Digest Journal of Nanomaterials and Biostructures Vol. 3, No.4, December 2008, p. 299 - 302

PI POLYNOMIAL OF ZIG-ZAG POLYHEX NANOTUBES

Amir Loghman•, and Leila Badakhshian
Department of Mathematics, Faculty of Science,
University of Isfahan, Isfahan 81746-73441, Iran

The PI polynomial of a molecular graph G is defined as $A+\sum x^{|E(G)|-N(e)}$, where N(e) is the number of edges parallel to e, $A=\frac{|V(G)|(|V(G)|+1)}{2}-|E(G)|$ and summation goes over all edges of G. In this paper, the PI polynomial of the Zig-Zag Polyhex Nanotubes is computed.

(Received December 11, 2008; accepted December 15 2008)

Keywords: PI index, PI polynomial, molecular graph, zig-zag polyhex nanotubes.

1. Introduction

Let G be a 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 denoted by d(u, v) and it is defined as the number of edges in a minimal path connecting the vertices u and v.

A topological index is a real number related to a graph. It must be a structural invariant, i.e., it is fixed by any automorphism of the graph. There are several topological indices have been defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of molecules.

The Wiener index W is the first topological index to be used in chemistry. It was introduced in 1947 by Harold Wiener, as the path number for characterization of alkanes, [15]. In a graph theoretical language, the Wiener index is equal to the count of all shortest distances in a graph. For a survey in this topic we encourage the reader to consult [8,15].

Let G be a graph and f = uv an edge of G. $n_{fu}(f|G)$ denotes the number of edges lying closer to the vertex u than the vertex v, and $n_{fv}(f|G)$ is the number of edges lying closer to the vertex v than the vertex u. The Padmakar-Ivan (PI) index of a graph G is defined as PI(G) = $\sum[n_{fu}(f|G)+ n_{fv}(f|G)]$ where summation goes over all edges of G see for details [7,9-11]. On can see that, for every f = uv $\in$ E(G) we define PI(f) = $n_{fu}(f|G) + n_{fv}(f|G)$ and N(f) = |E(G)| - PI(f), Therefore $PI(G)=|E(G)|^2-\sum_{f\in E(G)} N(f)$.

In [6], Ashrafi, Manoochehrian and Yousefi-Azari. defined a new polynomial and they named the Padmakar-Ivan polynomial. They abbreviated this new polynomial as PI(G,x), for a molecular graph G and investigate some of the elementary properties of this polynomial.

Definition. Let G be a connected graph and u, v be vertices of G. We define:

$$N(u,v)=\begin{cases} \mathrm{n}_{\mathrm{fu}}(\mathrm{f}\mid \mathrm{G})+\mathrm{n}_{\mathrm{fv}}(\mathrm{f}\mid \mathrm{G}) & f=uv\in E(G) \\ 0 & \text{otherwise} \end{cases}$$

• Corresponding author: aloghman@math.ui.ac.ir , loghmanamir@yahoo.com

Then PI polynomial of G is defined as $PI(G,x)=\sum_{\{u,v\}\subseteq V(G)} x^{|E(G)|-N(u,v)}$ and we have:

$$PI(G,x)=\sum_{\{u,v\}\subseteq V(G)} x^{|E(G)|-N(u,v)}=\sum_{(u,v)\in E(G)} x^{|E(G)|-N(u,v)}+\sum_{(u,v)\notin E(G)}1$$
$$=\sum_{f\in E(G)} x^{PI(f)}+\binom{|V(G)|+1}{2}-|E(G)|$$
$$=\sum_{f\in E(G)} x^{|E(G)|-N(f)}+\binom{|V(G)|+1}{2}-|E(G)|$$

In a series of papers [1-5], Ashrafi and Loghman computed PI index of some nanotubes and nanotori. In [12] the authors computed polynomial of some benzenoid graphs. Here we continue this progress to compute the PI polynomial of the zig-zag polyhex nanotubes. Our notation is standard and mainly taken from [13,14]. Throughout this paper T = $TUHC_6[2p,q]$ denotes an arbitrary zig-zag polyhex nanotube, see Figure 1.

