

Szeged Index of armchair polyhex Nanotube

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Abstract

Topological indices of nanotubes are numerical descriptors that are derived from graph of chemical compounds. Such indices based on the distances in graph are widely used for establishing relationships between the structure of nanotubes and their physico-chemical properties. The Szeged index is obtained as a bond additive quantity where bond contributions are given as the product of the number of atoms closer to each of the two end points of each bond. In this paper we find an exact expression for Szeged index of armchair polyhex nanotube ($TUAC_6[p, k]$).

Keywords: Szeged index, $TUAC_6[p, k]$ Nanotube

1. Introduction

A graph G consists of a set of vertices $V(G)$ and a set of edges $E(G)$. In chemical graphs, each vertex represented an atom of the molecule and covalent bonds between atoms are represented by edges between the corresponding vertices. This shape derived from a chemical compound is often called its molecular graph, and can be a path, a tree or in general a graph.

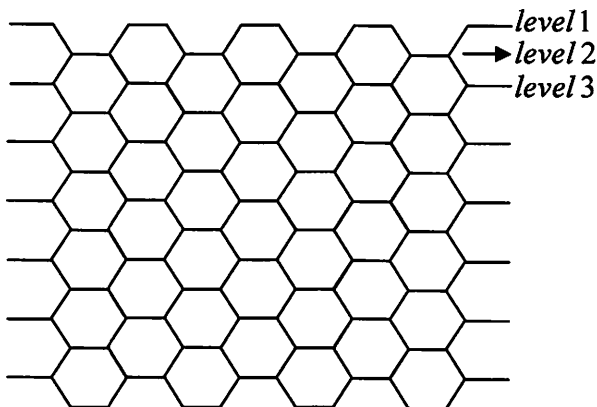
A topological index is a single number, derived following a certain rule, which can be used to characterize the molecule [18]. Usage of topological indices in biology and chemistry began in 1947 when chemist Harold Wiener [21] introduced Wiener index to demonstrate correlations between physico-

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chemical properties of organic compounds and the index of their molecular graphs. Wiener originally defined his index (W) on trees and studied its use for correlation of physico chemical properties of alkenes, alcohols, amines and their analogous compounds. A number of successful QSAR studies have been made based in the Wiener index and its decomposition forms [1].

In a series of papers, the Wiener index of some nanotubes are computed [3,4,5,7,9,19,20,22,23]. Another topological index was introduced by Gutman and called the Szeged index, abbreviated as Sz [8].

Let e be an edge of a graph G connecting the vertices u and v . Define two sets $N_1(e|G)$ and $N_2(e|G)$ as $N_1(e|G) = \{x \in V(G) | d(u,x) < d(v,x)\}$ and $N_2(e|G) = \{x \in V(G) | d(x,v) < d(x,u)\}$. The number of elements of $N_1(e|G)$ and $N_2(e|G)$ are denoted by $n_1(e|G)$ and $n_2(e|G)$ respectively. The Szeged index of the graph G is defined as $Sz(G) = Sz = \sum_{e \in E(G)} n_1(e|G)n_2(e|G)$. The Szeged index is a modification of the Wiener index to cyclic molecules. The Szeged index was conceived by Gutman at the Attila jozsef university in Szeged. This index received considerable attention. It has attractive mathematical characteristics. In [12,14,15,16] Szeged index and in [2,6,10,11,13,17], another topological index of some nanotubes are compute. In this paper, we computed the Szeged index of $TUAC_6[p, k]$ nanotube.



Two dimensional lattice of $TUAC_6[4,14]$ nanotube, $p = 4, k = 14$

Figure 1

According to Figure 1, we denote the number of horizontal lines in one row by p and the number of levels by k . Throughout this paper, our notation is standard. The notation $[f]$ is the greatest integer function.

2. The Szeged index of $TUAC_6[p, k]$ nanotube

In this section, the Szeged index of $T = TUAC_6[p, k]$ nanotube is computed.

