Szeged Related Indices of Unilateral Polyomino Chain and Unilateral Hexagonal Chain

Wei Gao, Li Shi

***Abstract*—In theoretical chemistry, the Szeged index and Szeged related indices were introduced to measure the stability of alkanes and the strain energy of cycloalkanes. In this paper, we determine the edge-vertex Szeged index and vertex-edge Szeged index of unilateral polyomino chain and unilateral hexagonal chain. Furthermore, the total Szeged indices, third atom bond connectivity indices, PI polynomials, vertex PI polynomials, Szeged polynomials and edge Szeged polynomials of these chemical structures are presented.**

***Index Terms*—molecular graph, edge-vertex Szeged index, vertex-edge Szeged index, total Szeged index, third atom bond connectivity index, unilateral polyomino chain, unilateral hexagonal chain.**

I. Introduction

One of the most important applications of chemical graph theory is to measure chemical, physical and pharmaceutical properties of molecules which is called alkanes. Several indices relied on the graphical structure of the alkanes are defined and employed to model both the melting point and boiling point of the molecules. Molecular graph is a topological representation of a molecule such that each vertex represents an atom of molecule, and covalent bounds between atoms are represented by edges between the corresponding vertices.

Specifically, topological index can be regarded as a score function $f : G \rightarrow \mathbb{R}^+$, with this property that $f(G_1) = f(G_2)$ if two molecular graphs G_1 and G_2 are isomorphic. There are several vertex distance-based and degree-based indices which are introduced to analyze the chemical properties of molecule graph, such as: Wiener index, PI index, Szeged index and atom-bond connectivity index. Several papers contributed to determine the indices of special molecular graphs and to be applied in engineering (See Yan et al. [1] and [2], Gao et al. [3] and [4], Gao and Shi [5], Xi and Gao [6], Gao and Wang [7], Reineix et al. [8], Liu and Zhang [9], and Okamoto and Itofor [10] for more details).

All (molecular) graphs considered in this paper are finite, loopless, and have no multiple edges. Let G be a (molecular) graph with vertex set $V(G)$ and edge set $E(G)$. All graph notations and terminologies used but undefined in this paper can be found in [11].

Let $e = uv$ be an edge of the molecular graph G. The number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $n_u(e)$. Analogously, $n_v(e)$ is the number of vertices of G whose distance to the vertex v is smaller than the distance to the vertex u. The number of edges of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $m_u(e)$. Analogously, $m_v(e)$ is the number of edges of G whose distance to the vertex v is smaller than the distance to the vertex u. The Szeged index is closely related to the Wiener index and defined as

$$Sz(G) = \sum_{e=uv} n_u(e)n_v(e).$$

Some conclusions for Szeged index applied in chemical engineering can refer to Yousefi-Azari et al. [12]. The edge Szeged index of G is defined as

$$Sz_e(G) = \sum_{e=uv} m_u(e)m_v(e).$$

Cai and Zhou [14] determined the n-vertex unicyclic graphs with the largest, the second largest, the smallest and the second smallest edge Szeged indices. Mahmiani and Iranmanesh [15] computed the edge-Szeged index of HAC5C7 nanotube. Chiniforooshan [16] presented the molecular graphs with maximum edge Szeged index. Khalifeh et. al. [17] studied the edge Szeged index of Hamming molecular graphs and C_4-nanotubes. Zhan and Qiao [18] determined the edge Szeged index of bridge molecular graph. Gutman and. Ashrafi [19] established the basic properties of edge Szeged index. Wang and Liu [20] proposed a method of calculating the edge-Szeged index of hexagonal chain.

The definition of edge-vertex Szeged index and vertex-edge Szeged index are stated as follows:

$$Sz_{ev}(G) = \frac{1}{2}\sum_{e=uv}(m_u(e)n_v(e) + m_v(e)n_u(e)),$$

$$Sz_{ve}(G) = \frac{1}{2}\sum_{e=uv}(m_u(e)n_u(e) + m_v(e)n_v(e)).$$

Results on edge-vertex Szeged index and vertex-edge Szeged index of bridge chemical structure can refer to Alaeiyan and Asadpour [21].

The number of edges and vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $t_u(e)$. Analogously, $t_v(e)$ is the number of edges and vertices of G whose distance to the vertex v is smaller than the distance to the vertex u. The total Szeged index of G is defined as

$$Sz_T(G) = \sum_{e=uv} t_u(e)t_v(e).$$

Manuel et. al., [22] determined the total Szeged index of C_4-Nanotubes, C_4-Nanotori and Dendrimer Nanostars.

The third atom bond connectivity index was introduced as

$$ABC_3(G) = \sum_{uv\in E}\sqrt{\frac{m_u(e) + m_v(e) - 2}{m_u(e)m_v(e)}}.$$

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W. Gao is with the School of Information and Technology, Yunnan Normal University, Kunming, 650500 China e-mail: gaowei@ynnu.edu.cn.

L. Shi is with the Institute of Medical Biology, Chinese Academy of Medical Sciences and Peking Union Medical College, Kunming, 650118 China e-mail: shili.imb@gmail.com.

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The PI index of molecular graph G is denoted by

$$PI(G) = \sum_{e=uv} (m_v(e) + m_u(e)).$$

The vertex PI index of molecular graph G is defined as

$$PI_v(G) = \sum_{e=uv} (n_v(e) + n_u(e)).$$

Khalifeh et. al., [23] presented the vertex PI indices of cartesian product molecular graphs. Ashrafi et. al., [24] studied the vertex PI index of an infinite family of fullerenes. Khalifeh et. al., [25] raised a matrix method for computing vertex PI index of molecular graphs.

As the extension of PI index and vertex PI index, the PI polynomial and vertex PI polynomial are introduced by Ashrafi et. al., [26] stated as

$$PI(G, x) = \sum_{e=uv} x^{(m_v(e)+m_u(e))}$$

and

$$PI_v(G, x) = \sum_{e=uv} x^{(n_v(e)+n_u(e))}.$$

Loghman and Badakhshiana [27] determined the PI polynomial of $TUC_4C_8(S)$ nanotubes and nanotorus. Alamian et. al., [28] presented the PI polynomial of V-phenylenic nanotubes and nanotori. Loghman and Badakhshiana [29] raised the PI polynomial of zig-zag polyhex nanotubes.

Similarly, like Szeged index and edge Szeged index, the Szeged polynomial and edge Szeged polynomial are defined as

$$Se_v(G, x) = \sum_{e=uv} x^{(m_v(e)m_u(e))}$$

and

$$Se_e(G, x) = \sum_{e=uv} x^{(n_v(e)n_u(e))},$$

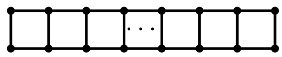
respectively. More results on Szeged polynomial and edge Szeged polynomial can refer to [30], [31] and [32].

Although there have been several advances in PI index, vertex PI index, Szeged index, edge Szeged index and atom bond connectivity index of molecular graphs, the study of edge-vertex Szeged index, vertex-edge Szeged index, total Szeged index, third atom bond connectivity index, PI polynomial, vertex PI polynomial, Szeged polynomial and edge Szeged polynomial of special chemical structures has been largely limited. In addition, as widespread and critical chemical structures, polyomino system, and hexagonal system are widely used in medical science and pharmaceutical field. As an example, polyomino chain is one of the basic chemical structures, and exists widely in benzene and alkali molecular structures. For these reasons, we have attracted tremendous academic and industrial interests to research the edge-vertex Szeged index, vertex-edge Szeged index, total Szeged index, third atom bond connectivity index, PI polynomial, vertex PI polynomial, Szeged polynomial and edge Szeged polynomial of these molecular structure from a mathematical point of view.

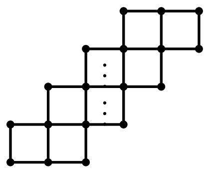
The contributions of our paper are two-fold. First, we compute the edge-vertex Szeged index, vertex-edge Szeged index, total Szeged index, third atom bond connectivity index, PI polynomial, vertex PI polynomial, Szeged polynomial and edge Szeged polynomial of unilateral polyomino chain. Second, the edge-vertex Szeged index, vertex-edge Szeged index, total Szeged index, third atom bond connectivity index, PI polynomial, vertex PI polynomial, Szeged polynomial and edge Szeged polynomial of unilateral hexagonal chain is calculated.

II. Szeged Related Indices of Unilateral Polyomino Chain

From the view of graph theory, polyomino is a finite 2-connected planar graph and each interior face is surrounded by a square with length 4. Polyomino chain is one class of polyomino such that the connection of centres for adjacent squares constitute a path $c_1c_2 \cdots c_n$, where c_i is the centre of i-th square. Polyomino chain H_n^4 is called a linear chain if the subgraph induced by all 3-degree vertices is a graph with $n-2$ squares. Furthermore, polyomino chain H_n^4 is called a Zig-zag chain if the subgraph induced by all vertices with degree > 2 is path with $n-1$ edges. In what follows, we use L_n^4 and Z_n^4 to denote linear polyomino chain and Zig-zag polyomino chain, respectively. The structure of L_n^4 and Z_n^4 can refer to Figure 1.



