Journal of Mathematical Chemistry Vol. 33, No. 1, January 2003 (© 2003)

Extremal k^*-cycle resonant hexagonal chains *

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Received 27 January 2002; revised 28 November 2002

Denote by $\mathcal{B}_n^*$ the set of all k^*-cycle resonant hexagonal chains with n hexagons. For any $B_n \in \mathcal{B}_n^*$, let $m(B_n)$ and $i(B_n)$ be the numbers of matchings (= the Hosoya index) and the number of independent sets (= the Merrifield–Simmons index) of B_n, respectively. In this paper, we give a characterization of the k^*-cycle resonant hexagonal chains, and show that for any $B_n \in \mathcal{B}_n^*$, $m(H_n) \leqslant m(B_n)$ and $i(H_n) \geqslant i(B_n)$, where H_n is the helicene chain. Moreover, equalities hold only if $B_n = H_n$.

KEY WORDS: k^*-cycle resonant hexagonal chain, helicene chain, Hosoya index, Merrifield–Simmons index

1. Introduction

A hexagonal system is a 2-connected plane graph whose every interior face is bounded by a regular hexagon. Hexagonal systems are of great importance for theoretical chemistry because they are the natural graph representation of benzenoid hydrocarbons [1]. A considerable amount of research in mathematical chemistry has been devoted to hexagonal systems [1–3]. A hexagonal chain with n hexagons is a hexagonal system consisting of n regular hexagons $C_1, C_2, \ldots, C_n$ with the properties that (a) for any k, j with $1 \leqslant k < j \leqslant n-1$, C_k and C_j have a common edge if and only if $j = k+1$, and (b) each vertex belongs to at most two hexagons. Hexagonal chains are the graph representation of an important subclass of benzenoid molecules, namely, of the so-called unbranched catacondensed benzenoids. A great deal of mathematical and mathematico-chemical results on hexagonal chains were obtained (see, for example, [1–10]).

Let $G = (V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. Let e and x be an edge and a vertex of G, respectively. We will denote by $G - e$ or $G - x$ the graph obtained from G by removing e or x, respectively. Denote by N_x the set $\{y \in V(G){:}\ xy \in E(G)\} \cup \{x\}$. Let S be a subset of $V(G)$. The subgraph of G induced

* The work was partially supported by the Hong Kong Baptist University Faculty Research Grant; National Natural Science Foundation of China (No. 10271105).

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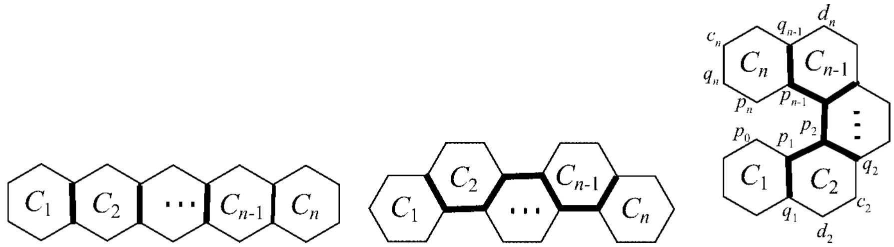


(a) L_n (b) Z_n (c) H_n

Figure 1.

by S is denoted by $G[S]$, and $G[V \setminus S]$ is denoted by $G - S$. Undefined concepts and notations of graph theory are referred to [11,12].

Two edges of a graph G are said to be *independent* if they are not incident. A subset M of $E(G)$ is called a *matching* of G if any two edges of M are independent in G. Denote by $m(G)$ the number of matchings of G. In chemical terminology, $m(G)$ is called the *Hosoya index*.

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 $i(G)$ the number of independent sets of G. In chemical terminology, $i(G)$ is called the *Merrifield–Simmons index*. Clearly, the Hosoya index or the Merrifield–Simmons index of a graph is larger than that of its proper subgraphs.

We denote by $\mathcal{B}_n$ the set of the hexagonal chains with n hexagons. Let $B_n \in \mathcal{B}_n$. We denote by $V_3 = V_3(B_n)$ the set of the vertices with degree 3 in B_n. Thus, the subgraph $B_n[V_3]$ is a 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. Figure 1(a), (b), and (c) illustrates L_n, Z_n and H_n, respectively, where $B_n[V_3]$ are indicated by heavy edges.

Note that the considered hexagonal chains include both geometrically planar (e.g., L_n and Z_n) and geometrically non-planar (e.g., H_n) species. It is easy to see that $\mathcal{B}_1 = \{L_1 = Z_1 = H_1\}$, $\mathcal{B}_2 = \{L_2 = Z_2 = H_2\}$ and $\mathcal{B}_3 = \{L_3, Z_3 = H_3\}$. Let $B_n \in \mathcal{B}_n$ and label its hexagons consecutively by $C_1, C_2, \ldots, C_n$. Thus, the hexagons C_1 and C_n are terminal and for $j = 1, 2, \ldots, n-1$, the hexagons C_j and C_{j+1} have a common edge. We also denote B_n by $C_1C_2 \ldots C_n$.

