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Hexagonal Chains with First Three Minimal Mostar Indices

Qiqi Xiao[1], Mingyao Zeng[1], Zikai Tang[1], Hanyuan Deng[1,*], Hongbo Hua[2]

[1] *Key Laboratory of Computing and Stochastic Mathematics (Ministry of Education), College of Mathematics and Statistics, Hunan Normal University, Changsha, Hunan 410081, P. R. China*

[2] *Faculty of Mathematics and Physics, Huaiyin Institute of Technology, 223003 Huai'an City, P. R. China*

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Abstract

The Mostar index of a graph G is defined as $Mo(G) = \sum_{e=uv\in E(G)} |n_u - n_v|$, where n_u denotes the number of vertices of G closer to u than to v and n_v denotes the number of vertices of G closer to v than to u. In this paper, we determine the first three minimal values of the Mostar index among all hexagonal chains with h hexagons, and characterize the corresponding extremal graphs by some transformations on hexagonal chains.

1 Introduction

Hexagonal systems are of great importance for theoretical chemistry because they are the molecular graphs of benzenoid hydrocarbons. A hexagonal system is a connected plane graph without cut-vertices in which all inner faces are hexagons (and all hexagons are faces), such that two hexagons are either disjoint or have exactly one common edge, and no three hexagons share a common edge.

A hexagonal system without any hexagon which has more than two neighboring hexagons is called a hexagonal chain. The set of all hexagonal chains with h hexagons is denoted by HC_h.

Let r be a hexagon of a hexagonal chain G. If r has only one neighboring hexagon, then it is said to be terminal. A hexagon r adjacent to exactly two other hexagons

*Corresponding author: hydeng@hunnu.edu.cn

possesses two vertices of degree 2 and r is angularly connected in G if these two vertices are adjacent. Each angularly connected hexagon in a hexagonal chain G is said to be a kink. The kink number of G is the number of kinks in G, denoted by $K(G)$ or K. A linear chain is a hexagonal chain without kinks. The linear chains with h hexagons is denoted by L_h. A segment is a maximal linear chain in a hexagonal chain, including the kinks and/or terminal hexagons at its end. A segment including a terminal hexagon is a terminal segment. A non-linear chain has at least two terminal segments. The number of hexagons in a segment S is called its length and is denoted by $\ell(S)$. A segment has a common kink with S is called a neighboring segment of S. The number of segments in G is called the segment number, denoted by $\ell(G)$. For any segment S of $G \in HC_h$, we have $2 \leq \ell(S) \leq h$. If $G \in HC_h$ consists of segments $S_1, S_2, \cdots, S_n$ with lengths $l_1, l_2, \cdots, l_n$, respectively, then the number of hexagons in G is equal to $h(G) = l_1 + l_2 + \cdots + l_n - n + 1$ since two neighboring segments have always one hexagon in common.

Let S be a non-terminal segment of a hexagonal chain G. If its two neighboring segments lie on different sides of the line through centers of all hexagons on S, then S is called a zigzag segment. If these segments lie on the same side of the line, then S is said to be a non-zigzag segment.

Throughout this paper, the notation and terminology of hexagonal systems are mainly taken from [1, 2].

Let $G \in HC_h$ with its vertex set $V(G)$ and edge set $E(G)$. $G - uv$ and $G + uv$ denote the graphs obtained from G by deleting an edge $uv \in E(G)$ or by adding an edge $uv \notin E(G)$, respectively. $|V(G)|$ and $|E(G)|$ denote the numbers of vertices and the number of edges of G, respectively. For any $G \in HC_h$, we have $|V(G)| = 4h + 2$ and $|E(G)| = 5h + 1$.

In 2018, Došlić et al. [3] introduced a new invariant of a connected graph G, i.e., the Mostar index, defined as

$$Mo(G) = \sum_{e=uv \in E(G)} |n_u - n_v|$$

where n_u denotes the number of vertices of G closer to u than to v, and n_v denotes the number of vertices of G closer to v than to u. They pointed out that the Mostar index measures how far a graph is from being distance-balanced [7, 8] and may be viewed of as a quantitative refinement of the distance-non-balancedness of a graph. They determined the extremal values and characterized extremal graphs for trees and unicyclic graphs, and showed how it can be efficiently computed for various classes of chemically interesting graphs using a variant of the cut method [4]. The Mostar index of bicyclic graphs was studied by Tepeh [5]. Hayat and Zhou [6] determined the cactus of order n with the largest Mostar index and gave a sharp upper bound of the Mostar index for all cacti of order n with k cycles.

Some conjectures and open problems were proposed in [3], where Problem 22 is concerned with benzenoid chains: find extremal benzenoid chains, catacondensed benzenoids and general benzenoid graphs with respect to the Mostar index. In this paper, we determine the first three minimal values of the Mostar index among all hexagonal chains with h hexagons, and characterize the corresponding extremal graphs by some transformations on hexagonal chains.

2 The hexagonal chains with the first three minimal Mostar indices

In this section, we will determine the hexagonal chains with the first three minimal Mostar indices. Firstly, we introduce some transformations on hexagonal chains and discuss the effect of the transformations on the Mostar index of hexagonal chains.

For a hexagonal chain $G \in HC_h$, let the hexagonal chains G_1 and G_2 be obtained from a hexagonal chain G by deleting a segment S_i, that is G_1 and G_2 are the connected components of $G \setminus S_i$ (see Figure 1). The number of hexagons of G_1 and G_2 will be denoted by n_1 and n_2, respectively, and $\ell(S_i) = l_i \geq 2$. Without loss of generality, we assume that $1 \leq n_1 \leq n_2$, and $h = n_1 + n_2 + l_i$.

