International Journal of Physical Sciences Vol. 7(9), pp. 1420 - 1423, 23 February, 2012
Available online at http://www.academicjournals.org/IJPS
DOI: 10.5897/IJPS11.796
ISSN 1992 - 1950 ©2012 Academic Journals

Full Length Research Paper

Connectivity, PI and vertex-PI indices and polynomials of an infinite class of dendrimer nanostars

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Accepted 07 February, 2012

A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. In this paper, we shall give the exact formulas for the first-connectivity, second-connectivity indices and polynomials, PI and vertex-PI indices and polynomials of an infinite class of dendrimer nanostars.

Key words: Connectivity index, connectivity polynomial, PI index, vertex-PI index, PI polynomial, vertex PI polynomial, dendrimer nanostar.

INTRODUCTION

Let *G* be a connected simple graph. The *m*-connectivity index and polynomial of *G* are defined as:

$$^{m}\chi(G) = \sum_{v_{i_1}v_{i_2}\ldots v_{i_{m+1}}} \frac{1}{\sqrt{d_{i_1}d_{i_2}\ldots d_{i_{m+1}}}},$$

where $v_{i_1}v_{i_2}\ldots v_{i_{m+1}}$ runs over all paths of length *m* in *G* and d_i is the degree of vertex v_i.

Let *e=uv* be an edge in *G*. Denote by $n_u(e)$ and $m_u(e)$ the number of vertex and edges lying closer to *u* than to *v* in *G*, respectively. Then, the well-studied PI and vertex-PI index of *G* are defined, respectively, as

$$PI(G) = \sum_{e=uv}[m_u(e) + m_v(e)]$$

and $PI_v(G) = \sum_{e=uv}[n_u(e) + n_v(e)]$. The PI and vertex-PI polynomials of *G* are defined as:

$$PI(G;x) = \sum_{e=uv} x^{m_u(e)+m_v(e)}$$

and

$$PI_v(G;x) = \sum_{e=uv} x^{n_u(e)+n_v(e)}$$

, respectively.

During the past several decades, there are many papers dealing with the connectivity index. The reader may consult these papers (Ahmadi and Sadeghimehr, 2009; Ashrafi and Nikzad, 2009; Li and Gutman, 2006; Wang and Hua, 2010) and the references cited therein. But there exist no papers concerning the connectivity of polynomial till now. About the PI and vertex-PI indices and polynomials, the reader is referred to these studies (Firozja and Gholamhossein, 2009; Loghman and Badakhshian, 2009; Seyedaliakbar and Faghani, 2010; Yazdani and Bahrami, 2010; Yousefi-Azari et al., 2008).

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MSC(2010): 05C07, 05C12, 05C90.

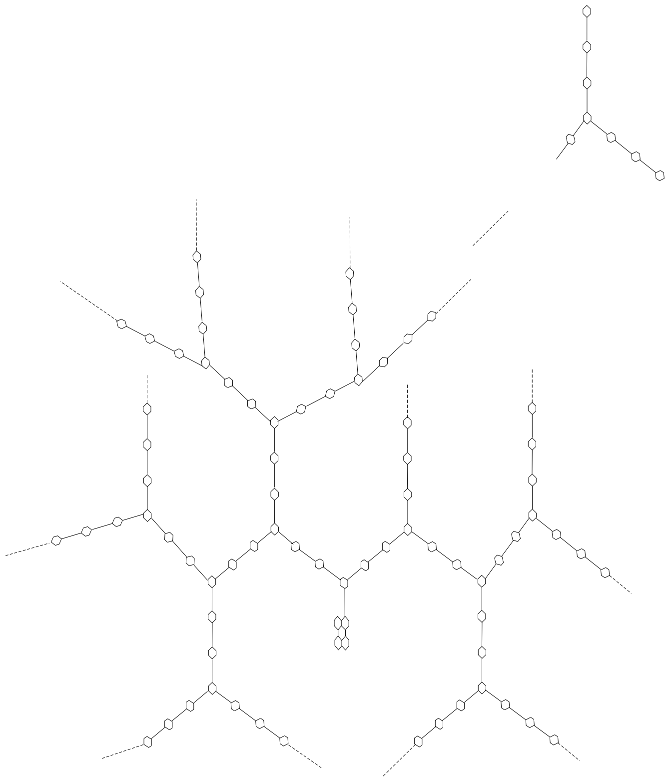

Figure 1. The dendrimer nanostar *NS[n]*.

