MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **80** (2018) 245-265

ISSN 0340 - 6253

Zhang–Zhang Polynomials of Multiple Zigzag Chains

Johanna Langner[a], Henryk A. Witek*[,a], Grzegorz Mość[b]

[a] *Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu, Taiwan*

[b] *Department of Mathematics, Silesian University, Katowice, Poland*

* hwitek@mail.nctu.edu.tw

(Received May 06, 2017)

Abstract

Generating functions of the Zhang–Zhang polynomials of multiple zigzag chains $Z(m,n)$ and generalized multiple zigzag chains $Z_k(m,n)$ are derived for arbitrary values of the indices. These generating functions can be expressed in the form of highly regular finite continued fractions,

$$\sum_{m=0}^{\infty} \mathrm{ZZ}(Z(m,n),z)t^m = \left[0; -t, (-1)^2 zt, (-1)^3 zt, \ldots, (-1)^n zt, 1 + (-1)^{n+1} zt\right],$$

or, in the case of $Z_k(m,n)$, products of such continued fractions. For the particularly important case of the multiple zigzag chains $Z(m,n)$, the generating functions are expanded to yield a closed form for the Zhang-Zhang polynomials of multiple zigzag chains $Z(m,n)$ that is valid for arbitrary values of m and n.

1 Introduction

Zhang-Zhang polynomials (*aka* ZZ polynomials or Clar covering polynomials) [1–5] occupy a pronounced position in the chemical graph theory of benzenoid structures. ZZ polynomials were first introduced by Zhang and Zhang to enable robust and convenient enumeration of Clar covers [6] for benzenoid structures. A Clar cover of a benzenoid structure S can be defined as a generalized resonance structure of S, such that every carbon atom is part of either a double bond or an aromatic sextet. [6] The ZZ polynomial for the benzenoid S is usually expressed in the form

$$\mathrm{ZZ}(S,x) = \sum_{k=0}^{Cl} c_k x^k, \tag{1}$$

where c_k is the number of Clar covers of order k, (i.e., Clar covers containing exactly k aromatic sextets) and Cl is the maximal number of aromatic sextets that can be accommodated inside S. Denoting the sequence of the number of Clar covers of S of each order by $(c_0, c_1, \ldots, c_{Cl})$, the Zhang-Zhang polynomial $\mathrm{ZZ}(S,x)$ is simply the generating function of this sequence. The ZZ polynomials possess a number of inviting structural properties, which make their evaluation rather straightforward [1, 4, 7–9]. In particular, ZZ polynomials can be evaluated recursively. Appropriate algorithms have been developed [7–10] and a computer program called ZZCalculator [8] based on these recursive decomposition has been reported. The brute force, recursive determination of ZZ polynomials is applicable to small and medium-size pericondensed benzenoid structures with up to 500 carbon atoms; for catacondensed benzenoids, this limit is much higher and can be estimated as 10^4 carbon atoms. It is clear that for both classes of structures one necessarily encounters size limitations, which prevent him/her from determination of the ZZ polynomial.

In order to resolve this problem, the chemical graph theory community invested considerable time and effort in pursuit of closed form formulas applicable to arbitrarily sized structures within a given benzenoid family. Such formulas have been reported for the ZZ polynomials of the following structures:

- polyacenes $L(n)$ (Eq. (2.3) of [1])
- multiple segment polyacenes $L(m,n)$ (Eq. (4.12) in [1], Eq. (12) of [11] as well as Eqs. (7) and (21) of [9])

