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Zhang–Zhang polynomials of cyclo-polyphenacenes

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Abstract The Zhang–Zhang polynomial (i.e., Clar covering 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 recurrence expression for the Zhang–Zhang polynomials of the cyclo-polyphenacenes, and determine their Clar numbers, numbers of Kekulé structures and their first Herndon numbers.

Keywords Zhang–Zhang polynomial · Clar covering polynomial · Kekulé structure · Clar number · Herndon number · Cyclo-polyphenacene

1 Introduction

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

In the theoretical chemistry of benzenoid hydrocarbons, one of important directions is Kekulé structures and Kekulé number. Scores of papers report results on the calculation of Kekulé number, both in the general case and for special classes of benzenoid systems; for details on this matter see the book [1] and the references quoted therein.

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Another important direction is the diagrammatic approach put forward by Clar [4]. The number of aromatic sextets in (any of the) Clar formulas of a benzenoid system is said to be its Clar number. It is pointed out in [5] that determining the value of Clar number in the case of large benzenoid systems may be a rather difficult task. And counting the number of Clar formulas of large benzenoids is an equally perplexing problem [6–8], and a pertinent algorithm for this purpose was put forward by Randić and El-Basil [7]. Hosoya and Yamaguchi introduced a significant concept in Clar theory-the sextet polynomial [9]. In these papers it is known how to compute Kekulé number, Clar number, the number of Clar formulas and the sextet polynomial, but each of these theoretical characteristics of a benzenoid molecule would have to be determined by a separate algorithm. 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 [10–12], 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 [13] and has become aware of its numerous chemical applications. An application to S,T-isomers can been found in [14]. In [11], they established a relation between Zhang–Zhang polynomial and sextet polynomial of hexagonal systems. In [12], Zhang further studied the relation between Zhang–Zhang polynomials of hexagonal systems and the chromatic polynomial.

In a series of papers [5,13,15–18], Gutman and his co-workers showed that Zhang–Zhang polynomial $P(w)$ of benzenoid hydrocarbons is related to resonance energy (RE), and that ln $P(w)$ and RE are best correlated when $w = 1$. This indicates that $P(1)$ could be viewed as a novel structure-descriptor, playing a role analogous to the Kekulé structure count in Kekulé-structure-based theories. They also showed that there are some significant differences between the structure-dependencies of Dewar-type resonance energy (DRE) and topological resonance energy (TRE). In particular, in the case of benzenoid molecules, DRE and TRE are found to be linearly related to ln $P(0)$ and ln $P(1)$, respectively. It was shown that there is a remarkable difference between the Kekulé-and Clar-structure-dependence of the total π-electron energy of catafusenes and perifusenes (catacondensed and pericondensed benzenoid molecules) by using the Zhang–Zhang polynomial.

Recently, Gutman and Borouićanin [19] obtained an explicit combinatorial expression for the Zhang–Zhang polynomial of the multiple linear hexagonal chains $M_{n;m}$. Zhou et al. [20] obtained the Zhang–Zhang polynomials of some hexagonal systems by constructing Clar covers without alternating hexagons.

After the discovery of carbon nanotube [21], the nonplane compounds with condensed benzene rings became an attractive topic for chemists and physicians, since it is expect that the carbon nanotube as an artificial material has nice electrical conductivity and strength. Stimulated by this fact, many researchers considered the tubulene [22–24]. The carbon skeleton of a tubulene is a benzenoid system embedded in a cylinder with two open ends (all its dangling bonds at both ends saturated with hydrogen atoms). One of the simplest tubulenes is said to be cyclo-polyphenacenes (a wide type of molecules including prim tubulenes and prim coronenes) which can be considered as a hexagonal chains embedded around a cylinder.

For the cyclo-polyphenacenes with small number of hexagons, many results are obtained by Dobrowolski [25], Hook et al. [26], Choi and Kim [27] and Turker [28] which could be a useful aid in the broader field of chemistry in the future. Another approach is to study the cyclo-polyphenacenes by using some invariant. For example, Misra and Klein [29] considered the case of cyclo-polyphenacenes with arbitrary number of hexagons and introduced the invariant combinatorial curvature and studied its plausible relation to structural stresses, as manifested in thermodynamic stability. Also, in order to compare the stability of the cyclo-polyphenacenes, Wang et al. [30] introduced a new quasiodering to rank the cyclo-polyphenacenes with respect to their number of Clar aromatic sextets.