In the topological theory of unbranched catacondensed hydrocarbons, mathematical chemists are interested in investigating extremal hexagonal chains with respect to some topological indices, such as the number of Kekulé structures, Wiener index, Hosoya index, Merrifield–Simmons index, graph eigenvalue and total π-electron energy (the total absolute values of eigenvalues of a graph) etc. [3,4,7,8,13–23]. Those topological indices of molecular graphs are of great importance in theoretical chemistry [14,16,24]. Among hexagonal chains with extremal properties on topological indices, L_n, Z_n and H_n play important roles. We list some of them in theorems 1.1–1.4.

Theorem 1.1 (Gutman [4], Zhang [7]). For any $n \geqslant 1$ and any $B_n \in \mathcal{B}_n$, if B_n is neither L_n nor Z_n, then

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

Theorem 1.2 (Gutman [4], Zhang [7]). For any $n \geqslant 1$ and any $B_n \in \mathcal{B}_n$, if B_n is neither L_n nor Z_n, then

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

Theorem 1.3 (Gutman [4], Zhang and Tian [8]). Denote by $\lambda_1(G)$ the largest eigenvalue of a graph G. Then for any $n \geqslant 1$ and any $B_n \in \mathcal{B}_n$, if B_n is neither L_n nor H_n, then

$$\lambda_1(L_n) < \lambda_1(B_n) < \lambda_1(H_n).$$

Theorem 1.4 (Zhang et al. [9,10]). Denote by $\pi(G)$ the total π-electron energy of a molecular graph G. Then for any $n \geqslant 1$ and any $B_n \in \mathcal{B}_n$, if B_n is neither L_n nor Z_n, then

$$\pi(L_n) < \pi(B_n) < \pi(Z_n).$$

Let M be a perfect matching of G. A cycle C in G is an *M-alternating cycle* if edges of C belongs to M and does not belong to M alternatively. A number of disjoint cycles in a graph G are *mutually resonant* if there is a perfect matching M of G such that each cycle is an M-alternating cycle. A connected graph G with perfect matching is said to be *k-cycle resonant* if G contains at least k ($\geqslant 1$) disjoint cycles, and any t disjoint cycles in G, $1 \leqslant t \leqslant k$, are mutually resonant. The concept of k-cycle resonant graph was introduced by Guo and Zhang [25]. It is a generalization of k-coverable hexagonal system induced by Zheng [26].

A graph G is called *k^*-cycle resonant* if G is k-cycle resonant and k is the maximum number of disjoint cycles in G. Denote by $\mathcal{B}_n^*$ the set of all k^*-cycle resonant hexagonal chains with n hexagons.

In this paper, we give a characterization of the k^*-cycle resonant hexagonal chains, and show that for any $B_n \in \mathcal{B}_n^*$, $m(H_n) \leqslant m(B_n)$ and $i(H_n) \geqslant i(B_n)$, where H_n is the helicene chain. Moreover, equalities hold only if $B_n = H_n$.

2. k^*-cycle resonant hexagonal chains

Any element B_n of $\mathcal{B}_n$ can be obtained from an appropriately chosen graph $B_{n-1} \in \mathcal{B}_{n-1}$ by attaching to it a new hexagon. Let B be a hexagonal chain, C a hexagon and rs an edge of C. It is easy to see that there are three types of attaching: (i) $r \equiv a,\ s \equiv b$; (ii) $r \equiv b,\ s \equiv c$ and (iii) $r \equiv c,\ s \equiv d$ as shown in figure 2. We call them *α-type*, *β-type* and *γ-type attaching*, respectively. Following [4], we denote by $[B]_\theta$ the hexagonal chain obtained from B by θ-type attaching to it a new hexagon C, where $\theta \in \{\alpha, \beta, \gamma\}$.

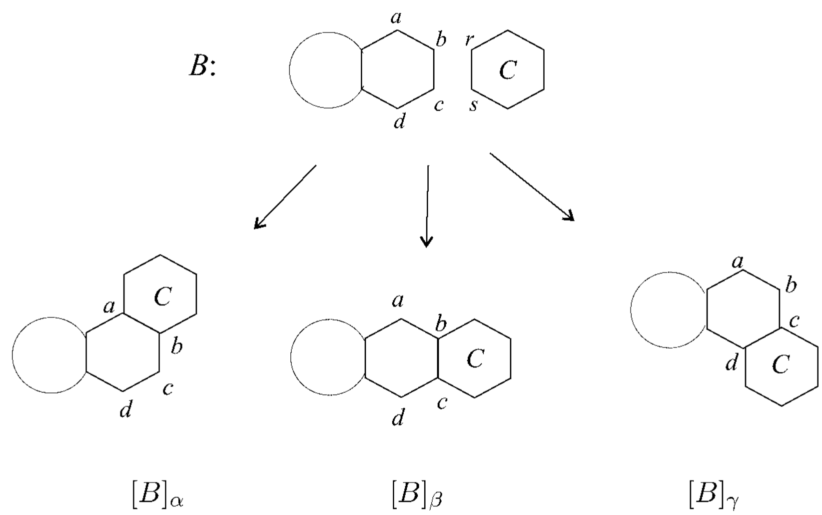


Figure 2.