Linear polyomino chain



Zig-zag polyomino chain

Fig.1. The structure of L_n^4 and Z_n^4

Use the similar technology raised in Gutman and Klavzar [13], we define elementary cut as follows. Choose an edge e of the polyomino system and draw a straight line through the center of e, orthogonal on e. This line will intersect the perimeter in two end points P_1 and P_2. The straight line segment C whose end points are P_1 and P_2 is the elementary cut, intersecting the edge e. A fragment S in polyomino chain is just maximal linear chain which includes the squares in start and end vertices. Let $l(S)$ be the length of fragment which denotes the number of squares it is contained. Let H_n^4 be a polyomino chain with n squares and consist of fragment sequence $S_1, S_2, \cdots, S_m (m \geq 1)$. Denote $l(S_i) = l_i (i = 1, \cdots, m)$. It is not difficult to verify that $l_1 + l_2 + \cdots + l_m = n + m - 1$ and $|V(H_n^4)| = 2n + 2$, $|E(H_n^4)| = 3n + 1$. For the k-th fragment of polyomino chain, the cut of this fragment is the cut which intersects with $l_k + 1$ parallel edges of squares in this fragment. A fragment called horizontal fragment if its cut parallels to the horizontal direction, and called vertical fragment if its cut parallels to the vertical direction. Unilateral polyomino chain is a special kind of polyomino chain such that for each vertical fragment, two horizontal fragments (if exists) adjacent it appear in the left and right sides, respectively.

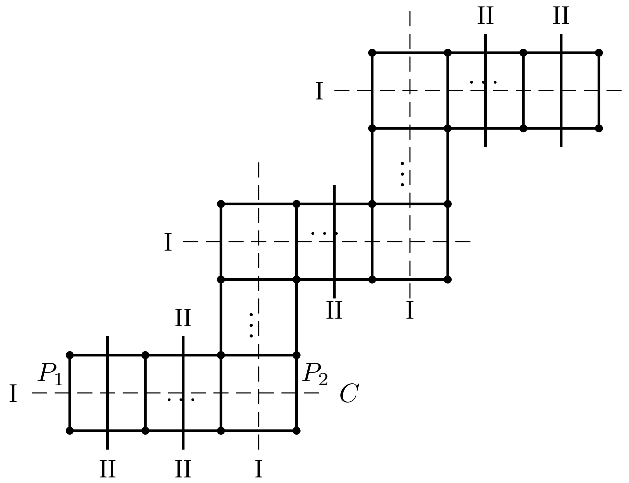


Fig.2. I-type cut and II-type cut of unilateral polyomino chain

Our main result in this section stated as follows presents the edge-vertex Szeged index, vertex-edge Szeged index and total Szeged index of unilateral polyomino chain.

Theorem 1: Let H_n^4 be a unilateral polyomino chain consisted of m fragment S_1, S_2, $\cdots$, $S_m (m \geq 1)$, and $l(S_i) = l_i (i = 1, \cdots, m)$ be the length of each fragment. Then, we have

$$
\begin{aligned}
& Sz_{ev}(H_n^4) \\
= & \sum_{j=1}^{l_1-1}[(12j-4)\sum_{i=2}^{m} l_i - (12j-4)m \\
& +(12j-4)(l_1-j)+(20j-8)] \\
& +\sum_{j=2}^{l_m}[(12l_m-12j+8)\sum_{i=1}^{m-1} l_i - (12l_m-12j \\
& +8)m+(12l_m-12j+8)j+(8l_m-8j+4))] \\
& +\sum_{k=2}^{m-1}\sum_{j=2}^{l_k-1}[(2\sum_{i=1}^{k-1} l_i - 2k+2j+2)(3\sum_{i=k+1}^{m} l_i \\
& -3(m-k)+3(l_k-j)+1)+(3\sum_{i=1}^{k-1} l_i - 3k \\
& +3j+1)(2\sum_{i=k+1}^{m} l_i - 2(m-k)+2(l_k-j)+2)] \\
& +\frac{1}{2}\sum_{k=1}^{m}(l_k+1)[(2\sum_{i=1}^{k-1} l_i - 2k+l_k+3)(3\sum_{i=k+1}^{m} l_i \\
& -3(m-k)+l_k)+(3\sum_{i=1}^{k-1} l_i - 3k+l_k \\
& +3)(2\sum_{i=k+1}^{m} l_i - 2(m-k)+l_k+1)].
\end{aligned}
$$

$$
\begin{aligned}
& Sz_{ve}(H_n^4) \\
= & \sum_{j=1}^{l_1-1}[(2\sum_{i=2}^{m} l_i - 2m+2(l_1-j)+4)(3\sum_{i=2}^{m} l_i \\
& -3m+3(l_1-j)+4)+6j^2-4j] \\
& +\sum_{j=2}^{l_m}[(2\sum_{i=1}^{m-1} l_i - 2m+2j+2)(3\sum_{i=1}^{m-1} l_i - 3m \\
& +3j+1)+(2l_m-2j+2)(3l_m-3j+1)] \\
& +\sum_{k=2}^{m-1}\sum_{j=2}^{l_k-1}[(2\sum_{i=1}^{k-1} l_i - 2k+2j+2)(3\sum_{i=1}^{k-1} l_i - 3k \\
& +3j+1)+(3\sum_{i=k+1}^{m} l_i - 3(m-k)+3(l_k-j) \\
& +1)(2\sum_{i=k+1}^{m} l_i - 2(m-k)+2(l_k-j)+2)] \\
& +\frac{1}{2}\sum_{k=1}^{m}(l_k+1)[(2\sum_{i=1}^{k-1} l_i - 2k+l_k+3)(3\sum_{i=1}^{k-1} l_i \\
& -3k+l_k+3)+(3\sum_{i=k+1}^{m} l_i - 3(m-k) \\
& +l_k)(2\sum_{i=k+1}^{m} l_i - 2(m-k)+l_k+1)].
\end{aligned}
$$

$$
\begin{aligned}
& Sz_T(H_n^4) \\
= & 2\sum_{j=1}^{l_1-1}[(5j-2)(5\sum_{i=2}^{m} l_i - 5m+5(l_1-j)+8)] \\
& +2\sum_{j=2}^{l_m}[(5\sum_{i=1}^{m-1} l_i - 5m+5j+3)(5l_m-5j+3)] \\
& +2\sum_{k=2}^{m-1}\sum_{j=2}^{l_k-1}[(5\sum_{i=1}^{k-1} l_i - 5k+5j+3)(5\sum_{i=k+1}^{m} l_i \\
& -5(m-k)+5(l_k-j)+3)] \\
& +\sum_{k=1}^{m}(l_k+1)[(5\sum_{i=1}^{k-1} l_i - 5k+2l_k+6)(5\sum_{i=k+1}^{m} l_i \\
& -5(m-k)+2l_k+1)].
\end{aligned}
$$

Proof. The cuts in H_n^4 are divided into two types: I-type and II-type (see Figure 2). An edge is called I-type (or, II-type) if it intersects with I-type (or, II-type) cut. Now, we consider the following two cases.

Case 1. If edge e is I-type in j-th square of k-th fragment (i.e., e is edge which is passed by dotted line in Figure 2). We observe that there $l_k + 1$ such edges in k-th fragment.

Subcase 1.1. If $k = 1$. Then, we have

$$n_1(e) = l_1 + 1,$$

$$n_2(e) = 2\sum_{i=2}^{m} l_i - 2m + l_1 + 3,$$

$$m_1(e) = l_1,$$

and

$$m_2(e) = 3\sum_{i=2}^{m} l_i - 3m + l_1 + 3.$$

Subcase 1.2. If $k = m$. Then, we obtain

$$n_1(e) = 2\sum_{i=1}^{m-1} l_i - 2m + l_m + 3,$$

$$n_2(e) = l_m + 1,$$

$$m_1(e) = 3\sum_{i=1}^{m-1} l_i - 3m + l_m + 3,$$

and

$$m_2(e) = l_m.$$

Subcase 1.3. If $2 \leq k \leq m-1$. Then, we get

$$n_1(e) = 2\sum_{i=1}^{k-1} l_i - 2k + l_k + 3,$$

$$n_2(e) = 2\sum_{i=k+1}^{m} l_i - 2(m-k) + l_k + 1,$$

$$m_1(e) = 3\sum_{i=1}^{k-1} l_i - 3k + l_k + 3,$$

and

$$m_2(e) = 2\sum_{i=k+1}^{m} l_i - 3(m-k) + l_k.$$

Case 2. If edge e is II-type in j-th square of k-th fragment (i.e., e is edge which is passed by real line in Figure 2).