In this paper, we will consider the Zhang–Zhang polynomial of the cyclo-polyphenacenes. We will give out an explicit recurrence expression for the Zhang–Zhang polynomial of the cyclo-polyphenacenes, 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. Let $h(C)$ denote the number of hexagons of C and $\sigma(H) = \max\{h(C) | C \text{is a Clar covering of} H\}$. $\sigma(H)$ is called the Clar number of H. The Zhang–Zhang polynomial (or Clar covering polynomial) [12] of H is defined as

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

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

Now we recall the concept in Clars aromatic sextet theory [4]. Let H be a benzenoid system with Kekulé structures (perfect matching). A Clar aromatic sextet (or a sextet 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. Clars theory 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. Since many isomers of benzenoid chains have the same Clar number, the accuracy is not enough to order the benzenoid chains (in general) with respect to their Clar numbers. Hosoya and Yamaguchi (see [9] and the excellent survey in [31, p. 255]) introduced the following sextet polynomial for benzenoid systems

$$S(H, x) = \sum_{i=0}^{\sigma(H)} s(H, i) x^i,$$

where $s(H, i)$ is the number of Clar aromatic sextets of H having i hexagons and $s(H, 0) = 1$.

Some basic properties of the Zhang–Zhang polynomial are the following ([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 $h_1(H) = \sum_s K(H - s)$ is the first Herndon number ([32]) of H, the summation goes over all the hexagons of H and $H - s$.

3 Cyclo-polyphenacenes

The cyclo-polyphenacenes (or cyclic hexagonal chain) can be obtained by identifying two edges in two end hexagons respective where each hexagon is adjacent to exactly two hexagons. In this section we will use the lengths of its maximal linear hexagonal chains to represent the cyclo-polyphenacenes and the graph (i.e., cyclic hexagonal chain) corresponding to its carbon skeleton. For the sake of brevity, we do not distinguish a cyclo-polyphenacene, its carbon skeleton and its graph.

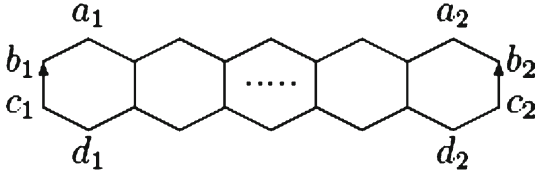
A maximal linear hexagonal chain in a cyclic hexagonal chain C is called a segment of C. The number of hexagons in a segment is called its length, and a cyclic hexagonal chain can be denoted by $C(r_1, r_2, \ldots, r_t)$, where r_i is the length of the ith segment, $2 \le r_i \le n$, $i = 1, 2, \ldots, t$, n is the number of hexagons. Since any segment can be chosen as the first, we have

$$C(r_1, r_2, \ldots, r_t) \cong C(r_2, r_3, \ldots, r_t, r_1) \cong \cdots \cong C(r_t, r_1, r_2, \ldots, r_{t-1}).$$

Let $C(r_1, r_2, \ldots, r_t)$ be a cyclic hexagonal chain with n hexagons, then $r_i \ge 2$ and $r_1 + r_2 + \cdots + r_t = n + t$. If $t = 1$, the cyclic hexagonal chain is called a linear cyclic hexagonal chain (i.e., the carbon skeleton (graph) of a cyclo-polyacene). Just identifying the edge b_1c_1 with the edge b_2c_2 will get it, see Fig. 1.

If $r_1 = r_2 = \cdots = r_t = 2$, $t \ge 3$, the cyclic hexagonal chain $C(2, 2, \ldots, 2)$ is called a zigzag cyclic hexagonal chain (a wide type of molecules including cyclo-polyphenathrenes), see Fig. 2.

Fig. 1 A linear hexagenal chain



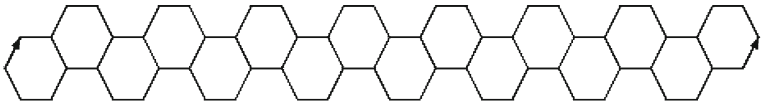


Fig. 2 A zigzag cyclic hexagonal chain $C(2, 2, 2, 2, 2, 2, 2, 2,)$ i.e., the carbon skeleton (graph) of a cyclo-polyphenathrene

4 The Zhang–Zhang polynomials of cyclo-polyphenacenes

In this section, we study the Zhang–Zhang polynomials of cyclo-polyphenacenes. The following lemmas will be used in calculating the Zhang–Zhang polynomials of cyclo-polyphenacenes.

Lemma 4.1 ([10]) *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 (see Fig. 3), then*

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

Lemma 4.2 ([10]) *Let H be a generalized hexagonal system, and xy be an edge not belonging to any hexagon of H (see Fig. 4), then*

$$P(H) = P(H - x - y) + P(H - xy).$$

Like the cyclic hexagonal, we use $L(r_1, r_2, \ldots, r_t)$ denote the hexagonal chain with t segments (i.e., maximal linear hexagonal chains) of lengths $r_1, r_2, \ldots, r_t$, respectively. Without danger of confusion we also use $L(r_1, r_2, \ldots, r_t)$ denote its Zhang–Zhang polynomial.

