Iranian Journal of Mathematical Chemistry, Vol. 2, No. 1, September 2011, pp. 71 − 79 **IJMC**

Hosoya Polynomial of an Infinite Family of Dendrimer Nanostar

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(Received July 6, 2011)

ABSTRACT

Let G 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. In this paper we compute the Hosoya polynomial for an infinite family of dendrimer nanostar. As a consequence we obtain the Wiener index and the hyper-Wiener index of this dendrimer.

Keywords: Hosoya polynomial; Wiener Index; Dendrimer nanostar; Diameter.

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 about distance distributing, introduced by Hosoya [6] in 1988 and for a connected graph G is defined as:

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

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where $d(u,v)$ denotes the distance between vertices u and v. The Hosoya polynomial has many chemical applications [4, 5] . Especially, the two well−known topological indices, i.e. Wiener index and hyper−Wiener index, can be directly obtained from the polynomial.

The Wiener index of a connected graph G is denoted by $W(G)$ and defined as the sum of distances between all pairs of vertices in G [7] , 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 [9] . Recently some people investigated the mathematical properties of this nanostructures in [1, 2, 3, 8 ,10, 11].

In Section 2 we present a method to compute the Hosoya polynomial of an infinite family of dendrimer nanostar. As a consequence we obtain the Wiener index and the hyper−Wiener index of this dendrimer nanostart in Section 3.

2. HOSOYA POLYNOMIAL OF AN INFINITE FAMILY OF DENDRIMER

In this section we shall compute the Hosoya polynomial of a dendrimer nanostar. We consider the first kind of dendrimer which has grown n steps denoted $D_1[n]$. Figure 1 show $D_1[4]$. Note that there are three edges between each two hexagon in this dendrimer.

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.

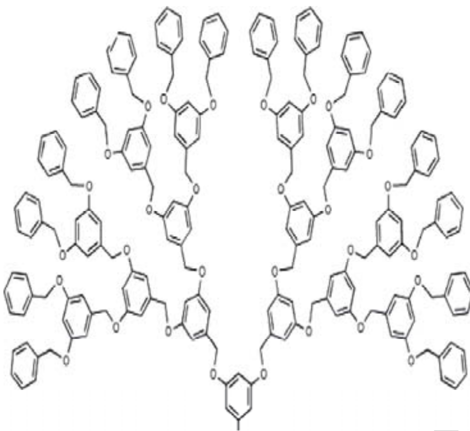

Figure 1. The First Kind of Dendrimer of Generation 1–3 Has Grown 4 Stages.

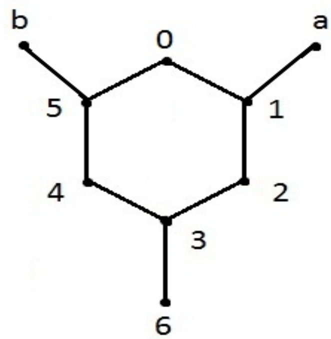

Figure 2: Labeled Hexagon.

We label every vertices of hexagon with three pendant edges as shown 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 until $(k-1)$–th stage. 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 $x, y \in \{0,1,\ldots,6,a,b\}$. 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 reader.

Theorem 1. The distance of two arbitrary vertices $x(O(x_1...x_i))$ and $y(O(y_1...y_j))$ obtain as follows:

1. $d(x(O), y(O(y_1...y_j)) = \begin{cases} d(x,a) + d(y,6) + 5j - 4; & y_1 = 1, \\ d(x,b) + d(y,6) + 5j - 4; & y_1 = 2; \end{cases}$

2. $d(x(O(x_1...x_k)), y(O(x_1...x_k x_{k+1}...x_j)) = d(x(O), y(O(x_{k+1}...x_j)))$.

3. $d(x(O(x_1...x_k)), y(O(y_1...y_j)) = d(x,6) + d(y,6) + 5(j+i-2r) + 6$, where r is defined as $r = min\{i : x_i \neq y_i\}$ (if there exist).

Now we try to compute the Hosoya polynomial of $D_1[n]$. We need the following lemma which is easy to obtain

Lemma 1.
1. The number of vertices of $D_1[n]$ is $2^{n+4} - 9$.
2. The number of edges of $D_1[n]$ is $2^{n+4} - 9$.
3. The number of hexagons of $D_1[n]$ is $2^{n+1} - 1$.

The following theorem gives the coefficient of x^i of $H(D_1[n], x)$ for $0 \le i \le 5$. 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 $i \ge 6$ in Theorem 4.

