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Zhang-Zhang Polynomials of a Class of Pericondensed Benzenoid Graphs[1]

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Abstract

The Zhang-Zhang polynomial of hexagonal systems is introduced by H. Zhang and F. Zhang, which can be used to calculate many important invariants such as the Clar number, the number of Kekulé structures and the first Herndon number, etc. In this paper, we give out an explicit expression for the Zhang-Zhang polynomials of a class of pericondensed benzenoid graphs, and determine their numbers of Kekulé structures and Clar formulas, their Clar numbers and their first Herndon numbers.

1 Introduction

Various topological properties of hexagonal systems were extensively treated by mathematicians and chemists, since a hexagonal system with perfect matchings is the skeleton of a benzenoid hydrocarbon molecule. Here, a hexagonal system is a 2-connected plane graph whose every interior face is bounded by a regular hexagon of unit length. The interested reader may refer to books [1-3].

In the theoretical chemistry of benzenoid hydrocarbons, the Kekulé structure, Kekulé number, Clar number and the number of Clar formulas are very important. It is pointed out in [4] that the Clar number of benzenoid systems (or plane bipartite graphs) can be calculated in linear program. And counting the number of Clar formulas of large benzenoids is an equally perplexing problem [5-7]. Nowadays it is

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known how to compute the numbers of Kekulé structures, Clar formulas and the Clar numbers, but each of these theoretical characteristics of a benzenoid molecule would have to be determined by a separate algorithm [6,8]. In 1996, the Chinese mathematicians Heping Zhang and Fuji Zhang introduced a combinatorial polynomial (i.e., the Clar covering polynomial of hexagonal systems) in the mathematical literature [9-11], from which Kekulé number, Clar number, the number of Clar formulas and the sextet polynomial, can be directly deduced, and which can be computed by an easy recursive technique. Therefore, it is also called Zhang-Zhang polynomial [12] and has become aware of its numerous chemical applications [10-17].

Recently, Gutman and Borovićanin [18] obtained an explicit combinatorial expression for the Clar covering polynomial of the multiple linear hexagonal chains $M_{n;m}$. Guo, Deng and Chen [19] gave out an explicit recurrence expression for the Zhang-Zhang polynomials of the cyclo-polyphenacenes.

In this paper, we will consider the Zhang-Zhang polynomials of a class of pericondensed benzenoid graphs consisting of three rows of hexagons of various lengths (in a chemical language, a subclass of pericondensed benzenoid), which was introduced by Vukičević and Trinajstić. They [20] obtained formulae for Wiener indices of these chemical graphs. Deng and Chen [21], Ashrafi and Loghman [22] calculated the PI indices of these chemical graphs. Here we continue this study to calculate the Zhang-Zhang polynomials of these chemical graphs with Kekulé structures, and obtain the Clar number, the number of Kekulé structures and the first Herndon number.

2 Definitions and basic results

Let H be a hexagonal system with perfect matchings. A Clar cover C of H is a spanning subgraph of H, each component of which is either a hexagon or an edge. $h(C)$ is the number of hexagons of C and $\sigma(H) = \max\{h(C)|C \text{ is a Clar cover of } H\}$. $\sigma(H)$ is called the Clar number of H. The Zhang-Zhang polynomial [8] of H is defined as

$$P(H,w) = \sum_{i=0}^{\sigma(H)} \sigma(H,i)w^i,$$

where $\sigma(H,i)$ is the number of Clar covers having precisely i hexagons and w is an indeterminate or weight associated with hexagons of H.

Let H be a benzenoid system with Kekulé structures. A sextet pattern or Clar pattern of H is a set of disjoint hexagons such that the remainder of the benzenoid system obtained by deleting the vertices of these hexagons must have a Kekulé structure or must be empty. A set of Clar aromatic sextets is said to be a Clar formula if it has the maximum number (i.e., the Clar number) of hexagons. Clar's theory [23] asserts that for two benzenoid systems H_1 and H_2, if the Clar number of H_1 is greater than that of H_2, then H_1 is more stable.

The Zhang-Zhang ploynomial has the following basic properties ([4,5]):

(1) The coefficient $\sigma(H,0)$ is equal to the number of Kekulé structures, $K(H)$;

(2) The power of $P(H,w)$ is equal to the Clar number $\sigma(H)$;

(3) The coefficient of the highest degree term, $\sigma(H,\sigma(H))$ equals the number of Clar formulas of H;

(4) $\sigma(H,1) = h_1(H)$, where $h_1(H) = \sum\limits_{s} K(H-s)$ is the first Herndon number ([12]) of H, the summation goes over all the hexagons s of H.

