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PI INDEX OF NANOTUBES AND NANOTORI

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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. In this paper, we survey some results on the PI index of a C_5C_7 nanotube is computed.

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1. Introduction and preliminaries

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which are represented by V(G) and E(G), respectively. A topological index of a graph G is a numeric quantity related to G. The oldest topological index is the Wiener index. Numerous of its chemical applications were reported and its mathematical properties are well understood, [1-2].

Khadikar and co-authors [3-6], defined a new topological index and named it Padmakar-Ivan index. Here Padmakar comes from Padmakar Khadikar, and Ivan from Ivan Gutman. They abbreviated this new topological index as PI. This newly proposed topological index does not coincide with the Wiener index for acyclic molecules. It is defined as $PI(G) = \sum_{e\in G}[n_{eu}(e|G) + n_{ev}(e|G)]$, where $n_{eu}(e|G)$ is the number of edges of G lying closer to u than to v and $n_{ev}(e|G)$ is the number of edges of G lying closer to v than to u.

The most important works on the geometric structures of nanotubes and its topological indices was done by Diudea and his co-authors, [7-9]. In some research papers they computed the Wiener index of some nanotubes and nanotori. Ashrafi and his co-workers [10-20] computed the PI index of some nanotubes and nanotori for the first time. In this paper, we continue this program to compute the PI index of a class of VC_5C_7 single and multi-walled nanotubes. Here, we only consider connected graphs. Our notation is standard and mainly taken from [21].

2. Main results and discussion

The aim of this section is to compute the PI index of single and multi-walled $VC_5C_7[4p,8]$ nanotubes A and B, respectively. To do this, we assume that T = (V(T),E(T)) and B = (V(B),E(B)). Then for an arbitrary edge $e \in T$, $N(e) = |E(T)| - (n_{eu}(e|T) + n_{ev}(e|T))$. Then $PI(T) = |E(T)|^2 - \Sigma_{e\in E(T)} N(e)$. Therefore, for computing the PI index of T, it is enough to calculate N(e), for every $e \in T$. A similar method is applied for computing the PI index of B.

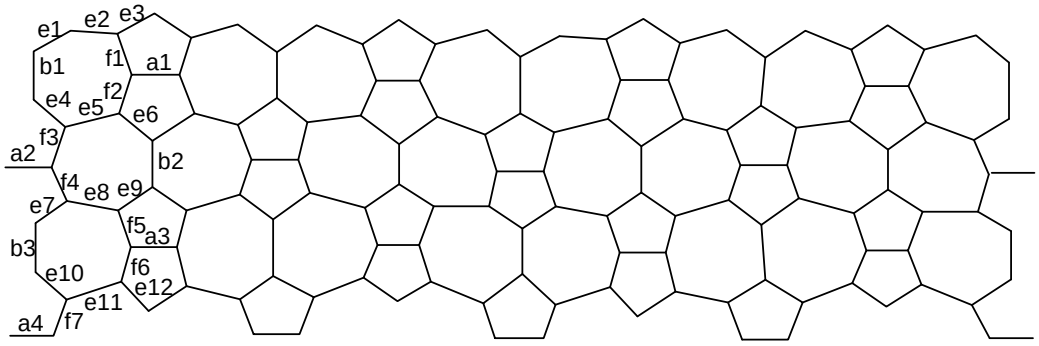

Fig. 1. A $VC_5C_7[12,8]$ Nanotube.

To compute the PI index of T, Figure 1, we first consider the set of edges $X = \{a_1, \ldots, a_4, b_1, b_2, b_3\}$ and $Y = \{e_1, e_2, \ldots, e_{12}, f_1, \ldots, f_7\}$. It is easy to see that T is constructed from X and Y with a repeation of G and then gluing the edges b_1, b_3, a_2 and a_4 of the first piece with appropriate edges of the end piece of A, see Figure 1. Thus by symmetry of T, it is enough to compute N(e) for every edge e of $X \cup Y$. Hence $PI(T) = |E(T)|^2 - \Sigma_{e\in E(T)}N(e) = |E(T)|^2 - p\Sigma_{e\in X}N(e) - 2p\Sigma_{e\in Y}N(e)$. A simple calculation shows that $N(b_1) = N(b_2) = N(b_3) = 2p$. On the other hand, one can see that $N(e_2) = 17$, $N(e_5) = 10$, $N(e_8) = 12$, $N(e_{11}) = 14$, $N(f_1) = 17p-16$, $N(f_2) = 20p - 21$, $N(f_3) = 21p-21$, $N(f_4) = 24p - 29$, $N(f_5) = 20p - 25$, $N(f_6) = 23p - 32$, $N(f_7) = 21p - 34$, and

$$N(e_1) = \begin{cases} 28 & 2 \nmid p \\ 27 & 2 \mid p \end{cases}, \qquad N(e_3) = \begin{cases} 33 & 2 \nmid p \\ 34 & 2 \mid p \end{cases}, \qquad N(e_4) = \begin{cases} 23 & 2 \nmid p \\ 22 & 2 \mid p \end{cases},$$

$$N(e_6) = \begin{cases} 19 & 2 \nmid p \\ 20 & 2 \mid p \end{cases}, \qquad N(e_7) = \begin{cases} 21 & 2 \nmid p \\ 20 & 2 \mid p \end{cases}, \qquad N(e_9) = \begin{cases} 18 & 2 \nmid p \\ 19 & 2 \mid p \end{cases},$$

Therefore, by our first equation, we have:

$$PI(T) = \begin{cases} 1639 & p = 1 \\ 6592 & p = 2 \\ 14916 & p = 3 \\ 1727p^2 - 210p & p > 3 \text{ and } 2 \mid p \\ 1727p^2 - 219p & \text{Otherwise} \end{cases}.$$

In what follows, we also compute the PI index of a polyhex nanotorus T = T[p,q] depicted in Figure 2.

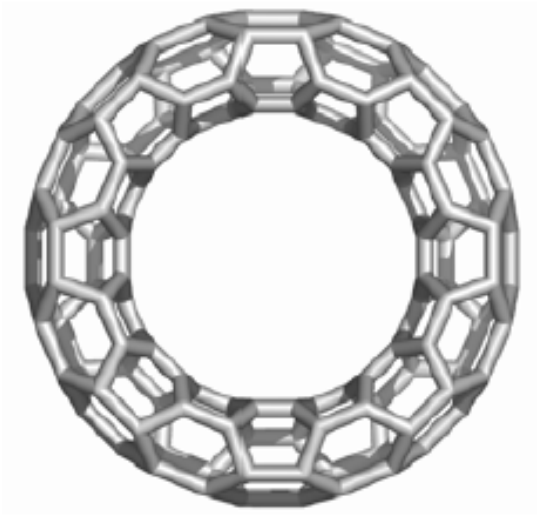

Fig. 2. A Polyhex Nanotorus.

To compute PI index of the graph T = T[p,q], 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 $e \in E$. Let A and B be the set of all horizontal and non-horizontal edges, respectively. Then we have:

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

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