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Hosoya Polynomial of Dendrimer Nanostar $D_3[n]$

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Abstract

Let $G=(V,E)$ be a simple graph. The Hosoya polynomial of G is

$$H(G,x)=\sum_{\{u,v\}\subseteq V(G)} x^{d(u,v)},$$

where $d(u,v)$ denotes the distance between vertices u and v. The dendrimer nanostar is a part of a new group of macromolecules that seem photon funnels just like artificial antennas and also is a great resistant of photo bleaching. In this paper we compute the Hosoya polynomial of an infinite family of dendrimer nanostar denoted by $D3[n]$.

1. Introduction

A simple graph $G=(V,E)$ is a finite nonempty set $V(G)$ of objects called vertices together with a (possibly empty) set $E(G)$ of unordered pairs of distinct vertices of G called edges. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds.

The Hosoya polynomial of a graph is a generating function for distance distribution, introduced by Hosoya [8] in 1988 and for a connected graph G is defined as:

$$H(G,x)=\sum_{\{u,v\}\subseteq V(G)} x^{d(u,v)}$$

where $d(u,v)$ denotes the distance between vertices u and v. The Hosoya polynomial has many chemical applications [5,6,7]. Especially, the two well-known topological indices, i.e. Wiener index and hyper-Wiener index, can be directly obtained from the Hosoya polynomial.

The Wiener index of a connected graph G is denoted by $W(G)$, is defined as the sum of distances between all pairs of vertices in G (see [9]), i.e.,

$$W(G,x) = \sum_{\{u,v\}\subseteq V(G)} d(u,v)$$

The hyper-Wiener index is denoted by $WW(G)$ and defined as follows:

$$WW(G) = \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d(u,v) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d^2(u,v)$$

Note that the first derivative of the Hosoya polynomial at $x=1$ is equal to the Wiener index:

$$W(G) = (H(G,x))'|_{x=1}$$

Also we have the following relation:

$$WW(G) = \frac{1}{2}(xH(G,x))''|_{x=1}$$

Dendrimers are a new class of polymeric materials. They are highly branched, mono-disperse macromolecules. The structure of these materials has a great impact on their physical and chemical properties. As a result of their unique behavior dendrimers are suitable for a wide range of biomedical and industrial applications [11]. Recently some people investigated the mathematical properties of this nanostructures in [1-4,10,12,14].

Xu and Zhang [13], computed the Hosoya polynomial of $TUC_4C_8(S)$ nanotubes. In this paper similar to [5] we compute the Hosoya polynomial of another family of dendrimer.

In Section 2 we compute the Hosoya polynomial of a graph with inductive structure denoted by $D_1'[n]$ which is a branch of an infinite family of dendrimer $D_3[n]$. In Section 3 we use results in Section 2 to compute the Hosoya polynomial of an infinite family of dendrimer nanostar $D_3[n]$.

2. Hosoya polynomial of $D_1'[n]$

In this section we introduce a graph with inductive structure denoted by $D_1'[n]$ which is useful for the study of an infinite family of dendrimer. We need some definitions.

We recall that in computer science, a binary tree is a tree data structure in which each node has at most two child nodes, usually distinguished as ``left" and ``right". Nodes with children are parent nodes, and child nodes may contain references to their parents. Outside the tree, there is often a reference to the "root" node (the ancestor of all nodes), if it exists. Any node in the data structure can be reached by starting at root node and repeatedly following references to either the left or right child.

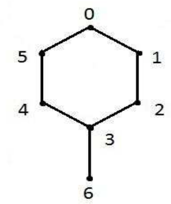

Figure 1. Labeled hexagon.