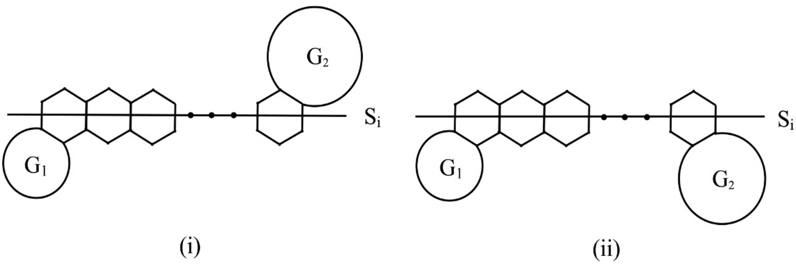

Figure 1. A hexagonal chain G with (i) a zigzag segment S_i, (ii) a non-zigzag segment S_i.

Note that a adjacent segment of S_i is a terminal segment, or a non-zigzag segment or a zigzag segment. If S_i' is a adjacent segment of S_i, and the subgraph $G_1 = (S_i' \bigcup G_1') - (S_i \bigcap S_i')$, then there are four possible structures of the hexagonal chain G, see Figure 2, where the segment of S_i' is the adjacent segment of S_i, G_1' is a subgraph of G_1, $\ell(S_i) = l_i$, $\ell(S_i') = l_i'$, G_1' contains $n_1 - l_i' + 1$ hexagons, $n_1 \geq l_i' - 1$.

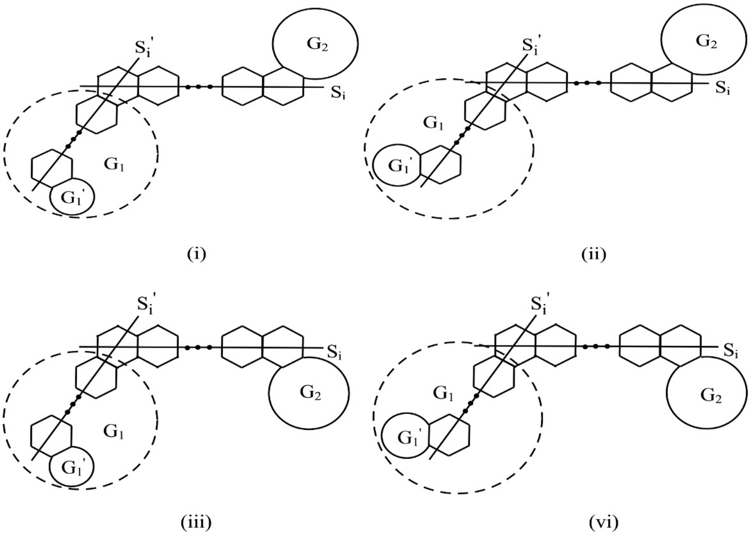

Figure 2. The four possible structures of G.

Let G be a hexagonal chain and a segment S of G. Draw a straight line through the centers of hexagons on the segment S and the edge-cut formed by all edges in S orthogonal to the straight line is called the orthogonal cut of S, which is recorded as $O(S)$. And the two components obtained by removing edges of the orthogonal edge-cut of S are its shores. The orthogonal cut of S is balanced if its shores have the same number of vertices. The contribution to the Mostar index for any edge in a balanced orthogonal cut is zero.

Two edges in the orthogonal cut of S contributes the same value to the Mostar index, i.e. for arbitrary $e_1 = v_1u_1$, $e_2 = v_2u_2 \in O(S)$, $|n_{v_1} - n_{u_1}| = |n_{v_2} - n_{u_2}|$.

In the following, we introduce some transformations on hexagonal chains and discuss the changes of their Mostar indices.

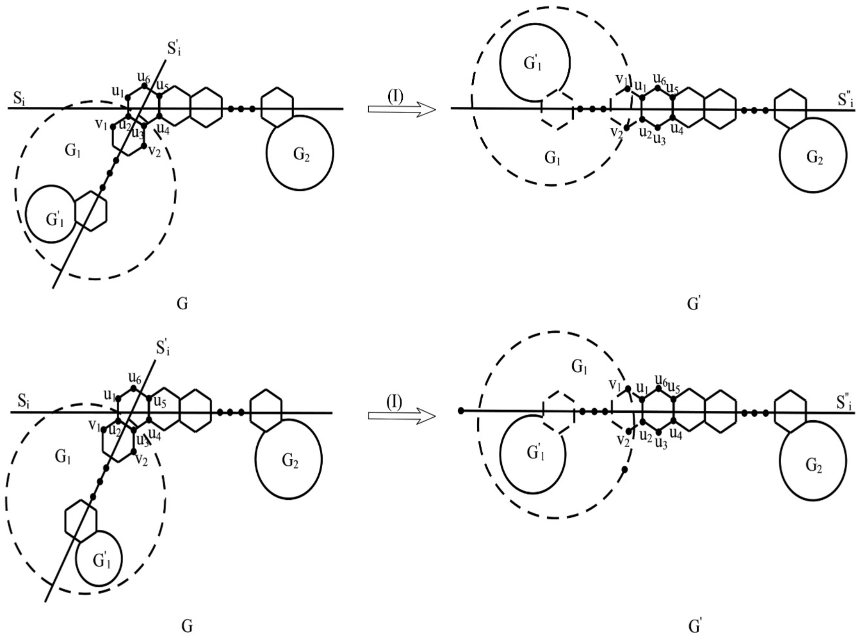

Figure 3. The kink transformation (I).