Obviously, each B_n with $n \geqslant 2$ can be written as $[\ldots[[[L_2]_{\theta_2}]_{\theta_3}]\ldots]_{\theta_{n-1}}$, where $\theta_j \in \{\alpha, \beta, \gamma\}$. We set $B_n = \beta\theta_2\theta_3\ldots\theta_{n-1}$ for short.

For each j, if $\theta_j = \beta$ then $B_n = L_n$; if $\theta_j \in \{\alpha, \gamma\}$ and $\theta_j \neq \theta_{j+1}$, then $B_n = Z_n$; and if $\theta_j = \alpha$ (or γ) then $B_n = H_n$.

Set

$$\overline{\theta} = \begin{cases} \gamma & \text{if } \theta = \alpha, \\ \beta & \text{if } \theta = \beta, \\ \alpha & \text{if } \theta = \gamma. \end{cases}$$

Obviously, the hexagonal chain $B_n = \beta\theta_2\theta_3\ldots\theta_{n-1}$ is isomorphic to the hexagonal chain $\overline{B}_n = \beta\overline{\theta}_2\overline{\theta}_3\ldots\overline{\theta}_{n-1}$.

In [25], Guo and Zhang give some necessary and sufficient conditions for a graph to be k-cycle resonant. We mention the following results which will be useful for our results.

Theorem 2.1 (Guo and Zhang [25]). A connected graph with at least k disjoint cycles is k-cycle resonant if and only if G is bipartite and, for $1 \leqslant t \leqslant k$ and any t disjoint cycles $W_1, W_2, \ldots, W_t$ in G, $G - \bigcup_{j=1}^{t} W_j$ contains no component of odd order.

Theorem 2.2 (Guo and Zhang [25]). Every 2-cycle resonant hexagonal system is k^*-cycle resonant, where k is the maximum number of disjoint cycles in the hexagonal system.

By theorems 2.1 and 2.2, we can show that

Theorem 2.3. A hexagonal chain B_n ($n \geqslant 3$) belongs to $\mathcal{B}_n^*$ if and only if $B_n = C_1C_2 \ldots C_n = \beta\theta_2\theta_3 \ldots \theta_{n-1}$, where $\theta_j \in \{\alpha, \gamma\}$, $2 \leqslant j \leqslant n-1$.

Proof. First, notice that each hexagonal chain is bipartite. Suppose that $B_n = \beta\theta_2\theta_3 \ldots \theta_{n-1}$ belongs to $\mathcal{B}_n^*$. If there is some j, $2 \leqslant j \leqslant n-1$, such that $\theta_j = \beta$, then it is easy to see that $B_n - C_{j-1} - C_{j+1}$ contains two components of order one. This contradicts that B_n is k^*-cycle resonant.

Now, suppose that $B_n = \beta\theta_2\theta_3 \ldots \theta_{n-1}$ is a hexagonal chain with $\theta_j \in \{\alpha, \gamma\}$, $2 \leqslant j \leqslant n-1$. First, we show that B_n is 2-cycle resonant. Let C be any cycle of B_n. Obviously, $B_n - C$ contains no component of odd order. Let C, C' be any two disjoint cycles of B_n, and let $B_n(C)$ and $B_n(C')$ be the sub-chains of B_n whose boundary are C and C', respectively. Assume that $B_n(C) = C_iC_{i+1} \ldots C_j$ and $B_n(C') = C_kC_{k+1} \ldots C_l$, $1 \leqslant i \leqslant j \leqslant k-2 \leqslant l-2 \leqslant n-2$. It is easy to see that in this case, $B_n - C - C'$ contains three components of orders $4(i-1)$, $4(k-j-2)+2$ and $4(n-l)$, respectively. Thus, by theorem 2.1, B_n is 2-cycle resonant, and hence, B_n is k^*-cycle resonant by theorem 2.2. □

By theorem 2.3, every element B_n of $\mathcal{B}_n^*$ can be written as $B_n = \beta\theta_2\theta_3 \ldots \theta_{n-1}$ with $\theta_j \in \{\alpha, \gamma\}$, $2 \leqslant j \leqslant n-1$. Clearly, H_n and Z_n are k^*-resonant.

Denote by $K(G)$ the number of perfect matchings (in chemical terminology, it is called the number of Kekulé structures) of G. In [4], Gutman pointed out that it is well known that all fully-angularly annulated hexagonal chains (with a given n) have equal and maximal K-value. Hence, by theorem 2.3, all k^*-cycle resonant hexagonal chains have equal and maximal K-value. It is easy to see that the equal and maximal K-values $K(B_n)$, $n = 1, 2, \ldots$, are Fibonacci numbers with the initial values $K(B_1) = 2$ and $K(B_2) = 3$.

