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Double hexagonal chains with minimal total π-electron energy

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The total energy of all π-electrons in a conjugated hydrocarbon (within the framework of HMO approximation) is the sum of the absolute value of all the eigenvalues of its corresponding graph. In this paper, we consider "double hexagonal chains" as benzenoids constructed by successive fusions of successive naphthalenes along a zig–zag sequence of triples of edges as appear on opposite sides of each naphthalene unit. It is shown that if the fusions are such as to give a polyaceacene then the total π-electron energy is the minimum from among all the double hexagonal chains with the same number of naphthalene units.

KEY WORDS: the total π-electron energy, double hexagonal chain, quasi-ordering

AMS subject classification: 05C50, 05C35

1. Introduction

A hexagonal system is a 2-connected plane graph whose every interior face is bounded by a regular hexagon of unit length 1. A hexagonal system H is said to be catacondensed if all its vertices are on the outerface, otherwise H is said to be pericondensed. The HMO total π-electron energy E is a well-known topological index in theoretical chemistry, which is related to the thermodynamic stability of conjugated structures [1–3]. From a chemical point of view, it is of great interest to find the extremal values of E for significant classes of graphs. For example, in Ref. [4], Gutman determines the trees with the minimal and maximal energy. More recent results in this direction can be found in Refs. [5–11], all of which concentrated on acyclic system or catacondensed hexagonal system.

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This work deals with pericondensed hexagonal system. Let us recall some notations and terminologies.

A hexagonal chain is a catacondensed hexagonal system which has no hexagon adjacent to more than two hexagons. An m-tuple hexagonal chain consists of m condensed identical hexagonal chains [1,2]. When $m = 2$, we call it a double hexagonal chain. Let us orient naphthalene so that its interior edges are horizontal. There are two types of triple-edge 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 α-type fusing and β-type fusing, respectively.

Let $\Phi_{2\times n} = \{D_{2\times n} | D_{2\times n}$ is a double hexagonal chain with n naphthalene units$\}$. The double hexagonal chain $D_{2\times n}$ can be obtained from a naphthalene by a stepwise triple-edge fusion of new naphthalene, and each type of fusion is selected from θ-type fusing, where $\theta \in \{\alpha, \beta\}$. So, we write $D_{2\times n} = \theta_1\theta_2\cdots\theta_{n-1}$ in short, where $\theta_j \in \{\alpha, \beta\}$. For each j, if $\theta_j = \theta_{j+1}$ then the double hexagonal chain $D_{2\times n}$ is denoted by $L_{2\times n}$; and if $\theta_j \neq \theta_{j+1}$ then the double hexagonal chain $D_{2\times n}$ is denoted by $Z_{2\times n}$(see figure 2). Set

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

It can be 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 $\overline{D_{2\times n}} = \overline{\theta_1}\;\overline{\theta_2}\cdots\overline{\theta_{n-1}}$. For $n \geqslant 2$, $D_{2\times n}$ is a pericondensed hexagonal system. There have been several previous works for double hexagonal chains with a regular repetition-both in MO & resonance-theoretic frameworks. In particular, two general classes of regular polymer graphs of a fixed number of hexagons width – "zig-zag" and "arm–chair" edges have been compared before in an alternative resonating VB framework. They showed that the species of the polypolyacene class is less stable than the corresponding members of the polypolyphenanthrene class [12,13]. In this paper, we consider the total π-electron energies of double hexagonal chains within the framework of HMO approximation. It is shown that if the fusions are such as to give a poly-

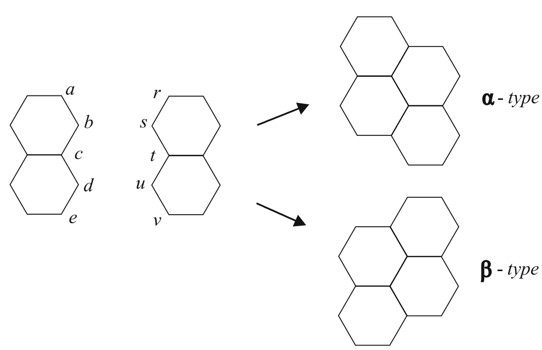


Figure 1. Two types of triple-edge fusion of two naphthalenes.

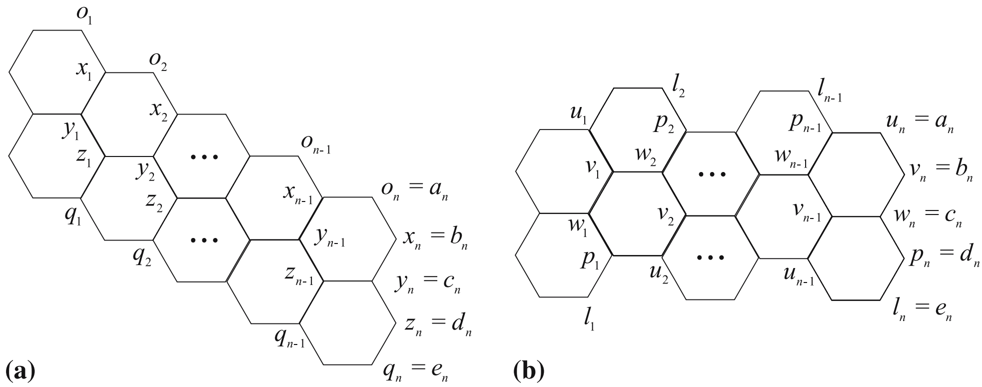


Figure 2. (a) $L_{2\times n}$; (b) $Z_{2\times n}$.

aceacene then the H*ü*ckel π-electron energy is the minimum from among all the double hexagonal chains with the same number of naphthalene units, i.e.

Theorem A. For any $D_{2\times n} \in \Phi_{2\times n}$ with n naphthalene units, $L_{2\times n} \preceq D_{2\times n}$, where the equality holds only if $L_{2\times n} = D_{2\times n}$.

2. Auxiliary results

The characteristic polynomial of a graph G, denoted by $\phi(G) = \phi(G, x)$, is defined as $\phi(G) = det(xI - A)$, where I is the identity matrix and A is the adjacency matrix of G [14]. If G is a bipartite graph then $\phi(G)$ can be written as

$$\phi(G) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k b(G,k) x^{n-2k}, \tag{1}$$

where n is the number of vertices of G. Note that $b(G,0) = 1$ and $b(G,k) \geqslant 0$ for each $k = 0, 1, \ldots, \lfloor n/2 \rfloor$. For other k, we assume $b(G,k) = 0$ for convenience.

The total π-electron energy of the molecule (within the framework of the HMO approximation) is defined to be $E(G) = \Sigma_{j=1}^{n} |\lambda_j|$, where $\lambda_j (j = 1, 2, \ldots, n)$ are the eigenvalues of its corresponding graph G. The energy of bipartite graph G is a strictly monotonously increasing function of the coefficients of its characteristic polynomial. Inspired by this fact, Gutman defined a quasi-ordering relation "$\succeq$"(i.e. a reflexive and transitive relation) over the set of all bipartite graphs: If G_1 and G_2 are bipartite graphs whose characteristic polynomials are of the form (1) then

$$G_1 \succeq G_2 \Longleftrightarrow b(G_1,k) \geqslant b(G_2,k) \quad \text{for all } k \geqslant 0.$$

If $G_1 \succeq G_2$ and there exists a k such that $b(G_1, k) > b(G_2, k)$ then we write $G_1 \succ G_2$. Thus, if $G_1 \succeq G_2$ then $E(G_1) \geqslant E(G_2)$; and if $G_1 \succ G_2$ then $E(G_1) > E(G_2)$ [3,4].

