Journal of Applied Sciences

ISSN 1812-5654

Journal of Applied Sciences 7 (23): 3606-3617, 2007
ISSN 1812-5654

Szeged Index of $HAC_5C_6C_7[k, p]$ Nanotube

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Abstract: A $C_5C_6C_7$ net is a trivalent decoration made by alternating C_5, C_6 and C_7. It can cover either a cylinder or a torus. In this study we compute the Szeged index of $HAC_5C_6C_7[k, p]$ nanotube.

Key words: Nanotube, molecular graph, szeged index

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 (Khadikar and Karmakar, 2002). Usage of topological indices in biology and chemistry began in 1947 when chemist Harold Wiener (Wiener, 1947) 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 (Agrawal *et al.*, 2000).

In a series of papers, the Wiener index of some nanotubes is computed (Deng, 2007; Diudea *et al.*, 2004; Randic, 2002; Stefu and Diudea, 2004; Yousefi and Ashrafi, 2006). Another topological index was introduced by Gutman and called the Szeged index, abbreviated as Sz (Gutman, 1994).

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 $Sz(G) = Sz = \Sigma_{e \in E(G)} n_1(e|G) n_2(e|G)$. 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 (Iranmanesh and Khormali, 2007a; Iranmanesh *et al.*, 2007) Szeged index and in (Ashrafi and Loghman, 2006; Deng, 2007; Iranmanesh and Ashrafi, 2007; Iranmanesh and Khormali, 2007b; Iranmanesh and Pakravesh, 2007; Iranmanesh and Solemani, 2007), another topological index of some nanotubes is computed. In this study, we computed the Szeged index of $HAC_5C_6C_7[k, p]$ nanotube. In Fig. 1, an $HAC_5C_6C_7[2, 2]$ lattice is shown.

We denote the number of pentagons in one row by p, the number of the periods by k and each period consist of three rows as in Fig. 2, which shows the m-th period, $1 \le m \le k$.

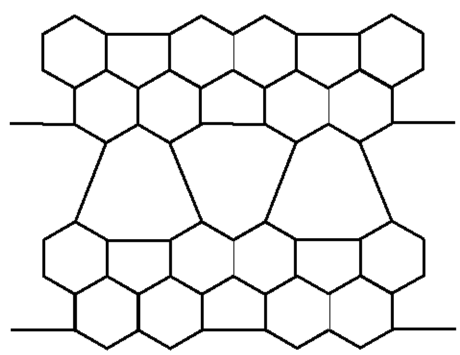

Fig. 1: $HAC_5C_6C_7[2, 2]$ nanotube, p = 2, k = 2

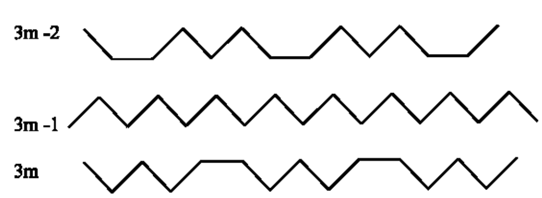

Fig. 2: m-th period of $HAC_5C_6C_7[k, p]$

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THE SZEGED INDEX OF $HAC_5C_6C_7[k, p]$ NANOTUBE

Let e be an edge in Fig. 1. Denote:

E_1 = {$e \in E(G)$| e is a vertical edge between hexagon and pentagon}
E_2 = {$e \in E(G)$| e is an oblique edge between pentagon and hexagon}
E_3 = {$e \in E(G)$| e is an oblique edge between heptagon and hexagon}
E_4 = {$e \in E(G)$| e is an oblique edge between heptagon and hexagon adjacent with pentagon}
E_5 = {$e \in E(G)$| e is an oblique edge between two heptagons}
E_6 = {$e \in E(G)$| e is a horizontal edge}
E_7 = {$e \in E(G)$| e is a vertical edge between two hexagons}
E_8 = {$e \in E(G)$| e is an oblique edge between two hexagons}.

And the number of vertices in each period of this nanotube is equal to 16p. In the hole of paper, the notation [f] is the greatest integer function. For computing the Szeged index, we must discus in two cases:

Case 1: p is even.

Let e = uv be an edge denoted in Fig. 3.

a) If $e \in E_1$, then according to Fig. 3, the region R has vertices belong to $N_1(e|G)$ and the region of R' has vertices belong 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). Then

$$n_e(v) = 16p(k-m) + \frac{19}{2}p - 14.$$

In this study for simplicity we define:

$$A(j) = \left[\frac{5p+j}{20}\right] \text{ and } B(j) = \left[\frac{3p+j}{12}\right]$$

Where:

$j = 0, \pm1, \pm2, \ldots$, also $C = \left[\frac{k-m}{2}\right]$, $D = \left[\frac{k-m+1}{2}\right]$ and $E = \left[\frac{m-1}{2}\right]$.

If $m \le A(-4)+1$ then $n_e(u) = 8pm - \frac{11}{2}p + 16m^2 - 19m + 11$.

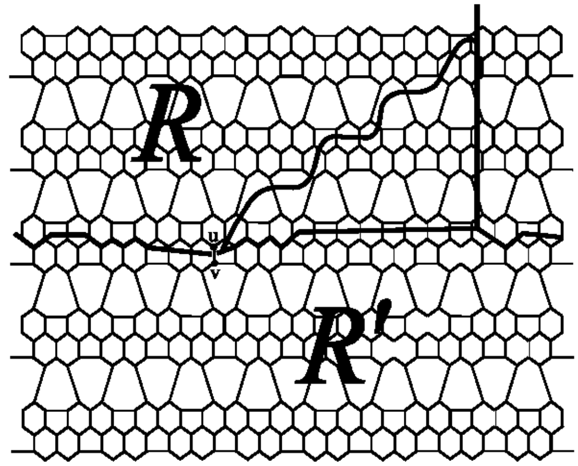

Fig. 3: e = uv belong to E_1

If m>A(-4)+1, then $n_e(u) = p(16m-11) + 25 + (7 + \frac{5}{2}p) \times A(-4) + 5(A(-4))^2 + (12 - \frac{21}{2}p) \times A(-4) + 5(A(-4))^2 + 16 \times B(-10) + 6(B(-10))^2$.

b) If $e \in E_2$, then according to Fig. 4, the region R has the vertices that belongs to $N_1(e|G)$ and the region of R' has vertices belong to $N_2(e|G)$. Then