3. Extremal properties of H_n

Among many properties of $m(G)$ and $i(G)$ [16,24]; we mention the following results which will be used later.

Claim 3.1. Let G be a graph consisting of two components G_1 and G_2. Then

(a) $m(G) = m(G_1)m(G_2)$;

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

Claim 3.2. Let G be a graph.

(a) Suppose $uv \in E(G)$. Then $m(G) = m(G - uv) + m(G - u - v)$.

(b) Suppose $u \in V(G)$. Then $i(G) = i(G - u) + i(G - N_u)$.

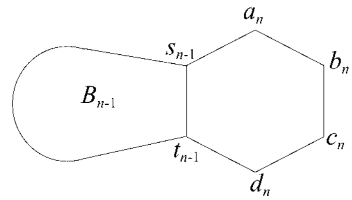


Figure 3.

Claim 3.3. Let G be a graph. For each $uv \in E(G)$,

(a) $m(G) - m(G-u) - m(G-u-v) \geqslant 0$;

(b) $i(G) - i(G-u) - i(G-u-v) \leqslant 0$.

Moreover, equalities hold only if v is the unique neighbor of u.

Let $B_n = C_1C_2 \ldots C_n$ be a any given hexagonal chain. For each $k,\ 1 \leqslant k \leqslant n-1$, we set $B_k = C_1C_2 \ldots C_k$. We use $s_{k-1}, t_{k-1}, a_k, b_k, c_k$ and d_k to label the vertices of C_k such that $s_{k-1}t_{k-1}$ is the common edge of C_{k-1} and C_k, and $s_{k-1}a_k, a_kb_k, b_kc_k, c_kd_k$ and d_kt_{k-1} are the edges of C_k. The case $k = n$ is shown in figure 3.

By claims 3.1 and 3.2, we obtain the following recurrences:

$$\begin{pmatrix} m(B_n) \\ m(B_n - a_n) \\ m(B_n - b_n) \\ m(B_n - c_n) \\ m(B_n - d_n) \\ m(B_n - a_n - b_n) \\ m(B_n - c_n - d_n) \end{pmatrix} = \begin{pmatrix} 5 & 3 & 3 & 2 \\ 3 & 0 & 2 & 0 \\ 2 & 2 & 1 & 1 \\ 2 & 1 & 2 & 1 \\ 3 & 2 & 0 & 0 \\ 2 & 0 & 1 & 0 \\ 2 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} m(B_{n-1}) \\ m(B_{n-1} - s_{n-1}) \\ m(B_{n-1} - t_{n-1}) \\ m(B_{n-1} - s_{n-1} - t_{n-1}) \end{pmatrix} \tag{1}$$

and

$$\begin{pmatrix} i(B_n) \\ i(B_n - a_n) \\ i(B_n - b_n) \\ i(B_n - a_n - b_n) \\ i(B_n - N_{a_n}) \\ i(B_n - N_{b_n}) \end{pmatrix} = \begin{pmatrix} 3 & 2 & 2 & 1 \\ 3 & 0 & 2 & 0 \\ 2 & 2 & 1 & 1 \\ 2 & 0 & 1 & 0 \\ 0 & 2 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} i(B_{n-1}) \\ i(B_{n-1} - s_{n-1}) \\ i(B_{n-1} - t_{n-1}) \\ i(B_{n-1} - s_{n-1} - t_{n-1}) \end{pmatrix}. \tag{2}$$

To demonstrate how to obtain the above relations, we prove the first identity. By applying claims 3.1(a) and 3.2(a) repeatedly we have

$$\begin{aligned} m(B_n) &= m(B_n - s_{n-1}a_n) + m(B_n - s_{n-1} - a_n) \\ &= m(B_n - s_{n-1}a_n - t_{n-1}d_n) + m(B_n - s_{n-1}a_n - t_{n-1} - d_n) \\ &\quad + m(B_n - s_{n-1} - a_n - t_{n-1}d_n) + m(B_n - s_{n-1} - a_n - t_{n-1} - d_n) \end{aligned}$$

$$\begin{aligned}
&= m(B_{n-1})m(P_4) + m(B_{n-1} - t_{n-1})m(P_3) \\
&\quad + m(B_{n-1} - s_{n-1})m(P_3) + m(B_{n-1} - s_{n-1} - t_{n-1})m(P_2) \\
&= 5m(B_{n-1}) + 3m(B_{n-1} - t_{n-1}) + 3m(B_{n-1} - s_{n-1}) \\
&\quad + 2m(B_{n-1} - s_{n-1} - t_{n-1}),
\end{aligned}$$

where P_m is the path with m vertices.

