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PI INDEX OF THE C_4C_8(S)–NANOTORUS

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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 the C_4C_8(S)-nanotorus T = T[2p,2q] is computed. We prove that:

$$\mathrm{PI(T)} = \begin{cases} 36p^2q^2 - 8p^2q - 10pq^2 + 4pq & q \le 2p \\ 36p^2q^2 - 20p^2q - 4pq^2 + 4pq & q > 2p \end{cases}.$$

INTRODUCTION

Throughout this paper, graphs are finite, undirected, simple and connected, 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 and the distance between a pair of vertices u and w of G is denoted by d(u,w).

A chemical graph is a graph in which every vertex has a degree ≤ 4. Each molecule is described by a chemical graph. The vertices of this graph denote the atoms and the edges are the bonds of the molecule.

A topological index is a real number related to a chemical 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 chemical, pharmaceutical and other properties of molecules.[1] The Wiener index W is the first topological index proposed to be used in Chemistry.[2] It was introduced in 1947 by Harold Wiener, as the path number for characterization of alkanes. We encourage the reader to consult papers by Dobrynin and co-authors[3,4] and references therein for computing Wiener index of some important chemical graphs.

Here, we consider a new topological index, named Padmakar-Ivan index[5-10] and abbreviated as PI index. 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 some earlier papers, the PI index of a zig-zag and armchair polyhex nanotube, a catacondensed hexagonal systems, a C_4C_8 nanotube and a polyhex nanotorus are computed.[11-15] In this paper we continue this study to find the PI index of a C_4C_8 torus. For topological properties of tori, we encourage the reader to consult papers by Diudea and co-authors.[16-20]

Definition 1. Suppose G is a bipartite graph, e = xy, f = uv ∈ E(G) and w ∈ V(G). Define d(w,e) = 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 ‖ f.

Lemma 1 ([13]). ‖ is reflexive and symmetric but not transitive.

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

Throughout this paper T = T[2p,2q], denotes the C_4C_8(S)–nanotorus. Our notation is standard.

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They are appearing as in the same way as in the following.[21,22] The main result of this paper is as follows:

Theorem. The PI index of $C_4C_8(S)$–nanotorus T, Figure 1, is as follows:

$$PI(T) = \begin{cases} 36p^2q^2 - 8p^2q - 10pq^2 + 4pq & q \le 2p \\ 36p^2q^2 - 20p^2q - 4pq^2 + 4pq & q > 2p \end{cases}.$$

RESULTS AND DISCUSSION

In this section, the PI index of the graph T = T[2p,2q] (Figure 1) was computed. 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 $|E(T)| = 6pq$ and so $PI(T) = 36p^2q^2 - \sum_{e\in E} N(e)$. Therefore, for computing the PI index of T, it is enough to calculate N(e), for every $e \in E$. To calculate N(e), we consider three cases that e is horizontal, vertical or oblique.

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

Proof. It is obvious that, if e and f are two horizontal edges of 2-dimensional lattice of T then N(e) = N(f). Hence it is enough to compute N(e), for $e = u_{21}u_{2(2p)}$. To do this we consider two cases that p is odd and even.

Case 1. p is odd. Define four sets A_1, A_2, A_3 and A_4, as follows:

$$A_1 = \{u_{(4k)p}u_{(4k)(p+1)} \mid 1 \le k \le q/2\},$$

$$A_2 = \{u_{(4k+1)p}u_{(4k+1)(p+1)} \mid 0 \le k \le q/2-1\},$$

$$A_3 = \{u_{(4k-1)1}u_{(4k-1)(2p)} \mid 1 \le k \le q/2\},$$

$$A_4 = \{u_{(4k-2)1}u_{(4k-2)(2p)} \mid 1 \le k \le q/2\}.$$

If $U = A_1\cup A_2\cup A_3\cup A_4$ then $U \subseteq P(e)$. We claim that U = P(e). To prove this, we assume that f is an arbitrary edge of T. Suppose f is a vertical or oblique edge in the s^{th} column of 2-dimensional lattice of T such that $f \notin U$, Figure 1. If $1 \le s \le p$ then $d(f,u_{21}) < d(f,u_{2(2p)})$ and if $p+1 \le s \le 2p$ then $d(f,u_{21}) > d(f,u_{2(2p)})$. Therefore f is not parallel to e and so $f \notin P(e)$. We now assume that $f = u_{is}u_{i(s+1)}$ is an arbitrary horizontal edge of T such that $f \notin U$. If s = p or s = 2p then $f \in U$, as desired. If $1 \le s < p$ then again $d(f,u_{21}) < d(f,u_{2(2p)})$ and if $p < s \le 2p$ then $d(f,u_{21}) > d(f,u_{2(2p)})$. This shows that U = P(e) and so N(e) = |P(e)| = |U| = 2q.

Case 2. p is even. Set

$$B = \{u_{(4k-1)p}u_{(4k-1)(p+1)}, u_{(4k-2)p}u_{(4k-2)(p+1)}, u_{(4k-1)1}u_{(4k-1)(2p)}, u_{(4k-2)1}u_{(4k-2)(2p)} \mid 1 \le k \le q/2\}.$$

Then a similar argument as Case 1 shows that N(e) = 2q, proving the lemma.

Lemma 3. If e is a vertical edge then N(e) = 4p.

