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$\Pi(G,x)$ polynomial and $\Pi(G)$ index of Armchair Polyhex Nanotubes $TUAC_6[m,n]$

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ABSTRACT

Let G be a simple connected graph with the vertex set $V = V(G)$ and the edge set $E = E(G)$, without loops and multiple edges. For counting *qoc* strips in G, Omega *polynomial* was introduced by *Diudea* and was defined as $\Omega(G,x) = \sum_c m(G,c).x^c$, where $m(G,c)$ be the number of *qoc* strips of length c in the graph G. Following Omega polynomial, the Sadhana polynomial was defined by *Ashrafi* et al as $Sd(G,x) = \sum_c m(G,c)x^{|E(G)|-c}$. In this paper we compute the *Pi* polynomial $\Pi(G,x) = \sum_c m(G,c).c.x^{|E(G)|-c}$ and *Pi* index $\Pi(G) = \sum_c c\times m(G,c)\left(|E(G)|-c\right)$ of an infinite class of "*Armchair Polyhex Nanotubes* $TUAC_6[m,n]$".

Keywords: Molecular Graph; Armchair Polyhex Nanotubes and Nanotori; Omega polynomial; Pi polynomial; Pi index.

1. INTRODUCTION

Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which being denoted by $V(G)$ and $E(G)$, respectively. Suppose G is a connected molecular graph and $u,v\in V(G)$. The distance $d(u,v)$ between u and v is defined as the length of a minimum path between u and v. Two edges $e = uv$ and $f = xy$ of G e co f if and only if $d(u,x) = d(v,y) = k$ and $d(u,y) = d(v,x) = k+1$ or vice versa, for a non-negative integer k.

The relation "*co*" is reflexive and symmetric but it is not necessary to be transitive, obviously. Set $C(e) := \{f\in E(G) \mid e \text{ co } f\}$), denote the subset of edges in G, *c*o-distant to the edge e. If the relation "*co*" is transitive on $C(e)$ then $C(e)$ is called an *orthogonal cut* (denoted by *oc*) of G [1-10]. The graph G is called *co-graph* if and only if the edge set $E(G)$ a union of disjoint orthogonal cuts. Observe *co* is a theta Θ relation, (*Djoković* [11], and *Winkler* [12]):

$$d(x,u) + d(y,v) \neq d(x,v) + d(y,u)$$

Theta Θ is a *co*-relation if and only if G is a partial cube, as *Klavžar* [13] correctly stated in a recent paper. Relation Θ is reflexive and symmetric but need not be transitive.

If any two consecutive edges of an edge-cut sequence are topologically parallel within the same face of the covering, such a sequence is called a *quasi-orthogonal cut qoc* strip.

Let $m(G,c)$ be the number of *qoc* strips of length c in the graph G. For counting "opposite edge strips" qocs of $E(G)$, *M.V. Diudea* introduced the Omega *polynomial* of G [1-10] and was defined as

$$\Omega(G,x) = \sum_c m(G,c)x^c$$

It is easy to see that the first derivative of Omega polynomial $\Omega(G, x)$ (in $x = 1$) equals the number of edges in the graph. Following Omega polynomial, the Sadhana polynomial was defined by *Ashrafi* and co-authors [14] in 2008, as

$$Sd(G,x) = \sum_c m(G,c)x^{|E(G)|-c}.$$

The Sadhana index $Sd(G)$ for counting *qoc* strips in G was defined by *Khadikar et. al* [15-17] as first derivative of sadhana polynomial evaluated at $x=1$

$$Sd(G) = Sd'(G, x) = \sum_{i=1}^{k}\left(\left|E(G)\right|-c_i\right)$$

Another polynomial also related to the Sadhana polynomial is the *Pi* polynomial $\Pi(G, x)$ and defined as:

$$\Pi(G,x) = \sum_c m(G,c).c.x^{|E(G)|-c}$$

The first derivative (computed at $x=1$) of this counting polynomial provide its topological index:

$$\Pi(G)=\Pi'(G,x) = \sum_c c\times m(G,c)\left(\left|E(G)\right|-c\right)$$

$\Omega(G,x)$ polynomial count codistant edges in G while $Sd(G,x)$ and $\Pi(G,x)$, non-codistant edges.