- If $m \le A(-2)+1$ and $k-m \le p$, then $n_e(v) = k(8p+5) + m(18-16m) - 9 + (16(k-m)-10) \times C - 16 \times C^2$.
- If $m > A(-2)+1$ and $k-m \le p$, then $n_e(v) = (8p+5)(k-m) + \frac{27}{2}p - 16 + (\frac{5}{2}p - 6) \times A(-2) - 5(A(-2))^2 + (\frac{5}{2}p - 11) \times A(-12) - 5(A(-12))^2 + (3p-14) \times B(-8) - 6(B(-8))^2 + (16(k-m)-10) \times C - 16C^2$.
- If $m \le A(-2)+1$ and $k-m > p$, then $n_e(v) = 8p(2k - m - \frac{1}{2}p) - 16m^2 + 23m - 9$.
- If $m \le A(-2)+1$ and $k-m > p$, then $n_e(v) = 16p(k-m) - 4p^2 + \frac{27}{2}p - 16 + (\frac{5}{2}p - 6) \times A(-2) - 5(A(-2))^2 + (\frac{5}{2}p - 11) \times A(-12) - 5(A(-2))^2 + (3p-14) \times B(-8) - 6(B(-8))^2$.

And for $n_e(u)$ we have:

- If $m \le p$, then $n_e(u) = 4p(2m-1) + 9m - 3 + (16m-22) \times E - 16E^2$.
- If $m > p$, then $n_e(u) = 4p(2m+p-1) - 2m + 3$.

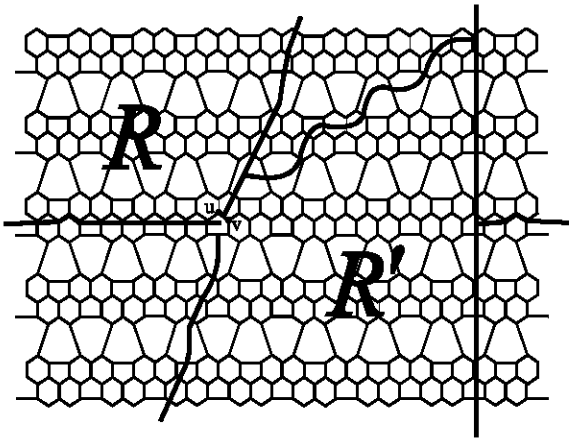

Fig. 4: e = uv belong to E_2

c) If $e \in E_3$, then according to Fig. 5, the region R has the vertices that belongs to $N_1(e|G)$ and the region of R' has vertices belong to $N_2(e|G)$.

In Fig. 5, 6 and 10 the symbol ∘ means that, the vertex that assigned with this symbol, have the same distance from u and v. Then

- If m≤p and k-m≤p, then $n_e(v) = 8pk + 3k - 16m + 9 + (16(k-m) - 6)\times C - 16C^2 + (26 - 16m)\times E + 16E^2$.
- If m>p and k-m≤p, then $n_e(v) = (8p+3)(k-m) + 4p^2 - 1 + (16(k-m) - 6)\times C - 16C^2$.
- If m≤p and k-m>p, then $n_e(v) = 8p(2k-m) - 4p^2 + 9 - 13m + (26 - 16m)\times E + 16E^2$.
- If m>p and k-m>p, then $n_e(v) = 16p(k-m) - 1$.

And for $n_e(u)$ we have:

- If m≤p and k-m≤p, then $n_e(u) = 8pk - 6k + 18m - 11 + (6 - 16(k-m))\times C + 16C^2 - 4D + (16m - 30)\times E - 16E^2$.
- If m>p and k-m≤p, then $n_e(u) = 8p(k+m) + 6(m-k) - 4p^2 - 3p + 3 + (6 - 16(k-m))\times C - 4D + 16C^2$.
- If m≤p and k-m>p, then $n_e(u) = 8pm + 4p^2 - 5p - 11 + 12m + (16m - 30)\times E - 16E^2$.
- If m>p and k-m>p, then $n_e(u) = 16pm - 8p + 3$.

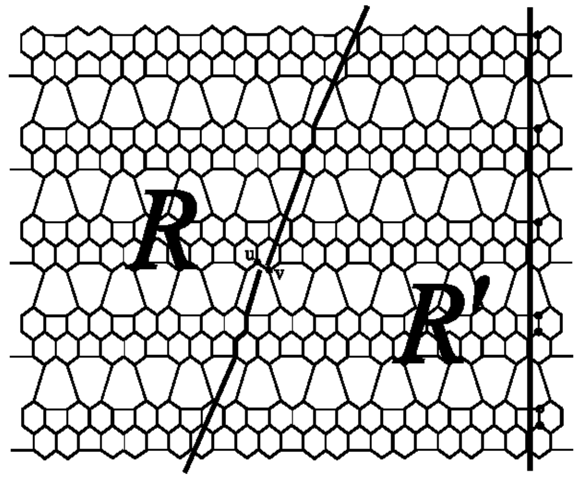

Fig. 5: e = uv belong to E_3

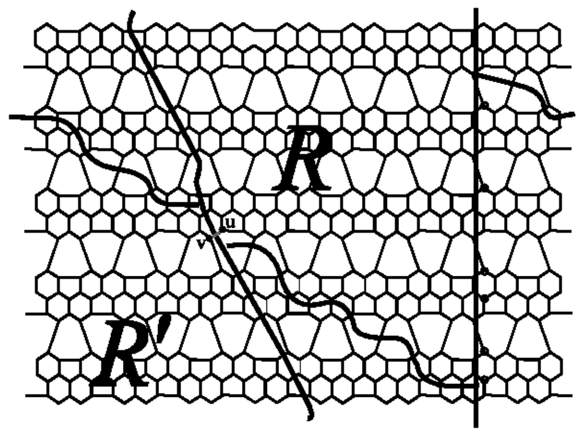

Fig. 6: e = uv belong to E_4

d) If $e \in E_4$, then according to Fig. 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:

- If m≤A(-10)+1 and k-m≤p, then $n_e(v) = 8k(p+1) - 16m^2 + m - 1 + (16(k-m) - 6)\times C - 16C^2$.
- If m≤A(-10)+1 and k-m>p, then $n_e(v) = 8p(2k-m) - 4p^2 + 5p + 9m - 16m^2 + 7$.
- If m>A(-10)+1 and k-m≤p, then $n_e(v) = (8p+8)(k-m) + 8p - 8 + (16(k-m) - 6)\times C - 16C^2 + (\frac{5}{2}p - 11)\times A(-10) - 5(A(-10))^2 + (\frac{5}{2}p - 5)\times A(0) - 5(A(0))^2 + (3p-7)\times B(-1) - 6(B(-1))^2$.
- If m>A(-10)+1 and k-m>p, then $n_e(v) = 16p(k-m) + 5p - 4p^2 + (\frac{5}{2}p - 11)A(-10) - 5(A(-10))^2 + (\frac{5}{2}p - 5)\times A(0) - 5(A(0))^2 + (3p-7)\times B(-1) - 6(B(-1))^2$.