Let G be a graph and uv an edge of G. We denote by $G - uv$ (resp. $G - u$) the graph obtained from G by deleting uv (resp. the vertex u and edges adjacent to it). Denote by $N(x)$ the set $\{y \in V(G)\colon\ xy \in E(G)\}$. Let S be a subset of $V(G)$, the subgraph of G induced by S is denoted by $G[S]$, and $G[V \setminus S]$ is denoted by $G - S$. Let $C_u(G)$ and $C_{uv}(G)$ denote the sets of cycles of G containing the vertex u and edge uv, respectively.

The following lemmas 2.1–2.5 can be found in Ref. [14]:

Lemma 2.1. Let G be composed of two components G_1 and G_2, then the characteristic polynomial of G is $\phi(G) = \phi(G_1)\phi(G_2)$.

Lemma 2.2. Let G be a graph and uv an edge of G, then the characteristic polynomial

$$\phi(G) = \phi(G - uv) - \phi(G - u - v) - 2\Sigma_{C_j \in C_{uv}} \phi(G - C_j).$$

Lemma 2.3. Let G be a graph and u a vertex of G, then the characteristic polynomial

$$\phi(G) = x\phi(G - u) - \Sigma_{w \in N(u)} \phi(G - u - w) - 2\Sigma_{C_j \in C_u} \phi(G - C_j).$$

Lemma 2.4. Let u and v be adjacent vertices in a graph G. Then

$$\phi(G) = \phi(G - uv) - \phi(G - u - v) \\ -2\sqrt{\phi(G - u)\phi(G - v) - \phi(G - uv)\phi(G - u - v)},$$

where the square root is interpreted as a polynomial with a positive coefficient in the highest term.

Lemma 2.5. Let u and v be vertices of a graph G. Let P_{uv} be the set of all paths which connect u and v. Then

$$\phi(G - u)\phi(G - v) - \phi(G)\phi(G - u - v) = (\Sigma_{T \in P_{uv}} \phi(G - T))^2.$$

For brevity, we denote $\Sigma_{T \in P_{uv}} \phi(G - T)$ by $T_{uv}(G)$.

The following lemma 2.6 is obvious (slightly different to lemma 4 given in Ref. [10]).

Lemma 2.6. Let G and G' be two bipartite graphs of order n and m, resp., where $n = m + 2k$ and $k \geqslant 0$. If the characteristic polynomials of G and G' are written as $\phi(G) = \sum_{i=0}^{\lfloor n/2 \rfloor} b_i x^{n-2i}$ and $\phi(G') = \sum_{j=0}^{\lfloor m/2 \rfloor} b'_j x^{m-2j}$, resp., then $G \succeq G'$ iff $(-1)^i(b_i - b'_{i-k}) \geqslant 0$ for $i = 0, 1, 2, \ldots, \lfloor n/2 \rfloor$; $G \succ G'$ iff $G \succeq G'$ and there is an $i \in \{0, 1, 2, \ldots, \lfloor n/2 \rfloor\}$ such that $(-1)^i(b_i - b'_{i-k}) > 0$.

Definition 2.1. Let G be a graph, and let s, g and h be the vertices of G. Define the characteristic polynomial vector of G with respect to the vertices s, g and h, denoted by $A(G; sgh)$, as the vector $A(G; sgh) = [\phi(G), \phi(G - s), \phi(G - g), \phi(G - h), \phi(G - s - g), \phi(G - g - h), \phi(G - s - h), \phi(G - s - g - h), 1]$.

Let $D_{2\times(n-1)}$ be a double hexagonal chain with $n - 1$ naphthalene units. $D_{2\times n}$ is obtained from $D_{2\times(n-1)}$ by θ-type fusing a new naphthalene B, where $\theta \in \{\alpha, \beta\}$. If $\theta = \alpha$, then the vertices of $D_{2\times n}$ are labelled as in figure 3a(1); and if $\theta = \beta$, then the vertices of $D_{2\times n}$ are labelled as in figure 3a(2). Thus, from figure 3a it follows that $rstgh \in \{abcde, edcba\}$. Note that $\overline{\beta} = \alpha$. Then the case

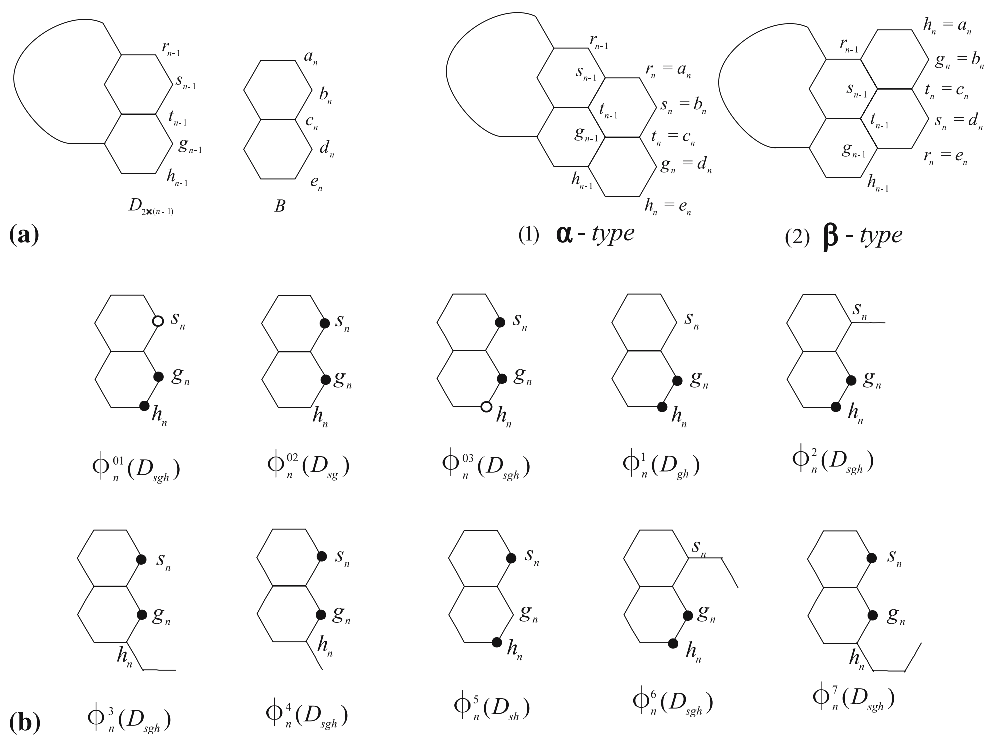


Figure 3. (a) The two types of double hexagonal chain $D_{2\times n}$ obtained from $D_{2\times(n-1)}$. (b) In each graph G only the n-th naphthalene is shown, and the black vertices denote the end-vertices of paths in $T_{uv}(G)$ and the white circle denotes the deleted vertex, where $uv \in \{g_n h_n, s_n g_n, s_n h_n\}$.

of figure 3a(2) is equivalent to the case of figure 3a(1). Hence, without loss of generality, in the following we only need to consider the case of figure 3a(1).

3. Main results and proofs

Let G be a graph and $u, v \in V(G)$. By the relations of $T_{uv}(G)$ with the characteristic polynomials of graphs G, $G - u$, $G - v$ and $G - u - v$ (see Lemma 2.5), we introduce some further notations (Definition 3.1) that will be used throughout the paper.