Subcase 2.1. If $k = 1$. Then, we yield

$$n_1(e) = 2j,$$

$$n_2(e) = 2\sum_{i=2}^{m} l_i - 2m + 2(l_1 - j) + 4,$$

$$m_1(e) = 3j - 2,$$

and

$$m_2(e) = 3\sum_{i=2}^{m} l_i - 3m + 3(l_1 - j) + 4.$$

Subcase 2.2. If $k = m$. Then, we infer

$$n_1(e) = 2\sum_{i=1}^{m-1} l_i - 2m + 2j + 2,$$

$$n_2(e) = 2l_m - 2j + 2,$$

$$m_1(e) = 3\sum_{i=1}^{m-1} l_i - 3m + 3j + 1,$$

and

$$m_2(e) = 3l_m - 3j + 1.$$

Subcase 2.3. If $2 \leq k \leq m-1$. Then, we deduce

$$n_1(e) = 2\sum_{i=1}^{k-1} l_i - 2k + 2j + 2,$$

$$n_2(e) = 2\sum_{i=k+1}^{m} l_i - 2(m-k) + 2(l_k - j) + 2,$$

$$m_1(e) = 3\sum_{i=1}^{k-1} l_i - 3k + 3j + 1,$$

and

$$m_2(e) = 3\sum_{i=k+1}^{m} l_i - 3(m-k) + 3(l_k - j) + 1.$$

Hence, by combining the above cases and the definition of the edge-vertex Szeged index, vertex-edge Szeged index and total Szeged index, we obtain

$$\begin{aligned}
& Sz_{ev}(H_n^4) \\
= \; & \frac{1}{2}\{2\sum_{j=1}^{l_1-1}[2j(3\sum_{i=2}^{m} l_i - 3m + 3(l_1 - j) + 4) \\
& +(3j-2)(2\sum_{i=2}^{m} l_i - 2m + 2(l_1 - j) + 4)] \\
& +2\sum_{j=2}^{l_m}[(2\sum_{i=1}^{m-1} l_i - 2m + 2j + 2)(3l_m - 3j + 1) \\
& +(3\sum_{i=1}^{m-1} l_i - 3m + 3j + 1)(2l_m - 2j + 2)] \\
& +2\sum_{k=2}^{m-1}\sum_{j=2}^{l_k-1}[(2\sum_{i=1}^{k-1} l_i - 2k + 2j + 2)(3\sum_{i=k+1}^{m} l_i \\
& -3(m-k) + 3(l_k - j) + 1) \\
& +(3\sum_{i=1}^{k-1} l_i - 3k + 3j + 1)(2\sum_{i=k+1}^{m} l_i \\
& -2(m-k) + 2(l_k - j) + 2)] \\
& +\sum_{k=1}^{m}(l_k + 1)[(2\sum_{i=1}^{k-1} l_i - 2k + l_k + 3)(3\sum_{i=k+1}^{m} l_i \\
& -3(m-k) + l_k) \\
& +(3\sum_{i=1}^{k-1} l_i - 3k + l_k + 3)(2\sum_{i=k+1}^{m} l_i - 2(m-k) \\
& +l_k + 1)]\}.
\end{aligned}$$

$$\begin{aligned}
& Sz_{ve}(H_n^4) \\
= \; & \frac{1}{2}\{2\sum_{j=1}^{l_1-1}[2j(3j-2) + (2\sum_{i=2}^{m} l_i - 2m + 2(l_1 - j) \\
& +4)(3\sum_{i=2}^{m} l_i - 3m + 3(l_1 - j) + 4)] \\
& +2\sum_{j=2}^{l_m}[(2\sum_{i=1}^{m-1} l_i - 2m + 2j + 2)(3\sum_{i=1}^{m-1} l_i \\
& -3m + 3j + 1) + (2l_m - 2j + 2)(3l_m - 3j + 1)] \\
& +2\sum_{k=2}^{m-1}\sum_{j=2}^{l_k-1}[(2\sum_{i=1}^{k-1} l_i - 2k + 2j + 2)(3\sum_{i=1}^{k-1} l_i \\
& -3k + 3j + 1) + (3\sum_{i=k+1}^{m} l_i - 3(m-k) + 3(l_k - j) \\
& +1)(2\sum_{i=k+1}^{m} l_i - 2(m-k) + 2(l_k - j) + 2)] \\
& +\sum_{k=1}^{m}(l_k + 1)[(2\sum_{i=1}^{k-1} l_i - 2k + l_k + 3)(3\sum_{i=1}^{k-1} l_i \\
& -3k + l_k + 3) + (3\sum_{i=k+1}^{m} l_i - 3(m-k) + \\
& l_k)(2\sum_{i=k+1}^{m} l_i - 2(m-k) + l_k + 1)]\}.
\end{aligned}$$

$$\begin{aligned}
& Sz_T(H_n^4) \\
= \;& 2\sum_{j=1}^{l_1-1}[(2j+3j-2)\times(2\sum_{i=2}^{m}l_i-2m+2(l_1-j) \\
& +4+3\sum_{i=2}^{m}l_i-3m+3(l_1-j)+4)] \\
& +2\sum_{j=2}^{l_m}[(2\sum_{i=1}^{m-1}l_i-2m+2j+2+3\sum_{i=1}^{m-1}l_i-3m \\
& +3j+1)\times(2l_m-2j+2+3l_m-3j+1)] \\
& +2\sum_{k=2}^{m-1}\sum_{j=2}^{l_k-1}[(2\sum_{i=1}^{k-1}l_i-2k+2j+2+3\sum_{i=1}^{k-1}l_i \\
& -3k+3j+1) \\
& \times(3\sum_{i=k+1}^{m}l_i-3(m-k)+3(l_k-j)+1 \\
& +2\sum_{i=k+1}^{m}l_i-2(m-k)+2(l_k-j)+2)] \\
& +\sum_{k=1}^{m}(l_k+1)[(2\sum_{i=1}^{k-1}l_i-2k+l_k+3 \\
& +3\sum_{i=1}^{k-1}l_i-3k+l_k+3) \\
& \times(3\sum_{i=k+1}^{m}l_i-3(m-k)+l_k+2\sum_{i=k+1}^{m}l_i \\
& -2(m-k)+l_k+1)].
\end{aligned}$$

The desired conclusion is yielded by arranging above formulas. □

Corollary 2: Let L_n^4 be the linear chain with n squares. Then, we have

$$Sz_{ev}(L_n^4)=3n^3+4n^2-7n+4,$$

$$Sz_{ve}(L_n^4)=5n^3-2n^2+3n-2,$$

$$Sz_T(L_n^4)=\frac{37}{3}n^3+13n^2-\frac{61}{3}n+13.$$

Proof. Using the definition of linear chain, we have $m=1$, $l_1=n$, $l_2=\cdots=l_m=0$. In terms of Theorem 1, we immediately get the result. □

Corollary 3: Let Z_n^4 be the Zig-zag chain with n squares. Then, we get

$$Sz_{ev}(Z_n^4)=3m^3+\frac{21}{2}m^2+\frac{41}{2}m+8,$$

$$Sz_{ve}(Z_n^4)=6m^3+\frac{45}{2}m^2+\frac{35}{2}m+8,$$

$$Sz_T(Z_n^4)=\frac{25}{2}m^3+\frac{75}{2}m^2+85m+36.$$

Proof. By virtue of the definition of Zig-zag chain, we have $m=n-1$, and $l_1=l_2=\cdots=l_m=2$. In view of Theorem 1, the result is immediately obtained. □

By what we obtained in the proving procedures, we infer the following conclusions on the third atom bond connectivity index.

Theorem 4: Let H_n^4 be a unilateral polyomino chain consisted of m fragment S_1, S_2, $\cdots$, $S_m (m\geq 1)$, and $l(S_i)=l_i (i=1,\cdots,m)$ be the length of each fragment. Then, we have

$$\begin{aligned}
& ABC_3(H_n^4) \\
= \;& 2\sum_{j=1}^{l_1-1}\sqrt{\frac{3\sum_{i=1}^{m}l_i-3m}{(3j-2)(3\sum_{i=1}^{m}l_i-3m-3j+4)}} \\
& +2\sum_{j=2}^{l_m}\{(3\sum_{i=1}^{m}l_i-3m)/((3\sum_{i=1}^{m-1}l_i-3m+3j \\
& +1)(3l_m-3j+1))\}^{\frac{1}{2}} \\
& +2\sum_{k=2}^{m-1}\sum_{j=2}^{l_k-1}\{(3\sum_{i=1}^{m}l_i-3m)/((3\sum_{i=1}^{k-1}l_i-3k+3j \\
& +1)(3\sum_{i=k}^{m}l_i-3(m-k+j)+1))\}^{\frac{1}{2}} \\
& +\sum_{k=1}^{m}(l_k+1)\{(3\sum_{i=1}^{k-1}l_i+2l_k+3\sum_{i=k+1}^{m}l_i-3m \\
& +1)/((3\sum_{i=1}^{k-1}l_i-3k+3+l_k)(3\sum_{i=k+1}^{m}l_i-3(m-k) \\
& +l_k))\}^{\frac{1}{2}}.
\end{aligned}$$

Corollary 5: Let L_n^4 be the linear chain with n squares. Then, we have

$$\begin{aligned}
ABC_3(L_n^4) \;=\; & 2\sum_{j=1}^{n-1}\sqrt{\frac{3n-3}{(3j-2)(3n-3j+1)}} \\
& +2\sum_{j=2}^{n}\sqrt{\frac{3n-3}{(3j-2)(3n-3j+1)}} \\
& +\frac{(n+1)\sqrt{2n-2}}{n}.
\end{aligned}$$

Corollary 6: Let Z_n^4 be the Zig-zag chain with n squares. Then, we have

$$\begin{aligned}
ABC_3(Z_n^4) \;=\; & 2\sqrt{\frac{3m}{3m+1}} \\
& +3\sum_{k=1}^{m}\sqrt{\frac{3m-1}{(3k-1)(3(m-k)+2)}}.
\end{aligned}$$

Furthermore, we get the following conclusions on PI and Szeged polynomials.

