

THE PI AND VERTEX PI POLYNOMIAL OF A T-BENZYL-TERMINATED AMIDE-BASED DENDRIMERS

MOHAMMAD ADABITABAR FIROZJA^a, GHOLAMHOSSEIN FATH-TABAR^{b*}

^a*Department of Mathematics, Qaemshahr Branch, Islamic Azad University, Qaemshahr, I. R. Iran*

^b*Department of Mathematics, Faculty of Science, University of Kashan, Kashan 87317-51167, I. R. Iran*

Let $G = (V, E)$ be a simple connected graph. Let $e = uv \in E(G)$ and $m_u(e)$ be the number of edges closer to u than v and $m_v(e)$ be the number of edges closer to v than u . Then the $PI(G, x)$ of the graph G is defined as $PI(G) = \sum_{e=uv} x^{m_u(e)+m_v(e)}$. We compute the PI vertex PI polynomial of this dendrimer.

(Received October 2, 2009; accepted November 23, 2009)

Keywords: PI Index, PI Polynomial, Dendrimer

1. Introduction

Let G be a simple connected 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 [1-7].

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 [3].

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 [12,13].

Let G be a simple graph. The $PI(G)$ defined as $PI(G) = \sum_{e=uv} m_u + m_v$. 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 [8]. The PI polynomial of G defined as $PI(G, x) = \sum_{e=uv} x^{m_u(e)+m_v(e)}$. It is clear that the derivation of $PI(G, x)$ for $x=1$ is $PI(G)$.

The $PI_v(G)$ defined as $PI_v(G) = \sum_{e=uv} n_u + n_v$. 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_v polynomial of G defined as $PI_v(G, x) = \sum_{e=uv} x^{n_u(e)+n_v(e)}$. It is clear that the derivation of $PI_v(G, x)$ for $x=1$ is $PI_v(G)$ [8-13]. Throughout this paper our notation is standard and taken mainly from the standard book of graph theory and [14, 15]. We present some theorems that we need in this paper.

* Corresponding author. e-mail: fathtabar@kashanu.ac.ir

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

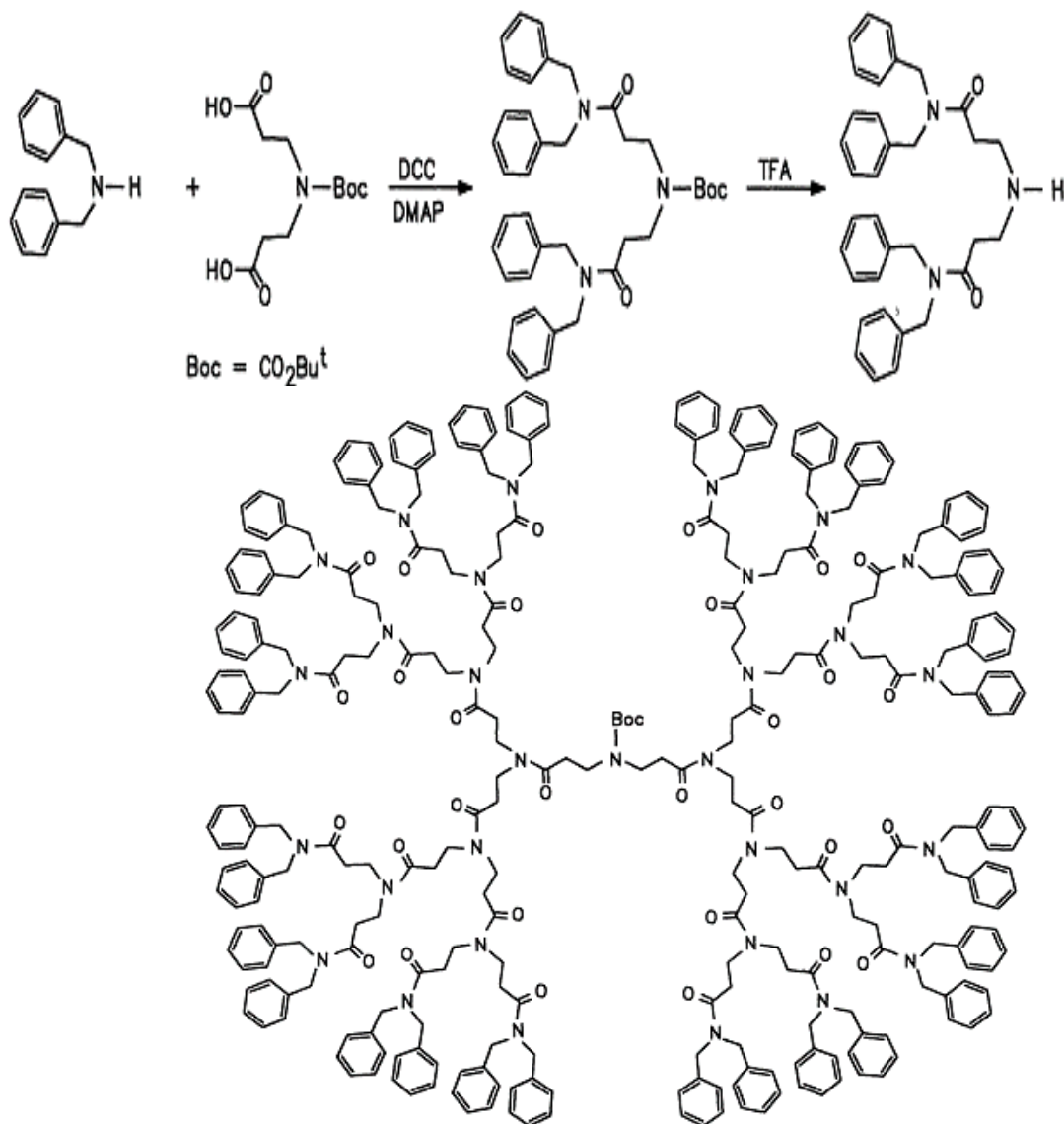
Theorem B. $PI(G, x) = x^{|E|} \sum_{e=uv} x^{-N(e)}$.