Lemma 1. (Kink transformation (I)). *Let G be a hexagonal chain with h hexagons and a non-zigzag segment S_i. $G^{'} = G - \{v_1u_2, v_2u_3\} + \{v_1u_1, v_2u_2\}$ is obtained by changing the angularly connected hexagon $u_1u_2u_3u_4u_5u_6u_1$ in $S_i \cap S_i'$ into a linearly connected hexagon, see Figure 3. Then*

$$Mo(G) > Mo(G^{'}).$$

Proof. Note that the hexagon $u_1u_2u_3u_4u_5u_6u_1$ is a kink hexagon of G, $S_i^{''}$ is a new segment of $G^{'} = G - \{v_1u_2, v_2u_3\} + \{v_1u_1, v_2u_2\}$ and G' consists of the segment $S^{''}$, $G_1^{'}$ and G_2, and the number of kinds of $G^{'}$ is one less than that of G.

From the structure of G, we know that $G_1^{'}$ contains $(n_1 - l_i^{'} + 1)$ hexagons. Two cases will be considered below. By the transformation, we can see that the contributions of edges to the Mostar index in G are changed for the orthogonal cut of S_i and $S_i^{'}$, and the contributions of the other edges to the Mostar index are not changed.

Case 1. $S_i^{'}$ is a zigzag segment or a terminal segment.

In G, the contribution of each edge uv in the orthogonal cut of S_i to $Mo(G)$ is

$$|n_u - n_v| = 4(h - l_i).$$

Since the orthogonal cut of S_i has (l_i+1) edges, the contributions of the orthogonal cut of S_i to $Mo(G)$ are

$$\sum_{uv\in O(S_i)\subseteq E(G)} |n_u - n_v| = 4(l_i+1)(h-l_i).$$

The contribution of each edge in the orthogonal cut of $S_i^{'}$ to $Mo(G)$ is

$$|n_u - n_v| = 4(n_2 + l_i + l_i^{'} - n_1 - 2).$$

And the orthogonal cut of $S_i^{'}$ have $(l_i^{'}+1)$ edges, so the contributions of the orthogonal cut of $S_i^{'}$ to $Mo(G)$ are

$$\sum_{uv\in O(S_i^{'})\subseteq E(G)} |n_u - n_v| = 4(l_i^{'}+1)(n_2 + l_i + l_i^{'} - n_1 - 2).$$

In G', the contribution of each edge in the orthogonal cut of $S_i^{''}$ to $Mo(G')$ is

$$|n_u - n_v| = 4(n_2 - n_1 + l_i^{'} - 1)$$

and the orthogonal cut of $S_i^{''}$ has $l_i+l_i^{'}$ edges, so the contributions of the edges of orthogonal cut of $S_i^{''}$ to $Mo(G^{'})$ are

$$\sum_{uv\in O(S_i^{''})\subseteq E(G^{'})} |n_u - n_v| = 4(l_i + l_i^{'})(n_2 + l_i^{'} - n_1 - 1).$$

Note that the edges of $e_1 = u_2u_3, e_2 = u_5u_6 \in S_i'$ in G, but $e_1, e_2 \notin S_i''$ in $G^{'}$, and the contributions of e_1, e_2 to $Mo(G^{'})$ are

$$\sum_{uv\in \{e_1,e_2\}\subseteq E(G^{'})} |n_u - n_v| = 2\times 4(n_2 - n_1 + l_i - 1).$$

So, we have

$$\begin{aligned}
Mo(G) - Mo(G^{'}) &= \{\sum_{uv\in O(S_i)\subseteq E(G)} |n_u - n_v| + \sum_{uv\in O(S_i^{'})\subseteq E(G)} |n_u - n_v|\} \\
&\quad - \{\sum_{uv\in O(S'')} |n_u - n_v| + \sum_{uv\in \{e_1,e_2\}\subseteq E(G^{'})} |n_u - n_v|\} \\
&= [4(l_i+1)(h-l_i) + 4(l_i^{'}+1)(n_2 + l_i + l_i^{'} - n_1 - 2)] \\
&\quad - [4(l_i + l_i^{'})(n_2 + l_i^{'} - n_1 - 1) + 2\times 4(n_2 - n_1 + l_i - 1)] \\
&= 8n_1(l_i+1) > 0
\end{aligned}$$

and $Mo(G) > Mo(G^{'})$.

Case 2. $S_i^{'}$ is a non-zigzag segment.

