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Merrifield–Simmons Index of Tree–Type Hexagonal Systems

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Abstract

Some results with respect to Merrifield-Simmons index of tree-type hexagonal systems are shown. Using these results, the tree-type hexagonal system with lower bound of Merrifield-Simmons index is determined. These results generalize some known results on hexagonal chains and hexagonal spiders.

1. Introduction

A hexagonal system is a 2-connected planar graph whose every interior face is bounded by a regular hexagon. Hexagonal systems are of great importance for theoretical chemistry because they are natural graph representations of benzenoid hydrocarbons [2]. A hexagonal system is a tree-type one if it has no inner vertex. Tree-type hexagonal systems are graph representations of an important subclass of benzenoid molecules. A considerable amount of research in mathematical chemistry has been devoted to hexagonal systems [2–14].

In order to describe our results, we need some graph-theoretic notations and terminologies. Our standard reference for any graph theoretical terminology is [1].

Let $G = (V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. Let e and u be an edge and a vertex of G, respectively. We will denote by $G - e$ or $G - u$ the graph

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obtained from G by removing e or u, respectively. Denote by N_u the set $\{v \in V(G) : uv \in E(G)\} \cup \{u\}$. Let H be a subset of $V(G)$. The subgraph of G induced by H is denoted by $G[H]$, and $G[V \setminus H]$ is denoted by $G - H$. Undefined concepts and notations of graph theory can be found in [9–14].

Two vertices of a graph G are said to be independent if they are not adjacent. A subset I of $V(G)$ is called an independent set of G if any two vertices of I are independent. Denote $i(G)$ by the number of independent sets of G. In chemical terminology, $i(G)$ is called the Merrifield-Simmons index. Clearly, the Merrifield-Simmons index of a graph is larger than that of its proper subgraphs.

We denote by Ψ_n the set of hexagonal chains with n hexagons. Let $B_n \in \Psi_n$. We denote by $V_3 = V_3(B_n)$ the set of vertices with degree 3 in B_n. Thus, the subgraph $B_n[V_3]$ is an acyclic graph. If the subgraph $B_n[V_3]$ is a matching with $n-1$ edges, then B_n is called a linear chain and denoted by L_n. If the subgraph $B_n[V_3]$ is a path, then B_n is called a zig-zag chain and denoted by Z_n. If the subgraph $B_n[V_3]$ is a comb, then B_n is called a helicene chain and denoted by H_n.

Denote by $\mathbf{T}_n$ the set of tree-type hexagonal systems containing n hexagons. Let $\mathbf{T} = \bigcup_1^\infty \mathbf{T}_n$, and $T \in \mathbf{T}$. Let H be a hexagon of T. Obviously, H has at most three adjacent hexagons in T; if H has exactly three adjacent hexagons in T, then H is called a full-hexagon of T; if H has two adjacent hexagons in T, and, moreover, if its two vertices with degree two are adjacent, then call H a turn-hexagon of T; and if H has at most one adjacent hexagon in T, then H is called an end-hexagon of T. It is easy to see that the number of end-hexagons of a tree-type hexagonal system of $n \geq 2$ hexagons is two more than the number of its full-hexagons. Let $T \in \mathbf{T}$ and $B = H_1H_2 \ldots H_k, k \geq 2$ be a hexagonal chain of T. If the end-hexagon H_1 of B is also an end-hexagon of T, the other end-hexagon H_k is a full-hexagon of T, and for $2 \leq i \leq k-1$, H_i is not a full-hexagon of T, then B is called a branch of T. Let $\Upsilon = H_1H_2 \ldots H_k, k \geq 2$ be a hexagonal chain of T. If both the end-hexagon H_1 and H_k of Υ are full-hexagons of T, and for $2 \leq i \leq k-1$, H_i is not a full-hexagon of T, then Υ is called a $\Upsilon-$ subgraph of T. If any branch and any $\Upsilon-$ subgraph of T are linear chains, then T is called linear tree-type hexagonal system. If any branch and any $\Upsilon-$ subgraph of T are zig-zag chains, then T is called zig-zag tree-type hexagonal system. A zig-zag hexagonal chain and a zig-zag hexagonal spider are zig-zag tree-type hexagonal systems with no full-hexagon and only one full-hexagon, respectively.

A graph G is called a spider if it is a tree and contains only one vertex of degree greater than 2. For positive integer n_1, n_2, n_3, we use $S(n_1, n_2, n_3)$ to denote a hexagonal spider with three legs of lengths n_1, n_2 and n_3, respectively.

