Szeged Index of a Zig-zag Polyhex Nanotube

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Abstract

The Szeged index extends the Wiener index for cyclic graphs by counting the number of atoms on both sides of each bond and sum these counts. This index introduced by Ivan Gutman at the Attila Jozsef University in Szeged, 1994, and so called Szeged index. In this paper, we introduce a novel method for enumerating by cuts. Using this method an exact formula for the Szeged index of a zig-zag polyhex nanotube T = $TUHC_6[p,q]$ is computed for the first time.

Keywords: Szeged index, chemical graph, zig-zag polyhex nanotube.

1. Introduction

A graph G is defined as a pair G = (V,E), where V is a finite, non-empty set of vertices and E is a set of edges. The term chemical graph was introduced by Cullen in 1758. He used those graphs for affinity diagrams showing a relationship between chemical substances. Those results have never been published officially. In a chemical graph, vertices represent atoms and edges represent bonds.

Numbers reflecting certain structural features of a molecule that are obtained from its chemical graph are usually called topological indices. Wiener index (W) is one of the oldest and most thoroughly examined molecular graph-based structural descriptor of organic molecule, [19]. This quantity is equal to

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the sum of distances between all pairs of vertices of the respective molecular graph.

Let G be a graph and e is an edge of G. If e is connecting the vertices i and j then we write e = i–j. The distance between a pair of vertices a and b of G is denoted by d(a,b). For acyclic molecular graphs, Wiener discovered a remarkably simple method for the calculation of W. For an edge e = i–j, let N(i) be the number of vertices of G lying closer to i than to j and N(j) be the number of vertices of G lying closer to j than to i, that is $N(i) = |\{u \in V(G) \mid d(u,i) < d(u,j)\}|$ and $N(j) = |\{u \in V(G) \mid d(u,j) < d(u,i)\}|$. Then the Szeged index of the graph G is defined as $Sz(G) = \sum_{e=ij \in E(G)} N(i)N(j)$.

This generalization was conceived by Gutman at the Attila Jozsef University in Szeged, and so it was called the Szeged index, [13]. It is usefule to mention here that Gutman in his 1994 paper proposed the existence of the cyclic index and abbreviated it by W*. In that paper he has not given any name to this index. It was in [16] the index named Szeged index and abbreviated as Sz. For more information about Szeged index we encourage the reader to consult [1-2,15-18,21-22].

Diudea and co-authors [8-12] computed the Wiener index of some nanotubes. In [14], John and Diudea computed the Wiener index of a zig-zag polyhex nanotube. They proved that:

$$W(T) = \begin{cases} \frac{qp^2}{24}\left(4q^2 + 3qp - 4\right) + \frac{q^2p}{12}\left(q^2 - 1\right) & q \le \frac{p}{2} + 1 \\ \frac{qp^2}{24}\left(8q^2 + p^2 - 6\right) - \frac{p^3}{192}\left(p^2 - 4\right) & q > \frac{p}{2} + 1 \end{cases}.$$

In [3-6,23-24], one of us (ARA) computed the PI and Wiener indices of some nanotubes and nanotori. In this paper, we continue this program to compute the Szeged index of a zig-zag polyhex nanotube. We mention here that computing PI and also Wiener indices of nanotubes is very simpler than computing Szeged index, because of the symmetry of nanotubes and nanotori.

In literature, there is a paper by Diudea in which Szeged index is tested in QSPR, see [12]. In this paper, he examined use of Szeged index and several other distance-based indices on correlation with the boiling points (BP) of 45 cycloalkanes. On the other hand, Khadikar et. al. [15] described various applications of Szeged index for modeling physicochemical properties as well as physiological activities of organic compounds acting as drugs or possess pharmacological activity. The authors of this paper reviewed 175 papers published on the subject of Szeged index. This shows that the subject of Szeged index is more and more growing in chemistry, physics and also biology.

