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Extremal catacondensed benzenoids *

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Some results with respect to Hosoya index and Merrifield–Simmons index of tree-type hexagonal systems (catacondensed hydrocarbons) are shown. Using the results, the tree-type hexagonal systems with minimum, second minimum Hosoya index and maximum, second maximum Merrifield–Simmons index are determined. These results generalize some known results on extremal hexagonal chains.

1. Introduction

A hexagonal system (benzenoid hydrocarbon) is regarded as a 2-connected plane graph in which every finite region is a regular hexagon of unit side length. Hexagonal systems are of great importance for theoretical chemistry because they are the natural graph representations of benzenoid hydrocarbons [1]. A hexagonal system is a *tree-type* one if it has no inner vertex. The tree-type hexagonal systems are the graph representations of an important subclass of benzenoid molecules, namely of the so called catacondensed benzenoids.

In order to describe our results, we need some graph-theoretic notation and terminology. Our standard reference for any graph theoretical terminology is [2].

Let $G = (V, E)$ be a graph and A be a subset of V. The subgraph of G whose vertex set is A and whose edge set is the set of those edges of G that have both end-vertices in A is called the subgraph of G induced by A, and is denoted by $G[A]$. The induced subgraph $G[V - A]$ is denoted by $G - A$. If $A = \{v\}$ we write $G - v$ for $G - \{v\}$. Denote by $N[A]$ the union of A and the set of neighbors of A in G. If $A = \{a_1, a_2, \dots, a_m\}$, then we write $N[a_1, a_2, \dots, a_m]$ instead of $N[\{a_1, a_2, \dots, a_m\}]$.

A subset M of E is called a matching if no two edges of M are incident in G. It is both consistent and convenient to regard the empty edge set as a matching. A subset I of V is called an independent set if no two vertices of I are adjacent in G. We also regard

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the empty vertex set as an independent set. We denote by $\mu(G)$ and $\sigma(G)$ the numbers of matchings of G and the number of independent sets of G, respectively.

Hosoya in [3] proposed the graph-theoretical invariant $\mu(G)$ for quantifying certain structural features of organic molecules. Numerous studies of $\mu(G)$ have been undertaken (see [4–6]). The invariant μ is nowadays commonly called "Hosoya index". Merrifield and Simmons in [7] developed a topological approach to structural chemistry. The cardinality of the topological space in their theory turns out to be equal to $\sigma(G)$ of the respective molecular graph G. In [5], Gutman first use "Merrifield–Simmons index" to name the quantity.

Denote by $\mathcal{T}_n$ the set of tree-type hexagonal systems containing n hexagons. Let $\mathcal{T} = \bigcup_1^\infty \mathcal{T}_n$, and $T \in \mathcal{T}$. 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. Figure 1 illustrates a tree-type hexagonal system with 19 hexagons, in which H_3, H_6 and H_{12} are its full-hexagons, H_2, H_8, H_9, H_{11}, H_{13}, H_{16}, H_{17} and H_{18} are its turn-hexagons, and H_1, H_4, H_{10}, H_{15} and H_{19} are its end-hexagons. It is easy to see that the number of the end-hexagons of a tree-type hexagonal system of $n \geqslant 2$ hexagons is more two than the number of its full-hexagons.

A *hexagonal chain* is a tree-type hexagonal system without full-hexagons. Let C be a hexagonal chain with n hexagons $H_1, H_2, \ldots, H_n$, where H_i and H_{i+1} have a common edge for each $i = 1, 2, \ldots, n-1$. We may denote the hexagonal chain by $C = H_1H_2\ldots H_n$. A hexagonal chain with at least two hexagons has two end-hexagons. Let $T \in \mathcal{T}$ and let $B = H_1H_2\ldots H_k$, $k \geqslant 2$ 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 $2 \leqslant i \leqslant k-1$, H_i is not a full-hexagon of T, then B is called a *branch* of T. For example, $B = H_{19}H_{18}H_{17}H_{16}H_{12}$ is a branch of the tree-type hexagonal system illustrated in figure 1. If $T \in \mathcal{T}$ is not a hexagonal chain, then the number of branches of T is equal to the number of end-hexagons of T. A *linear chain* is a hexagonal chain without turn-hexagons. Denote by L_n the linear chain with

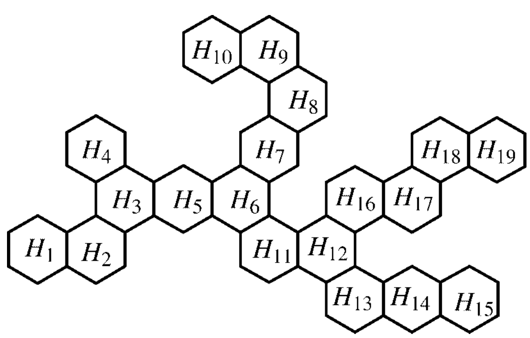

Figure 1. A tree-type hexagonal system.

n hexagons. A *single-angular hexagonal chain* is a hexagonal chain with exactly one turn-hexagon. Suppose that C is a single-angular hexagonal chain. By the definition of single-angular hexagonal chain, its turn-hexagon connects two linear chains, say L_i, L_j. Denote by L_j^i the singly-angular hexagonal chain of $i + j + 1$ hexagons. Obviously, we have $L_j^i = L_i^j$. For convenience, we always suppose that $j \geqslant i$ and $L_j^0 = L_{j+1}$.

