

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 Ω -polynomial of G and was defined as $\Omega(G, x) = \sum_{i=1}^k x^{c_i}$, where C_1, C_2, \dots, C_k be the “opposite edge strips” ops of G and $c_i = |C_i|$ ($i = 1, 2, \dots, k$). One can obtain the Sd -polynomial by replacing x^c with $x^{|E(G)|-c}$ in Ω -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]:

$$e \text{ co } e$$

$$e \text{ co } f \Leftrightarrow f \text{ co } e$$

$$e \text{ co } f \ \& \ f \text{ co } h \Rightarrow e \text{ co } h$$

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: $E(G) = \cup_{i=1}^k C_i$ and $C_i \cap C_j = \emptyset$, for $i \neq j$ and $i, j = 1, 2, \dots, k$.

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

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]

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

By definition of Ω -polynomial, one can obtain the Sd -polynomial by replacing x^c with $x^{|E(G)|-c}$ in Ω -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-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 [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 equal to

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

and

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

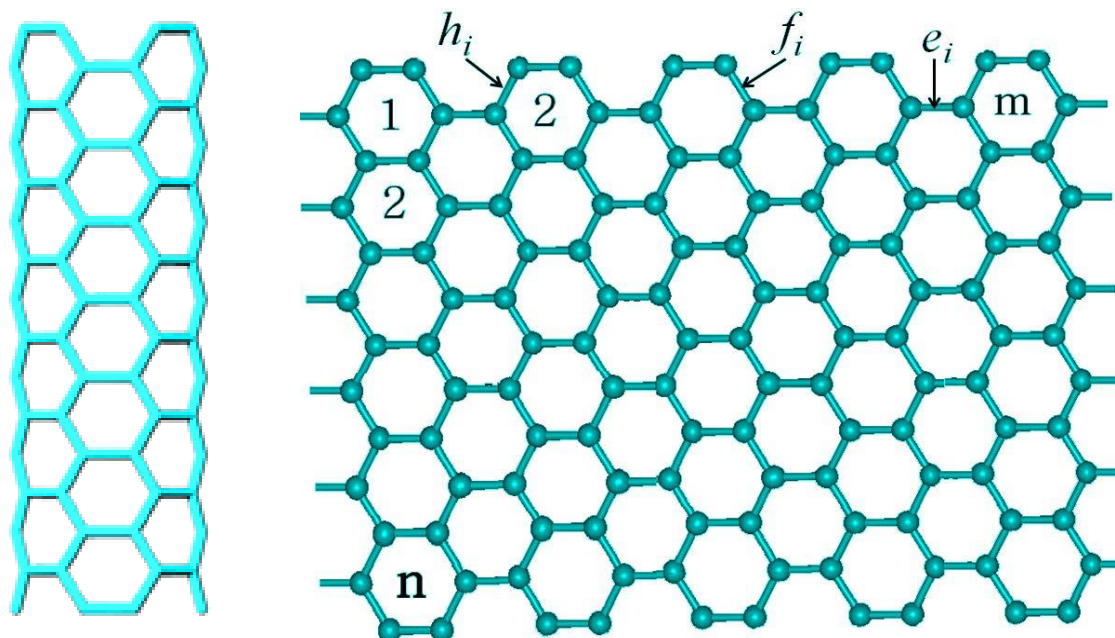


Fig. 1. A 3-dimensional (left) and 2-dimensional (right) lattices of Armchair Polyhex Nanotubes $TUAC_6[m,n]$.

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, \dots, C_{2m} , $C_i = C(e_i)$ and also for all *quasi-orthogonal cuts* $C_{2m+1}, C_{2m+2}, \dots, C_{3m}$, $C_{2m+j} = C(f_j)$ and alternatively, for all *qocs* $C_{3m+1}, C_{3m+2}, \dots, C_{4m}$, $C_{3m+l} = C(h_l)$.

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

Thus, *Sd*-polynomial of Armchair polyhex nanotubes $G = TUAC_6[m,n]$ is equal to

$$\begin{aligned} Sd(TUAC_6[m,n], x) &= \sum_{i=1}^k x^{|E(G)|-c_i} \\ &= 2m \times x^{6mn+4m-n-1} + m \times x^{6mn+4m-2n-1} + m \times x^{6mn+4m-2n-1} \end{aligned}$$

The *Sd*-polynomial of G implies that the *Sd*-index of $TUAC_6[m,n]$ is equal to

$$\begin{aligned} Sd(TUAC_6[m,n]) &= Sd'(TUAC_6[m,n], x) = \left. \frac{\partial Sd(TUAC_6[m,n], x)}{\partial x} \right|_{x=1} \\ &= 2m \times (6mn + 4m - n - 1) + m \times (6mn + 4m - 2n - 1) + m \times (6mn \\ &\quad + 4m - 2n - 1) = 24m^2n + 16m^2 - 6mn - 4m \end{aligned}$$

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.

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