Szeged Index of $HC_5C_7[r, p]$ Nanotube

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Abstract
A C_5C_7 net is a trivalent decoration made by alternating pentagons C_5 and heptagons C_7. It can cover either a cylinder or a torus. In this paper we compute the Szeged index of $HC_5C_7[r, p]$ nanotube.

Keywords: Nanotube, Molecular graph, Szeged index.

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 form 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-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 is 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 $N_2(e|G)=\{x\in V(G)|d(x,v)<d(x,u)\}$.

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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 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 is computed. In this paper, we computed the Szeged index of $HC_5C_7[r, p]$ nanotube.

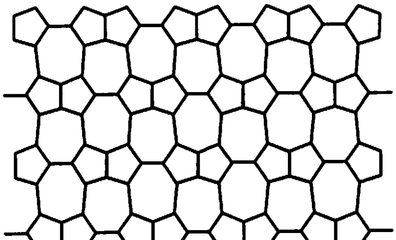

$HC_5C_7[4, 8]$ nanotube, $p = 8, k = 4$

Figure 1

In $HC_5C_7[r, p]$ nanotubes, we denote the number of pentagons in one row by p and number of the rows by k. In Figure 1, an $HC_5C_7[4, 8]$ lattice is illustrated. In the hole of paper, the notation $[f]$ is the greatest integer function.

2. The szeged index of $HC_5C_7[r, p]$ nanotube

Let e be an edge in Figure 1. Denote:

$E_1 = \{ e\in E(G)|$ e is a oblique edge between heptagon and pentagon adjacent a vertical edge$\}$

$E_2 = \{ e\in E(G)|$ e a oblique edge between heptagon and pentagon adjacent a horizontal edge$\}$

$E_3 = \{ e\in E(G)|$ e is an oblique edge between two heptagons$\}$

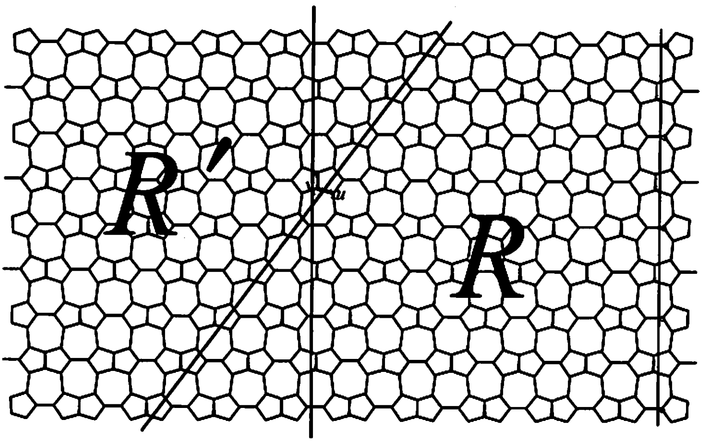
$E_4 = \{ e\in E(G)|$ e is an vertical edge between two pentagons$\}$

$E_5 = \{ e\in E(G)|$ e is a horizontal edge$\}$.

And the number of vertices in each period of this nanotube is equal to $4p$. For computing the Szeged index of above nanotube, we have the following cases:

a) If $e\in E_1$, then

according to Figure 2, the region R has the vertices that belongs to $N_1(e|G)$ and the region of R' has vertices that belongs to $N_2(e|G)$. (The notations $n_1(e|G)$ and $n_2(e|G)$ are indicated with $n_e(u)$ and $n_e(v)$, respectively).



$e = uv$ is an edge belong to E_1 in $m = 4$th row.

Figure 2

In Figure 2, the vertex that assigned by symbol $*$, is closer to v and the vertices that assigned by symbol $\circ$, have the same distance from u and v.

