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# COMPUTING THE HOSOYA INDEX AND THE WIENER INDEX OF AN INFINITE CLASS OF DENDRIMERS

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A dendrimer is a tree-like highly branched polymer molecule, which has some proven applications, and numerous potential applications. The Hosoya index of a graph is defined as the total number of the independent edge sets of the graph, while the Wiener index is the sum of distances between all pairs of vertices of a connected graph. In this paper, we give a relation for computing Hosoya index and a formula for computing Wiener index, of an infinite family of dendrimers.

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*Keywords*: Dendrimer, Molecule, Hosoya Index, Wiener Index

## 1. Intoduction

Dendrimers are nanostructures that can be precisely designed and manufactured for a wide variety of applications, such as drug delivery, gene delivery and diagnostics etc. The name “dendrimer” comes from the Greek word "δένδρον", which translates to "tree". A dendrimer is generally described as a macromolecule, which is characterized by its highly branched 3D structure that provides a high degree of surface functionality and versatility. The first dendrimers were made by divergent synthesis approaches by Vögtle in 1978 [1]. Dendrimers thereafter experienced an explosion of scientific interest because of their unique molecular architecture.

A topological index is a numerical quantity derived in a unambiguous manner from the structure graph of a molecule. As a graph structural invariant, i.e. it does not depend on the labeling or the pictorial representation of a graph. Various topological indices usually reflect molecular size and shape. One topological index is Hosoya index, which was first introduced by H. Hosoya [2]. It plays an important role in the so-called inverse structure–property relationship problems. For detais of mathematical properties and applications, the readers are suggested to refer to [3,4] and the references therein. As an oldest topological index in chemistry, Wiener index first introduced by H. Wiener [5] in 1947 to study the boiling points of paraffins. Other properties and applications of Wiener index can be found in [3, 6, 7]. For other tological indices, please see [8-11].

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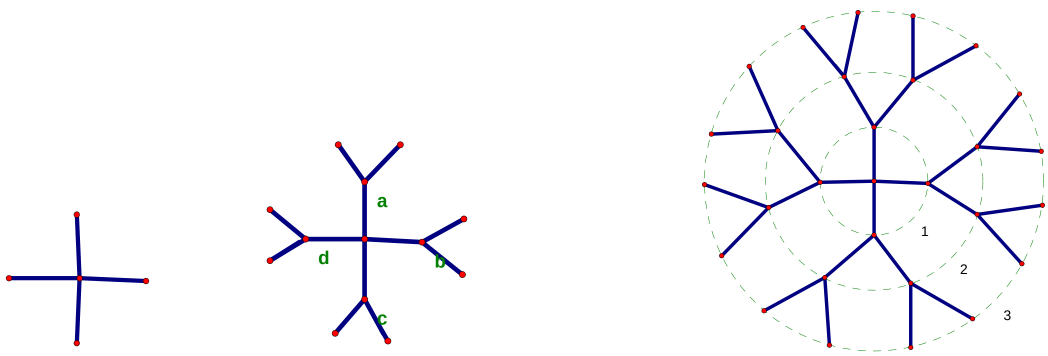
Let $G$ be a graph with vertex set $V(G)$ and edge set $E(G)$. For a vertex $v \in V(G)$, we denote by $N_G(v)$ the neighbors of $v$ in $G$. $d_G(v) = |N_G(v)|$ is called the degree of v in G or written as d(v) for short. A vertex *v* of a tree *T* is called a branching point of *T* if $d(v) \geq 3$, and a vertex in a tree $T$ is called a leaf when $d(v) = 1$. A matching of $G$ is a edge subset in which any two edges can not share a common vertex. A matching in $G$ with k edges is called a k- matching of $G$. The Hosoya index of molecular graph $G$, denoted by $z(G)$, is defined as [6]:

$$z(G) = \sum_{k=0}^{\left\lfloor \frac{n}{2} \right\rfloor} m(G,k),$$

where $m(G,k)$ denotes the number of k-matchings in $G$ for $k \geq 1$, and $m(G,0) = 1$. The Wiener index of a molecular graph *G* was defined as [5]:

$$W(G) = \sum_{u,v \in V(G)} d_G(u,v),$$

where the summation goes over all pairs of vertices of *G* and $d_G(u,v)$ denotes the distance of the two vertices *u* and *v* in the graph *G* (i.e., the number of edges in a shortest path connecting *u* and *v*). For other undefined notations and terminology from graph theory, the readers are referred to [8]. In this paper we study the Hosoya index and the Wiener index of an infinite class of dendrimers. Structure of dendrimer D[n] is shown in Fig. 1 for $n = 1,2,3$, where $n$ denotes the step of growth in this type of dendrimer.