Theorem 2.
1. The constant coefficient of $H(D_1[n], x)$ is $2^{n+4} - 9$.
2. The coefficient of x in $H(D_1[n], x)$ is $2^{n+4} - 9$.
3. The coefficient of x^2 in $H(D_1[n], x)$ is $24 \times 2^n - 16$.
4. The coefficient of x^3 in $H(D_1[n], x)$ is $27 \times 2^n - 22$.
5. The coefficient of x^4 in $H(D_1[n], x)$ is $23 \times 2^n - 22$.
6. The coefficient of x^5 in $H(D_1[n], x)$ is $28(2^n - 1)$.

Proof.
1. The constant coefficient of $H(D_1[n], x)$ is exactly the number of its vertices. Therefore by Lemma 1(i) we have the result.
2. The coefficient of x in $H(D_1[n], x)$ is the number of its edges which is $2^{n+4} - 9$. So we have the result by Lemma 1(ii).
3. To compute the coefficient of x^2, we compute the number of pair of vertices which

have distance 2 and are in different hexagons. So we have to consider two cases of Part (i) of Theorem 1, that is $d(x,a)+d(y,6)+5j-4=2$ or $d(x,b)+d(y,6)+5j-4=2$. In the both cases $j=1$. In the first case $\{d(x,a),d(y,6)\}=\{0,1\}$ or for the second case $\{d(x,b),d(y,6)\}=\{0,1\}$. Obviously $y=6$ is one of the answer. For this case there are two cases $(1,6)$ and $(5,6)$. Also if $d(y,6)=1$, then $y=3$ and $x=a$ or $x=b$. Therefore we have four solutions $(a(O),3(O(1)),(b(O),3(O(2))),(1(O),6(O(1)))$ and $(5(O),6(O(2)))$. Now by considering the Part (ii) of the Theorem 1 all of the pair of the vertices of distance 2 are in form:

$$\begin{matrix}(a(O(x_1...x_k)),3(O(x_1...x_k1))),(1(O(x_1...x_k)),6(O(x_1...x_k1))),\\(b(O(x_1...x_k)),3(O(x_1...x_k2))),(5(O(x_1...x_k)),6(O(x_1...x_k2)))\end{matrix}\quad(1\le k\le n-1).$$

Therefore the number of solutions are $4(2^n-1)$. In other hand there are 12 pairs of vertices of distance 2 in any hexagon, and so the coefficient of x^2 is $4(2^n-1)+12(1+2+...+2^{n-1})+8(2^n)=4(2^n-1)+12(2^n-1)+8(2^n)=24\times2^n-16$.

4. The proof of part (iv), (v), and (vi) are similar to proof of part(iii). ■

Theorem 3.

1. The diameter of $D_1[n]$ is $10n+4$.
2. The radius of $D_1[n]$ is $5n+4$.

Proof.

1. It is obvious that the most distances between two vertices of this graph is between $x\in O(x_1...x_n)$ and $y\in O(y_1...y_n)$, where $x_1\neq y_1$ and $x=y=0$. By Theorem 1(iii) we have $d(0O(x_1,...x_n),0O(y_1,...y_n))=2d(0,6)+5((2n-2)+6)=10n+4$.
2. 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 $x=6\in O$ and the maximum of $\{d(6,y)\mid y\in V(D_1[n])\}=5n+4$ and this occur when $y=0O(x_1...x_n))$ by Theorem 1(i). ■

Now we shall compute the coefficient of x^l in $H(D_1[n],x))=\sum_{u,v}x^{d(u,v)}$, where $l\ge6$. We need to the following lemma which its proof can be obtain directly by considering all the possibilities.

Lemma 2. Let x,y,a and 6 be vertices of hexagons of $D_1[n]$ with position shown in Figure 2. Then we have the following table:

Case	Equation	The number of solutions
1	$d(x,a)+d(y,6)=4$	13
2	$d(x,6)+d(y,6)=4$	14
3	$d(x,a)+d(y,6)=0$	1
4	$d(x,a)+d(y,6)=5$	13
5	$d(x,6)+d(y,6)=5$	14
6	$d(x,a)+d(y,6)=6$	18
7	$d(x,6)+d(y,6)=1$	2
8	$d(x,6)+d(y,6)=6$	16
9	$d(x,a)+d(y,6)=2$	5
10	$d(x,6)+d(y,6)=7$	12
11	$d(x,6)+d(y,6)=2$	5
12	$d(x,6)+d(y,6)=7$	12
13	$d(x,a)+d(y,6)=3$	8
14	$d(x,a)+d(y,6)=8$	9
15	$d(x,6)+d(y,6)=3$	8
16	$d(x,6)+d(y,6)=8$	9