In this paper for simplicity we define: $B = \left[\frac{m}{2}\right]$, $C = \left[\frac{m-1}{2}\right]$, $D = \left[\frac{k-m}{2}\right]$, $E = \left[\frac{k-m+1}{2}\right]$, $A(j) = \left[\frac{2p+j}{12}\right]$, $A(j,i) = \left[\frac{A(j)+i}{2}\right]$ where $i, j = 0, \pm 1, \pm 2, \ldots$.

i) If $m \le \frac{p}{2}$, then $a_1 = n_e(u) = 2pk - 2m^2 + m - 1 - B - 2C + 2D.$

ii) If $m > \frac{p}{2}$, then $a_2 = n_e(u) = 2p(k-m) + \frac{1}{2}p^2 - p + 2D.$

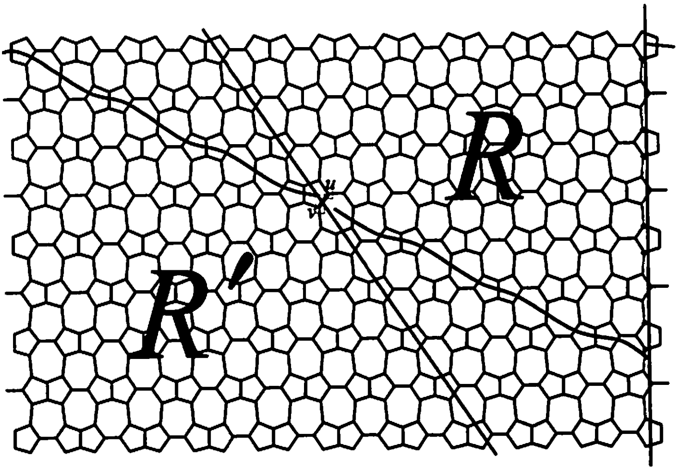
And for $n_e(v)$ we have:

i) If $k - m \le \frac{p}{2}$, then $a_3 = n_e(v) = k(2p - 2k + 4m - 1) - 2m^2 + m - 1 - B - 2C.$

ii) If $k - m > \frac{p}{2}$, then $a_4 = n_e(v) = 2pm + \frac{1}{2}p^2 + \frac{3}{2}p - 1 - B - 2C.$

b) If $e \in E_2$, then

according to Figure 3, the region R has the vertices that belongs to $N_1(e|G)$ and the region of R' has vertices that belongs to $N_2(e|G)$.



$e = uv$ is an edge belong to E_2 in $m = 4$th row.

Figure 3

In Figure 3, the vertices that assigned by symbol $\circ$, have the same distance from u and v. Then:

i) If $m \le A(-3)$ and $k - m \le A(3)$, then

$$b_1 = n_e(u) = k(2p + 12m - 6k - 3) - 4m^2 + 2m - 1 - 2C - 2E.$$

ii) If $A(-3) < m \le \frac{p}{2}$ and $k - m \le A(3)$, then

$$b_2 = n_e(u) = k(2p + 12m - 6k - 3) - 4m^2 + 2m - 1 - A(-3) - 2E.$$

iii) If $m > \frac{p}{2}$ and $k - m \le A(3)$, then

$$b_3 = n_e(u) = k(2p + 12m - 6k - 4) + m(4 - 6m + 2p) - \frac{3}{2}p^2 - \frac{1}{2}p - 1 - A(-3) - 2E.$$

iv) If $m \le A(-3)$ and $k - m > A(3)$, then

$$b_4 = n_e(u) = m(2p + 2m - 1) - 1 - 2C + (2p - 3) \times A(3) - 6(A(3))^2 - 2A(3,1).$$

v) If $A(-3) < m \le \frac{p}{2}$ and $k - m > A(3)$, then

$$b_5 = n_e(u) = m(2p + 2m - 1) - 1 + (2p - 3) \times A(3) - 6(A(3))^2 - A(-3) - 2A(3,1).$$

vi) If $m > \frac{p}{2}$ and $k - m > A(3)$, then

$$b_6 = n_e(u) = p(2m + \frac{1}{2}p + 1) + (2p - 3) \times A(3) - 6(A(3))^2 - A(-3) - 2A(3,1).$$

