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PI POLYNOMIAL OF V-PHENYLENIC NANOTUBES

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Let *G* be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets. The PI polynomial of a molecular graph G is defined as the sum of $x^{|E(G)|-N(e)}$ +|V(G)|(|V(G)|+1)/2 – |E(G)| over all edges of G, where N(e) is the number of edges parallel to e. In this paper, the PI polynomial of the V-phenylenic nanotubes is determined.

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1. Introduction

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 is a numeric quantity from the structural graph of a molecule. Usage of topological indices in chemistry began in 1947 when chemist Harold Wiener developed the most widely known topological descriptor, the Wiener index, and used it to determine physical properties of types of alkanes known as paraffin [1]. The Hosoya polynomial of a graph *G* is defined as $W(G;x) = \Sigma_{\{u,v\}\subseteq V(G)} x^{d(u,v)}$, where $d(u,v)$ denotes the length of a minimum path between u and v. In the paper [2] Hosoya used the name Wiener polynomial while some authors later used the name Hosoya polynomial.

Let *G* be a connected molecular 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

$$(G) = \Sigma_{e\in E(G)}[n_{eu}(e|G) + n_{ev}(e|G)], [3,4].$$

In series of papers Ashrafi and co-authors [5, 6], defined a new polynomial and named it Padmakar-Ivan polynomial.

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They abbreviated this new polynomial as PI (G,x), for a molecular graph G.

The PI polynomial of a graph G as $PI(G;X) = \Sigma_{\{u,v\}\subseteq V(G)} x^{N(u,v)}$, where for an edge $e = uv$, $N(u,v) = n_{eu}(e|G) + n_{ev}(e|G)$ and zero otherwise and we defined for the edge $e = uv$ of G two quantities $n_{eu}(e|G)$ and $n_{ev}(e|G)$. $n_{eu}(e|G)$ 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. This polynomial is most important to compute the PI index.

This newly proposed polynomial, $PI(G,X)$, does not coincide with the Wiener polynomial $(W(G,X))$ for acyclic molecules.

In a series of papers, Diudea and co-authors [7,8] investigated the structure and Hosoya polynomial of some nanotubes and nanotori. They computed the Hosoya polynomial and Winer polynomial of some nanotubes and nanotori. Also Ivan Gutman and co-authors [9] computed the and co-authors investigated the Xu. ShoujunHosoya polynomials of benzenoid graphs. In [10] Hosoya polynomials of armchair open-ended nanotubes.

Also, Ashrafi and co-authors [5, 6], computed the PI and Wiener Polynomial of some nanotubes and nanotori. In this paper we continue this program to compute the PI polynomial of V-phenylenic nanotubes, see Figure 1.

Throughout this paper, our notation is standard. They are appearing as in the same way as in [14].

We encourage the readers to consult [15-19] for background materials as well as basic.

2. Main results and discussion

In this section, the PI polynomial of a V-Phenylenic nanotube and nanotorus were computed. Following M.V. Diudea [13], we denote a V-Phenylenic nanotube by $T=VPHX[4n,2m]$. Let G be an arbitrary graph. For every edge e define :

$$N(e) = |E(G)| - (n_{eu}(e|G) + n_{ev}(e|G)).$$

By [6, Theorem.1], we have:

$$PI(G,X) = \sum_{e\in E(G)} X^{|E(G)|-N(e)} + \binom{|V(G)|+1}{2} - |E(G)|.$$

So it is enough to compute $N(e)$, for every edge $e \in E(G)$. From above the argument and Figures 1 and 2, it is easy to see that $|E(T)|=36mn-2n$.

PI polynomial of a V-Phenylenic nanotube

In the following theorem we compute the PI polynomial of T, Figure 1

THEOREM 1. $PI(T,X)=(X^{(36mn-6n)})(8mn)+(X^{(36mn-4n)})(4mn-2n)+(X^{(36mn-2n-8m)})(8mn)$

$$\begin{cases} X^{36mn-6n}(16mn) & ,if\ m \le \dfrac{n}{2} \\ 2\left(\sum_{i=1}^{4m-2n}\{2n(X^{36mn-6n-2i+2})\} + (n-m)(4n)X^{36mn-2n-8m}\right) & if\ m > \dfrac{n}{2} \text{ and } m < n+ \\ 2\left(\sum_{i=1}^{2n}\{2n(X^{36mn-6n-2i+2})\} + (m-n)(4n)X^{36mn-10n+2}\right) & ,m \ge n \end{cases}$$

$$+(24mn+1)(12mn+1)-36mn+2n.$$

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 in [21, Lemma 1], shows that N(e)=8m. Also, if e is a vertical edge in one hexagon or octagon then N(e) = 4n, 2n, respectively.

We consider set A(T) as oblique edges in T. For every e in A(T), we have two cases:

Case 1: $m \le \frac{n}{2}$

Similar argument as [21, Lemma 2], gives that N(e)=4n.

