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PI POLYNOMIAL OF $TUC_4C_8(S)$ NANOTUBES AND NANOTORUS

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A C_4C_8 net is a trivalent decoration made by alternating squares C_4 and octagons C_8. Such a covering can be derived from square net by the leapfrog operation. The PI polynomial of a molecular graph G is defined as A $+\Sigma x^{|E(G)|-N(e)}$, where N(e) is the number of edges parallel to e, A=1/2|V(G)|(|V(G)|+1)-|E(G)| and summation goes over all edges of G. In this paper, the PI polynomial of $TUC_4C_8(S)$ Nanotubes and Nanotorus are computed.

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1. Introduction

A graph G consists of a set of vertices V(G) and a set of edges E(G). The vertices in G are connected by an edge if there exists an edge $U_iU_j \in E(G)$ connecting the vertices U_i and U_j in G such that $U_i, U_j \in V(G)$. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds. The number of vertices and edges in a graph will be denoted by |V(G)| and |E(G)|, respectively. The distance between a pair of vertices u and w of G is denoted by d(u,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, [16]. In a graph theoretical language, the Wiener index is equal to the count of all shortest distances in a graph, [9,16].

Let G be a graph and e = uv an edge of G. $n_{eu}(e|G)$ denotes 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. The Padmakar–Ivan (PI) index of a graph G is defined as PI(G) = $\sum_{f\in E(G)} PI(f)$ where PI(f) = $n_{fu}(f|G) + n_{fv}(f|G)$ see for details [8,10-12]. In this definition, edges equidistant from the two ends of the edge e = uv are not counted. We call such edges parallel to e. The number of edges parallel to e is denoted by N(e).

The PI polynomial, introduced by Ashrafi, Manoochehrian and Yousefi-Azari [5], of a connected graph G is defined as PI(G,x)= $\sum_{\{u,v\}\subseteq V(G)} x^{|E(G)|-N(u,v)}$ where N(u,v)=N(f) if f=uv$\in$E(G) and N(u,v)=0 if uv$\notin$E(G). We can see that (1)

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

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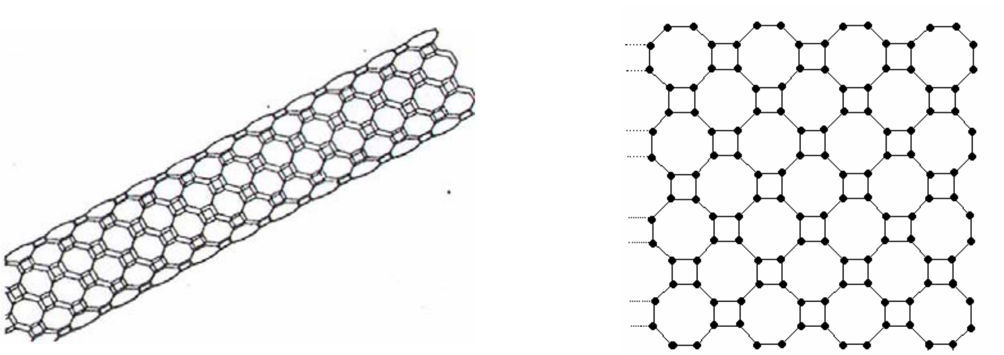
In a series of papers [1-4,6], Ashrafi and Loghman computed PI index of some nanotubes and nanotori. In [7,13] we computed polynomial of zig-zag and armchair polyhex nanotubes and nanotori. Here we continue this progress to compute the PI polynomial of the $TUC_4C_8(S)$ polyhex nanotubes and nanotorus. Our notation is standard and mainly taken from [14,15]. Throughout this paper T = $TUC_4C_8(S)[4p,q]$ an arbitrary C_4C_8 nanotubes and $T' = T[2p,2q]$ denotes a C_4C_8 nanotorus, see Figure 1, 2.