If a hexagonal spider $S(n_1, n_2, n_3)$ whose 3 legs are linear chains, then such a graph is called a linear hexagonal spider and denoted by $L(n_1, n_2, n_3)$.

Similarly if each leg of $S(n_1, n_2, n_3)$ attached to the central hexagon is a zig-zag chain, then such graph is called a zig-zag hexagonal spider and denoted by $Z(n_1, n_2, n_3)$.

2. Some useful results

Among tree-type hexagonal systems with extremal properties on topological indices, L_n and Z_n play important roles. We list some of them about the Merrifield-Simmons index as follows.

Theorem 2.1. ([5]). For any $n \geq 1$ and any $B_n \in \Psi_n$, if B_n is neither L_n nor Z_n, then

$$i(Z_n) < i(B_n) < i(L_n).$$

Theorem 2.2. ([14]). For any $n \geq 1$ and any $T \in \mathbf{T}_\mathrm{n}$, if T is not L_n, then

$$i(T) < i(L_n).$$

Theorem 2.3. ([9]). If $S(n_1, n_2, n_3)$ is neither $L(n_1, n_2, n_3)$ nor $Z(n_1, n_2, n_3)$, then

$$i(Z(n_1, n_2, n_3)) < i(S(n_1, n_2, n_3)) < i(L(n_1, n_2, n_3)).$$

Among many properties of $i(G)$, we mention the following results which will be used later.

Lemma 2.1. ([1]). Let G be a graph consisting of two components G_1 and G_2. Then

$$i(G) = i(G_1)i(G_2).$$

Lemma 2.2. ([1]). Let G be a graph and any $uv \in E(G)$. Then

$$i(G) = i(G - u) + i(G - N_u).$$

Lemma 2.3. ([1]). Let G be a graph. For each $uv \in E(G)$, then

$$i(G) - i(G - u) - i(G - u - v) \leq 0.$$

Moreover, the equality holds only if v is the unique neighbor of u.

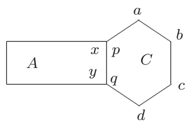


Fig. 2.1.$A(x, y) \otimes C(p, q)$.

Suppose G is the union of a graph A and a 6-cycle C in which A and C have only one common edge. Let this common edge be xy and the cycle C be $abcdqpa$ (*i.e.*, a, b, c, d, q and p are vertices of C and $x = p, y = q$) (see Fig. 2.1). We shall denote G by $A(x, y) \otimes C(p, q)$.

Let A and B be any graph, C be a hexagon and $G = A(x, y) \otimes C(p, q)$. Denote by $G(a, b) \otimes B(r, s)$ the graph obtained from G and B by identifying the edge ab with rs; by $G(b, c) \otimes B(r, s)$ the graph obtained from G and B by identifying the edge bc with rs; by $G(c, d) \otimes B(r, s)$ the graph obtained from G and B by identifying the edge cd with rs, where r and s are two adjacent vertices of B of at least degree two.

Lemma 2.4. ([9]). Let A and B be any graph and $G = A(x, y) \otimes C(p, q)$. If $i(A - x) < i(A - y)$, then $i(G(c, d) \otimes B(r, s)) < i(G(a, b) \otimes B(r, s))$.

Lemma 2.5. ([9]). Let A and B be any graph and $G = A(x, y) \otimes C(p, q)$. Then

(a) $i(G(a, b) \otimes B(r, s)) < i(G(b, c) \otimes B(r, s))$,

(b) $i(G(c, d) \otimes B(r, s)) < i(G(b, c) \otimes B(r, s))$.

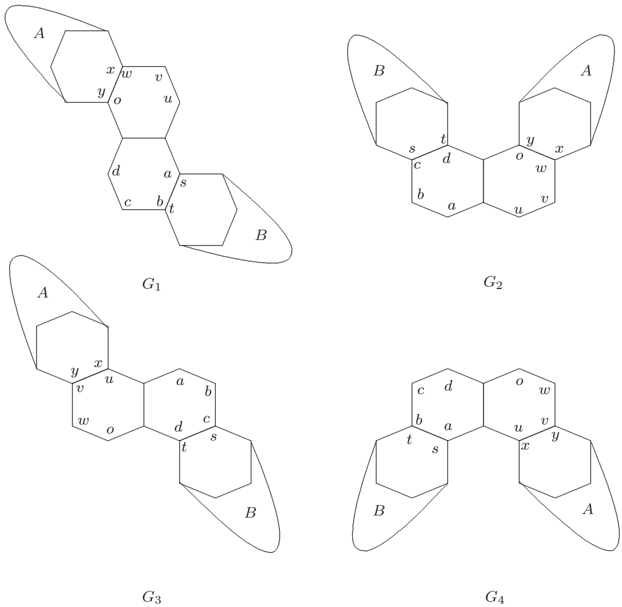


Fig. 2.2.