Case 2: m > n/2

We call i^th^ row of oblique edges in A(T) by A_i. (See Figure.1). It is easy to see that by symmetry of 2(m-|n-m|), by $\le$ i $\le$ A_i and 1 $\in$ graph each element of A_i has same number of parallels. If e 2m then N(e)=8n-2 if m>n and $\le$ i $\le$ computations, we have N(e)=4n+2i-2, also if 2(m-|n-m|)+1 N(e)=8m if n>m. For i>2m because of symmetry computations are similar to upper part of graph. So we have:

$$\sum_{e \text{ is vertical}} X^{|E|-N(e)} = (X^{(36mn-6n)})(8mn) + (X^{(36mn-4n)})(4mn-2n).$$

and

$$\sum_{e \text{ is horizontal}} X^{|E|-N(e)} = (X^{(36mn-2n-8m)})(8mn).$$

also

$$\sum_{e \text{ is oblique}} X^{|E|-N(e)} = \begin{cases} X^{36mn-6n}(16mn) & , if\ m \le \frac{n}{2} \\ 2\left(\sum_{i=1}^{4m-2n}\{2n(X^{36mn-6n-2i+2})\} + (n-m)(4n)X^{36mn-2n-8m}\right) & if\ m > \frac{n}{2} \text{ and } m < n \\ 2\left(\sum_{i=1}^{2n}\{2n(X^{36mn-6n-2i+2})\} + (m-n)(4n)X^{36mn-10n+2}\right) & , m \ge n \end{cases}$$

.

Thus

$$\mathrm{PI}(T,X) = \sum_{e\in E(T)} X^{|E(T)|-N(e)} + \binom{|V(T)|+1}{2} - |E(T)|$$

$$+ (|V(T)|+1)(|V(T)|+2)/2 - |E(T)| \sum_{e \text{ is oblique}} X^{|E|-N(e)} + \sum_{e \text{ is vertical}} X^{|E|-N(e)} + \sum_{e \text{ is horizontal}} X^{|E|-N(e)} =$$

$$= (X^{(36mn-6n)})(8mn) + (X^{(36mn-4n)})(4mn-2n) + (X^{(36mn-2n-8m)})(8mn) +$$

$$. \begin{cases} X^{36mn-6n}(16mn) & , if\ m \le \frac{n}{2} \\ 2\left(\sum_{i=1}^{4m-2n}\{2n(X^{36mn-6n-2i+2})\} + (n-m)(4n)X^{36mn-2n-8m}\right) & if\ m > \frac{n}{2} \text{ and } m < n \\ 2\left(\sum_{i=1}^{2n}\{2n(X^{36mn-6n-2i+2})\} + (m-n)(4n)X^{36mn-10n+2}\right) & , m \ge n \end{cases}$$

$$+(24mn+1)(12mn+1)-36mn+2n$$

which completed the proof. ■

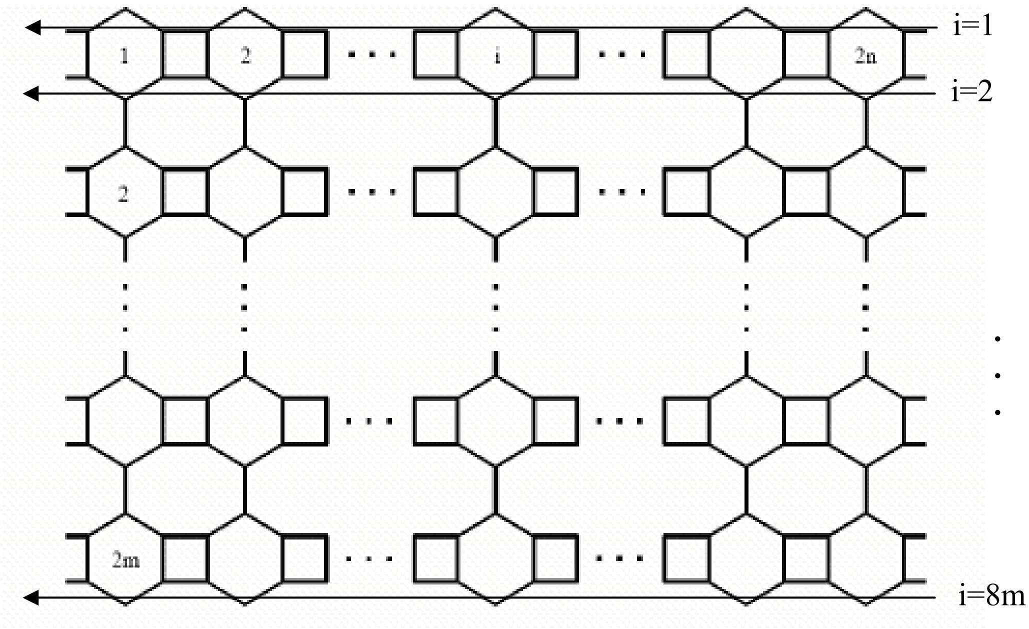

Fig. 1. A V-Phenylenic nanotube.

3. Conclusions

Graph polynomials are invariants of graphs (i.e. functions of graphs that are invariant with respect to graph isomorphism); they are usually polynomials in one or two variables with integer coefficients.In the article, by mathematical modeling, one Graph polynomial (PI) for some nanotubes is computed.

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