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The PI and vertex PI Polynomial of dendimers

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ABSTRACT. Let G be a simple connected graph. The vertex PI polynomial of G is defined as $PI_v(G,x)=\sum_{e=uv}x^{n_u(e)+n_v(e)}$, where $n_u(e)$ is the number of vertices closer to u than v and $n_v(e)$ is the number of vertices closer to v than u. The PI polynomial of G is defined as $PI(G,x)=\sum_{e=uv}x^{m_u(e)+m_v(e)}$, where $m_u(e)$ is the number of edges closer to u than v and $m_v(e)$ is the number of edges closer to v than u. In this paper, the PI and vertex PI polynomials of two types of dendrimers are computed.

Keywords: PI polynomial, vertex PI polynomial, Szeged index.

1. INTRODUCTION

Dendrimers are large and complex molecules with very well-defined chemical structures. They consist of three major architectural components: core, branches and end groups. Nanostar dendrimers are part of a new group of macromolecules. The topological study of these macromolecules is the subject of some recent papers [1,13].

Let G be a connected simple molecular graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. As usual, the distance between the vertices u and v of G is

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denoted by $d_G(u,v)$ (or $d(u,v)$ for short) and it is defined as the number of edges in a minimal path connecting vertices u and v.

The PI index of a graph G is defined as $PI(G)=\sum_{e=uv}[m_u(e)+m_v(e)]$, where $m_u(e)$ is the number of edges lying closer to u than to v and $m_v(e)$ is defined analogously. The vertex PI index of a graph G is defined as $PI_v(G)=\sum_{e=uv}[n_u(e)+n_v(e)]$, where $n_u(e)$ is the number of vertices lying closer to u than to v and $n_v(e)$ is de ined analogously [2–8]. The PI and vertex PI polynomial of G are defined as:

$$PI_v(G,x)=\sum_{e=uv}x^{n_u(e)+n_v(e)},\ PI(G,x)=\sum_{e=uv}x^{m_u(e)+m_v(e)}.$$

The mathematical properties of these topological indices can be found in some recent papers [9–20].In this paper, our notation is standard and taken mainly from the standard book of graph theory. The goal of this article is to compute the PI and vertex PI polynomial of two classes of dendrimeric nanostars.

2. THE PI AND VERTEX PI POLYNOMIAL OF NS[N] AND DENDRIMER D[N].

In this section, we compute the PI and vertex PI polynomial of dendrimer NS[n], where NS[n] is the following nanostar.

We begin by stating some general theorem in graph theory.

Theorem A ([12]). $PI(G)=|E|^2-\sum_{e=uv}N(e)$, where $N(e)=|\{xy\mid d(x,e)=d(y,e)\}|$.

Theorem B. $PI(G,x)=x^{|E|}\sum_{e=uv}x^{-N(e)}$.

Theorem C. $PI_v(G)=|E||V|-\sum_{e=uv}N(e)$, where $N(e)$ is the number of vertices of G with $d(x,u)=d(x,v)$, $x\in V(G)$.

Theorem D. $PI_v(G,x)=x^{|V|}\sum_{e=uv}x^{-N(e)}$ where N(e) is the number of vertices of G with $d(x,u)=d(x,v)$.

Lemma 1. $|V(NS[n])|=3\times 2^{n+4}-8$ and $|E(NS[n])|=52\times 2^{n}-8$.