It is useful to mention here that Randic [18] introduced a novel index named "revised Wiener index", RW, which as will be seen shows better descriptor than Szeged index for structure – property relationship for cyclic molecules. To define, we augment Szeged index with contributions from vertices not considered in the definition of Sz index as proposed by Gutman. A simple remedy to deficiency of Sz is to divide equally the count vertices at the same distance from vertices at both ends of an edge.

Throughout this paper T = $TUHC_6[p,q]$ denotes an arbitrary zig-zag polyhex nanotube, in the terms of their circumference (p) and the number of zig-zags (q), see Figure 1. Our notation is standard and taken mainly from [7,19]. We prove that:

Theorem. With notation as above, we have:

$$Sz(T)=\begin{cases} \frac{8}{3}p^3q^3-\frac{2}{3}p^3q+\frac{1}{6}pq^3-\frac{1}{6}pq^5 & q\le p \\ \frac{5}{2}p^6+\frac{43}{6}p^5+\frac{35}{6}p^4+\frac{5}{6}p^3-\frac{1}{3}p^2 & q=p+1 \\ \frac{2}{3}p^3q^3+\frac{2}{3}p^3q-\frac{2}{15}pq+\frac{2}{15}p^2-\frac{1}{5}pq^5+\frac{4}{3}p^2q^4 & p+1<q<2p \\ -\frac{5}{3}pq^3+\frac{8}{3}p^2q^2-\frac{1}{3}p^4-\frac{4}{3}p^5q+\frac{1}{5}p^6 & \\ \frac{89}{5}p^6-\frac{5}{3}p^4-\frac{1}{15}p^2 & q=2p \\ 2p^3q^3-\frac{4}{3}p^3q-\frac{2}{15}p^2+\frac{4}{3}p^5q-\frac{13}{15}p^6+p^4 & q>2p \end{cases}$$

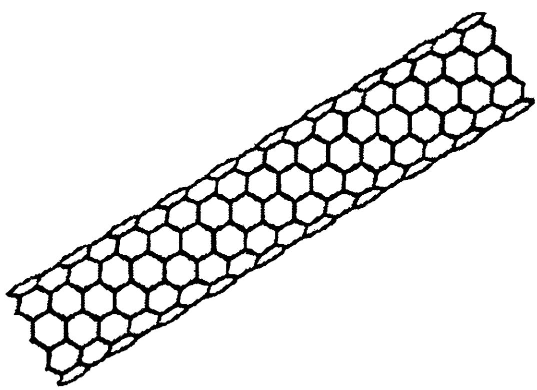

Figure 1. Zig-zag TUHC6[10,20] Nanotube.

2. Main Results and Discussion

The aim of this section is computing the Szeged index of the zig-zag polyhex nanotube T = $TUHC_6[p,q]$. It is clear that T has exactly 2pq vertices and p(3q-1) edges. Suppose A and B are the set of all vertical and oblique edges of T, respectively. Then $Sz(T)=\sum_{e=ij\in E(T)}N(i)N(j)=\sum_{e=ij\in A}N(i)N(j)$

$+\sum_{e=ij\in B} N(i)N(j)$. We assume that $Sz_1(T) = \sum_{e=ij\in A} N(i)N(j)$ and $Sz_2(T) = \sum_{e=ij\in B} N(i)N(j)$. To compute Sz(T), we first compute $Sz_1(T)$.

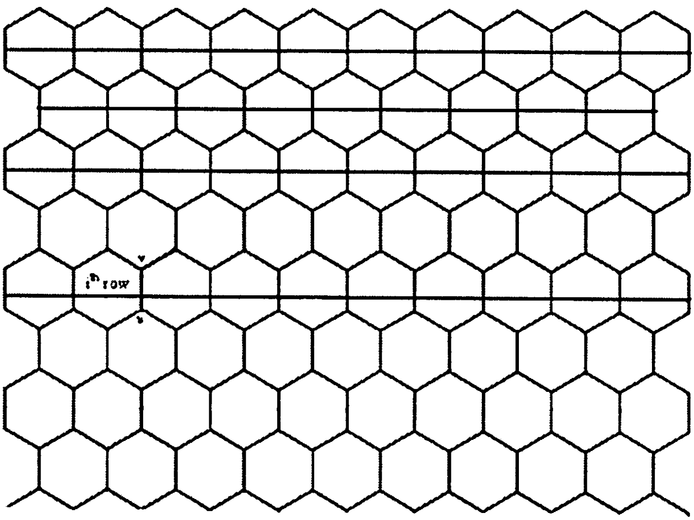

Figure 2. 2-Dimensional Graph of $T = TUHC_6[p,q]$.