In chemical, physics and nano sciences, we have the appealing structure, especially symmetric structure with chemical constitution purporting [18,19]. One of the nanotube is *Polyhex Nanotubes,* that the structure of polyhex nanotubes is consisting of the cycles with length six C_6 in columns. Since polyhex nanotubes have more practical in the chemical, physics and nano science (see Figure 1). In Figures 1 and 2, one can see that the 3-dimentional and 2-dimentional graph of Armchair polyhex nanotubes $TUAC_6[m,n]$, where m,n are the numbers of rows/columns of hexagon (C_6) in 2-dimentional perception $TUAC_6[m,n]$. In a series of papers [18-30], some properties and applications and more historical details of nanotubes are presented and studed.

In the present work we compute the *Pi* polynomial $\Pi(G,x)$ and *Pi* index $\Pi(G)$ for an infinite class of Nano-structure "*Armchair Polyhex Nanotubes* $TUAC_6$". Throghout this paper our notation is standard and mainly taken from standard book of graph theory such as [31-36].

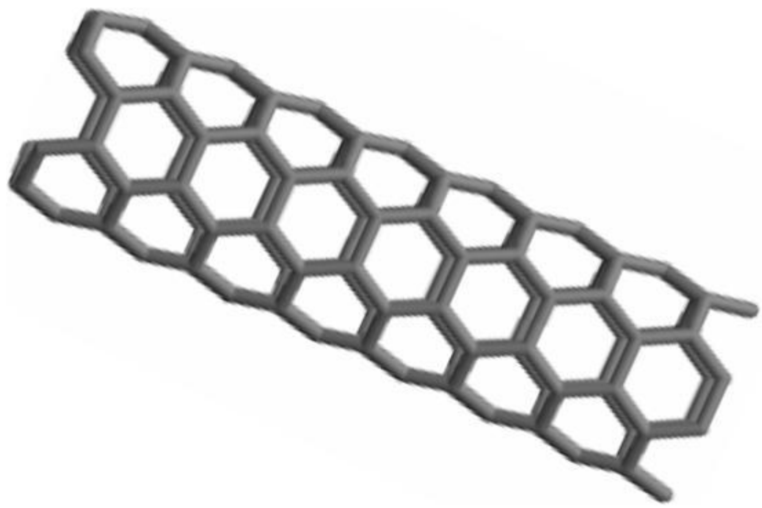

Figure 1. A 3-dimentional lattice of *Armchair Polyhex Nanotubes* $TUAC_6$.

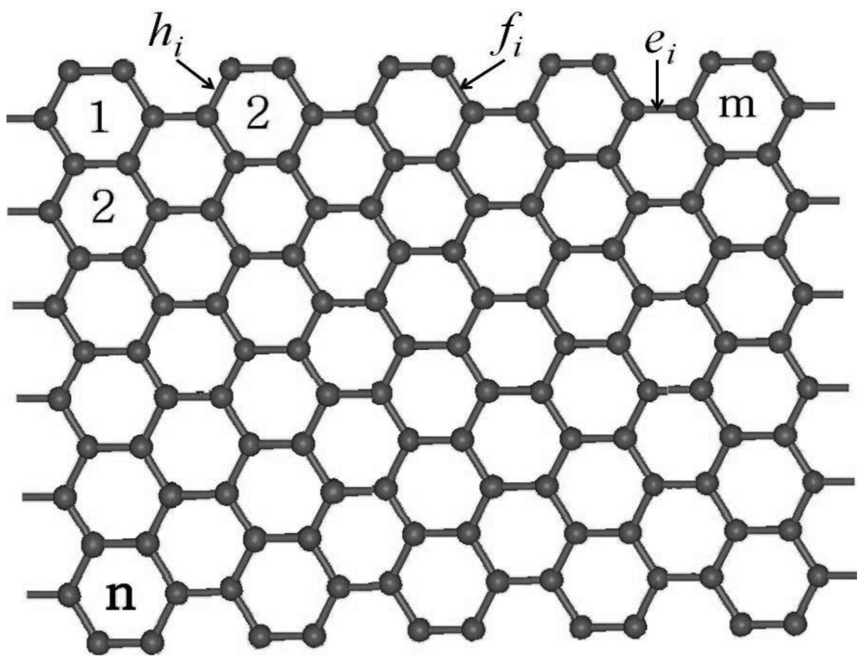

Figure 2. A 2-dimentional lattice of *Armchair Polyhex Nanotubes* $TUAC_6[m,n]$ and its hotizontal edge e_i and oblique edges f_i and h_i.