Over the years a variety of related properties of hexagonal chains with respect to some indices have been widely studied (for example, [5,6,8–18]). As for the extremal properties, two extremal hexagonal chains with respect to Hosoya index and Merrifield–Simmons index are linear chain and zigzag chain determined in [5] and [6], respectively. If hexagonal chains are restricted in k^*-cycle resonant chains, their two extremal chains are zigzag chain and helicene chain determined in [14]. Gutman, in [5], pointed out the linear hexagonal chain L_n is the unique hexagonal chain with minimum Hosoya index and maximum Merrifield–Simmons index among all the hexagonal chains with n hexagons. He proved the following.

Theorem 1 [5]. For any $n \geqslant 1$ and any hexagonal chain C with n hexagons,

(a) $\mu(L_n) \leqslant \mu(C)$ with the equality only if $C = L_n$,

(b) $\sigma(L_n) \geqslant \sigma(C)$ with the equality only if $C = L_n$.

In [16] and [17], the hexagonal chains with the second minimum Hosoya index and the second maximum Merrifield–Simmons index are determined.

Theorem 2. For any $n \geqslant 3$ and any hexagonal chain C with n hexagons,

(a) if $C \neq L_n$, then $\mu(L_{n-2}^1) \leqslant \mu(C)$ with the equality only if $C = L_{n-2}^1$ [17],

(b) if $C \neq L_n$, then $\sigma(L_{n-2}^1) \geqslant \sigma(C)$ with the equality only if $C = L_{n-2}^1$ [16].

In this paper, extending the class of hexagonal chains to the class of tree-type hexagonal systems, we offer some results with respect to Hosoya index and Merrifield–Simmons index of tree-type hexagonal systems. Using these results, we verify the linear chain L_n and the singly-angular hexagonal chain L_{n-2}^1 are also extremal on the two indices among tree-type hexagonal systems with n hexagons by showing the followings.

Theorem 3. For any $n \geqslant 1$ and any $T \in \mathcal{T}_n$,

(a) $\mu(L_n) \leqslant \mu(T)$ with the equality only if $T = L_n$.

(b) $\sigma(L_n) \geqslant \sigma(T)$ with the equality only if $T = L_n$.

Theorem 4. For any $n \geqslant 3$ and any $T \in \mathcal{T}_n$,

(a) if $T \neq L_n$, then $\mu(L_{n-2}^1) \leqslant \mu(T)$ with the equality only if $T = L_{n-2}^1$,

(b) if $T \neq L_n$, then $\sigma(L_{n-2}^1) \geqslant \sigma(T)$ with the equality only if $T = L_{n-2}^1$.

Note that the hexagonal chains belong to the class of tree-type hexagonal systems. Therefore, theorems 3 and 4 generalize theorems 1 and 2, respectively.

2. Auxiliary lemmas

The following recurrence relations are basic, and can be found in [3–5].

(a) If $G = G_1 \cup G_2$, (that is, G is a graph composed of disjoint components G_1 and G_2), then

$$\mu(G) = \mu(G_1)\mu(G_2), \tag{1}$$

$$\sigma(G) = \sigma(G_1)\sigma(G_2). \tag{2}$$

(b) Let $e = uv$ be an edge of G, and x be a vertex of G. Then

$$\mu(G) = \mu(G - e) + \mu(G - u - v), \tag{3}$$

$$\sigma(G) = \sigma(G - x) + \sigma\big(G - N[x]\big). \tag{4}$$

We add some notations which are convenient to express useful results. For a given linear chain L_n, denote by x'_n, x_n, y_n, y'_n the four clockwise successful vertices with degree two in one of end-hexagons. The turn-hexagon in a singly-angular hexagonal chain L^i_j has two vertices with degree two. Denote by u_i, v_j the two vertices such that u_i links L_i by an edge and v_j links L_j by another edge, (see figure 2(b)). For $L^0_j = L_{j+1}$, let $u_0 = x_{j+1}$ and $v_j = x'_{j+1}$.

For $k \geqslant 1$, set

$$\lambda_k = \mu(L_k), \qquad \xi_k = \mu(L_k - x_k) = \mu(L_k - y_k), \qquad \eta_k = \mu(L_k - x_k - y_k),$$
$$\xi'_k = \mu\big(L_k - x'_k\big) = \mu\big(L_k - y'_k\big), \qquad \eta'_k = \mu\big(L_k - x'_k - x_k\big) = \mu\big(L_k - y_k - y'_k\big).$$

Let $\lambda_0 = 2$, $\xi_0 = 1$ and $\eta_0 = 1$. Noting that $\lambda_1 = 18$, $\xi_1 = 8$ and $\eta_1 = 5$, and using the formulas (1) and (3) (referring to figure 2), we can deduce that for $k \geqslant 1$,

$$\lambda_k = 5\lambda_{k-1} + 6\xi_{k-1} + 2\eta_{k-1},$$
$$\xi_k = 2\lambda_{k-1} + 3\xi_{k-1} + \eta_{k-1},$$

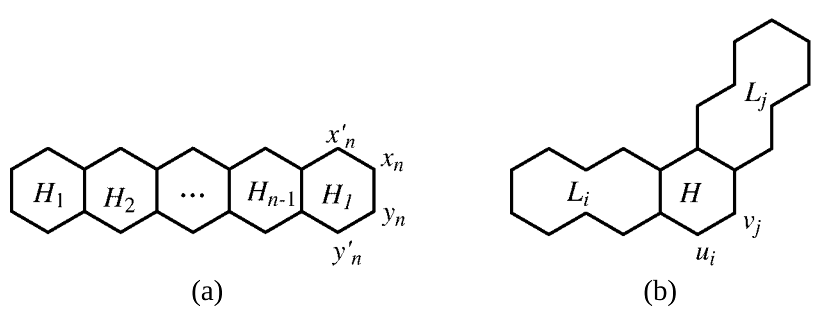

Figure 2. (a) L_n, (b) L^i_j.