For $n_e(u)$ we have:

- If k-m $\leq$A(0) and m$\leq$p, then
$$n_e(u) = 8k(p + 4m - 2k) - 16m^2 + 14m - 6k - 7 + (16m - 22)\times E - 16E^2.$$
- If m$\leq$p and k-m>A(0), then
$$n_e(u) = 8pm + 8m - 7 + (16m - 22)\times E - 16E^2 + (\frac{5}{2}p)\times A(10) - 5(A(10))^2 + (\frac{5}{2}p - 5)\times A(0) - 5(A(0))^2 + (3p - 1)\times B(5) - 6(B(5))^2.$$
- If m>p and k-m$\leq$A(0), then
$$n_e(u) = 8p(k + m) - 4p^2 - 3p + 6(m - k) - 16(m^2 + k^2) + 32km - 7.$$
- If m>p and k-m>A(0), then
$$n_e(u) = 16pm - 3p - 4p^2 - 1 + (\frac{5}{2}p)\times A(10) - 5(A(10))^2 + (\frac{5}{2}p - 5)\times A(0) - 5(A(0))^2 + (3p - 1)\times B(5) - 6(B(5))^2.$$

e) If e $\in E_5$, then according to Fig. 7, 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: $n_e(v)$ = 16p(k-m)-1

And for $n_e(u)$ we have:

- If m$\leq$A(4), then
$$n_e(u) = m(8p + 16m - 2).$$
- If m>A(4), then
$$n_e(u) = 24pm - 11p + 6 + (3 - 5p)\times A(4) + 5(A(4))^2 + (7 - 11p)\times A(-4) + 5(A(-4))^2 + 10\times B(-4) + 6(B(-4))^2.$$

f) If e $\in E_6$, then according to Fig. 8, 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:

- If m$\leq$p and k-m$\leq$p, then
$$n_e(v) = 8pk - 5k - 8m + 9 + (10 + 16(m - k))\times C + 16C^2 + (26 - 16m)\times E + 16E^2.$$
- If m>p and k-m$\leq$p, then
$$n_e(v) = (8p - 5)(k - m) + 4p^2 - 1 + (10 + 16(m - k))\times C + 16C^2.$$
- If m$\leq$p and k-m>p, then
$$n_e(v) = 8pm + 4p^2 + 9 - 13m + (26 - 16m)\times E + 16E^2.$$
- If m>p and k-m>p, then
$$n_e(v) = 8p^2 - 1. \text{ And } n_e(u) = n_e(v).$$

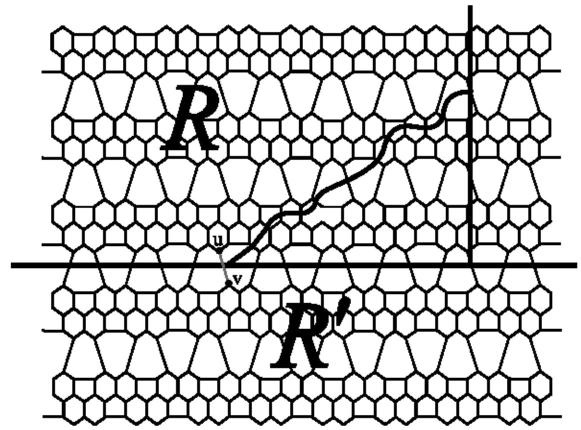

Fig. 7: e = uv belong to E_5

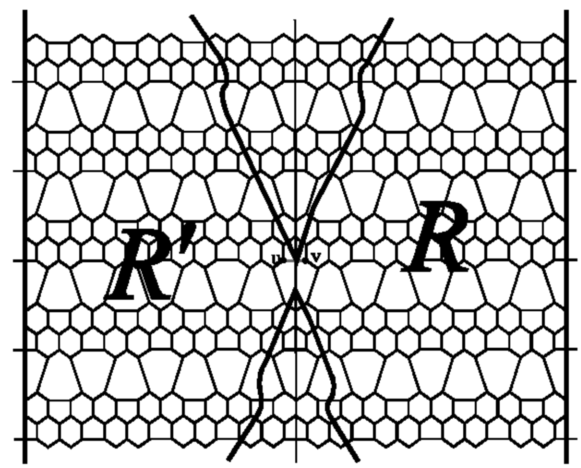

Fig. 8: e = uv belong to E_6

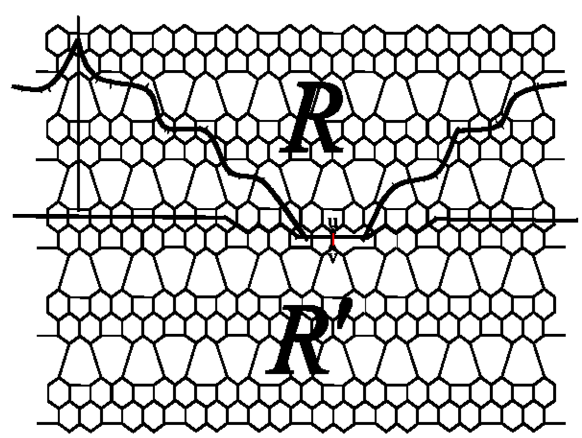

Fig. 9: e = uv belong to E_7

g) If e $\in E_7$, then according to Fig. 9, 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:

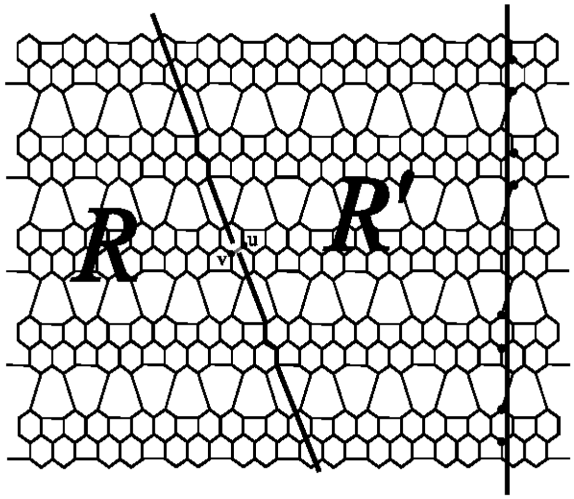

Fig. 10: e = uv belong to E_8

If p<3, then
$n_e(v) = 16p(k-m) + 5p - 1.$
And if $p \geq 3$, then
$n_e(v) = 16p(k-m) + 11p - 20.$