In G, the contribution of each edge uv in the orthogonal cut of S_i to $Mo(G)$ is

$$|n_u - n_v| = 4(h - l_i)$$

and the contributions of the orthogonal cut of S_i to $Mo(G)$ are

$$\sum_{uv \in O(S_i) \subseteq E(G)} |n_u - n_v| = 4(l_i + 1)(h - l_i).$$

The contribution of each edge in the orthogonal cut of $S_i^{'}$ to $Mo(G)$ is

$$|n_u - n_v| = 4(h - l_i^{'})$$

and the contributions of the orthogonal cut of $S_i^{'}$ to $Mo(G)$ are

$$\sum_{uv \in O(S_i^{'}) \subseteq E(G)} |n_u - n_v| = 4(l_i^{'} + 1)(h - l_i^{'}).$$

In G', the contribution of each edge in the orthogonal cut of $S_i^{''}$ to $Mo(G')$ is

$$|n_u - n_v| = 4(h - l_i - l_i^{'} + 1)$$

and the orthogonal cut of $S_i^{''}$ has $l_i + l_i^{'}$ edges, so the contributions of the edges of orthogonal cut of $S_i^{''}$ to $Mo(G^{'})$ are

$$\sum_{uv \in O(S_i^{''}) \subseteq E(G^{'})} |n_u - n_v| = 4(l_i + l_i^{'})(h - l_i - l_i^{'} + 1).$$

Note that the edges of $e_1 = u_2u_3, e_2 = u_5u_6 \in S_i^{\prime}$ in G, but $e_1, e_2 \notin S_i{}''$ in $G^{'}$, and the contributions of e_1, e_2 to $Mo(G^{'})$ are

$$\sum_{uv \in \{e_1, e_2\} \subseteq E(G^{'})} |n_u - n_v| = 2 \times 4(n_2 - n_1 + l_i - 1).$$

So, we have

$$\begin{aligned} Mo(G) - Mo(G^{'}) &= \{ \sum_{uv \in O(S_i) \subseteq E(G)} |n_u - n_v| + \sum_{uv \in O(S_i^{'}) \subseteq E(G)} |n_u - n_v| \} \\ &\quad - \{ \sum_{uv \in O(S'')} |n_u - n_v| + \sum_{uv \in \{e_1, e_2\} \subseteq E(G^{'})} |n_u - n_v| \} \\ &= [4(l_i + 1)(h - l_i) + 4(l_i^{'} + 1)(h - l_i^{'})] \\ &\quad - [4(l_i + l_i^{'})(h - l_i - l_i^{'} - n_1 + 1) + 2 \times 4(n_2 - n_1 + l_i - 1)] \\ &= 8 \times [2n_1 - l_i^{\prime} + l_i(l_i^{\prime} - 1)] > 0 \end{aligned}$$

and $Mo(G) > Mo(G^{'})$. ■

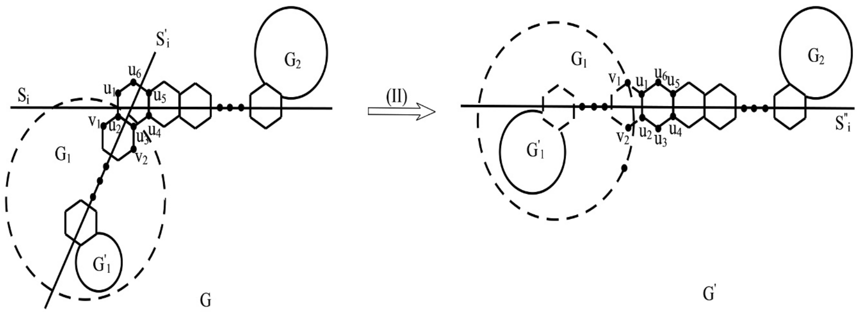

Figure 4. The kink transformation (II).

Lemma 2. (Kink transformation (II)). *Let G be a hexagonal chain with h hexagons and a zigzag segment S_i. $G^{'} = G - \{v_1u_2, v_2u_3\} + \{v_1u_1, v_2u_2\}$ is obtained by changing the angularly connected hexagon $u_1u_2u_3u_4u_5u_6u_1$ in $S_i \cap S_i'$ into a linearly connected hexagon, see Figure 4. If S_i' is a non-zigzag segment or a terminal segment, then*

$$Mo(G) \geq Mo(G^{'})$$

with equality if and only if S_i' is a terminal segment.

Proof. As in the proof of Lemma 1, the contribution of each edge uv in the orthogonal cut of S_i in G to $Mo(G)$ is

$$|n_u - n_v| = 4(n_2 - n_1)$$

and the contributions of the orthogonal cut of S_i to $Mo(G)$ are

$$\sum_{uv \in O(S_i) \subseteq E(G)} |n_u - n_v| = 4(l_i + 1)(n_2 - n_1).$$

The contribution of each edge in the orthogonal cut of $S_i^{'}$ to $Mo(G)$ is

$$|n_u - n_v| = 4(h - l_i^{'})$$

and the contributions of the orthogonal cut of $S_i^{'}$ to $Mo(G)$ are

$$\sum_{uv \in O(S_i^{'}) \subseteq E(G)} |n_u - n_v| = 4(l_i^{'} + 1)(h - l_i^{'}).$$

In G', the contribution of each edge in the orthogonal cut of $S_i^{''}$ to $Mo(G')$ is

$$|n_u - n_v| = 4(n_2 - n_1 + l_i' - 1)$$

and the contributions of the edges of orthogonal cut of $S_i^{''}$ to $Mo(G^{'})$ are

$$\sum_{uv\in O(S_i^{''})\subseteq E(G^{'})} |n_u - n_v| = 4(l_i + l_i^{'})(n_2 - n_1 + l_i^{\prime} - 1).$$

The contributions of e_1, e_2 to $Mo(G^{'})$ are

$$\sum_{uv\in\{e_1,e_2\}\subseteq E(G^{'})} |n_u - n_v| = 2 \times 4(n_2 - n_1 + l_i - 1).$$