Theorem 7: Let H_n^4 be a unilateral polyomino chain consisted of m fragment S_1, S_2, $\cdots$, $S_m (m\geq 1)$, and $l(S_i)=l_i (i=1,\cdots,m)$ be the length of each fragment. Then, we have

$$\begin{aligned}
& PI(H_n^4) \\
= \;& 2(l_1+l_m-2)(3\sum_{i=1}^{m}l_i-3m+2) \\
& +2\sum_{k=2}^{m-1}\sum_{j=2}^{l_k-1}(3\sum_{i=1}^{m}l_i-3m+2) \\
& +\sum_{k=1}^{m}(l_k+1)(3\sum_{i=1}^{k-1}l_i+2l_k+3\sum_{i=k+1}^{m}l_i-3m+3).
\end{aligned}$$

Corollary 8: Let L_n^4 be the linear chain with n squares. Then, we have

$$PI(L_n^4) = 14n^2 - 14n + 4.$$

Corollary 9: Let Z_n^4 be the Zig-zag chain with n squares. Then, we have

$$PI(Z_n^4) = 9m^2 + 15m + 8.$$

Theorem 10: Let H_n^4 be a unilateral polyomino chain consisted of m fragment S_1, S_2, $\cdots$, $S_m (m \geq 1)$, and $l(S_i) = l_i (i = 1, \cdots, m)$ be the length of each fragment. Then, we have

$$\begin{aligned} PI_v(H_n^4) &= 2(l_1 + l_m - 2)(2n+2) \\ &+ 2\sum_{k=2}^{m-1}\sum_{j=2}^{l_k-1}(2n+2) + \sum_{k=1}^{m}(l_k+1)(2n+2). \end{aligned}$$

Corollary 11: Let L_n^4 be the linear chain with n squares. Then, we have

$$PI_v(L_n^4) = 10n^2 + 4n - 6.$$

Corollary 12: Let Z_n^4 be the Zig-zag chain with n squares. Then, we have

$$PI_v(Z_n^4) = 6m^2 + 20m + 16.$$

Theorem 13: Let H_n^4 be a unilateral polyomino chain consisted of m fragment S_1, S_2, $\cdots$, $S_m (m \geq 1)$, and $l(S_i) = l_i (i = 1, \cdots, m)$ be the length of each fragment. Then, we have

$$\begin{aligned} & PI(H_n^4, x) \\ = \; & 2(l_1 + l_m - 2)x^{3\sum_{i=1}^m l_i - 3m + 2} \\ & + 2\sum_{k=2}^{m-1}\sum_{j=2}^{l_k-1} x^{3\sum_{i=1}^m l_i - 3m + 2} \\ & + \sum_{k=1}^{m}(l_k+1)x^{3\sum_{i=1}^{k-1} l_i + 2l_k + 3\sum_{i=k+1}^m l_i - 3m + 3}. \end{aligned}$$

Corollary 14: Let L_n^4 be the linear chain with n squares. Then, we have

$$PI(L_n^4, x) = 4(n-1)x^{3n-1} + (n+1)x^{2n}.$$

Corollary 15: Let Z_n^4 be the Zig-zag chain with n squares. Then, we have

$$PI(Z_n^4, x) = 4x^{3m+2} + 3mx^{3m+1}.$$

Theorem 16: Let H_n^4 be a unilateral polyomino chain consisted of m fragment S_1, S_2, $\cdots$, $S_m (m \geq 1)$, and $l(S_i) = l_i (i = 1, \cdots, m)$ be the length of each fragment. Then, we have

$$\begin{aligned} PI_v(H_n^4, x) &= 2(l_1 + l_m - 2)x^{(2n+2)} \\ &+ 2\sum_{k=2}^{m-1}\sum_{j=2}^{l_k-1} x^{(2n+2)} + \sum_{k=1}^{m}(l_k+1)x^{(2n+2)}. \end{aligned}$$

Corollary 17: Let L_n^4 be the linear chain with n squares. Then, we have

$$PI_v(L_n^4, x) = (5n-3)x^{2n+2}.$$

Corollary 18: Let Z_n^4 be the Zig-zag chain with n squares. Then, we have

$$PI_v(Z_n^4, x) = (3m+4)x^{2m+4}.$$

Theorem 19: Let H_n^4 be a unilateral polyomino chain consisted of m fragment S_1, S_2, $\cdots$, $S_m (m \geq 1)$, and $l(S_i) = l_i (i = 1, \cdots, m)$ be the length of each fragment. Then, we have

$$\begin{aligned} & Se_v(H_n^4, x) \\ = \; & 2\sum_{j=1}^{l_1-1} x^{2j(2\sum_{i=1}^m l_i - 2m - 2j + 4)} \\ & + 2\sum_{j=2}^{l_m} x^{(2\sum_{i=1}^m l_i - 2m + 2)(2l_m - 2j + 2)} \\ & + 2\sum_{k=2}^{m-1}\sum_{j=2}^{l_k-1}\{x^{2\sum_{i=1}^m l_i - 2k + 2j + 2} \\ & \cdot x^{2\sum_{i=k}^m l_i - 2(m-k+j) + 2}\} \\ & + \sum_{k=1}^{m}(l_k+1)\{x^{2\sum_{i=1}^{k-1} l_i + l_k - 2k + 3} \\ & \cdot x^{2\sum_{i=k+1}^m l_i - 2(m-k) + l_k + 1}\}. \end{aligned}$$

Corollary 20: Let L_n^4 be the linear chain with n squares. Then, we have

$$\begin{aligned} Se_v(L_n^4, x) &= 2\sum_{j=1}^{n-1} x^{2j(2\sum_{i=1}^m l_i - 2j + 2)} \\ &+ 2\sum_{j=2}^{n} x^{(2\sum_{i=1}^m l_i)(2n - 2j + 2)} + (n+1)x^{2n+2}. \end{aligned}$$

Corollary 21: Let Z_n^4 be the Zig-zag chain with n squares. Then, we have

$$\begin{aligned} Se_v(Z_n^4, x) &= 2x^{2(2m+2)} + 2x^{6(2m+2)} \\ &+ \sum_{k=1}^{m} 3x^{(2k+1)(2m-2k-1)}. \end{aligned}$$

Theorem 22: Let H_n^4 be a unilateral polyomino chain consisted of m fragment S_1, S_2, $\cdots$, $S_m (m \geq 1)$, and $l(S_i) = l_i (i = 1, \cdots, m)$ be the length of each fragment. Then, we have

$$\begin{aligned} & Se_e(H_n^4) \\ = \; & 2\sum_{j=1}^{l_1-1} x^{(3j-2)(3\sum_{i=1}^m l_i - 3m - 3j + 4)} \\ & + 2\sum_{j=2}^{l_m} x^{((3\sum_{i=1}^{m-1} l_i - 3m + 3j + 1)(3l_m - 3j + 1))} \\ & + 2\sum_{k=2}^{m-1}\sum_{j=2}^{l_k-1} x^{3\sum_{i=1}^{k-1} l_i - 3k + 3j + 1} \\ & \cdot x^{3\sum_{i=k}^m l_i - 3(m-k+j) + 1} \\ & + \sum_{k=1}^{m}(l_k+1)x^{3\sum_{i=1}^{k-1} l_i - 3k + 3 + l_k} \\ & \cdot x^{3\sum_{i=k+1}^m l_i - 3(m-k) + l_k}. \end{aligned}$$

Corollary 23: Let L_n^4 be the linear chain with n squares. Then, we have

$$Se_e(L_n^4,x) = 2\sum_{j=1}^{n-1} x^{(3j-2)(3n-3j+1)} +2\sum_{j=2}^{n} x^{(3j-2)(3n-3j+1)} + (n+1)x^{2n}.$$

Corollary 24: Let Z_n^4 be the Zig-zag chain with n squares. Then, we have

$$Se_e(Z_n^4,x) = 4x^{3m+1} + \sum_{k=1}^{m} 3x^{(3k-1)(3m-3k-4)}.$$

III. Szeged Related Indices of Unilateral Hexagonal Chain

Hexagonal chain is one class of hexagonal system which is made up of hexagonal. In hexagonal chain, each two hexagonals has one common edge or no common vertex. Two hexagonals are adjacented if they have common edge. No three or more hexagonals share one vertex. Each hexagonal has two adjacent hexagonals except hexagonals in terminus, and each hexagonal chain has two hexagonals in terminus.

