On the Quasi-Ordering of Catacondensed Hexagonal Systems with Respective to their Clar Covering Polynomials

Liqiong Xu[a] and Fuji Zhang[b]

[a] School of Sciences, Jimei University, Fujian 361023, P.R. China
[b] School of Mathematics Sciences, Xiamen University, Fujian 361005, P.R. China

Reprint requests to L. X.; Fax: 008605926181044, E-mail: xuliqiong@jmu.edu.cn

Z. Naturforsch. **67a,** 550 – 558 (2012) / DOI: 10.5560/ZNA.2012-0057
Received May 3, 2012 / published online August 20, 2012

In this paper, we discuss the quasi-ordering of hexagonal systems with respective to the coefficients of their Clar covering polynomials (also known as Zhang–Zhang polynomials). The last six minimal catacondensed hexagonal systems and the hexagonal chains with the maximum Clar covering polynomial are determined. Furthermore, the smallest pair of incomparable catacondensed hexagonal systems is given.

Key words: Catacondensed Hexagonal Systems; Clar Covering Polynomials; Zhang–Zhang Polynomials; k^*-Resonant Graph.

1. Introduction

A hexagonal system is a finite connected plane graph with no cut vertex in which every interior region is surrounded by a regular hexagon of side length 1. A hexagonal system without internal vertex is called catacondensed hexagonal system. Let H be a hexagonal system. A spanning subgraph C of H is said to be a Clar cover of H if each of its components is either a hexagon or an edge [1].

Heping Zhang and Fuji Zhang [2] first defined the Clar covering polynomial (i.e., Zhang–Zhang polynomial) of H as

$$P(H,w) = \sum_{i=0}^{C(H)} z(H,i)w^i\,, \qquad (1)$$

where $z(H,i)$ denotes the number of Clar covers of H having precisely i hexagons, and $C(H)$ is the Clar number, the maximum number of hexagons in Clar covers of H [2 – 6]. The Clar covering polynomial was used to conveniently compare Clar number and perfect matching number of some types of benzenoid isomers [4]. It is also called Zhang–Zhang polynomial in a series of papers due to Gutman et al. [7 – 13].

Throughout this paper, the following notations and terminology will be used. Let C_h be the set of catacondensed hexagonal systems with h hexagons. For a hexagonal system H, its dualist graph $D(H)$ is the graph whose vertex set is the set of hexagons of H, and two vertices of which are adjacent if the corresponding hexagons have a common edge. Clearly, the dualist graph of a catacondensed hexagonal system is a tree. Let $C'_h \subseteq C_h$ denote the set of all the hexagonal systems whose dualist graphs are paths. C'_h is also called the set of hexagonal chains, and $C_h \setminus C'_h$ is the set of branched catacondensed hexagonal systems. Let $H \in C'_h$ and label its hexagons consecutively by $c_1, c_2, \ldots, c_h$. Thus the hexagons c_1 and c_h are terminal and for $j = 1, 2, \ldots, h-1$, the hexagons c_j and c_{j+1} have a common edge. We also denote H by $c_1 c_2 \ldots c_h$.

For $H \in C_h$, a hexagon s of H is called a kink of H if s has exactly two consecutive vertices with degree 2 in H, and s is called a branched hexagon if s has no vertex with degree 2. The catacondensed hexagonal systems having no kink and branched hexagon are called single linear hexagonal chains. For two catacondensed hexagonal systems H_1 and H_2 with two adjacent vertices of degree two, say u and v for H_1 and u' and v' for H_2, they can be fused with each other in the following way: identify u and u' as well as v and v' to obtain a new catacondensed hexagonal system $H_1 : H_2$. We define D_h (resp. E_h) to be the set of the hexagonal chains with exactly one (resp. two) kink(s) and without branched hexagon, and F_h to be the set of the catacon-

© 2012 Verlag der Zeitschrift für Naturforschung, Tübingen · http://znaturforsch.com

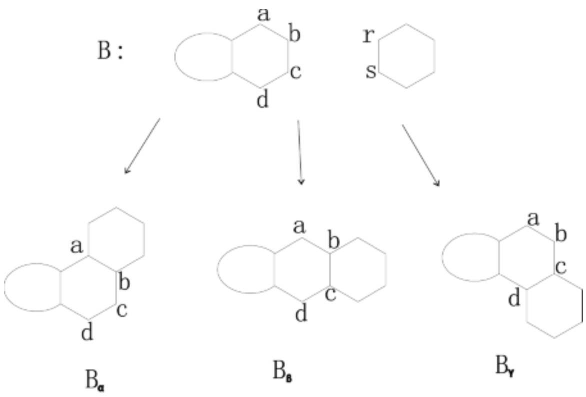


Fig. 1. θ-type attaching.

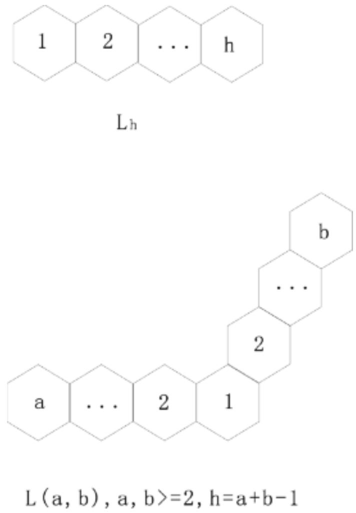


Fig. 2. Example of kinks and chains in catacondensed hexagonal systems.

densed hexagonal systems with exactly one branched hexagon and without kink.