$$\begin{aligned} \xi'_k &= 3\lambda_{k-1} + 2\xi_{k-1}, \\ \eta_k &= \lambda_{k-1} + 2\xi_{k-1} + \eta_{k-1}, \\ \eta'_k &= 2\lambda_{k-1} + \xi_{k-1}, \end{aligned} \tag{5}$$

And for $i \geqslant 0$,

$$\begin{aligned} \mu(L^i_j) &= 2\lambda_i\lambda_j + \lambda_i\xi_j + \xi_i\lambda_j + 3\xi_i\xi_j + \xi_i\eta_j + \eta_i\xi_j + \eta_i\eta_j, \\ \mu(L^i_j - u_i) &= \lambda_i\lambda_j + \lambda_i\xi_j + \xi_i\xi_j + \xi_i\eta_j, \\ \mu(L^i_j - v_j) &= \lambda_i\lambda_j + \xi_i\lambda_j + \xi_i\xi_j + \eta_i\xi_j, \\ \mu(L^i_j - u_i - v_j) &= \lambda_i\lambda_j + \xi_i\xi_j. \end{aligned} \tag{6}$$

For $k \geqslant 1$, set

$$\begin{aligned} &\overline{\lambda}_k = \sigma(L_k), \qquad \overline{\xi}_k = \sigma(L_k - x_k) = \sigma(L_k - y_k), \qquad \overline{\eta}_k = \sigma(L_k - x_k - y_k), \\ &\overline{\xi}'_k = \sigma\big(L_k - x'_k\big) = \sigma\big(L_k - y'_k\big), \qquad \overline{\eta}'_k = \sigma\big(L_k - x'_k - x_k\big) = \sigma\big(L_k - y_k - y'_k\big). \end{aligned}$$

Let $\overline{\lambda}_0 = 3$, $\overline{\xi}_0 = 2$ and $\overline{\eta}_0 = 1$. Noting that $\overline{\lambda}_1 = 18$, $\overline{\xi}_1 = 13$ and $\overline{\eta}_1 = 8$, and using the formulas (2) and (4) (referring to figure 2), we get that for $k \geqslant 1$,

$$\begin{aligned} \overline{\lambda}_k &= 3\overline{\lambda}_{k-1} + 4\overline{\xi}_{k-1} + \overline{\eta}_{k-1}, \\ \overline{\xi}_k &= 2\overline{\lambda}_{k-1} + 3\overline{\xi}_{k-1} + \overline{\eta}_{k-1}, \\ \overline{\xi}'_k &= 3\overline{\lambda}_{k-1} + 2\overline{\xi}_{k-1}, \\ \overline{\eta}_k &= \overline{\lambda}_{k-1} + 2\overline{\xi}_{k-1} + \overline{\eta}_{k-1}, \\ \overline{\eta}'_k &= 2\overline{\lambda}_{k-1} + \overline{\xi}_{k-1}. \end{aligned} \tag{7}$$

Similarly, for $i \geqslant 1$, we have

$$\begin{aligned} \sigma\big(L^i_j\big) &= \big(\overline{\lambda}_{i-1} + 2\overline{\xi}_{i-1} + \overline{\eta}_{i-1}\big)\big(2\overline{\lambda}_j + \overline{\xi}_j\big) \\ &\quad + \big(\overline{\lambda}_{i-1} + \overline{\xi}_{i-1}\big)\big(\overline{\lambda}_j + 3\overline{\xi}_j + \overline{\eta}_j\big), \\ \sigma\big(L^i_j - u_i\big) &= \overline{\xi}_i\big(\overline{\lambda}_j + \overline{\xi}_j\big) + \big(\overline{\lambda}_{i-1} + \overline{\xi}_{i-1}\big)\big(\overline{\xi}_j + \overline{\eta}_j\big), \\ \sigma\big(L^i_j - v_j\big) &= \overline{\lambda}_j\big(\overline{\xi}_i + \overline{\eta}_i\big) + 2\overline{\xi}_j\big(\overline{\lambda}_{i-1} + \overline{\xi}_{i-1}\big), \\ \sigma\big(L^i_j - u_i - v_j\big) &= \overline{\xi}_i\overline{\lambda}_j + \big(\overline{\lambda}_{i-1} + \overline{\xi}_{i-1}\big)\overline{\xi}_j. \end{aligned}$$

Noting that $\overline{\lambda}_0 = 3$, $\overline{\xi}_0 = 2$ and $\overline{\eta}_0 = 1$, and by (7), we get that for $i \geqslant 0$

$$\begin{aligned} \sigma\big(L^i_j\big) &= \overline{\eta}_i\big(2\overline{\lambda}_j + \overline{\xi}_j\big) + \big(\overline{\xi}_i - \overline{\eta}_i\big)\big(\overline{\lambda}_j + 3\overline{\xi}_j + \overline{\eta}_j\big), \\ \sigma\big(L^i_j - u_i\big) &= \overline{\xi}_i\big(\overline{\lambda}_j + \overline{\xi}_j\big) + \big(\overline{\xi}_i - \overline{\eta}_i\big)\big(\overline{\xi}_j + \overline{\eta}_j\big), \\ \sigma\big(L^i_j - v_j\big) &= \big(\overline{\xi}_i + \overline{\eta}_i\big)\overline{\lambda}_j + 2\big(\overline{\xi}_i - \overline{\eta}_i\big)\overline{\xi}_j, \\ \sigma\big(L^i_j - u_i - v_j\big) &= \overline{\xi}_i\overline{\lambda}_j + \big(\overline{\xi}_i - \overline{\eta}_i\big)\overline{\xi}_j. \end{aligned} \tag{8}$$

From (5) and (7), we have the following.