2. RESULTS AND DISCUSSION

In this section we present explicit formulas for the *Pi* polynomial $\Pi(G,x)$ and *Pi* index $\Pi(G)$ of an *Armchair Polyhex Nanotubes* $TUAC_6$.

Theorem 1. Consider the Armchair polyhex nanotubes $TUAC_6[m,n]$ $\forall\, m,n \in \mathbf{N}$; the Pi polynomials and its index are calculated by formulas:

$$\Pi(TUAC_6[m,n], x) = 2m[(n+1)x^{6mn+4m-n-1} + (2n+1)x^{6mn+4m-2n-1}]$$

and $$\Pi(TUAC_6[m,n]) = 23[18mn^2 + 24mn\ -5n^2 + 8m - 6n - 2]$$

Proof. Let $G = TUAC_6[m,n]$ be the the Armchair polyhex nanotubes and m and n be the number of hexagons in rows and columns of G.

From Figures 1 and 2, it is easy to see that the number of vertices/carbon atoms and edges/chemical bonds of $TUAC_6[m,n]$, are equal to $|V(TUAC_6[m,n])| = 4m(n+1)$ and $|E(TUAC_6[m,n])| = 6mn+4m$.

By according to Figure 2, we denote all hotizontal edge in i^{th} column by e_i and all oblique edges in i^{th} column by f_i (right) and h_i (left), then one can see that for all *quasi-orthogonal cuts* $C(e_i)$, $C(f_j)$ and $C(h_l)$:

There are $2m$ number of $C(e_i)$ with size $|C(e_i)| = n+1$ and m number of $C(f_j)$ and $C(h_l)$ with same size $|C(f_i)| = |C(h_i)| = 2n+1$. So we have the following relations for Armchair polyhex nanotubes $G = TUAC_6[m,n]$:

$$\Pi(TUAC_6[m,n],x) = \sum_c c\times m\left(TUAC_6[m,n],c\right)x^{|E(TUAC_6[m,n])|-c}$$

$$= \sum_c 2m\times|C(e_i)|.x^{6mn+4m-|C(e_i)|} + \sum_c m\times|C(f_i)|.x^{6mn+4m-|C(f_i)|} + \sum_c m\times|C(h_i)|.x^{6mn+4m-|C(h_i)|}$$

$$= 2m\times(n+1)x^{6mn+4m-n-1} + m\times(2n+1)x^{6mn+4m-2n-1} + m\times(2n+1)x^{6mn+4m-2n-1}$$

$$= 2m[(n+1)x^{6mn+4m-n-1} + (2n+1)x^{6mn+4m-2n-1}]$$

The first derivative (computed at $x=1$) of $\Pi(TUAC_6[m,n],x)$ polynomial provide the *Pi* index of an *Armchair Polyhex Nanotubes* $TUAC_6$ as follows:

$$\Pi(TUAC_6[m,n]) = \Pi'(TUAC_6[m,n],1)$$

$$= \sum_c c\times m\left(TUAC_6[m,n],c\right)\left(\left|E\left(TUAC_6[m,n]\right)\right|-c\right)$$

$$= 2m[(n+1)(6mn+4m-n-1) + (2n+1)(6mn+4m-2n-1)]$$

$$= 23[18mn^2 + 24mn - 5n^2 + 8m - 6n - 2]$$

and this completes the proof.

3. CONCLUSION

In this paper, I was counting a new counting topological polynomial and its index for a family of carbon nanotubes" Armchair polyhex nanotubes $TUAC_6[m,n]$". $\Pi(G,x)$ polynomial and its index are useful for counting the *quasi-orthogonal cut qoc* strip in structure of connected nanotubes and connected nanostructures.

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