Here we state the main theorem of this paper which gives the coefficients of x^l in $H(D_1[n],x)$ for $l \geq 6$. First we use the following notations:

$$A=2^{n+1}-2^q,\ B=2^{n+1}-2^{q+1},\ C=2^{n+1}-2^{q+2},$$

$$D=\sum_{r=0}^{\lfloor\frac{2n-q+3}{2}\rfloor}(2n-q-2r+1),$$

$$E=\sum_{r=0}^{\lfloor\frac{2n-q+2}{2}\rfloor}(2n-q-2r-2).$$

Theorem 4. Suppose that the Hosoya polynomial of $D_1[n]$ is $H(D_1[n],x)=\sum_{u,v\in V}x^{d(u,v)}=\sum_{l=0}^{10n+4}a_l x^l$. Then for every $l \geq 6$, we have

$$a_l = \begin{cases} 13A + 14D; & if\ l \equiv 0\ (\ mod\ 5), \\ B + 13C + 14D; & if\ l \equiv 1\ (\ mod\ 5) \\ 18A + 16D + 2E; & if\ l \equiv 2\ (\ mod\ 5) \\ 12A + 5B + 12D + 5E; & if\ l \equiv 3\ (\ mod\ 5) \\ 8B + 9D + 8E; & if\ l \equiv 4\ (\ mod\ 5)\ . \end{cases}$$

Proof. We prove the theorem for case $l \equiv 0(\ mod\ 5)$. Another cases prove similarly. Let $l = 5q$, for some $q \in \mathbb{N}$. Therefore we have $d(x,a) + d(y,6) + 5j - 4 = 5q$ and so $d(x,a) + d(y,6) = 4$. By Lemma 2 there are 13 cases. By solving of the equation of Theorem 1 (i) we will have $q = j$, and by Part (ii) of this theorem the number of all possibilities cases is

$$13 \times 2^q (1 + 2 + \ldots + 2^{n-q}) = 13(2^{n+1} - 2^q) = 13A.$$

Now by considering the part (iii) of Theorem 1, we have to find the number of solution of $d(x,6) + d(y,6) + 5(i + j - 2r) + 6 = 5q$. When $d(x,6) + d(y,6) = 4$ this equation has solution, and this occur for 14 different cases by Lemma 2. With substituting in equation we have $i + j = q + 2r - 2$, where $r \le i, j \le n$. This equation is equivalent to $i' + j' = q - 2$, $(0 \le i', j' \le n - r)$ or equivalent to $i'' + j'' = 2n - 2r - q + 2$, where i'' and j'' are non-negative. By inclusion-exclusion principle the number of solutions of this equation is

$$D = \sum_{r=0}^{\lfloor \frac{2n-q+3}{2} \rfloor} (2n - q - 2r + 1).$$

Since there are 14 cases for this part, we have $a_l = 13A + 14D$ and proof is complete. ■

3. WIENER INDEX AND HYPER–WIENER INDEX OF $D_1[n]$

In this section we use our result is Section 2 to obtain the Wiener index and hyper Wiener index of dendrimer $D_1[n]$. We obtained the following result in Section 2:

Corollary 1. The Hosoya polynomial of $D_1[n]$ is

$$H(D_1[n], x) = (2^{n+4} - 9) + (2^{n+4} - 9)x + (24 \times 2^n - 16)x^2 + (27 \times 2^n - 22)x^3 +$$
$$(23 \times 2^n - 22)x^4 + (28(2^n - 1))x^5 + \sum_{l=6}^{10n+4} a_l x^l$$

where a_l is obtained in Theorem 4.

The following theorem compute the Wiener index and hyper Wiener index of dendrimer $D_1[n]$.

Theorem 5.

1. The Wiener index of $D_1[n]$ is

$$W(D_1[n]) = (2^{n+4} - 9) + (24 \times 2^{n+1} - 32) + (81 \times 2^n - 66) + (23 \times 2^{n+2} - 88) + 140(2^n - 1) + \sum_{l=6}^{10n+4} l a_l x^{l+1},$$

2. The hyper Wiener index of $D_1[n]$ is

$$WW(D_1[n]) = (2^{n+4} - 9) + 3(24 \times 2^n - 16) + 6(27 \times 2^n - 22) + 10(23 \times 2^n - 22) + 15(28(2^n - 1)) + \frac{1}{2}\sum_{l=6}^{10n+4} l(l+1)a_l.$$

Proof.

1. Since $W(G) = (H(G,x))'|_{x=1}$, we have the result by Corollary 1.
2. Since $WW(G) = \frac{1}{2}(xH(G,x))''|_{x=1}$, we have the result by Corollary 1. ■

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