Lemma 1. (a) For $k \geqslant 1$, $\lambda_k > \xi_k + \eta_k$ and $\overline{\lambda}_k < \overline{\xi}_k + \overline{\eta}_k$.

(b) For $k \geqslant 2$, $\lambda_k > \xi'_k > \xi_k > \eta'_k > \eta_k$ and $\overline{\lambda}_k > \overline{\xi}_k > \overline{\xi}'_k > \overline{\eta}_k > \overline{\eta}'_k$.

Lemma 2. For $k \geqslant 0$, we have

(a) ξ_k/λ_k, η_k/λ_k, η_k/ξ_k are three strict decrease functions of k ([17]),

(b) $\overline{\xi}_k/\overline{\lambda}_k$, $\overline{\eta}_k/\overline{\lambda}_k$, $\overline{\eta}_k/\overline{\xi}_k$ are three strict increase functions of k.

Proof. In [16], it is proved that $\overline{\xi}_k/\overline{\lambda}_k$ is a strict increase function of k. So we only need to prove that $\overline{\eta}_k/\overline{\lambda}_k$ and $\overline{\eta}_k/\overline{\xi}_k$ are strict increase functions of k.

Noting that $2\overline{\xi}_0 = \overline{\lambda}_0 + \overline{\eta}_0$, and by (7), we obtain that for $k \geqslant 0$,

$$2\overline{\xi}_k = \overline{\lambda}_k + \overline{\eta}_k.$$

Thus, we get that for $k \geqslant 1$,

$$\begin{aligned} \overline{\lambda}_k &= 5\overline{\lambda}_{k-1} + 3\overline{\eta}_{k-1}, \\ \overline{\xi}_k &= \frac{7}{2}\overline{\lambda}_{k-1} + \frac{5}{2}\overline{\eta}_{k-1}, \\ \overline{\eta}_k &= 2\overline{\lambda}_{k-1} + 2\overline{\eta}_{k-1}. \end{aligned} \tag{9}$$

Therefore

$$\begin{aligned} \overline{\eta}_{k+1}\overline{\lambda}_k - \overline{\eta}_k\overline{\lambda}_{k+1} &= \left(2\overline{\lambda}_k + 2\overline{\eta}_k\right)\overline{\lambda}_k - \overline{\eta}_k\left(5\overline{\lambda}_k + 3\overline{\eta}_k\right) \\ &= 2\overline{\lambda}_k^2 - 3\overline{\lambda}_k\overline{\eta}_k - 3\overline{\eta}_k^2 \\ &= 4\left(2\overline{\lambda}_{k-1}^2 - 3\overline{\lambda}_{k-1}\overline{\eta}_{k-1} - 3\overline{\eta}_{k-1}^2\right) \\ &= 4^k\left(2\overline{\lambda}_0^2 - 3\overline{\lambda}_0\overline{\eta}_0 - 3\overline{\eta}_0^2\right) \\ &= 6 \cdot 4^k > 0. \end{aligned}$$

Thus

$$\frac{\overline{\eta}_{k+1}}{\overline{\lambda}_{k+1}} > \frac{\overline{\eta}_k}{\overline{\lambda}_k},$$

i.e., $\overline{\eta}_k/\overline{\lambda}_k$ is a strict increase function of k.

By (9), we can see that

$$\overline{\eta}_{k+1}\overline{\xi}_k - \overline{\xi}_{k+1}\overline{\eta}_k = \frac{1}{2}\left(\overline{\eta}_{k+1}\overline{\lambda}_k - \overline{\eta}_k\overline{\lambda}_{k+1}\right) = 3 \cdot 4^k > 0.$$

Hence $\overline{\eta}_k/\overline{\xi}_k$ is also a strict increase function of k.

The proof of lemma 2 is complete. □

3. Preliminary results and proofs

Suppose $T_1, T_2 \in \mathcal{T}$, and p_i, q_i are two adjacent vertices with degree two in T_i, $i = 1, 2$. Denote by $T_1(p_1, q_1) \oplus T_2(p_2, q_2)$ the tree-type hexagonal system obtained from T_1 and T_2 by identifying p_1 with p_2, and q_1 with q_2, respectively.

In the present section, for a given $T \in \mathcal{T}$, we always assume that s, t are two adjacent vertices with degree two in T, s_1 is the vertex of T adjacent to s but not to t, and t_1 is the vertex of T adjacent to t but not to s.

Theorem 5. For any $T \in \mathcal{T}$ and $k \geqslant 2$,

(a) $\mu(T(s,t) \oplus L_k(x_k, y_k)) < \mu(T(s,t) \oplus L_k(x_k', x_k)) = \mu(T(s,t) \oplus L_k(y_k', y_k))$,

(b) $\sigma(T(s,t) \oplus L_k(x_k, y_k)) > \sigma(T(s,t) \oplus L_k(x_k', x_k)) = \sigma(T(s,t) \oplus L_k(y_k', y_k))$.

