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The computation of total Szeged index of $TUC_4C_8(R)$ nanotube

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The total version of Szeged index was introduced very recently in 2010. In this paper, at first we compute the total Szeged index for hexagonal chains. Finally, the total Szeged index of $TUC_4C_8(R)$ nanotubes is computed.

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1. Introduction

Let G be a simple molecular graph without directed and multiple edges and without loops. The graph G consists of the set of vertices $V(G)$ and the set of edges $E(G)$. In molecular graph, each vertex represented an atom of the molecule and bonds between atoms are represented by edges between corresponding vertices. The first topological index was Wiener index which is

$$W(G) = W_v(G) = \sum_{\{x,y\}\subseteq V(G)} d(x,y) \qquad (1)$$

where $d(x,y)$ is the distance between to vertices x and y [1]. Numerous articles were published in the chemical and mathematical literature, devoted to the Wiener index and various methods for its calculation [2-5].

Another topological index was introduced by Gutman and called the Szeged index, abbreviated as Sz [6]. The Szeged index is a modification of Wiener index to cyclic molecules. This was the vertex version of Sz index which had been defined as

$$Sz_v(G) = \sum_{e=uv\in E(G)} n_e(u).n_e(v) \qquad (2)$$

where $n_e(u)$ is the number of vertices of G which are closer to u than to v and $n_e(v)$ is the number of vertices of G which are closer to v than to u. In [7-9], you can find computations of this index for some graphs.

The edge version of Szeged index introduced by Gutman and Ashrafi [10] that it is defined as

$$Sz_e(G) = \sum_{e=uv\in E(G)} m_e(u).m_e(v) \qquad (3)$$

where $m_e(u)$ is the number of edges of G which are closer to u than to v and $m_e(v)$ is the number of edges of G which are closer to v than to u. In [11-13], you can find computations of this index for some graphs.

The total version of Szeged index was introduced very recently in [14] and it is

$$Sz_T(G) = \sum_{e=uv\in E(G)} t_e(u).t_e(v) \qquad (4)$$

where $t_e(u)$ is the number of vertices and edges of G which are closer to u than to v and $t_e(v)$ is the number of vertices and edges of G which are closer to v than to u. Also $t_e(u) = n_e(u) + m_e(u)$ and $t_e(v) = n_e(v) + m_e(v)$.

In the rest of this paper, we compute the total Szeged index for hexagonal chains and $TUC_4C_8(R)$ nanotubes.

2. Discussion and results

Now, according to the definition of total Szeged index, we are ready to compute it for hexagonal chains L_h and H_h with h hexagons. A hexagonal chain G with h rings has $|V(G)| = n = 4h+2$ vertices and $|E(G)| = m = 5h+1$ edges. In Fig. 1, the hexagonal chains L_6 and H_h are depicted.

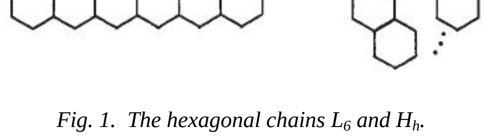

Fig. 1. The hexagonal chains L_6 and H_h.

Theorem 2-1. The total Szeged index of linear hexagonal chain with h hexagon, L_h, is

$$Sz_T(L_h) = 2h(27h^2 + 90h + 23) + (h+1)(4h+1)^2$$

Proof. According to the Fig. 1, there are two types of edges, vertical and oblique edges. We consider these edges separately.

If $e = uv$ is a vertical edge, then we have

$$t_e(u) = n_e(u) + m_e(u) = 2\mathrm{h} + (2\mathrm{h}+1) = 4\mathrm{h}+1$$
$$t_e(v) = n_e(v) + m_e(v) = 2\mathrm{h} + (2\mathrm{h}+1) = 4\mathrm{h}+1$$

Therefore $t_e(u) \times t_e(v) = (4\mathrm{h}+1)^2$.

If $e = uv$ is an oblique edge, then we have

$$t_e(u) = n_e(u) + m_e(u) = (4\mathrm{i}+3) + (5i+2) = 9i+5$$
$$t_e(v) = n_e(v) + m_e(v) = (5h - 5i + 2) + (4h - 4i + 3)$$
$$= 9h - 9i + 5$$

Therefore $t_e(u) \times t_e(v) = (9h - 9i + 5).(9i+5)$

Then,

$$Sz_T(L_h) = \sum_{i=0}^{h} 4(9h - 9i + 5).(9i+5) + (h+1)(4h+1)^2$$
$$= 2h(27h^2 + 90h + 23) + (h+1)(4h+1)^2.$$

Before computing the total Szeged index of hexagonal chain helicene H_h, $h \geq 3$, we introduce the set A which we use it for computation.