We add some notations which are convenient to express useful results. For a hexagonal chain L_2 of length two, denote by a, b, c, d and u, v, w, o four vertices of degree two in two end-hexagons respectively. In the present section, for a given $T \in \mathbf{T}$, we always assume that s, t or x, y are two adjacent vertices with degree two in T. By Lemma 2.1 and 2.2, we have the following lemma.

Lemma 2.6. Let $G_1 = \{A(x, y) \otimes L_2(w, o)\}(a, b) \otimes B(s, t)$, $G_2 = \{A(x, y) \otimes L_2(w, o)\}(c, d) \otimes B(s, t)$, $G_3 = \{A(x, y) \otimes L_2(u, v)\}(c, d) \otimes B(s, t)$ and $G_4 = \{A(x, y) \otimes L_2(u, v)\}(a, b) \otimes B(s, t)$ be defined above (see Fig. 2.2). Then

$$i(G_1) = \begin{pmatrix} i(A - x - y) \\ i(A - N_y) \\ i(A - N_x) \end{pmatrix}^T \begin{pmatrix} 21 & 13 & 15 \\ 15 & 10 & 9 \\ 13 & 8 & 10 \end{pmatrix} \begin{pmatrix} i(B - s - t) \\ i(B - N_t) \\ i(B - N_s) \end{pmatrix},$$

$$i(G_2) = \begin{pmatrix} i(A-x-y) \\ i(A-N_y) \\ i(A-N_x) \end{pmatrix}^T \begin{pmatrix} 22 & 13 & 14 \\ 13 & 13 & 8 \\ 14 & 8 & 9 \end{pmatrix} \begin{pmatrix} i(B-s-t) \\ i(B-N_t) \\ i(B-N_s) \end{pmatrix},$$

$$i(G_3) = \begin{pmatrix} i(A-x-y) \\ i(A-N_y) \\ i(A-N_x) \end{pmatrix}^T \begin{pmatrix} 21 & 15 & 13 \\ 13 & 10 & 8 \\ 15 & 9 & 10 \end{pmatrix} \begin{pmatrix} i(B-s-t) \\ i(B-N_t) \\ i(B-N_s) \end{pmatrix}$$

and

$$i(G_4) = \begin{pmatrix} i(A-x-y) \\ i(A-N_y) \\ i(A-N_x) \end{pmatrix}^T \begin{pmatrix} 22 & 14 & 13 \\ 14 & 9 & 8 \\ 13 & 8 & 13 \end{pmatrix} \begin{pmatrix} i(B-s-t) \\ i(B-N_t) \\ i(B-N_s) \end{pmatrix}.$$

By applying Lemma 2.1 and Lemma 2.2, it is easy to obtain the result.

Lemma 2.7. Suppose $G_i (i = 1, 2, 3, 4)$ is defined in Lemma 2.6 . Then

(*a*) $i(G_1) < i(G_2)$ or $i(G_3) < i(G_2)$,

(*b*) $i(G_1) < i(G_4)$ or $i(G_3) < i(G_4)$.

Proof. (a) We assume that $i(B - N_t) \geq i(B - N_s)$. By Lemma 2.6, we have

$$\Delta_1 = i(G_2) - i(G_1) = \begin{pmatrix} i(A-x-y) \\ i(A-N_y) \\ i(A-N_x) \end{pmatrix}^T \begin{pmatrix} 1 & 0 & -1 \\ -2 & 3 & -1 \\ 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} i(B-s-t) \\ i(B-N_t) \\ i(B-N_s) \end{pmatrix}$$

and

$$\Delta_2 = i(G_2) - i(G_3) = \begin{pmatrix} i(A-x-y) \\ i(A-N_y) \\ i(A-N_x) \end{pmatrix}^T \begin{pmatrix} 1 & -2 & 1 \\ 0 & 3 & 0 \\ -1 & -1 & -1 \end{pmatrix} \begin{pmatrix} i(B-s-t) \\ i(B-N_t) \\ i(B-N_s) \end{pmatrix}.$$