Proof. (a) Notice that if $\{e_1, e_2\}$ is a matching of a graph G, then the set of matchings of G can be partitioned into three subsets: the set of matchings containing no e_1 and e_2; the set of matchings containing exact one of e_1 and e_2; and the set of matchings containing e_1 and e_2.

Since $\{ss_1, tt_1\}$ is a matching of the graph illustrated in figure 3(a), by the argument mentioned above and (1), (3), we get

$$\begin{aligned}
&\mu\bigl(T(s,t) \oplus L_k(x_k, y_k)\bigr)\\
&\quad = \mu(T - s - t)\mu(L_k) + \bigl[\mu\bigl(T - N[s]\bigr)\mu(L_k - x_k) + \mu\bigl(T - N[t]\bigr)\mu(L_k - y_k)\bigr]\\
&\qquad + \mu\bigl(T - N[s,t]\bigr)\mu(L_k - x_k - y_k)\\
&\quad = \mu(T - s - t)\lambda_k + \bigl[\mu\bigl(T - N[s]\bigr)\xi_k + \mu\bigl(T - N[t]\bigr)\xi_k\bigr] + \mu\bigl(T - N[s,t]\bigr)\eta_k.
\end{aligned}$$

Similarly, referring to figure 3(b),

$$\begin{aligned}
&\mu\bigl(T(s,t) \oplus L_k\bigl(x_k', x_k\bigr)\bigr)\\
&\quad = \mu(T - s - t)\mu(L_k) + \bigl[\mu\bigl(T - N[s]\bigr)\mu\bigl(L_k - x_k'\bigr) + \mu\bigl(T - N[t]\bigr)\mu(L_k - x_k)\bigr]\\
&\qquad + \mu\bigl(T - N[s,t]\bigr)\mu\bigl(L_k - x_k' - x_k\bigr)\\
&\quad = \mu(T - s - t)\lambda_k + \bigl[\mu\bigl(T - N[s]\bigr)\xi_k' + \mu\bigl(T - N[t]\bigr)\xi_k\bigr] + \mu(T - N[s,t]\bigr)\eta_k'.
\end{aligned}$$

Since $\xi_k < \xi_k'$ and $\eta_k < \eta_k'$ by lemma 1(b), we have

$$\mu\bigl(T(s,t) \oplus L_k(x_k, y_k)\bigr) - \mu\bigl(T(s,t) \oplus L_k\bigl(x_k, x_k'\bigr)\bigr)$$

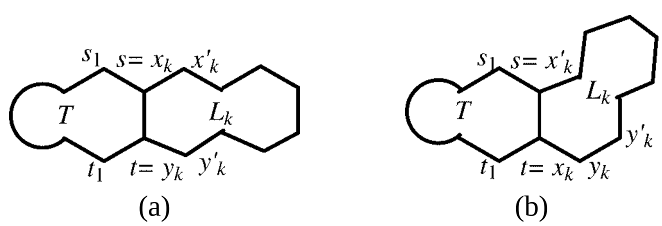

Figure 3. (a) $T(s,t) \oplus L_k(x_k, y_k)$, (b) $T(s,t) \oplus L_k(x_k', x_k)$.

$$= \mu\big(T - N[s]\big)\big(\xi_k - \xi_k'\big) + \mu\big(T - N[s,t]\big)\big(\eta_k - \eta_k'\big) < 0.$$

(b) Note that $\{s_1, t_1\}$ is an independent set of the graph illustrated in figure 3(a). Similar to the proof of (a), considering the sets of independent sets containing no s_1 and t_1, containing exact one of s_1 and t_1, and containing the s_1 and t_1, respectively, by (2) and (4), we get

$$\begin{aligned}
&\sigma\big(T(s,t) \oplus L_k(x_k, y_k)\big)\\
&\quad = \sigma(T - s_1 - t_1)\sigma(L_k) + \big[\sigma\big(T - N[s_1]\big)\sigma(L_k - x_k) + \sigma\big(T - N[t_1]\big)\sigma(L_k - y_k)\big]\\
&\qquad + \sigma\big(T - N[s_1, t_1]\big)\sigma(L_k - x_k - y_k)\\
&\quad = \sigma(T - s_1 - t_1)\overline{\lambda}_k + \big[\sigma\big(T - N[s_1]\big)\overline{\xi}_k + \sigma\big(T - N[t_1]\big)\overline{\xi}_k\big] + \sigma\big(T - N[s_1, t_1]\big)\overline{\eta}_k.
\end{aligned}$$

Similarly, referring to figure 3(b),

$$\begin{aligned}
&\sigma\big(T(s,t) \oplus L_k\big(x_k', x_k\big)\big)\\
&\quad = \sigma(T - s_1 - t_1)\sigma(L_k) + \big[\sigma\big(T - N[s_1]\big)\sigma\big(L_k - x_k'\big)\\
&\qquad + \sigma\big(T - N[t_1]\big)\sigma(L_k - x_k)\big] + \sigma\big(T - N[s_1, t_1]\big)\sigma\big(L_k - x_k' - x_k\big)\\
&\quad = \sigma(T - s_1 - t_1)\overline{\lambda}_k + \big[\sigma\big(T - N[s_1]\big)\overline{\xi}_k' + \sigma\big(T - N[t_1]\big)\overline{\xi}_k\big] + \sigma\big(T - N[s_1, t_1]\big)\overline{\eta}_k'.
\end{aligned}$$