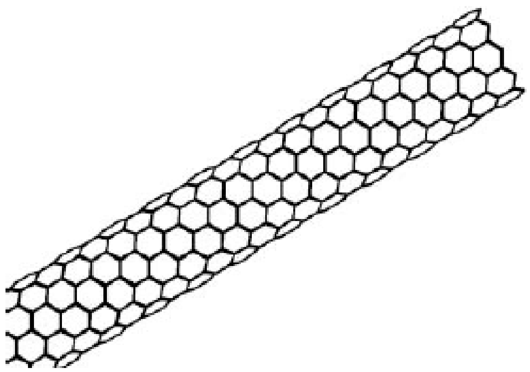

Fig. 1: Zig-zag $TUHC_6[20,q]$.

2. PI Polynomial of $TUHC_6[2p,q]$

In this section, the PI polynomial of the graph T = $TUHC_6[2p,q]$ were computed. From Figures 1 and 2, it is easy to see that |E(T)| = p(3q-1). In the following theorem we compute the PI polynomial of the molecular graph T in Figure 1.

Theorem. The PI polynomial of zig-zag polyhex nanotube is computed as follows:

$$PI(T,x)=\begin{cases} 2px^{|E(T)|-2(2p-1)}\left(\dfrac{2(x^{2p}-1)}{x^2-1}+q-2p\right)+p(q-1)x^{p(3q-2)}+A & q\ge 2p \\ 2px^{|E(T)|-2q}\left(\dfrac{2(x^{2(q-p+1)}-1)}{x^2-1}+2p-q-2\right)+p(q-1)x^{p(3q-2)}+A & p<q<2p, \\ 2pqx^{|E(T)|-2q}+p(q-1)x^{p(3q-2)}+A & q\le p \end{cases}$$

where $A=\binom{|V(T)|+1}{2}-|E(T)|$.

Proof. To compute the PI polynomial of T, it is enough to calculate N(e). To do this, we consider two cases: that e is horizontal or oblique edge. If e is horizontal a similar proof as Lemma 1 in [1] shows that N(e)=p. Also, by Lemma 2 in [1], if e is an oblique edge in the k^{th} column, 1≤ k ≤ p, then N(e) = $\begin{cases} 2p+2(k-1) & q\ge p+k-1 \\ 2q & q\le p+k-1 \end{cases}$. Therefore we consider E_{ij} denote the oblique edge of T in the i[th] row and j[th] column. We first notice that for every i, $1 \le i \le q-1$, $N(E_{i1}) = N(E_{i2}) = \cdots = N(E_{i(2p)})$, Figure 2.

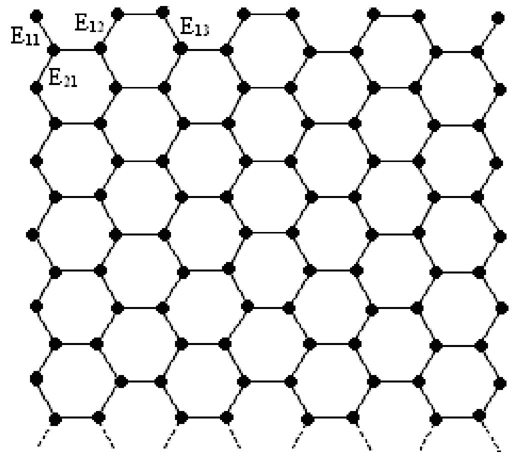

Fig. 2. A Zig-Zag Polyhex Lattice with p=6 and q=8.

Let X and Y are the set of all horizontal and oblique edges of T. It is easy to see that $|X|=p(q-1)$ and $|Y|=2pq$. Then Since T is symmetric, we have:

$$\begin{aligned} PI(T,x) &= \sum_{f\in E(T)} x^{|E(T)|-N(f)} + A = \sum_{f\in X} x^{|E(T)|-N(f)} + \sum_{f\in Y} x^{|E(T)|-N(f)} + A \\ &= \sum_{f\in X} x^{|E(T)|-p} + \sum_{f\in Y} x^{|E(T)|-N(f)} + A \\ &= p(q-1)x^{p(3q-2)} + \sum_{f\in Y} x^{|E(T)|-N(f)} + A \end{aligned}$$

For every *e* in Y, we have three cases:

Case 1. $q \ge 2p$. In this case by Figure 2, we have:

$$\begin{aligned} \sum_{f\in Y} x^{|E(T)|-N(f)} &= 4p(x^{|E(T)|-N(E_{11})} + x^{|E(T)|-N(E_{12})} + \ldots + x^{|E(T)|-N(E_{1p})}) + 2p(q-2p)x^{|E(T)|-N(E_{1p})} \\ &= 4px^{|E(T)|-N(E_{11})}(1 + x^{-2} + x^{-4} + \ldots + x^{-2(p-1)}) + 2p(q-2p)x^{|E(T)|-N(E_{11})-2(p-1)} \\ &= 2px^{|E(T)|-4p+2}\left(\frac{2(x^{2p}-1)}{x^2-1} + q - 2p\right) \end{aligned}$$