Let M be a perfect matching of a graph H. A cycle C in H 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 H are mutually resonant if there is a perfect matching M of H such that each cycle is an M-alternating cycle. A connected graph H with perfect matching is said to be k-cycle resonant if H contains at least $k(\geq 1)$ disjoint cycles, and any t disjoint cycles in H, $1 \leq t \leq k$, are mutually resonant. A graph H is called k^*-cycle resonant if H is k-cycle resonant, and k is the maximum number of disjoint cycles in H. Denote by $C_h^{\prime *}$ the set of all k^*-cycle resonant hexagonal chains with h hexagons. The concept of k-cycle resonant and k^*-cycle resonant graph were introduced by Guo and Zhang [14].

An element B_h of $C_h^\prime$ can be obtained from an appropriately chosen graph $B_{h-1} \in C_{h-1}^\prime$ 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 1. We call them α-type, β-type, and γ-type attaching, respectively. Following [14], we denote by $[B]_\theta$ the hexagonal chain obtained from B by θ-type attaching to it a new hexagon c, where $\theta \in \{\alpha, \beta, \gamma\}$. Obviously, each B_h with $h \geq 2$ can be written as $B_h = \beta\theta_2\theta_3 \ldots \theta_{h-1}$ for short, where $\theta_j \in \{\alpha, \beta, \gamma\}$.

Now we introduced a quasi-ordering relation $\succeq$ on the set of all hexagonal systems with h hexagons to compare their Clar covering polynomials: If H_1 and H_2 are two hexagonal systems with h hexagons and with Clar covering polynomials in the above form, and $z(H_1, i) \geq z(H_2, i)$ for all $i = 0, 1, \ldots, C(H)$, we say $P(H_1)$ is greater than $P(H_2)$ and write $P(H_1) \succeq P(H_2)$. If $P(H_1) \succeq P(H_2)$ and there exist a j such that $z(H_1, j) > z(H_2, j)$, then we write $P(H_1) \succ P(H_2)$. If neither $P(H_1) \succeq P(H_2)$ nor $P(H_1) \preceq P(H_2)$ holds, then $P(H_1)$ and $P(H_2)$ are incomparable. Obviously, $P(H) \succeq 0$ if and only if $z(H, i) \geq 0$ for all $i = 0, 1, \ldots, C(H)$; $P(H_1) \succeq P(H_2)$ if and only if $P(H_1) - P(H_2) \succeq 0$.

2. Some Related Lemmas

Lemma 1. [2] *Let L_h be the single linear hexagonal chain, let $L(a,b)$ (resp. $L(a,b,c)$, $L(a,b,c,d)$) be an unbranched hexagonal chain with exactly one (resp. two, three) kink(s), and let $B(a,b,c)$ be a branched catacondensed hexagonal system with exactly one branched hexagon and without kink (see Figs. 2 and 3). Then $P(L_h) = hw + h + 1$; $P(L(a,b)) = ((a-1)w + a)((b-1)w + b) + w + 1$; $P(L(a,b,c)) = (aw + a + 1)((c-1)w + c) + ((a-1)w + a)(cw + c + 1) + ((b-2)w + b - 3)((c-1)w + c)((a-1)w + a)$; $P(B(a,b,c)) = ((a-1)w + a)((b-1)w + b)((c-1)w + c) + w + 1$; where $P(H)$ denote the Clar covering polynomial of H.*

Lemma 2. [2] *Let H be a generalized hexagonal system, and xy be an edge not belonging to any hexagon of H. Then $P(H) = P(H - x - y) + P(H - xy)$.*

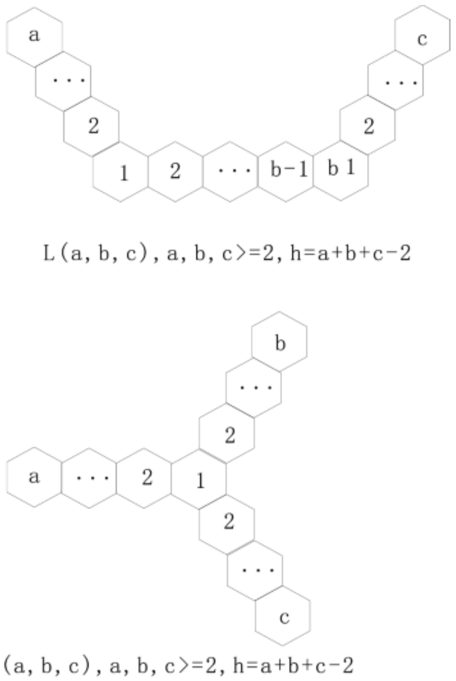


Fig. 3. Example of kinks and chains in catacondensed hexagonal systems.

Lemma 3. [2] *Let H be a catacondensed hexagonal system, and xy is an edge of a hexagon s of H which lies on the periphery of H, then $P(H) = wP(H-s) + P(H-x-y) + P(H-xy)$.*

In the following, we prove two lemmas, which are vital in our investigation of hexagonal systems presented in Section 3.

Let $h \geq 4$ be an integer and $D = \{$ integral points $(a,b,c) | a+b+c = h+2, a,b,c \geq 2\}$.

Let

$$p_1 = \min_{(a,b,c)\in D} P(B(a,b,c)),$$
$$p_2 = \min_{(a,b,c)\in D} P(L(a,b,c)),$$
$$P_1 = \max_{(a,b,c)\in D} P(B(a,b,c)),$$
$$P_2 = \max_{(a,b,c)\in D} P(L(a,b,c)),$$
$$p_2' = \min_{(a,b,c)\in D} P(L(a,b,c)) \setminus p_2 .$$

Then the polynomials of p_1, p_2, p_2', P_1, P_2, and the points (a,b,c) at which these polynomials are reached can be determined by Lemmas 4 and 5.