It is easy to verify that the hexagonal chain with n hexagonals has $4n+2$ vertices and $5n+1$ edges. Let L_n^6 and Z_n^6 be the linear hexagonal chain and Zig-zag hexagonal chain, respectively. The chemical structure of L_n^6 and Z_n^6 can refer to Figure 3 for more details.

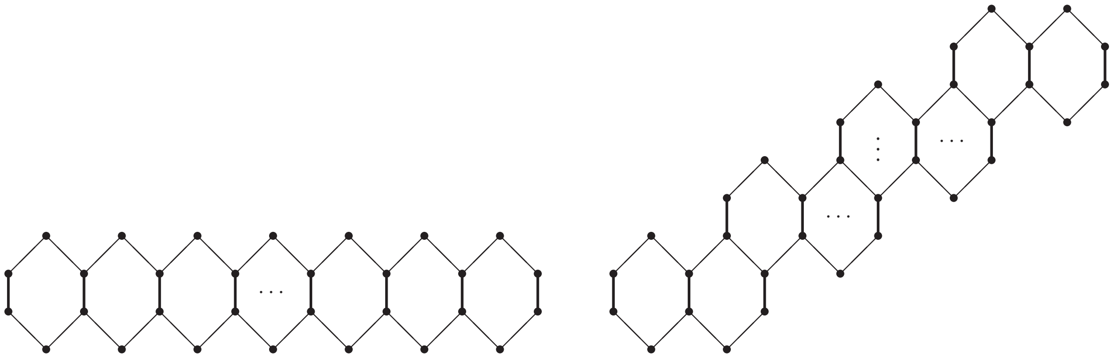
Again, we use the similar trick which was presented in Gutman and Klavzar [13], and we define elementary cut as follows. Choose an edge e of the hexagonal system and draw a straight line through the center of e, orthogonal on e. This line will intersect the perimeter in two end points P_1 and P_2. The straight line segment C whose end points are P_1 and P_2 is the elementary cut, intersecting the edge e. A fragment S in hexagonal chain is just maximal linear chain which include the hexagonals in start and end vertices. Let $l'(S)$ be the length of fragment which denotes the number of hexagonals it is contained. Let H_n^6 be a hexagonal chain with n hexagonals and consist of fragment sequence S_1, S_2, $\cdots$, $S_m (m \geq 1)$. Denote $l'(S_i) = l_i^{'} (i = 1, \cdots, m)$. Then, we verify that $l_1^{'} + l_2^{'} + \cdots + l_m^{'} = n+m-1$ since each two adjacent fragment have one common hexagonal. For the k-th fragment of hexagonal chain, the cut of this fragment is the cut which intersects with $l_k^{'}+1$ parallel edges of hexagonals in this fragment. A fragment called horizontal fragment if its cut parallels to the horizontal direction, otherwise called inclined fragment. Unilateral hexagonal chain is a special class of hexagonal chain such that the cut for each inclined fragment at the same angle with a horizontal direction. As an example, Figure 4 shows a structure of unilateral hexagonal chain. Clearly, linear hexagonal chain L_n^6 is a unilateral hexagonal chain with one fragment, and Zig-zag is a unilateral hexagonal chain with $n-1$ fragments.

We now show the edge-vertex Szeged index, vertex-edge Szeged index and total Szeged index of unilateral hexagonal chain.

Theorem 25: Let H_n^6 be a unilateral hexagonal chain consisted of m fragment S_1, S_2, $\cdots$, $S_m (m \geq 1)$, and $l'(S_i) = l_i^{'} (i = 1, \cdots, m)$ be the length of each fragment. Then, we have

$$\begin{aligned}
&Sz_{ev}(H_n^6)\\
=\ & 2\sum_{j=1}^{l_1^{'}-1}\{(4j-1)(5(\sum_{i=k+1}^{m} l_i^{'} - m + k) + 2l_k)\\
&+(5(\sum_{i=1}^{k-1} l_i^{'} - k + 1) + 2l_k^{'})(4(\sum_{i=2}^{m} l_i^{'} - m + 1)\\
&+4l_1^{'} - 4j + 3)\}\\
&+\sum_{k=1}^{m-1}\{(4(\sum_{i=1}^{k} l_i^{'} - k + 1) - 1)(5(\sum_{i=k+1}^{m} l_i^{'} - m + k)\\
&+2l_k^{'}) + (5(\sum_{i=1}^{k-1} l_i^{'} - k + 1) + 2l_k^{'})(4(\sum_{i=k+1}^{m} l_i^{'}\\
&-m + k) + 3)\}\\
&+2\sum_{k=2}^{m-1}\sum_{j=2}^{l_k^{'}-1}\{(4(\sum_{i=1}^{k-1} l_i^{'} - k + 1) + 4j - 1)\times\\
&(5(\sum_{i=k+1}^{m} l_i^{'} - m + k) + 2l_k^{'}) + (5(\sum_{i=1}^{k-1} l_i^{'} - k + 1)\\
&+2l_k^{'})(4(\sum_{i=k+1}^{m} l_i^{'} - m + k) + 4l_k^{'} - 4j + 3)\}\\
&+2\sum_{j=2}^{l_m^{'}}\{(4(\sum_{i=1}^{m-1} l_i^{'} - m + 1) + 4j - 1)(5(\sum_{i=k+1}^{m} l_i^{'}\\
&-m + k) + 2l_k^{'}) + (5(\sum_{i=1}^{k-1} l_i^{'} - k + 1)\\
&+2l_k^{'})(4l_m^{'} - 4j + 3)\}\\
&+\frac{1}{2}\sum_{k=2}^{m-1}(l_k^{'} + 1)\{((4(\sum_{i=1}^{k-1} l_i^{'} - k + 1) + 2l_k^{'}\\
&+1)(5(\sum_{i=k}^{m} l_i^{'} - m + k) - 5j + 2) + (5(\sum_{i=1}^{k-1} l_i^{'}\\
&-k + 1) + 5j - 3)(4(\sum_{i=k+1}^{m} l_i^{'} - m + k) + 2l_k^{'}\\
&+1))\}.
\end{aligned}$$

$$\begin{aligned}
&Sz_{ve}(H_n^6)\\
=\ & 2\sum_{j=1}^{l_1^{'}-1}\{(4j-1)(5(\sum_{i=1}^{k-1} l_i^{'} - k + 1) + 2l_k^{'})\\
&+(4(\sum_{i=2}^{m} l_i^{'} - m + 1) + 4l_1^{'} - 4j + 3)(5(\sum_{i=k+1}^{m} l_i^{'}\\
&-m + k) + 2l_k^{'})\}\\
&+\sum_{k=1}^{m-1}\{(4(\sum_{i=1}^{k} l_i^{'} - k + 1) - 1)(5(\sum_{i=1}^{k-1} l_i^{'} - k + 1)\\
&+2l_k^{'}) + (4(\sum_{i=k+1}^{m} l_i^{'} - m + k) + 3)(5(\sum_{i=k+1}^{m} l_i^{'} - m
\end{aligned}$$



Linear hexagonal chain   Zig-zag hexagonal chain

Fig.3. The structure of L_n^6 and Z_n^6

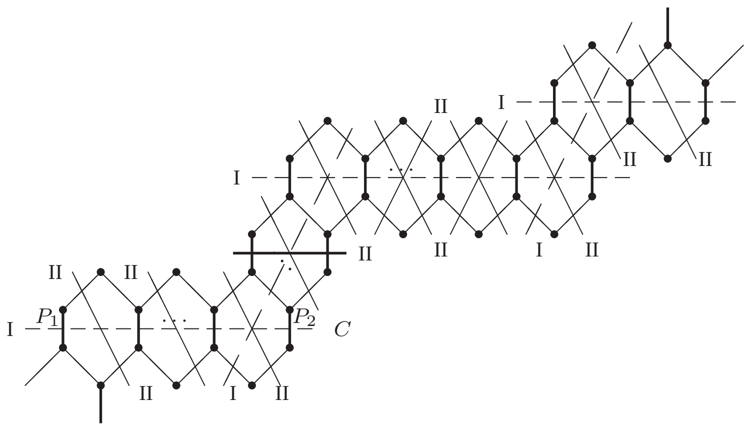


Fig. 4. I-type cut and II-type cut of unilateral hexagonal chain

$$+k)+2l_k^{'})\}$$

$$+2\sum_{k=2}^{m-1}\sum_{j=2}^{l_k^{'}-1}\{(4(\sum_{i=1}^{k-1}l_i^{'}-k+1)+4j-1)(5(\sum_{i=1}^{k-1}l_i^{'}-k$$