For $n_e(u)$ we have:

- If $m \leq A(-8)+1$, then
$n_e(u) = 32m^2 - 28m + 10.$
- If $m > A(-8)+1$, then
$n_e(u) = 16p(m-1) + (18-5p)\times A(-8) + 10(A(-8))^2 + (7-11p)\times A(4) + 10(A(4))^2 + 11\times B(1) + 12(B(1))^2.$

h) If $e \in E_8$, then according to Fig. 10, 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:

For $n_e(v)$ we have:

- If $m \leq p$ and $k\text{-}m \leq p$, then
$n_e(v) = 8pk + 6k - 18m + 11 + (16(k-m)-6)\times C - 16C^2 + (26-16m)\times E + 16E^2.$
- If m>p and $k\text{-}m \leq p$, then
$n_e(v) = (8p+6)(k-m) + 4p^2 + p + 1 + (16(k-m)-6)\times C - 16C^2.$
- If $m \leq p$ and k-m>p, then
$n_e(v) = 8p(2k-m) - 4p^2 + 3p + 11 - 12m + (26-16m)\times E + 16E^2.$
- If m>p and k-m>p, then
$n_e(v) = 16p(k-m) + 4p + 1.$

And for $n_e(u)$ we have:

- If m>p and $k\text{-}m \leq p$, then
$n_e(u) = 8pk - 6k + 18m - 13 + (4-16(k-m))\times C + 16C^2 - 6D + (16m-32)\times E - 16E^2.$
- If m>p and $k\text{-}m \leq p$, then
$n_e(u) = 8p(k+m) - 4p^2 - 4p + 3 + 6(m-k) + (4-16(k-m))\times C + 16C^2 - 6D.$
- If $m \leq p$ and k-m>p, then
$n_e(u) = 8pm + 4p^2 - 7p - 13 + 12m + (16m-32)\times E - 16E^2.$
- If m>p and k-m>p, then
$n_e(u) = 16pm - 11p + 3.$

For simplicity we define

In sub case a:

$$a_1 = 16p(k-m) + \frac{19}{2}p - 14.$$

$$a_2 = 8pm - \frac{11}{2}p + 16m^2 - 19m + 11.$$

$$a_3 = p(16m-11) + 25 + (7+\frac{5}{2}p)\times A(-4) + 5(A(-4))^2 + (12-\frac{21}{2}p)\times A(-14) + 5(A(-14))^2 + 16\times B(-10) + 6(B(-10))^2.$$

In sub case b:

$$b_0 = (\frac{5}{2}p-6)\times A(-2) - 5(A(-2))^2 + (\frac{5}{2}p-11)\times A(-12) - 5(A(-12))^2 + (3p-14)\times B(-8) - 6(B(-8))^2.$$

$$b'_0 = (16(k-m)-10)\times C - 16C^2.$$

$$b_1 = k(8p+5) + m(18-16m) - 9 + b'_0.$$

$$b_2 = (8p+5)(k-m) + \frac{27}{2}p - 16 + b_0 + b'_0.$$

$$b_3 = 8p(2k-m-\frac{1}{2}p) - 16m^2 + 23m - 9.$$

$$b_4 = 16p(k-m) - 4p^2 + \frac{27}{2}p - 16 + b_0.$$

$$b_5 = 4p(2m-1) + 9m - 3 + (16m-22)\times E - 16E^2.$$

$$b_6 = 4p(2m+p-1) - 2m + 3.$$

In sub case c:

$$c_0 = (16(k\text{-}m)\text{-}6)\times C\text{-}16C^2.$$

$$c'_0 = (26-16m)\times E+16E^2.$$

$$c_1 = 8pk+3k-16m+9+c_0+c'_0.$$

$$c_2 = (8p+3)(k-m)+4p^2-1+c_0.$$

$$c_3 = 8p(2k-m)-4p^2+9-13m+c'_0.$$

$$c_4 = 16p(k-m)-1.$$

$$c_5 = 8pk-6k+18m-11-c_0-4D+ (16m-30)\times E-16E^2.$$

$$c_6 = 8p(k+m)+6(m-k)-4p^2-3p+3-c_0-4D.$$

$$c_7 = 8pm+4p^2-5p-11+12m+(16m-30)\times E-16E^2.$$

$$c_8 = 16pm-8p+3.$$

In sub case d:

$$d_0 = (\frac{5}{2}p-11)\times A(-10)-5(A(-10))^2+(\frac{5}{2}p-5)\times A(0)-5(A(0))^2+(3p-7)\times B(-1)-6(B(-1))^2.$$

$$d'_0 = (\frac{5}{2}p)\times A(10)-5(A(10))^2+(\frac{5}{2}p-5)\times A(0)-5(A(0))^2+(3p-1)\times B(5)-6(B(5))^2.$$

$$d_1 = 8k(p+1)-16m^2+m-1+c_0.$$

$$d_2 = 8p(2k-m)-4p^2+5p+9m-16m^2+7.$$

$$d_3 = (8p+8)(k-m)+8p-8+c_0+d_0.$$

$$d_4 = 16p(k-m)+5p-4p^2+d_0.$$

$$d_5 = 8k(p+4m-2k)-16m^2+14m- 6k-7+(16m-22)\times E-16E^2.$$

$$d_6 = 8pm+8m-7+(16m-22)\times E-16E^2+d'_0.$$

$$d_7 = 8p(k+m)-4p^2-3p+6(m-k)- 16(m^2+k^2)+32km-7.$$

$$d_8 = 16pm-3p-4p^2-1+d'_0.$$

In sub case e:

$$e_0 = (3-5p)\times A(4)+5(A(4))^2+(7-11p)\times A(-4)+5(A(-4))^2+10\times B(-4)+6(B(-4))^2.$$

$$e_1 = 16p(k-m)-1.$$

$$e_2 = m(8p+16m-2).$$

$$e_3 = 24pm-11p+6+e_0.$$

In sub case f:

$$f_0 = (10+16(m-k))\times C+16C^2.$$

$$f_1 = 8pk-5k-8m+9+f_0+c'_0.$$

$$f_2 = (8p-5)(k-m)+4p^2-1+f_0.$$

$$f_3 = 8pm+4p^2+9-13m+c'_0.$$

$$f_4 = 8p^2-1.$$

In sub case g:

$$g_0 = (18-5p)\times A(-8)+10(A(-8))^2+(7-11p)\times A(4)+10(A(4))^2+11\times B(1)+12(B(1))^2.$$