Vukičević and Trinajstić [20] obtained formulae for Wiener indices of a class of pericondensed benzenoid graphs consisting of three linear hexagonal chains with lengths n_1, n_2, n_3, respectively. They introduced the graph $G(n_1,n_2,n_3)$ to be the pericondensed benzenoid graph given by Figure 1, in which n_1 is a positive integer and n_2, n_3 are non-negative integers. In the case that $n_3 = 0$, we denote this graph by $G(n_1,n_2)$ consisting of two linear hexagonal chains with lengths n_1, n_2, respectively, in Figure 2. Note that not all graphs $G(n_1,n_2,n_3)$ and $G(n_1,n_2)$ have Kekulé structure. We now give the conditions for $G(n_1,n_2,n_3)$ and $G(n_1,n_2)$ with Kekulé structure.

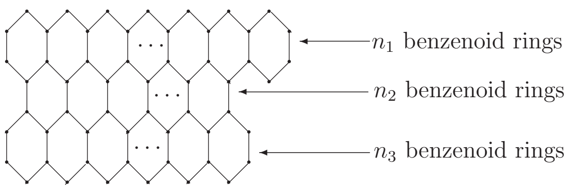

Figure 1. The graph $G(n_1,n_2,n_3)$.

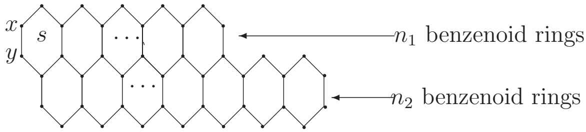

Figure 2. The graph $G(n_1, n_2)$ with $n_2 \geq n_1$.

For the graph $G(n_1, n_2)$, if $n_1 > n_2$, then the number of vertices of $G(n_1, n_2)$ is odd and $G(n_1, n_2)$ has no Kekulé structure; If $n_1 \leq n_2$, then a path with odd length is obtained by deleting n_2 hexagons in the same row, and $G(n_1, n_2)$ has a Kekulé structure. So, we have

Lemma 1. $G(n_1, n_2)$ has a Kekulé structure if and only if $n_1 \leq n_2$.

For the graph $G(n_1, n_2, n_3)$, if $n_2 \geq \max\{n_1, n_3\}$, then two paths with odd length are obtained by deleting n_2 hexagons in the middle row, and $G(n_1, n_2, n_3)$ has a Kekulé structure; If $n_2 < \min\{n_1, n_3\}$, then two linear chains with n_1 and n_3 hexagons, respectively, are obtained by deleting $n_2 + 1$ edges in the middle, and $G(n_1, n_2, n_3)$ has a Kekulé structure; Otherwise, the number of vertices of $G(n_1, n_2, n_3)$ is odd and $G(n_1, n_2, n_3)$ has no Kekulé structure. So, we have

Lemma 2. $G(n_1, n_2, n_3)$ has a Kekulé structure if and only if $n_2 \geq \max\{n_1, n_3\}$ or $n_2 < \min\{n_1, n_3\}$.

3 The Zhang-Zhang polynomials of $G(n_1, n_2)$ and $G(n_1, n_2, n_3)$ with Kekulé structures

In this section, we study the Zhang-Zhang polynomials of the pericondensed benzenoid graphs $G(n_1, n_2)$ and $G(n_1, n_2, n_3)$ with Kekulé structures. The following basic lemmas will be used in calculating the Zhang-Zhang polynomials.

Lemma 3([9]). Let H be a generalized hexagonal system. Assuming that xy is an edge of a hexagon s of H which lies on the periphery of H, then

$$P(H, w) = wP(H - s, w) + P(H - x - y, w) + P(H - xy, w).$$

Lemma 4([9]). Let L_m denote a linear hexagonal chain with $m \geq 0$ hexagons. Then

$$P(L_m, w) = mw + (m+1).$$

Theorem 5. Let $n_2 \geq n_1$. Then

(i) $P(G(n_1,n_2),w) = (n_1n_2 - \frac{1}{2}n_1^2 - \frac{1}{2}n_1)w^2 + (2n_1n_2 - n_1^2 + n_2)w + (n_1n_2 - \frac{1}{2}n_1^2 + n_2 + \frac{1}{2}n_1 + 1)$;

