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PI Index of Polyhex Nanotori

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Abstract

The Padmakar–Ivan (PI) index of a graph G is defined as PI(G) = $\sum[n_{eu}(e|G)+ n_{ev}(e|G)]$, where $n_{eu}(e|G)$ is the number of edges of G lying closer to u than to v, $n_{ev}(e|G)$ is the number of edges of G lying closer to v than to u and summation goes over all edges of G. In this paper, the PI index of a polyhex nanotorus T is computed. We prove that:

$$PI(T) = \begin{cases} 9p^2q^2 - pq^2 - 12p^2q + 4pq & q \geq 2p \\ 9p^2q^2 - 7pq^2 + 4pq & q < 2p \end{cases}.$$

1. INTRODUCTION

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. The graph G is said to be connected if for every vertices x and y in V(G) there exists a path between x and y. In this paper we only consider connected graphs. If e is an edge of G, connecting the vertices u and v then we write e=uv and the distance between a pair of vertices u and w of G is denoted by d(u,w).

A topological index is a real number related to a molecular graph. It must be a structural invariant, i.e., it does not depend on the labelling or the pictorial representation of a graph. There are several topological indices have been defined and many of them have found applications as means to model

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chemical, pharmaceutical and other properties of molecules[1]. The Wiener index W is the first topological index to be used in chemistry[2]. It was introduced in 1947 by Harold Wiener, as the path number for characterization of alkanes. In a chemical language, the Wiener index is equal to the sum of all shortest carbon carbon bond paths in a molecule. In a graph theoretical language, the Wiener index is equal to the count of all shortest distances in a graph. For a nice survey in this topic we encourage the reader to consult Refs. [3,4].

Here, we consider a new topological index, named Padmakar-Ivan index, which is abbreviated by PI index. This newly proposed topological index, is defined by Khadikar and co-authors[5-10]. To define PI index, we consider two quantities $n_{eu}(e|G)$ and $n_{ev}(e|G)$ related to an edge e = uv of a graph 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. Then the Padmakar–Ivan (PI) index of a graph G is defined as $PI(G) = \sum[n_{eu}(e|G)+ n_{ev}(e|G)]$.

In an earlier paper, the first author computed the PI index of a zig-zag polyhex nanotube, see Ref. [11]. Also, Dend[12,13] computed the PI index of the catacondensed hexagonal systems and some other nanotubes. In this paper we continue this study to find the PI index of a polyhex torus. For topological property of tori, we encourage the reader to consult Refs. [14-18] by Diudea and co-authors.

Definition 1. Suppose G is a hexagonal system, e = xy, f = uv $\in$ E(G) and w $\in$ V(G). Define $d(w,e) = \mathrm{Min}\{d(w,x) , d(w,y)\}$. We say that e is parallel to f if $d(x,f) = d(y,f)$. In this case, we write $e \parallel f$.

Lemma 1. $\parallel$ is a reflexive and symmetric relation, but it is not transitive.

Proof. Reflexivity is trivial. To prove $\parallel$ is symmetric, we assume that e = xy is parallel to f = uv. By definition $d(x,f) = d(y,f)$. If $d(x,u) = d(x,v)$ then we obtain a cycle of odd length containing the edge f, a contradiction. Hence $d(x,u) \neq d(x,v)$ and similarly $d(y,u) \neq d(y,v)$. Without loss of generality we can assume that $d(x,u) < d(x,v)$. Then by assumption $d(y,v) < d(y,u)$ and we can see that $d(x,u) = d(y,v)$, $d(x,v) = d(y,u)$. On the other hand, $d(x,u) < d(x,v)$ and $d(y,v) < d(y,u)$ imply that $d(x,v) = d(x,u) + 1$ and $d(y,u) = d(y,v) + 1$. This shows that d(u,e) = Min{d(u,x),d(u,y)} = Min{d(x,v) - 1,d(y,v) + 1} = Min{d(y,u) – 1, d(x,u) + 1} = Min{d(y,v),d(x,v)} = d(v,e), as desired. Finally, we show that || is not transitive. To do this, we consider the graph of a polyhex nanotorus with p = 2 and q = 6, Figure 1(a). In this graph, e||f and f||g but e is not parallel to g. ■

Definition 2. Suppose G is a hexagonal system and $e \in E(G)$. We define P(e) to be the set of all edges parallel to e and N(e) = |P(e)|.