We label every vertex of hexagon with one pendant edge as shown in Figure 1. Suppose that $D_1'[n]$ is obtained by replacing this hexagon to every vertex of a complete binary tree such that the vertex 0 of a parent connect to vertex 6 of its child (see $D_1'[3]$ in Figure 2). Let to denote the first hexagon (root) of $D_1'[n]$ by symbol o. We also denote the right child and the left child of O by $O(1)$ and $O(2)$, respectively. Let $O(x_1...x_{k-1})$ be dendrimer which has grown $(k-1)$-stages. As know we shall denote its left and right child by $O(x_1...x_{k-1}1)$ and $O(x_1...x_{k-1}2)$, respectively. Now suppose that $x, y \in \{0,1,\dots,6\}$. We mean $x(O(x_1...x_i))$ a vertex x in hexagon $O(x_1...x_i)$. We shall compute the distance of two arbitrary vertices $x(O(x_1...x_i))$ and $y(O(y_1...y_j))$. We obtain the following theorem which its proof follows from the construction of $D_1'[n]$ and left to the reader. Note that in the following theorem we consider two vertices which are not in the same hexagon.

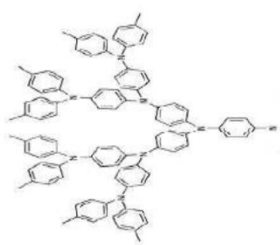

Figure 2. The graph $D_1'[3]$.

Theorem 1 .

1. $d(x(O), y(O(x_1...x_k)) = d(x,0) + d(y,6) + 5k - 4$;
2. $d(x(O(x_1...x_k)), y(O(x_1...x_k x_{k+1}...x_l)) = d(x,0) + d(y,6) + 5(l-k) - 4$
3. $d(x(O(x_1...x_k)), y(O(y_1...y_l)) = d(x,6) + d(y,6) + 5(k+l-2r)$, where r is defined as $r = min\{i : x_i \neq y_i\}$.

Now we try to compute the Hosoya polynomial of $D_1'[n]$. We need the following lemma.

Lemma 1 .

1. The number of vertices of $D_1'[n]$ is $15 \times 2^n - 8$.
2. The number of edges of $D_1'[n]$ is $16 \times 2^n - 8$.
3. The number of hexagons of $D_1'[n]$ is $2^{n+1} - 1$.
4. The diameter of $D_1'[n]$ is $10n$.
5. The radius of $D_1'[n]$ is $5n + 5$.

Proof. The parts (1), (2), (3) are easy to prove.

4. It is obvious that the maximum distances between two vertices of this graph is between $6(O(x_1...x_n,1))$ and $6(O(y_1...y_n,1))$, where $x_1 \neq y_1$. By Theorem 1(iii) we have $d(6O(x_1,...x_n,1), 6O(y_1,...y_n,1)) = d(6,6) + 5((2n+2)-2) = 10n$.

5. Note that the radius of a graph G is $r(G) = min_x max_y \{d(x,y) \mid y \in V(G)\}$. This minimum occur when $x = 6(O)$ and the maximum of $\{d(6(O), y) \mid y \in V(D_1'[n])\}$ by Theorem 1(i) occur while $y = 6O(y_1...y_n,1))$. So, the radius of $D_1'[n]$ is $5n + 5$. ■

Now we shall compute the coefficient of $x^{d(u,v)}$ in $H(D_1'[n], x)) = \sum_{u,v} x^{d(u,v)}$. We need the following lemma which its proof can be obtain directly by considering of all the possibilities.

Lemma 2 . *Let* x *and* y *be two vertices of a hexagon of* $D_1'[n]$ *with position shown in Figure 1. We have the following table:*

Case	Equation	The number of solutions
1	$d(x,0)+d(y,6)=4$	13
2	$d(x,6)+d(y,6)=5$	10
3	$d(x,0)+d(y,6)=5$	9
4	$d(x,6)+d(y,6)=1$	2
5	$d(x,6)+d(y,6)=6$	8
6	$d(x,0)+d(y,6)=1$	3
7	$d(x,0)+d(y,6)=6$	6
8	$d(x,6)+d(y,6)=2$	5
9	$d(x,6)+d(y,6)=7$	4
10	$d(x,0)+d(y,6)=2$	6
11	$d(x,6)+d(y,6)=7$	3
12	$d(x,6)+d(y,6)=3$	8
13	$d(x,6)+d(y,6)=8$	1
14	$d(x,0)+d(y,6)=3$	9
15	$d(x,0)+d(y,6)=8$	1
16	$d(x,6)+d(y,6)=4$	10

The following theorem gives the coefficient of x^i of $H(D_1'[n],x)$ for $0\le i\le 4$. Our method in the following theorem lead us to follow an approach for computing of the coefficient x^i of $H(D_1'[n],x)$ for $i \geq 5$ in Theorem 3.