Lemma 4.3 ([10]) *If $t \geq 2$, then*

$$\begin{aligned} L(r_1, r_2, \ldots, r_t) &= L(r_1, r_2, \ldots, r_{t-1}) + (r_t - 1)(w + 1)L(r_1, r_2, \ldots, r_{t-1} - 1) \\ &= L(r_2, r_3, \ldots, r_t) + (r_1 - 1)(w + 1)L(r_2 - 1, r_3, \ldots, r_t). \end{aligned}$$

Fig. 3 The graph in Lemma 4.1

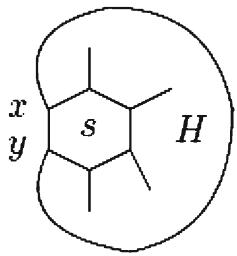
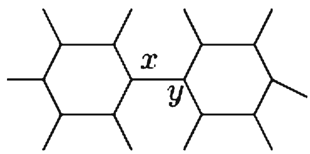


Fig. 4 The graph in Lemma 4.2



Lemma 4.4 ([10]) *If $t \geq 3$, then*

$$L(r_1, r_2, \ldots, r_t) = \left[(r_t - 1)w + r_t - \frac{r_t - 1}{r_{t-1} - 1}(w+1)\right] L(r_1, r_2, \ldots, r_{t-1}) + \frac{r_t - 1}{r_{t-1} - 1}(w+1) L(r_1, r_2, \ldots, r_{t-2}),$$

where $L(r_1) = r_1 w + r_1 + 1$, $L(r_1, r_2) = [(r_1 - 1)w + r_1][(r_2 - 1)w + r_2] + w + 1$.

Applying the above Lemma 4.3 and Lemma 4.4, we immediately have

Corollary 4.1

$$L(r_1, r_2, \ldots, r_{t-1} - 1) = \frac{r_{t-1} - 2}{r_{t-1} - 1} L(r_1, r_2, \ldots, r_{t-1}) + \frac{1}{r_{t-1} - 1} L(r_1, r_2, \ldots, r_{t-2}).$$

Lemma 4.5 ([10]) *For all $t \geq 3$,*

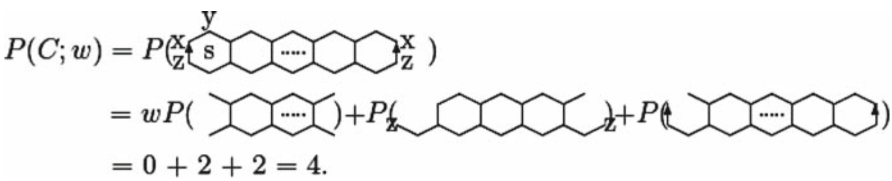
(i) $K(L(r_1, r_2, \ldots, r_t)) = \left(r_t - \frac{r_t - 1}{r_{t-1} - 1}\right) K(L(r_1, r_2, \ldots, r_{t-1})) + \frac{r_t - 1}{r_{t-1} - 1} K(L(r_1, r_2, \ldots, r_{t-2}))$,
with initial conditions $K(L(r_1)) = r_1 + 1$ and $K(L(r_1, r_2)) = r_1 r_2 + 1$;

(ii) $h_1(L(r_1, r_2, \ldots, r_t)) = \left(r_t - \frac{r_t - 1}{r_{t-1} - 1}\right) h_1(L(r_1, r_2, \ldots, r_{t-1})) + \frac{r_t - 1}{r_{t-1} - 1} \times h_1(L(r_1, r_2, \ldots, r_{t-2})) + (K(L(r_1, r_2, \ldots, r_t)) - K(L(r_1, r_2, \ldots, r_{t-1})))$,
with initial conditions $h_1(L(r_1)) = r_1$ and $h_1(L(r_1, r_2)) = 2r_1 r_2 - r_1 - r_2 + 1$.

4.1 The linear cyclic hexagonal chains

Theorem 4.1 *Let C be a linear cyclic hexagonal chains with n hexagons, $n \geq 3$. Then $P(C; w) = 4$.*

Proof of Theorem 4.1 By Lemmas 4.1 and 4.2,



□

From the basic properties of the Zhang–Zhang polynomial, we have

Corollary 4.2 *Let C be a linear cyclic hexagonal chain, then*

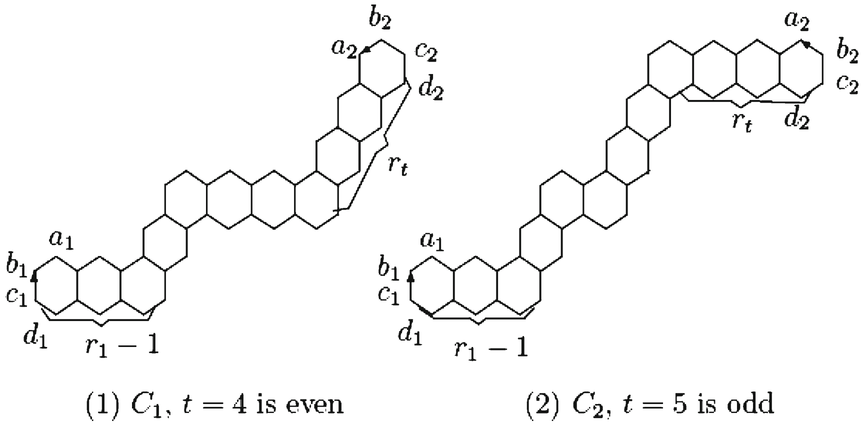


Fig. 5 Two cyclic hexagonal chains

(i) *the number of Kekulé structures of C is* $K(C) = 4$;
(ii) *the number of Clar formulas of C is* $\sigma(C, \sigma(C)) = 0$, *where* $\sigma(C) = 0$;
(iii) *the first Herndon number of C is* $h_1(C) = 0$.