$$g_1 = 16p(k-m)+11p-20.$$

$$g''_1 = 16p(k-m)+5p-1$$

$$g_2 = 32m^2-28m+10.$$

$$g_3 = 16p(m-1)+g_0.$$

In sub case h:

$$h_0 = (4-16(k-m))\times C+16C^2-6D.$$

$$h'_0 = (16m-32)\times E-16E^2.$$

$$h_1 = 8pk+6k-18m+11+c_0+c'_0.$$

$$h_2 = (8p+6)(k-m)+4p^2+p+1+c_0.$$

$$h_3 = 8p(2k-m)-4p^2+3p+11-12m+c'_0.$$

$$h_4 = 16p(k-m)+4p+1.$$

$$h_5 = 8pk-6k+18m-13+h_0+h'_0.$$

$h_6 = 8p(k+m) - 4p^2 - 4p + 3 + 6(m-k) + h_0.$

$h_7 = 8pm + 4p^2 - 7p - 13 + 12m + h'_0.$

$h_8 = 16pm - 11p + 3.$

Case 2: p is odd.

a) If $e \in E_2$, then $n_e(v) = 16p(k-m) + \frac{19}{2}p - \frac{25}{2}.$

If $m \le A(-4)+1$, then $n_e(u) = 8pm - \frac{11}{2}p + 16m^2 - 19m + \frac{23}{2}$

If $m > A(-4)+1$, then

$n_e(u) = p(8m - \frac{11}{2}) + \frac{17}{2} + (\frac{15}{2} - \frac{5}{2}p) \times A(-5) + 5(A(-5))^2$
$+(\frac{5}{2} - \frac{11}{2}p) \times A(5) + 5(A(5))^2 + 4 \times B(2) + 6(B(2))^2$

b) If $e \in E_2$, then

- If $m > A(-3)+1$ and $k-m \le p$, then $n_e(v) = k(8p+5) + m(18-16m) - 9 + (16(k-m)-10) \times C - 16C^2.$
- If $m > A(-3)+1$ and $k-m \le p$, then $n_e(v) = (8p+5)(k-m) + 8p - 2 + (\frac{5}{2}p - \frac{13}{2}) \times A(-3) - 5(A(-3))^2 + (\frac{5}{2}p - \frac{1}{2}) \times A(9) - 5(A(9))^2 + (3p-2) \times B(4) - 6(B(4))^2 + (16(k-m)-10) \times C - 16C^2.$
- If $m \le A(-2)+1$ and $k-m > p$, then $n_e(v) = 8p(2k-m-p+1) - 16m^2 + 23m - 12.$
- If $m > A(-2)+1$ and $k-m > p$, then $n_e(v) = 16p(k-m) - 4p^2 + 8p - 1 + (\frac{5}{2}p - \frac{13}{2}) \times A(-3) - 5(A(-3))^2 + (\frac{5}{2}p - \frac{1}{2}) \times A(9) - 5(A(9))^2 + (3p-2) \times B(4) - 6(B(4))^2.$

And for $n_e(u)$ we have:

- If $m \le p$, then $n_e(u) = 4p(2m-1) + 11m - 4 + (16m-22) \times E - 16E^2.$
- If $m > p$, then $n_e(u) = 4p(2m+p-1) + 3.$

c) If $e \in E_3$, then

- If $m \le p$ and $k-m \le p$, then $n_e(v) = 8pk + 3k - 16m + 9 + (16(k-m)-6) \times C - 16C^2 + (26-16m) \times E + 16E^2.$
- If $m > Ap$ and $k-m \le p$, then $n_e(v) = (8p+3)(k-m) + 4p^2 - 1 + (16(k-m)-6) \times C - 16C^2.$
- If $m \le p$ and $k-m > p$, then $n_e(v) = 8p(2k-m) - 4p^2 + 2 - 13m + (26-16m) \times E + 16E^2.$
- If $m > p$ and $k-m > p$, then $n_e(v) = 16p(k-m) - 1.$

And for $n_e(u)$ we have:

- If $m \le p$ and $k-m \le p$, then $n_e(u) = 8pk - 3k + 16m - 11 + (6-16(k-m)) \times C + 16C^2 - 4D + (16m-30) \times E - 16E^2.$
- If $m > p$ and $k-m \le p$, then $n_e(u) = 8p(k+m) + 3(m-k) - 4p^2 - 2p + 1 + (6-16(k-m)) \times C - 4D + 16C^2.$
- If $m \le p$ and $k-m > p$, then $n_e(u) = 8pm + 4p^2 - 3p - 5 + 13m + (16m-30) \times E - 16E^2.$
- If $m > p$ and $k-m > p$, then $n_e(u) = 16pm - 5p$

d) If $e \in E_4$, then

- If $m \le A(-11)+1$ and $k-m \le p$, then $n_e(v) = 8k(p+1) - 16m^2 + 2m - 1 + (16(k-m)-6) \times C - 16C^2.$
- If $m \le p$ and $k-m > A(-1)$, then $n_e(v) = 8p(2k-m) - 4p^2 + 5p + 10m - 16m^2 + 6.$
- If $m > A(-11)+1$ and $k-m \le p$, then $n_e(v) = (8p+8)(k-m) + 8p - 7 + (16(k-m) - 6) \times C - 16C^2 + (\frac{5}{2}p - \frac{21}{2}) \times A(-11) - 5(A(-11))^2 + (\frac{5}{2}p - \frac{9}{2}) \times A(1) - 5(A(1))^2 + (3p-7) \times B(-1) - 6(B(-1))^2.$
- If $m > A(-11)+1$ and $k-m > p$, then $n_e(v) = 8p(k-m) + 13p - 4p^2 - 8 + (\frac{5}{2}p - \frac{21}{2}) \times A(-11) - 5(A(-11))^2 + (\frac{5}{2}p - \frac{9}{2}) \times A(1) - 5(A(1))^2 + (3p-7) \times B(-1) - 6(B(-1))^2.$

For $n_e(u)$ we have:

- If $k-m \le A(-1)$ and $m \le p$, then $n_e(u) = 8k(p+4m-2k) - 16m^2 + 14m - 6k - 7 + (16m-22) \times E - 16E^2.$