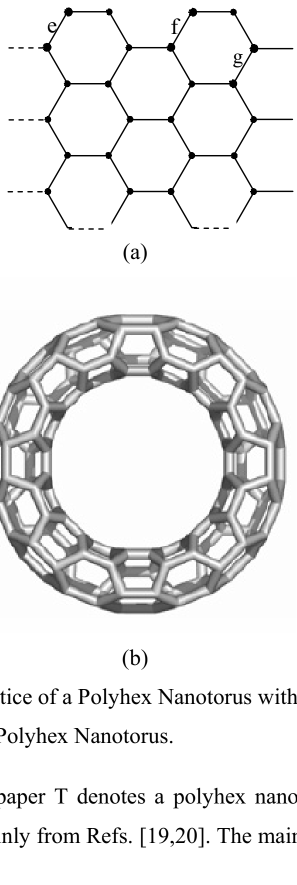

Figure 1. (a) Lattice of a Polyhex Nanotorus with p=2 and q=6.
(b) A Polyhex Nanotorus.

Throughout this paper T denotes a polyhex nanotorus. Our notation is standard and is taken mainly from Refs. [19,20]. The main result of this paper is as follows:

Theorem. Suppose T is a polyhex nanotorus. Then we have:

$$PI(T)=\begin{cases} 9p^2q^2-pq^2-12p^2q+4pq & q\ge 2p \\ 9p^2q^2-7pq^2+4pq & q<2p \end{cases}.$$

2. MAIN RESULT

In this section, the PI index of the graph T = T[p,q] were computed, Figure 1(b). We first notice that q must be even, say q = 2m. To compute the PI index of this graph, we note that N(e) = |P(e)| = |E| - (n_{eu}(e|G) + n_{ev}(e|G)), where E = E(T) is the set of all edges of T. Therefore PI(T) = $|E|^2$ - $\sum_{e\in E}$N(e). But |E(T)| = 3pq and so PI(T) = $9p^2q^2$ - $\sum_{e\in E}$N(e). Therefore, for computing the PI index of T, it is enough to calculate N(e), for every e ∈ E. To calculate N(e), we consider two cases that e is horizontal or non-horizontal.

Lemma 2. *If e is an horizontal edge then N(e) = q.*

Proof. Let u_{ij} be the $(i,j)^{th}$ entry and e_{ij} be the $(i,j)^{th}$ horizontal edge of the 2-dimensional lattice of T, Figure 2(a). It is easy to see that:

$$e_{ij}=\begin{cases} u_{i(2j-1)}u_{i(2j)} & i \text{ is odd} \\ u_{i(2j)}u_{i(2j+1)} & i \text{ is even} \end{cases} \tag{1}$$

For the symmetry of a polyhex nanotorus, it is enough to compute N(e_{11}). To do this we consider horizontal edges e_{11}, e_{31}, …, $e_{(q-1)1}$. We claim that these are q/2 edges parallel to e_{11}. Since $e_{(2k+1)1} = u_{(2k+1)1}u_{(2k+1)2}$, for 0 ≤ k ≤ q/2-1 we have:

$$d(u_{(2k+1)1},u_{11}) = \text{Min}\{2k,q-2k\},$$
$$d(u_{(2k+1)1},u_{12}) = \text{Min}\{2k,q-2k\} + 1,$$
$$d(u_{(2k+1)2},u_{11}) = \text{Min}\{2k,q-2k\} + 1,$$
$$d(u_{(2k+1)2},u_{12}) = \text{Min}\{2k,q-2k\}.$$

Thus $e_{(2k+1)1} \parallel e_{11}$. Suppose p is even. Set $L_1 = \{e_{1(1+p/2)}, e_{3(1+p/2)}, \ldots, e_{(q-1)(1+p/2)}\}$. We claim that every element of L_1 is parallel to e_{11}. If q < p + 2 then

$$d(u_{(2k+1)(p+2)},u_{11}) = 2p - 1,$$
$$d(u_{(2k+1)(p+1)},u_{12}) = 2p - 1,$$
$$d(u_{(2k+1)(p+1)},u_{11}) = 2p,$$
$$d(u_{(2k+1)(p+2)},u_{12}) = 2p,$$