4.2 The cyclic hexagonal chains with at least two segments

Let $C(r_1, r_2, \ldots, r_t)$ *be a cyclic hexagonal chain with at least two segments (i.e.,* $t \geq 2$*). Then it can be obtained from the hexagonal chain* $L(r_1 - 1, r_2, \ldots, r_t)$ *by identifying the edge* b_1c_1 *with the edge* a_2b_2 *(or* c_2d_2*), see Fig. 5.*

First, we consider the non-zigzag cyclic hexagonal chain. If $C(r_1, r_2, \ldots, r_t)$ $(t \geq 2)$ *is not a zigzag cyclic hexagonal chain, then there exits a* $r_i \geq 3$, $1 \leq i \leq t$. *Without loss of generality, we always assume that* $r_t \geq 3$.

Theorem 4.2 *Let* $C(r_1, r_2, \ldots, r_t)$ *be a cyclic hexagonal chains with n hexagons and* $r_t \geq 3$.

(i) *If* $t \geq 2$ *is even, then*

$$\begin{aligned} C(r_1, r_2, \ldots, r_t) = & \left[\frac{(r_t - 2)w + r_t - 3}{r_{t-1} - 1} + 1\right] L(r_1 - 1, r_2, \ldots, r_{t-1}) \\ & + \frac{(r_t - 2)w + r_t - 3}{r_{t-1} - 1} L(r_1 - 1, r_2, \ldots, r_{t-2}) \\ & + \frac{1}{r_{t-1} - 1}[(r_{t-1} - 2)L(r_1, r_2, \ldots, r_{t-1}) \\ & + L(r_1, r_2, \ldots, r_{t-2})] + 2; \end{aligned}$$

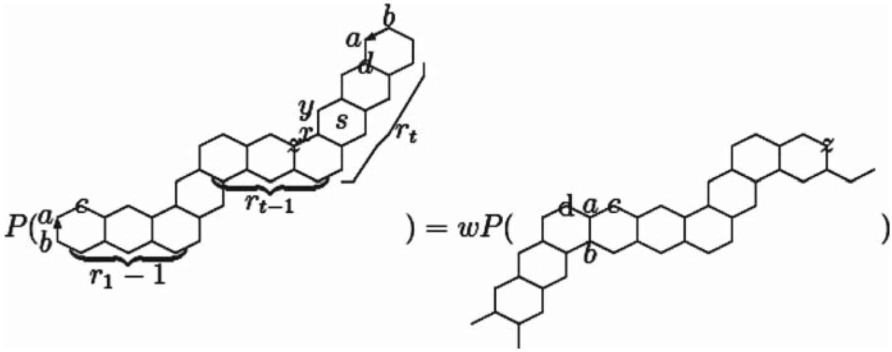
(ii) *If* $t \geq 2$ *is odd, then*

$$\begin{aligned} C(r_1, r_2, \ldots, r_t) = & \left[\frac{(r_t - 2)w + r_t - 3}{r_{t-1} - 1} + 1\right] L(r_1 - 1, r_2, \ldots, r_{t-1}) \\ & + \frac{(r_t - 2)w + r_t - 3}{r_{t-1} - 1} L(r_1 - 1, r_2, \ldots, r_{t-2}) \end{aligned}$$

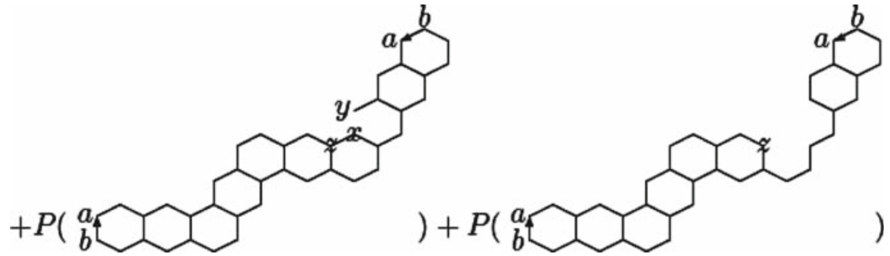
$$+\frac{1}{r_{t-1}-1}[(r_{t-1}-2)L(r_1,r_2,\ldots,r_{t-1})$$
$$+L(r_1,r_2,\ldots,r_{t-2})].$$

Proof of theorem 4.2 Without danger of confusion we also use $c(r_1,r_2,\ldots,r_t)$ denote its Clar covering polynomial.