- If m≤p and k-m>A(-1), then
$$n_e(u)=8pm+8m-7+(16m-22)\times E-16E^2+(\frac{5}{2}p-\frac{11}{2})\times A(-1)-5(A(-1))^2+(\frac{5}{2}p+\frac{1}{2})\times A(11)-5(A(11))^2+(3p-1)\times B(5)-6(B(5))^2.$$
- If m>p and k-m≤A(-1), then
$$n_e(u)=8p(k+m)-4p^2-3p+6(m-k)-16(m^2+k^2)+32km.$$
- If m>p and k-m>A(-1), then
$$n_e(u)=16pm-3p-4p^2-1+(\frac{5}{2}p-\frac{11}{2})\times A(-1)-5(A(-1))^2+(\frac{5}{2}p+\frac{1}{2})\times A(11)-5(A(11))^2+(3p-1)\times B(5)-6(B(5))^2.$$

e) If $e\in E_5$, then $n_e(v)$ = 16p(k-m). And for $n_e(u)$ we have:

- If m≤A(5), then $n_e(u)=m(8p+16m-2)$.
- If m>A(5), then
$$n_e(u)=24pm-11p+6+(3-5p)\times A(5)+5(A(5))^2+(7-11p)\times A(-5)+5(A(-5))^2+10\times B(-4)+6(B(-4))^2.$$

f) If $e\in E_6$, then

- If m≤p and k-m≤p, then
$$n_e(v)=8pk-5k-8m+9+(10+16(m-k))\times C+16C^2+(26-16m)\times E+16E^2.$$
- If m>p and k-m≤p, then
$$n_e(v)=(8p-5)(k-m)+4p^2+(10+16(m-k))\times C+16C^2.$$
- If m≤p and k-m>p, then
$$n_e(v)=8pm+4p^2+8p-13m+(26-16m)\times E+16E^2.$$
- If m>p and k-m>p, then $n_e(v)$ = $8p^2$-1. And $n_e(u)=n_e(v)$.

g) If $e\in E_7$, then $n_e(v)$ = 16p(k-m)+11p-20.

For $n_e(u)$ we have:

- If m≤A(-7)+1, then
$$n_e(u)=32m^2-28m+10.$$
- If m>A(-7)+1, then
$$n_e(u)=16p(m-1)+14+(18-5p)\times A(-7)+10(A(-7))^2+(7-11p)\times A(5)+10(A(5))^2+11\times B(1)+12(B(1))^2.$$

h) If $e\in E_8$, then

For $n_e(v)$ we have:
- If m≤p and k-m≤p, then
$$n_e(v)=8pk+5k-15m+9+(16(k-m)-4)\times C-16C^2+(26-16m)\times E+16E^2.$$
- If m>p and k-m≤p, then
$$n_e(v)=(8p+5)(k-m)+4p^2+3p+1+(16(k-m)-4)\times C-16C^2.$$
- If m≤p and k-m>p, then
$$n_e(v)=8p(2k-m)-4p^2+3p+8-10m+(26-16m)\times E+16E^2.$$
- If m>p and k-m>p, then
$$n_e(v)=16p(k-m)+6p-1.$$

And for $n_e(u)$ we have:

- If m≤p and k-m≤p, then
$$n_e(u)=8pk-5k+13m-11+(4-16(k-m))\times C+16C^2-4D+(16m-30)\times E-16E^2.$$
- If m>p and k-m≤p, then
$$n_e(u)=8p(k+m)-4p^2-7p-1+5(m-k)+(4-16(k-m))\times C+16C^2-4D.$$
- If m≤p and k-m>p, then
$$n_e(u)=8pm+4p^2-5p-12+8m+(16m-30)\times E-16E^2.$$
- If m>p and k-m>p, then $n_e(u)$ = 16pm-12p-1

For simplicity we define:

In sub case a:

$$a'_1=16p(k-m)+\frac{19}{2}p-\frac{25}{2}.$$

$$a'_2=8pm-\frac{11}{2}p+16m^2-19m+\frac{23}{2}.$$

$$a'_3=p(8m-\frac{11}{2})+\frac{17}{2}+(\frac{15}{2}-\frac{5}{2}p)\times A(-5)+5(A(-5))^2+(\frac{5}{2}-\frac{11}{2}p)\times A(5)+5(A(5))^2+4\times B(2)+6(B(2))^2.$$

In sub case b:

$$b''_0=(\frac{5}{2}p-\frac{13}{2})\times A(-3)-5(A(-3))^2+(\frac{5}{2}p-\frac{1}{2})\times A(9)-5(A(9))^2+(3p-2)\times B(4)-6(B(4))^2.$$

$b'_1 = k(8p+5) + m(18-16m) - 9 + b'_0.$

$b'_2 = (8p+5)(k-m) + 8p - 2 + b''_0 + b'_0.$

$b'_3 = 8p(2k-m-p+1) - 16m^2 + 23m - 12.$

$b'_4 = 16p(k-m) - 4p^2 + 8p - 1 + b''_0.$

$b'_5 = 4p(2m-1) + 11m - 4 + (16m-22)\times E - 16E^2.$

$b'_6 = 4p(2m+p-1) + 3.$

In sub case c:

$c'_1 = 8pk + 3k - 16m + 9 + c_0 + c'_0.$

$c'_2 = (8p+3)(k-m) + 4p^2 - 1 + c_0.$

$c'_3 = 8p(2k-m) - 4p^2 + 2 - 13m + c'_0.$

$c'_4 = 16p(k-m) - 1.$

$c'_5 = 8pk - 3k + 16m - 11 - c_0 - 4D + (16m-30)\times E - 16E^2.$

$c'_6 = 8p(k+m) + 3(m-k) - 4p^2 - 2p + 1 - c_0 - 4D.$

$c'_7 = 8pm + 4p^2 - 3p - 5 + 13m + (16m-30)\times E - 16E^2.$

$c'_8 = 16pm - 5p.$

In sub case d:

$$d''_0 = (\frac{5}{2}p - \frac{21}{2})\times A(-11) - 5(A(-11))^2 + (\frac{5}{2}p - \frac{9}{2})\times A(1) - 5(A(1))^2 + (3p-7)\times B(-1) - 6(B(-1))^2.$$

$$d'''_0 = (\frac{5}{2}p - \frac{11}{2})\times A(-1) - 5(A(-1))^2 + (\frac{5}{2}p + \frac{1}{2})\times A(11) - 5(A(11))^2 + (3p-1)\times B(5) - 6(B(5))^2.$$