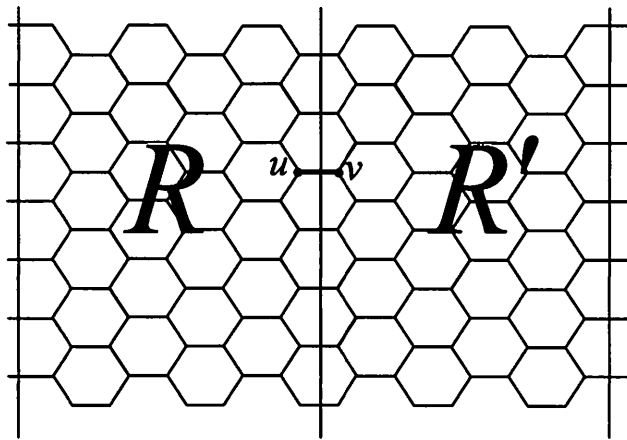
Let e be an arbitrary edge of nanotube. Suppose $n_1(e|G)$ counts the vertices of G lying closer to one vertex than to other vertex and the meaning of $n_2(e|G)$ is analogues. For computing the Szeged index of T , we assume two cases:

Case 1: p is even.

Lemma 1. If e is a horizontal edge of T , then $n_1(e|G)n_2(e|G) = p^2k^2$.

Proof. Suppose that e is a horizontal edge of T , for example $e = uv$ in Figure 2. In this Figure the region R has the vertices that belong to $N_1(e|G)$ and the region R' has the vertices that belong to $N_2(e|G)$. So we have

$n_1(e|G) = n_2(e|G) = pk$, therefore $n_1(e|G)n_2(e|G) = p^2k^2$. By the symmetry of $TUAC_6[p, k]$ nanotube for every horizontal edges the above relations is hold.



$e = uv$ is a horizontal edge in level $m = 6$.

Figure 2

For simplicity, we define $a = \left\lfloor \frac{k-m-1}{2} \right\rfloor$ and $b = \left\lfloor \frac{m-1}{2} \right\rfloor$.

Lemma 2. Suppose p is even. If e is an oblique edge in level $m(1 \leq m \leq k)$, then we have

i) If $m \leq p$ and $k - m \leq p$ then

$$n_1(e|G) = p(k+m-1) + 2b(5-2m+3b-p) + 2a(k-m-a-2) + 2k-6m+2. \quad (I)$$

ii) If $m \leq p$ and $k - m > p$,

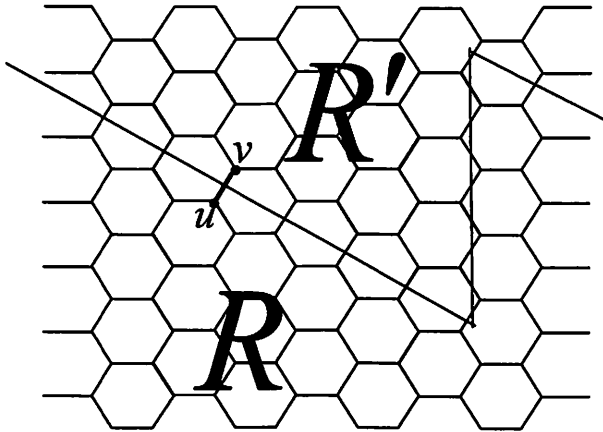
$$\text{then } n_1(e|G) = p(2k-1/2p-1) + 2b(5-p+3b-2m) - 4m + 4. \quad (II)$$

iii) If $m > p$ and $k - m \leq p$, then

$$n_1(e|G) = p(k-m+1/2p) + 2a(k-a-m-2) + 2(k-m-1). \quad (III)$$

iv) If $m > p$ and $k - m > p$, then $n_1(e|G) = 2p(k-m) + 2. \quad (IV)$

Proof. Let e be an oblique edge of T , for example $e = uv$ in Figure 3. In this figure, the region R has the vertices that belongs to $N_1(e|G)$ and the region R' has the vertices that belongs to $N_2(e|G)$.