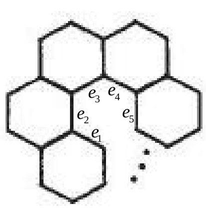

Fig. 2. The hexagonal chain helicene H_h.

The set A is the edges of e_i and the edges which are parallel with e_i in the Fig. 2 and $3 \leq i \leq h$.

Theorem 2-2. The total Szeged index of helicene H_h with h hexagon is

$$Sz_T(L_h) = h(27h^2 + 90h + 23) + (81h - 81)(5h - 3)$$

Proof. According to the Fig. 1, we consider two types of edges, edges of set A and other edges. We consider these edges separately.

If $e = uv$ is an edges of set A, then we have

$$t_e(u) = n_e(u) + m_e(u) = (4\mathrm{i}+3) + (5i+2) = 9i+5$$
$$t_e(v) = n_e(v) + m_e(v) = (5h - 5i + 2) + (4h - 4i + 3)$$
$$= 9h - 9i + 5$$

Therefore $t_e(u) \times t_e(v) = (9h - 9i + 5).(9i+5)$

If $uv = e$ is an edge which is not in set A, then we have

$$t_e(u) = n_e(u) + m_e(u) = 5 + 4 = 9$$
$$t_e(v) = n_e(v) + m_e(v) = (4\mathrm{h}\text{-}3) + (5h - 6) = 9h - 9$$

Therefore $t_e(u) \times t_e(v) = 81h - 81$.

Then,

$$Sz_T(H_h) = \sum_{i=0}^{h} 2(9h - 9i + 5).(9i+5) + (81h - 81)(5h - 3)$$
$$= h(27h^2 + 90h + 23) + (81h - 81)(5h - 3).$$

Now, we compute the total Szeged index of $TUC_4C_8(R)$ nanotubes. In Fig. 3, the $TUC_4C_8(R)$ nanotube is shown.

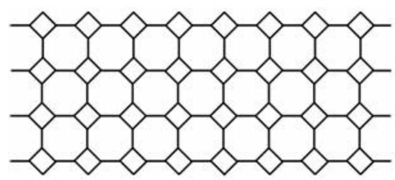

Fig. 3. Two dimensional lattice of $TUC_4C_8(R)$ nanotube, $k = 4, p = 8$.

According to Fig. 3, k is the number of rows of rhombus and p is the number of rhombus in a row (that p indicates the number of columns of rhombus in Figure 3). Therefore, we indicate the rhombus which located in $i-th\ row\ and\ j-th\ column$ with S_{ij}. Also, we have $|V(G)| = 4pk$. We show the molecular graph of $TUC_4C_8(R)$ nanotube with G in following computation.

Lemma 2-3. Let $uv = e \in E(G)$ be the vertical edge of G between rows i and $i+1$, $1 \leq i \leq k-1$. Then we have:

$$t_e(u) = 10pi - p$$

and

$$t_e(v) = 10p(k-i) - p.$$

Proof. According to the Fig. 3, we have

$$t_e(u) = n_e(u) + m_e(u) = 4pi + (5pi + p(i-1))$$
$$= 10pi - p$$

and

$$t_e(v) = n_e(v) + m_e(v) = 4p(k-i) + (5p(k-i) + p(k-i-1))$$
$$= 10p(k-i) - p$$

Lemma 2-4. Let $uv = e \in E(G)$ be the horizontal edge of G in row i, $1 \le i \le k$. Then we have:

If p is even:

$$t_e(u) = t_e(v) = 5pk - \frac{p}{2} - k$$

If p is odd:

$$t_e(u) = t_e(v) = 5pk - \frac{p+1}{2} - 2k$$

Proof. Let $uv = e \in E(G)$ be the horizontal edge of G in row i, $1 \le i \le k$. According to the Fig. 3, we have

If p is even:

The number of edges and vertices which are in the equidistance with edge e if $2k$. Therefore according to $|E(G)| = 10pk - p$, we have

$$t_e(u) = t_e(v) = \frac{|E(G)| - 2k}{2} = 5pk - k - \frac{p}{2}$$

If p is odd:

The number of edges and vertices which are in the equidistance with edge e if $4k - 1$. Therefore according to $|E(G)| = 10pk - p$, we have

$$t_e(u) = t_e(v) = \frac{|E(G)| - 4k + 1}{2} = 5pk - k - \frac{p+1}{2} \quad .$$

Lemma 2-5. Let $uv = e \in E(G)$ be the oblique edge of G in row m, $1 \le m \le k$. Then we have:

If p is even:

$$t_e(u) = \begin{cases} 10km - \frac{p}{2} - 9k + 5kp - 5k^2 & , m \le \frac{p}{2} + 1 \ \& \ q - m \le \frac{p}{2} \\ 5mp + 5m^2 - 9m + 5\frac{p^2}{4} - 5p & , m \le \frac{p}{2} + 1 \ \& \ q - m > \frac{p}{2} \\ 10km - 5k^2 + 5pk - 9k - 5m^2 + 5mp + 7m - 5\frac{p^2}{4} + 4p - 2 & , m > \frac{p}{2} + 1 \ \& \ q - m \le \frac{p}{2} \\ 10mp - 2m - \frac{p}{2} - 2 & , m > \frac{p}{2} + 1 \ \& \ q - m > \frac{p}{2} \end{cases}$$

and

$$t_e(v) = \begin{cases} 5kp - 10km - \frac{p}{2} + 5k + 5k^2 & , m \le \frac{p}{2} + 1 \ \& \ q - m \le \frac{p}{2} \\ 10pk - 5mp - 5m^2 + 5m - 5\frac{p^2}{4} + 2p & , m \le \frac{p}{2} + 1 \ \& \ q - m > \frac{p}{2} \\ 5k^2 - 10km + 5pk + 5k + 5m^2 - 5mp - 5m + 5\frac{p^2}{4} + 2p & , m > \frac{p}{2} + 1 \ \& \ q - m \le \frac{p}{2} \\ \frac{p}{2}(20k - 20m + 9) & , m > \frac{p}{2} + 1 \ \& \ q - m > \frac{p}{2} \end{cases}$$

If p is odd:

$$t_e(u) = \begin{cases} 10km - \frac{p}{2} - 8k + 5kp - 5k^2 + \frac{1}{2} & , m \le \frac{p+1}{2} \ \& \ q - m \le \frac{p-1}{2} \\ 5mp + 5m^2 - 8m + 5\frac{p^2}{4} - 9\frac{p}{2} + \frac{13}{4} & , m \le \frac{p+1}{2} \ \& \ q - m > \frac{p-1}{2} \\ 10km - 5k^2 + 5pk - 8k - 5m^2 + 5mp + 7m - 5\frac{p^2}{4} - 4p - \frac{7}{4} & , m > \frac{p+1}{2} \ \& \ q - m \le \frac{p-1}{2} \\ 10mp - 8p - m + 1 & , m > \frac{p+1}{2} \ \& \ q - m > \frac{p-1}{2} \end{cases}$$

and

$$t_e(v) = \begin{cases} 5kp - 10km - \frac{p}{2} + 4k + 5k^2 + \frac{1}{2} & , m \le \frac{p+1}{2} \ \& \ q - m \le \frac{p-1}{2} \\ 10pk - 5mp - 5m^2 + 4m - 5\frac{p^2}{4} + 3\frac{p}{2} - \frac{1}{4} & , m \le \frac{p+1}{2} \ \& \ q - m > \frac{p-1}{2} \\ 5k^2 - 10km + 5pk + 4k + 5m^2 - 5mp - 4m + 5\frac{p^2}{4} + 3\frac{p}{2} + \frac{5}{4} & , m > \frac{p+1}{2} \ \& \ q - m \le \frac{p-1}{2} \\ \frac{7p}{2} + 10kp - 10mp + \frac{1}{2} & , m > \frac{p+1}{2} \ \& \ q - m > \frac{p-1}{2} \end{cases}$$