So, we have

$$\begin{aligned} Mo(G) - Mo(G^{'}) &= \{\sum_{uv\in O(S_i)\subseteq E(G)} |n_u - n_v| + \sum_{uv\in O(S_i^{'})\subseteq E(G)} |n_u - n_v|\} \\ &\quad - \{\sum_{uv\in O(S^{''})} |n_u - n_v| + \sum_{uv\in\{e_1,e_2\}\subseteq E(G^{'})} |n_u - n_v|\} \\ &= [4(l_i + 1)(n_2 - n_1) + 4(l_i^{'} + 1)(n_2 + n_1 + l_i - l_i^{'})] \\ &\quad - [4(l_i + l_i^{'})(n_2 - n_1 + l_i^{\prime} - 1) + 2 \times 4(n_2 - n_1 + l_i - 1)] \\ &= 8 \times [n_1 + n_1 l_i^{\prime} - l_i^{\prime 2} + 1] \\ &\geq 8 \times [(l_i^{'} - 1) + (l_i^{'} - 1)l_i^{'} - (l_i^{'})^2 + 1] \\ &= 8 \times [l_i^{'} - 1 - l_i^{'} + 1 + (l_i^{'})^2 - (l_i^{'})^2] \\ &= 0 \end{aligned}$$

and $Mo(G) \geq Mo(G^{'})$ with equality if and only if $n_1 = l_i^{\prime} - 1$, i.e., $S_i^{\prime}$ is a terminal segment. ■

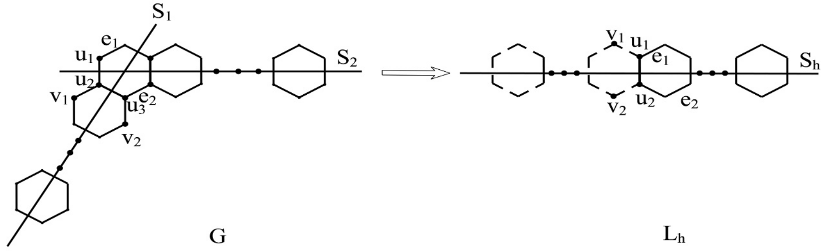

Figure 5. A hexagonal chain G with $K(G) = 1$ and L_h.

Lemma 3. *Let $G \in HC_h$ with $K(G) = 1$. Then $Mo(G) > Mo(L_h)$.*

Proof. From $G \in HC_h$ with $K(G) = 1$, we know that G has only two segments S_1, S_2, see Figure 5. Let $\ell(S_1) = l_1$ and $\ell(S_2) = l_2$, where $l_2 \geq l_1 \geq 2$ and $h = l_1 + l_2 - 1$. Then $L_h = G - \{v_1u_2, v_2u_3\} + \{v_1u_1, v_2u_2\}$. It can be seen by direct calculation that

$$\begin{aligned} Mo(G) - Mo(L_h) = \{ & \sum_{uv \in O(S_1) \subseteq E(G)} |n_u - n_v| + \sum_{uv \in O(S_2) \subseteq E(G)} |n_u - n_v| \} \\ & - \sum_{uv \in \{u_2u_3, u_5u_6\} \subseteq E(L_h)} |n_u - n_v| \\ & = [4 \times (l_1 + 1)(l_2 - 1) + 4 \times (l_2 + 1)(l_1 - 1)] - 8 \times (l_2 - l_1) \\ & = 8 \times (l_1 - 1)(l_2 + 1) > 0. \end{aligned}$$

i.e., $Mo(G) > Mo(L_h)$. ■

Lemma 4. *Let $G \in HC_h$ with $K(G) = k \geq 1$ and its segments $S_1, S_2, \cdots, S_{k+1}$, where S_1 and S_{k+1} are its terminal segments with $\ell(S_1) \leq \ell(S_{k+1})$. If $k = 1$ or at least one of $S_i (2 \leq i \leq k)$ is a non-zigzag segment, then there exists a hexagonal chain $G^{'} \in HC_h$ with $K(G^{'}) = k - 1$ such that $Mo(G^{'}) < Mo(G)$; otherwise, there exists a hexagonal chain $G^{'} \in HC_h$ with $K(G^{'}) = k - 1$ such that $Mo(G^{'}) = Mo(G)$, where G' is obtained by the kink transformation (II) on the zigzag segment S_2.*

Proof. From Lemma 3, we know the result is true for $k = 1$.

Now, let $G \in HC_h$ with $K(G) = k > 1$ and its segments $S_1, S_2, \cdots, S_{k+1}$, where S_1 and S_{k+1} are its terminal segments with $\ell(S_1) \leq \ell(S_{k+1})$. If there is $2 \leq i \leq k$ such that S_i is a non-zigzag segment, then by the kink transformation (I) on the segment S_i, we can get $G' \in HC_h$ with $K(G^{'}) = k - 1$ such that $Mo(G') < Mo(G)$. Otherwise, S_2 is a zigzag segment, then by the kink transformation (II) on S_2, we can get $G' \in HC_h$ with $K(G^{'}) = k - 1$ such that $Mo(G^{'}) = Mo(G)$. ■

Lemma 5. *[3] Let L_h be the linear chain with h hexagons. Then*

$$Mo(L_h) = 32 \lfloor \frac{h}{2} \rfloor \lceil \frac{h}{2} \rceil.$$

From Lemmas 3,4 and 5, we can obtain the following theorem.