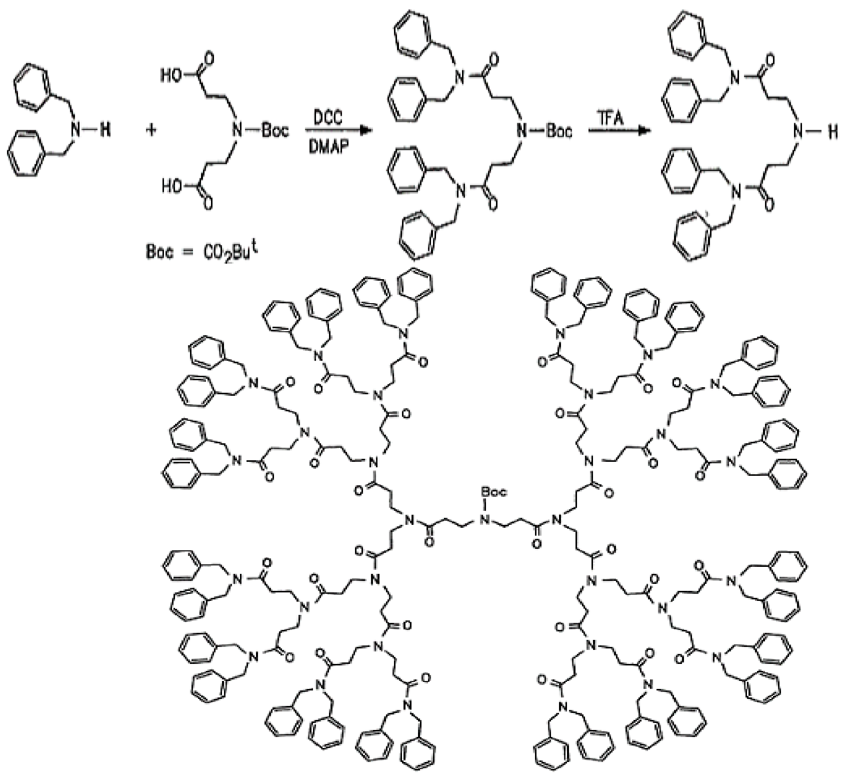

Figure 1. The Nanostar Dendrimer NS[4].

Theorem 2. If $G = NS[n]$ then

$$PI(NS[n], x) = 6 \times 2^{n+2} x^{52 \times 2^n - 10} + (28 \times 2^n - 8) x^{52 \times 2^n - 9},$$

$$PI(NS[n]) = (52 \times 2^n - 8)(52 \times 2^n - 9) - 6 \times 2^{n+2}.$$

Proof. Let $e = uv$ be an edge on hexagon then,

$$m_u(e) + m_v(e) = m - 2 = 52 \times 2^n - 8 - 2 = 52 \times 2^n - 10.$$

A simple computation shows that if $e = uv$ is not an edge of hexagon then

$$m_u(e) + m_v(e) = m - 1 = 52 \times 2^n - 8 - 1 = 52 \times 2^n - 9.$$

Thus,

$$PI(NS[n], x) = 6 \times 2^{n+2} x^{52 \times 2^n - 10} + (28 \times 2^n - 8) x^{52 \times 2^n - 9}$$

$$PI(NS[n]) = (52 \times 2^n - 8)(52 \times 2^n - 9) - 6 \times 2^{n+2},$$

which completes the proof.

Theorem 3. $PI_v(NS[n],x) = x^{3\times 2^{n+4}-8}$ and $PI_v(NS[n]) = (3\times 2^{n+4}-8)(52\times 2^n - 8)$.

Theorem 4. If G be a connected graph with k disjoint even r-cycle then $PI(G) = m^2 - m - kr$.

Proof. If $e \in E(G)$ then $N(e)=1$, otherwise $N(e)=0$. By Theorem A, $PI(G) = m^2 - m - kr$.

Now we are ready to compute the PI and vertex PI polynomials of dendrimer D(n), depicted in Figure 2.

Lemma 5. If N is the number of vertices of $D[n]$, then

$$n_u(e_i)n_v(e_i) = (\frac{3^{n+1-i}-1}{2})(N - \frac{3^{n+1-i}-1}{2}).$$

Proof. From Figure 2, one can see that there are $\frac{3^{n+1-i}-1}{2}$ vertices on one side of e_i that are farther from the center. In this case, those are closer to a vertex of e_i that is farther from the center and the rest vertices are closer to the other vertex of e_i. Thus

$$n_u(e_i)n_v(e_i) = (\frac{3^{n+1-i}-1}{2})(N - \frac{3^{n+1-i}-1}{2}).$$

Lemma 6. If N is the number of vertices $D[n]$, then

$$m_u(e_i)m_v(e_i) = (\frac{3^{n+1-i}-1}{2} - 1)(N - 1 - \frac{3^{n+1-i}-1}{2}).$$