$$+1)+2l_k^{'})+(4(\sum_{i=k+1}^{m}l_i^{'}-m+k)+4l_k^{'}-4j$$

$$+3)(5(\sum_{i=k+1}^{m}l_i^{'}-m+k)+2l_k^{'})\}$$

$$+2\sum_{j=2}^{l_m^{'}}\{(4(\sum_{i=1}^{m-1}l_i^{'}-m+1)+4j-1)(5(\sum_{i=1}^{k-1}l_i^{'}$$

$$-k+1)+2l_k^{'})+(4l_m^{'}-4j+3)(5(\sum_{i=k+1}^{m}l_i^{'}$$

$$-m+k)+2l_k^{'})\}$$

$$+\frac{1}{2}\sum_{k=2}^{m-1}(l_k^{'}+1)\{(4(\sum_{i=1}^{k-1}l_i^{'}-k+1)+2l_k^{'}$$

$$+1)(5(\sum_{i=1}^{k-1}l_i^{'}-k+1)+5j-3)+(4(\sum_{i=k+1}^{m}l_i^{'}$$

$$-m+k)+2l_k^{'}+1)(5(\sum_{i=k}^{m}l_i^{'}-m+k)-5j+2)\}.$$

$$Sz_T(H_n^6)$$

$$=4\sum_{j=1}^{l_1^{'}-1}(5(\sum_{i=1}^{k-1}l_i^{'}-k+1)+2l_k^{'}+4j-1)\times(4\sum_{i=1}^{m}l_i^{'}$$

$$+5\sum_{i=k+1}^{m}l_i^{'}-4j+7-9m+5k+2l_k^{'})$$

$$+2\sum_{k=1}^{m-1}(9\sum_{i=1}^{k-1}l_i^{'}-9k+8+6l_k^{'})\times(9\sum_{i=k+1}^{m}l_i^{'}$$

$$-9m+9k+3+2l_k^{'})$$

$$+4\sum_{k=2}^{m-1}\sum_{j=2}^{l_k^{'}-1}(9(\sum_{i=1}^{k-1}l_i^{'}-k+1)+4j-1+2l_k^{'})$$

$$\times(9(\sum_{i=k+1}^{m}l_i^{'}-m+k)+6l_k^{'}-4j+3)$$

$$+4\sum_{j=2}^{l_m^{'}}(4\sum_{i=1}^{m-1}l_i^{'}+5\sum_{i=1}^{k-1}l_i^{'}-4m+4j-5k+8$$

$$+2l_k^{'})(9l_m^{'}-4j+3+5\sum_{i=k+1}^{m-1}l_i^{'}-5m+5k+2l_k^{'})$$

$$+\sum_{k=2}^{m-1}(l_k^{'}+1)(9\sum_{i=1}^{k-1}l_i^{'}-9k+2l_k^{'}+7+5j)$$

$$\times(9\sum_{i=k+1}^{m}l_i^{'}-9m+9k+6l_k^{'}+3-5j).$$

Proof. The cuts in H_n^6 are divided into two types: I-type and II-type (see Figure 4). An edge is called I-type if it intersects with I-type cut. Also, an edge is called II-type if it intersects with II-type cut. In what follows, we consider two situations according to the type of edge.

Case 1. If edge e is I-type in j-th square of k-th fragment (i.e., e is edge which is passed by dotted line in Figure 4). Then, the value of $m_1(e)$ and $m_2(e)$ is calculated as follows:

$$m_1(e) = 5(\sum_{i=1}^{k-1} l_i^{'} - k + 1) + 5j - 3,$$

$$m_2(e) = 5(\sum_{i=k}^{m} l_i^{'} - m + k) - 5j + 2.$$

Subcase 1.1. If $k = 1$. Then, we have

$$n_1(e) = 2l_1^{'} + 1$$

and

$$n_2(e) = 4\sum_{i=2}^{m}(l_i^{'} - m + 1) + 2l_1^{'} + 1.$$

Subcase 1.2. If $k = m$. Then, we obtain

$$n_1(e) = 4\sum_{i=1}^{m-1}(l_i^{'} - m + 1) + 2l_k^{'} + 1$$

and

$$n_2(e) = 2l_m^{'} + 1.$$

Subcase 1.3. If $2 \le k \le m - 1$. Then, we get

$$n_1(e) = 4\sum_{i=1}^{k-1}(l_i^{'} - k + 1) + 2l_k^{'} + 1$$

and

$$n_2(e) = 4\sum_{i=k+1}^{m}(l_i^{'} - m + k) + 2l_k^{'} + 1.$$

Case 2. If edge e is II-type in j-th square of k-th fragment (i.e., e is edge which is passed by real line in Figure 4). Then, we deduce

$$m_1(e) = 5(\sum_{i=1}^{k-1} l_i^{'} - k + 1) + 2l_k^{'},$$

$$m_2(e) = 5(\sum_{i=k+1}^{m} l_i^{'} - m + k) + 2l_k^{'}.$$

Subcase 2.1. If $k = 1$. Then, we yield

$$n_1(e) = 4j - 1$$

and

$$n_2(e) = 4\sum_{i=2}^{m} l_i^{'} + 4l_1^{'} - 4j + 3.$$

Subcase 2.2. If $k = m$. Then, we infer

$$n_1(e) = 4\sum_{i=1}^{m-1}(l_i^{'} - k + 1) + 4j - 1$$

and

$$n_2(e) = 4l_m^{'} - 4j + 3.$$

Subcase 2.3. If $2 \le k \le m - 1$. Then, we deduce

$$n_1(e) = 4\sum_{i=1}^{k-1}(l_i^{'} - k + 1) + 4j - 1$$

and

$$n_2(e) = 4\sum_{i=k+1}^{m} l_i^{'} + 4(l_k^{'} - j) + 3.$$

In particular, if $j = l_k^{'}$ in Subcase 2.3, we have $n_1(e) = 4\sum_{i=1}^{k}(l_i^{'} - k + 1) - 1$ and $n_2(e) = 4\sum_{i=k+1}^{m}(l_i^{'} - m + k) + 3$.

Hence, by combining the above cases and the definition of the the edge-vertex Szeged index, vertex-edge Szeged index and total Szeged index, we get

$$\begin{aligned}
& Sz_{ev}(H_n^6) \\
= \quad & \frac{1}{2}\{4\sum_{j=1}^{l_1^{'}-1}\{(4j-1)[5(\sum_{i=k+1}^{m} l_i^{'} - m + k) + 2l_k^{'}] \\
& +(5(\sum_{i=1}^{k-1} l_i^{'} - k + 1) + 2l_k^{'})[4(\sum_{i=2}^{m} l_i^{'} - m + 1) \\
& +4l_1^{'} - 4j + 3]\} \\
& +2\sum_{k=1}^{m-1}\{[4(\sum_{i=1}^{k} l_i^{'} - k + 1) - 1][5(\sum_{i=k+1}^{m} l_i^{'} - m \\
& +k) + 2l_k^{'}] + (5(\sum_{i=1}^{k-1} l_i^{'} - k + 1) + 2l_k^{'})[4(\sum_{i=k+1}^{m} l_i^{'} \\
& -m + k) + 3]\} \\
& +4\sum_{k=2}^{m-1}\sum_{j=2}^{l_k^{'}-1}\{[4(\sum_{i=1}^{k-1} l_i^{'} - k + 1) + 4j - 1] \times \\
& [5(\sum_{i=k+1}^{m} l_i^{'} - m + k) + 2l_k^{'}] + (5(\sum_{i=1}^{k-1} l_i^{'} - k + 1) \\
& +2l_k^{'})[4(\sum_{i=k+1}^{m} l_i^{'} - m + k) + 4l_k^{'} - 4j + 3]\} \\
& +4\sum_{j=2}^{l_m^{'}}\{[4(\sum_{i=1}^{m-1} l_i^{'} - m + 1) + 4j - 1][5(\sum_{i=k+1}^{m} l_i^{'} \\
& -m + k) + 2l_k^{'}] + (5(\sum_{i=1}^{k-1} l_i^{'} - k + 1) + 2l_k^{'})(4l_m^{'} \\
& -4j + 3)\} \\
& +\sum_{k=2}^{m-1}(l_k^{'} + 1)\{[4(\sum_{i=1}^{k-1} l_i^{'} - k + 1) + 2l_k^{'} + 1] \times \\
& (5(\sum_{i=k}^{m} l_i^{'} - m + k) - 5j + 2) + (5(\sum_{i=1}^{k-1} l_i^{'} - k + 1) \\
& +5j - 3)[4(\sum_{i=k+1}^{m} l_i^{'} - m + k) + 2l_k^{'} + 1]\}\}.
\end{aligned}$$