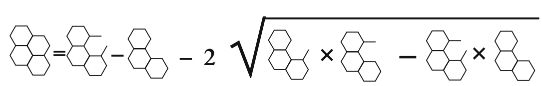
Definition 3.1. Let $D_{2\times n} \in \Phi_{2\times n}$ and s_n, g_n and h_n be its vertices. We define $\phi_n^{01}(D_{sgh}) = T_{g_nh_n}(D_{2\times n} - s_n)$, $\phi_n^{02}(D_{sg}) =, T_{s_ng_n}(D_{2\times n})$, $\phi_n^{03}(D_{sgh}) = T_{s_ng_n}(D_{2\times n} - h_n)$, $\phi_n^{1}(D_{gh}) = T_{g_nh_n}(D_{2\times n})$, $\phi_n^{2}(D_{sgh}) = x\phi_n^{1}(D_{gh}) - \phi_n^{01}(D_{sgh})$, $\phi_n^{3}(D_{sgh}) = x\phi_n^{4}(D_{sgh}) - \phi_n^{02}(D_{sg})$, $\phi_n^{4}(D_{sgh}) = x\phi_n^{02}(D_{sg}) - \phi_n^{03}(D_{sgh})$, $\phi_n^{5}(D_{sh}) = T_{s_nh_n}(D_{2\times n})$, $\phi_n^{6}(D_{sgh}) = x\phi_n^{2}(D_{sgh}) - \phi_n^{1}(D_{gh})$ and $\phi_n^{7}(D_{sgh}) = x\phi_n^{3}(D_{sgh}) - \phi_n^{4}(D_{sgh})$, which be illustrated, respectively, by these corresponding graphs (see figure 3b).

Lemma 3.1. Let the vertices of $D_{2\times n}$ be labelled as in figure 3a(1). If G is a graph concerning with $D_{2\times n}$ which is listed in table 1. Then the characteristic polynomial of G can be written as the scalar product of two vectors, i.e.

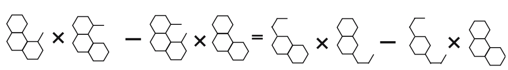
$$\phi(G) = B(G) \cdot A(D_{2\times(n-1)}; s_{n-1}g_{n-1}h_{n-1}),$$

where $B(G)$ denotes the vector in x with 9 entries represented in table 1.

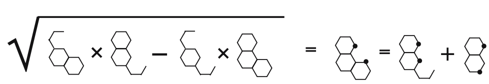
Proof. We only compute the characteristic polynomial $\phi(D_{2\times n})$, and omit the others. By lemma 2.4, we have



And by lemmas 2.1–2.3 and 2.5, we get



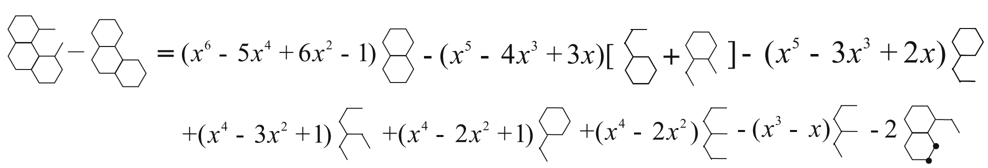
and



where the black vertices denote the end-vertices of paths. Similarly, by lemmas 2.1–2.5,

Table 1
The vector $B(G)$ of graph G.

G	B(G)
$D_{2\times n} - a_n$	$[x^5 - 4x^3 + 3x, 0, -x^4 + 2x^2, -x^4 + 3x^2 - 1,$ $0, x^3 - x, 0, 0, -2x\phi^1_{n-1}(D_{gh})]$
$D_{2\times n} - b_n$	$[x^5 - 3x^3 + x, -x^4 + 3x^2 - 1, -x^4 + 2x^2, -x^4 + 2x^2,$ $x^3 - 2x, x^3 - x, x^3 - 2x, -x^2 + 1, -2\phi^2_{n-1}(D_{sgh})]$
$D_{2\times n} - d_n$	$[x^5 - 3x^3 + 2x, -x^4 + 2x^2 - 1, -x^4 + 2x^2 - 1, -x^4 + 2x^2,$ $x^3 - x, x^3 - x, x^3 - x, -x^2, -2\phi^3_{n-1}(D_{sgh})]$
$D_{2\times n} - e_n$	$[x^5 - 3x^3 + x, -x^4 + 2x^2, -x^4 + x^2, -x^4 + 3x^2 - 1, x^3, x^3 - x,$ $x^3 - 2x, -x^2, -2x\phi^4_{n-1}(D_{sgh})]$
$D_{2\times n} - a_n - d_n$	$[x^4 - 2x^2 + 1, 0, -x^3 + x, -x^3 + x, 0, x^2, 0, 0, 0]$
$D_{2\times n} - b_n - e_n$	$[x^4 - x^2, -x^3 + x, -x^3, -x^3 + x, x^2, x^2, x^2 - 1, -x, 0]$
$D_{2\times n} - d_n - e_n$	$[x^4 - 2x^2, -x^3 + x, -x^3 + x, -x^3 + 2x, x^2, x^2 - 1, x^2 - 1, -x,$ $-2\phi^4_{n-1}(D_{sgh})]$
$D_{2\times n} - a_n - b_n$	$[x^4 - 3x^2 + 1, 0, -x^3 + 2x, -x^3 + 2x, 0, x^2 - 1, 0, 0, -2\phi^1_{n-1}(D_{gh})]$
$D_{2\times n} - b_n - d_n$	$[x^4 - x^2, -x^3 + x, -x^3 + x, -x^3, x^2 - 1, x^2, x^2, -x, 0]$
$D_{2\times n} - b_n - c_n$	$[x^4 - 2x^2, -x^3 + 2x, 0, -x^3 + x, 0, 0, x^2 - 1, 0, 0]$
$D_{2\times n} - d_n - c_n$	$[x^4 - 2x^2 + 1, -x^3 + x, 0, -x^3 + x, 0, 0, x^2, 0, 0]$
$D_{2\times n} - a_n - b_n - d_n$	$[x^3 - x, 0, -x^2 + 1, -x^2, 0, x, 0, 0, 0]$
$D_{2\times n} - b_n - d_n - e_n$	$[x^3, -x^2, -x^2, -x^2, x, x, x, -1, 0]$
$D_{2\times n} - b_n - c_n - d_n$	$[x^3 - x, -x^2 + 1, 0, -x^2, 0, 0, x, 0, 0]$
$D_{2\times n} - a_n - b_n - c_n - d_n$	$[x^2 - 1, 0, 0, -x, 0, 0, 0, 0, 0]$
$D_{2\times n} - b_n - c_n - d_n - e_n$	$[x^2, -x, 0, -x, 0, 0, 1, 0, 0]$
$D_{2\times n}$	$[x^6 - 5x^4 + 6x^2 - 1, -x^5 + 4x^3 - 3x, -x^5 + 3x^3 - 2x,$ $-x^5 + 4x^3 - 3x, x^4 - 2x^2, x^4 - 2x^2 + 1, x^4 - 3x^2 + 1, -x^3 + x,$ $-2(\phi^5_{n-1}(D_{sh}) + \phi^6_{n-1}(D_{sgh}) + \phi^7_{n-1}(D_{sgh}))]$



Thus, by definition 2.1, the above four equalities yield

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

where $B(D_{2\times n})$ is represented in table 1.

Lemma 3.2. If the vertices of $D_{2\times n}$ are labelled as in figure 3a(1). Then the recursion formulas of $\phi^{01}_n(D_{sgh})$, $\phi^{02}_n(D_{sg})$, $\phi^{03}_n(D_{sgh})$, $\phi^1_n(D_{gh})$ and $\phi^5_n(D_{sh})$ can, respectively, be represented in table 2, where $sgh \in \{bde, dba\}$.