(ii) the number of Kekulé structures of $G(n_1,n_2)$ is $K(G(n_1,n_2)) = n_1n_2 - \frac{1}{2}n_1^2 + n_2 + \frac{1}{2}n_1 + 1$;

(iii) the first Herndon number of $G(n_1,n_2)$ is $h_1(G(n_1,n_2)) = 2n_1n_2 - n_1^2 + n_2$;

(iv) the Clar number of $G(n_1,n_2)$ is $\sigma(G(n_1,n_2)) = 2$;

(v) the number of Clar formulas of $G(n_1,n_2)$ is $\sigma(G(n_1,n_2),2) = n_1n_2 - \frac{1}{2}n_1^2 - \frac{1}{2}n_1$.

Proof. (i) From Lemma 1, $G(n_1,n_2)$ has a Kekulé structure since $n_2 \geq n_1$. Let s be the upper left-most hexagon and xy the upper left-most vertical edge, see Figure 2. Using Lemmas 3-4, we have the following recurrence relation

$$\begin{aligned}
& P(G(n_1,n_2),w) \\
= \; & wP(G(n_1,n_2)-s,w) + P(G(n_1,n_2)-x-y,w) \\
& +P(G(n_1,n_2)-xy,w) \\
= \; & wP(L_{n_2-1},w) + P(L_{n_2},w) + P(G(n_1-1,n_2-1),w) \\
= \; & (n_2-1)w^2 + 2n_2w + (n_2+1) + P(G(n_1-1,n_2-1),w)
\end{aligned}$$

with the initial condition

$$P(G(n_1-n_2,0),w) = P(L_{n_1-n_2},w) = (n_1-n_2)w + n_1 - n_2 + 1.$$

It can give out the result (i).

(ii)-(v) follow the basic properties of Zhang-Zhang polynomial and (i).

Remark. (i) If $n_1 = n_2 = n$, then $G(n_1,n_2) = G(n,n)$ is a double linear hexagonal chain, and

$$P(G(n,n),w) = \frac{1}{2}(n^2-n)w^2 + (n^2+n)w + \frac{1}{2}(n^2+3n+2);$$

(ii) If $n_1 = 0$ and $n_2 = n$, then $G(n_1, n_2) = G(0, n) = L_n$ is a linear hexagonal chain, and

$$P(G(0,n), w) = nw + (n+1).$$

These results are the same as in [18] and [9], respectively.

For the pericondensed benzenoid graph $G(n_1, n_2, n_3)$, we have $G(n_1, n_2, n_3) \cong G(n_3, n_2, n_1)$. In the following, we may assume $n_1 \geq n_3$.

Theorem 6. If $n_2 \geq n_1 \geq n_3$, then

(i) $P(G(n_1, n_2, n_3), w) = (1 + \frac{1}{2}n_1 - \frac{1}{2}n_1^2 + n_2 + n_1n_2 + \frac{2}{3}n_3 + \frac{1}{2}n_1n_3 - \frac{1}{2}n_1^2n_3 + n_2n_3 + n_1n_2n_3 - \frac{1}{2}n_3^2 - \frac{1}{6}n_3^3) + (-n_1^2 + n_2 + 2n_1n_2 + \frac{1}{2}n_3 + \frac{1}{2}n_1n_3 - \frac{3}{2}n_1^2n_3 + 2n_2n_3 + 3n_1n_2n_3 - n_3^2 - \frac{1}{2}n_3^3)w + (-\frac{1}{2}n_1 - \frac{1}{2}n_1^2 + n_1n_2 - \frac{1}{2}n_1n_3 - \frac{3}{2}n_1^2n_3 + n_2n_3 + 3n_1n_2n_3 - \frac{1}{2}n_3^2 - \frac{1}{2}n_3^3)w^2 + (\frac{1}{6}n_3 - \frac{1}{2}n_1n_3 - \frac{1}{2}n_1^2n_3 + n_1n_2n_3 - \frac{1}{6}n_3^3)w^3$;