Theorem 2 .

1. The constant coefficient of $H(D_1'[n],x)$ is $15\times 2^n - 8$.
2. The coefficient of x in $H(D_1'[n],x)$ is $2^{n+4} - 8$.
3. The coefficient of x^2 in $H(D_1'[n],x)$ is $22\times 2^n - 12$.
4. The coefficient of x^3 in $H(D_1'[n],x)$ is $22\times 2^n - 15$
5. The coefficient of x^4 in $H(D_1'[n],x)$ is $20\times 2^n - 18$.

Proof.

1. The constant coefficient of $H(D_1'[n],x)$ is exactly the number of its vertices. Therefore we have the result by Lemma 1(i).

2. The coefficient of x in $H(D_1'[n],x)$ is the number of its edges which is $2^{n+4} - 8$. So we have the result by Lemma 1(ii).

3. To obtain the coefficient of x^2, we compute the number of pair of vertices which have distance two. Note that these two vertices can be in the same hexagon, which there are eight pairs of vertices with this property. Also they may are in different hexagons, one of them in the parent's hexagon and another one in the child's hexagon. We have four pairs of this kind of vertices. For the hexagon in level n of $D_1'[n]$ we have two vertices which have distance two with the last vertices of $D_1'[n]$. Since the number of hexagons is $2^{n+1} - 1$ and the number of parent's and child's hexagon is $1 + 2 + ... + 2^{n-1} = 2^n - 1$, we have

$a_2 = 6(2^{n+1} - 1) + 4(2^n - 1) + 2\times 2^n = 222^n - 12$.

Similarly we can compute the values of a_3 and a_4. ■

The following theorem gives the coefficients of x^l in $H(D_1'[n],x)$ for $l \geq 5$. We put $x_* = Max\{x,0\}$, and use the following notations:

$$A = \sum_{r=0}^{n}(2n - t - 2r + 1)_*$$

$$B = \sum_{r=0}^{n}(2n - t - 2r + 2)_*$$

$$C = 2^t + ... + 2^n,\ D = 2^{t+1} + ... + 2^n$$

Theorem 3 . *Suppose that the Hosoya polynomial of* $D_1'[n]$ *is* $H(D_1'[n],x)=\sum_{u,v\in V} x^{d(u,v)}=\sum_{i=0}^{10n} a_i x^i$. *For every* $i \geq 5$ *, we have*

$$a_i=\begin{cases} A+10B+13C; & if\ i\equiv 0\ (\ mod\,5), \\ 2A+8B+D+9C; & if\ i\equiv 1\ (\ mod\,5) \\ 5A+4B+6C+3D; & if\ i\equiv 2\ (\ mod\,5) \\ 8A+B+3C+6D; & if\ i\equiv 3\ (\ mod\,5) \\ A+C+9D; & if\ i\equiv 4\ (\ mod\,5)\ . \end{cases}$$

Proof. We prove the theorem for case $i\equiv 0(\ mod\,5)$. Another cases prove with similar approach. Let $i=5t$, for some $t\in \mathbb{N}$. Therefore we have to consider three cases of Theorem 1. By Theorem 1 (i), there are x,y and k such that $d(x,0)+d(y,6)+5k-4=5t$. So $k=t$ and $d(x,0)+d(y,6)=4$. By Lemma 2(i) the number of solutions is 13. The number of pairs which satisfy Parts (i) and (ii) of Theorem 1 is $13C=13(2^t+...+2^n)$. Now we shall compute the number of pairs which their distance is $5t$ and satisfy in Theorem 1(iii). We have $d(x,6)+d(y,6)+5(k+l-2r)=5t.$ We have two cases as follows:

Case 1:

$$\begin{cases} d(x,6)+d(y,6)=0, \\ k+l-2r=t; \quad where\ r\leq k\leq n\ and\ r\leq l\leq n\ . \end{cases}$$