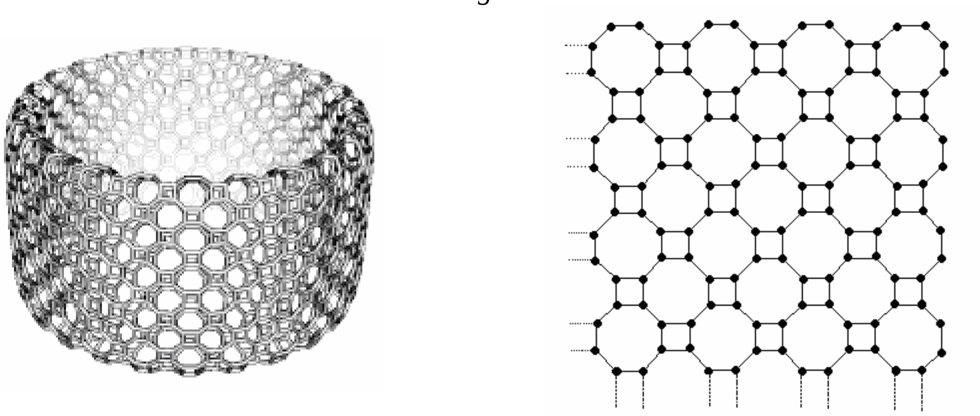
2. PI Polynomial of $TUC_4C_8[4p,q]$

In this section, the PI polynomial of the graph T = $TUC_4C_8[4p,q]$ were computed. From Figures 1(a) and 1(b), it is easy to see that $|E(T)| = 2p(3q-1)$. In the following theorem we compute the PI polynomial of the molecular graph T in Figure 1.



(a). The $TUC_4C_8(S)$ Nanotubes *(b). A $TUC_4C_8(S)$ Lattice with p = 4 and q = 8*

Fig. 1



(a). The $C_4C_8(S)$ nanotorus *(b). A $C_4C_8(S)$ nanotorus Lattice*

Fig. 2

Theorem 1. The PI polynomial of $TUC_4C_8(S)[4p,q]$ nanotube is as follows:

$$\mathrm{PI(T,x)} = \mathrm{f(x)} + \begin{cases} 2pqx^{6pq-2(p+q)} & q \le p \\ 2px^{6pq-2(p+q)}\left(\dfrac{2(x^{2(q-p+1)}-1)}{x^2-1} + 2p - q - 2\right) & p < q < 2p, \\ 2px^{6p(q-1)+2}\left(\dfrac{2(x^{2p}-1)}{x^2-1} + q - 2p\right) & q \ge 2p \end{cases}$$

where $f(x)=2p(q-1)x^{2p(3q-2)}+2pqx^{6pq-2(p+q)}+\binom{|V(T)|+1}{2}-|E(T)|$.

Proof. To compute the PI polynomial of T, it is enough to calculate N(e). To do this, we consider three cases that e is vertical, horizontal or oblique. If e is horizontal a similar proof as Lemma 1,2 in [2] shows that N(e)=2q and N(e)=2p for vertical edge e. Also, by Lemma 3 in [2], if e is an oblique edge in the $(2k-1)^{th}$ row, $1\le k\le p$, of the $TUC_4C_8(S)[4p,q]$ lattice of T, then N(e) $=\begin{cases} 2p+2k-2 & q\ge p+k-1 \\ 2q & q\le p+k-1 \end{cases}$.

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, $1\le i\le q$, $N(E_{(2i-1)1}) = N(E_{(2i-1)2}) = \cdots = N(E_{(2i-1)(2p)})$, Figure 1(b). Suppose A, B and C are the set of all horizontal, vertical and oblique edges of T. It is easy to see that |A|=|C|=2pq and |B|=2p(q-1). Then Since T is symmetric, we have:

$$\begin{aligned}
\mathrm{PI}(T,x) &= \sum_{f\in E(T)} x^{|E(T)|-N(f)} + \underbrace{\binom{|V(T)|+1}{2}-|E(T)|}_{K} \\
&= \sum_{f\in A} x^{|E(T)|-N(f)} + \sum_{f\in B} x^{|E(T)|-N(f)} + \sum_{f\in C} x^{|E(T)|-N(f)} + K \\
&= \sum_{f\in A} x^{|E(T)|-2q} + \sum_{f\in B} x^{|E(T)|-2p} + \sum_{f\in C} x^{|E(T)|-N(f)} + K \\
&= 2p(q-1)x^{2p(3q-2)} + 2pqx^{6pq-2(p+q)} + \sum_{f\in C} x^{|E(T)|-N(f)}
\end{aligned}$$

For every e in C, we have three cases:

Case 1. q≤p. In this case, we have:

$$\sum_{f\in Y} x^{|E(T)|-N(f)} = \sum_{f\in Y} x^{|E(T)|-N(E_{11})} = 2pqx^{6pq-2(p+q)}$$

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

$$\begin{aligned}
\sum_{f\in Y} x^{|E(T)|-N(f)} &= 4p(x^{|E(T)|-N(E_{11})} + x^{|E(T)|-N(E_{12})} + \ldots + x^{|E(T)|-N(E_{1(q-p+1)})}) \\
&\quad + 2p(2p-q-2)x^{|E(T)|-N(E_{1(q-p+1)})} \\
&= 4px^{|E(T)|-N(E_{11})}(1+x^{-2}+x^{-4}+\ldots+x^{-2(q-p)}) \\
&\quad + 2p(2p-q-2)x^{|E(T)|-N(E_{11})-2(q-p)} \\
&= 2px^{6pq-2(p+q)}\left(\frac{2(x^{2(q-p+1)}-1)}{x^2-1}+2p-q-2\right)
\end{aligned}$$