Since $\overline{\xi}_k > \overline{\xi}_k'$ and $\overline{\eta}_k > \overline{\eta}_k'$ by lemma 1(b), we have

$$\begin{aligned}
&\sigma\big(T(s,t) \oplus L_k(x_k, y_k)\big) - \sigma\big(T(s,t) \oplus L_k\big(x_k', x_k\big)\big)\\
&\quad = \sigma\big(T - N[s_1]\big)\big(\overline{\xi}_k - \overline{\xi}_k'\big) + \sigma\big(T - N[s_1, t_1]\big)\big(\overline{\eta}_k - \overline{\eta}_k'\big) > 0. \qquad \square
\end{aligned}$$

Using of recurrence method leads immediately to

Corollary 1. Suppose C is a hexagonal chain with k hexagons, $k \geqslant 1$, and u, v are two adjacent vertices with degree two of its one end-hexagon. Then for any $T \in \mathcal{T}$ the following inequalities hold:

(a) $\mu(T(s,t) \oplus L_k(x_k, y_k)) \leqslant \mu(T(s,t) \oplus C(u,v))$,

(b) $\sigma(T(s,t) \oplus L_k(x_k, y_k)) \geqslant \sigma(T(s,t) \oplus C(u,v))$.

In the following theorem, as we note before, when $i = 1$, $L_{j+1}^{i-1} = L_{j+2}$, $u_{i-1} = x_{j+2}$ and $v_{j+1} = x_{j+2}'$.

Theorem 6. For any $T \in \mathcal{T}$ and $j \geqslant i \geqslant 1$, we have

(a) $\mu(T(t,s) \oplus L_{j+1}^{i-1}(u_{i-1}, v_{j+1})) < \mu(T(s,t) \oplus L_j^i(u_i, v_j))$,

(b) $\sigma(T(t,s) \oplus L_{j+1}^{i-1}(u_{i-1}, v_{j+1})) > \sigma(T(s,t) \oplus L_j^i(u_i, v_j))$.

Proof. The proof of theorem 6 follows a similar pattern of reasoning as the proof of theorem 5 and will be outlined in an abbreviated form.

(a) Note that

$$\begin{aligned}&\mu\big(T(s,t)\oplus L_j^i(u_i,v_j)\big)\\&\quad=\mu(T-s-t)\mu\big(L_j^i\big)+\big[\mu\big(T-N[s]\big)\mu\big(L_j^i-u_i\big)\\&\qquad+\mu\big(T-N[t]\big)\mu\big(L_j^i-v_j\big)\big]+\mu\big(T-N[s,t]\big)\mu\big(L_j^i-u_i-v_j\big)\end{aligned}$$

and

$$\begin{aligned}&\mu\big(T(t,s)\oplus L_{j+1}^{i-1}(u_{i-1},v_{j+1})\big)\\&\quad=\mu(T-s-t)\mu\big(L_{j+1}^{i-1}\big)+\big[\mu\big(T-N[s]\big)\mu\big(L_{j+1}^{i-1}-v_{j+1}\big)\\&\qquad+\mu\big(T-N[t]\big)\mu\big(L_{j+1}^{i-1}-u_{i-1}\big)\big]+\mu\big(T-N[s,t]\big)\mu\big(L_{j+1}^{i-1}-u_{i-1}-v_{j+1}\big).\end{aligned}$$

Thus

$$\begin{aligned}&\mu\big(T(s,t)\oplus L_j^i(u_i,v_j)\big)-\mu\big(T(t,s)\oplus L_{j+1}^{i-1}(u_{i-1},v_{j+1})\big)\\&\quad=\mu(T-s-t)\big[\mu\big(L_j^i\big)-\mu\big(L_{j+1}^{i-1}\big)\big]\\&\qquad+\mu\big(T-N[s]\big)\big[\mu\big(L_j^i-u_i\big)-\mu\big(L_{j+1}^{i-1}-v_{j+1}\big)\big]\\&\qquad+\mu\big(T-N[t]\big)\big[\mu\big(L_j^i-v_j\big)-\mu\big(L_{j+1}^{i-1}-u_{i-1}\big)\big]\\&\qquad+\mu\big(T-N[s,t]\big)\big[\mu\big(L_j^i-u_i-v_j\big)-\mu\big(L_{j+1}^{i-1}-u_{i-1}-v_{j+1}\big)\big].\end{aligned}$$

Applications of the formulas (5) and (6) lead

$$\begin{aligned}&\mu\big(L_j^i\big)-\mu\big(L_{j+1}^{i-1}\big)=3(\xi_{i-1}\lambda_j-\lambda_{i-1}\xi_j)+2(\eta_{i-1}\lambda_j-\lambda_{i-1}\eta_j)+(\eta_{i-1}\xi_j-\xi_{i-1}\eta_j),\\&\mu\big(L_j^i-u_i\big)-\mu\big(L_{j+1}^{i-1}-v_{j+1}\big)=-(\xi_{i-1}\lambda_j-\lambda_{i-1}\xi_j),\\&\mu\big(L_j^i-v_j\big)-\mu\big(L_{j+1}^{i-1}-u_{i-1}\big)=6(\xi_{i-1}\lambda_j-\lambda_{i-1}\xi_j)+3(\eta_{i-1}\lambda_j-\lambda_{i-1}\eta_j)\\&\qquad\qquad+2(\eta_{i-1}\xi_j-\xi_{i-1}\eta_j)\end{aligned}$$

and

$$\begin{aligned}&\mu\big(L_j^i-u_i-v_j\big)-\mu\big(L_{j+1}^{i-1}-u_{i-1}-v_{j+1}\big)\\&\quad=4(\xi_{i-1}\lambda_j-\lambda_{i-1}\xi_j)+2(\eta_{i-1}\lambda_j-\lambda_{i-1}\eta_j)+(\eta_{i-1}\xi_j-\xi_{i-1}\eta_j).\end{aligned}$$