Proof. We compute only $t_e(u)$ when p is even, because computation of $t_e(v)$ is similar to computation of $t_e(u)$, also the computations of $t_e(u)$ and $t_e(v)$ when p are odd and even is very similar to each other. By the Fig. 3, we have, if p is even:

$$n_e(u)=\begin{cases} (\frac{4p}{2}-1)m+2m(m-1)+(\frac{4p}{2}-5)(k-m)- \\ 2(k-m)(k-m-1) & ,m\le\frac{p}{2}+1\ \&\ q-m\le\frac{p}{2} \\ (\frac{4p}{2}-1)m+2m(m-1)+(\frac{4p}{2}-5)\frac{p}{2}-p(\frac{p}{2}-1) & ,m\le\frac{p}{2}+1\ \&\ q-m<\frac{p}{2} \\ (\frac{4p}{2}-1)(\frac{p}{2}+1)+2p(\frac{p}{2}+1)+4p(m-\frac{p}{2}+1)+ \\ (\frac{4p}{2}-1)(k-m)-2(k-m)(k-m-1) & ,m>\frac{p}{2}+1\ \&\ q-m\le\frac{p}{2} \\ (\frac{4p}{2}-1)(\frac{p}{2}+1)+2p(\frac{p}{2}+1)+4p(m-\frac{p}{2}+1)+ \\ (\frac{4p}{2}-5)\frac{p}{2}-p(\frac{p}{2}-1) & ,m>\frac{p}{2}+1\ \&\ q-m>\frac{p}{2} \end{cases}$$

and

$$m_e(u)=\begin{cases} (\frac{5p}{2}-3)+(\frac{6p}{2}+3)(m-1)+3(m-1)(m-2)+ \\ (\frac{6p}{2}-9)(k-m)-3(k-m)(k-m-1) & ,m\le\frac{p}{2}+1\ \&\ q-m\le\frac{p}{2} \\ (\frac{5p}{2}-3)+(\frac{6p}{2}+3)(m-1)+3(m-1)(m-2)+ \\ (\frac{6p}{2}-9)\frac{p}{2}-3\frac{p}{2}(\frac{p}{2}-1) & ,m\le\frac{p}{2}+1\ \&\ q-m<\frac{p}{2} \\ (\frac{5p}{2}-3)+(\frac{6p}{2}+3)(\frac{p}{2})+3(\frac{p}{2}-1)(\frac{p}{2}-2)+ \\ (6p-2)(m-\frac{p}{2}-1)+(\frac{6p}{2}-9)(k-m)- \\ 3(k-m)(k-m-1) & ,m>\frac{p}{2}+1\ \&\ q-m\le\frac{p}{2} \\ (\frac{5p}{2}-3)+(\frac{6p}{2}+3)(\frac{p}{2})+3(\frac{p}{2}-1)(\frac{p}{2}-2)+ \\ (6p-2)(m-\frac{p}{2}-1)+(\frac{6p}{2}-9)(\frac{p}{2})-3(\frac{p}{2})(\frac{p}{2}-1) & ,m>\frac{p}{2}+1\ \&\ q-m>\frac{p}{2} \end{cases}$$

According to the definition of total Szeged index, $t_e(u)$ and $t_e(v)$ can be concluded when p are even and odd.

For simplifying following computations, we use the following notations.

