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# Double hexagonal chains with maximal Hosoya index and minimal Merrifield–Simmons index

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It is well known that the two graph invariants, "the Hosoya index" and "the Merrifield–Simmons index" are important ones in structural chemistry. The extremal hexagonal chains with respect to the Hosoya index and Merrifield–Simmons index are determined by Gutman and Zhang (J. Math. Chem., 12 (1993) 197–210, 27 (2000) 319–329 and J. Sys. Sci. Math. Sci., 18 (4) (1998) 460–465). In this paper, we will consider a type of the pericondensed hexagonal system. The double hexagonal chains with maximal Hosoya index and minimal Merrifield Simmons index are determined.

**KEY WORDS:** double hexagonal chain, Hosoya index, Merrifield–Simmons index

## 1. Introduction

Let $G = (V, E)$ be a graph with the vertex set $V(G)$ and edge set $E(G)$. Let $uv$ be an edge of $G$ we write $G - uv$ for the graph obtained from $G$ by deleting $uv$. For $v \in V(G)$, $G - v$ denotes the graph obtained from $G$ by deleting the vertex $v$ and all edges incident with $v$. More generally, for $S \subseteq V(G)$, $G - S$ is the subgraph of $G$ induced by $V(G) \backslash S$.

Two edges of a graph $G$ are said to be independent if they are not adjacent. 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(=the Hosoya index) of $G$. 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 in $G$. Denote by $i(G)$ the number of independent sets(=the Merrifield–Simmons index) of $G$.

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A hexagonal system is a 2-connected plane graph whose every interior face is bounded by a regular hexagon of unit length 1. Hexagonal systems are of considerable importance in theoretical chemistry because they are the natural graph representation of benzenoid hydrocarbons [1, 3–5]. A vertex of a hexagonal system belongs to, at most, three hexagons. A vertex shared by three hexagons is called an internal vertex of the respective hexagonal system. A hexagonal system $H$ is said to be catacondensed if it does not possess internal vertices, otherwise $H$ is said to be pericondensed. A hexagonal chain is a catacondensed hexagonal system which has no hexagon adjacent to more than two hexagons. An $n$-tuple hexagonal chain consists of $n$ condensed identical hexagonal chains. When $n = 2$, we call it double hexagonal chain [1–2]. The double hexagonal chain can be constructed inductively. Let us orient the naphthalene so that its interior edges is horizontal. There are two types of fusion of two naphthalenes: (i) $b \equiv r, c \equiv s, d \equiv t, e \equiv u$; (ii) $a \equiv s, b \equiv t, c \equiv u, d \equiv v$ as shown in figure 1. We call them $\alpha$-type and $\beta$-type fusing, respectively.

A double hexagonal chain can be obtained from a naphthalene by a stepwise fusion of new naphthalene, and at each step a type of fusion is selected from $\theta$-type fusing, where $\theta \in \{\alpha, \beta\}$. If $D$ is a double hexagonal chain, we denote that by $[D]_\theta$ the double hexagonal chain obtained from $D$ by $\theta$-type fusing to it a new naphthalene $B$. Let $\Phi_{2\times n} = \{D_{2\times n} | D_{2\times n}$ is a double hexagonal chain with $2n$ hexagons$\}$. Obviously, each $D_{2\times n}$ with $n \geqslant 2$ can be written as $[\cdots[[[B]_{\theta_1}]_{\theta_2}]\cdots]\theta_{n-1}$, where $\theta_j \in \{\alpha, \beta\}$. We set $D_{2\times n} = \theta_1\theta_2\cdots\theta_{n-1}$ for short. For each $j, \theta_j \in \{\alpha, \beta\}$, if $\theta_j = \theta_{j+1}$ then $D_{2\times n}$ is called the double linear hexagonal chain and denoted by $L_{2\times n}$; if $\theta_j \neq \theta_{j+1}$ then $D_{2\times n}$ is called the double zig-zag hexagonal chain and denoted by $Z_{2\times n}$ (see figure 2).
Set

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

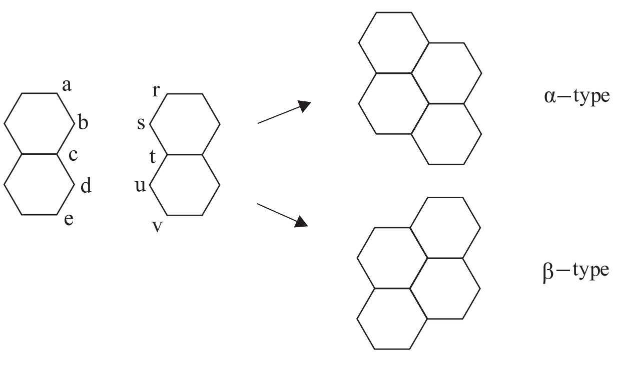


Figure 1.

