

$\Pi(G,x)$ 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 $\Pi(G) = \sum_c c \times m(G,c) (|E(G)|-c)$ 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 are co 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 $C(e) = \{f \in E(G) \mid e \text{ } co \text{ } f\}$, denote the subset of edges in G , co -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 $x=1$

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

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:

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

$\Omega(G,x)$ 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-dimensional and 2-dimensional graph of Armchair polyhex nanotubes $TUAC_6[m,n]$, where m,n are the numbers of rows/columns of hexagon (C_6) in 2-dimensional 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 studied.

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 TUAC₆*”. Throughout this paper our notation is standard and mainly taken from standard book of graph theory such as [31-36].

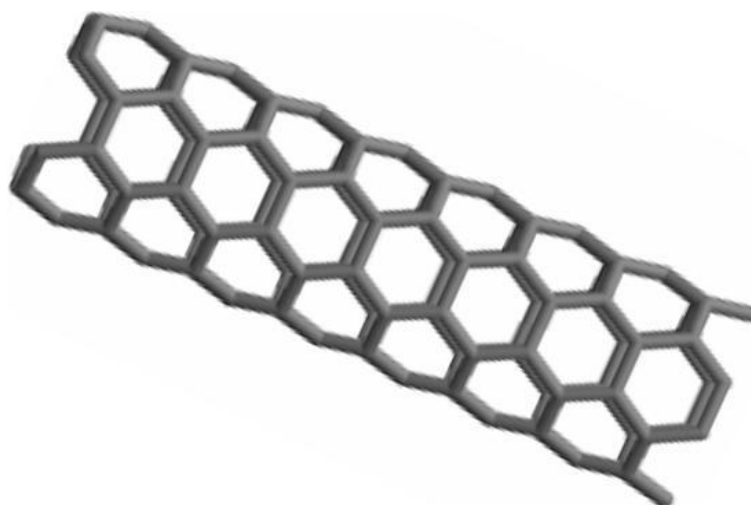


Figure 1. A 3-dimentional lattice of *Armchair Polyhex Nanotubes TUAC₆*.

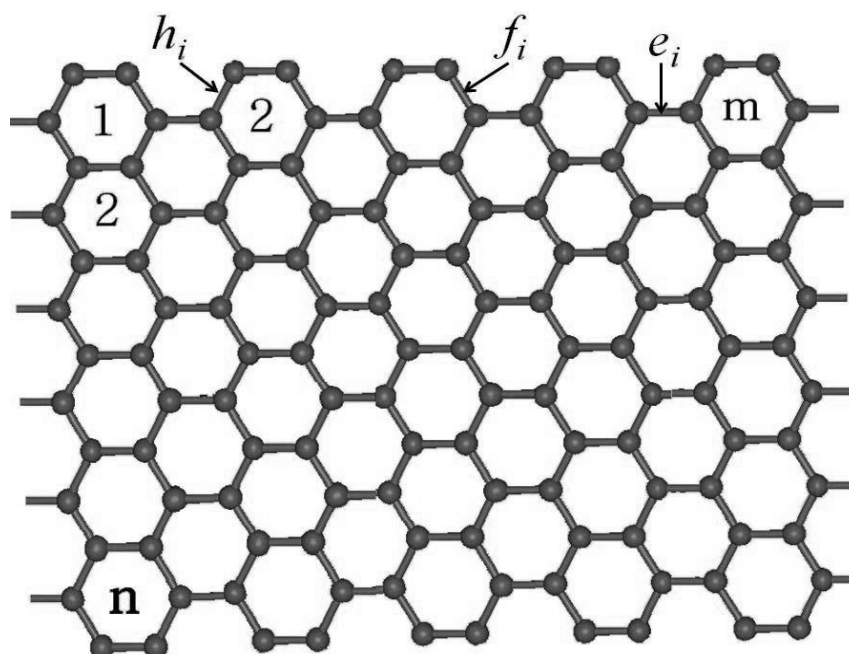


Figure 2. A 2-dimentional lattice of *Armchair Polyhex Nanotubes TUAC₆[m,n]* and its hozizontal edge e_i and oblique edges f_i and h_i .

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 TUAC₆*.

Theorem 1. Consider the Armchair polyhex nanotubes $TUAC_6[m,n] \forall m,n \in N$; 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 horizontal 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 $C(h_i)$:

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

$$\begin{aligned} \Pi(TUAC_6[m,n],x) &= \sum_c c \times m(TUAC_6[m,n],c) x^{|E(TUAC_6[m,n])|-c} \\ &= \sum_c 2m \times |C(e_i)| \cdot x^{6mn+4m-|C(e_i)|} + \sum_c m \times |C(f_i)| \cdot x^{6mn+4m-|C(f_i)|} + \sum_c m \times |C(h_i)| \cdot x^{6mn+4m-|C(h_i)|} \\ &= 2m \times (n+1)x^{6mn+4m-n-1} + m \times (2n+1)x^{6mn+4m-2n-1} + m \times (2n+1)x^{6mn+4m-2n-1} \\ &= 2m[(n+1)x^{6mn+4m-n-1} + (2n+1)x^{6mn+4m-2n-1}] \end{aligned}$$

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

$$\begin{aligned} \Pi(TUAC_6[m,n]) &= \Pi'(TUAC_6[m,n],1) \\ &= \sum_c c \times m(TUAC_6[m,n],c) (|E(TUAC_6[m,n])|-c) \\ &= 2m[(n+1)(6mn+4m-n-1) + (2n+1)(6mn+4m-2n-1)] \\ &= 23[18mn^2 + 24mn - 5n^2 + 8m - 6n - 2] \end{aligned}$$

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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