$$\begin{aligned}
& Sz_{ve}(H_n^6) \\
= \quad & \frac{1}{2}\{4\sum_{j=1}^{l_1^{'}-1}\{(4j-1)(5(\sum_{i=1}^{k-1} l_i^{'} - k + 1) + 2l_k^{'})
\end{aligned}$$

$$+[4(\sum_{i=2}^{m} l_i^{'}-m+1)+4l_1^{'}-4j+3][5(\sum_{i=k+1}^{m} l_i^{'}$$
$$-m+k)+2l_k^{'}]\}+2\sum_{k=1}^{m-1}\{[4(\sum_{i=1}^{k} l_i^{'}-k+1)$$
$$-1](5(\sum_{i=1}^{k-1} l_i^{'}-k+1)+2l_k^{'})+[4(\sum_{i=k+1}^{m} l_i^{'}$$
$$-m+k)+3][5(\sum_{i=k+1}^{m} l_i^{'}-m+k)+2l_k^{'}]\}$$
$$+4\sum_{k=2}^{m-1}\sum_{j=2}^{l_k^{'}-1}\{[4(\sum_{i=1}^{k-1} l_i^{'}-k+1)+4j-1](5(\sum_{i=1}^{k-1} l_i^{'}$$
$$-k+1)+2l_k^{'})+[4(\sum_{i=k+1}^{m} l_i^{'}-m+k)+4l_k^{'}-4j$$
$$+3][5(\sum_{i=k+1}^{m} l_i^{'}-m+k)+2l_k^{'}]\}$$
$$+4\sum_{j=2}^{l_m^{'}}\{[4(\sum_{i=1}^{m-1} l_i^{'}-m+1)+4j-1](5(\sum_{i=1}^{k-1} l_i^{'}$$
$$-k+1)+2l_k^{'})+(4l_m^{'}-4j+3)[5(\sum_{i=k+1}^{m} l_i^{'}$$
$$-m+k)+2l_k^{'}]\}$$
$$+\sum_{k=2}^{m-1}(l_k^{'}+1)\{[4(\sum_{i=1}^{k-1} l_i^{'}-k+1)+2l_k^{'}+1]\times$$
$$(5(\sum_{i=1}^{k-1} l_i^{'}-k+1)+5j-3)+[4(\sum_{i=k+1}^{m} l_i^{'}-m+k)$$
$$+2l_k^{'}+1](5(\sum_{i=k}^{m} l_i^{'}-m+k)-5j+2)\}\}.$$

$$\begin{aligned}
&Sz_T(H_n^6)\\
=\ &4\sum_{j=1}^{l_1^{'}-1}\{(4j-1+5(\sum_{i=1}^{k-1} l_i^{'}-k+1)+2l_k^{'})\\
&\times[4(\sum_{i=2}^{m} l_i^{'}-m+1)+4l_1^{'}-4j+3+5(\sum_{i=k+1}^{m} l_i^{'}\\
&-m+k)+2l_k^{'}]\}\\
&+2\sum_{k=1}^{m-1}\{(4(\sum_{i=1}^{k} l_i^{'}-k+1)-1+5(\sum_{i=1}^{k-1} l_i^{'}\\
&-k+1)+2l_k^{'})\times[4(\sum_{i=k+1}^{m} l_i^{'}-m+k)+3\\
&+5(\sum_{i=k+1}^{m} l_i^{'}-m+k)+2l_k^{'}]\}\\
&+4\sum_{k=2}^{m-1}\sum_{j=2}^{l_k^{'}-1}\{(4(\sum_{i=1}^{k-1} l_i^{'}-k+1)+4j-1+5(\sum_{i=1}^{k-1} l_i^{'}\\
&-k+1)+2l_k^{'})\times(4(\sum_{i=k+1}^{m} l_i^{'}-m+k)+4l_k^{'}\\
&-4j+3+5(\sum_{i=k+1}^{m} l_i^{'}-m+k)+2l_k^{'})\}\\
&+4\sum_{j=2}^{l_m^{'}}\{(4(\sum_{i=1}^{m-1} l_i^{'}-m+1)+4j-1+5(\sum_{i=1}^{k-1} l_i^{'}\\
&-k+1)+2l_k^{'})\times(4l_m^{'}-4j+3+5(\sum_{i=k+1}^{m} l_i^{'}\\
&-m+k)+2l_k^{'})\}\\
&+\sum_{k=2}^{m-1}(l_k^{'}+1)\{(4(\sum_{i=1}^{k-1} l_i^{'}-k+1)+2l_k^{'}+1\\
&+5(\sum_{i=1}^{k-1} l_i^{'}-k+1)+5j-3)\times(4(\sum_{i=k+1}^{m} l_i^{'}-m\\
&+k)+2l_k^{'}+1+5(\sum_{i=k}^{m} l_i^{'}-m+k)-5j+2)\}.
\end{aligned}$$

The desired conclusion is yielded by arranging above formulas. □

As we presented in Corollary 2 and Corollary 3, we can calculate the the edge-vertex Szeged index, vertex-edge Szeged index and total Szeged index of linear chain L_n^6 with n hexagonals and Zig-zag chain Z_n^6 with n hexagonals by virtue of the same tricks. These computations are left to the readers.

According to what we obtained in the proving procedures, we deduce the following results on third atom bond connectivity index.

Theorem 26: Let H_n^6 be a unilateral hexagonal chain consisted of m fragment S_1, S_2, $\cdots$, $S_m (m \geq 1)$, and $l'(S_i) = l_i^{'} (i = 1, \cdots, m)$ be the length of each fragment. Then, we have

$$\begin{aligned}
&ABC_3(H_n^6)\\
=\ &4\sqrt{\frac{5\sum_{i=1}^{m} l_i^{'}-5m+4}{4(5(\sum_{i=1}^{m} l_i^{'}-m+1)-3)}}\\
&+2\sum_{k=1}^{m-1}\{(5\sum_{i=1}^{m} l_i^{'}-5m+2)/((5(\sum_{i=1}^{k} l_i^{'}-k+1)\\
&-3)(5(\sum_{i=k+1}^{m} l_i^{'}-m+k)+2))\}^{\frac{1}{2}}\\
&+4\sum_{k=1}^{m}\sum_{j=2}^{l_k^{'}-1}\{(5\sum_{i=1}^{m} l_i^{'}-5m+2)/((5(\sum_{i=1}^{k-1} l_i^{'}-k+1)\\
&+5j-3)(5(\sum_{i=k}^{m} l_i^{'}-m+k)-5j+2))\}^{\frac{1}{2}}\\
&+\sum_{k=1}^{m}(l_k^{'}+1)\{(5\sum_{i=1}^{k-1} l_i^{'}+5\sum_{i=k+1}^{m} l_i^{'}+4l_k^{'}-5m\\
&+3)/((5(\sum_{i=1}^{k-1} l_i^{'}-k+1)+2l_k^{'})(5(\sum_{i=k+1}^{m} l_i^{'}-m+k)\\
&+2l_k^{'}))\}^{\frac{1}{2}}.
\end{aligned}$$

Corollary 27: Let L_n^6 be the linear chain with n hexagonals. Then, we have

$$\begin{aligned}ABC_3(L_n^6) &= 4\sqrt{\frac{5n-1}{4(5n-3)}} \\ &+4\sum_{j=2}^{n-1}\sqrt{\frac{5n-3}{(5j-3)(5n-5j+2)}} \\ &+\frac{(n+1)\sqrt{2n-2}}{n}.\end{aligned}$$

Corollary 28: Let Z_n^6 be the Zig-zag chain with n hexagonals. Then, we have

$$\begin{aligned}ABC_3(Z_n^6) &= 4\sqrt{\frac{5m+4}{4(5m+2)}} \\ &+2\sum_{k=1}^{m-1}\sqrt{\frac{5m+2}{(5k+2)(5m-5k+2)}} \\ &+3\sum_{k=1}^{m}\sqrt{\frac{5m+1}{(5k-1)(5m-5k+4)}}.\end{aligned}$$

At last, we present the following conclusions.