- variable-length multiple segment polyacenes $L([r_1, r_2, \ldots, r_n])$ (recurrence relations given by Eq. (4.6) of [3] and Lemma 4.4 of [12])
- catacondensed ladders $\Theta(m_1, m_2, n)$ (Eq. (4.26) of [1])
- catacondensed all-benzenoids $U(n)$ and $Z(n)$ (Eqs. (4.32) and (4.34) of [1])
- single zigzag chains $N(n)$ (p.167 of [3], Eqs. (11) and (12) of [8])
- polyphenylenes $P(n)$ and cyclic polyphenylenes $AC(n, m, l)$ (Eqs. (20, 22) of [8])
- cyclo-polyphenacenes $C(r_1, r_2, \ldots, r_n)$ (Theorem 4.2 of [12], corrected in [13])
- zigzag-edge coronoids $ZC(n, m, l)$ (Eq. (32) of [11]; Eq. (3) of [14] formally derived)
- armchair-edge coronoids $AC(n, m, l)$ (Eq. (22) of [8])
- hammer-like structures $H(n)$ (Eq. (15) of [11])
- starphenes $St(n, m, l)$ (Eq. (4.17) of [1] and Eq. (22) of [11])
- tripods $T(n, m, l)$ (for $m = 1$ given by Eq. (4.4) of [1], for general m by Eq. (27) of [11], formally derived in [15])
- zigzag-edge coronoids fused with starphene $ZCS(n, m, l)$ (Eqs. (65) and (66) of [11], formally derived in [15])
- fenestrenes $F(n, m)$ (Eq. (33) of [11], Eqs. (5) and (6) of [14])
- the $S(n)$ structures of Randić [16] (generating function given by Eq. (25) of [8], closed form by Eq. (15) of [15])
- parallelograms $M(m, n)$ (Eq. (16) of [17], Eqs. (18, 19) of [8], Eqs. (2–5) of [18])
- prolate rectangles $Pr(m, n)$ (Thm. 10 of [4], Eq. (62) of [11], formal derivation in [19])
- generalized prolate rectangles $Pr([m_1, m_2, \ldots, m_n], n)$ (Eq. (63) of [11])
- chevrons $Ch(k, m, n)$ (for $k = 1, 2, 3$ given by Eqs. (10, 40, 43) of [11], general closed form given by Eqs. (15) and (16) of [18])
- generalized chevrons $Ch(k, m, n_1, n_2)$ (Eqs. (19–21) of [18])

- irregular 2- and 3-tier benzenoid strips (Thms. 5, 6 and 7 of [20])
- regular 3-, 4- [21], and 5-tier [22] benzenoid strips

Many of these formulas were discovered using the ZZDecomposer computer environment [9], which has been designed for the particular purpose of finding recurrence relations between ZZ polynomials of isostructural benzenoids. Despite of this quite long list of achievements of the general ZZ polynomial theory, there still remains a long list of unsolved problems. We believe that the greatest challenges in the general theory of ZZ polynomials concern obtaining closed-form formulas of ZZ polynomials for the oblate rectangles $Or(m,n)$, ribbons $Rb(k,m,n)$, multiple zigzag chains $Z(m,n)$, and hexagons $O(m,k,n)$. For these structures, ZZ polynomials are available in the literature only in a few special cases, in particular for

- oblate rectangles $Or(m,n)$
  - with $m = 1$ and arbitrary n (Eq. (12) of [7]),
  - with $n = 1$ and arbitrary m (Eq. (35) of [11]),
  - with $n = 2$ and arbitrary m (Eq. (58) of [11], formal derivation in [15]),
- ribbons $Rb(k,m,n)$ with $n = 2,3$ and $k = m \geq n$ (Eqs. (54, 56) of [11]),
- multiple zigzag chains $Z(m,n)$ with $m = 4,\ldots,9$ and arbitrary n (Eqs. (44–46) of [11] and Eqs. (32, 35, 37, 39–41) with formal derivation in [15]),
- and hexagons $O(m,k,n)$
  - with $m = k = 1,2,3$ and arbitrary n (Eqs. (10, 35, 37) of [11], formal derivation in [15]),
  - with $m = 2$, $k = 3$ and arbitrary n (Eq. (65) with formal derivation in [15]).

The current paper reports a solution to one of these four problems. Namely, we present a formal derivation of the ZZ polynomials for the multiple zigzag chains $Z(m,n)$ valid for arbitrary values of the indices m and n. The derivation process is closely related to the generating function technique of solving recurrence relations and—somewhat surprisingly—to the theory of continued fractions. Expansion of the resulting generating function in power series yields the sought closed-form formulas of the ZZ polynomials for the multiple zigzag chains $Z(m,n)$.

2 Generating functions for generalized multiple zigzag chains $Z_k(m,n)$

Define the generalized multiple zigzag chain $Z_k(m,n)$ to be a multiple zigzag chain $Z(m,n)$ merged with a polyacene $L(k)$ in the way shown in Figure 1.

