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A Method of Calculating the Edge–Szeged Index of Hexagonal Chain

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Abstract

The edge-Szeged index is recently introduced graph invariant, having applications in chemistry. In this paper, a method of calculating the edge-Szeged index of hexagonal chain is proposed, and the results of the index are presented.

1 Introduction

In theoretical chemistry, the physico-chemical properties of chemical compounds are often modeled by the molecular graph based molecular structure descriptors which are also referred to as topological indices. Among the variety of those indices, the Wiener index is the best known one [1]. The first reported use of a topological index in chemistry was by wiener in the study of paraffin boiling points. From then on, in order to model various molecular properties, many topological indices have been designed. I. Gutman extended the Wiener index to Szeged index and edge-Szeged index to all connected graph [1–4]. The main advantage of the Szeged index and edge-Szeged index is that it is a modification of Wiener index. Under the condition of tree, the two indexes are coincident. I. Gutman and S. Klavzar gave a good algorithm for the calculation of the Szeged index of benzenoid hydrocarbons [5]. This cut-method was shown to be applicable to all sorts of benzenoids. The method was eventually extended by Klavzar to a number of other topological indices [6]. It plays an important role in the theory of benzenoid systems.

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Hexagonal chains are of great importance of theoretical chemistry because they are the natural graph representations of benzenoid hydrocarbons, a great deal of investigations in mathematical chemistry has been developed to hexagonal chains(benzenoid hydrocarbons) [7].

Let $G = (V(G), E(G))$ be a graph, where $|V(G)|$ and $|E(G)|$ are respectively referred to as the order and the size of G. The length of the shortest path of two vertices $u, v \in V(G)$ is called their distance $d(u, v)$. Let $w \in V(G)$ and $e = uv \in E(G)$. The distance between w and e is denoted by $d(w, e)$, which is defined as $min\{d(w, u), d(w, v)\}$. Furthermore, $m_1(e)$ is the number of edges whose distance to u is smaller than that to v , $m_2(e)$ is the number of edges whose distance to v is smaller than that to u. Define the edge Szeged index of graph G as

$$Sz_e(G) = \sum_{e \in E(G)} m_1(e)m_2(e).$$

Hexagonal chains are exclusively constructed by hexagons of length one. In a hexagonal chain, any two hexagons either have one common edge or have no common vertices. The two hexagons which have one common edge is said to be adjacent. No three or more hexagons share one common vertex. Each hexagon except the terminal ones has two adjacent hexagons. A hexagonal chain has exactly two terminal hexagons.

The vertex number of a hexagonal chain with n hexagons is $4n + 2$, and the edge number of which is $5n + 1$ [7]. The linear hexagonal chain is a hexagonal chain without kinks, where the kinks are the angularly connected or branched hexagons. The linear hexagonal chain with n hexagons is denoted by L_n(as shown in Fig. 1). The hexagonal chain with n hexagons shown in Fig. 2 is called zig-zag hexagonal chain, which is denoted by Z_n.

Fig. 1: linear chain L_n

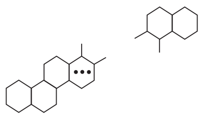

Fig. 2: zig-zag chain Z_n

The cut of a hexagonal chain is defined as follows: Choose an edge e of the hexagonal chain and draw a line through the center of e, orthogonal on e. This line will intersect the perimeter in two points P_1 and P_2 . The straight line segment C whose end points are P_1 and P_2 is the cut, intersecting the edge e [5]. Some cuts of the hexagonal chain are illustrated in Figure.3.

The primary aim of the investigation is to introduce a new method to calculate the edge-Szeged index of hexagonal chain with the help of cut-method. Moreover, by this new method, we can simplify some complex calculations of edge-Szeged index of hexagonal chains.

2 Main results

The maximal linear chain of a hexagonal chain, including the kinks and/or terminal hexagons at its end, is called a segment S. The number of hexagons in the segment S is refered to as the length of segment S , which is denoted by $l(S)$. For any segment S of a hexagonal chain with $n \geq 2$ hexagons, $2 \leq l(S) \leq n$.

A hexagonal chain consists of a series of segments $S_1, S_2, \ldots, S_m$, $m \geq 1$, with lengths $l(S_i) = l_i$, $i = 1, 2 \ldots, m$, where $l_1 + l_2 + \cdots + l_m = n + m - 1$, where n is the number of hexagons of a hexagonal chain, since two neighboring segments have always one hexagon in common.