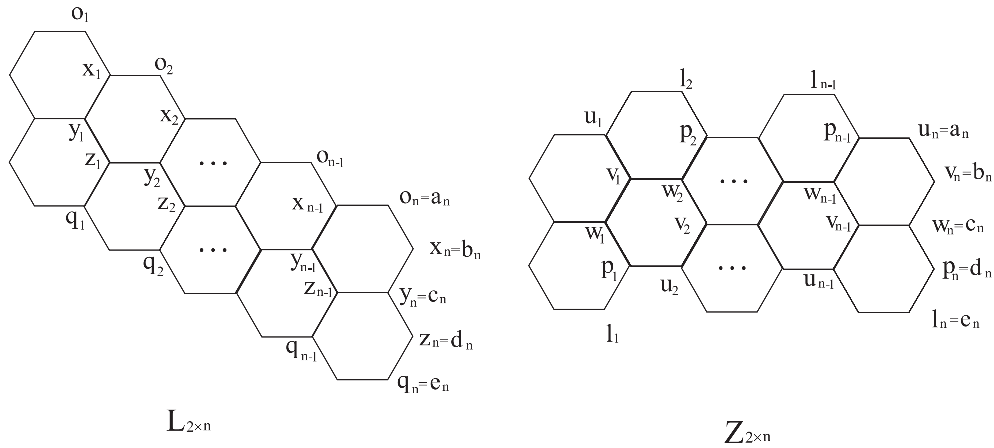


Figure 2.

It is seen that the double hexagonal chain $D_{2\times n} = \theta_1\theta_2\cdots\theta_{n-1}$ is isomorphic to the double hexagonal chain $\overline{D_{2\times n}} = \overline{\theta_1}\,\overline{\theta_2}\cdots\overline{\theta_{n-1}}$. Clearly when $n \geqslant 2$, the double hexagonal chain $D_{2\times n}$ is a pericondensed hexagonal system.

The topological indices, the Hosoya index and Merrifield-Simmons index of molecular graphs are importance ones in structural chemistry [1, 2, 6–10]. For the hexagonal chains, Gutman showed that the linear chain had possessed the minimal Hosoya index and maximal Merrifield–Simmons index. He also proposed the conjectures on the zig-zag chain with maximal Hosoya index and minimal Merrifield–Simmons index [9], which was verified in [10]. It is natural to conjecture that similar results exist for the $n$-tuple hexagonal chains as well, but a proof seems to be not easy. So, we first consider the double hexagonal chains. In the manuscript - "Double hexagonal chains with minimal $k$-matching numbers and maximal $k$-independent set number" proved by Rex and Zhand (submitted) we showed that the double linear hexagonal chain had possessed the minimal Hosoya index and maximal Merrifield–Simmons index. In this paper, we will show that the double zig-zag hexagonal chain possesses the maximal Hosoya index and minimal Merrifield–Simmons index. The main results are the following two theorems:

**Theorem A.** For any double hexagonal chain $D_{2\times n} \in \Phi_{2\times n}$, we have $m(D_{2\times n}) \leqslant m(Z_{2\times n})$ with relevant equality holding only if $D_{2\times n} = Z_{2\times n}$.

**Theorem B.** For any double hexagonal chain $D_{2\times n} \in \Phi_{2\times n}$, we have $i(D_{2\times n}) \geqslant i(Z_{2\times n})$ with relevant equality holding only if $D_{2\times n} = Z_{2\times n}$.

Since $\Phi_{2\times 1} = \{L_{2\times 1}\} = \{Z_{2\times 1}\}$, $\Phi_{2\times 2} = \{L_{2\times 2}\} = \{Z_{2\times 2}\}$, $\Phi_{2\times 3} = \{L_{2\times 3}, Z_{2\times 3}\}$. Obviously, theorems A and B hold for $n = 1, 2$. Thus, we suppose that $n \geqslant 3$ below.

## 2. Preliminaries

The following Lemmas 2.1–2.3 will be used in sequel ([6]–[8]).

**Lemma 2.1.** Let $G$ be a graph consisting of two components $G_1$ and $G_2$. Then

(i) $m(G) = m(G_1) \cdot m(G_2)$, (ii) $i(G) = i(G_1) \cdot i(G_2)$.

**Lemma 2.2.** Let $G$ be a graph.

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

(ii) Suppose $u \in V(G)$ and $N_u$ be the subset of $V(G)$ containing the vertex $u$ and its neighbors. Then $i(G) = i(G - u) + i(G - N_u)$.