Noting that $j>i-1$ and by lemma 2(a), we have $\xi_{i-1}\lambda_j-\lambda_{i-1}\xi_j>0$, $\eta_{i-1}\lambda_j-\lambda_{i-1}\eta_j>0$, and $\eta_{i-1}\xi_j-\xi_{i-1}\eta_j>0$.

Since $\mu(T-s-t)>\mu(T-N[s])$, we get

$$\mu\big(T(s,t)\oplus L_j^i(u_i,v_j)\big)-\mu\big(T(t,s)\oplus L_{j+1}^{i-1}(u_{i-1},v_{j+1})\big)>0,$$

and hence theorem 6(a) is verified.

(b) Similarly, note that

$$\begin{aligned}
&\sigma\big(T(s,t)\oplus L_j^i(u_i,v_j)\big)\\
&\quad=\sigma(T-s_1-t_1)\sigma\big(L_j^i\big)+\big[\sigma\big(T-N[s_1]\big)\sigma\big(L_j^i-u_i\big)\\
&\qquad+\sigma\big(T-N[t_1]\big)\sigma\big(L_j^i-v_j\big)\big]+\sigma\big(T-N[s_1,t_1]\big)\sigma\big(L_j^i-u_i-v_j\big)
\end{aligned}$$

and

$$\begin{aligned}
&\sigma\big(T(t,s)\oplus L_{j+1}^{i-1}(u_{i-1},v_{j+1})\big)\\
&\quad=\sigma(T-s_1-t_1)\sigma\big(L_{j+1}^{i-1}\big)+\big[\sigma(T-N[s_1])\sigma\big(L_{j+1}^{i-1}-v_{j+1}\big)\\
&\qquad+\sigma\big(T-N[t_1]\big)\sigma\big(L_{j+1}^{i-1}-u_{i-1}\big)\big]+\sigma\big(T-N[s_1,t_1]\big)\sigma\big(L_{j+1}^{i-1}-u_{i-1}-v_{j+1}\big).
\end{aligned}$$

Thus

$$\begin{aligned}
&\sigma\big(T(s,t)\oplus L_j^i(u_i,v_j)\big)-\sigma\big(T(t,s)\oplus L_{j+1}^{i-1}(u_{i-1},v_{j+1})\big)\\
&\quad=\sigma\big(T-s_1-t_1\big)\big[\sigma\big(L_j^i\big)-\sigma\big(L_{j+1}^{i-1}\big)\big]\\
&\qquad+\sigma\big(T-N[s_1]\big)\big[\sigma\big(L_j^i-u_i\big)-\sigma\big(L_{j+1}^{i-1}-v_{j+1}\big)\big]\\
&\qquad+\sigma\big(T-N[t_1]\big)\big[\sigma\big(L_j^i-v_j\big)-\sigma\big(L_{j+1}^{i-1}-u_{i-1}\big)\big]\\
&\qquad+\sigma\big(T-N[s_1,t_1]\big)\big[\sigma\big(L_j^i-u_i-v_j\big)-\sigma\big(L_{j+1}^{i-1}-u_{i-1}-v_{j+1}\big)\big],
\end{aligned}$$

By (7) and (8), we get

$$\begin{aligned}
&\sigma\big(L_j^i\big)-\sigma\big(L_{j+1}^{i-1}\big)=\big(\overline{\xi}_{i-1}\overline{\lambda}_j-\overline{\lambda}_{i-1}\overline{\xi}_j\big)+\big(\overline{\eta}_{i-1}\overline{\lambda}_j-\overline{\lambda}_{i-1}\overline{\eta}_j\big),\\
&\sigma\big(L_j^i-u_i\big)-\sigma\big(L_{j+1}^{i-1}-v_{j+1}\big)=0,\\
&\sigma\big(L_j^i-v_j\big)-\sigma\big(L_{j+1}^{i-1}-u_{i-1}\big)=3\big(\overline{\xi}_{i-1}\overline{\lambda}_j-\overline{\lambda}_{i-1}\overline{\xi}_j\big)+2\big(\overline{\eta}_{i-1}\overline{\lambda}_j-\overline{\eta}_j\overline{\lambda}_{i-1}\big)
\end{aligned}$$

and

$$\sigma\big(L_j^i-u_i-v_j\big)-\sigma\big(L_{j+1}^{i-1}-u_{i-1}-v_{j+1}\big)=2\big(\overline{\xi}_{i-1}\overline{\lambda}_j-\overline{\lambda}_{i-1}\overline{\xi}_j\big)+\big(\overline{\eta}_{i-1}\overline{\lambda}_j-\overline{\lambda}_{i-1}\overline{\eta}_j\big).$$

Therefore, by lemma 2(b), we get

$$\sigma\big(T(s,t)\oplus L_j^i(u_i,v_j)\big)-\sigma\big(T(t,s)\oplus L_j^i(u_{i-1},v_{j+1})\big)<0. \qquad \square$$