If $i(A - N_x) \geq i(A - N_y)$, we get

$$\Delta_1 > i(A - N_y)[3i(B - N_t) - 3i(B - N_s)] \geq 0.$$

Otherwise, in order to prove that $\Delta_1 > 0$ or $\Delta_2 > 0$, it suffices to show that $\Delta_1 + \Delta_2 > 0$. Note that

$$\Delta_1 + \Delta_2 = \begin{pmatrix} i(A-x-y) \\ i(A-N_y) \\ i(A-N_x) \end{pmatrix}^T \begin{pmatrix} 2 & -2 & 0 \\ -2 & 6 & -1 \\ 0 & -1 & -2 \end{pmatrix} \begin{pmatrix} i(B-s-t) \\ i(B-N_t) \\ i(B-N_s) \end{pmatrix}.$$

Both $A - x$ and $A - y$ are proper subgraphs of $A - xy$ and by Lemma 2.3, we obtain

$$\Delta_1 + \Delta_2 > i(A - N_y)[3i(B - N_t) - 3i(B - N_s)] \geq 0.$$

If $i(B - N_t) < i(B - N_s)$, the proof of (a) is similar as above.

(b) A similar proof as in (a), we have $i(G_1) < i(G_4)$ or $i(G_3) < i(G_4)$ and the proof of Lemma 2.7 is complete.

3. Preliminary results and proofs

Suppose $B_n \in \Psi_n$. Let $C_1, C_2, ..., C_n$ be n hexagons of B_n such that C_{k-1} and C_k are adjacent for $k = 2, ..., n$. We use $x_{k-1}, y_{k-1}, a_k, b_k, c_k$ and d_k to denote vertices of C_k such that $x_{k-1}y_{k-1}$ is the common edge of C_k and C_{k-1}, and $x_{k-1}a_k, a_kb_k, b_kc_k, c_kd_k$ and d_ky_{k-1} are edges of C_k. Moreover, we require that x_k and x_{k-1} have the distance two.

Suppose T_1, $T_2 \in \mathbf{T}$ and $B_n \in \Psi_n$. p_i, q_i and u_i, v_i are two adjacent vertices with degree two in T_i and B_n $i = 1, 2$, respectively. Firstly, we denote by $T_1(p_1, q_1) \otimes B_n(u_1, v_1)$ the tree-type hexagonal system obtained from T_1 and B_n by identifying p_1 with u_1, and q_1 with v_1, respectively. Secondly, we denote by $\{T_1(p_1, q_1) \otimes B_n(u_1, v_1)\}(u_2, v_2) \otimes T_2(p_2, q_2)$ the tree-type hexagonal system obtained from $T_1(p_1, q_1) \otimes B_n(u_1, v_1)$ and T_2 by identifying u_2 with p_2, and v_2 with q_2, respectively (see Fig. 3.1). For given T_1, $T_2 \in \mathbf{T}$ and any $B_n \in \Psi_n$, we shall use Φ to denote the set of all tree-type hexagonal systems of the form $\{T_1(p_1, q_1) \otimes B_n(u_1, v_1)\}(u_2, v_2) \otimes T_2(p_2, q_2)$.

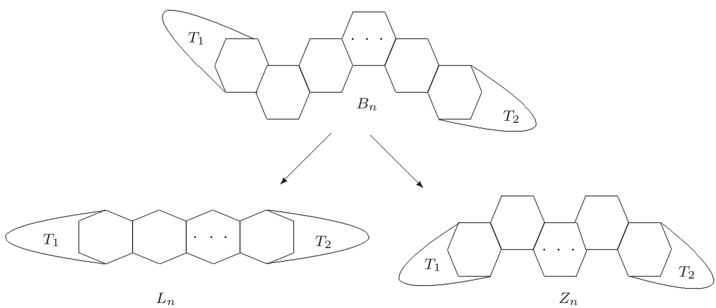


Fig. 3.1.

Theorem 3.1. Suppose $T_{min} \in \Phi$ has the minimum Merrifield-Simmons index among all tree-type hexagonal systems of Φ. Then B_n is a zig-zag hexagonal chain.