And for $n_e(v)$ we have:

i) If $m \le A(-3)$ and $k - m \le \frac{p}{2}$, then $b_7 = n_e(v) = k(2p - 4m + 2k + 1) - 4m^2 + 2m - 1.$

ii) If $m > A(-3)$ and $k - m \le \frac{p}{2}$, then

$$b_8 = n_e(v) = (2p+1)(k-m) + k(2k-4m) + 2m^2 + 2p - 4 + (2p-8)\times A(-3) - 6(A(-3))^2 - 2A(-3,0).$$

iii) If $m \le A(-3)$ and $k - m > \frac{p}{2}$, then

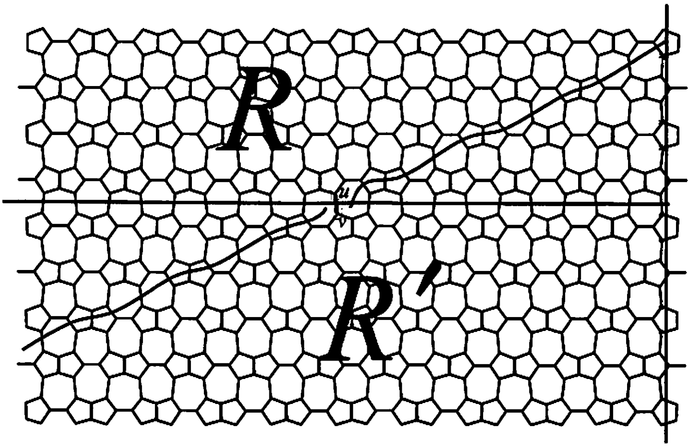
$$b_9 = n_e(v) = 2p(2k-m) + 3m - 6m^2 - \frac{1}{2}p^2 + \frac{1}{2}p - 1.$$

iv) If $m > A(-3)$ and $k - m > \frac{p}{2}$, then

$$b_{10} = n_e(v) = 4p(k-m) + \frac{5}{2}p - \frac{1}{2}p^2 - 4 + (2p-8)\times A(-3) - 6(A(-3))^2 - 2A(-3,0).$$

c) If $e \in E_3$, then

according to Figure 4, the region R has the vertices that belongs to $N_1(e|G)$ and the region of R' has vertices that belongs to $N_2(e|G)$.



$e = uv$ is an edge belong to E_3 in m = 4th row.

Figure 4

In Figure 4, the vertices that assigned by symbol $*$, is closer to u and the vertices that assigned by symbol $\circ$, have the same distance from u and v. Then:

i) If $m \le A(-5)$, then $c_1 = n_e(u) = m(2p + 6m - 1) - 1 + B.$

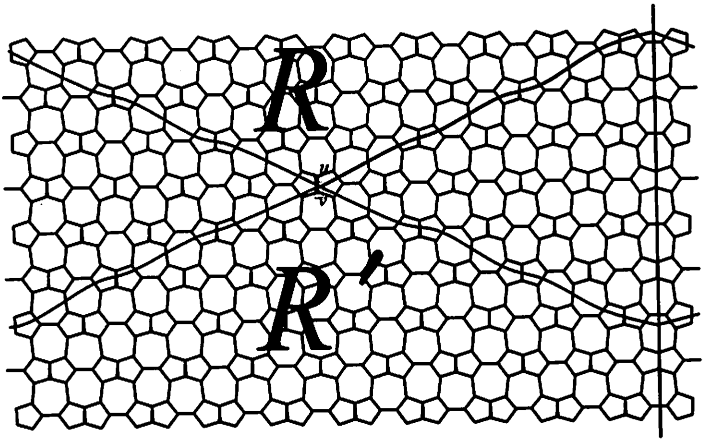
ii) If $m > A(-5)$, then $c_2 = n_e(u) = 4pm - 1 + 6(A(-5))^2 - (2p+1)\times A(-5) + A(-5,0).$

And for $n_e(v)$ we have:

i) If $k - m \le A(-5)$, then $c_3 = n_e(v) = k(2p - 12m + 6k - 1) + m(6m - 2p + 1) - 1 - 2E.$

ii) If $k - m > A(-5)$, then

$$c_4 = n_e(v) = 4p(k-m) - 1 + 6(A(-5))^2 - (2p+1)\times A(-5) - 2A(-5,0).$$



$e = uv$ is an edge belong to E_4 in $m = 4$th row.