Case 3. q≥2p. In this case by Figure 1, we have:

$$\begin{aligned}
\sum_{f\in Y} x^{|E(T)|-N(f)} &= 4p(x^{|E(T)|-N(E_{11})} + x^{|E(T)|-N(E_{12})} + \ldots + x^{|E(T)|-N(E_{1p})}) + 2p(q-2p)x^{|E(T)|-N(E_{1p})} \\
&= 4px^{|E(T)|-N(E_{11})}(1+x^{-2}+x^{-4}+\ldots+x^{-2(p-1)}) + 2p(q-2p)x^{|E(T)|-N(E_{11})-2(p_1)} \\
&= 2px^{6p(q-1)+2}\left(\frac{2(x^{2p}-1)}{x^2-1}+q-2p\right)
\end{aligned}$$

which completes the proof.

Corollary 1. The PI index of $TUC_4C_8(S)[4p,q]$ nanotube is as follows:

$$\mathrm{PI}(TUC_4C_8(S)[4p,q]) = \frac{d}{dx}\mathrm{PI}(T,x)\Big|_{x=1} = \begin{cases} X & q\le p \\ Y & q\ge p \end{cases},$$

where $X = 36p^2q^2 - 28p^2q + 8p^2 - 8pq^2$ and $Y = 36p^2q^2 - 36p^2q - 4pq^2 + 4pq + 4p^3 + 4p^2$.

3. PI Polynomial of $C_4C_8(S)$ nanotorus

In this section, the PI polynomial of the graph $T^{'}$ = T[2p,2q] were computed. From Figures 2(a) and 2(b), we can see that |E(T)| = 6pq. In the following theorem we compute the PI polynomial of the $C_4C_8(S)$ nanotorus.

Theorem 2. The PI polynomial of $C_4C_8(S)$ nanotorus is computed as follows:

$$\mathrm{PI}(\mathrm{T}^{'},\mathrm{x})=\begin{cases}2pq(x^{2q(3p-1)}+x^{2p(3q-1)}+x^{6p(q-1)+2})+A & q\geq p\\ 2pq(x^{2q(3p-1)}+x^{2p(3q-1)}+x^{6q(p-1)+2})+A & q\leq p\end{cases}.$$

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

Proof. To compute the PI polynomial of $T^{'}$, it is enough to calculate N(e). By Lemma 2, 3 and 4 in [6] we have:

$$\mathrm{N(e)}=\begin{cases}2p & if \quad \text{e is vertical}\\ 2q & if \quad \text{e is horizontal}\\ 6p-2 & if \quad \text{e is an oblique and q} \geq \text{p}\\ 6q-2 & if \quad \text{e is an oblique and q} \leq \text{p}\end{cases}$$

Let X, Y and Z are the set of all horizontal, vertical and oblique edges of $T^{'}$. It is easy to see that |X|=|Y|=|Z|=2pq. Then Since $T^{'}$ is symmetric, we have:

$$\mathrm{PI(G,x)}=\sum_{f\in X}x^{|E(G)|-N(f)}+\sum_{f\in Y}x^{|E(G)|-N(f)}+\sum_{f\in Z}x^{|E(G)|-N(f)}+A$$

$$=2pqx^{2q(3p-1)}+2pqx^{2p(3q-1)}+A+\begin{cases}2pqx^{6q(p-1)+2} & q\leq p\\ 2pqx^{6p(q-1)+2} & q\geq p\end{cases}$$

$$=\begin{cases}2pq(x^{2q(3p-1)}+x^{2p(3q-1)}+x^{6p(q-1)+2})+A & q\geq p\\ 2pq(x^{2q(3p-1)}+x^{2p(3q-1)}+x^{6q(p-1)+2})+A & q\leq p\end{cases}$$

which completes the proof.

Corollary 2. Suppose $T^{'}$ is a $C_4C_8(S)$ nanotorus. Then we have:

$$\mathrm{PI}(\mathrm{T}^{'})=\frac{d}{dx}\mathrm{PI}(\mathrm{T}^{'},\mathrm{x})\Big|_{\mathrm{x}=1}=\begin{cases}36p^2q^2-8p^2q-10pq^2+4pq & q\geq p\\ 36p^2q^2-20p^2q-4pq^2+4pq & q<p\end{cases}$$

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