where 0 ≤ k ≤ q/2 – 1. This shows that $e_{(2k+1)(1+p/2)} \parallel e_{11}$. If q ≥ p + 2 then we have:

$$\underbrace{d(u_{12},u_{1(p+1)})=d(u_{12},u_{3(p+1)})=.....=d(u_{12},u_{(p+1)(p+1)})=2p-1}_{p/2+1}$$

$$\underbrace{d(u_{11},u_{1(p+2)}) = d(u_{11},u_{3(p+2)}) = ... = d(u_{11},u_{(p+1)(p+2)}) = 2p-1}_{p/2+1}$$

$$d(u_{12},u_{(p+3)(p+1)}) = d(u_{11},u_{(p+3)(p+2)}) = 2p+1$$

$$d(u_{12},u_{(p+5)(p+1)}) = d(u_{11},u_{(p+5)(p+2)}) = 2p+3$$

$$\vdots$$

$$d(u_{12},u_{(q-p+3)(p+1)}) = d(u_{11},u_{(q-p+3)(p+2)}) = 2p+3$$

$$d(u_{12},u_{(q-p+1)(p+1)}) = d(u_{11},u_{(q-p+1)(p+2)}) = 2p+1$$

$$\underbrace{d(u_{12},u_{(q-1)(p+1)}) = d(u_{12},u_{(q-3)(p+1)}) = ... = d(u_{12},u_{(q-p-1)(p+1)}) = 2p-1}_{p/2}$$

$$\underbrace{d(u_{11},u_{(q-1)(p+2)}) = d(u_{11},u_{(q-3)(p+2)}) = ... = d(u_{11},u_{(q-p-1)(p+2)}) = 2p-1}_{p/2}.$$

Thus, every element of L_1 is parallel to e_{11}. When p is odd, a similar argument shows that every element of the set $L_2 = \{ e_{2(1+p)/2}, e_{4(1+p)/2}, \ldots, e_{q(1+p)/2}\}$ is parallel to e_{11}. Therefore $N(e) \geq q$. Let $e = e_{rs}$ be an arbitrary horizontal edge of T. If $1 < s < 1 + p/2$ then e is closer than to u_{12} than u_{11} and if $1 + p/2 < s \leq p$ then e is closer than to u_{11} than u_{12}, as desired. Finally, there is no non-horizontal edge parallel to e_{rs}, which completes the proof. ■

Lemma 3. *If e is a non-horizontal edge then N(e) =* $\begin{cases} 3q-2 & q<2p \\ 6p-2 & q\geq 2p \end{cases}$.

Proof. Suppose f_{ij} is the $(i,j)^{th}$ non-horizontal edge of the 2-dimensional lattice of T, Figure 2(b). Define $X = \{f_{11}, f_{22}, \ldots, f_{pp}, f_{1(p+1)}, f_{2(p+1)}, \ldots, f_{p(p+1)}, f_{(m+1)1}, f_{(m+1)2}, \ldots, f_{(m+1)(2p)}, f_{q(p+1)}, f_{(q-1)(p+1)}, \ldots, f_{(q-p+1)(p+1)}, f_{q(2p)}, f_{(q-1)(2p-1)}, \ldots, f_{(q(p+1)(p+1)}\}$ and $Y = \{f_{11}, f_{22}, \ldots, f_{mm}, f_{1(p+1)}, f_{2(p+1)}, \ldots, f_{q(p+1)}, f_{(m+1)1}, f_{(m+1)2}, \ldots, f_{(m+1)(m)}, f_{(m+1)(2p)}, f_{(m+1)(2p-1)}, \ldots, f_{(m+1)(2p-m+1)}, f_{q(2p)}, f_{(q-1)(2p-1)}, \ldots, f_{(q-m+1)(2p-m+1)}\}$. If $f_{ii} = u_{ii}u_{(i+1)i}$, $1\leq i \leq p$, then we have:

$$\begin{aligned} d(u_{11},f_{ii}) &= \mathrm{Min}\{d(u_{11},u_{ii}), d(u_{11},u_{(i+1)i})\} \\ &= \mathrm{Min}\{2(i-1), 2i-1\} = 2i-2 \\ d(u_{21},f_{ii}) &= \mathrm{Min}\{d(u_{21},u_{ii}), d(u_{21},u_{(i+1)i})\} \\ &= \mathrm{Min}\{2i-1, 2(i-1)\} = 2i-2. \end{aligned}$$