Lemma 3.1. For any $B_n \in \mathcal{B}_n^*$ $(n \geqslant 1)$ and $\{u, v\} = \{a_n, b_n\}$ (see figure 3), we have

(a) $m(B_n) + m(B_n - u) - 2m(B_n - v) - m(B_n - u - v) > 0$;

(b) $i(B_n - u - v) + i(B_n - N_u) - 2i(B_n - N_v) > 0$.

Proof. Since $m(B_1) = 18$, $m(B_1 - u) = 8$, $m(B_1 - u - v) = 5$, $i(B_1 - u - v) = 8$ and $i(B_1 - N_u) = 5 = i(B_1 - N_v)$, the lemma holds when $n = 1$. So we assume $n \geqslant 2$.

(a) Suppose that $u = a_n$ and $v = b_n$. By (1) we have

$$\begin{aligned}
&m(B_n) + m(B_n - a_n) - 2m(B_n - b_n) - m(B_n - a_n - b_n) \\
&\quad = 2m(B_{n-1}) - m(B_{n-1} - s_{n-1}) + 2m(B_{n-1} - t_{n-1}).
\end{aligned}$$

Since $B_{n-1} - s_{n-1}$ is a proper subgraph of B_{n-1}, thus, $m(B_{n-1}) > m(B_{n-1} - s_{n-1})$, and hence, $m(B_n) + m(B_n - a_n) - 2m(B_n - b_n) - m(B_n - a_n - b_n) > 0$.

Suppose that $u = b_n$ and $v = a_n$. By (1) we have

$$\begin{aligned}
&m(B_n) + m(B_n - b_n) - 2m(B_n - a_n) - m(B_n - a_n - b_n) \\
&\quad = -m(B_{n-1}) + 5m(B_{n-1} - s_{n-1}) - m(B_{n-1} - t_{n-1}) + 3m(B_{n-1} - s_{n-1} - t_{n-1}).
\end{aligned}$$

In order to prove that $m(B_n) + m(B_n - b_n) - 2m(B_n - a_n) - m(B_n - a_n - b_n) > 0$, it suffices to show that $5m(B_{n-1} - s_{n-1}) > m(B_{n-1})$ and $3m(B_{n-1} - s_{n-1} - t_{n-1}) > m(B_{n-1} - t_{n-1})$.

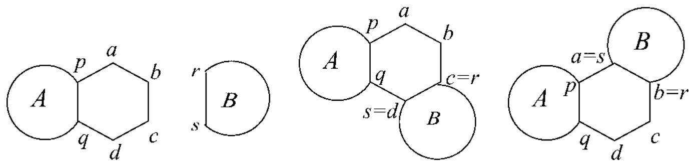
Note that, since B_n is a k^*-cycle resonant hexagonal chain, we must have that either $s_{n-1} = a_{n-1}, t_{n-1} = b_{n-1}$ or $s_{n-1} = c_{n-1}, t_{n-1} = d_{n-1}$. Moreover, $B_{n-1} \in \mathcal{B}_{n-1}^*$.

If $s_{n-1} = a_{n-1}, t_{n-1} = b_{n-1}$, then by (1), we get that

$$\begin{aligned}
&5m(B_{n-1} - s_{n-1}) - m(B_{n-1}) \\
&\quad = 5m(B_{n-1} - a_{n-1}) - m(B_{n-1}) \\
&\quad = 5\big[3m(B_{n-2}) + 2m(B_{n-2} - t_{n-2})\big] \\
&\qquad - \big[5m(B_{n-2}) + 3m(B_{n-2} - s_{n-2}) + 3m(B_{n-2} - t_{n-2}) + 2m(B_{n-2} - s_{n-2} - t_{n-2})\big] \\
&\quad = 10m(B_{n-2}) - 3m(B_{n-2} - s_{n-2}) + 7m(B_{n-2} - t_{n-2}) - 2m(B_{n-2} - s_{n-2} - t_{n-2}).
\end{aligned}$$

Since $B_{n-2} - s_{n-2}$ and $B_{n-2} - s_{n-2} - t_{n-2}$ are the proper subgraphs of B_{n-2} and $B_{n-2} - t_{n-2}$, respectively, we can get $5m(B_{n-1} - s_{n-1}) - m(B_{n-1}) > 0$ in this case.

Similarly, we can show that $5m(B_{n-1} - s_{n-1}) > m(B_{n-1})$ in the case $s_{n-1} = c_{n-1}, t_{n-1} = d_{n-1}$, and that $3m(B_{n-1} - s_{n-1} - t_{n-1}) > m(B_{n-1} - t_{n-1})$.



(a) A^* and B (b) G_γ (c) G_α

Figure 4.