Proof. By repeatedly using lemma 2.5, we can get table 2.

We define the operation O_1 to the polynomial equality A, i.e. O_1: Check the highest order of each term on both sides of A, and denote this process by $O_1 \longrightarrow A$ in short.

Lemma 3.3. If the vertices of $D_{2\times n}$ are labelled as in figure 3a(1). Let $sgh \in \{bde, dba\}$. Then $\phi_n^{01}(D_{sgh})$, $\phi_n^{02}(D_{sg})$, $\phi_n^{03}(D_{sgh})$, $\phi_n^{1}(D_{gh})$, $\phi_n^{2}(D_{sgh})$, $\phi_n^{3}(D_{sgh})$, $\phi_n^{4}(D_{sgh})$, $\phi_n^{5}(D_{sh})$, $\phi_n^{6}(D_{sgh})$ and $\phi_n^{7}(D_{sgh})$ are of the form (1) with orders $6n+1, 6n+1, 6n, 6n+2, 6n+3$, $6n+3$, $6n+2, 6n, 6n+4$ and $6n+4$, resp.

Proof. According to definition 3.1 and lemma 2.6, it is seen that we only need to prove that $\phi_n^{01}(D_{sgh}), \phi_n^{02}(D_{sg}), \phi_n^{03}(D_{sgh}), \phi_n^{1}(D_{gh})$ and $\phi_n^{5}(D_{sh})$ are of the form (1) with orders $6n+1, 6n+1, 6n, 6n+2$ and $6n$, resp.

Using induction on n. When $n=1$, by lemma 2.5 and a routine computation we obtain that $\phi_n^{01}(D_{sgh}) = x^7 - 6x^5 + 10x^3 - 5x$, $\phi_n^{02}(D_{sg}) = x^7 - 6x^5 + 12x^3 - 7x$, $\phi_n^{03}(D_{sgh}) = x^6 - 5x^4 + 7x^2 - 2$, $\phi_n^{1}(D_{gh}) = x^8 - 8x^6 + 20x^4 - 19x^2 + 6$ and $\phi_n^{5}(D_{sh}) = x^6 - 4x^4 + 6x^2 - 3$, which imply Lemma 3.3 holding.
When $n \geqslant 2$, suppose that lemma 3.3 is true for $n-1$. we first prove Fact 1. *Fact 1.*

(i) $\phi(D_{2\times n} - b_n - c_n - d_n) \succ -x\phi_{n-1}^{5}(D_{sh})$;

(ii) $\phi(D_{2\times n} - b_n - c_n - d_n - e_n) \succ -x\phi_{n-1}^{2}(D_{sgh})$,
$\phi(D_{2\times n} - a_n - b_n - c_n - d_n) \succ -x\phi_{n-1}^{3}(D_{sgh})$.

The proof of fact 1. Suppose that $s_{n-1} \equiv b_{n-1}$, $g_{n-1} \equiv d_{n-1}$ and $h_{n-1} \equiv e_{n-1}$(for $s_{n-1} \equiv d_{n-1}$, $g_{n-1} \equiv b_{n-1}$ and $h_{n-1} \equiv a_{n-1}$, the proof being similar). From tables

Table 2
The recursion formulas of $\phi_n^{01}(D_{sgh}), \phi_n^{02}(D_{sg}), \phi_n^{03}(D_{sgh})$, $\phi_n^{1}(D_{gh})$ and $\phi_n^{5}(D_{sh})$, where $sgh \in \{bde, dba\}$.

	The recursion formulas
$\phi_n^{01}(D_{bde})$	$\phi(D_{2\times n} - b_n - d_n - e_n) + \phi_{n-1}^{2}(D_{sgh})$
$\phi_n^{01}(D_{dba})$	$\phi(D_{2\times n} - a_n - b_n - d_n) + \phi_{n-1}^{3}(D_{sgh})$
$\phi_n^{03}(D_{bde})$	$\phi(D_{2\times n} - b_n - c_n - d_n - e_n) + \phi_{n-1}^{4}(D_{sgh})$
$\phi_n^{03}(D_{dba})$	$\phi(D_{2\times n} - a_n - b_n - c_n - d_n) + \phi_{n-1}^{1}(D_{gh})$
$\phi_n^{1}(D_{ba})$	$\phi(D_{2\times n} - a_n - b_n) + \phi_{n-1}^{7}(D_{sgh}) + \phi_{n-1}^{5}(D_{sh})$
$\phi_n^{1}(D_{de})$	$\phi(D_{2\times n} - d_n - e_n) + \phi_{n-1}^{6}(D_{sgh}) + \phi_{n-1}^{5}(D_{sh})$
$\phi_n^{02}(D_{db})$	$\phi(D_{2\times n} - b_n - c_n - d_n) + \phi_{n-1}^{3}(D_{sgh}) + x\phi_{n-1}^{5}(D_{sh}) + \phi_{n-1}^{2}(D_{sgh})$
$\phi_n^{5}(D_{da})$	$\phi(D_{2\times n} - a_n - b_n - c_n - d_n) + x\phi_{n-1}^{3}(D_{sgh}) + (x^2-1)\phi_{n-1}^{5}(D_{sh}) + \phi_{n-1}^{1}(D_{gh})$
$\phi_n^{5}(D_{be})$	$\phi(D_{2\times n} - b_n - c_n - d_n - e_n) + x\phi_{n-1}^{2}(D_{sgh}) + (x^2-1)\phi_{n-1}^{5}(D_{sh}) + \phi_{n-1}^{4}(D_{sgh})$

1 and 2, it follows that

$$\begin{aligned}
&\phi(D_{2\times n} - b_n - c_n - d_n) + x\phi^5_{n-1}(D_{be}) \\
&\quad = x\phi(D_{2\times(n-1)} - b_{n-1} - c_{n-1} - d_{n-1} - e_{n-1}) + x\phi^4_{n-2}(D_{sgh}) + (x^3 - x)\phi^5_{n-2} \\
&\qquad (D_{sh}) + x^2\phi^2_{n-2}(D_{sgh}) + (x^3 - x)\phi(D_{2\times(n-1)}) - (x^2 - 1)\phi(D_{2\times(n-1)} - b_{n-1}) \\
&\qquad - x^2\phi(D_{2\times(n-1)} - e_{n-1}) + x\phi(D_{2\times(n-1)} - b_{n-1} - e_{n-1}) \qquad (2)
\end{aligned}$$

And, by definition 3.1, lemma 2.6 and the expression of $\phi(D_{2\times(n-1)})$ we know that

$$-x\phi^4_{n-2}(D_{sgh}) - (x^3 - x)\phi^5_{n-2}(D_{sh}) \prec (x^3 - x)\phi(D_{2\times(n-1)}).$$

Since $\phi(D_{2\times(n-1)} - b_{n-1} - e_{n-1}) = x\phi(D_{2\times(n-1)} - b_{n-1} - d_{n-1} - e_{n-1}) - \phi(D_{2\times(n-1)} - b_{n-1} - c_{n-1} - d_{n-1} - e_{n-1})$ by Lemmas 2.1–2.2. Then, substituting the expression of $\phi(D_{2\times(n-1)} - b_{n-1} - e_{n-1})$ into (2) and by $O_1 \longrightarrow$(2), we know that (i) holds by Lemma 2.6. The proof of (ii) is similar. Completing the proof of fact 1.