Proof. In Figure 2 for the edge e_i there are $\frac{3^{n+1-i}-1}{2} - 1$ edges on one side e_i that are farther from the center. In this case, those are closer to a vertex of e_i that is farther from the center and the rest edges are closer to the other vertex of e_i. Thus

$$m_u(e_i)m_v(e_i) = (\frac{3^{n+1-i}-1}{2} - 1)(N - 1 - \frac{3^{n+1-i}-1}{2}).$$

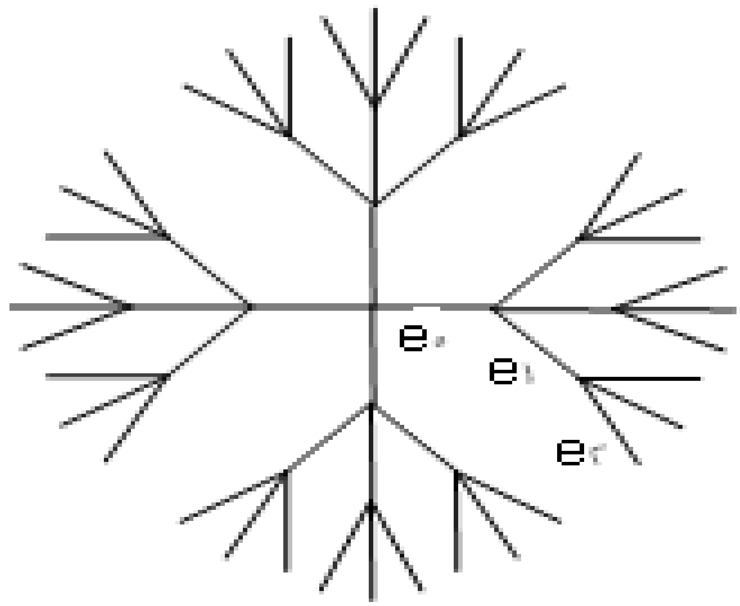

Figure 2. DendrimerD[2].

Theorem 7. If N is the number of vertices $D[n]$, then

$$P(Sz(G),x)=\sum_{i=0}^{n}(4\times 3^{i})x^{(\frac{3^{n+1-i}-1}{2})(N-\frac{3^{n+1-i}-1}{2})},$$

$$P(Sz_{e}(G),x)=\sum_{i=0}^{n}(4\times 3^{i})x^{(\frac{3^{n+1-i}-1}{2}-1)(N-1-\frac{3^{n+1-i}-1}{2})}.$$

Proof. This dendrimer has exactly 4×3^{i} edges in the i^{th} stage. By two previous lemmas, $n_u(e_i)n_v(e_i)$ and $m_u(e_i)m_v(e_i)$ are computed as:

$$P(Sz(G),x)=\sum_{i=0}^{n}(4\times 3^{i})x^{(\frac{3^{n+1-i}-1}{2})(N-\frac{3^{n+1-i}-1}{2})},$$

$$P(Sz_{e}(G),x)=\sum_{i=0}^{n}(4\times 3^{i})x^{(\frac{3^{n+1-i}-1}{2}-1)(N-1-\frac{3^{n+1-i}-1}{2})},$$

this completes the proof.

Corollary 8. If N is the number of vertices $D[n]$, then

$$\mathrm{Sz(G)} = \sum_{i=0}^{n}(4\times 3^{i})(\frac{3^{\mathrm{n+1-i}}-1}{2})(N-\frac{3^{\mathrm{n+1-i}}-1}{2}),$$
$$\mathrm{Sz_e(G)} = \sum_{i=0}^{n}(4\times 3^{i})(\frac{3^{\mathrm{n+1-i}}-1}{2}-1)(N-1-\frac{3^{\mathrm{n+1-i}}-1}{2}).$$

The two indices are easily obtained by the calculated value of N .

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