(ii) the number of Kekulé structures of $G(n_1, n_2, n_3)$ is $K(G(n_1, n_2, n_3)) = 1 + \frac{1}{2}n_1 - \frac{1}{2}n_1^2 + n_2 + n_1n_2 + \frac{2}{3}n_3 + \frac{1}{2}n_1n_3 - \frac{1}{2}n_1^2n_3 + n_2n_3 + n_1n_2n_3 - \frac{1}{2}n_3^2 - \frac{1}{6}n_3^3$;

(iii) the first Herndon number of $G(n_1, n_2, n_3)$ is $h_1(G(n_1, n_2, n_3)) = -n_1^2 + n_2 + 2n_1n_2 + \frac{1}{2}n_3 + \frac{1}{2}n_1n_3 - \frac{3}{2}n_1^2n_3 + 2n_2n_3 + 3n_1n_2n_3 - n_3^2 - \frac{1}{2}n_3^3$;

(iv) the Clar number of $G(n_1, n_2, n_3)$ is $\sigma(G(n_1, n_2, n_3)) = 3$;

(v) the number of Clar formulas of $G(n_1, n_2)$ is $\sigma(G(n_1, n_2, n_3), 3) = \frac{1}{6}n_3 - \frac{1}{2}n_1n_3 - \frac{1}{2}n_1^2n_3 + n_1n_2n_3 - \frac{1}{6}n_3^3$.

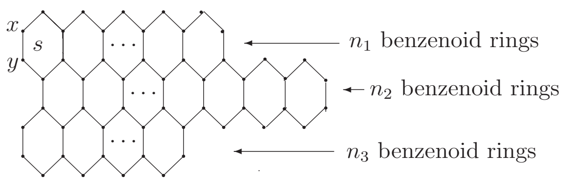

Figure 3. The graph $G(n_1, n_2, n_3)$ with $n_2 \geq \max\{n_1, n_3\}$.

Proof. (i) From Lemma 2, $G(n_1, n_2, n_3)$ has a Kekulé structure since $n_2 \geq$

$\max\{n_1, n_3\}$. Let s be the upper left-most hexagon and xy the upper left-most vertical edge, see Figure 3. Then $P(G(n_1, n_2, n_3) - s, w) = P(G_1, w)$, $P(G(n_1, n_2, n_3) - xy, w) = P(G_2, w)$, $P(G(n_1, n_2, n_3) - x - y, w) = P(G(n_3, n_2), w)$, where G_1 and G_2 are shown in Figure 4.

Using Lemma 3, we have the following recurrence relation

$$\begin{aligned}
& P(G(n_1, n_2, n_3), w) \\
= \; & wP(G(n_1, n_2, n_3) - s, w) + P(G(n_1, n_2, n_3) - xy, w) \\
& + P(G(n_1, n_2, n_3) - x - y, w) \\
= \; & wP(G_1, w) + P(G_2, w) + P(G(n_3, n_2), w) \\
= \; & w[wP(G_1 - s', w) + P(G_1 - x' - y', w) + P(G_1 - x'y', w)] \\
& + [wP(G_2 - s'', w) + P(G_2 - x'' - y'', w) + P(G_2 - x''y'', w)] \\
& + P(G(n_3, n_2), w) \\
= \; & w[wP(L_{n_2-1}, w) + P(L_{n_2-1}, w) + P(G(n_3 - 1, n_2 - 1), w)] \\
& + [wP(G(n_1 - 1, n_2 - 1), w) + P(G(n_1 - 1, n_2 - 1), w) \\
& + P(G(n_1 - 1, n_2 - 1, n_3 - 1), w)] + P(G(n_3, n_2), w) \\
= \; & (w+1)^2 P(L_{n_2-1}, w) + (w+1)P(G(n_1 - 1, n_2 - 1), w) \\
& + (w+1)P(G(n_3 - 1, n_2 - 1), w) + (w+1) \\
& + P(G(n_1 - 1, n_2 - 1, n_3 - 1), w) \\
= \; & (1 + \tfrac{1}{2}n_1 - \tfrac{1}{2}n_1^2 + n_2 + n_1 n_2 + \tfrac{1}{2}n_3 + n_2 n_3 - \tfrac{1}{2}n_3^2) \\
& + (\tfrac{1}{2}n_1 - \tfrac{3}{2}n_1^2 + n_2 + 3n_1 n_2 + \tfrac{1}{2}n_3 + 3n_2 n_3 - \tfrac{3}{2}n_3^2)w \\
& + (-\tfrac{1}{2}n_1 - \tfrac{3}{2}n_1^2 - n_2 + 3n_1 n_2 - \tfrac{1}{2}n_3 + 3n_2 n_3 - \tfrac{3}{2}n_3^2)w^2 \\
& + (1 - \tfrac{1}{2}n_1 - \tfrac{1}{2}n_1^2 - n_2 + n_1 n_2 - \tfrac{1}{2}n_3 + n_2 n_3 - \tfrac{1}{2}n_3^2)w^3 \\
& + P(G(n_1 - 1, n_2 - 1, n_3 - 1), w)
\end{aligned}$$