Case 2. $p<q<2p$. In this case, we have:

$$\begin{aligned} \sum_{f\in Y} x^{|E(T)|-N(f)} &= 4p(x^{|E(T)|-N(E_{11})} + x^{|E(T)|-N(E_{12})} + \ldots + x^{|E(T)|-N(E_{1(q-p+1)})}) \\ &\quad + 2p(2p-q-2)x^{|E(T)|-N(E_{1(q-p+1)})} \\ &= 4px^{|E(T)|-N(E_{11})}(1 + x^{-2} + x^{-4} + \ldots + x^{-2(q-p)}) \\ &\quad + 2p(2p-q-2)x^{|E(T)|-N(E_{11})-2(q-p)} \\ &= 2px^{|E(T)|-2q}\left(\frac{2(x^{2(q-p+1)}-1)}{x^2-1} + 2p - q - 2\right) \end{aligned}$$

Case 3. $q \le p$. In this case, we have:

$$\sum_{f\in Y} x^{|E(T)|-N(f)} = \sum_{f\in Y} x^{|E(T)|-N(E_{11})} = 2pqx^{|E(T)|-2q}$$

which completes the proof.

Corollary. If T = TUHC$_6$[2p,q] is a zig-zag polyhex nanotube and p,q are positive integer then $\mathrm{PI(T)} = \frac{d}{dx}\mathrm{PI(T,x)}\Big|_{x=1} = \begin{cases} p^2(9q^2 - 7q + 2) - 4pq^2 & q \le p \\ p^2(9q^2 - 15q + 4p - 2) + 4pq & q \ge p \end{cases}$.

Acknowledgement

This research was in part supported by the Center of Excellence for Mathematics, University of Isfahan.

References

[1] A.R. Ashrafi, A. Loghman, PI Index of Zig-Zag Polyhex Nanotubes, MATCH Commun. Math. Comput. Chem., **55**(2), 447 (2006).
[2] A.R. Ashrafi, A. Loghman, Padmakar-Ivan Index of TUC$_4$C$_8$(S) Nanotubes, J. Comput. Theor. Nanosci., **3**(3), 378 (2006).
[3] A. R. Ashrafi, A. Loghman, PI Index of Armchair Polyhex Nanotubes, Ars Combinatoria, **80,** 193 (2006).
[4] A.R. Ashrafi, A. Loghman, Computing Padmakar-Ivan Index of TUC4C8(R) Nanotorus, J. Comput. Theor. Nanosci. (in press).
[5] A.R. Ashrafi, F. Rezaei, PI Index of Polyhex Nanotori, MATCH Commun. Math. Comput. Chem., **57**(1), 243 (2007).
[6] A.R. Ashrafi, B. Manoochehrian, H. Yousefi-Azari, On the PI Polynomial of a Graph, Util. Math., **71,** 97 (2006).
[7] H. Deng, Extremal Catacondensed Hexagonal Systems with Respect to the PI Index, MATCH Commun. Math. Comput. Chem., **55**(2), 453 (2006).
[8] A. Graovac and T. Pisanski, On the Wiener index of a graph, J. Math. Chem. **8,** 53 (1991).
[9] P.V. Khadikar, On a Novel Structural Descriptor PI, Nat. Acad. Sci. Lett., **23,** 113 (2000).
[10] P.V. Khadikar, P.P. Kale, N.V. Deshpande, S. Karmarkar and V.K. Agrawal, Novel PI Indices of Hexagonal Chains, J. Math. Chem., **29,** 143 (2001).
[11] P.V. Khadikar, S. Karmarkar and R.G. Varma, The Estimation of PI Index of Polyacenes, Acta Chim. Slov., **49,** 755 (2002).
[12] B. Manoochehrian, H. Yousefi-Azari, A. R Ashrafi, PI polynomial of some benzenoid graphs. MATCH Commun. Math. Comput. Chem., **57,** 653 (2007).
[13] R. Todeschini and V. Consonni, Handbook of Molecular De- scriptors, Wiley, Weinheim, 2000.
[14] N. Trinajstic, Chemical Graph Theory, CRC Press, Boca Raton, FL. 1992.
[15] H. Wiener, Structural determination of the paraffin boiling points, J. Am. Chem. Soc., **69,** 17 (1947).