$e = uv$ is an oblique edge in level $m = 6$

Figure 3

Number of vertices that is closer to u than to v is as follows: If $m \leq p$ and $k - m \leq p$, then

$$\begin{aligned}
 n_1(e|G) &= p(k - m + 1) + \sum_{i=1}^a (4i) + \\
 &\sum_{i=1}^b (2p - 4i) + (k - m - 2a - 1)(2a + 2) + \\
 &(m - 2b - 1)(2p - 4b - 4) = \\
 &p(k+m-1) + 2b(5-2m+3b-p) + 2a(k-m-a-2) + 2k-6m+2.
 \end{aligned}$$

If $m \leq p$ and $k - m > p$, then

$$\begin{aligned}
 n_1(e|G) &= p(2k - 2m - p + 2) + \sum_{i=1}^{\lfloor \frac{p-2}{2} \rfloor} (4i) + \sum_{i=1}^b (2p - 4i) + \\
 &(m - 2b - 1)(2p - 4b - 4) \\
 &= p(2k-1/2p-1) + 2b(5-p+3b-2m) - 4m + 4.
 \end{aligned}$$

If $m > p$ and $k - m \leq p$, then

$$n_1(e|G) = p(k-m+1) + \sum_{i=1}^a (4i) + \sum_{i=1}^{\frac{p-2}{2}} (2p-4i) + (k-m-2a-1)(2a+2) + 2 = p(k-m+1/2p) + 2a(k-a-m-2) + 2(k-m-1).$$

And if $m > p$ and $k - m > p$, then

$$n_1(e|G) = p(2k-2m-p+2) + \sum_{i=1}^{\frac{(p-2)}{2}} (4i) + \sum_{i=1}^{\frac{(p-2)}{2}} (2p-4i) + 2 = 2p(k-m)+2.$$

By the symmetry of $TUAC_6[p, k]$ nanotube for every oblique edge this relations is hold. ■

Remark 3. According to Figure 3, let e be an oblique edge in level $m(1 \leq m \leq k)$, then

$$n_2(e|G) = 2pk - n_1(e|G).$$

Theorem 4. If p is even, then the Szeged index of $TUAC_6[p, k]$ nanotube is given as follows:

1. k is even

i) If $k \leq p$, then we have

$$Sz(T) = p^3(2k^3 - k^2 - k + 2) + p^2(k^2 - 2k) + p(-1/6k^5 + 1/3pk^4 + 1/3k^3 - 1/3k^2 - 2/3k).$$

ii) If $p < k \leq 2p$, then we have

$$Sz(T) = p^5(91/12 - 31/3k) + p^4(14/3k^2 - 22/3k - 10/3) + p^3(2k^3 + 1/2k^2 + 4/3k - 4/3) + p^2(11/3k^3 - 4k^2 - 2/3k^4 - 4/3k + 2/15) + p(-1/30k^5 - 7/12k^4 + 7/3k^3 - 5/3k^2 - 4/5k) + 31/5p^6.$$

iii) If $k > 2p$, then we have

$$Sz(T) = p(1/4k^4 - 1/5k^5 + 2/3k^3 - 22/15k) + p^2(+1/3k^4 + 2/3k^3 + 2/3k^2 - 14/3k + 22/15) + p^3(-2k^3 + 5/2k^2 - 8/3k + 8/3) + p^4(10k^2 - 6k - 2/3) + p^5(91/12 - 31/3k) + 31/5p^6.$$

2. k is odd.

i) If $k \leq p$, then we have

$$Sz(T) = p(-1/6k^5 + 1/3k^4 - 2/3k^3 - 4/3k^2 + 5/6k + 1) + p^2(2k^2 - 2) + p^3(2k^3 - k^2 - k + 1).$$

ii) If $p < k \leq 2p$, then we have

$$Sz(T) = p^3(2k^3+1/2k^2+13/3k+13/6)+p^4(+14/3k^2-22/3k-7/3)+$$

$$p(-1/30k^5-1/12k^4+1/3k^3+5/6k^2-3/10k-3/4)$$

$$+p^2(-2/3k^4+5/3k^3-3k^2-13/3k+17/15)+91/12p^5+31/5p^6.$$

iii) If $k > 2p$, then we have

$$Sz(T) = p^3(-2k^3+5/2k^2-11/3k+1/6)+p^4(+10k^2-6k+1/3)+31/5p^6+p(-1/5k^5+1/4k^4-$$

$$1/3k^3-1/2k^2+8/15k+1/4)+p^2(1/3k^4+2/3k^3+5/3k^2-8/3k+22/15)+p^5(-31/3k+91/12).$$