Lemma 4. *p_1 is reached only at points (a,b,c) with two of a,b,c having values 2, and $p_1 = (w+2)^2((h-3)w+h-2)+w+1$;*

when $h \equiv 0 (mod\ 3)$, $P_1 = (\frac{h}{3}w + \frac{h}{3} + 1)^2((\frac{h}{3} - 1)w + \frac{h}{3}) + w + 1$, which is reached only at $(a,b,c) = (h/3, h/3+1, h/3+1), (h/3+1, h/3, h/3+1), (h/3+1, h/3+1, h/3)$;

when $h \equiv 1 (mod\ 3)$, $P_1 = (\lceil \frac{h}{3} \rceil w + \lceil \frac{h}{3} \rceil + 1)^3 + w + 1$, which is reached only at $(a,b,c) = (\lceil h/3 \rceil, \lceil h/3 \rceil, \lceil h/3 \rceil)$;

when $h \equiv 2 (mod\ 3)$, $P_1 = ((\lceil \frac{h}{3} \rceil - 1)w + \frac{h}{3})^2(\lceil \frac{h}{3} \rceil w + \lceil \frac{h}{3} \rceil + 1) + w + 1$, which is reached only at $(a,b,c) = (\lceil h/3 \rceil, \lceil h/3 \rceil, \lceil h/3 \rceil + 1), (\lceil h/3 \rceil, \lceil h/3 \rceil + 1, \lceil h/3 \rceil), (\lceil h/3 \rceil + 1, \lceil h/3 \rceil, \lceil h/3 \rceil)$.

Proof. Since a, b, c are symmetric in $P(B(a,b,c))$, we may assume without loss of generality that $2 \leq a \leq b$.

Suppose that $a > 2$. Then $(a-1, b+1, c) \in D$, and $P(B(a,b,c)) - P(B(a-1,b+1,c)) = (b-a+1)((c-1)w+c)(w+1)^2 \succ 0$. Therefore, p_1 can only be reached at $(2,b,c) \in D$. When $a = 2$, assume that $b > 2$ and $b \leq c$, then $P(B(2,b,c)) - P(B(2,b-1,c+1)) = (c-b+1)(w+2)(w+1)^2 \succ 0$.

Thus, p_1 is reached only at $(2,2,h-2)$. By the symmetry of a,b,c in $P(B(a,b,c))$, in any case p_1 is reached only at (a,b,c) with two of a, b, c having values 2. This proves the conclusion about p_1.

We now turn to deal with P_1. We still assume $2 \leq a \leq b$. Suppose that $b - a \geq 2$. Then $(a+1, b-1, c) \in D$, and $P(B(a+1,b-1,c)) - P(B(a,b,c)) = (b-a+1)((c-1)w+c)(w+1)^2 \succ 0$. Thus, $P(B(a+1,b-1,c)) \succ P(B(a,b,c))$. Therefore, by the symmetry of a, b, c in $P(B(a,b,c))$ and in D, if P_1 is reached at (a,b,c), then $|a-b| \leq 1$, $|a-c| \leq 1$, $|b-c| \leq 1$. From this fact, we know that when $h = 3n$, M_1 is reached only at $(a,b,c) = (n, n+1, n+1), (n+1, n, n+1), (n+1, n+1, n)$.

When $h = 3n+1$, P_1 is reached only at $(a,b,c) = (n+1, n+1, n+1)$.

When $h = 3n+2$, P_1 is reached only at $(a,b,c) = (n+1, n+1, n+2), (n+1, n+2, n+1), (n+2, n+1, n+1)$.

From these results, it is trivial to get the conclusion about P_1. This complete the proof of the lemma. □

Lemma 5. *p_2 is reached only at points $(a,b,c) = (2,2,h-2)$ and $(h-2,2,2)$, and $p_2 = (2w+3)((h-3)w+h-2) + (w+1)(w+2)$; p_2' is reached only at points $(a,b,c) = (3,2,h-3)$ and $(h-3,2,3)$;*

when $h \equiv 1 (mod\ 3)$, P_2 *is reached only at* $(a,b,c) = (\lceil h/3 \rceil, \lceil h/3 \rceil, \lceil h/3 \rceil)$*;*

when $h \equiv 2 (mod\ 3)$, P_2 *is reached only at* $(a,b,c) = (\lceil h/3 \rceil, \lceil h/3 \rceil + 1, \lceil h/3 \rceil)$*;*

when $h \equiv 0 (mod\ 3)$, P_2 *is reached only at* $(a,b,c) = (h/3, h/3+1, h/3+1), (h/3+1, h/3+1, h/3)$.

Proof. Since a,c are symmetric in $P(L(a,b,c))$, we may assume without loss of generality that $2 \le a \le c$.

Suppose that $a > 2$. Then $(a-1,b,c+1) \in D$, and $P(L(a,b,c)) - P(L(a-1,b,c+1)) = (c-a+1)((b-2)w+b-1)(w+1)^2 \succ 0$. Therefore, p_2 can only be reached at $(2,b,c) \in D$. When $a = 2$, then $P(L(2,b,c)) = (b-2)(c-1)w^3 + (c(4b-3)-3h+5)w^2 + (b(5c+3)-5h+4)w + 2bc - c + 2$.

The coefficient of w^3 is $(b-2)(c-1)$, ie. $(h-2-c)(c-1)$. Let $f(c) = (h-2-c)(c-1), c \in [2,h-2]$, then $f(c)$ is quadratic in c with negative leading coefficient -1. Hence, its minimum value over the interval $[2,h-2]$ can only be reached at the endpoints of the interval. Simple calculation gives that $f(2) = h-4$, $f(h-2) = 0$. When $h \ge 4$, it is always true that $f(h-2) \le f(2)$.