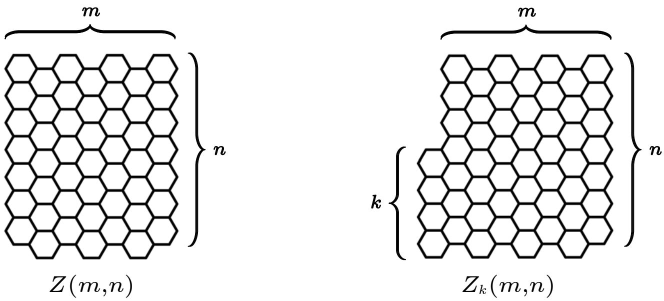

Figure 1. Definition of the benzenoids $Z(m,n)$ and $Z_k(m,n)$

Note that $Z_0(m,n) = Z_n(m-1,n) = Z(m,n)$. The Zhang-Zhang polynomials of the benzenoid structures $Z_k(m,n)$ fulfill the recurrence relation originating from the following recurrence diagram

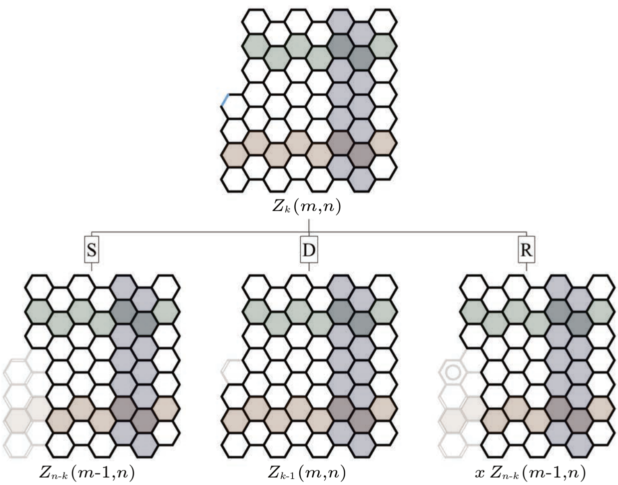

Figure 2. Recurrence diagram for $Z_k(m,n)$. The shaded rows and columns are placeholders for $n-k-2$ rows, $k-3$ rows and $m-5$ columns, respectively.

valid for arbitrary positive values of m, n, and for $k = 1, ..., n$. This shows that

$$\mathrm{ZZ}(Z_k(m,n),x) = \mathrm{ZZ}(Z_{k-1}(m,n),x) + (1+x)\,\mathrm{ZZ}(Z_{n-k}(m-1,n),x), \tag{2}$$

which can be rewritten as

$$\mathrm{ZZ}(Z_k(m,n),z) = \mathrm{ZZ}(Z_{k-1}(m,n),z) + z\mathrm{ZZ}(Z_{n-k}(m-1,n),z), \tag{3}$$

after introducing the shorthand notation $z = 1 + x$. The initialization conditions are $\mathrm{ZZ}(Z_k(0,n),z) = \mathrm{ZZ}(L(k),z) = kz+1$ and $\mathrm{ZZ}(Z_0(1,n),z) = \mathrm{ZZ}(L(n),z) = nz+1$. Multiplying Eq. (3) by t^m and summing over all values of $m \in \mathbb{N}$ gives

$$\sum_{m=1}^{\infty} \mathrm{ZZ}(Z_{k-1}(m,n),z)t^m + z\sum_{m=1}^{\infty} \mathrm{ZZ}(Z_{n-k}(m-1,n),z)t^m - \sum_{m=1}^{\infty} \mathrm{ZZ}(Z_k(m,n),z)t^m = 0. \tag{4}$$

This expression can be rewritten in a more compact form after introducing a generating function $F_{k,n}(t)$ defined as

$$F_{k,n}(t) = \frac{1}{t} + \sum_{m=0}^{\infty} \mathrm{ZZ}(Z_k(m,n),z)t^m \tag{5}$$

for the sequence of Zhang-Zhang polynomials $\mathrm{ZZ}(Z_k(m,n),z)$. It follows directly from this definition that the following condition is satisfied for the generating function $F_{k,n}(t)$

$$tF_{n,n}(t) = F_{0,n}(t) - \frac{1}{t}. \tag{6}$$

The new, concise form of Eq. (4) is given by

$$-F_{k,n}(t) + F_{k-1,n}(t) + ztF_{n-k,n}(t) = 0, \tag{7}$$

where we have used the fact that $\mathrm{ZZ}(Z_k\,(0,n)\,,z) = \mathrm{ZZ}(L(k),z) = zk+1$. The family of recurrence relations given by Eq. (7) is valid for $k = 1, ..., n$. For $k = n$, due to Eq. (6), Eq. (7) reduces to

$$-\frac{1}{t}F_{0,n}(t) + F_{n-1,n}(t) + ztF_{0,n}(t) = -\frac{1}{t^2}, \tag{8}$$

so that the system of n linear equations defining the generating functions

$F_{0,n}$, $F_{1,n}$,. . .,$F_{n-1,n}$ for an arbitrary value of n is given by

$$-F_{k,n}(t) + F_{k-1,n}(t) + ztF_{n-k,n}(t) = 0 \qquad \text{for } k \in \{1, 2, \ldots, n-1\} \tag{9a}$$

$$-\frac{1}{t}F_{0,n}(t) + F_{n-1,n}(t) + ztF_{0,n}(t) = -\frac{1}{t^2}. \tag{9b}$$

The solutions of Eqs. (9) have a somewhat complex and rather unexpected form. For this reason, we find it appropriate to give two introductory examples illustrating how the structure of the solution naturally emerges in the solution process.