(b) Similar to the proof of (a), by (2) we get

$$\begin{aligned} &i(B_n) + i(B_n - N_{a_n}) - 2i(B_n - N_{b_n}) \\ &\quad = i(B_{n-1}) + 4i(B_{n-1} - s_{n-1}) + 2i(B_{n-1} - s_{n-1} - t_{n-1}), \end{aligned}$$

and

$$\begin{aligned} &i(B_n) + i(B_n - N_{b_n}) - 2i(B_n - N_{a_n}) \\ &\quad = 4i(B_{n-1}) + 3i(B_{n-1} - t_{n-1}) - 2i(B_{n-1} - s_{n-1}) - i(B_{n-1} - s_{n-1} - t_{n-1}). \end{aligned}$$

Notice that $B_{n-1} - s_{n-1}$ and $B_{n-1} - s_{n-1} - t_{n-1}$ are the proper subgraphs of B_{n-1} and $B_{n-1} - s_{n-1}$, respectively. Therefore, $i(B_n) + i(B_n - N_u) - 2i(B_n - N_v) > 0$ for $\{u, v\} = \{a_n, b_n\}$. □

Let A^* and B be two hexagonal chains, where A^* is obtained from the hexagonal chain A by attaching a hexagon H. The vertices of H are labeled a, b, c, d, q and p as shown in figure 4(a). Let r and s be two adjacent vertices of B of degree two. Now, we denote by G_γ the hexagonal chain obtained from A^* and B by identifying c and r, and d and s, respectively (figure 4(b)); and by G_α the hexagonal chain obtained from A^*, B by identifying a and s, and b and r, respectively (figure 4(c)).

Lemma 3.2. Let A, B, G_γ and G_α be the k^*-cycle resonant hexagonal chains shown in figure 4. We have

(a) if $m(A - p) > m(A - q)$, then $m(G_\gamma) > m(G_\alpha)$;

(b) if $i(A - p) < i(A - q)$, then $i(G_\gamma) < i(G_\alpha)$.

Proof. (a) By claims 3.1(a) and 3.2(a), we have the following:

$$\begin{aligned} m(G_\gamma) = &\big\{m(A) + m(A - p)\big\}\big\{m(B) + m(B - r)\big\} \\ &+ \big\{m(A - q) + m(A - p - q)\big\}\big\{m(B - s) + m(B - r - s)\big\} \\ &+ m(A)m(B) + m(A - q)m(B - s) \end{aligned}$$

and

$$\begin{aligned} m(G_\alpha) = &\big\{m(A) + m(A - q)\big\}\big\{m(B) + m(B - r)\big\} \\ &+ \big\{m(A - p) + m(A - p - q)\big\}\big\{m(B - s) + m(B - r - s)\big\} \\ &+ m(A)m(B) + m(A - p)m(B - s). \end{aligned}$$

Thus,

$$\begin{aligned} &m(G_\gamma) - m(G_\alpha) \\ &\quad = \big\{m(A-p) - m(A-q)\big\}\big\{m(B) + m(B-r) - 2m(B-s) - m(B-r-s)\big\}. \end{aligned}$$

By lemma 3.1(a), $m(B) + m(B-r) - 2m(B-s) - m(B-r-s) > 0$. Therefore, if $m(A-p) > m(A-q)$, then $m(G_\gamma) > m(G_\alpha)$.

(b) By claims 3.1(b) and 3.2(b), we have the following:

$$\begin{aligned} i(G_\gamma) = &\big\{2i(A) + i(A-p)\big\}i(B-r-s) + \big\{i(A) + i(A-p)\big\}i(B-N_r) \\ &+ \big\{2i(A-q) + i(A-p-q)\big\}i(B-N_s) \end{aligned}$$

and

$$\begin{aligned} i(G_\alpha) = &\big\{2i(A) + i(A-q)\big\}i(B-r-s) + \big\{i(A) + i(A-q)\big\}i(B-N_r) \\ &+ \big\{2i(A-p) + i(A-p-q)\big\}i(B-N_s). \end{aligned}$$

Thus,

$$i(G_\gamma) - i(G_\alpha) = \big\{i(A-p) - i(A-q)\big\}\big\{i(B-r-s) + i(B-N_r) - 2i(B-N_s)\big\}.$$

By lemma 3.1(b), $i(B-r-s) + i(B-N_r) - 2i(B-N_s) > 0$. Hence, if $i(A-p) < i(A-q)$, then $i(G_\gamma) < i(G_\alpha)$. $\square$