This means that the coefficient of w^3 has minimum value iff $c = h-2$. By similar argument, $c(4b-3) - 3h + 5$, $b(5c+3) - 5h + 4$ and $2bc - c + 2$ have minimum value if $c = h-2$. Therefore, p_2 is reached at $(2,2,h-2)$. By the symmetry of a,c in $P(L(a,b,c))$ and in D, in any case, p_2 is reached only at $(a,b,c) = (2,2,h-2)$ or $(h-2,2,2)$. We now consider p'_2.

When $a = 2$, by a similar argument, the coefficients of $P(L(2,b,c))$ reached the second minimum values when $c = 2$. Therefore, when $a = 2$, the hexagonal chain with exactly two kinks, which have the second minimum Clar covering polynomial is $L(2,h-2,2)$.

When $a \ge 3$, by a similar argument, the hexagonal chain with exactly two kinks, which have minimum Clar covering polynomial is $L(3,2,h-3)$.

By simple calculation, $P(L(2,h-2,2)) \succ P(L(3,2,h-3))$. Thus p'_2 is reached only at $(a,b,c) = (3,2,h-3)$ or $(h-3,2,3)$. We now turn to deal with P_2.

Suppose that $c - a \ge 2$. Then $(a+1,b,c-1) \in D$, and $P(L(a+1,b,c-1)) - P(L(a,b,c)) = (c-a-1)((b-2)w+b-1)(w+1)^2 \succ 0$.

Therefore, by the symmetry of a,c in $P(L(a,b,c))$ and in D, if P_2 is reached at $(a,b,c) \in D$, then $|a-c| \le 1$.

Suppose that $b - c \ge 2$. Then $(a,b-1,c+1) \in D$, and $P(L(a,b-1,c+1)) - P(L(a,b,c)) = ((b-c-2)((a-1)w+a)+1)(w+1)^2 \succ 0$.

Therefore, if P_2 is reached at $(a,b,c) \in D$ with $b-c \ge 0$, then $c \le b \le c+1$.

Suppose that $c - b \ge 2$. Then $(a,b+1,c-1) \in D$, and $P(L(a,b+1,c-1)) - P(L(a,b,c)) = (w+1)((a-1)w+a)((c-b)w+2) \succ 0$.

Therefore, if P_2 is reached at $(a,b,c) \in D$ with $c-b \ge 0$, then $b \le c \le b+1$.

Suppose that $b - a \ge 2$. Then $(a+1,b-1,c) \in D$, and $P(L(a+1,b-1,c)) - P(L(a,b,c)) = (w+1)^2((b-a-2)(c-1)w + (b-a-2)c + 1) \succ 0$.

Therefore, if P_2 is reached at $(a,b,c) \in D$ with $b-a \ge 0$, then $a \le b \le a+1$.

Thus, P_2 is reached when $c = a$, $c = a-1$, or $a+1$. Then we have to consider the following three cases.

Case I. $c = a$.

If $b \ge a$, we have $b = a$ or $a+1$. If $a \ge b$, i.e. $c \ge b$, then we also have $b = a$ or $a-1$.

Case II. $c = a+1$.

If $b \ge c$, we have $b = c$ or $c+1$. If $b = c+1$, then $b = a+2$, contradicting to that when $b-a \ge 0$, then $a \le b \le a+1$.

If $b \le c$, then we have $b = c$ or $c-1 = a$.

Case III. $c = a-1$.

By the symmetry of a and c in $P(L(a,b,c))$ and in D, this case is dual to Case II.

In all these cases, we conclude that the absolute values of the differences of any two of a, b, and c are at most 1. From this fact, we can obtain the value of P_2 and at where it is reached. We need to consider three cases.

Case I. If $h+2 = 3n$, where n is an integer, then $a = b = c = n$. Because if one of them is greater n, then one of them must be smaller than n, and then the difference of these two is greater than 1. Therefore, P_2 is reached only at $(a,b,c) = (n,n,n) = (\lceil h/3 \rceil, \lceil h/3 \rceil, \lceil h/3 \rceil)$.

Case II. If $h+2 = 3n+1$, where n is an integer, then exactly two of a, b, and c are n and the other is $n+1$.

The reason is as follows. If the largest of a, b, and c is greater than or equal to $n+2$, then the smaller of the three must be greater than or equal to $n+1$, and then the sum of the three is greater than $3n+1$. If the smallest of a, b, and c is smaller than or equal to $n-1$, then the largest of the three must be smaller than or equal to n, and then the sum of the three is smaller than $3n+1$. Therefore, the largest of the three is at most $n+1$ and the smallest is at least n. Since the sum of the three numbers is $3n+1$, then exactly two of the three are n, and the other is $n+1$. Since $P(L(n,n+1,n)) - P(L(n,n,n+1)) = (n-1)(w+1)^3 \succ 0$, we have P_2 which is reached only at $(a,b,c) = (\lceil h/3 \rceil, \lceil h/3 \rceil + 1, \lceil h/3 \rceil)$.

Case III. If $h+2 = 3n+2$, where n is an integer, then exactly two of a, b, and c are $n+1$, and the other is n.

The reason is as follows. If the largest of a, b, and c is greater than or equal to $n+2$, then the smaller of the three must be greater than or equal to $n+1$, and then the sum of the three is greater than $3n+2$. If the smallest of a, b, and c is smaller than or equal to $n-1$, then the largest of the three must be smaller than or equal to n, and then the sum of the three is smaller than $3n+2$. Therefore, the largest of the three is at most $n+1$ and the smallest is at least n. Since the sum of the three numbers is $3n+2$, then exactly two of the three are $n+1$, and the other is n. Since $P(L(n,n+1,n+1)) - P(L(n+1,n,n+1)) = n(w+1)^3 \succ 0$, we have P_2 which is reached only at $(a,b,c) = (h/3, h/3+1, h/3+1), (h/3+1, h/3+1, h/3)$.