Lemma 1. $Sz_1(T) = \sum_{e=ij\in A} N(i)N(j) = 2/3p^3q(q^2-1)$.

Proof. Suppose e = uv is an arbitrary vertical edge in the i^{th} row, Figure 2. One can see that T has exactly p vertical edges in each row and so there are 2pi vertices above the i^{th} row, which are all closer to v than u. Therefore,

$$Sz_1(T) = \sum_{i=1}^{q-1} p(2pi)(2pq-2pi) = 2/3p^3q(q^2-1).$$

To calculate $Sz_2(T)$, we consider six cases that are explained in the following lemmas. We explain our method for computing summations which are needed for calculating Szeged index of T. Without loss of generality, suppose $e = x_{33}-x_{34}$. To calculate the number of closer vertices to x_{34}, we first draw two copies of 2-dimensional lattice of T and then cut e by an oblique line and pass a vertical line through $x_{3(p+4)}$, oblique and vertical heavy lines of Figure 4. Then vertices closer to x_{34} lie in the triangular region between those two lines. In general, to calculate $N(x_{i(i+1)})$, we compute the number of vertices in the triangular or trapezoidal region, Figures 3 and 4, surrounded by the vertical line passes through $x_{i,p+i+2}$ and oblique line passes through $e_{ii} = x_{ii}-x_{i(i+1)}$.

Lemma 2. If $q \le p$ then $Sz_2(T) = 2p^3q^3 + 1/6pq^3 - 1/6pq^5$.

Proof. Suppose $e_{is} = x_{is}\text{-}x_{i(s+1)}$ and $e_{ir} = x_{ir}\text{-}x_{i(r+1)}$ are two arbitrary oblique edges of T, Figure 3. Notice that $N(x_{ir})N(x_{i(r+1)}) = N(x_{is})N(x_{i(s+1)})$. Since T is bipartite, $N(x_{ir}) + N(x_{i(r+1)}) = N(x_{is}) + N(x_{i(s+1)}) = 2pq$. So, it is sufficient to consider one oblique edge in each zig-zag. Without loss of generality, we can consider e_{ii} in the i^{th} zig-zag. Let M denote the set of all vertices closer to x_{ii} than $x_{i(i+1)}$. Then $M = \{x_{12},\ldots,x_{1(p+i)},x_{23},\ldots,x_{2(p+i)},\ldots,x_{q(q+1)},\ldots,x_{q(p+i)}\}$. So, $N(x_{ii}) = 1 + 2 + \ldots + q + q(p - q + i - 1) = T_q + q(p - q + I - 1)$, where $T_q = 1 + 2 + \ldots + q$ is the q^{th} triangular number. And $N(x_{i(i+1)}) = 2pq - (T_q + q(p - q + i - 1)) = T_q + q(p - i)$. Therefore,

$$Sz_2(T) = 2p\sum_{i=1}^{q}[q(p+i-T_q)][T_q + q(p-i)] = 2p^3q^3 + 1/6pq^3 - 1/6pq^5.$$

Lemma 3. If $p+1 < q < 2p$ then $Sz_2(T) = 1/6pq^3 - 4/3p^5q + 4/3p^3q - p^2q^2 + 8/3p^4q^2 + 1/5p^6 - 2/15pq - 1/30pq^5 - 1/3p^4 + 2/15p^2 + 1/3p^2q^4$.