Combining theorem 6 and corollary 1, we have

Corollary 2. For any $T\in\mathcal{T}$ and $j\geqslant i>0$:

(a) At least one of the following two inequalities holds:

$$\mu\big(T(s,t)\oplus L_j^i(u_i,v_j)\big)>\mu\big(T(s,t)\oplus L_{i+j+1}\big(x_{i+j+1},x'_{i+j+1}\big)\big)$$

and

$$\mu\big(T(s,t)\oplus L_j^i(u_i,v_j)\big)>\mu\big(T(t,s)\oplus L_{i+j+1}\big(x_{i+j+1},x'_{i+j+1}\big)\big).$$

(b) At least one of the following two inequalities holds:

$$\sigma\big(T(s,t)\oplus L_j^i(u_i,v_j)\big) < \sigma\big(T(s,t)\oplus L_{i+j+1}\big(x_{i+j+1},x'_{i+j+1}\big)\big)$$

and

$$\sigma\big(T(s,t)\oplus L_j^i(u_i,v_j)\big) < \sigma\big(T(t,s)\oplus L_{i+j+1}\big(x_{i+j+1},x'_{i+j+1}\big)\big).$$

4. Proofs of main results

Now we give the proofs of theorems 3 and 4 as follows.

Proof of theorem 3. Denote by $f(T)$ the number of full-hexagons of T.

If $f(T)=0$, then, by theorem 1, we know that theorem 3 holds. Assume the conclusion of the theorem holds for any $T\in\mathcal{T}_n$ with $f(T)=k\geqslant 0$. We now show that the conclusion holds for any $T\in\mathcal{T}_n$ with $f(T)=k+1$.

Let $T\in\mathcal{T}_n$ with $f(T)=k+1>0$. Thus $n\geqslant 4$ and T has at least three branches. Choose two branches $B_1=H_{i+1}H_i\ldots H_1$ and $B_2=H'_{j+1}H'_j\ldots H'_1$ such that $H_{i+1}=H'_{j+1}$ is a full-hexagon in T. Assume, without loss of generality, that $j\geqslant i\geqslant 1$.

Denote by T' the tree-type hexagonal system obtained from T by replacing B_1 with L_{i+1} and B_2 with L_{j+1}, respectively. In this case, obviously, the union of L_{i+1} and L_{j+1} forms a singly-angular hexagonal chain L_j^i with $i+j+1$ hexagons.

Denote by T'' the tree-type hexagonal system obtained from T' by replacing L_j^i with L_{i+j+1}.

By corollaries 1 and 2, we have

$$\mu(T)>\mu\big(T'\big)>\mu\big(T''\big)\quad\text{and}\quad\sigma(T)<\sigma\big(T'\big)<\sigma\big(T''\big). \tag{10}$$

Note that $f(T')=f(T)=k+1$ and $f(T'')=f(T')-1=k$. By the inductive hypothesis, we get that $\mu(L_n)\leqslant\mu(T'')$ with the equality only if $T''=L_n$; and $\sigma(L_n)\geqslant\sigma(T'')$ with the equality only if $T''=L_n$. From (10), we deduce that $\mu(L_n)<\mu(T)$ and that $\sigma(L_n)>\sigma(T)$. The proof of theorem 3 is complete. □

Proof of theorem 4. Let T be any tree-type hexagonal system with n hexagons. If $f(T)=0$, i.e., T is a hexagonal chain, then theorem 6 holds according to theorem 2. So we may assume that $f(T)\neq 0$. Thus $n\geqslant 4$ and T has at least three branches. Suppose $B_1=H_{i+1}H_i\ldots H_1$ and $B_2=H'_{j+1}H'_j\ldots H'_1$ are two branches of T such that $H_{i+1}=H'_{j+1}=H$ is a full-hexagon in T. Let s and t be two vertices of the full-hexagon H but not in $H_iH_{i-1}\ldots H_1$ and $H'_jH'_{j-1}\ldots H'_1$. Set $T_1=T[V(T-(B_1\cup B_2))\cup\{s,t\}]$. Then by theorem 5,

$$\mu(T)\geqslant\mu\big(T_1(s,t)\oplus L_j^i(u_i,v_j)\big)\quad\text{and}\quad\sigma(T)\leqslant\sigma\big(T_1(s,t)\oplus L_j^i(u_i,v_j)\big).$$

Using induction on $f(T)$ and by corollary 2, there is a hexagonal chain C with n hexagons such that $C\neq L_n$ and

$$\mu\big(T_1(s,t)\oplus L_j^i(u_i,v_j)\big)>\mu(C)\quad\text{and}\quad\sigma\big(T_1(s,t)\oplus L_j^i(u_i,v_j)\big)<\sigma(C).$$

Therefore, theorem 4 holds by theorem 2. □

5. Question

From the theorems and corollaries of preceding sections, we can see that if we denote by T_1 and T_2 the two corresponding tree-type hexagonal systems appeared in a theorem or a corollary, then both $\mu(T_1) > \mu(T_2)$ and $\sigma(T_1) < \sigma(T_2)$ hold simultaneously. We do not know if it is true for *any* two tree-type hexagonal systems containing the same number of hexagons. Thus we would like to propose naturally the following question:

For any $T_1, T_2 \in \mathcal{T}_n$, is it true that $\mu(T_1) > \mu(T_2)$ if and only if $\sigma(T_1) < \sigma(T_2)$?

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