**Lemma 2.3.** Let $G$ be a graph. For each $uv \in E(G)$,

(i) $m(G) - m(G-u) - m(G-u-v) \geqslant 0$, (ii) $i(G) - i(G-u) - i(G-u-v) \leqslant 0$.

Moreover, the equalities of (i) and (ii) hold only if $v$ is the unique neighbor of $u$.

**Corollary 2.4.** Let $u$ be a vertex of $G$ and $N_G(u) = N_u - \{u\}$. Then

$$m(G) = m(G - u) + \sum_{v_i \in N_G(u)} m(G - u - v_i).$$

*Proof.* It is easy to see that corollary 2.4 holds by repeatedly using Lemma 2.2(i).

Let $D_{2\times(n-1)}$ be a double hexagonal chain with $n-1$ naphthalenes and $D_{2\times n}$ is obtained from $D_{2\times(n-1)}$ by $\theta$-type fusing to it a new naphthalene, where $\theta \in \{\alpha, \beta\}$ (see figure 3). If $\theta = \alpha$ then the vertices of $D_{2\times n}$ are labelled as in figure 3 (a); and if $\theta = \beta$ then the vertices of $D_{2\times n}$ are labelled as in figure 3(b). Thus from figure 3 it follow that $rstgh \in \{abcde, edcba\}$. Note that $\bar{\beta} = \alpha$, it is clear that the case of figure 3(b) is equivalent to the case of figure 3(a). Hence, without loss of generality, in the following we only need to consider figure 3(a).

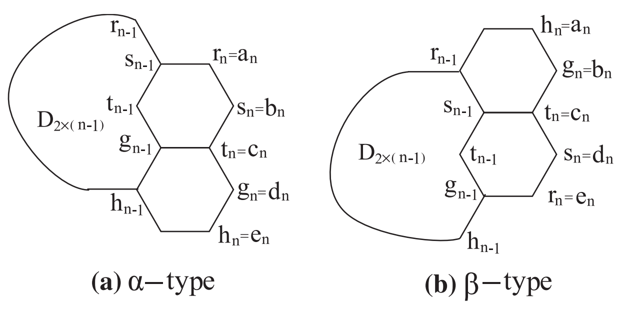


Figure 3. (a) $\alpha$-type, (b) $\beta$-type.

Let $G$ be a graph and $s, g, h \in V(G)$, Define $A(\Psi(G), sgh)$ as the index vector of $G$ with respect to $s, g$ and $h$, i.e., $A(\Psi(G), sgh) = [\Psi(G), \Psi(G - s), \Psi(G-g), \Psi(G-h), \Psi(G-s-g), \Psi(G-g-h), \Psi(G-s-h), \Psi(G-s-g-h)]$, where $\Psi \in \{m, i\}$.

**Lemma 2.5.** If the vertices of $D_{2\times n}$ are labelled as in figure 3(a). Let $G \in \{D_{2\times n}, D_{2\times n}, -\gamma_n, D_{2\times n} - \delta_n - \varepsilon_n, D_{2\times n} - \zeta_n - \eta_n - \theta_n | \gamma \in \{a, b, d, e\}, \delta\varepsilon \in \{bd, ab, bc, cd, de, ad, be\}, \zeta\eta\theta \in \{abd, bde\}\}$. Then the recurrence relation for $m(G)$(resp. $i(G)$) can be written as the scalar product of two vectors, i.e.

$$\Psi(G) = B(\Psi(G)) \cdot A(\Psi(D_{2\times(n-1)}), s_{n-1}g_{n-1}h_{n-1}),$$

where $\Psi = m$(resp. $\Psi = i$) and $B(\Psi(G))$ (see table 1) denotes the vector in $x$ with 8 entries determined by the coefficients of $A(\Psi(D_{2\times(n-l)}), s_{n-1}g_{n-1}h_{n-1})$ in $\Psi(G)$.

*Proof.* For $\Psi = m$, by repeatedly using Lemma 2.1(i) and Corollary 2.4 to $G$, it is seen that $m(G) = B(m(G)) \cdot A(m(D_{2\times(n-1)}), s_{n-1}g_{n-1}h_{n-1})$, where $B(m(G))$ is listed in Table 1. For $\Psi = i$, by Lemmas 2.1(ii) and 2.2(ii) we can get similar results. Thus Lemma 2.5 holds. □

**Lemma 2.6.** If the vertices of $D_{2\times n}$ are labelled as in figure 3(a). Let

$$f_n(D_s) = m(D_{2\times n}) - m(D_{2\times n} - s_n) - m(D_{2\times n} - s_n - h_n)$$