Proof. By our discussion in the paragraph before Lemma 2, we have $N(x_{ii}) = 1 + 2 + \ldots + (p+i-1) = T_{p+i-1}$ and $N(x_{i(i+1)}) = 2pq - T_{p+i-1}$. Suppose $N = \sum_{e=ij\in A} N(i)N(j)$. To compute N, it is enough to calculate N for all oblique edges along an oblique cut and then multiply by 2p to obtain $Sz_2(T)$. Therefore,

$$\begin{aligned} Sz_2(T) &= 2p\sum_{i=1}^{q-p+1} T_{p+i-1}(2pq - T_{p+i-1}) \\ &+ 2p\sum_{i=q-p+2}^{p+1}(T_{p+i-1} - T_{p+i-1-q})(2pq - T_{p+i-1} + T_{p+i-1-q}) \\ &+ 2p\sum_{i=p+2}^{q}(T_{p+i-1} - T_{p+i-1-q} - T_{i-p-1})(2pq - T_{p+i-1} + T_{p+i-1-q} + T_{i-p-1}) \end{aligned}$$

Hence $$Sz_2(T) = 1/6pq^3 - 4/3p^5q + 4/3p^3q - p^2q^2 + 8/3p^4q^2 + 1/5p^6 - 2/15pq - 1/30pq^5 - 1/3p^4 + 2/15p^2 + 1/3p^2q^4.$$

Lemma 4. If $q = p+1$ then $Sz_2(T) = 11/6p^6 + 31/6p^5 + 9/2p^4 + 5/6p^3 - 1/3p^2$.

Proof. If $q = p+1$ then a similar argument as in Lemma 3 shows that

$$\begin{aligned} Sz_2(T) &= 2p\sum_{i=1}^{q-p+1} T_{p+i-1}(2pq - T_{p+i-1}) \\ &+ 2p\sum_{i=q-p+2}^{p+1}(T_{p+i-1} - T_{p+i-1-q})(2pq - T_{p+i-1} + T_{p+i-1-q}) \\ &= 11/6p^6 + 31/6p^5 + 9/2\,p^4 + 5/6p^3 - 1/3p^2. \end{aligned}$$

Lemma 5. Suppose $q = 2p$. Then $Sz_2(T) = 89/5p^6 - 5/3p^4 - 1/15p^2$.

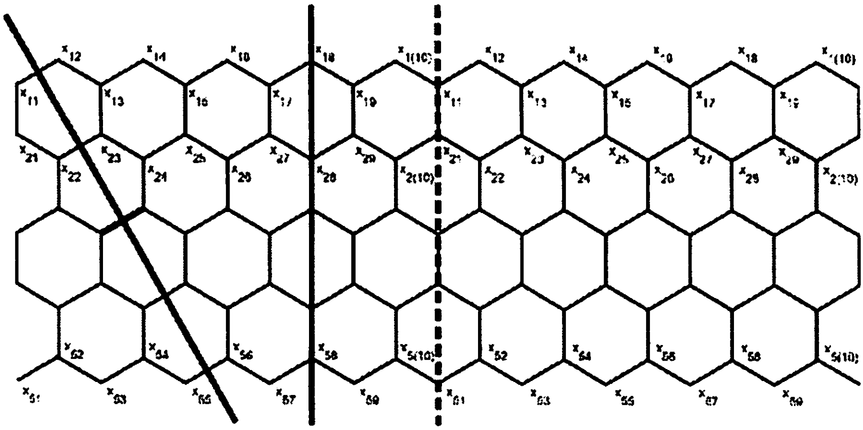

Figure 3. Oblique and Vertical Edges of T with p < q.

Proof. Since $q = 2p$, $T_{p+i-1-q} = T_{i-p-1}$. Therefore,

$$Sz_2(T) = 2p\sum_{i=1}^{p+1} T_{p+i-1}(2pq - T_{p+i-1}) + 2p\sum_{i=p+2}^{q}(T_{p+i-1} - 2T_{i-p-1})(2pq - T_{p+i-1} + 2T_{i-p-1}).$$

Therefore, $Sz_2(T) = -2/15p^2 - 293/15p^6 - 1/3p^4 + 16p^5q$.