By fact 1., lemma 2.6 and $O_1 \longrightarrow$ the recursion formulas in table 2, we know that $\phi^{01}_n(D_{sgh})$, $\phi^{02}_n(D_{sg})$, $\phi^{03}_n(D_{sgh})$, $\phi^1_n(D_{gh})$ and $\phi^5_n(D_{sh})$ are of the form (1) with orders $6n+1$,$6n+1$,$6n$,$6n+2$ and $6n$, resp. Thus, the proof of Lemma 3.3 is complete.

Lemma 3.4. If the vertices of $D_{2\times n}$ are labelled as in figure 3a(1). Let

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

and

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

where $sgh \in \{bde, dba\}$. Then we have

(i) $f_n(D_s) = \sum_{i=0}^{\lfloor m_1/2\rfloor} \psi'_i x^{m_1-2i}$, where $m_1 = 6n+4$, $\psi'_0 = 0$, $\psi'_1 < 0$ and $(-1)^i\psi'_i \geqslant 0$ for $i = 2, \ldots, \lfloor m_1/2\rfloor$.

(ii) $f_n(D_{sg}) = \sum_{i=0}^{\lfloor m_2/2\rfloor} \psi''_i x^{m_2-2i}$, where $m_2 = 6n+3$, $\psi''_0 = 0$, $\psi''_1 < 0$ and $(-1)^i\psi''_i \geqslant 0$ for $i = 2, \ldots, \lfloor m_2/2\rfloor$.

Proof. We only consider (i) (using the same methods, and by induction we can prove (ii)). By lemmas 2.1–2.5, if $s_n = b_n$, $g_n = d_n$ and $h_n = e_n$ then

$$\begin{aligned}
f_n(D_b) = {} & \phi(D_{2\times n} - b_n - e_n) - \phi(D_{2\times n} - b_n - a_n) \\
& - \phi(D_{2\times n} - b_n - c_n) - 2[\phi^5_{n-1}(D_{sh}) + \phi^7_{n-1}(D_{sgh})];
\end{aligned}$$

and if $s_n = d_n$, $g_n = b_n$ and $h_n = a_n$ then

$$f_n(D_d) = \phi(D_{2\times n} - d_n - a_n) - \phi(D_{2\times n} - d_n - e_n) \\ -\phi(D_{2\times n} - d_n - c_n) - 2[\phi^5_{n-1}(D_{sh}) + \phi^6_{n-1}(D_{sgh})].$$

Recall table 1. It is seen that $\phi(D_{2\times n} - b_n - e_n) \prec \phi(D_{2\times n} - b_n - a_n) + \phi(D_{2\times n} - b_n - c_n)$ and $\phi(D_{2\times n} - d_n - a_n) \prec \phi(D_{2\times n} - d_n - e_n) + \phi(D_{2\times n} - d_n - c_n)$. So, by Lemma 3.3 and $O_1 \longrightarrow$ the above two equalities, we know that the term of order $6n+4$ in $f_n(D_s)$ is 0, the term of order $6n+2$ in $f_n(D_s)$ is non-positive and the coefficients of its successive terms are non-negative and non-positive alternately. Lemma 2.6 thus proves our results.

Lemma 3.5. If the vertices of $D_{2\times n}$ are labelled as in figure 3a(1). Let $sgh \in \{bde, dba\}$. Then

(i) $f_n(D_s)+\alpha[\phi^1_n(D_{gh})-\phi^4_n(D_{sgh})] = \sum_{i=0}^{\lfloor n_1/2\rfloor} a_i x^{n_1-2i}$, where $n_1 = 6n+2, \alpha \in \{-2, -1, 1\}, a_0 < 0$ and $(-1)^i a_i \leqslant 0$ for $i = 1, \ldots, \lfloor n_1/2\rfloor$.

(ii) $-f_n(D_{sg}) + \beta[\phi^{02}_n(D_{sg}) - \phi^{01}_n(D_{sgh})] = \sum_{i=0}^{\lfloor n_2/2\rfloor} b_i x^{n_2-2i}$, where $n_2 = 6n+1, \beta \in \{\pm 1, \pm 2\}, b_0 > 0$ and $(-1)^i b_i \geqslant 0$ for $i = 1, \ldots, \lfloor n_2/2\rfloor$.

(iii) $f_n(D_s) + [\phi^6_n(D_{sgh}) - \phi^7_n(D_{sgh})] = \sum_{i=0}^{\lfloor n_3/2\rfloor} c_i x^{n_3-2i}$, where $n_3 = 6n+2, c_0 < 0$ and $(-1)^i c_i \leqslant 0$ for $i = 1, \ldots, \lfloor n_3/2\rfloor$.

Proof. Suppose that $s_n \equiv b_n, g_n \equiv d_n$ and $h_n \equiv e_n$ (for $s_n \equiv d_n, g_n \equiv b_n$ and $h_n \equiv a_n$, the proof being similar).

(i) From definition 3.1 and table 2, we have

$$\phi^1_n(D_{de}) = \phi(D_{2\times n} - d_n - e_n) + \phi^6_{n-1}(D_{sgh}) + \phi^5_{n-1}(D_{sh})$$

and

$$\phi^4_n(D_{bde}) = \phi(D_{2\times n} - b_n - c_n) + \phi^7_{n-1}(D_{sgh}) + x^2\phi^5_{n-1}(D_{sh}) + x\phi^2_{n-1}(D_{sgh})$$

Then, by lemma 3.4

$$\begin{aligned} &f_n(D_b) + \alpha[\phi^1_n(D_{de}) - \phi^4_n(D_{bde})] \\ &= \phi(D_{2\times n} - b_n - e_n) - \phi(D_{2\times n} - a_n - b_n) \\ &\quad +\alpha\phi(D_{2\times n} - d_n - e_n) - (\alpha+1)\phi(D_{2\times n} - b_n - c_n) - \alpha\phi^1_{n-1}(D_{gh}) \\ &\quad -(2+\alpha)\phi^7_{n-1}(D_{sgh}) + [-2+\alpha(1-x^2)]\phi^5_{n-1}(D_{sh}) \end{aligned} \tag{3}$$

Recall table 1. It is seen that $-\phi(D_{2\times n} - b_n - e_n) + \phi(D_{2\times n} - a_n - b_n) - \alpha\phi(D_{2\times n} - d_n - e_n) + (\alpha+1)\phi(D_{2\times n} - b_n - c_n)$ is of the form (1) with order $6n+2$.

If $\alpha = -1, -2$ then, by $O_1 \longrightarrow (3)$ we know from Lemma 2.6 that (i) follows. Similarly, if $\alpha = 1$, since $\phi(D_{2\times n} - b_n - c_n) \succ x\phi(D_{2\times n} - b_n - c_n - d_n)$, then by lemma 2.6, lemma 3.3 and Fact 1(given in lemma 3.3) we know that (i) is true.

Using the same methods, we can prove (ii) and (iii).

Lemma 3.6. If the vertices of $D_{2\times n}$ are labelled as in figure 3a(1). Then

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

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

(iii) $(D_{2\times n} - a_n - b_n - d_n) \succ (D_{2\times n} - b_n - d_n - e_n)$;
$(D_{2\times n} - a_n - b_n - c_n - d_n) \succ (D_{2\times n} - b_n - c_n - d_n - e_n)$;

(iv) $\phi_n^{01}(D_{dba}) \succ \phi_n^{01}(D_{bde}), \phi_n^{03}(D_{dba}) \succ \phi_n^{03}(D_{bde}), \phi_n^{1}(D_{ba}) \succ \phi_n^{1}(D_{de})$, $\phi_n^{5}(D_{da}) \succ \phi_n^{5}(D_{be})$.