Table 1
Two vectors $B(m(G))$ and $B(i(G))$ of graph $G$.

| G | B(m(G)) | B(i(G))) |
|---|---|---|
| $D_{2\times n} - a_n$ | [8,0,3,5,0,2,0,0] | [6,0,2,4,0,1,0,0] |
| $D_{2\times n} - b_n$ | [5,5,3,3,3,2,3,2] | [3,3,2,2,2,1,2,1] |
| $D_{2\times n} - d_n$ | [6,4,4,3,2,2,2,1] | [4,2,2,2,2,1,1,1] |
| $D_{2\times n} - e_n$ | [5,3,2,5,1,2,3,1] | [4,2,1,4,1,1,2,1] |
| $D_{2\times n} - b_n - d_n$ | [2,2,2,1,2,1,1,1] | [2,2,2,1,2,1,1,1] |
| $D_{2\times n} - a_n - b_n$ | [5,0,3,3,0,2,0,0] | [3,0,2,2,0,1,0,0] |
| $D_{2\times n} - b_n - c_n$ | [3,3,0,2,0,0,2,0] | [3,3,0,2,0,0,2,0] |
| $D_{2\times n} - c_n - d_n$ | [4,2,0,2,0,0,1,0] | [4,2,0,2,0,0,1,0] |
| $D_{2\times n} - d_n - e_n$ | [3,2,2,3,1,2,2,1] | [2,1,1,2,1,1,1,1] |
| $D_{2\times n} - a_n - d_n$ | [4,0,2,2,0,1,0,0] | [4,0,2,2,0,1,0,0] |
| $D_{2\times n} - b_n - e_n$ | [2,2,1,2,1,1,2,1] | [2,2,1,2,1,1,2,1] |
| $D_{2\times n} - a_n - b_n - d_n$ | [2,0,2,1,0,1,0,0] | [2,0,2,1,0,1,0,0] |
| $D_{2\times n} - b_n - d_n - e_n$ | [1,1,1,1,1,1,1,1] | [1,1,1,1,1,1,1,1] |
| $D_{2\times n}$ | [13,8,6,8,3,4,5,2] | [6,3,2,4,2,1,2,1] |

and

$$f_n(D_{sg}) = m(D_{2\times n} - g_n) - m(D_{2\times n} - s_n - g_n) - m(D_{2\times n} - s_n - g_n - h_n),$$

where $sgh \in \{bde, dba\}$. Then $f_n(D_s) > 0$ and $f_n(D_{sg}) > 0$.

*Proof.* We only need to prove $f_n(D_s) > 0$ (for $f_n(D_{sg}) > 0$, the proof being similar). By Corollary 2.4, if $s_n = b_n$ then

$$f_n(D_b) = m(D_{2\times n} - a_n - b_n) + m(D_{2\times n} - b_n - c_n) - m(D_{2\times n} - b_n - e_n);$$

and if $s_n = d_n$ then

$$f_n(D_d) = m(D_{2\times n} - d_n - c_n) + m(D_{2\times n} - d_n - e_n) - m(D_{2\times n} - d_n - a_n).$$

So by Lemma 2.5, we get

$$\begin{aligned} f_n(D_b) = \;& 6m(D_{2\times(n-1)}) + 2m(D_{2\times(n-1)} - g_{n-1}) + 3m(D_{2\times(n-1)} - h_{n-1}) \\ & + m(D_{2\times(n-1)} - g_{n-1} - h_{n-1}) + m(D_{2\times(n-1)} - s_{n-1}) \\ & - m(D_{2\times(n-1)} - s_{n-1} - g_{n-1}) \\ & - m(D_{2\times(n-1)} - s_{n-1} - g_{n-1} - h_{n-1}) \end{aligned}$$

and

$$\begin{aligned} f_n(D_d) = \;& 3m(D_{2\times(n-1)}) + 4[m(D_{2\times(n-1)} - s_{n-1}) + m(D_{2\times(n-1)} - h_{n-1})] \\ & + m(D_{2\times(n-1)} - s_{n-1} - g_{n-1}) + m(D_{2\times(n-1)} - g_{n-1} - h_{n-1}) \\ & + 3m(D_{2\times(n-1)} - s_{n-1} - h_{n-1}) + m(D_{2\times(n-1)} - s_{n-1} - g_{n-1} - h_{n-1}). \end{aligned}$$

Thus, $f_n(D_s) > 0$ by Lemma 2.3(i). □

**Lemma 2.6′.** If the vertices of $D_{2\times n}$ are labelled as in figure 3(a). Let

$$f'_n(D_s) = i(D_{2\times n}) - i(D_{2\times n} - s_n) - i(D_{2\times n} - s_n - h_n)$$

and

$$f'_n(D_{sg}) = i(D_{2\times n} - g_n) - i(D_{2\times n} - s_n - g_n) - i(D_{2\times n} - s_n - g_n - h_n),$$

where $sgh \in \{bde, dba\}$. Then $f'_n(D_s) < 0$ and $f'_n(D_{sg}) < 0$.