Figure 5

d) If $e \in E_4$, then

according to Figure 5, the region R has the vertices that belongs to $N_1(e|G)$ and the region of R' has vertices that belongs to $N_2(e|G)$. Then:

i) If $m \le A(0)+1$, then $d_1 = n_e(u) = 12m(m-1)+2-3C.$

ii) If $m > A(0)+1$, then

$$d_2 = n_e(u) = 4pm - 4p + 2 + 12(A(0))^2 + (12-4p)\times A(0) - 3A(0,0).$$

And for $n_e(v)$ we have:

i) If $k-m \le A(0)$, then $d_3 = n_e(v) = 12(k-m)(k-m+1)+2-3D.$

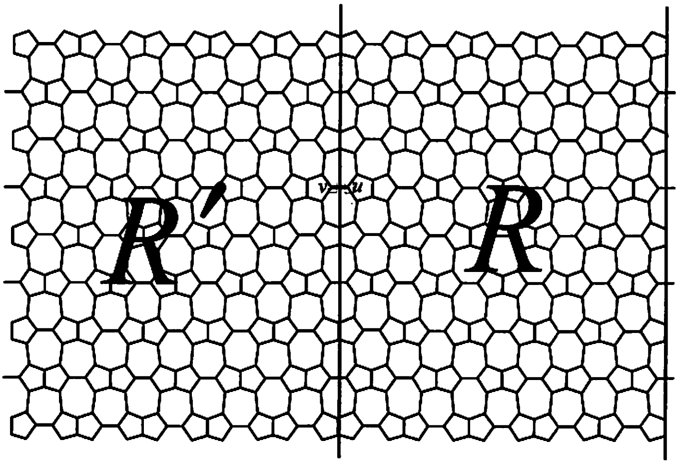
ii) If $k-m > A(0)+1$, then

$$d_4 = n_e(v) = 4p(k-m) + 2 + 12(A(0))^2 + (12-4p)\times A(0) - 3A(0,0).$$

e) If $e \in E_5$, then

according to Figure 6, the region R has the vertices that belongs to $N_1(e|G)$ and the region of R' has vertices that belongs to $N_2(e|G)$. Then:

$$e_0 = n_e(u) = n_e(v) = 4pk - 1 - 2(E+B).$$



$e = uv$ is an edge belong to E_5 in $m = 4$th row.

Figure 6

For simplicity we define:

$$S_0 = \sum_{m=1}^{k} \{2p(a_1a_2 + b_1b_7) + \frac{p}{2}(d_1d_3 + e_0{}^2)\}.$$

$$S_1 = p\{ \sum_{m=1}^{k-A(-5)-1} c_1c_4 + \sum_{m=k-A(-5)}^{A(-5)} c_1c_3 + \sum_{m=A(-5)+1}^{k-1} c_2c_3 \}.$$

$$S_2 = p\{ \sum_{m=1}^{A(-5)} c_1c_4 + \sum_{m=A(-5)+1}^{k-A(-5)-1} c_2c_4 + \sum_{m=k-A(-5)}^{k-1} c_2c_3 \}.$$

$$S_3 = 2p\{ \sum_{m=1}^{k-A(3)-1} b_4b_7 + \sum_{m=k-A(3)}^{A(3)} b_1b_7 + \sum_{m=A(3)+1}^{k} b_2b_8 \}.$$