Proof. Since $x(\phi_n^1(D_{gh}) - \phi_n^4(D_{sgh})) = (\phi_n^2(D_{sgh}) - \phi_n^3(D_{sgh})) + (\phi_n^{01}(D_{sgh}) - \phi_n^{02}(D_{sg}))$ by definition 3.1. Then, by lemmas 3.1 and 3.4 we get

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

$$\begin{aligned}
&\phi(D_{2\times n} - a_n - b_n - d_n) - \phi(D_{2\times n} - b_n - d_n - e_n) = -x f_{n-1}(D_s) + f_{n-1}(D_{sg}),\\
&\phi(D_{2\times n} - a_n - b_n - c_n - d_n) - \phi(D_{2\times n} - b_n - c_n - d_n - e_n) = -f_{n-1}(D_s),\\
&\phi(D_{2\times n} - a_n - b_n) - \phi(D_{2\times n} - d_n - e_n)\\
&\quad = (-x^2 + 1) f_{n-1}(D_s) + x f_{n-1}(D_{sg}) - 2[\phi_{n-1}^1(D_{gh}) - \phi_{n-1}^4(D_{sgh})],\\
&\phi(D_{2\times n} - a_n) - \phi(D_{2\times n} - e_n) = x f_{n-1}(D_s)\\
&\quad + x[\phi(D_{2\times n} - a_n - b_n) - \phi(D_{2\times n} - d_n - e_n)]
\end{aligned}$$

and

$$\phi(D_{2\times n} - d_n) - \phi(D_{2\times n} - b_n) = x f_{n-1}(D_s) - f_{n-1}(D_{sg}) - 2x[\phi_{n-1}^1(D_{gh}) - \phi_{n-1}^4(D_{sgh})] - [\phi_{n-1}^{02}(D_{sg}) - \phi_{n-1}^{01}(D_{sgh})].$$

By lemmas 3.5$(i)(ii)$ and $O_1 \longrightarrow$ the above six equalities, we know from lemma 2.6 that $(i) - (iii)$ follow.

(iv) Similarly, since $x(\phi_n^2(D_{sgh}) - \phi_n^3(D_{sgh})) = (\phi_n^1(D_{gh}) - \phi_n^4(D_{sgh})) + (\phi_n^6(D_{sgh}) - \phi_n^7(D_{sgh}))$ by definition 3.1. Then, from lemmas 3.1, 3.2 and 3.4 we deduce that

$$\begin{aligned}
[\phi_n^{01}(D_{dba}) - \phi_n^{01}(D_{bde})] &= -xf_{n-1}(D_s) + f_{n-1}(D_{sg}) - x[\phi_{n-1}^1(D_{gh}) - \phi_{n-1}^4(D_{sgh})] \\
&\quad +[\phi_{n-1}^{01}(D_{sgh}) - \phi_{n-1}^{02}(D_{sg})], \\
\phi_n^{03}(D_{dba}) - \phi_n^{03}(D_{bde}) &= -f_{n-1}(D_s) - [\phi_{n-1}^4(D_{sgh}) - \phi_{n-1}^1(D_{gh})], \\
\phi_n^1(D_{ba}) - \phi_n^1(D_{de}) &= \phi(D_{2\times n} - a_n - b_n) - \phi(D_{2\times n} - d_n - e_n) \\
&\quad +\phi_{n-1}^7(D_{sgh}) - \phi_{n-1}^6(D_{sgh}) = (-x^2+1)f_{n-1}(D_s) \\
&\quad +xf_{n-1}(D_{sg}) - (x^2+1)[\phi_{n-1}^1(D_{gh}) - \phi_{n-1}^4(D_{sgh})] \\
&\quad +x[\phi_{n-1}^{01}(D_{sgh}) - \phi_{n-1}^{02}(D_{sg})],
\end{aligned}$$

and

$$\phi_n^5(D_{da}) - \phi_n^5(D_{be}) = -f_{n-1}(D_s) + [\phi_{n-1}^7(D_{sgh}) - \phi_{n-1}^6(D_{sgh})].$$

Hence, (iv) is true by lemma 2.6 and lemma 3.5. So, the proof of lemma 3.6 is complete.

By lemma 3.6, it is seen that the following Lemma 3.7 holds.

Lemma 3.7. If the vertices of $L_{2\times n}(n \geqslant 2)$ are labelled as in figure 2(a). Then

(i) $(L_{2\times n} - o_n - x_n) \succ (L_{2\times n} - z_n - q_n), (L_{2\times n} - o_n - z_n) \succ (L_{2\times n} - x_n - q_n)$;

(ii) $(L_{2\times n} - o_n - x_n - z_n) \succ (L_{2\times n} - x_n - z_n - q_n)$;

(iii) $(L_{2\times n} - o_n) \succ (L_{2\times n} - q_n), (L_{2\times n} - z_n) \succ (L_{2\times n} - x_n)$;

(iv) $\phi_n^{01}(L_{zxo}) \succ \phi_n^{01}(L_{xzq}), \phi_n^{03}(L_{zxo}) \succ \phi_n^{03}(L_{xzq}), \phi_n^1(L_{ox}) \succ \phi_n^1(L_{zq})$, $\phi_n^5(L_{zo}) \succ \phi_n^5(L_{xq})$.

The proof of theorem A. If the vertices of $L_{2\times n}$, $Z_{2\times n}$ and $D_{2\times n}$ are labelled as in figure 2 and figure 3a, respectively. We only need to consider the figure 3a(1) (for figure 3a(2), the proof being similar). It is easy to see that $\Phi_{2\times 1} = \{L_{2\times 1}\} = \{Z_{2\times 1}\}$, $\Phi_{2\times 2} = \{L_{2\times 2}\} = \{Z_{2\times 2}\}$ and $\Phi_{2\times 3} = \{L_{2\times 3}, Z_{2\times 3}\}$. Obviously, theorem A holds as $n = 1, 2$. So, we suppose that $n \geqslant 3$ below. By lemma 3.1, we know that

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

where $B(D_{2\times n})$ is represented in table 1. Note that $r_{n-1}, s_{n-1}, t_{n-1}, g_{n-1}$ and h_{n-1} correspond to $o_{n-1}, x_{n-1}, y_{n-1}, z_{n-1}$ and q_{n-1} (or $l_{n-1}, p_{n-1}, w_{n-1}, v_{n-1}$ and u_{n-1}), respectively(see figures 2 and 3a(1)). Then,

$$\phi(L_{2\times n}) = B(L_{2\times n}) \cdot A(L_{2\times(n-1)}; x_{n-1}z_{n-1}q_{n-1}), \tag{4}$$

and

$$\phi(Z_{2\times n}) = B(Z_{2\times n}) \cdot A(Z_{2\times(n-1)}; p_{n-1}v_{n-1}u_{n-1}), \tag{5}$$

where

$$\begin{aligned} B(L_{2\times n}) = [&x^6 - 5x^4 + 6x^2 - 1, -x^5 + 4x^3 - 3x, -x^5 + 3x^3 - 2x, \\ &-x^5 + 4x^3 - 3x, x^4 - 2x^2, x^4 - 2x^2 + 1, x^4 - 3x^2 + 1, -x^3 + x, \\ &-2(\phi^5_{n-1}(L_{xq}) + \phi^6_{n-1}(L_{xzq}) + \phi^7_{n-1}(L_{xzq}))] \end{aligned}$$

and

$$\begin{aligned} B(Z_{2\times n}) = [&x^6 - 5x^4 + 6x^2 - 1, -x^5 + 4x^3 - 3x, -x^5 + 3x^3 - 2x, \\ &-x^5 + 4x^3 - 3x, x^4 - 2x^2, x^4 - 2x^2 + 1, x^4 - 3x^2 + 1, -x^3 + x, \\ &-2(\phi^5_{n-1}(Z_{pu}) + \phi^6_{n-1}(Z_{pvu}) + \phi^7_{n-1}(Z_{pvu}))] \end{aligned}$$

In order to use induction to prove Theorem A. Recall tables 1 and 2 and Definitions 2.1 and 3.1. Comparing $\phi(D_{2\times n})$ with $\phi(L_{2\times n})$, we know by Lemma 2.6 that it suffices to prove the following claim 1 which contains more contents than that of theorem A.

