of growth in the type of dendrimer.




D[1] D[2] D[3]

*Fig. 1. Structures of the dendrimer used in this study*

## 2. Main results and discussion

We give two important lemmas from [3, 10] which are helpful to the proofs of our main results.

***Lemma 1.*** [3] Let $G$ be a graph with $k$ components $G_1, G_2, \ldots, G_k$, then

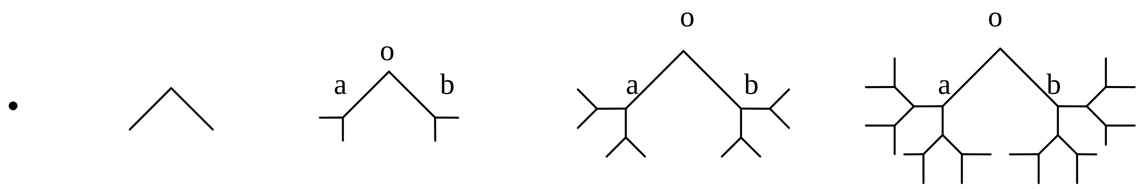
$$i(G) = \prod_{j=1}^{k} i(G_j).$$

***Lemma 2.*** [10] For any graph $G$ with any $v \in V(G)$, we have

$$i(G) = i(G - v) + i(G - [v]),$$

where $[v] = N_G(v) \cup v$.

Define $T_n$ as the binary tree whose step of growth is equal to $n$ [figure 2]. First, we try to find a recursive relation for computing $i(T_n)$.




$T_0$ $T_1$ $T_2$ $T_3$ $T_4$

*Figure 2.*

***Theorem 1*:** The Merrifield-Simmons index of $T_n$, is computed as follows:

$$i(T_n) = (i(T_{n-1}))^2 + (i(T_{n-2}))^4 \qquad for\ n \geq 2,$$

where $i(T_0) = 2$ and $i(T_1) = 5$.

***Proof:*** For $n=0$ and $n=1$, it's easy to realize that $i(T_0)=2$ and $i(T_1)=5$. For $n\geq 2$, assumes that $o$ is the first node of $T_n$ and $a$ and $b$ are vertices which are adjacent with $o$ [see figure 2]. From lemma1, we have:

$$i(T_n)=i(T_n-o)+i(T_n-[o]). \tag{1}$$

The graph $T_n-o$ consists of two subgraphs $T_{n-1}$. From lemma 2 we can say that:

$$i(T_n-o)=(i(T_{n-1}))^2. \tag{2}$$

The graph $T_n-[o]$ has four components that each of them is $T_{n-2}$. So we have

$$i(T_n-[o])=(i(T_{n-2}))^4. \tag{3}$$

Finally, from (1), (2) and (3) we obtain:

$$i(T_n)=(i(T_{n-1}))^2+(i(T_{n-2}))^4. \tag{4}$$

***Theorem 2*:** The Merrifield-Simmons index of $D[n]$ is computed as follows:

$$D[n]=\begin{cases}(i(T_{n-1}))^4+(i(T_{n-2}))^8 & n\geq 2\\ 17 & n=1\end{cases}$$

***Proof:*** It's easy to find out that $i(D[1])=17$. For $n\geq 2$ assumes that $o$ is the center vertex of $D[n]$ with which the vertices $c,d,e$ and $f$ are adjacent. From lemma 1, we have:

$$i(D[n])=i(D[n]-o)+i(D[n]-[o]), \tag{5}$$

where $[o]=N(G_o)\cup o=\{o,c,d,e,f\}$. $D[n]-o$ is a graph with 4 components that each of them is similar to $T_{n-1}$. The graph $D[n]-[o]$ consists of 8 subgraphs that each of them is similar to $T_{n-2}$. So, by lemma 2 we have:

$$i(D[n]-o)=(i(T_{n-1}))^4\ , \tag{6}$$

and

$$i(D[n]-[o])=(i(T_{n-2}))^8. \tag{7}$$

Finally, from (5), (6) and (7) we conclude that:

$$i(D[n])=(i(T_{n-1}))^4+(i(T_{n-2}))^8. \tag{8}$$

The proof is now complete.

Using theorem 1 and 2, In table 1, the values of the Merrifield-Simmons index of $D[n]$ for $2\leq n\leq 8$ are computed.

*Table 1. Computing the Merrifield-Simmons index of* $D[n]$ *for* $2 \le n \le 8$.

| Dendrimer | Merrifield-Simmons index |
|---|---|
| $D[2]$ | 881 |
| $D[3]$ | 3216386 |
| $D[4]$ | $3.6262 \times 10^{13}$ |
| $D[5]$ | $5.1973 \times 10^{27}$ |
| $D[6]$ | $9.9400 \times 10^{55}$ |
| $D[7]$ | $3.8129 \times 10^{112}$ |
| $D[8]$ | $5.4478 \times 10^{225}$ |

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