Proof. Suppose not. Let $T_{min} = \{T_1(p_1, q_1) \otimes B_n(u_1, v_1)\}(u_2, v_2) \otimes T_2(p_2, q_2)$ have the minimum Merrifield-Simmons index among all tree-type hexagonal systems of Φ, $B_n = C_1C_2...C_n$ and k be the least integer such that $B_k = C_1C_2...C_k(3 \leq k \leq n)$ is not a zig-zag chain. Then

$$B_n = \{Z_{k-3}(x_{k-3}, y_{k-3}) \otimes L_2(w, o)\}(c, d) \otimes \{B_n - Z_{k-1}\}(x_{k-1}, y_{k-1})$$

or

$$B_n = \{Z_{k-3}(x_{k-3}, y_{k-3}) \otimes L_2(w, o)\}(b, c) \otimes \{B_n - Z_{k-1}\}(x_{k-1}, y_{k-1}).$$

Let $A = T_1(p_1, q_1) \otimes Z_{k-3}(u_1, v_1)$ and $B = \{B_n - Z_{k-1}\}(u_2, v_2) \otimes T_2(p_2, q_2)$. Then

$$T_{min} = \{A(x_{k-3}, y_{k-3}) \otimes L_2(w, o)\}(b, c) \otimes B(x_{k-1}, y_{k-1})$$

or

$$T_{min} = \{A(x_{k-3}, y_{k-3}) \otimes L_2(w, o)\}(c, d) \otimes B(x_{k-1}, y_{k-1}).$$

By Lemma 2.5 and 2.7, we get

$$i(\{A(x_{k-3}, y_{k-3}) \otimes L_2(w, o)\}(a, b) \otimes B(x_{k-1}, y_{k-1})) < i(T_{min})$$

or

$$i(\{A(x_{k-3}, y_{k-3}) \otimes L_2(u, v)\}(c, d) \otimes B(x_{k-1}, y_{k-1})) < i(T_{min}).$$

Since $\{A(x_{k-3}, y_{k-3}) \otimes L_2(w, o)\}(a, b) \otimes B(x_{k-1}, y_{k-1})$ and $\{A(x_{k-3}, y_{k-3}) \otimes L_2(u, v)\}(c, d)$ $\otimes B(x_{k-1}, y_{k-1}) \in \Phi$, we obtain a contradiction.

By using Lemma 2.4, 2.5 and 2.7, and a similar proof as for Theorem 3.1, we have

Theorem 3.2. Suppose $T_{max} \in \Phi$ has the maximum Merrifield-Simmons index among all tree-type hexagonal systems of Φ. Then B_n is a linear hexagonal chain.

4. Tree–type hexagonal systems

Let $T \in \mathbf{T}$. Denote by L^* the linear tree-type hexagonal system obtained from T whose every branch and $\Upsilon-$ subgraph are replaced by linear hexagonal chains with same number of hexagons, respectively. We shall use $\mathbf{Z}^*$ to denote the set of zig-zag tree-type hexagonal systems obtained from T whose every branch and $\Upsilon-$ subgraph are replaced by zig-zag hexagonal chains with same number of hexagons, respectively.

Theorem 4.1. Suppose $T \in \mathrm{T}_n$ with n hexagons. There must exist a $Z^* \in \mathbf{Z}^*$ with n hexagons such that

$$i(T) \geq i(Z^*).$$

Proof. Suppose not. T must exist a branch or $\Upsilon-$ subgraph which is not a zig-zag chain. By Theorem 3.1, there exists the tree-type hexagonal system $T^{'}$ obtained from T by replacing this branch or $\Upsilon-$ subgraph by a zig-zag chain with the same number of hexagons such that $i(T^{'}) < i(T)$. Repeating this operation, we end up with a hexagonal system $Z^* \in \mathbf{Z}^*$ such that $i(Z^*) < i(T)$, which is a contradiction.

By using Theorem 3.2, and a similar proof as for Theorem 4.1, we have

Theorem 4.2. Suppose $T \in \mathrm{T}_n$ with n hexagons. Then

$$i(T) \leq i(L^*).$$

Moreover, the equality holds if and only if $T \cong L^*$.

Corollary 4.1. Suppose $S(n_1, n_2, n_3)$ has the minimum Merrifield-Simmons index among all hexagonal spiders. Then $S(n_1, n_2, n_3)$ is a zig-zag hexagonal spider.

Corollary 4.2. Suppose $S(n_1, n_2, n_3)$ has the maximum Merrifield-Simmons index among all hexagonal spiders. Then $S(n_1, n_2, n_3)$ is a linear hexagonal spider.

Corollary 4.3. Suppose $B_n \in \Psi_n$. If B_n is neither L_n nor Z_n, then

$$i(Z_n) < i(B_n) < i(L_n).$$

In next section, we want to establish the lower bound for Merrifield-Simmons index of tree-type hexagonal systems.