Claim 1. For $sgh \in \{bde, dba\}$,

$$\begin{gathered} (D_{2\times n} - s_n - g_n - h_n) \succeq (L_{2\times n} - x_n - z_n - q_n), \\ (D_{2\times n} - g_n - h_n) \succeq (L_{2\times n} - z_n - q_n), \\ (D_{2\times n} - s_n - h_n) \succeq (L_{2\times n} - x_n - q_n), \quad (D_{2\times n} - s_n - g_n) \succeq (L_{2\times n} - x_n - z_n), \\ (D_{2\times n} - h_n) \succeq (L_{2\times n} - q_n), \quad (D_{2\times n} - s_n) \succeq (L_{2\times n} - x_n), \\ \phi(D_{2\times n} - s_n) + \phi(D_{2\times n} - g_n) \succeq \phi(L_{2\times n} - x_n) + \phi(L_{2\times n} - z_n), \\ \phi^5_n(D_{sh}) \succeq \phi^5_n(L_{xq}), \quad \phi^1_n(D_{gh}) \succeq \phi^1_n(L_{zq}), \quad \phi^{01}_n(D_{sgh}) \succeq \phi^{01}_n(L_{xzq}), \\ \phi^{02}_n(D_{sg}) \succeq \phi^{02}_n(L_{xz}), \\ \phi^{03}_n(D_{sgh}) \succeq \phi^{03}_n(L_{xzq}), \quad L_{2\times n} \preceq D_{2\times n}. \end{gathered}$$

Note that if $D_{2\times n} = L_{2\times n}$ then claim 1 holds by lemma 3.7. Hence, we may assume that $D_{2\times n} \neq L_{2\times n}$ in the following. By lemmas 3.6 we know that for claim 1 holding it suffices to prove the following claim 2((i)–(v)).

(i) $(D_{2\times n} - b_n - d_n - e_n) \succ (L_{2\times n} - x_n - z_n - q_n)$;

(ii) $(D_{2\times n} - d_n - e_n) \succ (L_{2\times n} - z_n - q_n), (D_{2\times n} - b_n - e_n) \succ (L_{2\times n} - x_n - q_n), (D_{2\times n} - b_n - d_n) \succ (L_{2\times n} - x_n - z_n)$;

(iii) $(D_{2\times n} - e_n) \succ (L_{2\times n} - q_n), (D_{2\times n} - b_n) \succ (L_{2\times n} - x_n), \phi(D_{2\times n} - b_n) + \phi(D_{2\times n} - d_n) \succ \phi(L_{2\times n} - x_n) + \phi(L_{2\times n} - z_n)$;

(iv) $\phi^5_n(D_{be}) \succ \phi^5_n(L_{xq}), \phi^1_n(D_{de}) \succ \phi^1_n(L_{zq}), \phi^{01}_n(D_{bde}) \succ \phi^{01}_n(L_{xzq}), \phi^{02}_n(D_{db}) \succ \phi^{02}_n(L_{zx}), \phi^{03}_n(D_{bde}) \succ \phi^{03}_n(L_{xzq})$;

(v) $L_{2\times n} \prec D_{2\times n}$.

using induction on n. When $n = 3$. $\Phi_{2\times 3} = \{L_{2\times 3}, Z_{2\times 3}\}$. Then, applying computer algebra (*Mathematic* 4.0) techniques to (4) and (5) we can get $\phi(L_{2\times 3})$ and $\phi(Z_{2\times 3})$ (See appendix A). Using the same methods and referencing tables 1 and 2, we can get the rest of characterize polynomials in Appendix A. And recall figure 2, it is easy to see that Claim 2 holds as $n = 3$.

Suppose that claim 2 is true for all double hexagonal chains with fewer than n naphthalene units. We show that Claim 2 holds as $n \geqslant 4$. From table 1 it follows that

$$\begin{aligned}\phi(D_{2\times n} - b_n - d_n - e_n) &= x^3\phi(D_{2\times(n-1)}) - x^2[\phi(D_{2\times(n-1)} - s_{n-1})\\ &+\phi(D_{2\times(n-1)} - g_{n-1}) + \phi(D_{2\times(n-1)} - h_{n-1})]\\ &+x[\phi(D_{2\times(n-1)} - s_{n-1} - g_{n-1}) + \phi(D_{2\times(n-1)} - g_{n-1} - h_{n-1})\\ &+\phi(D_{2\times(n-1)} - s_{n-1} - h_{n-1})] - \phi(D_{2\times(n-1)} - s_{n-1} - g_{n-1} - h_{n-1}),\end{aligned}$$

where $sgh \in \{bde, dba\}$, and

$$\begin{aligned}\phi(L_{2\times n} - x_n - z_n - q_n) &= x^3\phi(L_{2\times(n-1)}) - x^2[\phi(L_{2\times(n-1)} - x_{n-1})\\ &+\phi(L_{2\times(n-1)} - z_{n-1}) + \phi(L_{2\times(n-1)} - q_{n-1})]\\ &+x[\phi(L_{2\times(n-1)} - x_{n-1} - z_{n-1}) + \phi(L_{2\times(n-1)} - z_{n-1} - q_{n-1})\\ &+\phi(L_{2\times(n-1)} - x_{n-1} - q_{n-1})] - \phi(L_{2\times(n-1)} - x_{n-1} - z_{n-1} - q_{n-1}).\end{aligned}$$

By the inductive hypotheses and Lemma 2.6, it is easy to see that (i) holds. The proof of (ii)–(iii) is similar to it. Now we prove $\phi_n^5(D_{be}) \succ \phi_n^5(L_{xq})$. From tables 1 and 2 we deduce that

$$\begin{aligned}\phi_n^5(D_{be}) &= \phi(D_{2\times n} - b_n - c_n - d_n - e_n) + x\phi_{n-1}^2(D_{sgh})\\ &+(x^2-1)\phi_{n-1}^5(D_{sh}) + \phi_{n-1}^4(D_{sgh}),\end{aligned}$$

where $sgh \in \{bde, dba\}$, and

$$\begin{aligned}\phi_n^5(L_{xq}) &= \phi(L_{2\times n} - x_n - y_n - z_n - q_n) + x\phi_{n-1}^2(L_{xzq})\\ &+(x^2-1)\phi_{n-1}^5(L_{xq}) + \phi_{n-1}^4(L_{xzq}).\end{aligned}$$

Similar to the proof of Fact 1 (given in lemma 3.3), by the inductive hypotheses, lemmas 2.6, 3.1–3.3, 3.6 and definition 3.1, we know that $\phi_n^5(D_{be}) \succ \phi_n^5(L_{xq})$. Using the same methods, we have $\phi_n^1(D_{de}) \succ \phi_n^1(L_{zq})$, $\phi_n^{01}(D_{bde}) \succ \phi_n^{01}(L_{xzq})$, $\phi_n^{02}(D_{db}) \succ \phi_n^{02}(L_{zx})$ and $\phi_n^{03}(D_{bde}) \succ \phi_n^{03}(L_{xzq})$. In the further, from (i)–(iv), (1), (4), definition 3.1 and lemma 2.6 it follows that $L_{2\times n} \prec D_{2\times n}$. Hence claim 2 holds as $n \geqslant 4$. So, the proof of theorem A is complete.