with the initial condition

$$\begin{aligned}
& P(G(n_1 - n_3, n_2 - n_3, 0), w) = P(G(n_1 - n_3, n_2 - n_3), w) \\
= \; & (1 + \tfrac{1}{2}n_1 - \tfrac{1}{2}n_1^2 + n_2 + n_1 n_2 - \tfrac{3}{2}n_3 - n_2 n_3 + \tfrac{1}{2}n_3^2) \\
& + (-n_1^2 + n_2 + 2n_1 n_2 - n_3 - 2n_2 n_3 + n_3^2)w \\
& + (-\tfrac{1}{2}n_1 - \tfrac{1}{2}n_1^2 + n_1 n_2 + \tfrac{1}{2}n_3 - n_2 n_3 + \tfrac{1}{2}n_3^2)w^2.
\end{aligned}$$

It can give out the result (i).

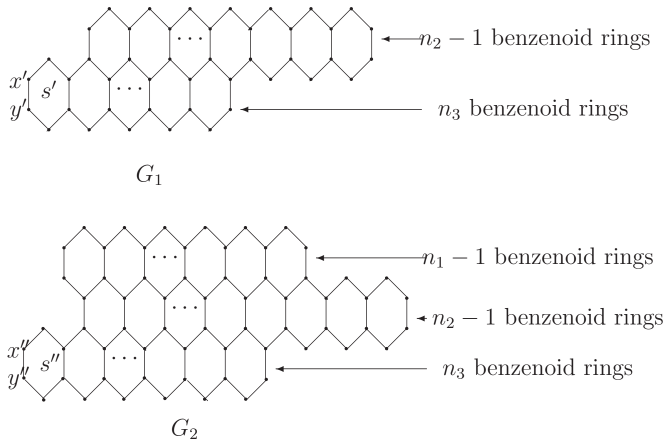

Figure 4. The graphs G_1 and G_2.

(ii)-(v) follow the basic properties of Zhang-Zhang polynomial and (i).

Theorem 7. Let $n_2 < \min\{n_1, n_3\}$. Then

(i) $P(G(n_1, n_2, n_3), w) = (1 + n_1 + n_3 + n_1n_3) + (n_1 + n_3 + 2n_1n_3)w + n_1n_3w^2$;

(ii) the number of Kekulé structures of $G(n_1, n_2, n_3)$ is $K(G(n_1, n_2, n_3)) = 1 + n_1 + n_3 + n_1n_3$;

(iii) the first Herndon number of $G(n_1, n_2, n_3)$ is $h_1(G(n_1, n_2, n_3)) = 1 + 2n_1 + 2n_3 + 4n_1n_3$;

(iv) the Clar number of $G(n_1, n_2, n_3)$ is $\sigma(G(n_1, n_2, n_3)) = 2$;

(v) the number of Clar formulas of $G(n_1, n_2)$ is $\sigma(G(n_1, n_2, n_3), 2) = n_1n_3$.

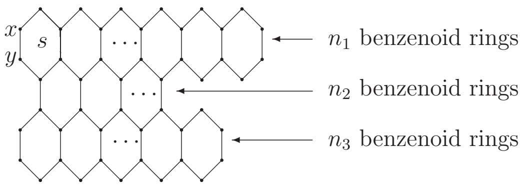

Figure 5. The graph $G(n_1, n_2, n_3)$ with $n_2 < \min\{n_1, n_3\}$

Proof. (i) Since the middle vertical edges in $G(n_1, n_2, n_3)$ are fixed single edges (i.e., do not belong to any Kekulé structure) for $n_2 < \min\{n_1, n_3\}$, we have

$P(G(n_1, n_2, n_3), w) = P(L_{n_1}, w)P(L_{n_3}, w)$ by Theorem 3 in [9], and the result is immediate.

Acknowledgement

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