This complete the proof of the lemma. □

3. Main Results

For convenience, we denote by X the set of hexagons of H, and for $S \subseteq X$, Let $H[S]$ denote the hexagon system induced by the hexagons in S.

Theorem 1. *The hexagonal chain in $C'_h \setminus (D_h \cup L_h)$ with the minimum Clar covering polynomial is $L(2,2,h-2)$ in E_h, with the second minimum Clar covering polynomial is $L(3,2,h-3)$ in E_h.*

Proof. Let H be a hexagonal chain in $C'_h \setminus (D_h \cup L_h)$ with minimum Clar covering polynomial. If $H \notin E_h$, then H has more than two kinks. Since H is a hexagonal chain, we can take a maximal single linear chain L_s in H containing a kink 1 and an end hexagon s (see Fig. 4). We can fuse L_s with $H[X \setminus \{1,2,\ldots,s\}]$ in another way to obtain the hexagonal chain H' such that H' contains one less kinks than H (see Fig. 4). We have $P(H) = wP(H-s) + P(H-\{u,v\}) + P(H-uv), P(H') = wP(H'-s) + P(H'-\{u,v\}) + P(H'-uv)$.

Let $(H-\{u,v\})^*$(resp.$(H'-\{u,v\})^*$) be the graph obtained from $H-\{u,v\}$ (resp. $H'-\{u,v\}$) by deleting a vertex of degree 1 together with its adjacent vertex consecutively. If $s=2$, then it is not difficult to see that

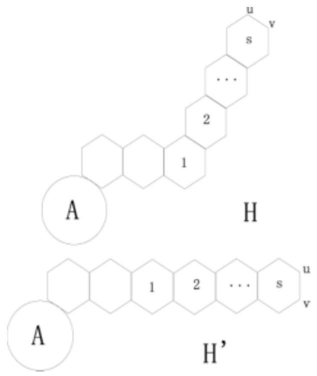


Fig. 4. Proof of Theorem 1.

$(H'-\{u,v\})^*$ is a subgraph of $(H-\{u,v\})^*$ and that $P(H-\{u,v\}) = P((H-\{u,v\})^*)$ and $P(H'-\{u,v\}) = P((H'-\{u,v\})^*)$. So $P(H-\{u,v\}) \succ P(H'-\{u,v\})$ by Lemma 3. By similar argument, we can deduce that $P(H-uv) = P(H'-uv)$, $P(H-s) \succ P(H'-s)$. Hence $P(H) \succ P(H')$, a contradiction.

Now suppose $P(H) \succ P(H')$ for $s = k > 1$. Let $s = k+1$. Similarly, $(H'-\{u,v\})^*$ is a subgraph of $(H-\{u,v\})^*$ and $(H'-s)^*$ is a subgraph of $(H-s)^*$, so $P(H-\{u,v\}) \succ P(H'-\{u,v\})$ and $P(H-s) \succ P(H'-s)$. By induction hypothesis, $P(H-uv) \succ P(H'-uv)$. It follows that $P(H) \succ P(H')$.

Now it follows from Lemma 4 that H must be $L(2,2,h-2)$.

By a similar argument, the hexagonal chain in $C'_h \setminus (D_h \cup L_h)$ with the second minimum Clar covering polynomial is $L(3,2,h-3)$ in E_h. □

Theorem 2. *The branched catacondensed hexagonal system with the minimum Clar covering polynomial is $B(2,2,h-2)$ in F_h.*

Proof. Let H be a branched catacondensed hexagonal system with the minimum Clar covering polynomial. If $H \notin F_h$, then H contains at least two branched hexagons or H contains exactly one branched hexagon and at least one kink. Let L_s be a maximal single linear chain in H containing an end hexagon s, and 1 is the other end hexagon of L_s. If hexagon 1 is a kink of H, then by a similar argument as in the proof of Theorem 1, we can deduce a contradiction. Otherwise, hexagon 1 is a branched hexagon of H (see Fig. 5), and H has at least two branched hexagons.

Let L_t be the single linear chain in H consisting of hexagons $(s+1)$,$(s+2)$,..., $(s+t)$. We fuse L_t with

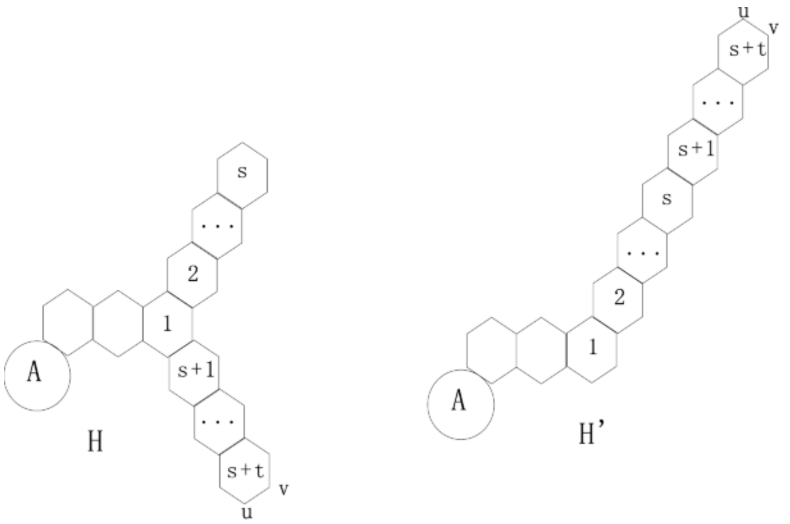


Fig. 5. Proof of Theorem 2.