Appendix

Appendix A
The characteristic polynomials of graphs concerning with $D_{2\times n}$, where $n = 3$.

$\phi_n^1(L_{zq})$	$40 - 837x^2 + 4079x^4 - 9186x^6 + 11623x^8 - 8956x^{10} + 4333x^{12} - 1313x^{14} + 240x^{16} - 24x^{18} + x^{20}$
$\phi_n^1(Z_{pl})$	$112 - 1167x^2 + 4699x^4 - 9796x^6 + 11958x^8 - 9058x^{10} + 4349x^{12} - 1314x^{14} + 240x^{16} - 24x^{18} + x^{20}$
$\phi_n^{01}(L_{xzq})$	$-55x + 730x^3 - 2691x^5 + 4710x^7 - 4616x^9 + 2699x^{11} - 954x^{13} + 198x^{15} - 22x^{17} + x^{19}$
$\phi_n^{01}(Z_{vpl})$	$-121x + 951x^3 - 2993x^5 + 4920x^7 - 4693x^9 + 2713x^{11} - 955x^{13} + 198x^{15} - 22x^{17} + x^{19}$
$\phi_n^{02}(L_{xz})$	$-160x + 1248x^3 - 3720x^5 + 5763x^7 - 5215x^9 + 2889x^{11} - 985x^{13} + 200x^{15} - 22x^{17} + x^{19}$
$\phi_n^{02}(Z_{pv})$	$-206x + 1424x^3 - 3979x^5 + 5952x^7 - 5288x^9 + 2903x^{11} - 986x^{13} + 200x^{15} - 22x^{17} + x^{19}$
$\phi_n^{03}(L_{xzq})$	$-4 + 248x^2 - 1331x^4 + 2875x^6 - 3247x^8 + 2108x^{10} - 808x^{12} + 179x^{14} - 21x^{16} + x^{18}$
$\phi_n^{03}(Z_{vpl})$	$-24 + 351x^2 - 1514x^4 + 3027x^6 - 3311x^8 + 2121x^{10} - 809x^{12} + 179x^{14} - 21x^{16} + x^{18}$
$\phi_n^5(L_{xq})$	$-10 + 266x^2 - 1227x^4 + 2491x^6 - 2759x^8 + 1804x^{10} - 709x^{12} + 163x^{14} - 20x^{16} + x^{18}$
$\phi_n^5(Z_{vl})$	$-42 + 385x^2 - 1394x^4 + 2601x^6 - 2795x^8 + 1809x^{10} - 709x^{12} + 163x^{14} - 20x^{16} + x^{18}$
$\phi(L_{2\times 3})$	$-100 + 1838x^2 - 9605x^4 + 24398x^6 - 35902x^8 + 33110x^{10} - 19831x^{12} + 7783x^{14} - 1973x^{16} + 309x^{18} - 27x^{20} + x^{22}$
$\phi(Z_{2\times 3})$	$-196 + 2358x^2 - 10792x^4 + 25862x^6 - 36968x^8 + 33580x^{10} - 19953x^{12} + 7800x^{14} - 1974x^{16} + 309x^{18} - 27x^{20} + x^{22}$
$\phi(L_{2\times 3} - x_3)$	$180x - 1995x^3 + 7601x^5 - 14708x^7 + 16670x^9 - 11779x^{11} + 5305x^{13} - 1512x^{15} + 262x^{17} - 25x^{19} + x^{21}$
$\phi(L_{2\times 3} - z_3)$	$278x - 2396x^3 + 8271x^5 - 15304x^7 + 16978x^9 - 11872x^{11} + 5320x^{13} - 1513x^{15} + 262x^{17} - 25x^{19} + x^{21}$
$\phi(L_{2\times 3} - q_3)$	$80x - 1313x^3 + 5916x^5 - 12607x^7 + 15187x^9 - 11164x^{11} + 5157x^{13} - 1493x^{15} + 261x^{17} - 25x^{19} + x^{21}$
$\phi(Z_{2\times 3} - l_3)$	$160x - 1692x^3 + 6620x^5 - 13278x^7 + 15543x^9 - 11269x^{11} + 5173x^{13} - 1494x^{15} + 261x^{17} - 25x^{19} + x^{21}$
$\phi(Z_{2\times 3} - v_3)$	$292x - 2434x^3 + 8312x^5 - 15330x^7 + 16989x^9 - 11874x^{11} + 5320x^{13} - 1513x^{15} + 262x^{17} - 25x^{19} + x^{21}$
$\phi(Z_{2\times 3} - p_3)$	$326x - 2628x^3 + 8732x^5 - 15786x^7 + 17260x^9 - 11963x^{11} + 5335x^{13} - 1514x^{15} + 262x^{17} - 25x^{19} + x^{21}$
$\phi(L_{2\times 3} - x_3 - q_3)$	$1 - 177x^2 + 1511x^4 - 4585x^6 + 7057x^8 - 6268x^{10} + 3380x^{12} - 1115x^{14} + 218x^{16} - 23x^{18} + x^{20}$
$\phi(L_{2\times 3} - z_3 - q_3)$	$16 - 598x^2 + 3309x^4 - 7998x^6 + 10623x^8 - 8477x^{10} + 4204x^{12} - 1295x^{14} + 239x^{16} - 24x^{18} + x^{20}$

Appendix A *(Continued)*

$\phi(L_{2\times3} - x_3 - z_3)$	$-215x^2 + 1615x^4 - 4693x^6 + 7110x^8 - 6280x^{10} + 3381x^{12} - 1115x^{14} + 218x^{16} - 23x^{18} + x^{20}$
$\phi(Z_{2\times3} - l_3 - v_3)$	$9 - 292x^2 + 1816x^4 - 4948x^6 + 7288x^8 - 6348x^{10} + 3394x^{12} - 1116x^{14} + 218x^{16} - 23x^{18} + x^{20}$
$\phi(Z_{2\times3} - p_3 - l_3)$	$64 - 830x^2 + 3770x^4 - 8480x^6 + 10905x^8 - 8568x^{10} + 4219x^{12} - 1296x^{14} + 239x^{16} - 24x^{18} + x^{20}$
$\phi(Z_{2\times3} - v_3 - p_3)$	$-255x^2 + 1762x^4 - 4913x^6 + 7278x^8 - 6347x^{10} + 3394x^{12} - 1116x^{14} + 218x^{16} - 23x^{18} + x^{20}$
$\phi(L_{2\times3} - x_3 - z_3 - q_3)$	$-18x + 467x^3 - 2088x^5 + 4060x^7 - 4247x^9 + 2587x^{11} - 937x^{13} + 197x^{15} - 22x^{17} + x^{19}$
$\phi(Z_{2\times3} - l_3 - v_3 - p_3)$	$-58x + 614x^3 - 2308x^5 + 4228x^7 - 4314x^9 + 2600x^{11} - 938x^{13} + 197x^{15} - 22x^{17} + x^{19}$

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