Let $H_n = C_1C_2\ldots C_n$ be a helicene chain. We label the common edge of C_1 and C_2 as p_1q_1; and for each k, $2 \leqslant k \leqslant n$, we label the vertices of $V(C_k) - V(C_{k-1})$ as $p_k,\ q_k,\ c_k$ and d_k such that $p_{k-1}p_k, p_kq_k, q_kc_k, c_kd_k$ and d_kq_{k-1} are edges in H_n (see figure 1(c)). In figure 3, if let $B_n = H_n$, $B_{n-1} = H_{n-1}$, $s_{n-1} = p_{n-1}$, $t_{n-1} = q_{n-1}$, then $a_n = p_n$ and $b_n = q_n$. By (1) and (2) we get

$$\begin{pmatrix} m(H_n) \\ m(H_n - p_n) \\ m(H_n - q_n) \\ m(H_n - p_n - q_n) \end{pmatrix} = \begin{pmatrix} 5 & 3 & 3 & 2 \\ 3 & 0 & 2 & 0 \\ 2 & 2 & 1 & 1 \\ 2 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} m(H_{n-1}) \\ m(H_{n-1} - p_{n-1}) \\ m(H_{n-1} - q_{n-1}) \\ m(H_{n-1} - p_{n-1} - q_{n-1}) \end{pmatrix} \tag{3}$$

and

$$\begin{pmatrix} i(H_n) \\ i(H_n - p_n) \\ i(H_n - q_n) \\ i(H_n - p_n - q_n) \end{pmatrix} = \begin{pmatrix} 3 & 2 & 2 & 1 \\ 3 & 0 & 2 & 0 \\ 2 & 2 & 1 & 1 \\ 2 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} i(H_{n-1}) \\ i(H_{n-1} - p_{n-1}) \\ i(H_{n-1} - q_{n-1}) \\ i(H_{n-1} - p_{n-1} - q_{n-1}) \end{pmatrix}. \tag{4}$$

Let

$$\Phi_n = m(H_n) - m(H_n - p_n) - m(H_n - p_n - q_n)$$

and

$$\Psi_n = i(H_n) - i(H_n - p_n) - i(H_n - p_n - q_n).$$

Lemma 3.3. For $n \geqslant 1$, we have

(a) Φ_n is a strictly increasing function of n;

(b) Ψ_n is a strictly decreasing function of n.

Proof. (a) It is easy to see that $\Phi_1 = 5$ and $\Phi_2 = 34$.

By (3), we can get

$$\Phi_n = 3m(H_{n-1} - p_{n-1}) + 2m(H_{n-1} - p_{n-1} - q_{n-1}).$$

For $n \geqslant 3$, we have

$$\begin{aligned}\Phi_n - \Phi_{n-1} = {} & 3\{m(H_{n-1} - p_{n-1}) - m(H_{n-2} - p_{n-2})\} \\ & + 2\{m(H_{n-1} - p_{n-1} - q_{n-1}) - m(H_{n-2} - p_{n-2} - q_{n-2})\}.\end{aligned}$$

Since $H_{n-2} - p_{n-2}$ and $H_{n-2} - p_{n-2} - q_{n-2}$ are the proper subgraphs of $H_{n-1} - p_{n-1}$ and $H_{n-1} - p_{n-1} - q_{n-1}$, respectively, $m(H_{n-1} - p_{n-1}) > m(H_{n-2} - p_{n-2})$ and $m(H_{n-1} - p_{n-1} - q_{n-1}) > m(H_{n-2} - p_{n-2} - q_{n-2})$. Therefore, $\Phi_n > \Phi_{n-1}$.

(b) It is easy to see that $i(H_1) = 18$, $i(H_1 - p_1) = 13$ and $i(H_1 - p_1 - q_1) = 8$. Thus, $\Psi_1 = -3$, $\Psi_2 = -10$ and $\Psi_3 = -190$.

By (4), we get that

$$\begin{aligned}\Psi_n &= -2i(H_{n-1}) + 2i(H_{n-1} - p_{n-1}) - i(H_{n-1} - q_{n-1}) + i(H_{n-1} - p_{n-1} - q_{n-1}) \\ &= -6i(H_{n-2} - p_{n-2}) - 3i(H_{n-2} - p_{n-2} - q_{n-2}).\end{aligned}$$

Thus, for $n \geqslant 4$, we have that

$$\begin{aligned}\Psi_n - \Psi_{n-1} = {} & 6\{i(H_{n-3} - p_{n-3}) - i(H_{n-2} - p_{n-2})\} \\ & + 3\{i(H_{n-3} - p_{n-3} - q_{n-3}) - i(H_{n-2} - p_{n-2} - q_{n-2})\}.\end{aligned}$$

Since $H_{n-3} - p_{n-3}$ and $H_{n-3} - p_{n-3} - q_{n-3}$ are the proper subgraphs of $H_{n-2} - p_{n-2}$ and $H_{n-2} - p_{n-2} - q_{n-2}$, respectively, we have that $i(H_{n-3} - p_{n-3}) < i(H_{n-2} - p_{n-2})$ and $i(H_{n-3} - p_{n-3} - q_{n-3}) < i(H_{n-2} - p_{n-2} - q_{n-2})$. Therefore $\Psi_n < \Psi_{n-1}$. □

Lemma 3.4. Let H_n be a helicene chain. Then

(a) $m(H_1 - p_1) = m(H_1 - q_1)$, and for each $n \geqslant 2$, $m(H_n - p_n) > m(H_n - q_n)$.

(b) $i(H_1 - p_1) = i(H_1 - q_1)$, and for each $n \geqslant 2$, $i(H_n - p_n) < i(H_n - q_n)$.