Proof. Suppose T′ = T′[p′,q′] is the rotation of the 2–dimensional lattice of T through π/2, where p′=q/2 and q′ = 2p. Then every vertical edge of T is a horizontal edge of T′ and by Lemma 1, N(e) = 2q′ = 4p, as desired.

Lemma 4. If e is an oblique edge then

$$N(e) = \begin{cases} 3q-2 & q < p \\ 6p-2 & q \ge p \end{cases}.$$

Proof. We first assume that $q \ge p$. Consider an oblique edge $e = u_{11}u_{21}$. Define

$$A_1 = \{ u_{(2p+3)j}u_{(2p+4)j} \mid 1 \le j \le 2p \},$$

$$A_2 = \{ u_{(2j-1)j}u_{(2j)j} \mid 1 \le j \le p \},$$

$$A_3 = \{ u_{(2q+2j-4p-1)j}u_{(2q+2j-4p)j} \mid p + 2 \le j \le 2p \},$$

$$A_4 = \{ u_{(2j-1)(p+1)}u_{(2j)(p+1)} \mid 1 \le j \le p \},$$

$$A_5 = \{ u_{(2q+2j-4p-1)(p+1)}u_{(2q+2j-4p)(p+1)} \mid p + 2 \le j \le 2p \}.$$

Set $U = A_1\cup A_2\cup A_3\cup A_4\cup A_5$. Since $d(u_{(2p+3)j},e) = d(u_{(2p+4)j},e)$, $1 \le j \le 2p$; $d(u_{(2j-1)j},e) = d(u_{(2j)j},e)$ and $d(u_{(2j-1)(p+1)},e) = d(u_{(2j)(p+1)},e)$, $1 \le j \le p$; $d(u_{(2q+2j-4p-1)(p+1)},e) = d(u_{(2q+2j-4p)(p+1)},e)$ and $d(u_{(2q+2j-4p-1)j},e) = d(u_{(2q+2j-4p)j},e)$, we have $U \subseteq P(e)$. Finally if $f \notin U$ then $d(u_{11},f) < d(u_{21},f)$ or $d(u_{11},f) > d(u_{21},f)$. This implies that U = P(e) and so N(e) = |P(e)| = 6p – 2. If q < p then we rotate T through π/2 to find another nanotorus T′ = T′[p′,q′]. Using our argument N(e) = 6p′ – 2 = 6(q/2) – 2 = 3q – 2.

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

Theorem. The PI index of $C_4C_8(S)$ – nanotorus, Figure 1, is as follows:

$$PI(T) = \begin{cases} 36p^2q^2 - 8p^2q - 10pq^2 + 4pq & q \le 2p \\ 36p^2q^2 - 20p^2q - 4pq^2 + 4pq & q > 2p \end{cases}.$$

Proof. The proof follows from Lemmas 1-3 and the first paragraph of this section.

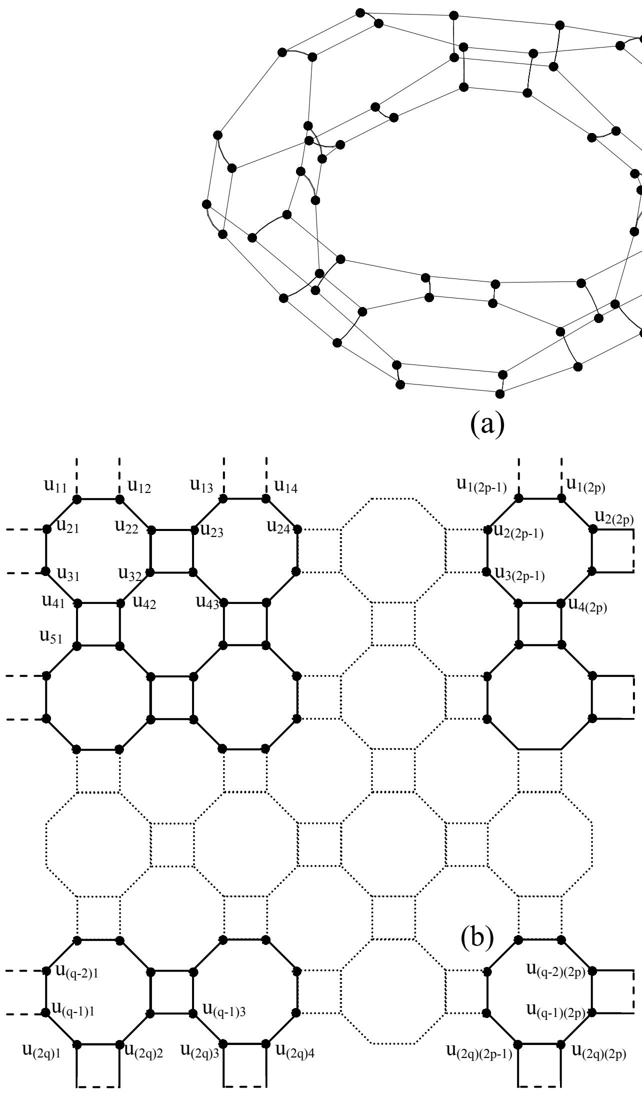

Fig. 1 – (a) A C_4C_8(S) Nanotorus; (b) The Vertex Labeled 2-Dimensional Lattice of T.

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