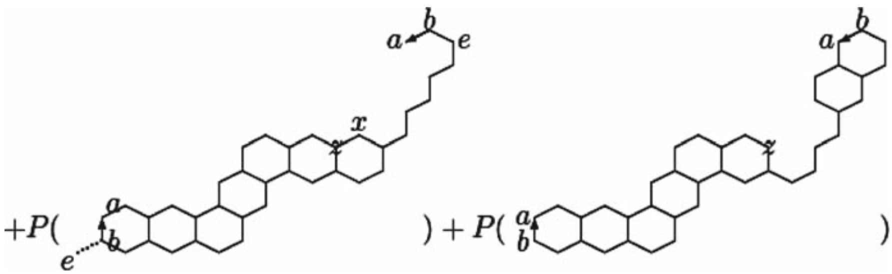
(i) Let $t \geq 2$ is even. By Lemmas 4.1 and 4.2, where we take the second hexagon on the last segment as the "s" of Lemma 4.1.



$$= wL(r_1-1,r_2,\ldots,r_{t-1}-1)$$



$$= wL(r_1-1,r_2,\ldots,r_{t-1}-1)$$



$$= wL(r_1-1,r_2,\ldots,r_{t-1}-1)$$
$$+[L(r_1-1,r_2,\ldots,r_{t-1})+1]+[L(r_t-2,r_1,r_2,\ldots,r_{t-1}-1)+1].$$

Applying Lemma 4.3, we have

$$L(r_1-2, r_1, r_2, \ldots, r_{t-1}-1) = (r_t-3)(w+1)L(r_1-1, r_2, \ldots, r_{t-1}-1) \\ + L(r_1, r_2, \ldots, r_{t-1}-1).$$

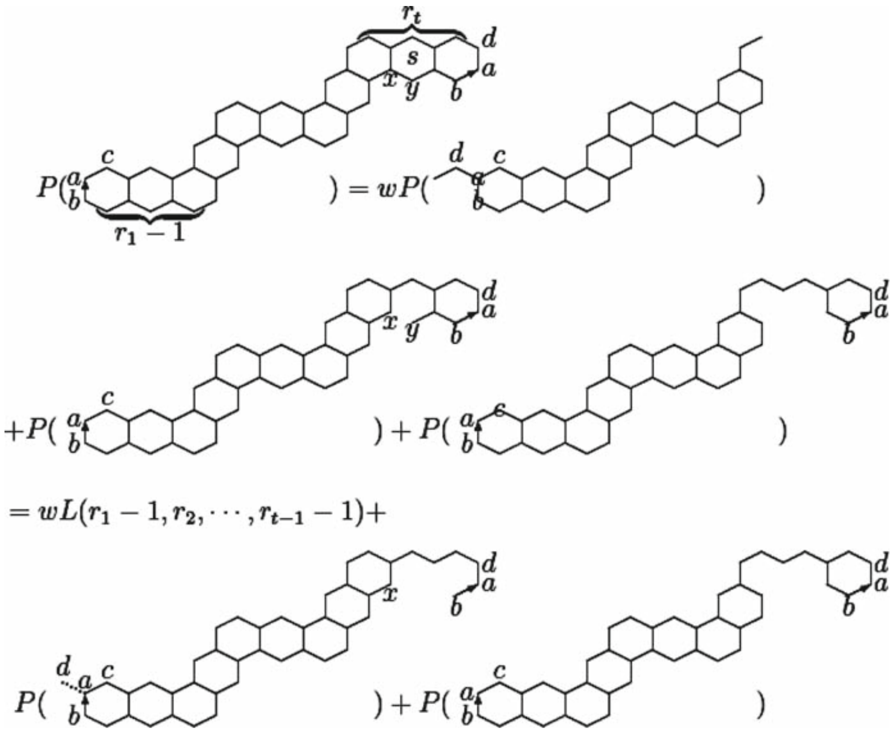
So,

$$C(r_1, r_2, \ldots, r_t) = [(r_t-2)w + (r_t-3)]L(r_1-1, r_2, \ldots, r_{t-1}-1) \\ + L(r_1-1, r_2, \ldots, r_{t-1}) + L(r_1, r_2, \ldots, r_{t-1}-1) + 2.$$

Combining the above equation with Corollary 4.1, we obtain the recurrence relation:

$$\begin{aligned} C(r_1, r_2, \ldots, r_t) = {} & \left[\frac{(r_t-2)w + r_t - 3}{r_{t-1}-1} + 1\right] L(r_1-1, r_2, \ldots, r_{t-1}) \\ & + \frac{(r_t-2)w + r_t - 3}{r_{t-1}-1} L(r_1-1, r_2, \ldots, r_{t-2}) \\ & + \frac{1}{r_{t-1}-1}[(r_{t-1}-2)L(r_1, r_2, \ldots, r_{t-1}) \\ & + L(r_1, r_2, \ldots, r_{t-2})] + 2. \end{aligned}$$

