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PADMAKAR-IVAN INDEX OF H-PHENYLENIC NANOTUBES AND NANOTORI

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The Padmakar-Ivan (PI) index of a molecular graph G is the sum over all edges uv of G , the number of edges which are not equidistant to u and v. In this paper, we determine the Padmakar-Ivan index of H-Phenylenic nanotubes and nanotori.

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1. Introduction

A graph G = (V, E) is a combinatorial object consisting of an arbitrary set V = V(G) of vertices and a set E = E(G) of unordered pairs {x, y} = xy of distinct vertices of G called edges. 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 labeling 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. The first topological index was introduced by Harold Wiener in 1947, as the half-sum of distances between atoms in the H-suppressed molecule.[1] However, it was after Randic[2,3] proposed a topological index for characterization of molecular branching, By definition, a topological index is a numeric quantity from the structural graph of a molecule. There are more than one thousand topological indices which enables us to characterize the physicochemical properties of most of molecules.

Khadikar and co-authors[4-8] defined a new topological index and named it Padmakar-Ivan (PI) index. This newly proposed topological index does not coincide with the Wiener index for acyclic molecules. The derived PI index is very simple to calculate and has a discriminating power similar to that of the Wiener index.

Diudea and his co-authors,[9-11] were the first scientists to take topological indices of nanotubes into account. Then Ashrafi and his co-authors,[12-14] continued Diudea's program[15-19] on geometric structure of nanotubes and nanotori to compute PI and Wiener indices of some important class of nanotubes and nanotori.

Throughout this paper, our notation is standard. They are appearing as in the same way as in the following[20,21].

2. Main Results and Discussion

In this section, the PI index of a H-Phenylenic nanotube and nanotorus were computed.

Following M.V. Diudea[22] , we denote a H-Phenylenic nanotube by G = HPHX[4n,2m].We also denote an H-Phenylenic nanotorus by H = HPHY[4n,2m]. Let G be a

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graph.Define $N(e) = |E(G)| - \sum (n_{eu}(e|G) + n_{ev}(e|G))$. Then $PI(G) = |E(G)|^2 - \sum_{e \in E(G)} N(e)$. So it is enough to compute N(e), for every edge $e \in E(G)$. From above argument and Figures 1 and 2, it is easy to see that $|E(G)| = 28mn + 2n$, $|E(H)| = 28mn + 4n$, $PI(G) = (28mn + 2n)^2 - \sum_{e \in E(G)} N(e)$ and $PI(H) = (28mn + 4n)^2 - \sum_{e \in E(G)} N(e)$.

In the following theorem we compute the PI index of G, Figure 1.

THEOREM 1. $PI(G) = 784m^2n^2-64m^2n-256n^2m -32\ r^2(2n+2m+1)$;Where $r = \mathrm{Min}\{2n,2m\}$.

Proof . for computing the PI index of G, it is enough to calculate N(e), for every e in E(G).

Consider the molecular graph of a linear H-phenylene Nanotube, Figure 1, $|E(G)| = 28mn$ and so $PI(G) = (28mn + 2n)^2 - \sum_{e \in E(G)} N(e)$. To calculate N(e), we consider three cases that e is vertical, horizontal or oblique. If e is horizontal or oblique, similar to [12] ; N(e) = 4m,4r ;Where $r = \mathrm{Min}\{2n,2m\}$. respectively. for vertical edges we have N(e) = 8n. Thus $PI(G) = 784m^2n^2-64m^2n-256n^2m -32\ r^2(2n+2m+1)$;Where $r = \mathrm{Min}\{2n,2m\}$.▲

THEOREM 2. $PI(H) = 784m^2n^2-32m^2n +16m^2-256n^2m -128\ r^2(2n+2m+1)$;Where $r = \mathrm{Min}\{2n,2m\}$.

Proof . We applying a similar argument ,as Theorem.1.We calculate That N(e) for every e in E(H). If e is horizontal or oblique; N(e) = 8m,8r ;Where $r = \mathrm{Min}\{2n,2m\}$, respectively. for vertical edges we have N(e) = 8n. Thus

$PI(H) = 784m^2n^2-32m^2n +16m^2-256n^2m -128\ r^2(2n+2m+1)$;Where $r = \mathrm{Min}\{2n,2m\}$ which complete the proof. ▲

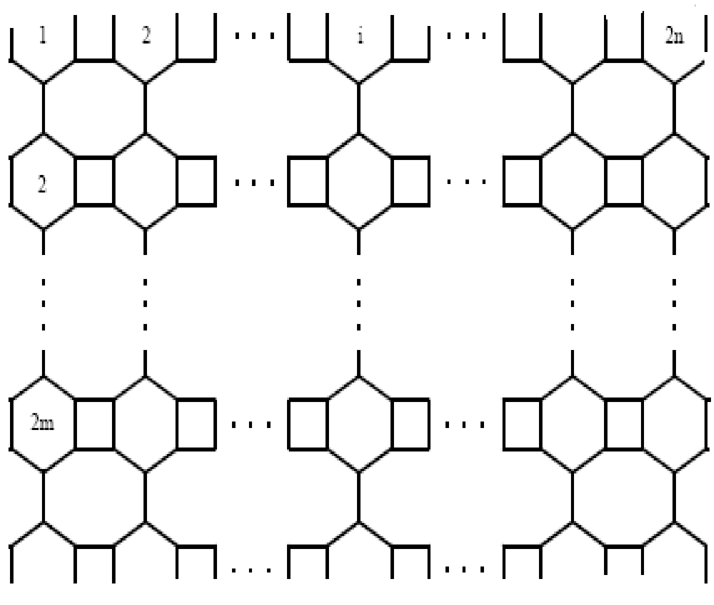

Fig.1. A H-Phenylenic Nanotube

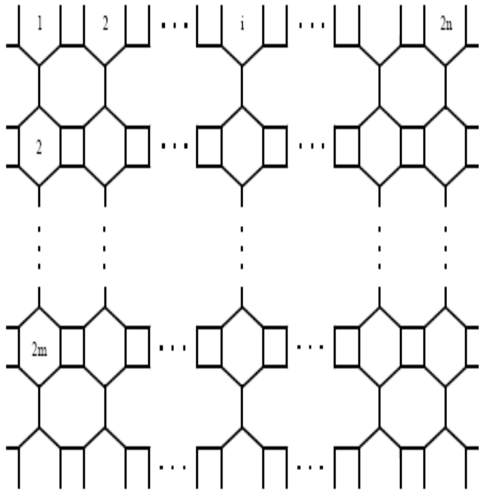

Fig.2. A H-Phenylenic Nanotorus.

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