This shows that $f_{ii} \parallel f_{11}$. Consider $f_{i(p+1)} = u_{i(p+1)}u_{(i+1)(p+1)}$, $1\leq i \leq p$. It is easy to see that $d(u_{11}, f_{i(p+1)}) = \mathrm{Min}\{d(u_{11},u_{i(p+1)}),d(u_{11},u_{(i+1)(p+1)})\} = 2p-1 = d(u_{21}, f_{(i+1)(p+1)})$ and so $f_{i(p+1)} \parallel f_{11}$. Using a similar argument, we can see that if $q \geq 2p$ then all the edges of X are parallel to f_{11}. Suppose $q < 2p$. In this case, $d(u_{11}, f_{(p+1)(j)}) = d(u_{21},$

$f_{(p+1)(j)}) - 1$, where $m + 1 \le j \le 2p - m$ and $j \ne p + 1$. Therefore $f_{(p+1)(j)}$, $m + 1 \le j \le 2p - m$ and $j \ne p + 1$, is not parallel to f_{11}. A similar argument as above, we can see that other type of elements of X are parallel to f_{11}. Finally, a tedious calculation shows that these are the only edges parallel to f_{11}. Therefore,

$$P(f_{11}) = \begin{cases} X & q \ge 2p \\ Y & q < 2p \end{cases},$$

which completes the proof. ■

We now ready to state the main result of the paper.

Theorem. Suppose T is a polyhex nanotorus. Then we have:

$$PI(T) = \begin{cases} 9p^2q^2 - pq^2 - 12p^2q + 4pq & q \ge 2p \\ 9p^2q^2 - 7pq^2 + 4pq & q < 2p \end{cases}.$$

Proof. Since T has 3pq edges, $PI(T) = 9p^2q^2 - \sum_{e\in E}N(e)$. Let A and B be the set of all horizontal and non-horizontal edges, respectively. Apply Lemmas 1 and 2, we have:

$$\begin{aligned} PI(T[p,q]) &= 9p^2q^2 - \sum_{e\in A}N(e) - \sum_{e\in B}N(e) \\ &= 9p^2q^2 - pq^2 - \begin{cases} 2pq(3q-2) & q < 2p \\ 2pq(6p-2) & q \ge 2p \end{cases} \\ &= \begin{cases} 9p^2q^2 - pq^2 - 12p^2q + 4pq & q \ge 2p \\ 9p^2q^2 - 7pq^2 + 4pq & q < 2p \end{cases}. \end{aligned}$$ ■

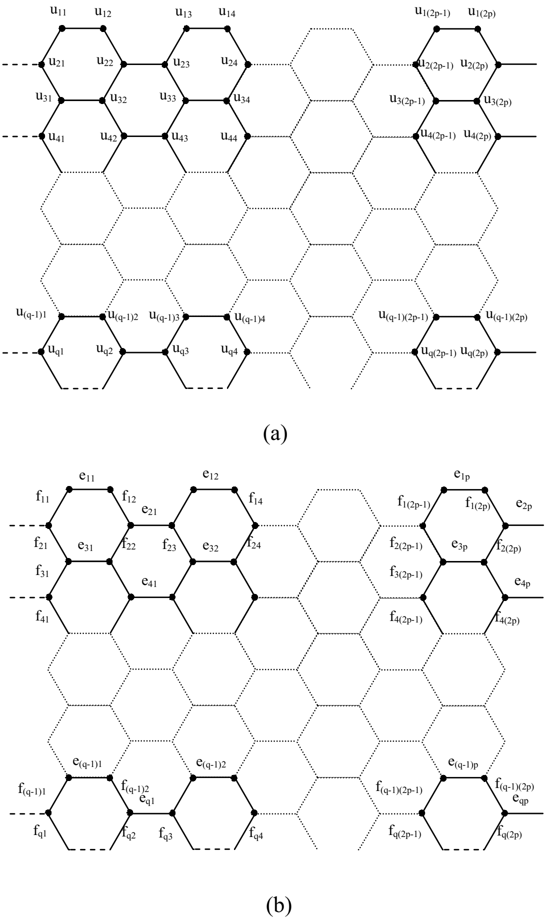

Figure 2. (a) The vertex labeled lattices of T[p,q].
(b) The edge labeled lattices of T[p,q].

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