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

Theorem D. $PI_V(G) \leq |E(G)| \cdot |V(G)|$ with equality if and only if G is a bipartite graph.

2. Main results

In this paper, we compute the PI index and PI Polynomial of Dendrimer $NS(n)$ where $NS(n)$ is the following Nano Star.



Construction of *N*-benzyl-terminated amide-based dendrimers.

Lemma. $|V(NS(n))| = 3 \cdot 2^{n+4} - 8$ and $|E(NS(N))| = 52 \cdot 2^n - 8$.

Theorem 1. If G is the Nano star $NS(n)$ then $PI(NS(n), x) = 6.2^{n+2}x^{52.2^n - 10} + (28.2^n - 8)x^{52.2^n - 9}$ and $PI(NS(n)) = (52.2^n - 8)(52.2^n - 8 - 1) - 6 \times 2^{n+2}$.

Proof. Let $e=uv$ be an edge on hexagon then $m_u(e) + m_v(e) = m - 2 = 52.2^n - 8 - 2 = 52.2^n - 10$. A simple computation shows that if $e=uv$ is not an edge on hexagon then we can see that $m_u(e) + m_v(e) = m - 1 = 52.2^n - 9$. Thus

$$PI(NS(n), x) = 6.2^{n+2}x^{52.2^n - 10} + (28.2^n - 8)x^{52.2^n - 9}$$

$$PI(NS(n)) = (52.2^n - 8)(52.2^n - 8 - 1) - 6 \times 2^{n+2} . \square$$

Theorem 2. $PI_v(NS(n), x) = x^{3.2^{n+4} - 8}$ and $PI_v(NS(n)) = (3.2^{n+4} - 8)(52.2^n - 8)$.

Theorem 3. If G be a connected graph with k disjoint even r -cycle then $PI(G) = m^2 - m - kr$.

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

References

- [1] Ashrafi A R & Alipour M A, Digest Journal of Nanomaterials and Biostructures **4**, 1 (2009).
- [2] Ashrafi A R & Nikzad P, Digest Journal of Nanomaterials and Biostructures **4**, 269 (2009).
- [3] A. R. Ashrafi, M. Faghani, S. M. Seyedaliakbar, A. R. Ashrafi, P. Nikzad, Digest Journal of Nanomaterials and Biostructures **4**, 59 (2009).
- [4] Ashrafi A R & Saati H, J Comput Theor Nanosci, **4**, 761 (2007).
- [5] Ashrafi A R & Loghman A, MATCH Commun Math Comput Chem, **55**, 447 (2006).
- [6] Ashrafi A R & Loghman A, J Comput Theor Nanosci, **3**, 378 (2006).
- [7] Ashrafi A R & Rezaei F, MATCH Commun Math Comput Chem, **57**, 243 (2007).
- [8] Ashrafi A R & Loghman A, Ars Combinatoria, **80**, 193 (2006).
- [9] Ashrafi A R and Rezaei F, MATCH Commun. Math. Comput. Chem., **57**, 243 (2007).
- [10] Diudea M V, MATCH Commun. Math. Comput. Chem., **45**, 109 (2002),.
- [11] Fath-Tabar G. H, Digest Journal of Nanomaterials and Biostructures **4**, 189 (2009).
- [12] Fath-Tabar G H, Najafi M J and Ashrafi A R, MATCH Commun Math Comput Chem(in press)
- [13] Fath-Tabar G H, Iranian Journal of Mathematical Sciences and Informatics, **2**(2007)29.
- [14] Wiene H.r , J. Am. Chem. Soc., **69**, 17 (1947)
- [15] Ashrafi A R, B. Bull. Iranian Math. Soc., **33**, 37 (2007).