*Proof.* Similar to the proof of Lemma 2.6, by Lemmas 2.2 (ii), 2.3(ii) and 2.5 we get Lemma 2.6′.

**Lemma 2.7.** If the vertices of $D_{2\times n}$ are labelled as in figure 3(a). Then

(i) $m(D_{2\times n} - a_n) > m(D_{2\times n} - e_n), m(D_{2\times n} - d_n) > m(D_{2\times n} - b_n)$;

(ii) $m(D_{2\times n} - a_n) + m(D_{2\times n} - b_n) > m(D_{2\times n} - d_n) + m(D_{2\times n} - e_n)$;

(iii) $m(D_{2\times n} - a_n - b_n) > m(D_{2\times n} - d_n - e_n), m(D_{2\times n} - d_n - a_n) > m(D_{2\times n} - b_n - e_n)$;

(iv) $m(D_{2\times n} - a_n - b_n - d_n) > m(D_{2\times n} - b_n - d_n - e_n)$.

*Proof.* By Lemmas 2.5 and 2.6, we have

$$m(D_{2\times n} - a_n) - m(D_{2\times n} - e_n) = 3f_{n-1}(D_s) + f_{n-1}(D_{sg});$$
$$m(D_{2\times n} - d_n) - m(D_{2\times n} - b_n) = f_{n-1}(D_s) + f_{n-1}(D_{sg});$$

$$\begin{aligned}&[m(D_{2\times n} - a_n) + m(D_{2\times n} - b_n)] - [m(D_{2\times n} - d_n) + m(D_{2\times n} - e_n)]\\ &\quad = 2f_{n-1}(D_s); m(D_{2\times n} - a_n - b_n) - m(D_{2\times n} - d_n - e_n)\\ &\quad = m(D_{2\times n} - a_n - d_n) - m(D_{2\times n} - b_n - e_n) = 2f_{n-1}(D_s) + f_{n-1}(D_{sg})\end{aligned}$$

and

$$m(D_{2\times n} - a_n - b_n - d_n) - m(D_{2\times n} - b_n - d_n - e_n) = f_{n-1}(D_s) + f_{n-1}(D_{sg}),$$

where $sgh \in \{bde, dba\}$. Lemma 2.7 thus holds.

**Lemma 2.7′.** If the vertices of $D_{2\times n}$ are labelled as in figure 3(a). Then

(i) $i(D_{2\times n} - a_n) < i(D_{2\times n} - e_n), i(D_{2\times n} - d_n) < i(D_{2\times n} - b_n)$;

(ii) $i(D_{2\times n} - a_n) + i(D_{2\times n} - b_n) < i(D_{2\times n} - d_n) + i(D_{2\times n} - e_n)$;

(iii) $i(D_{2\times n} - a_n - b_n) < i(D_{2\times n} - d_n - e_n), i(D_{2\times n} - d_n - a_n) < i(D_{2\times n} - b_n - e_n)$;

(iv) $i(D_{2\times n} - a_n - b_n - d_n) < i(D_{2\times n} - b_n - d_n - e_n)$.

*Proof.* By Lemmas 2.5 and 2.6′ we get

$$\begin{aligned}i(D_{2\times n} - a_n) - i(D_{2\times n} - e_n) &= i(D_{2\times n} - a_n - d_n) - i(D_{2\times n} - b_n - e_n)\\ &= 2f^1_{n-1}(D_s) + f^1_{n-1}(D_{sg});\end{aligned}$$
$$i(D_{2\times n} - d_n) - i(D_{2\times n} - b_n) = f^1_{n-1}(D_s);$$

and

$$\begin{aligned}
&[i(D_{2\times n}-a_n)+i(D_{2\times n}-b_n)]-[i(D_{2\times n}-d_n)+i(D_{2\times n}-e_n)]\\
&\quad = i(D_{2\times n}-a_n-b_n)-i(D_{2\times n}-d_n-e_n)\\
&\quad = i(D_{2\times n}-a_n-b_n-d_n)-i(D_{2\times n}-b_n-d_n-e_n)\\
&\quad = f^1_{n-1}(D_s)+f^1_{n-1}(D_{sg}),
\end{aligned}$$

where $sgh \in \{bde, dba\}$. Thus, Lemma 2.7′ holds.