For the kth segment of a hexagonal chain, the cut intersecting these $l_k + 1$ parallel edges of hexagons in this segment (the dotted line shown in Fig. 3) is called the cut of this segment. If the cut of this segment parallels the horizontal, then the segment is called horizontal, otherwise it is called oblique segment. If the angles always equal that the cut of every oblique segment in a hexagonal chain makes with the same horizontal direction, then the hexagonal chain is called one-sided hexagonal chain. The hexagonal chain shown in Fig. 3 is a one-sided hexagonal chain. It is obvious that Z_n is a one-sided hexagonal chain which has $n - 1$ segments, and the length of every segment equals 2; L_n is a one-sided hexagonal chain which has only one segment. In this paper, we shall be mainly concerned with one-sided hexagonal chain.

Let e be an edge of a hexagonal chain, we make a cut of hexagonal chain which intersects the edge e. These edges intersecting the cut are equidistant to the both ends of them. Because in all case of cyclic graphs there are edges equidistant to the both ends of the edges, such edges are not taken into account in $m_1(e)$ and $m_2(e)$ [7]. So these edges intersecting the cut are not taken account in $m_1(e)$ and $m_2(e)$ of hexagonal chain either.Then the number of those edges which are located at both sides of the cut are $m_1(e)$ and $m_2(e)$ respectively.

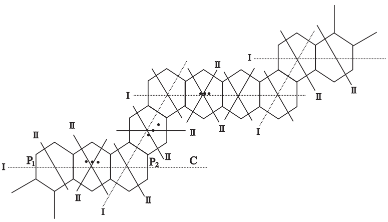

Fig. 3: I type cut (denoted by dotted lines) and II type cut (denoted by real lines) in one-sided hexagonal chain

Theorem 2.1. *Let G be a one-sided hexagonal chain with n hexagons. G consists of m segments S_1, S_2, …, S_m, where $m \geq 1$, $l(S_i) = l_i$ $(i = 1, 2 \cdots m)$. Then*

$Sz_e(G) = 16[5(\sum_{i=1}^{m} l_i - m + 1) - 3] + 2\sum_{k=1}^{m-1}[5(\sum_{i=1}^{k} l_i - k + 1) - 3][5(\sum_{i=k+1}^{m} l_i - m + k) + 2] + 4\sum_{k=1}^{m}\sum_{j=2}^{l_k - 1}[5(\sum_{i=1}^{k-1} l_i - k + 1) + 5j - 3][5(\sum_{i=k+1}^{m} l_i - m + k) + 5l_k - 5j + 2] + \sum_{k=1}^{m}(l_k + 1)[5(\sum_{i=1}^{k-1} l_i - k + 1) + 2l_k][5(\sum_{i=k+1}^{m} l_i - m + k) + 2l_k]$.

Proof. In order to describe convenience, these edges intersecting I type cut are called I type edges, these edges intersecting II type cut are called II type edges. The edges of the hexagonal chain are classified into two categories: I type and II type(as shown in Fig. 3).

Case 1. If e is the I type edge in the jth hexagon of the kth segment of a hexagonal chain (as shown in Fig. 3), then the calculation of $m_1(e)$ is as follows:
$m_1(e) = [5(\sum_{i=1}^{k-1} l_i - k + 1) + 1] - 1 + 5(j - 1) + 1 + 1 = 5(\sum_{i=1}^{k-1} l_i - k + 1) + 5j - 3$.
Especially, if $j = l_k$, $m_1(e) = 5(\sum_{i=1}^{k} l_i - k + 1) - 3$.
The calculation of $m_2(e)$ is as follows:
$m_2(e) = [5(\sum_{i=k+1}^{m} l_i - m + k) + 1] - 1 + 5(l_k - j) + 1 + 1 = 5(\sum_{i=k+1}^{m} l_i - m + k) + 5l_k - 5j + 2$.
Especially, if $j = l_k$, $m_2(e) = 5(\sum_{i=k+1}^{m} l_i - m + k) + 2$.