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

*Fig. 1 Structure of dendrimer D[n] for* $n = 1,2,3$

## 2. Main results and discussion

To obtain our main results, we list some important lemmas which will be used in the subsequent proofs.

**Lemma 1.** [3] Let G be a graph, and v ∈ V (G). Then we have

$$z(G) = z(G - v) + \sum_{w \in N_G(v)} z(G - \{v, w\}).$$

**Lemma 2.** [3] If $G_1, G_2, \cdots, G_k$ are the components of a graph G, then we have

$$z(G) = \prod_{i=1}^{k} z(G_i).$$

**Lemma 3.** [16,17] Let T be a tree of order n, $v_1, v_2, \cdots, v_k$ be the all branching points of T with $d(v_i) = m_i$ $(i = 1,2,\cdots,k)$, $T_{i1}, T_{i2}, \cdots, T_{im}$, be the components of $T - v_i$, and the order of $T_{ij}$ is equal to $n_{ij}$ $(j = 1,2,\cdots,m_i; i = 1,2,\cdots,k)$. Then

$$W(T) = \binom{n+1}{3} - \sum_{i=1}^{k} \sum_{1 \le p < q < r \le m_i} n_{ip} n_{iq} n_{ir} \quad \text{,where} \quad n_{i1} + n_{i2} + \cdots + n_{im_i} = n - 1 \quad , \quad \text{and}$$

$i = 1,2,\cdots,k$.

Let $T_n$ be the binary tree whose step of growth is equal to $n$ [see Fig. 2]. In the following theorem, we give the recursive formula for $z(T_n)$.

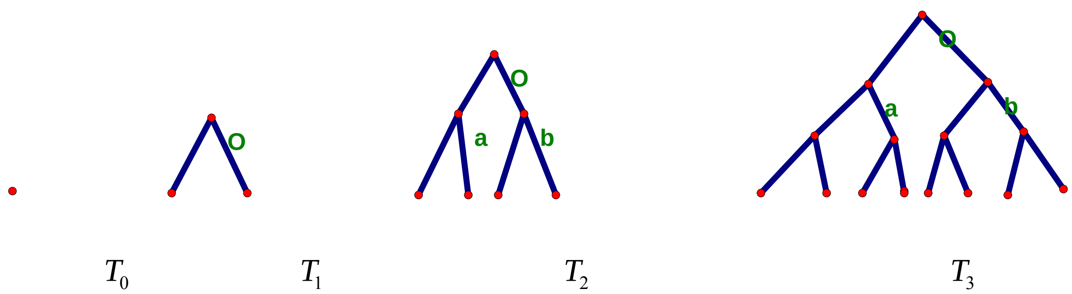



*Fig. 2 The trees* $T_n$ *for* $n = 0,1,2,3$

**Theorem 1.** $z(T_n) = z(T_{n-1})^2 + 2z(T_{n-2})z(T_{n-1})$, where $z(T_0) = 1, z(T_1) = 3$.

**Proof.** From the definition of Hosoya index, it is easy to check that $z(T_0) = 1, z(T_1) = 3$. When

$n \geq 2$, assume that $O$ is the first vertex of $T_n$ with $a,b$ as its only neighbors (see Fig. 2) , by Lemma 1, we have

$z(T_n) = z(T_n - O) + z(T_n - \{o,a\}) + z(T_n - \{o,b\})$.

Note that $T_n - O$ consists of two components, each of which is $T_{n-1}$ , and $T_n - \{o,a\}$ , $T_n - \{o,b\}$ are all isomorphic to $T_{n-1} \cup T_{n-2}$. By Lemma 2, we have

$z(T_n) = z(T_{n-1})^2 + 2z(T_{n-2})z(T_{n-1})$,

which completes the proof of this theorem. ■

**Theorem 2.** $z(D[n]) = z(T_{n-1})^4 + 4z(T_{n-2})^2 z(T_{n-1})^3$, where $z(D[1]) = 5$.

**Proof.** From the definition, we obtain $z(D[1]) = 5$ immediately. For $n \geq 2$, assume that $O$ is the center vertex of $D[n]$ with $a,b,c,d$ as its four neighbors. Obviously, $D[n] - o$ consists of four components, each of which is $T_{n-1}$ . By symmetry, we find that $D[n] - a$ , $D[n] - b$ , $D[n] - c$ and $D[n] - d$ are all isomorphic to $2T_{n-2} \cup 3T_{n-1}$. By Lemmas 1 and 2, we have

$$\begin{aligned} z(D[n]) &= z(D[n] - o) + z(D[n] - \{o,a\}) + z(D[n] - \{o,b\}) + z(D[n] - \{o,c\}) \\ &\quad + z(D[n] - \{o,d\}) \\ &= z(T_{n-1})^4 + 4z(T_{n-2})^2 z(T_{n-1})^3, \end{aligned}$$

which finishes the proof of this theorem. ■

Nest we consider the Wiener index of $D[n]$. In the following theorem we present the formula of $W(D[n])$. From the definition of Wiener index, $W(D[1]) = 16$.