Example 1. In the case $n = 1$, Eq. (9b) has the form

$$-\frac{1}{t}F_{0,1}(t) + F_{0,1}(t) + ztF_{0,1}(t) = -\frac{1}{t^2}, \tag{10}$$

which directly solves to

$$F_{0,1}(t) = \frac{-1}{\frac{-1}{1+zt} + t} + \frac{1}{t}, \tag{11}$$

giving the explicit formula for the generating function of the Zhang-Zhang polynomials of $Z(m, n)$ with $n = 1$ in the following form

$$\sum_{m=0}^{\infty} \mathrm{ZZ}(Z(m, 1), z)t^m = \frac{-1}{\frac{-1}{1+zt} + t}. \tag{12}$$

This generating function is consistent with the already known [8, 11] recurrence relation for ZZ polynomials of single zigzag chains. It will be demonstrated in Example 8 that the polynomials $\mathrm{ZZ}(Z(m, 1), z)$ produced by the generating function Eq. (12) agree with the previously reported [8, 11] explicit formula.

Example 2. In the case $n = 4$, the system of equations defined by Eqs. (9) has the form

$$-F_{1,4}(t) + F_{0,4}(t) + ztF_{3,4}(t) = 0 \tag{13a}$$

$$-F_{2,4}(t) + F_{1,4}(t) + ztF_{2,4}(t) = 0 \tag{13b}$$

$$-F_{3,4}(t) + F_{2,4}(t) + ztF_{1,4}(t) = 0 \tag{13c}$$

$$-\frac{1}{t}F_{0,4}(t) + F_{3,4}(t) + ztF_{0,4}(t) = -\frac{1}{t^2}. \tag{13d}$$

Solving Eqs. (13b), (13c), and (13a) in this particular order gives

$$F_{2,4}(t) = \underbrace{\frac{-1}{-1+zt}}_{A_2} F_{1,4}(t) \tag{14a}$$

$$F_{1,4}(t) = \underbrace{\frac{1}{A_2+zt}}_{A_1} F_{3,4}(t) \tag{14b}$$

$$F_{3,4}(t) = \underbrace{\frac{-1}{-A_1+zt}}_{A_3} F_{0,4}(t) \tag{14c}$$

Finally, substituting (14c) into Eq. (13d) and solving for $F_{0,4}(t)$ gives

$$F_{0,4}(t) = \frac{-1}{\frac{-1}{A_3+zt}+t} + \frac{1}{t}. \tag{15}$$

Back–substitution of the functional coefficients A_3, A_1, and A_2 defined by Eqs. (14c), (14b), and (14a), respectively, to Eq. (15) yields an explicit formula for the generating function of the Zhang-Zhang polynomials of $Z(m,n)$ with $n=4$ given by

$$\sum_{m=0}^{\infty} \mathrm{ZZ}(Z(m,4),z)t^m = \frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{-1+zt}+zt}+zt}+zt}+t}. \tag{16}$$

The generating functions for the Zhang-Zhang polynomials of $Z(m,n)$ with $n=1$ and with $n=4$ represented by Eqs. (12) and (16), respectively, have the form of a finite continued fraction. This somewhat unexpected result appears even more intriguing considering that this is not the first time for continued fraction expressions to appear in connection with resonance structures of zigzag chains: He *et al.* [23] discovered that Kekulé structure counts of nonbranched cata-condensed benzenoids can be written as products of continued fractions. We expect this connection between (generalized) resonance structures of zigzag chains and continued fractions to be more deep and profound than is currently evident. We will compare our result with the one given by He *et al.* in more detail in Section 4.