Theorem 6. *Let $G \in HC_h$. Then $Mo(G) \geq Mo(L_h) = 32 \lfloor \frac{h}{2} \rfloor \lceil \frac{h}{2} \rceil$ with equality if and only if $G \cong L_h$.*

Theorem 6 shows that the linear chain L_h is the unique graph with the minimum Mostar index among all hexagonal chains with h hexagons.

Now, we consider the hexagonal chains with the second minimal Mostar index among all hexagonal chains with h hexagons.

Let B_h^t denote the hexagonal chain with h hexagons and two segments of lengths t and $h-t+1$, where $2 \le t \le \lfloor \frac{h+1}{2} \rfloor$. Now, we compute the Mostar index of B_h^t and order all hexagonal chains with exactly one kink by their Mostar indices.

Theorem 7. *Let B_h^t be the hexagonal chain with h hexagons and two segments of lengths t and $h-t+1$, where $2 \le t \le \lfloor \frac{h+1}{2} \rfloor$. Then*

$$Mo(B_h^2) < Mo(B_h^3) < \cdots < Mo(B_h^{\lfloor \frac{h+1}{2} \rfloor}).$$

Proof. Let S_1 and S_2 be two segments of B_h^t, $\ell(S_1) = t$ and $\ell(S_2) = h-t+1$, see Figure 5. Then

$$\begin{aligned} Mo(B_h^t) - Mo(L_h) &= \{ \sum_{uv \in O(S_1) \subseteq E(B_h^t)} |n_u - n_v| + \sum_{uv \in O(S_2) \subseteq E(B_h^t)} |n_u - n_v| \} \\ &\quad - \{ \sum_{uv \in O(S_h) \subseteq E(L_h)} |n_u - n_v| + \sum_{uv \in \{u_2u_3, u_5u_6\} \subseteq E(L_h)} |n_u - n_v| \} \\ &= [4(t+1)(h-t) + 4(h-t+2)(t-1)] - [0 + 8(h-2t+1)] \\ &= 8[-t^2 + (h+3)t - h - 2]. \end{aligned}$$

So, $Mo(B_h^t) = Mo(L_h) + 8[-t^2 + (h+3)t - h - 2]$ and $Mo(B_h^2) < Mo(B_h^3) < \cdots < Mo(B_h^{\lfloor \frac{h+1}{2} \rfloor})$. ■

Let $B_h^{t_1,t_3}$ denote the hexagonal chain with h hexagons and exactly three segments S_1, S_2, S_3 of lengths t_1, $t_2 = h - t_1 - t_3 + 2$ and t_3, respectively, where $2 \le t_1 \le t_3$, S_1, S_3 are the terminal segments and S_2 is a zigzag segment.

Let $\bar{B}_h^{t_1,t_3}$ denote the hexagonal chain with h hexagons and exactly three segments S_1, S_2, S_3 of lengths t_1, $t_2 = h - t_1 - t_3 + 2$ and t_3, respectively, where $2 \le t_1 \le t_3$, S_1, S_3 are the terminal segments and S_2 is a non-zigzag segment.

Using Lemma 2, we can get the Mostar index of $B_h^{t_1,t_3}$.

Theorem 8. *For the hexagonal chain $B_h^{t_1,t_3}$, we have $Mo(B_h^{t_1,t_3}) = Mo(B_h^{mim\{t_3, h-t_3+1\}})$, i.e.,*

(1) $Mo(B_h^{t_1,t_3}) = Mo(B_h^{t_3})$ for $t_3 \le \frac{1}{2}(h+1)$;

(2) $Mo(B_h^{t_1,t_3}) = Mo(B_h^{h-t_3+1})$ for $t_3 > \frac{1}{2}(h+1)$.

Theorem 9. *If $G \in HC_h$ and $G \ncong L_h$, then $Mo(G) \geq Mo(B_h^2) = Mo(B_h^{2,2}) = 8h + 32\lfloor \frac{h}{2} \rfloor \lceil \frac{h}{2} \rceil$ with equality if and only if $G \cong B_h^2$ or $B_h^{2,2}$, see Figure 6.*

Proof. It can be calculated directly that $Mo(B_h^2) = Mo(B_h^{2,2}) = 8h + Mo(L_h) = 8h + 32\lfloor \frac{h}{2} \rfloor \lceil \frac{h}{2} \rceil$.

Let $K(G) = k$, $k \geq 1$ since $G \ncong L_h$.

If $k = 1$, then $G \cong B_h^t$, by Theorem 7, we have $Mo(G) \geq Mo(B_h^2)$ with equality if and only if $G \cong B_h^2$.

If $k = 2$, then $G \cong B_h^{t_1,t_3}$ or $\bar{B}_h^{t_1,t_3}$, where $t_1, t_2, t_3 \geq 2$ and $t_1 \leq t_3$. If $G \cong \bar{B}_h^{t_1,t_3}$, then $Mo(G) > Mo(B_h^2)$ by Lemma 2 and Theorem 7. If $G \cong B_h^{t_1,t_3}$, then, by Theorem 8, $Mo(B_h^{t_1,t_3}) = Mo(B_h^{min\{t_3,h-t_3+1\}}) \geq Mo(B_h^2)$ with equality if and only if $t_3 = 2$ since $h - t_3 + 1 = \ell(S_1) + \ell(S_2) - 1 \geq 3$, i.e., $G \cong B_h^{2,2}$ because $2 \leq t_1 \leq t_3$.