Proof. At first, suppose A and B are the sets of all horizontal and oblique edges of T , respectively. Then we have

$$Sz(T) = \sum_{e \in A} n_1(e|G)n_2(e|G) + \sum_{e \in B} n_1(e|G)n_2(e|G). \quad (*)$$

The number of horizontal edges are pk . Thus we have

$$\sum_{e \in A} n_1(e|G)n_2(e|G) = p^2k^2.p = p^3k^2.$$

The number of oblique edges are $2pk$.

Let k be even.

Now for $k \leq p$, we have :

$$\sum_{e \in B} n_1(e|G)n_2(e|G) = 2p \cdot \left\{ \sum_{m=1}^{k-1} \{(I)(2pk - (I))\} \right\} =$$

$$2p \{ (-1/12k^5 + 1/6k^4 + 1/6k^3 - 1/6k^2 - 1/3k) +$$

$$p^2(k^3 - k^2 - 1/2k + 1) + p(1/2k^2 - k) \}.$$

When $p < k \leq 2p$ we have :

$$\sum_{e \in C} n_1(e|G)n_2(e|G) = 2p \cdot \left\{ \sum_{m=1}^{k-p-1} \{(II)(2pk - (II))\} + \sum_{m=k-p}^p (I)(2pk - (I)) + \right.$$

$$\left. \sum_{m=p+1}^{k-1} (III)(2pk - (III)) \right\} =$$

$$2p \{ (-1/60k^5 - 5/6k^2 + 7/6k^3 - 2/5k +$$

$$p(-1/3k^4 + 11/6k^3 - 2k^2 - 2/3k + 1/15) - 11/3p^3k +$$

$$p^2(+k^3 - 1/4k^2 + 2/3k - 2/3)$$

$$+ p^3(7/3k^2 - 5/3) + p^4(91/24 - 31/6k) + 31/10p^5 \}.$$

And if $k > 2p$, then we have :

$$\begin{aligned} \sum_{e \in \mathcal{C}} n_1(e|G)n_2(e|G) &= 2p \cdot \left\{ \sum_{m=1}^{k-p-1} \{(II)(2pk - (II))\} + \sum_{m=k-p}^p (IV)(2pk - (IV)) + \right. \\ &\quad \left. \sum_{m=p+1}^{k-1} (III)(2pk - (III)) \right\} = \\ &= 2p\{-1/10k^5 + 1/8k^4 + 1/3k^3 - 11/15k\} + p\{+1/6k^4 + 1/3k^3 + 1/3k^2 - 7/3k + 11/15\} + \\ &\quad p^2\{-k^3 + 3/4k^2 - 4/3k + 4/3\} \\ &\quad + p^3\{+5k^2 - 3k - 1/3\}p^4\{-31/6k + 91/24\} + 31/10p^5\}. \end{aligned}$$

Suppose k is odd, in this case for $k \leq p$ we have :

$$\begin{aligned} \sum_{e \in \mathcal{C}} n_1(e|G)n_2(e|G) &= 2p\{-1/12k^5 + 1/6k^4 - 1/3k^3 - 2/3k^2 + 1/2 + 5/12k + p(k^2 - 1) + \\ &\quad p^2(1/2 - 1/2k - k^2 + k^3)\}. \end{aligned}$$

When $p < k \leq 2p$ we have :

$$\begin{aligned} \sum_{e \in \mathcal{C}} n_1(e|G)n_2(e|G) &= 2p\{-1/60k^5 - 1/24k^4 + 1/6k^3 + 5/12k^2 - 3/20k - 3/8 + \\ &\quad p(-1/3k^4 + 5/6k^3 - 3/2k^2 - 13/6k + 17/30) \\ &\quad + p^2(k^3 - 1/4k^2 + 13/6k + 13/12) + p^3(7/3k^2 - 11/3k - 7/6) + p^4(-31/6k + 91/24) + 31/10p^5\}. \end{aligned}$$

And if $k > 2p$, then we have :

$$\begin{aligned} \sum_{e \in \mathcal{C}} n_1(e|G)n_2(e|G) &= 2p\{-3/40k^5 - 1/12k^3 + 19/120k + \\ &\quad p(+1/8k^4 + 1/3k^3 + 5/4k^2 - 4/3k + 11/120) \\ &\quad p^2(-5/4k^3 + k^2 - 11/4k + 1/3) + p^3(19/4k^2 - 3k + 19/12) + p^4(-31/8k + 11/3) + 93/40p^5\}. \end{aligned}$$

So if p is even, then by using the above relations in (*) the result is hold. ■

Case 2. p is odd.