$$S_4 = 2p\{ \sum_{m=1}^{A(-3)} b_4b_7 + \sum_{m=A(-3)+1}^{k-A(3)-1} b_5b_8 + \sum_{m=k-A(3)}^{k} b_2b_8 \}.$$

$$S_5 = 2p\{ \sum_{i=1}^{k-\frac{p}{2}-1} b_4b_9 + \sum_{m=k-\frac{p}{2}}^{A(-3)} b_4b_7 + \sum_{m=A(-3)+1}^{k-A(3)-1} b_5b_8 + \sum_{m=k-A(3)}^{\frac{p}{2}} b_2b_8 + \sum_{m=\frac{p}{2}+1}^{k} b_3b_8 \}.$$

$$S_6 = 2p\{\sum_{m=1}^{A(-3)} b_4b_9 + \sum_{m=A(-3)+1}^{k-\frac{p}{2}-1} b_5b_{10} + \sum_{m=k-\frac{p}{2}}^{\frac{p}{2}} b_5b_8 + \sum_{m=\frac{p}{2}+1}^{k-A(3)-1} b_6b_8 + \sum_{m=k-A(3)}^{k} b_3b_8\}.$$

$$S_7 = \frac{p}{2}\{\sum_{m=1}^{k-A(0)-1} d_1d_4 + \sum_{m=k-A(0)}^{A(0)} d_1d_3 + \sum_{m=A(0)+1}^{k} d_2d_3\}.$$

$$S_8 = \frac{p}{2}\{\sum_{m=1}^{A(0)} d_1d_4 + \sum_{m=A(0)+1}^{k-A(0)-1} d_2d_4 + \sum_{m=k-A(0)}^{k-1} d_2d_3\}.$$

$$S_9 = \sum_{m=1}^{k}(2pa_1a_3 + \frac{p}{2}e_0^2).$$

$$S_{10} = 2p\{\sum_{m=1}^{k-\frac{p}{2}-1} a_1a_4 + \sum_{m=k-\frac{p}{2}}^{k} a_1a_3\}.$$

$$S_{11} = 2p\{\sum_{m=1}^{\frac{p}{2}} a_1a_4 + \sum_{m=\frac{p}{2}+1}^{k-\frac{p}{2}-1} a_2a_4 + \sum_{m=k-\frac{p}{2}}^{k} a_2a_3\}.$$

The Szeged index of $HC_5C_7[r, p]$ nanotube is given as follows:

If $k \le A(-5)$, then: $SZ = S_0 + \sum_{m=1}^{k-1} pc_1c_3$.

If $A(-5) < k \le A(-3)$, then: $SZ = S_1 + S_0$.

If $A(-3) < k \le A(0)+1$, then: $SZ = S_9 + S_3 + S_1 + \sum_{m=1}^{k} \frac{p}{2} d_1d_3$.

If $A(0)+1 < k \le 2A(-5)$, then: $SZ = S_9 + S_7 + S_1 + S_3$.

If $2A(-5) < k \le A(3) + A(-3)$, then: $SZ = S_9 + S_7 + S_2 + S_3$.

If $A(3) + A(-3) < k \le 2A(0)+1$, then: $SZ = S_9 + S_7 + S_4 + S_2$.

If $2A(0)+1 < k \le \frac{p}{2}$, then: $SZ = S_9 + S_8 + S_2 + S_4$.

If $\frac{p}{2} < k \le \frac{p}{2} + A(-3)$, then: $SZ = S_{10} + S_8 + S_2 + S_5 + \sum_{m=1}^{k} e_0^2$.

If $\frac{p}{2} + A(-3) < k \le p$, then: $SZ = S_{10} + S_8 + S_2 + S_6 + \sum_{m=1}^{k} e_0^2$.

If $k > p$, then: $SZ = S_{11} + S_8 + S_2 + S_6 + \sum_{m=1}^{k} e_0^2$.

Therefore the Szeged index of above nanotube is computed.

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