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PI POLYNOMIAL OF ARMCHAIR POLYHEX NANOTUBES AND NANOTORUS

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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 Armchair Polyhex Nanotubes and Nanotorus are computed.

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1. Introduction

Graph theory was successfully provided the chemist with a variety of very useful tools, namely, the topological index. A topological index is a numeric quantity from the structural graph of a molecule. With hundreds of topological indices one would expect that most molecules could be well characterized and their physicochemical properties correlated with the available descriptors.

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].

We now recall some algebraic definitions that will be used in the paper. Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-shapes of which are represented by V(G) and E(G), respectively. If e is an edge of G, connecting the vertices u and v then we write e=uv. The number of vertices of G is denoted by n. The distance between a pair of 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. We define for e=uv two quantities $n_{eu}(e|G)$ and $n_{ev}(e|G)$. $n_{eu}(e|G)$ is the number of edges lying closer to the vertex u than the vertex v, and $n_{ev}(e|G)$ is the number of edges lying closer to the vertex v than the vertex u. Edges equidistant from both ends of the edge uv are not counted. In fact, if $G_{u,e} = \{x \mid d(u,x) < d(v,x)\}$, $G_{v,e} = \{ x \mid d(u,x) > d(v,x)\}$ and $G_e = \{x \mid d(u,x) - d(v,x) = \pm 1\}$ then $n_{eu}(e|G) = |E(G_{u,e})|$, $n_{ev}(e|G) = |E(G_{v,e})|$ and

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N(e) = |E(G_e)|. Here for any subset U of the vertex set V = V(G), |E(U)| denotes the number of edges of G between the vertices of U.

The Padmakar-Ivan (PI) index of a graph G is defined as PI(G) = ∑[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 ∈ 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:

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

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 armchair polyhex nanotubes and nanotorus. Our notation is standard and mainly taken from [13,14]. Throughout this paper T = TUVC$_6$[2p,q] denotes an arbitrary armchair polyhex nanotubes and G=G[2p,q] denotes a polyhex nanotorus, see Figure 1.

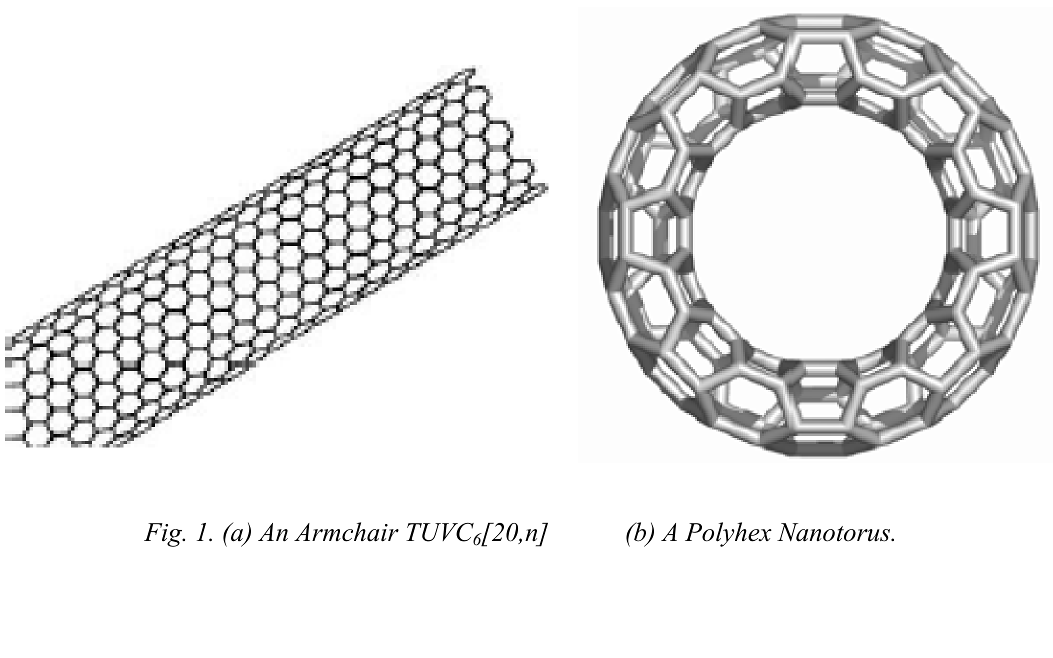

Fig. 1. (a) An Armchair TUVC$_6$[20,n] *(b) A Polyhex Nanotorus.*

2. PI Polynomial of $TUVC_6[2p,q]$

In this section, the PI polynomial of the graph T = $TUVC_6[2p,q]$ were computed. From Figs. 1(a) and 2(a), it is easy to see that $|E(T)| = p(3q-2)$. In the following theorem we compute the PI polynomial of the molecular graph T in Figure 1(a).