Case 2. If e is the II type edge in the jth hexagon of the kth segment of a hexagonal chain (as shown in Fig. 3), then the calculation of $m_1(e)$ is as follows:
$m_1(e) = [5(\sum_{i=1}^{k-1} l_i - k + 1) + 1] + 2l_k - 1 = 5(\sum_{i=1}^{k-1} l_i - k + 1) + 2l_k$.
And the calculation of $m_2(e)$ is as follows:
$m_2(e) = [5(\sum_{i=k+1}^{m} l_{i=1} - m + k) + 1] + 2l_k - 1 = 5(\sum_{i=k+1}^{m} l_i - m + k) + 2l_k$.
According to the discussion above, the theorem is proved. □

Corollary 2.2. *Let L_n be linear hexagonal chain with n hexagons, then*

$$Sz_e(L_n) = \frac{62}{3}n^3 - 6n^2 + \frac{28}{3}n \ .$$

Proof. L_n be linear hexagonal chain with n hexagons,then $m = 1, l_1 = n$. According to Theorem 2.1, we have

$Sz_e(L_n) = 16(5n-3) + 4\sum_{j=2}^{n-1}[(5j-3)(5n-5j+2)] + (n+1)(2n)^2$.

By calculating, we have

$$Sz_e(L_n) = \tfrac{62}{3}n^3 - 6n^2 + \tfrac{28}{3}n \ . \qquad \square$$

Corollary 2.3. *Let Z_n be zig-zag hexagonal chain with n hexagons, then*

$$Sz_e(Z_n) = \tfrac{125}{6}n^3 - 20n^2 + \tfrac{301}{6}n - 27 \ .$$

Proof. Because Z_n is zig-zag hexagonal chain with n hexagons,then $l_i = 2\ (i = 1, 2\cdots m)$, and $m = n-1$. According to theorem 2.1, we have

$Sz_e(Z_n) = 16[5(2(m-1+1)-3) + 2\sum_{k=1}^{m-1}[5(2k-k+1)-3][5(2m-2k+k)+2)] + \sum_{k=1}^{m}(2+1)[5(2k-2-k+1)+4][5(2m-2k-m+k)+4]$.

Because Z_n satisfies $n = m+1$, by calculating and simplifying, we have

$$Sz_e(Z_n) = \tfrac{125}{6}n^3 - 20n^2 + \tfrac{301}{6}n - 27 \ . \qquad \square$$

By the two corollaries above, we can draw a conclusion: If $n \leq 80$, then $Sz_e(L_n) > Sz_e(Z_n)$; if $n \geq 82$, then $Sz_e(L_n) < Sz_e(Z_n)$.

By this cut method, we can not only calculate the edge-Szeged index of one-sided hexagonal chains, but also calculate the edge-Szeged index of some benzenoid systems. We illustrate two benzenoid systems in figure.4. The helicenes H_n [7] and the hexagonal squeeze with seven hexagons HS_2 [8] are not one-sided hexagonal chains.

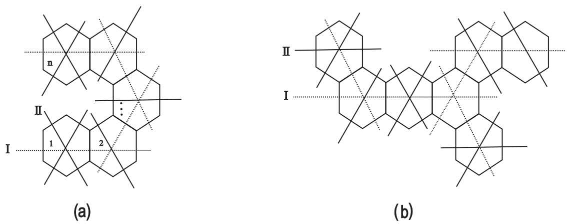

Fig. 4: (a)The helicenes H_n, (b)The hexagonal squeeze with seven hexagons HS_2 . I type cut (denoted by dotted lines), II type cut (denoted by real lines)

Now let's calculate the edge-Szeged index of the helicenes H_n and the hexagonal squeeze with seven hexagons HS_2.

Because the helicenes H_n has $n-1$ segments, and the length of every segment equals 2. It is obvious $m_1(e)$ of each edge of these edges intersecting I type cut in H_n is same, $m_2(e)$ of them equals too. And $m_1(e)$ of these edges intersecting II type cut in two terminal hexagons is same, so is $m_2(e)$ of them. Then we have:

$Sz_e(H_n) = (n-1)\cdot 3\cdot 4\cdot (5n-6) + 2\cdot 4\cdot 2\cdot [5(n-1)+1+1] + \sum_{i=2}^{n-1} 2\cdot [5(i-1)+1+1][5(n-i)+1+1] = 12(5n^2-11n+6) + 8(5n-3) + 2\sum_{i=1}^{n}(5i-3)(5n-5i+2)$.

By calculating, we have

$$Sz_e(H_n) = \frac{25}{3}n^3 + 55n^2 - \frac{262}{3}n + 48.$$

With regard to HS_2 with seven hexagons, $m_1(e)$ of these edges intersecting II type cut in three terminal hexagons equals, so is $m_2(e)$ of them. Then we have:

$Sz_e(HS_2) = 3\times 4\times 2\times 32 + 2\times 7\times 27 + 4\times 12\times 22 + 2\times 27\times 7 + 2\times 3\times 4\times 29 + 4\times 11\times 21 + 2\times 3\times 14\times 19 = 5796$.

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