Lemma 6. If $q > 2p$ then $Sz_2(T) = 2p^3q^3 - 4/3p^3q \; -2/15p^2 + 4/3p^5q - 13/15p^6 + p^4$.

Proof. To prove the lemma, we consider three cases that $2p < q < 2p + 4$ and $q \geq 2p + 4$ (q is odd or even).

Case 1. $2p < q < 2p + 4$. In this case we have:

$$\begin{aligned} Sz_2(T) = {} & 2p\sum_{i=1}^{p+1} T_{p+i-1}(2pq - T_{p+i-1}) \\ & +2p\sum_{i=p+2}^{q-p+1}(T_{p+i-1} - T_{i-p-1})(2pq - T_{p+i-1} + T_{i-p-1}) \\ & +2p\sum_{i=q-p+2}^{q}(T_{p+i-1} - T_{i-p-1} - T_{p+i-1-q})(2pq - T_{p+i-1} - T_{i-p-1} - T_{p+i-1-q}) \\ = {} & -2/15p^2 - 2/3p^3q + 4/3p^5q - 13/15p^6 + p^4 + 4/3\,p^3q^3. \end{aligned}$$

Case 2. $q \geq 2p + 4$ and q is even. Suppose $e_1 = x_{11}-x_{12}$, $e_2 = x_{22}-x_{23}$, …, $e_q = x_{qq} - x_{q(q+1)}$. Then it is clear that $N(x_{11})N(x_{12}) = N(x_{qq})N(x_{q(q+1)})$, …, $N(x_{q/2(q/2)})N(x_{q/2(q/2+1)}) = N(x_{(q/2+1)(q/2+1)})N(x_{(q/2+1)(q/2+2)})$, Figure 4. So it is sufficient to calculate one half of these values and then multiply by 2. Therefore,

$$\begin{aligned} Sz_2(T) = {} & 4p\sum_{i=1}^{p+1} T_{p+i-1}(2pq - T_{p+i-1}) \\ & +4p\sum_{i=p+2}^{q/2}(T_{p+i-1} - T_{i-p-1})(2pq - T_{p+i-1} + T_{i-p-1}) \\ = {} & -2/15p^2 - 2/3p^3q + 4/3p^5q - 13/15p^6 + p^4 + 4/3\,p^3q^3. \end{aligned}$$