$d'_1 = 8k(p+1) - 16m^2 + 2m - 1 + c_0.$

$d'_2 = 8p(2k-m) - 4p^2 + 5p + 10m - 16m^2 + 6.$

$d'_3 = (8p+8)(k-m) + 8p - 7 + c_0 + d''_0.$

$d'_4 = 8p(k-m) + 13p - 4p^2 - 8 + d''_0.$

$d'_5 = 8k(p+4m-2k) - 16m^2 + 14m - 6k - 7 + (16m-22)\times E - 16E^2.$

$d'_6 = 8pm + 8m - 7 + (16m-22)\times E - 16E^2 + d'''_0.$

$d'_7 = 8p(k+m) - 4p^2 - 3p + 6(m-k) - 16(m^2+k^2) + 32km.$

$d'_8 = 16pm - 3p - 4p^2 - 1 + d'''_0.$

In sub case e:

$e'_1 = 16p(k-m).$

$e'_2 = m(8p + 16m - 2).$

$e'_3 = 24pm - 11p + 6 + (3-5p)\times A(5) + 5(A(5))^2 + (7-11p)\times A(-5) + 5(A(-5))^2 + 10\times B(-4) + 6(B(-4))^2.$

In sub case f:

$f'_1 = 8pk - 5k - 8m + 9 + f_0 + c'_0.$

$f'_2 = (8p-5)(k-m) + 4p^2 + f_0.$

$f'_3 = 8pm + 4p^2 + 8p - 13m + c'_0.$

$f'_4 = 8p^2 - 1.$

In sub case g:

$g'_1 = 16p(k-m) + 11p - 20.$

$g'_2 = 32m^2 - 28m + 10.$

$g'_3 = 16p(m-1) + 14 + (18-5p)\times A(-7) + 10(A(-7))^2 + (7-11p)\times A(5) + 10(A(5))^2 + 11\times B(1) + 12(B(1))^2.$

In sub case h:

$h''_0 = (16(k-m) - 4)\times C - 16C^2.$

$h'''_0 = (16m-30)\times E - 16E^2.$

$h'_1 = 8pk + 5k - 15m + 9 + h''_0 + c'_0.$

$h'_2 = (8p+5)(k-m) + 4p^2 + 3p + 1 + h''_0.$

$h'_3 = 8p(2k-m) - 4p^2 + 3p + 8 - 10m + c'_0.$

$h'_4 = 16p(k-m) + 6p - 1.$

$h'_5 = 8pk - 5k + 13m - 11 + h_0 + h''''_0.$

$h'_6 = 8p(k+m) - 4p^2 - 7p - 1 + 5(m-k) + h_0.$

$h'_7 = 8pm + 4p^2 - 5p - 12 + 8m + h'''_0.$

$h'_8 = 16pm - 12p - 1.$

$S_1 = 4p(a_1a_2 + b_1b_5 + c_1c_5 + d_1d_5) + 2p(f_1^2 + g_1g_2).$

$S_2 = 2p\{\sum_{m=1}^{A(4)}(e_1e_2) + \sum_{m=A(4)+1}^{k-1}(e_1e_3)\}.$

$S_3 = 4p(b_1b_5 + c_1c_5) + 2p(h_1h_5 + f_1^2 + g_1g_2).$

$S_4 = 4p(b_2b_5 + c_1c_5 + d_3d_5) + 2p(h_1h_5 + f_1^2 + g_1g_3).$

$S_5 = 4p(b_3b_5 + c_3c_7 + d_2d_6) + 2p(h_3h_7 + f_3^2).$

$S_6 = 4p(b_2b_6 + c_2c_6 + d_3d_7) + 2p(h_2h_6 + f_2^2).$

$S_7 = 4p(b_2b_6 + c_2c_6 + d_3d_8).$

$S_8 = 2p\{\sum_{m=1}^{A(-8)+1}(g_1g_2) + \sum_{m=A(-8)+2}^{k}(g_1g_3)\}.$

$S_9 = 4pc_3c_7 + 2p(h_3h_7 + f_3^2).$

$S_{10} = 4pc_2c_6 + 2p(h_2h_6 + f_2^2).$

$S_{11} = 4pc_1c_5 + 2p(h_1h_5 + f_1^2).$

$S_{12} = 4pc_4c_8 + 2p(h_4h_8 + f_4^2).$

$$S_{13} = 4p\{\sum_{m=A(-2)+2}^{k-p-1}(d_4d_6) + \sum_{m=1}^{A(-2)+1}(d_2d_6) + \sum_{m=p+1}^{k-A(-2)-1}(d_3d_8) + \sum_{m=k-A(-2)}^{k}(d_3d_7)\}.$$

$$S_{14} = 4p\{\sum_{m=A(-2)+2}^{p}(b_2b_5) + \sum_{m=k-p}^{A(-2)+1}(d_1d_6 + b_1b_5) + \sum_{m=A(-2)+2}^{k-A(-2)-1}(d_3d_6) + \sum_{m=k-A(-2)}^{p}(d_3d_5)\}.$$

$$S_{15} = 4p\{\sum_{m=A(-2)+2}^{k-A(-2)-1}(d_3d_8) + \sum_{m=k-A(-2)}^{k}(d_3d_7)\}.$$

$S'_1 = 4p(a'_1a'_2 + b'_1b'_5 + c'_1c'_5 + d'_1d'_5) + 2p(f_1'^2 + g'_1g'_2).$

$S'_2 = 2p\{\sum_{m=1}^{A(5)}(e'_1e'_2) + \sum_{m=A(5)+1}^{k}(e'_1e'_3)\}.$

$S'_3 = 4p(b'_1b'_5 + c'_1c'_5) + 2p(h'_1h'_5 + f_1'^2 + g'_1g'_2).$

$S'_4 = 4p(b'_2b'_5 + c'_1c'_5 + d'_3d'_5) + 2p(h'_1h'_5 + f_1'^2 + g'_1g'_3).$

$S'_5 = 4p(b'_3b'_5 + c'_3c'_7 + d'_2d'_6) + 2p(h'_3h'_7 + f_3'^2).$

$S'_6 = 4p(b'_2b'_6 + c'_2c'_6 + d'_3d'_7) + 2p(h'_2h'_6 + f_2'^2).$

$S'_7 = 4p(b'_2b'_6 + c'_2c'_6 + d'_3d'_8).$

$S'_8 = 2p\{\sum_{m=1}^{A(-7)+1}(g'_1g'_2) + \sum_{m=A(-7)+2}^{k}(g'_1g'_3)\}.$

$S'_9 = 4pc'_3c'_7 + 2p(h'_3h'_7 + f_3'^2).$

$S'_{10} = 4pc'_2c'_6 + 2p(h'_2h'_6 + f_2'^2).$

$S'_{11} = 4pc'_1c'_5 + 2p(h'_1h'_5 + f_1'^2).$

$S'_{12} = 4pc'_4c'_8 + 2p(h'_4h'_8 + f_4'^2).$

$$S'_{13} = 4p\{\sum_{m=A(-1)+2}^{k-p-1}(d'_4d'_6) + \sum_{m=1}^{A(-1)+1}(d'_2d'_6) + \sum_{m=p+1}^{k-A(-1)-1}(d'_3d'_8) + \sum_{m=k-A(-1)}^{k}(d'_3d'_7)\}.$$

$$S'_{14} = 4p\{\sum_{m=A(-1)+2}^{p}(b'_2b'_5) + \sum_{m=k-p}^{A(-1)+1}(d'_1d'_6 + b'_1b'_5) + \sum_{m=A(-1)+2}^{k-A(-1)-1}(d'_3d'_6) + \sum_{m=k-A(-1)}^{p}(d'_3d'_5)\}.$$

$$S'_{15} = 4p\{\sum_{m=A(-1)+2}^{k-A(-1)-1}(d'_3d'_8) + \sum_{m=k-A(-1)}^{k}(d'_3d'_7)\}.$$