**Theorem 3.** For a dendrimer $D[n]$ with $n \geq 2$ , we have

$$W(D[n]) = \frac{(2^{n+2} - 2)(2^{n+2} - 3)(2^{n+1} - 2)}{3} - \frac{32}{3} 2^{3n} + 4n 2^{2n+2} - 4(n - \frac{11}{3}) 2^n - 4.$$

**Proof.** Note that the number of vertices in $D[n]$ is:

$4(2^0 + 2^1 + \cdots + 2^{n-1}) + 1 = 4(2^n - 1) + 1 = 2^{n+2} - 3$.

For $1 \leq i \leq n-1$, let $v_i$ be the vertex of $D[n]$ with the distance $i$ from the center vertex

$O$. We find that, for $1 \le i \le n-1$, the number of such $v_i$'s is $4 \times 2^{i-1} = 2^{i+1}$, and the graph $D[n] - v_i$ has three components, two of which have the same order: $2^0 + 2^1 + \cdots + 2^{n-i-1} = 2^{n-i} - 1$, while the remaining one of which has the order: $2^{n+2} - 3 - 1 - 2(2^{n-i} - 1) = 2^{n+2} - 2^{n-i+1} - 2$.

For the center vertex $o$, the graph $D[n] - o$ has four components, each of which has the same order $2^0 + 2^1 + \cdots + 2^{n-1} = 2^n - 1$. So by Lemma 3, we have

$$W(D[n]) = \binom{2^{n+2}-2}{3} - 4\sum_{i=1}^{n-1} 2^{i-1}(2^{n-i}-1)^2(2^{n+2} - 2^{n-i+1} - 2) - 4(2^n-1)^3$$

$$= \binom{2^{n+2}-2}{3} - 4\sum_{i=1}^{n-1} 2^{i}(2^{2n-2i} - 2^{n+1-i} + 1)(2^{n+1} - 2^{n-i} - 1) - 4(2^n-1)^3$$

$$= \binom{2^{n+2}-2}{3} - 4\sum_{i=1}^{n-1} 2^{i}[2^{-2i}(2^{3n+1} + 2^{2n}) - 2^{3n-3i} - 2^{-i}(2^{2n+2} - 2^n) + 2^{n+1} - 1] - 4(2^n-1)^3$$

$$= \binom{2^{n+2}-2}{3} - 4\sum_{i=1}^{n-1} [2^{-i}(2^{3n+1} + 2^{2n}) - 2^{3n-2i} - (2^{2n+2} - 2^n) + 2^{n+1+i} - 2^i] - 4(2^n-1)^3$$

$$= \frac{(2^{n+2}-2)(2^{n+2}-3)(2^{n+1}-2)}{3} - 4(2^{3n+1} + 2^{2n})(1 - 2^{-(n-1)}) + \frac{4}{3}2^{3n}(1 - 2^{-2(n-1)})$$
$$+ 4(n-1)(2^{2n+2} - 2^n) - 4(2^{n+1}-1)(2^n - 2) - 4(2^n-1)^3$$

$$= \frac{(2^{n+2}-2)(2^{n+2}-3)(2^{n+1}-2)}{3} - 4(2^{3n+1} - 3 \times 2^{2n} - 2^{n+1}) + \frac{4}{3}(2^{3n} - 2^{n+2}) + 4 \times 2^n - 8$$
$$+ 4(n-1)(2^{2n+2} - 2^n) - 4 \times 2^{n+1}(2^n - 2) - 4(2^n-1)^3$$

$$= \frac{(2^{n+2}-2)(2^{n+2}-3)(2^{n+1}-2)}{3} - \frac{4}{3}(5 \times 2^{3n} - 2 \times 2^n) + (4n-1)2^{2n+2} - 4(n-2)2^n$$
$$- 8 - 4(2^{3n} - 3 \times 2^{2n} + 3 \times 2^n - 1) - 2 \times 2^{2n+2} + 16 \times 2^n$$

$$= \frac{(2^{n+2}-2)(2^{n+2}-3)(2^{n+1}-2)}{3} - \frac{32}{3}2^{3n} + 4n2^{2n+2} - 4(n - \frac{11}{3})2^n - 4.$$

Thus we complete the proof of this theorem. ■

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