Theorem 1. The PI polynomial of armchair polyhex nanotube is computed as follows:

$$PI(T,x) = \binom{|V(T)|+1}{2} - |E(T)| + H(x) + O(x)$$

where $H(x) = \begin{cases} p(\frac{q-1}{2})x^{|E(T)|-q+1} + p(\frac{q+1}{2})x^{|E(T)|-q-1} & 2\,|\,p\ \&\ 2\,|\,q-1 \\ pqx^{|E(T)|-q} & otherwise \end{cases}$

and $O(x) = \begin{cases} 2px^{|E(T)|-4p+2}(\frac{2(x^{2p}-1)}{x^2-1} + q - 2p - 1) & q \ge 2p+1 \\ 2px^{|E(T)|-2q+2}(\frac{2(x^{2(q-p)}-1)}{x^2-1} + 2p - q - 1) & p+1 < q < 2p+1. \\ (q-1)x^{|E(T)|-2q+2} & q \le p+1 \end{cases}$

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 [3] shows that $N(e) = \begin{cases} \begin{cases} q-1 & e \in T_{2k} \\ q+1 & e \in T_{2k-1} \end{cases} & 2\,|\,p\ \&\ 2\,|\,q-1 \\ q & otherwise \end{cases}$ where T_i denotes the set of all horizontal edges of the i^th^ row of the armchair polyhex lattice. Also, by Lemma 2 in [3], if e is an oblique edge in the k^{th} row, $1 \le k \le p$, then N(e) = $\begin{cases} 2p+2(k-1) & q \ge p+k \\ 2q-2 & q \le p+k \end{cases}$. 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, $1 \le i \le q-1$, $N(E_{i1}) = N(E_{i2}) = \cdots = N(E_{i(2p)})$, Fig. 2(a).

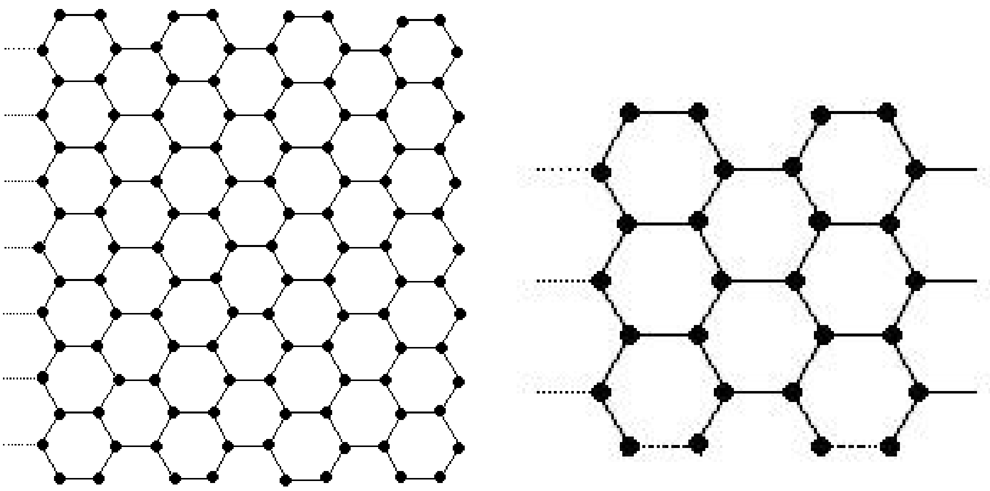

Fig. 2. (a) An Armchair Lattice with p = 4 and q = 15(b) Lattice of a Polyhex Nanotorus with p=2 and q=6.

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

$$PI(T,x) = \sum_{f\in E(T)} x^{|E(T)|-N(f)} + \binom{|V(T)|+1}{2} - |E(T)|$$

$$= \sum_{f\in X} x^{|E(T)|-N(f)} + \sum_{f\in Y} x^{|E(T)|-N(f)} + \binom{|V(T)|+1}{2} - |E(T)|$$

For every f in X, we have two cases:

Case 1. 2|p and 2|q-1. In this case by Lemma 1 in [3], we have:

$$\sum_{f\in X} x^{|E(T)|-N(f)} = \sum_{f\in T_{2k}} x^{|E(T)|-N(f)} + \sum_{f\in T_{2k+1}} x^{|E(T)|-N(f)}$$

$$= \sum_{f\in T_{2k}} x^{|E(T)|-q+1} + \sum_{f\in T_{2k+1}} x^{|E(T)|-q-1}$$

$$= p(\frac{q-1}{2})x^{|E(T)|-q+1} + p(\frac{q+1}{2})x^{|E(T)|-q-1}$$

Case 2. p is odd or q is even. In this case, we have:

$$\sum_{f\in X} x^{|E(T)|-N(f)} = pqx^{|E(T)|-q}$$

Then $PI(T,x) = H(x) + \sum_{f\in Y} x^{|E(T)|-N(f)} + \binom{|V(T)|+1}{2} - |E(T)|$. Finally, if f is an oblique edge then we have three cases:

Case 1. q≥2p+1. In this case by Figure 2(a), we have:

$$\sum_{f\in Y} x^{|E(T)|-N(f)} = 4p(x^{|E(T)|-N(E_{11})} + x^{|E(T)|-N(E_{21})} + ... + x^{|E(T)|-N(E_{p1})})$$

$$+ 2p(q-2p-1)x^{|E(T)|-N(E_{p1})}$$

$$= 4px^{|E(T)|-N(E_{11})}(1 + x^{-2} + x^{-4} + ... + x^{-2(p-1)})$$

$$+ 2p(q-2p-1)x^{|E(T)|-N(E_{11})-2(p\_1)}$$

$$= 2px^{|E(T)|-4p+2}(\frac{2(x^{2p}-1)}{x^2-1} + q - 2p - 1)$$

Case 2. p+1<q<2p+1. In this case, we have:

$$\sum_{f\in Y} x^{|E(T)|-N(f)} = 4p(x^{|E(T)|-N(E_{11})} + x^{|E(T)|-N(E_{21})} + ... + x^{|E(T)|-N(E_{(q-p)1})})$$

$$+ 2p(2p-q-1)x^{|E(T)|-N(E_{(q-p)1})}$$

$$= 4px^{|E(T)|-N(E_{11})}(1 + x^{-2} + x^{-4} + ... + x^{-2(q-p-1)})$$

$$+ 2p(2p-q-2)x^{|E(T)|-N(E_{11})-2(q-p-1)}$$

$$= 2px^{|E(T)|-2q+2}(\frac{2(x^{2(q-p)}-1)}{x^2-1} + 2p - q - 1)$$

Case 3. q≤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 1. The PI index of armchair polyhex nanotube is as follows:

$$\mathrm{PI(TUVC_6[2p,q])} = \frac{d}{dx}\mathrm{PI(T,x)}\Big|_{x=1} = \begin{cases} \begin{cases} A-p & q \le p+1 \\ B-p & q \ge p+1 \end{cases} & 2 \mid p \,\&\, 2 \mid q-1 \\ \begin{cases} A & q \le p+1 \\ B & q \ge p+1 \end{cases} & otherwise \end{cases}.$$

where A = 9p2q2 – 12p2q – 5pq2 + 8pq + 4p2 – 4p and B = 9p2q2 – 20p2q –pq2 + 4pq + 4p3 + 8p2 – 4p.

3. PI Polynomial of polyhex nanotorus

In this section, the PI polynomial of the graph G = G[2p,q] were computed. We first notice that q must be even, say q = 2m. From Figures 1(b) and 2(b), it is easy to see that |E(T)| = 3pq. In the following theorem we compute the PI polynomial of the polyhex nanotorus.

Theorem 2. The PI polynomial of armchair polyhex nanotorus is computed as follows:

$$PI(G,x) = \binom{|V(G)|+1}{2} - 3pq + \begin{cases} pqx^{q(3p-1)} + 2pqx^{3q(p-1)+2} & q \le 2p \\ pqx^{q(3p-1)} + 2pqx^{3p(q-2)+2} & q \ge 2p \end{cases}.$$

Proof. To compute the PI polynomial of G, it is enough to calculate N(e). By Lemma 1, 2 in [5] we have:

If e is a horizontal edge then N(e) = q and if e is a non-horizontal edge then N(e) = $\begin{cases} 3q-2 & q \le 2p \\ 6p-2 & q \ge 2p \end{cases}$. Let X and Y are the set of all horizontal and non-horizontal edges of G. It is easy to see that |X|=pq and |Y|=2pq. Then Since G is symmetric, we have:

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

$$= \sum_{f \in X} x^{|E(G)|-N(f)} + \sum_{f \in Y} x^{|E(G)|-N(f)} + \binom{|V(G)|+1}{2} - |E(G)|$$

$$= \sum_{f \in X} x^{3pq-q} + \begin{cases} \sum_{f \in Y} x^{3pq-(3q-2)} & q \le 2p \\ \sum_{f \in Y} x^{3pq-(6p-2)} & q \ge 2p \end{cases} + \binom{|V(G)|+1}{2} - |E(G)|$$

$$= pqx^{3pq-q} + \begin{cases} 2pqx^{3pq-(3q-2)} & q \le 2p \\ 2pqx^{3pq-(6p-2)} & q \ge 2p \end{cases} + \binom{|V(G)|+1}{2} - |E(G)|$$

$$= \binom{|V(G)|+1}{2} - 3pq + \begin{cases} pqx^{q(3p-1)} + 2pqx^{3q(p-1)+2} & q \le 2p \\ pqx^{q(3p-1)} + 2pqx^{3p(q-2)+2} & q \ge 2p \end{cases}$$

which completes the proof.

Corollary 2. Suppose G is a polyhex nanotorus. Then we have:

$$\mathrm{PI(G)} = \frac{d}{dx}\mathrm{PI(G,x)}\Big|_{x=1} = \begin{cases} 9p^2q^2 - pq^2 - 12p^2q + 4pq & q \ge 2p \\ 9p^2q^2 - 7pq^2 + 4pq & q \le 2p \end{cases}$$

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