Proof. It is easy to obtain that $m(H_1 - p_1) - m(H_1 - q_1) = 0$ and $m(H_2 - p_2) - m(H_2 - q_2) > 0$. For $n \geqslant 3$, by (3) and (4) we have

$$\begin{aligned}m(H_n - p_n) - m(H_n - q_n) &= m(H_{n-1}) - m(H_{n-1} - p_{n-1}) - m(H_{n-1} - p_{n-1} - q_{n-1}) \\ &\quad - \{m(H_{n-1} - p_{n-1}) - m(H_{n-1} - q_{n-1})\} \\ &= \Phi_{n-1} - \{m(H_{n-1} - p_{n-1}) - m(H_{n-1} - q_{n-1})\} \\ &= (\Phi_{n-1} - \Phi_{n-2}) + \{m(H_{n-2} - p_{n-2}) - m(H_{n-2} - q_{n-2})\}\end{aligned}$$

and

$$\begin{aligned} i(H_n - p_n) - i(H_n - q_n) &= \bigl\{i(H_{n-1}) - i(H_{n-1} - p_{n-1}) - i(H_{n-1} - p_{n-1} - q_{n-1})\bigr\} \\ &\quad - \bigl\{i(H_{n-1} - p_{n-1}) - i(H_{n-1} - q_{n-1})\bigr\} \\ &= \Psi_{n-1} + \bigl\{i(H_{n-1} - q_{n-1}) - i(H_{n-1} - p_{n-1})\bigr\} \\ &= (\Psi_{n-1} - \Psi_{n-2}) + \bigl\{i(H_{n-2} - p_{n-2}) - i(H_{n-2} - q_{n-2})\bigr\}. \end{aligned}$$

By lemma 3.3(a), we have $\Phi_{n-1} - \Phi_{n-2} > 0$. Hence, we get that for each $n \geqslant 3$, $m(H_n - p_n) > m(H_n - q_n)$.

Similarly, we can obtain $i(H_1 - p_1) - i(H_1 - q_1) = 0$ and $i(H_2 - p_2) - i(H_2 - q_2) < 0$. By lemma 3.3(b), we have $\Psi_{n-1} - \Psi_{n-2} < 0$. Hence, we get that for each $n \geqslant 3$, $i(H_n - p_n) < i(H_n - q_n)$. □

Theorem 3.5. For any $n \geqslant 1$ and any $B_n \in \mathcal{B}_n^*$, we have

(a) $m(H_n) \leqslant m(B_n) \leqslant m(Z_n)$;

(b) $i(H_n) \geqslant i(B_n) \geqslant i(Z_n)$,

with relevant equalities holding only if $B_n = H_n$, or only if $B_n = Z_n$.

Proof. We only need to verify the first inequalities of (a) and (b) according to theorems 1.1 and 1.2. Let $B_n \in \mathcal{B}_n^*$ be the hexagonal chain with the smallest number of matchings (the largest number of independent sets, respectively). By theorem 2.3, $B_n \in \mathcal{B}_n^*$ can be written as $B_n = \beta\theta_2\theta_3\ldots\theta_{n-1}$ with $\theta_j \in \{\alpha, \gamma\}$, $2 \leqslant j \leqslant n-1$. Assume, without loss of generality, that $\theta_2 = \alpha$ (otherwise, we consider $\overline{B}_n = \beta\overline{\theta}_2\overline{\theta}_3\ldots\overline{\theta}_{n-1}$). Suppose that $B_n \neq H_n$. Since $\mathcal{B}_1^* = \{H_1\}$, $\mathcal{B}_2^* = \{H_2\}$ and $\mathcal{B}_3^* = \{H_3\}$, we have that $n \geqslant 4$. Let θ_j be the first element of $\theta_2, \theta_3, \ldots, \theta_{n-1}$ such that $\theta_j = \gamma$. Thus, $j \geqslant 3$, and $B_n = \beta\alpha\ldots\alpha\gamma\theta_{j+1}\ldots\theta_{n-1}$.

Referring to figure 4, set $G_\gamma = B_n = \beta\alpha\ldots\alpha\gamma\theta_{j+1}\ldots\theta_{n-1}$, $A = \beta\alpha\ldots\alpha = H_{j-1}$, $p = p_{j-1}$ and $q = q_{j-1}$. Let $G_\alpha = \beta\alpha\ldots\alpha\alpha\overline{\theta}_{j+1}\ldots\overline{\theta}_{n-1}$.

By lemma 3.4(a) (lemma 3.4(b), respectively), we have $m(A-p) > m(A-q)$ (and $(A - p) < i(A - q)$, respectively). By lemma 3.2(a) (lemma 3.2(b), respectively), we have $m(B_n) > m(G_\alpha)$, (and $(B_n) < i(G_\alpha)$, respectively), which contradicts the choice of B_n. The proof of theorem 3.5 is complete. □

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