$$a_1=10km-\frac{p}{2}-9k+5kp-5k^2$$

$$a_2=5mp+5m^2-9m+5\frac{p^2}{4}-5p$$

$$a_3=10km-5k^2+5pk-9k-5m^2+5mp+7m-5\frac{p^2}{4}+4p-2$$

$$a_4=10mp-2m-\frac{p}{2}-2$$

$$b_1=5kp-10km-\frac{p}{2}+5k+5k^2$$

$$b_2=10pk-5mp-5m^2+5m-5\frac{p^2}{4}+2p$$

$$b_3=5k^2-10km+5pk+5k+5m^2-5mp-5m+5\frac{p^2}{4}+2p$$

$$b_4=\frac{p}{2}\left(20k-20m+9\right)$$

and

$$a'_1=10km-\frac{p}{2}-8k+5kp-5k^2+\frac{1}{2}$$

$$a'_2=5mp+5m^2-8m+5\frac{p^2}{4}-9\frac{p}{2}+\frac{13}{4}$$

$$a'_3=10km-5k^2+5pk-8k-5m^2+5mp+7m-5\frac{p^2}{4}-4p-\frac{7}{4}$$

$$a'_4=10mp-8p-m+1$$

$$b'_1=5kp-10km-\frac{p}{2}+4k+5k^2+\frac{1}{2}$$

$$b'_2=10pk-5mp-5m^2+4m-5\frac{p^2}{4}+3\frac{p}{2}-\frac{1}{4}$$

$$b'_3=5k^2-10km+5pk+4k+5m^2-5mp-4m+5\frac{p^2}{4}+3\frac{p}{2}+\frac{5}{4}$$

$$b'_4=\frac{7p}{2}+10kp-10mp+\frac{1}{2}$$

Now, we are ready to state the total Szeged index of $TUC_4C_8(S)$ nanotube.

Theorem 2-6. The total Szeged index of $TUC_4C_8(S)$ nanotube is

If p is even:

$$Sz_T(G)=\begin{cases} \sum_{m=1}^{q}2pa_1b_1+\frac{p^3}{3}(q-1)(50q^2+20q+3)+ \\ pq(5pq-\frac{p}{2}-q)^2 & ,q\le\frac{p}{2}+1 \\ \sum_{m=1}^{\frac{p}{2}+1}2pa_2b_2+\sum_{m=\frac{p}{2}+2}^{q}2pa_3b_3+ \\ \frac{p^3}{3}(q-1)(50q^2+20q+3)+pq(5pq-\frac{p}{2}-q)^2 & ,\frac{p}{2}+1<q\le p+2 \\ \sum_{m=1}^{\frac{p}{2}+1}2pa_2b_2+\sum_{m=\frac{p}{2}+2}^{q-\frac{p}{2}+1}2pa_4b_4+\sum_{m=q-\frac{p}{2}+2}^{q}2pa_3b_3+ \\ \frac{p^3}{3}(q-1)(50q^2+20q+3)+pq(5pq-\frac{p}{2}-q)^2 & ,q>p+2 \end{cases}$$

If p is odd:

$$Sz_T(G)=\begin{cases}\sum_{m=1}^{q}2pa'_1b'_1+\frac{p^3}{3}(q-1)(50q^2+20q+3)+ & ,q\le\frac{p+1}{2}\\ pq(5pq-\frac{p+1}{2}-2q)^2 & \\ \sum_{m=1}^{\frac{p+1}{2}}2pa'_2b'_2+\sum_{m=\frac{p+1}{2}+1}^{q}2pa'_3b'_3+ & ,\frac{p+1}{2}<q\le p+1\\ \frac{p^3}{3}(q-1)(50q^2+20q+3)+pq(5pq-\frac{p+1}{2}-2q)^2 & \\ \sum_{m=1}^{\frac{p+1}{2}}2pa'_2b'_2+\sum_{m=\frac{p+1}{2}+1}^{q-\frac{p+1}{2}}2pa'_4b'_4+\sum_{m=q-\frac{p+1}{2}+1}^{q}2pa'_3b'_3+ & ,q>p+1\\ \frac{p^3}{3}(q-1)(50q^2+20q+3)+pq(5pq-\frac{p+1}{2}-2q)^2 & \end{cases}$$

Proof. By the Lemmas (2-3) and (2-4), we have

$$\sum_{\substack{e=uv\in E(G)\\ \text{and } e \text{ is vertical edge}}}\left[t_e(u)\times t_e(v)\right]=\frac{p^3}{3}(q-1)(50q^2+20q+3)$$

and

If p is even:

$$\sum_{\substack{e=uv\in E(G)\\ \text{and } e \text{ is horizontal edge}}}\left[t_e(u)\times t_e(v)\right]=pq(5pq-\frac{p}{2}-q)^2$$

If p is odd:

$$\sum_{\substack{e=uv\in E(G)\\ \text{and } e \text{ is horizontal edge}}}\left[t_e(u)\times t_e(v)\right]=pq(5pq-\frac{p+1}{2}-2q)^2$$

Also, by the Lemma (2-5) and notation a_i, b_i, a'_i and b'_i where $1\le i\le 4$, the desire result can be concluded.

3. Conclusion

In this paper, we compute the total Szeged index of hexagonal chains and in particular the total Szeged index of $TUC_4C_8(R)$ nanotubes by concluding some techniques which are in graph theory.

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