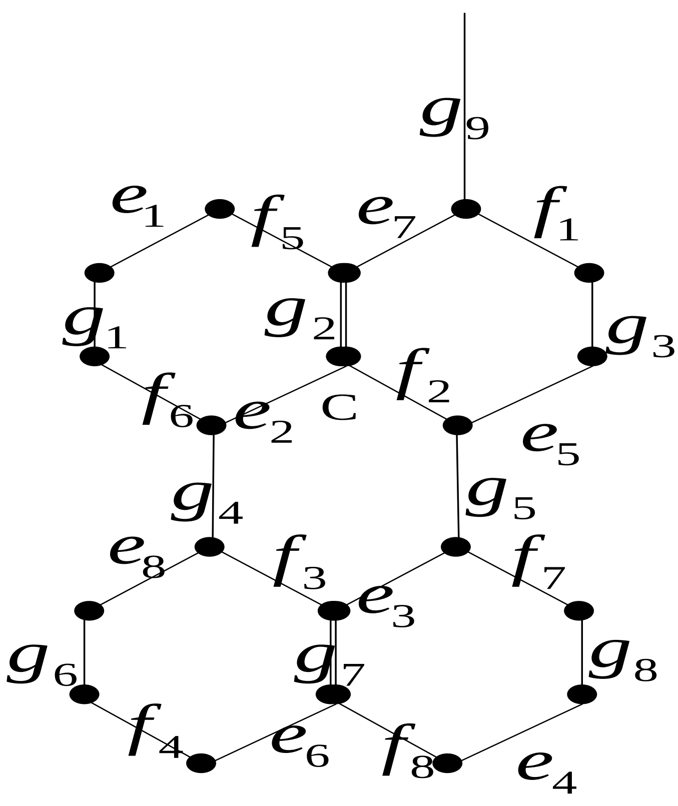

Figure 2. The nucleus of dendrimer nanostar *NS[n]*.

In this paper, we shall give explicit computing formulas for first and second connectivity indices and polynomials, the PI and vertex-PI indices and polynomials of a type of dendrimer nanostars with *n* growth stages.

MAIN RESULTS

Let *NS[n]* denote a kind of dendrimer nanostar with *n* growth stages (Figures 1 and 2). We first give an exact computing formula for the first-connectivity index and polynomial of this kind of dendrimer nanostar.

Theorem 1

Let *NS[n]* be the dendrimer nanostar as shown in Figure 1. Then,

$$^{1}\chi(NS[n];x)=(2^{n+3}-1)x^{\frac{1}{2}}+(3\cdot 2^{n+3}-14)x^{\frac{1}{\sqrt{6}}}+(5\cdot 2^{n+1}+4)x^{\frac{1}{3}},$$

$$^{1}\chi(NS[n])=(\frac{11}{3}+2\sqrt{6})2^{n+1}+\frac{5}{6}-\frac{7\sqrt{6}}{3}.$$

Proof

Let e_{ij} denote the edge in *NS[n]* whose two ends are of degree *i* and *j*, respectively. Also, we use d_{ij} to denote the number of edge e_{ij} in *NS[n]*. It is easy to see that there contains only three types of edges: e_{22}, e_{23} and e_{33}. By a simple computation, we obtain:

$$d_{22}=7+4(2^{1}+\cdots+2^{n})=2^{n+3}-1,$$

$$d_{23}=7+4(2^{1}+\cdots+2^{n})+10\cdot 2^{n}=3\cdot 2^{n+3}-14,$$

$$d_{33}=[31+21(2^{1}+\cdots+2^{n})]-(2^{n+3}-1)-(3\cdot 2^{n+3}-14)$$
$$=5\cdot 2^{n-1}+4.$$

So, we have:

$$^{1}\chi(NS[n];x)=(2^{n+3}-1)x^{\frac{1}{2}}+(3\cdot 2^{n+3}-14)x^{\frac{1}{\sqrt{6}}}+(5\cdot 2^{n+1}+4)x^{\frac{1}{3}},$$

$$^{1}\chi(NS[n])=(\frac{11}{3}+2\sqrt{6})2^{n+1}+\frac{5}{6}-\frac{7\sqrt{6}}{3}.$$

Now, we shall give the second-connectivity index and polynomial for the dendrimer nanostar as shown in Figure 1.