In the following formula:

$$SZ = \sum_{m=1}^{p}S_9 + \sum_{m=p+1}^{k-p-1}S_{12} + \sum_{m=k-p}^{k}(S_{10} - 2pf_2^2) + \sum_{m=k-p}^{p}(4pd_3d_6 + 2pf_2^2) + S_2 + S_{13} + S_8$$

if we substitute g''_1 to g_1 then we obtain the Szeged index of $HAC_5C_6C_7[k, p]$ nanotube for $p = 2$ and $k>4$. In fact, $Sz = 2048k^3 + 45080k^2 - 46136k - 57776$.

The Szeged index of $HAC_5C_6C_7[k, p]$ nanotube for $p \geq 3$ is given as follows:

a) p is even.

If $k \le A(4)$, then

$$SZ = \sum_{m=1}^{k} S_1 + \sum_{m=1}^{k-1} 2pe_1e_2.$$

If $A(4) < k \le A(-2)+1$, then

$$SZ = \sum_{m=1}^{k} (S_1) + S_2.$$

If $A(-2)+1 < k \le 2(A(-2)+1)$, then

$$SZ = \sum_{m=1}^{A(-2)+1} S_3 + \sum_{m=A(-2)+2}^{k} S_4 + 4p\{\sum_{m=1}^{k-A(-2)-1} (d_1d_6) + \sum_{m=k-A(-2)}^{A(-2)+1} (d_1d_5)\} + S_2.$$

If $2(A(-2)+1) < k \le p$, then

$$SZ = \sum_{m=1}^{A(-2)+1} (S_3 + 4pd_1d_6) + \sum_{m=A(-2)+2}^{k} (S_4 - 4pd_3d_5) + S_{15} + S_2.$$

If $k = p+1$, then

$$SZ = \sum_{m=1}^{A(-2)+1} (S_3 + 4pd_1d_6) + \sum_{m=A(-2)+2}^{p} (S_4 - 4pd_3d_5 - 2pg_1g_3) + \sum_{m=A(-2)+2}^{p+1} (2pg_1g_3) + S_{15} + S_2 + S_7.$$

If $p+1 < k \le p+A(-2)+1$, then

$$SZ = \sum_{m=1}^{k-p-1} S_5 + \sum_{m=p+1}^{k} S_6 + \sum_{m=k-p}^{p} S_{11} + S_{14} + S_2 + S_8.$$

If $p+A(-2)+1 < k \le 2p$, then

$$SZ = \sum_{m=1}^{k-p-1} S_9 + \sum_{m=p+1}^{k} S_{10} + \sum_{m=k-p}^{p} (S_{11} + d_3d_6) + S_{13} + S_2 + S_8.$$

If $k > 2p$, then

$$SZ = \sum_{m=1}^{p} S_9 + \sum_{m=p+1}^{k-p-1} S_{12} + \sum_{m=k-p}^{k} (S_{10} - 2pf_2^{\,2}) + \sum_{m=k-p}^{p} (4pd_3d_6 + 2pf_2^{\,2}) + S_2 + S_{13} + S_8.$$

b) p is odd.

If $k \le A(5)$, then

$$SZ = \sum_{m=1}^{k} S_1' + \sum_{m=1}^{k-1} e_1'e_2'.$$

If $A(5) < k \le A(-1)+1$, then

$$SZ = \sum_{m=1}^{k} (S_1') + S_2'.$$

If $A(-1)+1 < k \le 2(A(-1)+1)$, then

$$SZ = \sum_{m=1}^{A(-1)+1} S_3' + \sum_{m=A(-1)+2}^{k} S_4' + 4p\{\sum_{m=1}^{k-A(-1)-1} (d_1'd_6') + \sum_{m=k-A(-1)}^{A(-1)+1} (d_1'd_5')\} + S_2'.$$

If $2(A(-1)+1) < k \le p$, then

$$SZ = \sum_{m=1}^{A(-1)+1} (S_3' + 4pd_1'd_6') + \sum_{m=A(-1)+2}^{k} (S_4' - 4pd_3'd_5') + S_{15}' + S_2'.$$

If $k = p+1$, then

$$SZ = \sum_{m=1}^{A(-1)+1} (S_3' + 4pd_1'd_6') + \sum_{m=A(-1)+2}^{p} (S_4' - 4pd_3'd_5' - 2pg_1'g_3') + \sum_{m=A(-1)+2}^{p+1} (2pg_1'g_3') + S_{15}' + S_2' + S_7'.$$

If $p+1 < k \le p+A(-1)+1$, then

$$SZ = \sum_{m=1}^{k-p-1} S_5' + \sum_{m=p+1}^{k} S_6' + \sum_{m=k-p}^{p} S_{11}' + S_{14}' + S_2' + S_8'.$$

If $p+A(-1)+1 < k \le 2p$, then

$$SZ = \sum_{m=1}^{k-p-1} S_9' + \sum_{m=p+1}^{k} S_{10}' + \sum_{m=k-p}^{p} (S_{11}' + d_3'd_6') + S_{13}' + S_2' + S_8'.$$

If $k > 2p$, then

$$SZ = \sum_{m=1}^{p} S_9' + \sum_{m=p+1}^{k-p-1} S_{12}' + \sum_{m=k-p}^{k} (S_{10}' - 2pf_2'^{\,2}) + \sum_{m=k-p}^{p} (4pd_3'd_6' + 2pf_2'^{\,2}) + S_2' + S_{13}' + S_8'.$$

Therefore the Szeged index of above nanotube is computed.

ACKNOWLEDGMENT

This research is partially supported by Iran National Science Foundation (INSF) (Grant No. 83120).

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