Lemma 5. If e is an oblique edge in level m ($1 \leq m \leq k$), then we have :

i) If $m \leq p$ and $k - m \leq p$ then
 $n_1(e|G) = p(k+m-1) + 2b(5-2m+3b-p) + 2a(k-m-a-2) + 2k-6m+2.$

ii) If $m \leq p$ and $k - m > p$, then
 $n_1(e|G) = p(2k - 1/2p - 1) + 2b(5 - p + 3b - 2m) - 4m + 7/2$.

iii) If $m > p$ and $k - m \leq p$, then
 $n_1(e|G) = p(k - m + 1/2p) - 3/2 + 2a(k - a - m - 2) + 2(k - m)$.

iv) If $m > p$ and $k - m > p$, then $n_1(e|G) = 2p(k - m)$.

Proof. The proof is similar to the proof of lemma 2. ■

Theorem 6. If p is odd, then Szeged index of $TUAC_6[p, k]$ nanotube is given as follows:

1. k is even.

i) If $k \leq p$, then we have

$$Sz(T) = p^3(2k^3 - k^2 - k + 2) + p(-1/6k^5 + 1/3k^4 + 1/3k^3 - 1/3k^2 - 2/3k) + p^2(k^2 - 2k).$$

ii) If $p < k \leq 2p$, then we have:

$$Sz(T) = p^3(2k^3 + 1/2k^2 - 26/3k - 41/6) + p(-1/30k^5 - 7/12k^4 + 2/3k^3 + 11/6k^2 - 17/15k - 7/4) + p^2(-2/3k^4 + 11/3k^3 + 2k^2 - 10/3k - 128/15) + p^4(14/3k^2 - 22/3k + 4/3) + p^5(91/12 - 31/3k) + 31/5p^6.$$

iii) If $k > 2p$, then we have :

$$Sz(T) = p^3(-2k^3 + 5/2k^2 - 26/3k + 7/6) + p(-1/5k^5 + 1/4k^4 + 1/2k^2 - 4/5k + 1/4) + p^2(1/3k^4 + 2/3k^3 + 8/3k^2 - 8/3k - 6/5) + p^4(10k^2 - 6k + 4) + p^5(91/12 - 31/3k) + 31/5p^6.$$

2. k is odd.

i) If $k \leq p$, then we have

$$Sz(T) = p^3(2k^3 - k^2 - k + 1) + p(-1/6k^5 + 1/3k^4 - 2/3k^3 - 4/3k^2 + 5/6k + 1) + 2p^2(k^2 - 1).$$

ii) If $p < k \leq 2p$, then we have:

$$Sz(T) = p^3(+2k^3 - 17/3k + 1/2k^2 - 10/3) + p(-1/30k^5 - 1/12k^4 - 4/3k^3 - 2/3k^2 + 41/30k) + p^2(-2/3k^4 + 5/3k^3 + 3k^2 + 11/3k - 8/15) + p^4(14/3k^2 - 22/3k + 7/3) + p^5(91/12 - 31/3k) + 31/5p^6.$$

iii) If $k > 2p$, then we have :

$$Sz(T) = p^3(-2k^3 + 5/2k^2 - 29/3k - 4/3) + p(-1/5k^5 + 1/4k^4 - k^3 + 1/5k) + p^2(1/3k^4 + 2/3k^3 + 11/3k^2 - 2/3k - 1/5) + p^4(10k^2 - 6k + 5) + p^5(91/12 - 31/3k) + 31/5p^6.$$

Proof. The proof is similar to the proof of Theorem 4. ■

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