If $k \geq 3$, by the kink transformation (I) or (II) and Lemma 4, there exist $B_h^{t_1,t_3}$ or $\bar{B}_h^{t_1,t_3}$ (where $t_1 \geq 3$ or $t_3 \geq 3$) such that $Mo(G) \geq Mo(B_h^{t_1,t_3}) > Mo(B_h^{2,2})$ or $Mo(G) \geq Mo(\bar{B}_h^{t_1,t_3}) > Mo(B_h^{2,2})$.

So, we have $Mo(G) \geq Mo(B_h^2) = Mo(B_h^{2,2})$ with equality if and only if $G \cong B_h^2$ or $G \cong B_h^{2,2}$. ■

Theorem 9 shows that the hexagonal chain B_h^2 and $B_h^{2,2}$ are only the extremal graphs with the second minimal Mostar index among all hexagonal chains with h hexagons.

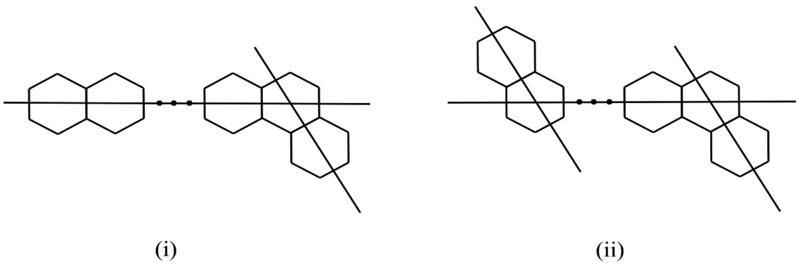

Figure 6. The graph of B_h^2 (i) and $B_h^{2,2}$ (ii)

In the following, we will characterize the hexagonal chains with the third minimal Mostar index among all hexagonal chains with h hexagons.

Let $B_h^{t_1,t_2,\cdots,t_{k+1}}$ be the hexagonal chain with h hexagons and exactly $k+1$ segments $S_1, S_2, \cdots, S_{k+1}$ of lengths $t_1, t_2, \cdots, t_{k+1}$, respectively, where S_1, S_{k+1} are the terminal segments, all S_i $(2 \leq i \leq k)$ are zigzag segments and $2 \leq t_1 \leq t_{k+1}$.

Theorem 10. *If $G \in HC_h$ and $G \notin \{L_h, B_h^2, B_h^{2,2}\}$, then $Mo(G) \geq 16(h-1) + 32\lfloor\frac{h}{2}\rfloor\lceil\frac{h}{2}\rceil$ with equality if and only if $G \in \{B_h^3, B_h^{2,h-2}, B_h^{2,3}, B_h^{3,3}, B_h^{2,2,h-3,2}, B_h^{2,2,h-4,3}, B_h^{2,2,h-4,2,2}\}$, see Figure 7.*

Proof. Firstly, it can be calculated that $Mo(B_h^3) = Mo(B_h^{2,h-2}) = Mo(B_h^{2,3}) = Mo(B_h^{3,3}) = Mo(B_h^{2,2,h-3,2}) = 16(h-1) + 32\lfloor\frac{h}{2}\rfloor\lceil\frac{h}{2}\rceil$ by Lemma 4.

Let $K(G) = k$, where $k \geq 1$ since $G \ncong L_h$.

Case 1. $k = 1$. Then $G \cong B_h^t$ and $t \geq 3$ since $G \ncong B_h^2$. By Theorem 7, we have $Mo(G) \geq Mo(B_h^3) = 16(h-1) + 32\lfloor\frac{h}{2}\rfloor\lceil\frac{h}{2}\rceil$ with equality if and only if $G \cong B_h^3$.

Case 2. $k = 2$. Let S_1, S_2, S_3 be the segments of G with lengths t_1, t_2, t_3, respectively, where $t_i \geq 2$ $(i = 1, 2, 3)$, $2 \leq t_1 \leq t_3$, S_1, S_3 are the terminal segments.

If S_2 is a non-zigzag segment and $t_3 \geq 3$, then $Mo(G) > Mo(B_h^3)$ by Lemma 1; If S_2 is a non-zigzag segment and $t_3 = 2$, then we have $t_1 = 2$ and $t_2 = h-2$ since $t_1 \leq t_3$, and $Mo(G) = Mo(B_h^2) + 8(t_1-1)(t_2+1)$ from the proof of Case 1 in Lemma 1. So, $Mo(G) = 8h + Mo(L_h) + 8(h-1) > 16(h-1) + Mo(L_h)$.

If S_2 is a zigzag segment, then $G \cong B_h^{t_1,t_3}$, by Theorem 8, $Mo(B_h^{t_1,t_3}) = Mo(B_h^{t_3}) \geq Mo(B_h^3)$ for $t_3 \leq \frac{1}{2}(h+1)$ and $Mo(B_h^{t_1,t_3}) = Mo(B_h^{h-t_3+1}) \geq Mo(B_h^3)$ for $t_3 > \frac{1}{2}(h+1)$, with equality if and only if $t_3 = 3$ or $t_3 = h-2$, respectively, i.e., $G \in \{B_h^{2,3}, B_h^{3,3}, B_h^{2,h-2}\}$.

Case 3. $k = 3$. Let S_1, S_2, S_3, S_4 be the segments of G with lengths t_1, t_2, t_3, t_4, respectively, where $t_i \geq 2$ $(i = 1, 2, 3, 4)$, $2 \leq t_1 \leq t_4$, S_1, S_4 are the terminal segments.

