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ZAGREB POLYNOMIAL AND PI INDICES OF SOME NANO STRUCTURES

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Let G be a graph, e = uv ∈ E(G), d (u) be degree of vertex u.. Then the $ZG_1(G)$ and Zagreb polynomials of the graph G are defined as $ZG_1(G,x)=\sum_{e=uv} x^{d(u)+d(v)}$ and $ZG_2(G,x)=\sum_{e=uv} x^{d(u)d(v)}$, respectively. These counting polynomials for an infinite family of dendrimers are computed.

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1. Introduction

By a graph, we mean a finite, undirected, simple graph. We denote the vertex set and the edge set of a graph G by V(G) and E(G), respectively. For notation and graph theory terminology not presented here, we follow[6].

Let G be a graph and P is a property on G. A counting polynomial for G is a polynomial as $P(G,x) = \sum_k P(G,k)x^k$, where P(G,k) is the frequency of occurrence of the property P of length k and x is simply a parameter to hold k[7]. A topological index of a graph is a number related to a graph which is invariant under graph automorphisms. It is easy to see that every topological index defines a counting polynomial and vice versa. The simplest topological indices are the number of vertices and edges of the graph. The Wiener index (W) is the oldest topological indices[8].

Let G be a connected graph. The SZ_1 and SZ_1 polynomials of G are defined as $ZG_1(G)=\sum_{e=uv} d(u)+d(v)$ and $ZG_1(G,x)=\sum_{e=uv} x^{d(u)+d(v)}$ respectively[4]. The SZ_2 and SZ_2 polynomials of G are defined as $ZG_2(G)=\sum_{e=uv} d(u)d(v)$ and $ZG_2(G,x)=\sum_{e=uv} x^{d(u)d(v)}$ respectively Throughout this paper our notation is standard and taken mainly from the standard book of graph theory.

The PI(G) is $\sum_{e=uv} m_u(e)+m_v(e)$ where $m_u(e)$[1-5] is the number of vertices of G lying closer to u and $m_v(e)$ is the number of vertices of G lying closer to v.

2. Main Results

In. this paper, we compute the Zagreb polynomial of Dendrimers NS(n) [5}and obtain the for x=1 $ZG_1(G)$. Zagreb index NS(n) where NS(n) is the following Nano star. A simple method . show that derivation of $ZG_1(G,x)$ is equal to

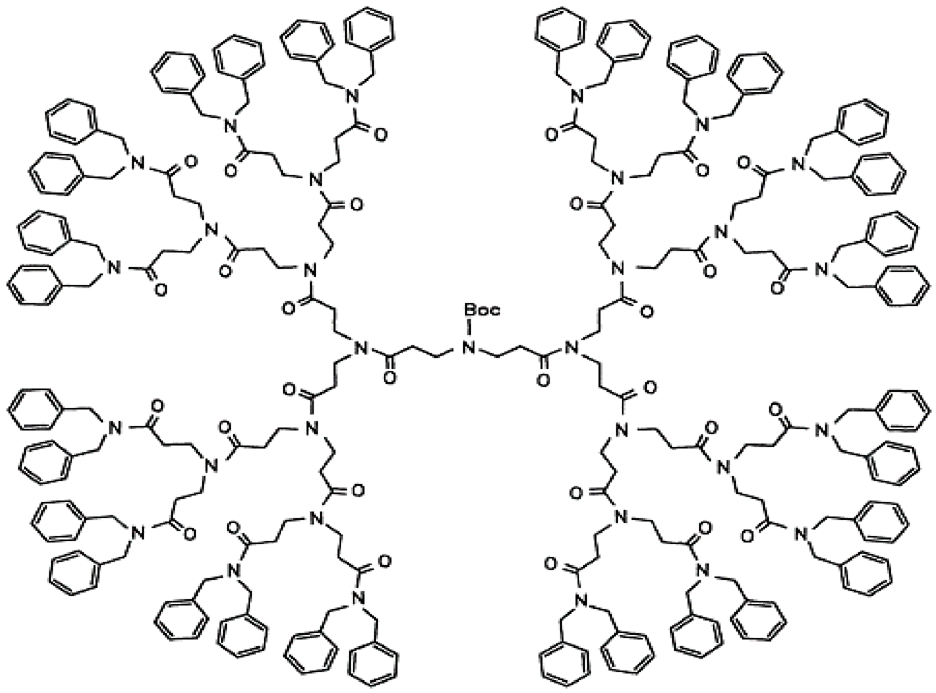

Fig. 1. Construction of N-benzy1-terminated amid-based dendrimers.

Theorem 1. Let **G** be the Nano star NS(n) then $ZG_1(G,x) = (12x^4 + 12x^5 + 2x^6) \times 2^n - 3x^4 - 4x^5 - 2x^6$.

Proof. We prove this theorem with reduction sequence method. If $Z_n(x)$ is Zagreb polynomial NS(n) then by simple computation $Z_1(x) = 21x^4 + 20x^5 + 2x^6$ and we can see that $Z_n(x) = 3x^4 + 4x^5 + 2x^6 + 2Z_{n-1}(x)$. By solution of this reduction sequence $ZG_1(G,x) = (12x^4 + 12x^5 + 2x^6) \times 2^n - 3x^4 - 4x^5 - 2x^6$.□

Corollary 1. Let **G** be the Nano star NS(n) then $ZG_1(G) = 120 \times 2^n - 34$.

Proof. By derivation, we can see that $ZG_1(G,x)' = (48x^3 + 60x^4 + 12x^5) \times 2^n - 12x^3 - 20x^4 - 12x^5$ thus ZG(G) is obtained. □

Benzenoid system is a molecular graph with hexagon cycles [6]. We copute the first Zagrep polynomial of this system.

Theorem 2. Suppose **G** is a benzenoid chain with n hexagon. Then first Zagreb indices of G is $26n - 2$ and $ZG_1(G,x) = (n-1)x^6 + 4(n-1)x^5 + 6x^4$.

Proof. The number of edges with e=uv and d(u)+d(v)=6, d(u)+d(v)=5, d(u)+d(v)=4 are n-1, 4(n-1), 6 respectively. Thus equalities are hold. □

Theorem 3. If **G** is the Nano star NS(n) then $PI(NS(n)) = m(m-1) - 6 \times 2^{n+2}$.

Proof. Let e=uv be an edge on hexagon then $m_u(e) + m_v(e) = m - 2$. A simple coputation shows that if e=uv is not an edge on hexagon then we can see that $m_u(e) + m_v(e) = m - 1$. Thus $PI(G) = 6 \times 2^{n+2}(m-2) + (m - 6 \times 2^{n+2})(m-1) = -6 \times 2^{n+2} + m(m-1)$.□

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