$H[X\backslash\{(s+1),(s+2),\dots,(s+t)\}]$ to obtain another catacondensed hexagonal system H' so that hexagons $1,2,\dots,s,(s+1),\dots,(s+t)$ form a single linear chain (see Fig. 5).

If $t=1$, then $P(H-uv)=P(H'-uv)$, $H_1=(H'-\{u,v\})^*$ is a subgraph of $H_2=(H-\{u,v\})^*$ and $(H'-s)^*$ is a subgraph of $(H-s)^*$. So $P(H)=wP(H-s)+P(H-\{u,v\})+P(H-uv)\succ wP(H'-s)+P(H'-\{u,v\})+P(H'-uv)=P(H')$ by Lemma 3. Now suppose $P(H)\succ P(H')$ for $t=k>1$. Let $t=k+1$. Similarly, $(H'-\{u,v\})^*$ is a subgraph of $(H-\{u,v\})^*$ and $(H'-s)^*$ is a subgraph of $(H-s)^*$, so $P(H-\{u,v\})\succ P(H'-\{u,v\})$ and $P(H-s)\succ P(H'-s)$. By induction hypothesis, $P(H-uv)\succ P(H'-uv)$. It follows that $P(H)\succ P(H')$.

In any case, we can find another branched catacondensed hexagonal system H' with smaller Clar covering polynomial, again a contradiction.

By Lemma 5, H can only be $B(2,2,h-2)$. □

Theorem 3. *[15] The elements of $L(a,b)$, $a+b=h+1$, can be ordered by their Clar covering polynomial as follows: $P(L(2,h-1))\prec P(L(3,h-2))\prec\dots\prec\dots\prec P(L(\lfloor h/2\rfloor,\lfloor h/2\rfloor+1))$.*

Theorem 4. *Let S_i, $i=1,2,\dots$, be the catacondensed hexagonal system with $h\geq 5$ hexagons and the ith smallest Clar covering polynomials. Then $S_1=L(h)$, $S_2=L(2,h-1)$, $S_3=L(3,h-2)$, $S_4=L(2,2,h-2)$; when $h\geq 7$, $S_5=L(4,h-3)$; when $h\geq 10$, $S_6=L(3,2,h-3)$.*

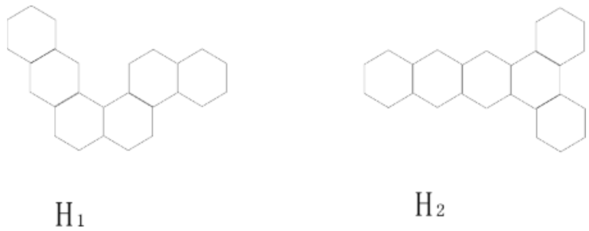
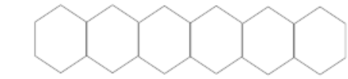
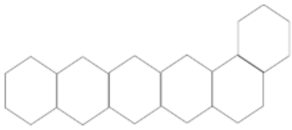


Fig. 6. Incomparable catacondensed hexagonal systems.

Proof. By Theorem 3, elements of $L(a,b)$ can be ordered. By Lemmas 4 and 5, we only need to compare $P(L(3,h-2))$, $P(L(4,h-3))$, $P(L(2,2,h-2))$ and $P(B(2,2,h-2))$, for $h\geq 5$. By Lemma 1, $P(L(3,h-2))=(2w+3)((h-3)w+h-2)+w+1$, $P(L(2,2,h-2))=(2w+3)((h-3)w+h-2)+(w+2)(w+1)$, $P(B(2,2,h-2))=(w+2)^2((h-3)w+h-2)+w+1$. Then $P(B(2,2,h-2))-P(L(2,2,h-2))=(h-3)(w+1)^3\succ 0$, $P(L(2,2,h-2))-P(L(3,h-2))=(w+1)^2\succ 0$, $P(L(4,h-3))-P(L(2,2,h-2))=(h-7)(w+1)^2\succeq 0$ for $h\geq 7$. In addition, if $h=5$, $L(2,h-1)=L(4,h-3)$, and if $h=6$, $L(4,h-3)=L(3,h-2)$. Now it is not difficult to verify that $S_4=L(2,2,h-2)$ for $h\geq 5$. Since $P(L(3,2,h-3))-P(L(4,h-3))=2(w+1)^2\succ 0$, $P(B(2,2,h-2))-P(L(4,h-3))=((h-3)w+4)(w+1)^2\succ 0$, then $S_5=L(4,h-3)$ when $h\geq 7$. Since $P(B(2,2,h-2))-P(L(3,2,h-3))=(w+1)^2((h-3)w+2)\succ 0$, $P(L(5,h-4))-P(L(3,2,h-3))=(h-10)(w+1)^2\succeq 0$ for $h\geq 10$, then $S_6=L(3,2,h-3)$ when $h\geq 10$. □