Theorem 2

Let *NS[n]* be the dendrimer nanostar as shown in Figure 1. Then,

$$^{2}\chi(NS[n];x)=3\cdot 2^{n}x^{\frac{1}{2\sqrt{2}}}+(15\cdot 2^{n+1}-18)x^{\frac{1}{2\sqrt{3}}}+2^{n}x^{\frac{1}{\sqrt{2}}}+12x^{\frac{1}{3\sqrt{3}}},$$

$$^{2}\chi(NS[n])=(\frac{5\sqrt{2}}{4}+5\sqrt{3})2^{n}-\frac{5\sqrt{3}}{3}.$$

Proof

Let d_{ijk} denote the number of 2 paths whose three consecutive vertices are of degree *i*, *j* and *k*, respectively. Also, we use $d_{ijk}^{(s)}$ to mean d_{ijk} in the s^{th} stage. Obviously, $d_{ijk}^{(s)}=d_{kji}^{(s)}$.

Firstly, we compute the value of $d_{ijk}^{(1)}$. It is easily seen that:

$$d_{222}^{(1)}=6,\quad d_{223}^{(1)}=28,\quad d_{232}^{(1)}=14,$$
$$d_{233}^{(1)}=40,\quad d_{323}^{(1)}=3,\quad d_{333}^{(1)}=12,$$

Now, we are ready to deduce the relation between $d_{ijk}^{(s)}$ and $d_{ijk}^{(s-1)}$ for $S\geq 2$.

$$d_{222}^{(s)}=d_{222}^{(s-1)}+3\cdot 2^{s}-3\cdot 2^{s-1}=d_{222}^{(s-1)}+3\cdot 2^{s-1}.$$

$$d_{223}^{(s)}=d_{223}^{(s-1)}+10\cdot 2^{s}-2\cdot 2^{s-1}=d_{223}^{(s-1)}+9\cdot 2^{s}.$$

$$d_{232}^{(s)}=d_{232}^{(s-1)}+5\cdot 2^{s}+2\cdot 2^{s-1}=d_{232}^{(s-1)}+3\cdot 2^{s+1}.$$

$$d_{233}^{(s)}=d_{233}^{(s-1)}+10\cdot 2^{s}+4\cdot 2^{s-1}=d_{232}^{(s-1)}+3\cdot 2^{s+2}.$$

$$d_{323}^{(s)}=d_{323}^{(s-1)}+3\cdot 2^{s-1}.$$

Obviously, for any $(i,j,k)\neq(2,2,2),(2,2,3),(2,3,2),(2,3,3),(3,2,3),$ we have:

$d_{ijk}^{(s)}=0$ or $d_{ijk}^{(s)}=d_{ijk}^{(s-1)}=\cdots=d_{ijk}^{(1)}$ for $s=2,\cdots,n.$

By the aforementioned recursive formulas for $d_{ijk}^{(s)}$, we obtain:

$$d_{222}^{(n)}=d_{222}^{(n-1)}+3\cdot 2^{n-1}=6+3(2^{n-1}+\cdots+2^{1})=3\cdot 2^{n}.$$
$$d_{223}^{(n)}=d_{223}^{(n-1)}+9\cdot 2^{n}=\cdots=28+9(2^{n}+\cdots+2^{2})=9\cdot 2^{n+1}-8.$$
$$d_{232}^{(n)}=d_{232}^{(n-1)}+3\cdot 2^{n+1}=\cdots=14+3(2^{n+1}+\cdots+2^{3})=6\cdot 2^{n+1}-10.$$
$$d_{233}^{(n)}=d_{233}^{(n-1)}+3\cdot 2^{n+2}=\cdots=40+3(2^{n+2}+\cdots+2^{4})=6\cdot 2^{n+2}-8.$$
$$d_{323}^{(n)}=d_{323}^{(n-1)}+3\cdot 2^{n-1}=\cdots=3+3(2^{n-1}+\cdots+2^{0})=3\cdot 2^{n}.$$
$$d_{333}^{(n)}=\cdots=d_{333}^{(1)}=12.$$

