\( \Pi(G,x) \) 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 \( Sd(G,x) = \sum_{c} m(G,c)x^{2c} \). In this paper we compute the Pi polynomial \( \Pi(G,x) = \sum_{c} m(G,c)x^{c+1} \) and Pi index \( \Pi(G) = \sum_{c \in m(G,c)} |E(G) - c| \) 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 \( C(e) = \{f \in E(G) \mid e \text{ co } f \} \), 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 \( \Theta \) relation, (Djoković [11], and Winkler [12]):

\[ d(x,u) + d(y,v) \neq d(x,v) + d(y,u) \]

Theta \( \Theta \) is a co-relation if and only if \( G \) is a partial cube, as Klavžar [13] correctly stated in a recent paper. Relation \( \Theta \) 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 \( x=1 \)

\[
Sd(G) = Sd'(G, x) = \sum_{c,l}(|E(G)|^c-1)
\]

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

\[
\Pi(G,x) = \sum_c m(G,c)x|E(G)-c|
\]

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

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

\( \Omega(G,x) \) 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-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}”. Throughout this paper our notation is standard and mainly taken from standard book of graph theory such as [31-36].
2. RESULTS AND DISCUSSION

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

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

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

\[
\Pi(TUAC_6[m,n],x) = \sum_{c} c \times m(TUAC_6[m,n],c)x^{\text{deg}(TUAC_6[m,n]) - c}
= \sum_{c} 2m \times |C(e_i)| \times x^{6mn+4m-6n-1} \times \sum_{c} m \times |C(f_i)| \times x^{6mn+4m-2n-1} + \sum_{c} m \times |C(h_i)| \times x^{6mn+4m-2n-1}
= 2m \times (n+1) \times x^{6mn+4m-n-1} + m \times (2n+1) \times x^{6mn+4m-2n-1} + m \times \times (2n+1) \times x^{6mn+4m-2n-1}
= 2m \times (n+1) \times x^{6mn+4m-n-1} + (2n+1) \times x^{6mn+4m-2n-1}
\]

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:

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

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.
References


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