From Lemmas 2.7 and 2.7′ it is seen that following Lemmas 2.8 and 2.8′ hold.

**Lemma 2.8.** If the vertices of $Z_{2\times n}(n \geqslant 2)$ are labelled as in figure 2. Then

(i) $m(Z_{2\times n}-u_n) > m(Z_{2\times n}-l_n), m(Z_{2\times n}-p_n) > m(Z_{2\times n}-v_n)$,

(ii) $m(D_{2\times n}-u_n)+m(D_{2\times n}-v_n) > m(D_{2\times n}-p_n)+m(D_{2\times n}-l_n)$;

(iii) $m(Z_{2\times n}-u_n-v_n) > m(Z_{2\times n}-p_n-l_n), m(Z_{2\times n}-u_n-p_n) > m(Z_{2\times n}-v_n-l_n)$;

(iv) $m(Z_{2\times n}-u_n-v_n-p_n) > m(Z_{2\times n}-v_n-p_n-l_n)$.

**Lemma 2.8′.** If the vertices of $Z_{2\times n}(n \geqslant 2)$ are labelled as in figure 2. Then

(i) $i(Z_{2\times n}-u_n) < i(Z_{2\times n}-l_n), i(Z_{2\times n}-p_n) < i(Z_{2\times n}-v_n)$,

(ii) $i(D_{2\times n}-u_n)+i(D_{2\times n}-v_n) < i(D_{2\times n}-p_n)+i(D_{2\times n}-l_n)$;

(iii) $i(Z_{2\times n}-u_n-v_n) < i(Z_{2\times n}-p_n-l_n), i(Z_{2\times n}-u_n-p_n) < i(Z_{2\times n}-v_n-l_n)$;

(iv) $i(Z_{2\times n}-u_n-v_n-p_n) < i(Z_{2\times n}-v_n-p_n-l_n)$.

## 3. The proofs of main results

*The proof of Theorem A.* Let the vertices of $L_{2\times n}$, $Z_{2\times n}$ and $D_{2\times n}$ are labelled as in figure 2 and figure 3, respectively. In the following we only need to consider figure 3(a) (similarly, for figure 3(b) we can get the same results). Suppose that $n \geqslant 3$. By Lemma 2.5 we get

$$\begin{aligned}
m(D_{2\times n}) = {}& 13m(D_{2\times(n-1)})+8m(D_{2\times(n-1)}-s_{n-1})+6m(D_{2\times(n-1)}-g_{n-1})\\
&+8m(D_{2\times(n-1)}-h_{n-1})+3m(D_{2\times(n-1)}-s_{n-1}-g_{n-1})\\
&+4m(D_{2\times(n-1)}-g_{n-1}-h_{n-1})\\
&+5m(D_{2\times(n-1)}-s_{n-1}-h_{n-1})+2m(D_{2\times(n-1)}-s_{n-1}-g_{n-1}-h_{n-1})
\end{aligned}$$

and

$$\begin{aligned} m(Z_{2\times n}) = {} & 13m(Z_{2\times(n-1)}) + 8m(Z_{2\times(n-1)} - p_{n-1}) + 6m(Z_{2\times(n-1)} - v_{n-1}) \\ & +8m(Z_{2\times(n-1)} - u_{n-1}) + 3m(Z_{2\times(n-1)} - p_{n-1} - v_{n-1}) \\ & +4m(Z_{2\times(n-1)} - v_{n-1} - u_{n-1}) \\ & +5m(Z_{2\times(n-1)} - p_{n-1} - u_{n-1}) + 2m(Z_{2\times(n-1)} - p_{n-1} - v_{n-1} - u_{n-1}), \end{aligned}$$

where $sgh \in \{bde, dba\}$. By comparing $m(D_{2\times n})$ with $m(Z_{2\times n})$ we know that it suffices to prove the following Claim 1.
*Claim 1*

(i) $m(Z_{2\times n}-u_n) \geqslant m(D_{2\times n}-h_n)$; $m(Z_{2\times n}-u_n)+m(Z_{2\times n}-v_n) \geqslant m(D_{2\times n}-g_n) + m(D_{2\times n}-h_n)$, $m(Z_{2\times n}-p_n)+m(Z_{2\times n}-v_n) \geqslant m(D_{2\times n}-s_n)+m(D_{2\times n}-g_n)$;

(ii) $m(Z_{2\times n}-u_n-v_n) \geqslant m(D_{2\times n}-g_n-h_n)$, $m(Z_{2\times n}-v_n-p_n) \geqslant m(D_{2\times n}-s_n-g_n)$, $m(Z_{2\times n}-p_n-u_n) \geqslant m(D_{2\times n}-s_n-h_n)$;

(iii) $m(Z_{2\times n}-p_n)+m(Z_{2\times n}-u_n-v_n-p_n) \geqslant m(D_{2\times n}-s_n)+m(D_{2\times n}-s_n-g_n-h_n)$;

(iv) $m(D_{2\times n}) \leqslant m(Z_{2\times n})$.