Theorem 29: Let H_n^6 be a unilateral hexagonal chain consisted of m fragment $S_1, S_2, \cdots, S_m (m \geq 1)$, and $l'(S_i) = l_i^{'}(i = 1, \cdots, m)$ be the length of each fragment. Then, we have

$$\begin{aligned}& PI(H_n^6) \\ = \; & 4(5\sum_{i=1}^{m} l_i^{'} - 5m + 6) + 2\sum_{k=1}^{m-1}(5\sum_{i=1}^{m} l_i^{'} - 5m + 4) \\ & +4\sum_{k=1}^{m}\sum_{j=2}^{l_k^{'}-1}(5\sum_{i=1}^{m} l_i^{'} - 5m + 4) \\ & +\sum_{k=1}^{m}(l_k^{'}+1)(5\sum_{i=1}^{k-1} l_i^{'} + 5\sum_{i=k+1}^{m} l_i^{'} + 4l_k^{'} - 5m + 5).\end{aligned}$$

Corollary 30: Let L_n^6 be the linear chain with n hexagonals. Then, we have

$$PI(L_n^6) = 24n^2 - 12n - 4.$$

Corollary 31: Let Z_n^6 be the Zig-zag chain with n hexagonals. Then, we have

$$PI(Z_n^6) = 25m^2 + 27m + 26.$$

Theorem 32: Let H_n^6 be a unilateral hexagonal chain consisted of m fragment $S_1, S_2, \cdots, S_m (m \geq 1)$, and $l'(S_i) = l_i^{'}(i = 1, \cdots, m)$ be the length of each fragment. Then, we have

$$\begin{aligned}PI_v(H_n^6) &= (4l_1^{'} + 4l_m^{'} + 2m - 10)(4n+2) \\ &+4\sum_{k=2}^{m-1}\sum_{j=2}^{l_k^{'}-1}(4n+2) \\ &+\sum_{k=2}^{m-1}(l_k^{'}+1)(4n+2).\end{aligned}$$

Corollary 33: Let L_n^6 be the linear chain with n hexagonals. Then, we have

$$PI_v(L_n^6) = 32n^2 - 16n - 16.$$

Corollary 34: Let Z_n^6 be the Zig-zag chain with n hexagonals. Then, we have

$$PI_v(Z_n^6) = 20n^2 - 10n - 10.$$

Theorem 35: Let H_n^6 be a unilateral hexagonal chain consisted of m fragment $S_1, S_2, \cdots, S_m (m \geq 1)$, and $l'(S_i) = l_i^{'}(i = 1, \cdots, m)$ be the length of each fragment. Then, we have

$$\begin{aligned}& PI(H_n^6, x) \\ = \; & 4x^{(5\sum_{i=1}^{m} l_i^{'} - 5m + 6)} + 2\sum_{k=1}^{m-1} x^{(5\sum_{i=1}^{m} l_i^{'} - 5m + 4)} \\ & +4\sum_{k=1}^{m}\sum_{j=2}^{l_k^{'}-1} x^{(5\sum_{i=1}^{m} l_i^{'} - 5m + 4)} \\ & +\sum_{k=1}^{m}(l_k^{'}+1)x^{(5\sum_{i=1}^{k-1} l_i^{'} + 5\sum_{i=k+1}^{m} l_i^{'} + 4l_k^{'} - 5m + 5)}.\end{aligned}$$

Corollary 36: Let L_n^6 be the linear chain with n hexagonals. Then, we have

$$PI(L_n^6, x) = 4(n-1)x^{5n+1} + (n+1)x^{4n}.$$

Corollary 37: Let Z_n^6 be the Zig-zag chain with n hexagonals. Then, we have

$$PI(Z_n^6, x) = 4x^{5m+6} + 2(m-1)x^{5m+4} + 3mx^{5m+3}.$$

Theorem 38: Let H_n^6 be a unilateral hexagonal chain consisted of m fragment $S_1, S_2, \cdots, S_m (m \geq 1)$, and $l'(S_i) = l_i^{'}(i = 1, \cdots, m)$ be the length of each fragment. Then, we have

$$\begin{aligned}PI_v(H_n^6, x) &= (4l_1^{'} + 4l_m^{'} + 2m - 10)x^{4n+2} \\ &+4\sum_{k=2}^{m-1}\sum_{j=2}^{l_k^{'}-1} x^{4n+2} \\ &+\sum_{k=2}^{m-1}(l_k^{'}+1)x^{4n+2}.\end{aligned}$$

Corollary 39: Let L_n^6 be the linear chain with n hexagonals. Then, we have

$$PI_v(L_n^6, x) = 8(n-1)x^{4n+2}.$$

Corollary 40: Let Z_n^6 be the Zig-zag chain with n hexagonals. Then, we have

$$PI_v(Z_n^6, x) = 5(n-1)x^{4n+2}.$$

Theorem 41: Let H_n^6 be a unilateral hexagonal chain consisted of m fragment $S_1, S_2, \cdots, S_m (m \geq 1)$, and $l'(S_i) = l_i^{'}(i = 1, \cdots, m)$ be the length of each fragment.

Then, we have

$$\begin{aligned} & Se_v(H_n^6,x) \\ = \; & 4\sum_{j=1}^{l_1'-1} x^{(4j-1)[4(\sum_{i=1}^{m} l_i'-m+1)-4j+3]} \\ & +2\sum_{k=1}^{m-1} x^{[4(\sum_{i=1}^{k} l_i'-k+1)-1][4(\sum_{i=k+1}^{m} l_i'-m+k)+3]} \\ & +4\sum_{k=2}^{m-1}\sum_{j=2}^{l_k'-1}\{x^{4(\sum_{i=1}^{k-1} l_i'-k+1)+4j-1} \\ & \cdot x^{4(\sum_{i=k}^{m} l_i'-m+k)-4j+3}\} \\ & +4\sum_{j=2}^{l_m'} x^{[4(\sum_{i=1}^{m-1} l_i'-m+1)+4j-1](4l_m'-4j+3)} \\ & +\sum_{k=2}^{m-1}(l_k'+1)\{x^{4(\sum_{i=1}^{k-1} l_i'-k+1)+2l_k'+1} \\ & \cdot x^{4(\sum_{i=k+1}^{m} l_i'-m+k)+2l_k'+1}\}. \end{aligned}$$

Corollary 42: Let L_n^6 be the linear chain with n hexagonals. Then, we have

$$\begin{aligned} Se_v(L_n^6,x) \;&=\; 4\sum_{j=1}^{n-1} x^{(4j-1)(4n-4j+3)} \\ & \quad +4\sum_{j=2}^{n} x^{(4j-1)(4n-4j+3)}. \end{aligned}$$

Corollary 43: Let Z_n^6 be the Zig-zag chain with n hexagonals. Then, we have

$$\begin{aligned} Se_v(Z_n^6,x) \;&=\; 8x^{3(4n-1)}+2\sum_{k=1}^{m-1} x^{(4k+3)(4m-4k+3)} \\ & \quad +3\sum_{k=2}^{m-1} x^{(4k+1)(4m-4k+5)}. \end{aligned}$$

Theorem 44: Let H_n^6 be a unilateral hexagonal chain consisted of m fragment S_1, S_2, $\cdots$, $S_m (m \geq 1)$, and $l'(S_i) = l_i' (i = 1, \cdots, m)$ be the length of each fragment. Then, we have

$$\begin{aligned} & Se_e(H_n^6,x) \\ = \; & 4x^{4(5(\sum_{i=1}^{m} l_i'-m+1)-3)} \\ & +2\sum_{k=1}^{m-1} x^{((5(\sum_{i=1}^{k} l_i'-k+1)-3)(5(\sum_{i=k+1}^{m} l_i'-m+k)+2))} \\ & +4\sum_{k=1}^{m}\sum_{j=2}^{l_k'-1}\{x^{5(\sum_{i=1}^{k-1} l_i'-k+1)+5j-3} \\ & \cdot x^{5(\sum_{i=k}^{m} l_i'-m+k)-5j+2}\} \\ & +\sum_{k=1}^{m}(l_k'+1)\{x^{5(\sum_{i=1}^{k-1} l_i'-k+1)+2l_k'} \\ & \cdot x^{5(\sum_{i=k+1}^{m} l_i'-m+k)+2l_k'}\}. \end{aligned}$$

Corollary 45: Let L_n^6 be the linear chain with n hexagonals. Then, we have

$$\begin{aligned} Se_e(L_n^6,x) \;&=\; 4x^{4(5n-3)}+4\sum_{j=2}^{n-1} x^{(5j-3)(5n-5j+2)} \\ & \quad +(n+1)x^{4n^2}. \end{aligned}$$

Corollary 46: Let Z_n^6 be the Zig-zag chain with n hexagonals. Then, we have

$$\begin{aligned} Se_e(Z_n^6,x) \;&=\; 4x^{4(5m+2)}+2\sum_{k=1}^{m-1} x^{((5k+2)(5m-5k+2))} \\ & \quad +\sum_{k=1}^{m} 3x^{(5k-1)(5m-5k+4)}. \end{aligned}$$

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Wei Gao , male, was born in the city of Shaoxing, Zhejiang Province, China on Feb. 13, 1981. He got two bachelor degrees on computer science from Zhejiang industrial university in 2004 and mathematics education from College of Zhejiang education in 2006. Then, he was enrolled in department of computer science and information technology, Yunnan normal university, and got Master degree there in 2009. In 2012, he got PhD degree in department of Mathematics, Soochow University, China.

Now, he acts as lecturer in the department of information, Yunnan Normal University. As a researcher in computer science and mathematics, his interests are covering two disciplines: Graph theory, Statistical learning theory, Information retrieval, and Artificial Intelligence.

Li Shi , female, is professor in department of research and development management, institute of medical biology, Chinese academy of medical sciences (CAMS) and Peking union medical college (PUMC).