5. Zig–zag tree–type hexagonal systems

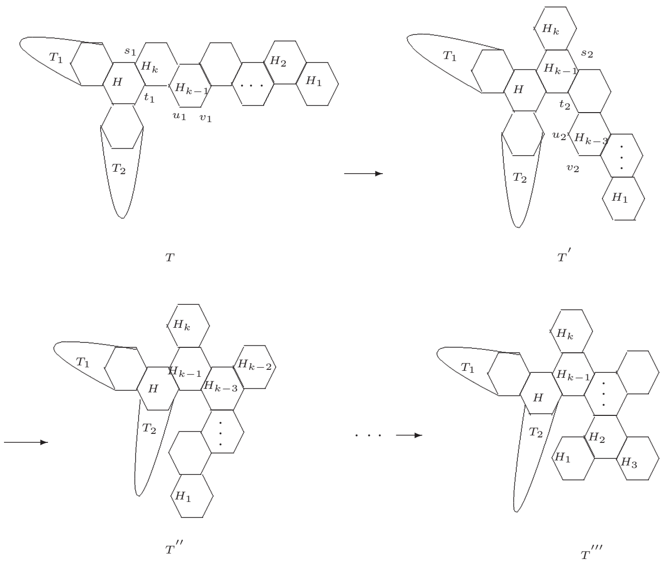
In the present section, for a zig-zag chain Z_k with k hexagons, denote by $x_k^{'}, x_k, y_k$ and $y_k^{'}$ four clockwise successive vertices with degree two in one of end-hexagons.

Theorem 5.1. ([15]). For any $T \in \mathbf{T}$ and any $k \geq 3$, then

(a) $i(T(s,t) \otimes Z_k(x_k, y_k)) > i(T(s,t) \otimes Z_k(x_{k-1}^{'}, x_{k-1}))$,
(b) $i(T(s,t) \otimes Z_k(x_k^{'}, x_k)) > i(T(s,t) \otimes Z_k(x_{k-1}^{'}, x_{k-1}))$,
(c) $i(T(s,t) \otimes Z_k(y_k, y_k^{'})) > i(T(s,t) \otimes Z_k(x_{k-1}^{'}, x_{k-1}))$.

The proof of this theorem can be found in [15] where it is given with full detail.

We shall use $\mathbf{Z}_{\rm n}^{*}$ to denote the set of all zig-zag tree-type hexagonal systems with n hexagons. For a zig-zag tree-type system $Z^{*}(\in \mathbf{Z}_{\rm n}^{*})$, we denote by $Z^{\perp}$ the graph obtained from Z^{*} whose every branch is transformed by transformation I.



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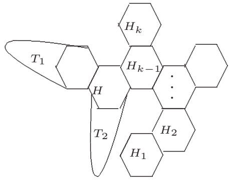

$Fig.5.1.\ Transformation\ I.$

Transformation I. Let $Z_k = H_1H_2\cdots H_k$ and $Z_k \bigotimes H$ be a branch of T. The graph T' is obtained from $T - Z_k$ and Z_k by identifying the edge u_1v_1 of H_{k-1} with the edge s_1t_1 of H. Repeating this operation, we end up with a graph T'''. If $T = Z_n$, we only let $H = H_1$(see Fig. 5.1).

Now we can establish the best currently known lower bound for Merrifield-Simmons index of tree-type hexagonal systems.

Theorem 5.2. For any $Z^* \in \mathbf{Z}_\mathrm{n}^*$ with n hexagons and any $n \geq 4$, then

$$i(Z^{\perp}) \leq i(Z^*).$$

Proof. Note that the graph $Z^{\perp}$ is obtained from Z^* whose every branch is transformed by transformation I, and by Theorem 5.1, we get $i(Z^{\perp}) \leq i(Z^*)$.

By repeating to apply transformation I on a hexagonal spider $Z(n_1, n_2, n_3)$ and Z_n, and according to Theorem 5.1, we will also obtain good lower bound of Merrifield-Simmons index of Z_n and $Z(n_1, n_2, n_3)$ as follows.

Theorem 5.3. For any $Z(n_1, n_2, n_3)$ with n hexagons and any $n \geq 4$, then

$$i(Z^{\perp}(n_1, n_2, n_3)) \leq i(Z(n_1, n_2, n_3)).$$

Moreover, the equality holds if and only if $Z^{\perp}(n_1, n_2, n_3) \cong Z(n_1, n_2, n_3)$.

Theorem 5.4. For any Z_n with n hexagons and any $n \geq 4$, then

$$i(Z^{\perp}) < i(Z_n).$$

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