(ii) Let $t \geq 2$ is odd. Calculating as in the case (i), we have



$$
\begin{aligned}
&= wL(r_1-1, r_2, \ldots, r_{t-1}-1) + L(r_1-1, r_2, \ldots, r_{t-1}) \\
&\quad + L(r_t-2, r_1, r_2, \ldots, r_{t-1}-1).
\end{aligned}
$$

Using Lemma 4.3, we can get the recurrence relation:

$$
\begin{aligned}
C(r_1, r_2, \ldots, r_t) = &\left[\frac{(r_t-2)w + r_t - 3}{r_{t-1}-1} + 1\right] L(r_1-1, r_2, \ldots, r_{t-1}) \\
&+ \frac{(r_t-2)w + r_t - 3}{r_{t-1}-1} L(r_1-1, r_2, \ldots, r_{t-2}) \\
&+ \frac{1}{r_{t-1}-1}[(r_{t-1}-2)L(r_1, r_2, \ldots, r_{t-1}) + L(r_1, r_2, \ldots, r_{t-2})].
\end{aligned}
$$

The proof of the theorem is completed. □

Combining the basic properties of the Zhang–Zhang polynomial with Theorem 4.2, we have the following recurrence relations of the number of Kekulé structures and the number of the first Herndon number of cyclic hexagonal chains.

Corollary 4.3 *Let* $t \geq 2, r_t \geq 3$,

(i) *If* t *is even, then*

$$
\begin{aligned}
K(C(r_1, r_2, \ldots, r_t)) = &\left(\frac{r_t-3}{r_{t-1}-1} + 1\right) K(L(r_1-1, r_2, \ldots, r_{t-1})) \\
&+ \frac{r_t-3}{r_{t-1}-1} K(L(r_1-1, r_2, \ldots, r_{t-2})) \\
&+ \frac{1}{r_{t-1}-1} K(L(r_1, r_2, \ldots, r_{t-1})) \\
&+ K(L(r_1, r_2, \ldots, r_{t-2})) + 2;
\end{aligned}
$$

(ii) *If* t *is odd, then*

$$
\begin{aligned}
K(C(r_1, r_2, \ldots, r_t)) = &\left(\frac{r_t-3}{r_{t-1}-1} + 1\right) K(L(r_1-1, r_2, \ldots, r_{t-1})) \\
&+ \frac{r_t-3}{r_{t-1}-1} K(L(r_1-1, r_2, \ldots, r_{-2})) \\
&+ \frac{1}{r_{t-1}-1} K(L(r_1, r_2, \ldots, r_{t-1})) \\
&+ K(L(r_1, r_2, \ldots, r_{t-2})),
\end{aligned}
$$

where $K(L(r_1, r_2, \ldots, r_t))$ *satisfy the recurrence relations of Lemma 4.5.*

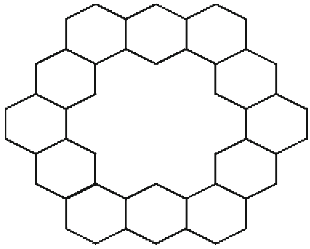


Fig. 6 A coronoid

Corollary 4.4 . *Let $t \geq 2$, $r_t \geq 3$, then*

$$\begin{aligned} h_1(C(r_1, r_2, \ldots, r_t)) = & \frac{r_t - 2}{r_{t-1} - 1}[K(L(r_1 - 1, r_2, \ldots, r_{t-1})) \\ & + K(L(r_1 - 1, r_2, \ldots, r_{n-2}))] \\ & + \left(\frac{r_t - 3}{r_{t-1} - 1} + 1\right) h_1(L(r_1 - 1, r_2, \ldots, r_{t-1})) \\ & + \frac{r_t - 3}{r_{t-1} - 1} h_1(L(r_1 - 1, r_2, \ldots, r_{t-2})) \\ & + \frac{1}{r_{t-1} - 1}[(r_{t-1} - 2) h_1(L(r_1, r_2, \ldots, r_{t-1})) \\ & + h_1(L(r_1, r_2, \ldots, r_{t-2}))], \end{aligned}$$

where $h_1(L(r_1, r_2, \ldots, r_t))$ satisfy the recurrence relations of Lemma 4.5.

For example, the graph $C(3, 3, 3, 3, 3, 3)$ in Fig. 6 is a a coronoid (see [33, p. 180]).

By Theorem 4.2, the Zhang–Zhang polynomial of the coronoid $C(3, 3, 3, 3, 3, 3)$ is

$$\begin{aligned} P(C(3, 3, 3, 3, 3, 3); w) = & \left[\frac{w}{2} + 1\right] L(2, 3, 3, 3, 3) + \frac{w}{2} L(2, 3, 3, 3) \\ & + \frac{1}{2}[L(3, 3, 3, 3, 3) + L(3, 3, 3, 3)] + 2 \\ = & w^6 + 18w^5 + 123w^4 + 408w^3 + 699w^2 + 594w + 200. \end{aligned}$$

The number of Kekulé is 200, which is consistent with the result enumerated by the two-step fragmentation method in [33].