If exactly one of S_2 and S_3 is a non-zigzag segment, then there is a hexagonal chain $B_h^{t_1',t_3'}$ such that $Mo(G) > Mo(B_h^{t_1',t_3'}) \geq Mo(B_h^3)$ by the kink transformation (I) on S_2 or S_3.

If S_2 and S_3 are non-zigzag segments, then there is a hexagonal chain G' with $K(G') = 2$ kinks and a non-zigzag segment such that $Mo(G) > Mo(G')$ by the kink transformation (I) on S_2, and $Mo(G') \geq Mo(B_h^3)$ from Case 2. So, $Mo(G) > Mo(B_h^3)$.

If S_2 and S_3 are zigzag segments, then we can get $Mo(G) = Mo(B_h^{t_1+t_2-1,t_4})$ by the kink transformation (II) on S_2. Moreover, $Mo(B_h^{t_1+t_2-1,t_4}) = Mo(B_h^{min\{t_1+t_2+t_3-2,t_4\}}) > Mo(B_h^3)$ for $t_4 > t_1+t_2-1$, and $Mo(B_h^{t_1+t_2-1,t_4}) = Mo(B_h^{min\{t_1+t_2-1,t_3+t_4-1\}}) \geq Mo(B_h^3)$ for $t_4 \leq t_1+t_2-1$ with equality if and only if $min\{t_1+t_2-1, t_3+t_4-1\} = 3$, i.e., $t_1 = t_2 = 2$ or $t_3 = t_4 = 2$, i.e., $G \in \{B_h^{2,2,h-3,2}, B_h^{2,2,h-4,3}\}$.

Case 4. $k = 4$. Let S_i be the segments of G with lengths t_i, respectively, where $t_i \geq 2$ $(i = 1, 2, 3, 4, 5)$,$2 \leq t_1 \leq t_5$, S_1, S_5 are the terminal segments.

If at least one of S_i $(2 \le i \le 4)$ is a non-zigzag segment, then there is a hexagonal chain G' with $K(G') = 3$ kinks such that $Mo(G) > Mo(G') \ge Mo(B_h^3)$ from Lemma 4 and Case 3.

If all S_i $(2 \le i \le 4)$ are zigzag segments, then we can get $Mo(G) = Mo(B_h^{t_1+t_2-1,t_3,t_4,t_5})$ by the kink transformation (II) on S_2. From Case 3, $Mo(B_h^{t_1+t_2-1,t_3,t_4,t_5}) \ge Mo(B_h^3)$ with equality if and only if $B_h^{t_1+t_2-1,t_3,t_4,t_5} \in \{B_h^{2,2,h-3,2}, B_h^{2,2,h-4,3}\}$, i.e., $t_1 + t_2 - 1 = 3$ and $t_4 = t_5 = 2$ since $t_1 + t_2 - 1 \ge 3$, i.e., $G \cong B_h^{2,2,h-4,2,2}$.

Case 5. $k \ge 5$. Let S_i be the segments of G with lengths t_i, respectively, where $t_i \ge 2$ $(i = 1, 2, \cdots, k+1)$, $2 \le t_1 \le t_{k+1}$, S_1, S_{k+1} are the terminal segments. Then there is a hexagonal chain G' with $K(G') = 4$ kinks such that $Mo(G) \ge Mo(G')$ from Lemma 4, and $G' \ncong B_h^{2,2,h-4,2,2}$. So, $Mo(G) \ge Mo(G') > Mo(B_h^3)$ by Case 4.

The proof is completed. ∎

Theorem 10 shows that the hexagonal chains B_h^3, $B_h^{2,h-2}$, $B_h^{2,3}$, $B_h^{3,3}$, $B_h^{2,2,h-3,2}$, $B_h^{2,2,h-4,3}$ and $B_h^{2,2,h-4,2,2}$ are only the graphs with the third minimal Mostar index among all hexagonal chains with h hexagons.

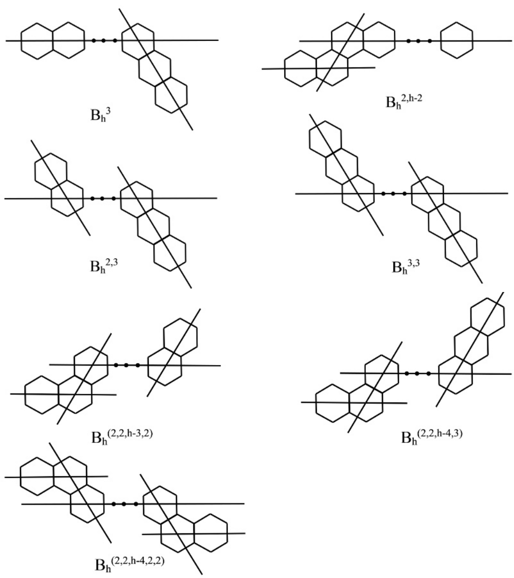

Figure 7. The hexagonal chains with the third minimal Mostar index

3 Conclusions

In this paper, we gave the first three minimal values of the Mostar index for hexagonal chains, and determined the corresponding extremal graphs. The proof techniques used the kink transformations of hexagonal chains and the structural properties of the Mostar index. In the future, we will continue to study the maximal values of the Mostar index for hexagonal chains and the extremal values of this topological index for more general graphs, such as catacondensed hexagonal systems and polymeric networks.

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