Case 2:

$$\begin{cases} d(x,6)+d(y,6)=5, \\ k+l-2r=t-1; \quad where\ r\leq k\leq n\ and\ r\leq l\leq n\ . \end{cases}$$

There exists one pair $x=y=6$ in Case 1 and we shall obtain the number of solutions of $k+l-2r=t$, where $r\leq k\leq n$ and $r\leq l\leq n$. This equation is equivalent to $k'+l'=t$, where $0\leq k'\leq n-r$ and $0\leq l'\leq n-r$. This equation has $(t+1)-2(t-n+r)=2n-t-2r+1$ solutions by Inclusion-Exclusion principle. Since r can choose every element between 0 and n , the number of possible cases is $\sum_{r=0}^{n}(2n-t-2r+1)_*$.

There exists 10 pair x,y in Case 2 and we shall obtain the number of solutions of $k+l-2r=t-1$, where $r\leq k\leq n$ and $r\leq l\leq n$. This equation is equivalent to $k'+l'=t+1$, where $0\leq k'\leq n-r$ and $0\leq l'\leq n-r$. This equation has $t-2(t-n+r-1)=2n-t-2r+2$ solutions by Inclusion-Exclusion principle. Since r can choose every element between 0 and

n, the number of possible cases is $10\sum_{r=0}^{n}(2n-t-2r+2)_*$. By considering all cases we have $a_{5t} = A+10B+13C$. ■

3 Hosoya polynomial of dendrimer $D_3[n]$

In this section we use our results in Section 2 to compute the Hosoya polynomial of a dendrimer nanostar. We consider the first kind of dendrimer which has grown n steps denoted $D_3[n]$. The dendrimer $D_3[3]$ is depicted in Figure 3. Note that there are two edges between each two hexagons in this dendrimer.

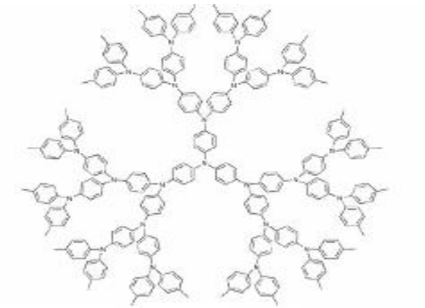

Figure 3. The first kind of dendrimer of generation 1-3 has grown 3 stages

First we construct $D_3[n]$ from $D_1'[n]$. Consider three copies of $D_1'[n]$ with roots O, P and Q. The dendrimer $D_3[n]$ is obtained by identifying the vertex 6 of one copy of $D_1'[n]$ with two vertices 6 of two another copy of $D_1'[n]$.

We have the following theorem:

Theorem 4 .

1. The number of vertices of $D_3[n]$ is $45\times 2^n - 26$ (see [1])
2. The number of edges of $D_3[n]$ is $48\times 2^n - 24$.
3. The number of hexagons of $D_3[n]$ is $3(2^{n+1}-1)$.
4. The diameter of $D_3[n]$ is $10n+10$.
5. The radius of $D_3[n]$ is $5n+5$.

Proof.

1. Since $D_3[n]$ is obtained by identifying vertex 6 of three copy of $D_1'[n]$, we have $|V(D_3[n])| = 3|V(D_1'[n])| - 2$. So we have the result by Lemma 1(i).

2. Obviously $|E(D_3[n])| = 3|E(D_1'[n])|$, so we have the result by Lemma 1(ii).

3. It is obvious that the number of hexagons in $D_3[n]$ is 3 times of the number of hexagons of $D_1'[n]$. Therefore, we have the result by Lemma 1(iii).

4. The maximum distances between two vertices of this graph is between $6(O(x_1 \ldots x_n, 1))$ and $6P(x_1 \ldots x_n, 1)$. By Theorem 1 we have

$d(6O(x_1, \ldots x_n, 1), 6P(x_1, \ldots x_n, 1)) = 2d(6O, 6O(x_1, \ldots, x_n, 1)) = 2(4 + 5n + 1) = 10n + 10$.