Note that if $D_{2\times n} = Z_{2\times n}$ then Claim 1 holds by Lemma 2.8. Hence, for Claim 1 holding we may assume that $D_{2\times n} \neq Z_{2\times n}$. Now we use induction on $n$.

When $n = 3$. In this case, $\Phi_{2\times 3} = \{L_{2\times 3}, Z_{2\times 3}\}$. Since $a, b, c, d$ and $e$ are correspond to $o, x, y, z$ and $q$ (or $u$, $v$, $w$, $p$ and $l$), respectively (see figure 2). Let $s_2 \equiv x_2, g_2 \equiv z_2, h_2 \equiv q_2$ and $D = L$ (or $s_2 \equiv p_2, g_2 \equiv v_2, h_2 \equiv u_2$ and $D = Z$). Then, by applying computer algebra (*Mathematic* 4.0) techniques to table 1 we deduce that

$$A(m(L_{2\times 3}), x_3z_3q_3) = [101217, 47004, 48892, 42742, 20769, 29070, 20540, 12404],$$
$$A(m(L_{2\times 3}), z_3x_3o_3) = [101217, 48892, 47004, 47206, 20769, 32246, 23716, 14292]$$

and

$$A(m(Z_{2\times 3}), p_3v_3u_3) = [103774, 49888, 48314, 48026, 21221, 32748, 24013, 14430].$$

It is easy to see that Claim 1 holds for $n = 3$.

Suppose that the Claim 1 is true for all double hexagonal chains with fewer than $n$ naphthalenes, and that $D_{2\times n} \neq Z_{2\times n}$. We show that Claim 1 holds for $n \geqslant 4$. Note that $rstgh \in \{abcde, edcba\}$. By Lemma 2.7, it suffices to show that

(i) $m(Z_{2\times n}-u_n) > m(D_{2\times n}-a_n)$; $m(Z_{2\times n}-u_n)+m(Z_{2\times n}-v_n) > m(D_{2\times n}-b_n) + m(D_{2\times n}-a_n)$, $m(Z_{2\times n}-p_n)+m(Z_{2\times n}-v_n) > m(D_{2\times n}-d_n) + m(D_{2\times n}-b_n)$;

(ii) $m(Z_{2\times n}-u_n-v_n) > m(D_{2\times n}-b_n-a_n)$, $m(Z_{2\times n}-v_n-p_n) > m(D_{2\times n}-b_n-d_n)$, $m(Z_{2\times n}-p_n-u_n) > m(D_{2\times n}-d_n-a_n)$;

(iii) $m(Z_{2\times n}-p_n)+m(Z_{2\times n}-u_n-v_n-p_n) > m(D_{2\times n}-d_n) + m(D_{2\times n}-d_n-b_n-a_n)$;

(iv) $m(D_{2\times n}) < m(Z_{2\times n})$.

Referring to table 1 (see $B(m(G))$), it is easy to see that the above (i)–(iv) hold by the inductive hypotheses. Thus Claim 1 holds for $n \geqslant 4$. Hence the proof of Theorem A is complete.

*The proof of Theorem B.* Similar to the proof of Theorem A, we only need to consider the figure 3(a). Assume that $n \geqslant 3$. By Lemma 2.5 we get

$$\begin{aligned} i(D_{2\times n}) = {} & 6i(D_{2\times(n-1)}) + 3i(D_{2\times(n-1)}-s_{n-1}) + 2i(D_{2\times(n-1)}-g_{n-1}) \\ & +4i(D_{2\times(n-1)}-h_{n-1}) + 2i(D_{2\times(n-1)}-s_{n-1}-g_{n-1}) \\ & +i(D_{2\times(n-1)}-g_{n-1}-h_{n-1}) \\ & +2i(D_{2\times(n-1)}-s_{n-1}-h_{n-1}) \\ & +i(D_{2\times(n-1)}-s_{n-1}-g_{n-1}-h_{n-1}) \end{aligned}$$

and

$$\begin{aligned} i(Z_{2\times n}) = {} & 6i(Z_{2\times(n-1)}) + 3i(Z_{2\times(n-1)}-p_{n-1}) + 2i(Z_{2\times(n-1)}-v_{n-1}) \\ & +4i(Z_{2\times(n-1)}-u_{n-1}) + 2i(Z_{2\times(n-1)}-p_{n-1}-v_{n-1}) \\ & +i(Z_{2\times(n-1)}-v_{n-1}-u_{n-1}) \\ & +2i(Z_{2\times(n-1)}-p_{n-1}-u_{n-1}) \\ & +i(Z_{2\times(n-1)}-p_{n-1}-v_{n-1}-u_{n-1}), \end{aligned}$$

where $sgh \in \{bde, dba\}$. By comparing $i(D_{2\times n})$ with $i(Z_{2\times n})$ we know that it suffices to show that the following Claim 1′.