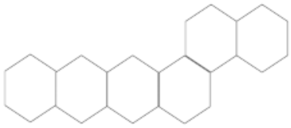


$P(L_6) = 6w+7$

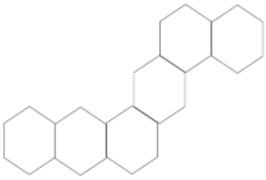


$P(L(5,2)) = 4w^2+14w+11$

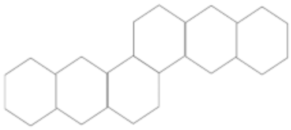
$P(L(4,3)) = 6w^2+18w+13$



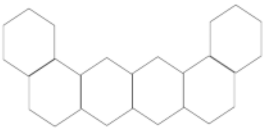
$P(L(4,2,2)) = 7w^2+20w+14$



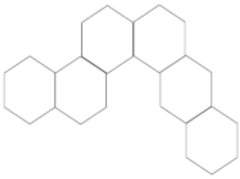
$P(L(3,3,2)) = 2w^3+14w^2+28w+17$



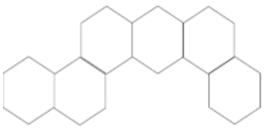
$P(L(3,2,3)) = 8w^2+22w+15$



$P(L(2,4,2)) = 2w^3+13w^2+26w+16$

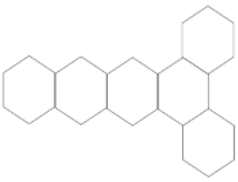


$P(L(2,2,2,3)) = 2w^3+15w^2+30w+18$



$P(L(2,2,3,2)) = w^3+18w^2+33w+19$

$P(L(2,2,2,2,2)) = 4w^3+22w^2+38w+21$



$P(B(2,2,4)) = 3w^3+16w^2+29w+17$

$P(B(2,3,3)) = 4w^3+20w^2+34w+19$

Fig. 7. Proof of Theorem 8.

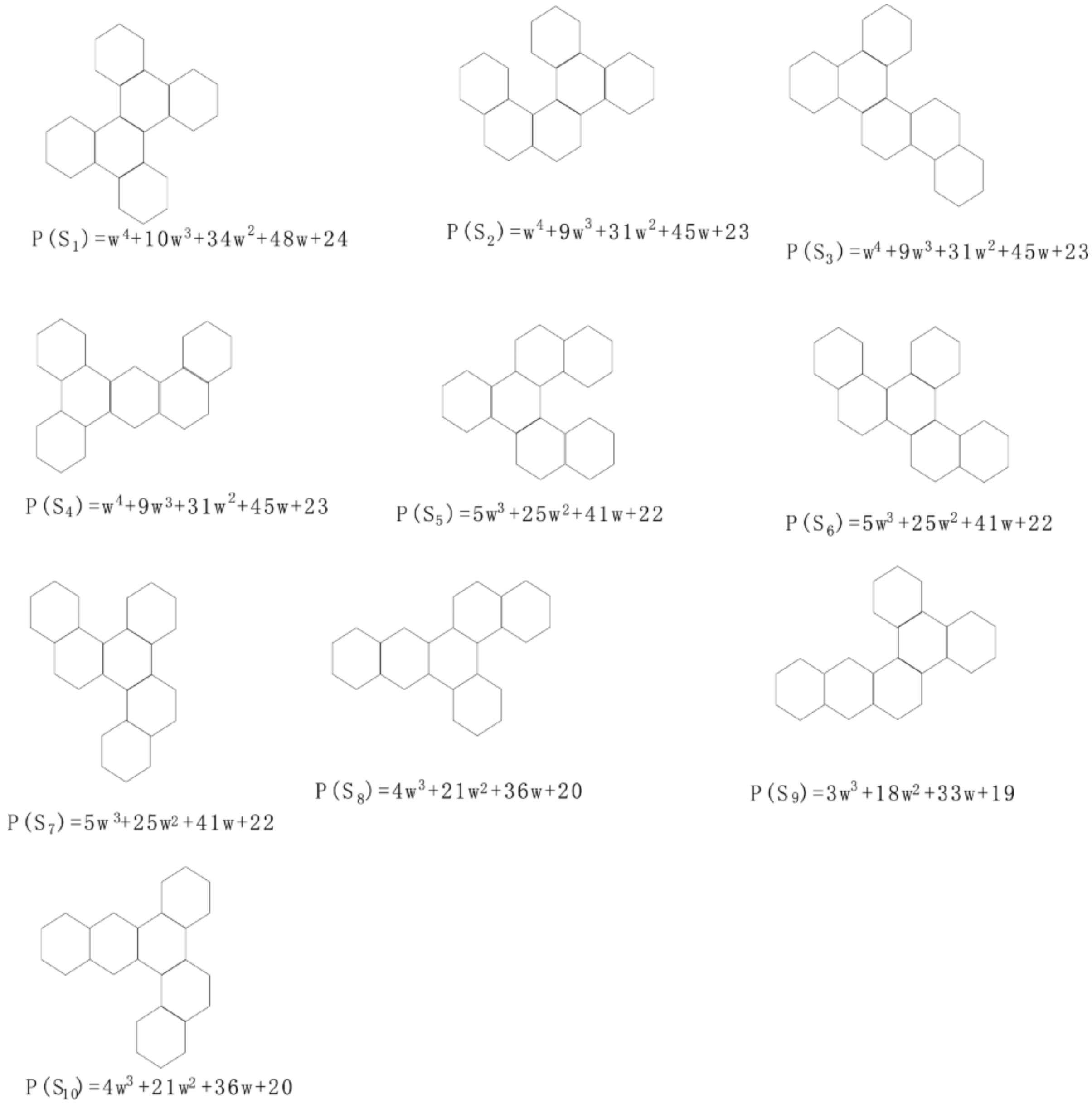


Fig. 7. Continued.

Now we turn to discuss the hexagonal chains with the maximum Clar covering polynomials. We mention the following results which will be useful for our results.