So, we arrive at:

$$^{2}\chi(NS[n];x)=3\cdot 2^{n}x^{\frac{1}{2\sqrt{2}}}+(15\cdot 2^{n+1}-18)x^{\frac{1}{2\sqrt{3}}}+2^{n}x^{\frac{1}{\sqrt{2}}}+12x^{\frac{1}{3\sqrt{3}}},$$

$$^{2}\chi(NS[n])=(\frac{5\sqrt{2}}{4}+5\sqrt{3})2^{n}-\frac{5\sqrt{3}}{3}.$$

In the following two theorems, we shall give the PI and vertex PI indices and polynomials for the dendrimer nanostar as shown in Figure 1.

Theorem 3

Let *NS[n]* be the dendrimer nanostar as shown in Figure 1. Then,

$$PI(NS[n];x)=(3\cdot 2^{n+1}-5)x^{21\cdot 2^{n+1}-12}+(9\cdot 2^{n+2}-20)x^{21\cdot 2^{n+1}-13}$$
$$+6x^{21\cdot 2^{n+1}-14}+8x^{21\cdot 2^{n+1}-15}.$$

$$PI(NS[n])=189\cdot 2^{2n+3}+63\cdot 2^{2n+2}-117\cdot 2^{n+2}-195\cdot 2^{n+1}+116.$$

Proof

From Figure 1, we know that *NS[n]* has exactly $18(2+2^{2}+\cdots+2^{n})+26=9\cdot 2^{n+2}-10$ vertices and $21(2+2^{2}+\cdots+2^{n})+31=21\cdot 2^{n+1}-11$ edges. Also, it can be seen that for any edge $e=uv\in E(NS[n])$ not belonging to the nucleus (Figure 2), $m(e)=m_{u}(e)+m_{v}(e)=|E(NS[n])|-1$ or $|E(NS[n])|-2$.

More precisely, there exist $3(2+2^2+\cdots+2^n)=3\cdot 2^{n+1}-6$ edges e such that and $9\cdot 2^{n+2}-30$ edges e such that;

$$m(e)=m_u(e)+m_v(e)=|E(NS[n])|-2=21\cdot 2^{n+1}-13.$$

Now, consider an edge e lying within the nucleus. Then, $e\in\{e_i, f_j, g_k\}$, $i=1,2,\cdots,8$, $j=1,2,\cdots,8$ and $k=1,2,\cdots,9$.

By an elementary calculation, we obtain:

$$m(e_i)=m(f_i)=|E(NS[n])|-4=21\cdot 2^{n+1}-15$$

for i=1, 2, 3, 4, and

$$m(e_i)=m(f_i)=|E(NS[n])|-2=21\cdot 2^{n+1}-13$$

for i=5, 6, 7, 8.
Also,

$$m(g_i)=|E(NS[n])|-3=21\cdot 2^{n+1}-14$$

for $i=1,\cdots,8,\ i\neq 4,5$

$$m(g_i)=|E(NS[n])|-2=21\cdot 2^{n+1}-13$$

for i=4, 5, and

$$m(g_i)=|E(NS[n])|-1=21\cdot 2^{n+1}-12.$$

So,

$$PI(NS[n];x)=(3\cdot 2^{n+1}-5)x^{21\cdot 2^{n+1}-12}+(9\cdot 2^{n+2}-20)x^{21\cdot 2^{n+1}-13}+6x^{21\cdot 2^{n+1}-14}+8x^{21\cdot 2^{n+1}-15}.$$

$$PI(NS[n])=189\cdot 2^{2n+3}+63\cdot 2^{2n+2}-117\cdot 2^{n+2}-195\cdot 2^{n+1}+116.$$

Since *NS[n]* is a bipartite plane graph, for any edge $e\in E(NS[n])$, we have $n_u(e)+n_v(e)=|V(NS[n])|$. Thus, we have the following.

Theorem 4

Let *NS[n]* be the dendrimer nanostar as shown in Figure 1. Then,

$$PI_v(NS[n];x)=(21\cdot 2^{n+1}-11)x^{9\cdot 2^{n+2}-10},$$

$$PI_v(NS[n])=189\cdot 2^{2n+3}-408\cdot 2^{n+1}+110.$$

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