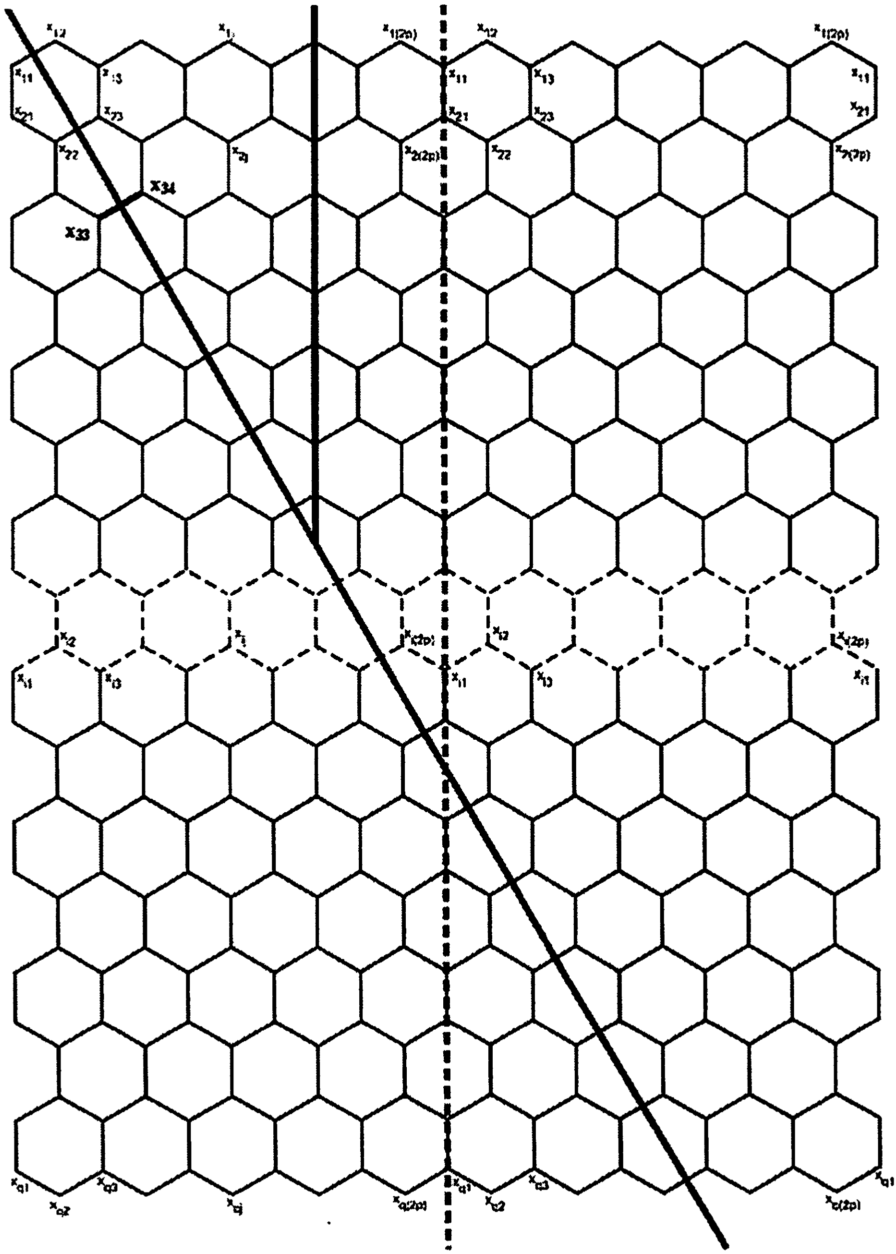

Figure 4. Oblique and Vertical Edges of T with p > q.

Case 3. $q \geq 2p + 4$ and q is odd. Using a similar argument as above $N(x_{11})N(x_{12}) = N(x_{qq})N(x_{q(q+1)})$, ..., $N(x_{(q-1)/2(q-1)/2})N(x_{(q-1)/2(q+1)/2}) = N(x_{(q+3)/2(q+3)/2})N(x_{(q+3)/2(q+5)/2})$, Figure 4. So we must calculate one half of these values and then add to $N(x_{(q+1)/2(q+1)/2})N(x_{(q+1)/2(q+3)/2})$. Therefore,

$$
\begin{aligned}
Sz_2(T) &= 4p\sum_{i=1}^{p+1} T_{p+i-1}(2pq - T_{p+i-1}) \\
&+4p\sum_{i=p+2}^{(q-1)/2}(T_{p+i-1} - T_{i-p-1})(2pq - T_{p+i-1} + T_{i-p-1}) \\
&+2p(T_{(q+1)/2+p-1} - T_{(q+1)/2-p-1})(2pq - T_{(q+1)/2+p-1} + T_{(q+1)/2-p-1}) \\
&= -2/15p^2 - 2/3p^3q + 4/3p^5q - 13/15p^6 + p^4 + 4/3\, p^3q^3.
\end{aligned}
$$

This completes the proof.

Proof of the Theorem. The proof is straightforward and follows from Lemmas 1-6.

Corollary. If T is a zig-zag polyhex nanotube then RW(T) = Sz(T).

Proof. Since a zig-zag polyhex nanotube is bipartite, T does not have a cycle of odd length. Therefore, RW(T) = Sz(T).

Acknowledgement. The third author, was in part supported by a grant from the Center of Excellence of Algebraic Methods and Applications of the Isfahan University of Technology.

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