Theorem 5. *[14] A hexagonal chain H in $C'_h(h \geq 3)$ belong to B^*_h if and only if $H = c_1c_2\ldots c_h = \beta\theta_2\theta_3\ldots\theta_{h-1}$, where $\theta_j \in \{\alpha,\gamma\}$, $2 \leq j \leq h-1$.*

Theorem 6. *[16] Let H be a catacondensed hexagonal system, C be an M-alternating cycle in H. Then there exist an M-resonant hexagon in the interior of C.*

Theorem 7. *The hexagonal chain H in C'_h with the maximum Clar covering polynomial if and only if $H = c_1c_2\ldots c_h = \beta\theta_2\theta_3\ldots\theta_{h-1}$, where $\theta_j \in \{\alpha,\gamma\}$, $2 \leq j \leq h-1$.*

Proof. Let H be a hexagonal chain with the maximum Clar covering polynomial in C'_h. By the definition of $C(H)$ and Theorem 6, $C(H)$ is no more than the maximum number of disjoint cycles in H; $Z(H,i)$ is no more than the maximum number of i disjoint cycles in H for $i = 1,\dots,C(H)$. For $H_1 \in C'_h$, if H_1 is k^*-cycle resonant, then $C(H_1)$ is equal to the maximum number of disjoint cycles in H_1 and $Z(H_1,i)$ is equal to the maximum number of i disjoint cycles in H_1 for $i = 1,\dots,C(H_1)$. And for all hexagonal chains in C'_h, the maximum number of disjoint cycles and the maximum number of i disjoint cycles in them are all equal, respectively. Thus H_1 is a hexagonal chain with the maximum Clar covering polynomial in C'_h and a hexagonal chain H with the maximum Clar covering polynomial is k^*-cycle resonant. Combined Theorem 5, we have the above result. □

Let H_1 and H_2 be hexagonal systems. It is clear that $P(H_1) \succ P(H_2)$ is the sufficient condition for the fact that the number of perfect matching of H_1 is greater or equal to the number of perfect matching of H_2. We would like to propose the following question: Whether or not the sufficient condition is also necessary. Our results in this paper seem to support the positive answer. But it is not true even for the case of catacondensed hexagonal systems. For example, let H_1 and H_2 be catacondensed hexagonal systems (see Fig. 6). Then the number of perfect matching of H_1 is greater than the number of perfect matching of H_2, but $P(H_1)$ and $P(H_2)$ are incomparable. Furthermore, we prove the following:

Theorem 8. *The smallest pair of incomparable catacondensed hexagonal systems H_1 and H_2 with $z(H_1,0) > z(H_2,0)$ is unique and is shown in Figure 6.*

Proof. According to Table 1 in [2], there is no catacondensed hexagonal systems pair with less than six hexagons fulfilling the condition of Theorem 8. Now we need to consider all catacondensed hexagonal systems with six hexagons. In fact the catacondensed hexagonal systems with six hexagons are listed in [17]. By Lemmas 1 and 3, we computed their Clar covering polynomials and arranged them in Figure 7. Checking the Clar covering polynomials in this figure, we find that H_1 and H_2 are the only pair of catacondensed hexagonal systems fulfilling the condition of the theorem.

From Theorem 8, we can see that the quasi-ordering problem of hexagonal systems is harder than the ordering problem of hexagonal systems with respect to their number of Kekule structures.

Note that we only listed one hexagonal chain in $L(l_1,l_2,\dots,l_n)$ in Figure 7, since the Clar covering polynomial of the hexagonal chain $L(l_1,l_2,\dots,l_n)$ depends only on the sequence $(l_1,l_2,\dots,l_n)$ by [2] [Remark 4]. □

Acknowledgement

The Project Supported by the National Natural Science Foundation of China (Grant No. 10831001, 11171134), the Natural Science Foundation of Fujian Province (Grant No. 2011J01015), and the Science Research Foundation of Jimei University, China.

[1] I. Gutman, Bull. Soc. Chim. Beograd **47**, 453 (1982).
[2] H. Zhang and F. Zhang, Discr. Appl. Math. **69**, 147 (1996).
[3] F. Zhang, H. Zhang, and Y. Liu, Chin. J. Chem. **14**, 321 (1996).
[4] H. Zhang, MATCH Commun. Math. Comput. Chem. **29**, 189 (1993).
[5] H. Zhang, Discr. Math. **172**, 163 (1997).
[6] H. Zhang and F. Zhang, Discr. Math. **212**, 261 (2000).
[7] I. Gutman and B. Borouicnin, Z. Naturforsch. **61a**, 73 (2006).
[8] I. Gutman, B. Furtula, and A. T. Balaban, Polyc. Arom. Comp. **26**, 17 (2006).
[9] I. Gutman, S. Gojak, and B. Furtula, Chem. Phys. Lett. **413**, 396 (2005).
[10] I. Gutman, S. Gojak, S. Radenkovic, and A. Vodopivec, J. Serb. Chem. Soc. **72**, 673 (2007).
[11] I. Gutman, S. Gojak, S. Radenkovic, and A. Vodopivec, Monatsh. Chem. **137**, 1127 (2006).
[12] I. Gutman, S. Gojak, S. Stankovic, and B. Furtula, J. Mol. Struct. (Theochem) **757**, 119 (2005).
[13] S. Gojak, I. Gutman, S. Radenkovic, and A. Vodopivec, J. Serb. Chem. Soc. **72**, 665 (2007).
[14] X. Guo and F. Zhang, Discr. Math. **69**, 147 (1996).
[15] L. Zhang, The extreme and ordering problems of regular polygon chains, Ph.D. thesis, Sicuan University, Chengdu, Sicuan, China 1999.
[16] H. Zhang and F. Zhang, Discr. Appl. Math. **105**, 291 (2000).
[17] J. Knop, W. Muller, K. Szymanski, and N. Trinajstic, Computer Generation of Certain Classes of Molecules, Editions Kemija u industriji, Zagreb 1985.