*Claim 1′*

(i) $i(Z_{2\times n}-u_n) \leqslant i(D_{2\times n}-h_n)$; $i(Z_{2\times n}-u_n)+i(Z_{2\times n}-v_n) \leqslant i(D_{2\times n}-g_n) + i(D_{2\times n}-h_n)$, $i(Z_{2\times n}-p_n)+i(Z_{2\times n}-v_n) \leqslant i(D_{2\times n}-s_n)+i(D_{2\times n}-g_n)$;

(ii) $i(Z_{2\times n}-u_n-v_n) \leqslant i(D_{2\times n}-g_n-h_n)$, $i(Z_{2\times n}-v_n-p_n) \leqslant i(D_{2\times n}-s_n-g_n)$, $i(Z_{2\times n}-p_n-u_n) \leqslant i(D_{2\times n}-s_n-h_n)$;

(iii) $i(Z_{2\times n}-p_n)+i(Z_{2\times n}-u_n-v_n-p_n) \leqslant i(D_{2\times n}-s_n)+i(D_{2\times n}-s_n-g_n-h_n)$;

(iv) $i(D_{2\times n}) \geqslant i(Z_{2\times n})$.

Note that if $D_{2\times n} = Z_{2\times n}$ then Claim 1′ holds by Lemma 2.8′. Hence, for Claim 1′ holding we may assume that $D_{2\times n} \neq Z_{2\times n}$. In the following we use induction on $n$.

When $n = 3$, $\Phi_{2\times 3} = \{L_{2\times 3}, Z_{2\times 3}\}$. Similar to the proof of Theorem A, let $s_2 \equiv x_2, g_2 \equiv z_2, h_2 \equiv q_2$ and $D = L$(or $s_2 \equiv p_2, g_2 \equiv v_2, h_2 \equiv u_2$ and $D = Z$). Then from table 1 it follows that

$$A(i(L_{2\times 3}), x_3z_3q_3) = [26500, 18729, 18345, 19716, 13593, 11561, 13678, 8542],$$
$$A(i(L_{2\times 3}), z_3x_3o_3) = [26500, 18345, 18729, 18701, 13593, 10930, 12663, 7911]$$

and

$$A(i(Z_{2\times 3}), p_3v_3u_3) = [26035, 18086, 18386, 18465, 13395, 10816, 12549, 7858].$$

It is easy to see that Claim 1′ holds for $n = 3$.

Suppose that Claim 1′ is true for all double hexagonal chains with fewer than $n$ naphthalenes, and that $D_{2\times n} \neq Z_{2\times n}$. We show that Claim 1′ holds for $n \geqslant 4$. By Lemma 2.7′, it suffices to show that

(i) $i(Z_{2\times n} - u_n) < i(D_{2\times n} - a_n)$; $i(Z_{2\times n} - u_n) + i(Z_{2\times n} - v_n) < i(D_{2\times n} - b_n) + i(D_{2\times n} - a_n)$, $i(Z_{2\times n} - p_n) + i(Z_{2\times n} - v_n) < i(D_{2\times n} - d_n) + i(D_{2\times n} - b_n)$;

(ii) $i(Z_{2\times n} - u_n - v_n) < i(D_{2\times n} - b_n - a_n)$, $i(Z_{2\times n} - v_n - p_n) < i(D_{2\times n} - b_n - d_n)$, $i(Z_{2\times n} - p_n - u_n) < i(D_{2\times n} - d_n - a_n)$;

(iii) $i(Z_{2\times n} - p_n) + i(Z_{2\times n} - u_n - v_n - p_n) < i(D_{2\times n} - d_n) + i(D_{2\times n} - d_n - b_n - a_n)$;

(iv) $i(D_{2\times n}) > i(Z_{2\times n})$.

Referring to table 1 see $B(i(G)))$, it is easy to see that the above (i) – (iv) hold by the inductive hypotheses. Thus Claim 1′ holds for $n \geqslant 4$. Hence the proof of Theorem B is complete.

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