Next, we consider the zigzag cyclic hexagonal chain $C(2, 2, \ldots, 2)$ with $t \geq 3$ segments.

Let f_t denote the Zhang–Zhang polynomial of zigzag hexagonal chain $L(2, 2, \ldots, 2)$ with $t \geq 3$ segments. Zhang and Zhang [10] obtained the following result:

Lemma 4.6 ([10]) *Let $t \geq 3$, then*

$$f_t = (2w+3) \sum_{k_1+2k_2=t-1} \binom{k_1+k_2}{k_1} (1+w)^{k_2}$$
$$+(w^2+3w+2) \sum_{k_1+2k_2=t-2} \binom{k_1+k_2}{k_1} (1+w)^{k_2}.$$

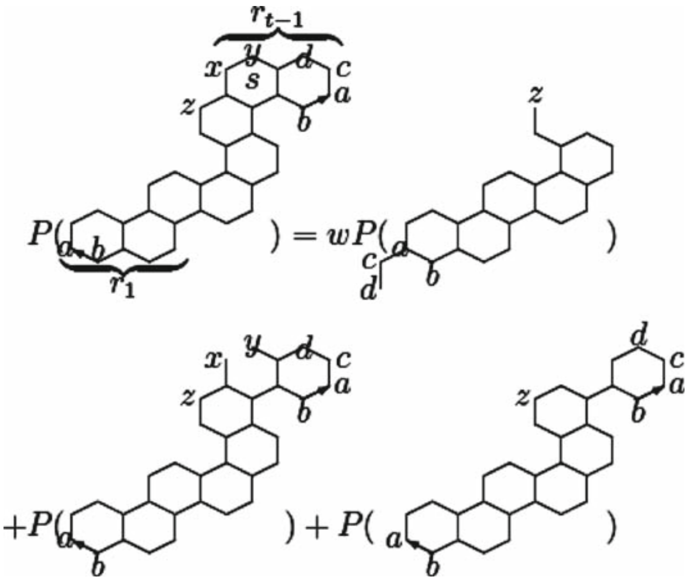
In the following, we give the recurrence relations of the Zhang–Zhang polynomial of a zigzag cyclic hexagonal chain $C(2, 2, \ldots, 2)$.

Theorem 4.3 *Let $C(2, 2, \ldots, 2)$ be a zigzag cyclic hexagonal chain with $t \geq 3$ segments,*

(i) *If $t > 6$ is even, then $C(2, 2, \ldots, 2) = (w+1) f_{t-4} + f_{t-2} + 2$;*
(ii) *If $t > 6$ is odd, then $C(2, 2, \ldots, 2) = (w+1) f_{t-4} + f_{t-2}$;*
(iii) $C(2, 2, 2) = 3w + 4$; $C(2, 2, 2, 2) = 2w^2 + 8w + 9$; $C(2, 2, 2, 2, 2) = 5w^2 + 15w + 11$; $C(2, 2, 2, 2, 2, 2) = 2w^3 + 15w^2 + 30w + 20$.

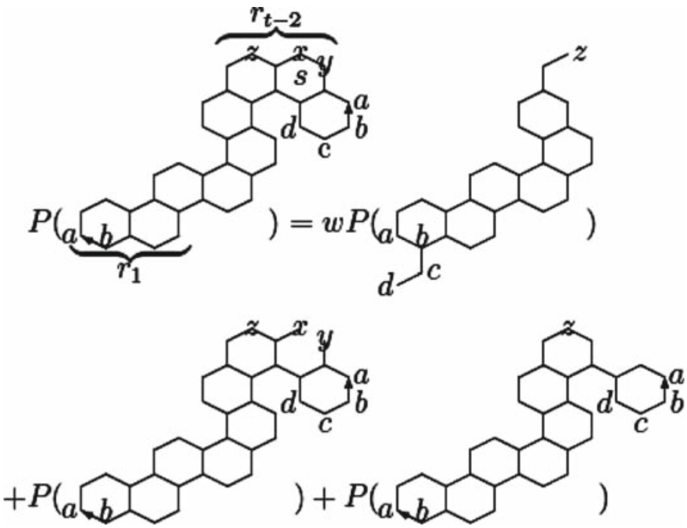
Proof of theorem 4.3

(i) Let $t > 6$ is even. By Lemmas 4.1 and 4.2, where we take the first hexagon on the $(t-1) - th$ segment as "s"of Lemma 4.1.



$$= wf_{t-4} + [f_{t-4} + 1] + [f_{t-2} + 1]$$
$$= (w+1) f_{t-4} + f_{t-2} + 2.$$

(ii) Similarly,



$$= wf_{t-4} + f_{t-4} + f_{t-2} = (w+1)f_{t-4} + f_{t-2}.$$

(iii) It can be obtained by calculating immediately.

