On the SD- polynomial and SD- index of an infinite class of “Armchair Polyhex Nanotubes”

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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 $G$, Diudea introduced the $\Omega$-polynomial of $G$ and was defined as $\Omega(G, x) = \sum_{i=1}^{k} x^{c_i}$, where $C_1, C_2, ..., C_k$ be the “opposite edge strips” ops of $G$ and $c_i = |C_i|$ ($l = 1, 2, ..., k$). One can obtain the $Sd$-polynomial by replacing $x$ with $x^{\frac{|E(G)|-c}{2}}$ in $\Omega$-polynomial. Then the $Sd$-index will be the first derivative of $Sd(x)$ evaluated at $x = 1$. In this paper we compute the $Sd$-polynomial and $Sd$-index of an infinite class of “Armchair Polyhex Nanotubes”.

Keywords: Omega and Sadhana polynomial; Sadhana index; Armchair Polyhex Nanotubes and Nanotori

1. INTRODUCTION

By a graph $G$ means a pair $G = (V, E)$ in which $V = V(G)$ and $E = E(G)$ denote to the set of vertices and edges, respectively. A chemical graph is a graph theoretical representation of a molecule whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. For two vertices $x$ and $y$ belong to $V$, $x$ is adjacent to $y$ if and only if $xy \in E(G)$. In a connected graph, there is a path between every pair $(x,y)$ of its vertices. The distance $d(x,y)$ between vertices/atoms $x$ and $y$ ($x,y \in V(G)$) is defined as the length of a shortest path between $x$ and $y$. Two edges $e = uv$ and $f = xy$ of $G$ are called co-distant, “$e$ co $f$”, if and only if they obey the following relation for a non-negative integer $d$: [1]

$$d(v, x) = d(v, y) + 1 = d(u, x) + 1 = d(u, y) = d$$

For some edges of $G$ there are the following relations satisfied [1,2]:

$$e \text{ co } e$$
though the last relation is not always valid. In other words, the relation “co” is reflexive and symmetric but it is not necessary to be transitive. 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 \( G \). The graph \( G \) is called co-graph if and only if the edge set \( E(G) \) a union of disjoint orthogonal cuts: \( E(G) = \bigcup_{i=1}^{k} C_i \) and \( C_i \cap C_j = \emptyset \), for \( i \neq j \) and \( i,j = 1, 2, \ldots, k \).

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. For counting “opposite edge strips” qocs \( C_i \) of \( E(G) \) (\( i, j = 1, 2, \ldots, k \), \( M.V. \) Diudea introduced the \( \Omega \)-polynomial of \( G \) [3-11] and was defined as \( \Omega(G, x) = \sum_{i=1}^{k} |C_i| \), where \( c_i \)'s is the size of opposite edge strips (= \( |C_i| \) \( i = 1, 2, \ldots, k \)).

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

\[
\Omega'(G, x) = \sum_{i=1}^{k} c_i = \sum_{i=1}^{k} |C_i| = |E(G)|
\]

Another polynomial also related to the ops in \( G \) was introduced by Ashrafi and co-authors [12] in 2008, that counting the non-opposite edges is the Sadhana polynomial \( Sd(G, x) \) defined as:

\[
Sd(G, x) = \sum_{i=1}^{k} x^{[E(G)]-c_i}
\]

The Sadhana index \( Sd(G) \) for counting \( qoc \) strips in \( G \) was defined by Khadikar et. al [13,14] as first derivative of sadhana polynomial evaluated at \( x = 1 \) [13-18]

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

By definition of \( \Omega \)-polynomial, one can obtain the \( Sd \)-polynomial by replacing \( x^c \) with \( x^{[E(G)]-c} \) in \( \Omega \)-polynomial.

In chemical, physics and nano sciences, we have the appealing structure, especially symmetric structure with chemical constitution purporting. Carbon exists in several forms in nature. One is the so-called nanotube which was discovered for the first time in 1991 [19,20]. 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, in this paper we focus on its structure and by using definition of \( Sd \)-polynomial and \( Sd \)-index, we compute these topological polynomial and index for an infinite class of Nano-structure “Armchair Polyhex Nanotubes TUAC6”, depicted in Figure 1.
Throughout this paper our notation is standard and mainly taken from standard book of graph theory such as [21-25].

2. RESULTS AND DISCUSSION

In this section we compute the $Sd$-polynomial and $Sd$-index of a family of Polyhex Nanotubes. In Figure 1, 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 [26-36], some properties and applications and more historical details of nanotubes are presented and studied.

By these terminologies and from Figure 1, we will have the following results for Armchair Polyhex Nanotubes $TUAC_6$.

Theorem 1.

$\forall m,n \in N$ let $G = TUAC_6[m,n]$ be the Armchair polyhex nanotubes, then the $Sd$-polynomial and $Sd$-index of $G$ are equale to

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

and

$$Sd(TUAC_6[m,n]) = 24m^2n + 16m^2 - 6mn - 4m$$

![Fig. 1. A 3-dimentional (left) and 2-dimentional (right) lattices of Armchair Polyhex Nanotubes $TUAC_6[m,n]$.](image-url)
Proof.

Consider the Armchair polyhex nanotubes \( G = TUAC_6[m,n] \) \( (m,n \in \mathbb{N}) \) (Figure 1). Let \( m, n, |V(G)| \) and \( |E(G)| \) be the hexagons in rows/columns, number of vertices/carbon atoms and edges/chemical bonds of \( G \). Then one can see that \( |V(G)| = 4m(n + 1) \) and \( |E(G)| = 6mn + 4m \). Now, if we denote all horizontal edge in \( i^{th} \) column by \( e_i \) and all left (or right) oblique edges in \( i^{th} \) column by \( f_i \) (or \( h_i \)), then it is easy to see that for all quasi-orthogonal cuts \( C_1, C_2, \ldots, C_{2m}, C_i = C(e_i) \) and also for all quasi-orthogonal cuts \( C_{2m+1}, C_{2m+2}, \ldots, C_{3m}, C_{2m+j} = C(f_j) \) and alternatively, for all qocs \( C_{3m+1}, C_{3m+2}, \ldots, C_{4m}, C_{3m+l} = C(h_l) \).

Now by according to Figure 1, one can see that \( \forall i=1, 2, \ldots, 2m: c_i = n + 1 \) and \( \forall j = 1, 2, \ldots, m: c_{m+j} = c_{3m+j} = 2n + 1 \).

Thus, \( Sd \)-polynomial of Armchair polyhex nanotubes \( G = TUAC_6[m,n] \) is equale to

\[
Sd(TUAC_6[m,n], x) = \sum_{i=1}^{k} [E(G)]_{-C_i} x
= 2m \times x^{6mn+4m-n-1} + m \times x^{6mn+4m-2n-1} + m \times x^{6mn+4m-2n-1}
\]

The \( Sd \)-polynomial of \( G \) implies that the \( Sd \)-index of \( TUAC_6[m,n] \) is equale to

\[
Sd(TUAC_6[m,n]) = Sd'(TUAC_6[m,n], x) = \frac{\partial Sd(TUAC_6[m,n], x)}{\partial x} |_{x=1}
= 2m \times (6mn + 4m - n - 1) + m \times (6mn + 4m - 2n - 1) + m \times (6mn + 4m - 2n - 1) = 24m^2n + 16m^2 - 6mn - 4m
\]

Here, the proof is completed.

3. CONCLUSION

In this paper, we obtained the Sadhana polynomial and Sadhana index of Armchair Polyhex Nanotubes and Nanotori for the first time.

References


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