5. In this case we have $x = 6O$ and therefore $r(D_3[n]) = 5n + 5$. ■

Here we compute the Hosoya polynomial of $D_3[n]$. For this purpose let $g(x) = \sum_i g_i x^i$, where g_i is the number of vertices which have distance i from $6(O)$ in $D_1'[n]$.

Remark 1. Obviously the degree of $g(x)$ is finite, but simply we suppose that its degree is infinite and we consider $g(x)$ as a series in the rest of paper.

We state and prove the following lemma which is about $g(x)$:

Lemma 3 . $g(x) = \dfrac{1 + x + 2x^2 + 2x^3 + x^4 - x^5}{1 - 2x^5}$.

Proof. Clearly we have $g_0 = 1$, $g_1 = g_2 = g_3 = 2$ and $g_4 = 0$. By Theorem 1 we have $d(6(O), yO(x_1, \ldots, x_k)) = 5k + d(6, y)$. Suppose that $i = 5k + d(6, y)$ $(i \geq 5)$. We have the following cases

(i) $i = 5k$. In this case $k = t$, $y = 6$.

(ii) $i = 5k + 1$. In this case $k = t$, $y = 3$.

(iii) $i = 5k + 2$. In this case $k = t$, $y \in \{2, 4\}$.

(iv) $i = 5k + 3$. In this case $k = t$, $y \in \{1, 5\}$.

(v) $i = 5k + 4$. In this case $k = t$, $y = 0$.

If $i = 5t$, then the number of possibilities of y is 2^{t-1}. For other cases, i.e., $i = 5t + r$, $1 \leq r \leq 4$, the number of possibilities of y is 2^t. Therefore

$$g(x) = 1 + 2x + 2x^2 + 2x^3 + x^4 + x^5(1 + 2x + 2^2x^2 + 2^2x^3 + 2x^4) +$$
$$2x^{10}(1 + 2x + 2^2x^2 + 2^2x^3 + 2x^4) + \ldots$$

If $l(x) = 1 + x + 2^2x^2 + 2^2x^3 + x^4$, then $g(x) = l(x) + x^5(2l(x) - 1) + 2x^{10}(2l(x) - 1) + \ldots$

$$= l(x) + \frac{2l(x) - 1}{2}(2x^5 + (2x^5)^2 + (2x^5)^3 + \ldots) = \frac{l(x) - x^5}{1 - 2x^5} = \frac{1 + x + 2x^2 + 2x^3 + x^4 - x^5}{1 - 2x^5}.$$

■

Now we are ready to state and prove the main theorem of this paper. Observe that the statement in the following theorem is a polynomial, because we need to consider the coefficients x^i of $g(x)$ just for $0 \le i \le 10n$.

Theorem 5 . $H(D_3[n], x) = 3H(D_1'[n], x) + 3(g(x))^2$, *where*

$$g(x) = \frac{1 + x + 2x^2 + 2x^3 + x^4 - x^5}{1 - 2x^5}.$$

Proof. Let $H(D_3[n], x) = \sum_{i=0}^{10n+10} b_i x^i$ and $H(D_1'[n], x) = \sum_{i=0}^{10n} a_i x^i$. By definition of Hosoya polynomial b_i is the number of pairs of vertices with distance i in $D_3[n]$. This pair can be in the one of the $D_1'[n]$. Since in every $D_1'[n]$ the number of these kind of pairs is a_i, we have $3a_i$ pairs of vertices with distance i in one of the $D_1'[n]$. Now we consider two vertices x and y such there are in different $D_1'[n]$. If $d(x,6) = j$ and $d(y,6) = l$, then $j + l = i$. The number of these kind of vertices is the coefficient of x^i in $(g(x))^2$. Since we are able to choose two vertices x, y in three ways from different $D_1'[n]$, the number of these kind of vertices is the coefficient of x^i in $3(g(x))^2$. Therefore $H(D_3[n], x) = 3H(D_1'[n], x) + 3(g(x))^2$. ■

Remark 2. Since $W(G) = (H(G, x))'|_{x=1}$, and $WW(G) = \frac{1}{2}(xH(G, x))''|_{x=1}$, , we are able to obtain the Wiener index and hyper Wiener index of dendrimer $D_3[n]$ easily by Theorem 5 and it left to the reader.

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