□

Combining the above result and Lemma 4.6, we have

Corollary 4.5 *Let* $C = C(2, 2, \ldots, 2)$ *be a zigzag cyclic hexagonal chain with* $t > 6$ *segments,*

(i) *If* t *is even, then*

$$\begin{aligned} P(C; w) = (w^3 + 4w^2 + 5w + 2) &\sum_{k_1+2k_2=t-6} \binom{k_1+k_2}{k_1} (1+w)^{k_2} \\ +(2w^2 + 5w + 3) &\sum_{k_1+2k_2=t-5} \binom{k_1+k_2}{k_1} (1+w)^{k_2} \\ +(w^2 + 3w + 2) &\sum_{k_1+2k_2=t-4} \binom{k_1+k_2}{k_1} (1+w)^{k_2} \\ +(2w + 3) &\sum_{k_1+2k_2=t-3} \binom{k_1+k_2}{k_1} (1+w)^{k_2} + 2; \end{aligned}$$

(ii) *If t is odd, then*

$$\begin{aligned}P(C;w) = (w^3+4w^2+5w+2)&\sum_{k_1+2k_2=t-6}\binom{k_1+k_2}{k_1}(1+w)^{k_2}\\&+(2w^2+5w+3)\sum_{k_1+2k_2=t-5}\binom{k_1+k_2}{k_1}(1+w)^{k_2}\\&+(w^2+3w+2)\sum_{k_1+2k_2=t-4}\binom{k_1+k_2}{k_1}(1+w)^{k_2}\\&+(2w+3)\sum_{k_1+2k_2=t-3}\binom{k_1+k_2}{k_1}(1+w)^{k_2}.\end{aligned}$$

By the basic properties of the Zhang–Zhang polynomial of $C(2,2,\ldots,2)$, we can easily derive the following Corollaries 4.6–4.8 from the above theorem.

Corollary 4.6 *Let $C(2,2,\ldots,2)$ be a zigzag cyclic hexagonal chain with $t \geq 3$ segments,*

(i) *If $t > 6$ is even, then*

$$\begin{aligned}K(C(2,2,\ldots,2)) = 2&\sum_{k_1+2k_2=t-6}\binom{k_1+k_2}{k_1}+3\sum_{k_1+2k_2=t-5}\binom{k_1+k_2}{k_1}\\&+2\sum_{k_1+2k_2=t-4}\binom{k_1+k_2}{k_1}+3\sum_{k_1+2k_2=t-3}\binom{k_1+k_2}{k_1}+2;\end{aligned}$$

(ii) *If $t > 6$ is odd,*

$$\begin{aligned}K(C(2,2,\ldots,2)) = 2&\sum_{k_1+2k_2=t-6}\binom{k_1+k_2}{k_1}+3\sum_{k_1+2k_2=t-5}\binom{k_1+k_2}{k_1}\\&+2\sum_{k_1+2k_2=t-4}\binom{k_1+k_2}{k_1}+3\sum_{k_1+2k_2=t-3}\binom{k_1+k_2}{k_1};\end{aligned}$$

(iii) $K(C(2,2,2)) = 4$*;* $K(C(2,2,2,2)) = 9$*;* $K(C(2,2,2,2,2)) = 11$*;*
$K(C(2,2,2,2,2,2)) = 20$*.*

Corollary 4.7 *Let $C(2,2,\ldots,2)$ be a zigzag cyclic hexagonal chain with $t \geq 3$ segments,*

(i) *If* $t > 6$*, then*

$$\begin{aligned} h_1(C(2,2,\ldots,2)) = &\sum_{k_1+2k_2=t-6}(5+2k_2)\binom{k_1+k_2}{k_1} \\ &+\sum_{k_1+2k_2=t-5}(5+3k_2)\binom{k_1+k_2}{k_1} \\ &+\sum_{k_1+2k_2=t-4}(3+2k_2)\binom{k_1+k_2}{k_1} \\ &+\sum_{k_1+2k_2=t-3}(2+3k_2)\binom{k_1+k_2}{k_1}; \end{aligned}$$

(ii) $h_1(C(2,2,2)) = 3$*;* $h_1(C(2,2,2,2)) = 8$*;* $h_1(C(2,2,2,2,2)) = 15$*;* $h_1(C(2,2,2,2,2,2)) = 30$*.*

Corollary 4.8 *Let* $C(2,2,\ldots,2)$ *be a zigzag cyclic hexagonal chain with* $t \geq 3$ *segments,*

(i) *If* t *is even, then* $\sigma(C(2,2,\ldots,2)) = \frac{t}{2}$*;* $\sigma\left(C(2,2,\ldots,2),\frac{t}{2}\right) = 2$*;*
(i) *If* t *is odd, then* $\sigma(C(2,2,\ldots,2)) = \frac{t-1}{2}$*;* $\sigma\left(C(2,2,\ldots,2),\frac{t-1}{2}\right) = t$*.*

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