Using a standard notation for finite continued fractions, in which

$$x = a_0 + \cfrac{1}{a_1 + \cfrac{1}{a_2 + \cfrac{1}{a_3 + \cfrac{1}{a_4 + \frac{1}{a_5}}}}} \tag{17}$$

is written as $x = [a_0; a_1, a_2, a_3, a_4, a_5]$, we can express Eqs. (12) and (16) in the following form

$$\sum_{m=0}^{\infty} \mathrm{ZZ}(Z(m,1),z)t^m = [0; -t, 1+zt] \tag{18}$$

$$\sum_{m=0}^{\infty} \mathrm{ZZ}(Z(m,4),z)t^m = [0; -t, zt, -zt, zt, 1-zt] \, . \tag{19}$$

It is natural to expect that the generating functions for the Zhang-Zhang polynomials of $Z(m,n)$ with an arbitrary value of n is given by the following finite continued fraction

$$\sum_{m=0}^{\infty} \mathrm{ZZ}(Z(m,n),z)t^m = \left[0; -t, (-1)^2 zt, (-1)^3 zt, \ldots, (-1)^n zt, 1 + (-1)^{n+1} zt\right] . \tag{20}$$

Formal demonstration of this fact requires introducing certain tools.

Let τ be a linear fractional transformation given by

$$\tau(a) = -\frac{1}{a + zt}. \tag{21}$$

Using this transformation, it is possible to rewrite Eqs. (12) and (16) in the following form

$$\sum_{m=0}^{\infty} \mathrm{ZZ}(Z(m,1),z)t^m = \frac{-1}{\tau(1) + t}, \tag{22}$$

$$\sum_{m=0}^{\infty} \mathrm{ZZ}(Z(m,4),z)t^m = \frac{-1}{\tau^4(-1) + t}, \tag{23}$$

where $\tau^4(a)$ represents $\tau(\tau(\tau(\tau(a))))$. We will demonstrate below that this transformation allows one to express the generating function for the Zhang-Zhang polynomials of $Z(m,n)$ with an arbitrary value of n in the following simple form

$$\sum_{m=0}^{\infty} \mathrm{ZZ}(Z(m,n),z)t^m = \frac{-1}{\tau^n((-1)^{n+1}) + t}. \tag{24}$$

Lemma 3. *The functions $F_{k,n}(t)$ (i.e., the solutions to Eqs. (9)) fulfill the following relations:*

$$F_{k,n}(t) = A_k F_{n-k,n}(t) \qquad \text{with } 1 \le k < \tfrac{n}{2}, \tag{25a}$$

$$F_{n-k,n}(t) = A_{n-k} F_{k-1,n}(t) \qquad \text{with } 1 \le k \le \tfrac{n}{2}, \tag{25b}$$

where

$$A_k = -\tau^{n-2k}\left((-1)^{n+1}\right) \qquad \text{with } 1 \le k < \tfrac{n}{2}, \tag{26a}$$

$$A_{n-k} = \tau^{n-2k+1}\left((-1)^{n+1}\right) \qquad \text{with } 1 \le k \le \tfrac{n}{2}. \tag{26b}$$

Proof. The set of the indices enumerating the coefficients A_k is given by $\{1, 2, \ldots, n-1\}$. We introduce a new order $\prec$ on this index set related to the absolute distance of a given index to $\frac{n}{2} - \frac{1}{4}$,

$$k_1 \prec k_2 \iff \left|\tfrac{n}{2} - \tfrac{1}{4} - k_1\right| < \left|\tfrac{n}{2} - \tfrac{1}{4} - k_2\right|. \tag{27}$$

It is easy to see that the sequence c of indices following this order is given by

$$c = \begin{cases} \left(\frac{n}{2}, \frac{n}{2} - 1, \frac{n}{2} + 1, \frac{n}{2} - 2, \frac{n}{2} + 2, ..., 1, n-1\right) & \text{for even } n, \\ \left(\frac{n}{2} - \frac{1}{2}, \frac{n}{2} + \frac{1}{2}, \frac{n}{2} - \frac{3}{2}, \frac{n}{2} + \frac{3}{2}, ..., 1, n-1\right) & \text{for odd } n. \end{cases} \tag{28}$$

with the j^{th} element explicitly expressed as

$$c_j = \left\lfloor \frac{n}{2} \right\rfloor - (-1)^{n+j} \left\lceil \frac{j-1}{2} \right\rceil \qquad \text{for} \qquad 1 \le j \le n-1. \tag{29}$$

Note that for every $k < \frac{n}{2}$ we have $\frac{n}{2} - k > \frac{1}{4}$ and thus

$$\begin{aligned} & \left|\tfrac{n}{2} - k - \tfrac{1}{4}\right| < \left|\tfrac{n}{2} - k + \tfrac{1}{4}\right| \\ \Longrightarrow\ & \left|\tfrac{n}{2} - \tfrac{1}{4} - k\right| < \left|-\left(\tfrac{n}{2} - \tfrac{1}{4} - (n-k)\right)\right| \\ \Longrightarrow\ & k \prec n-k \end{aligned} \tag{30}$$

Similarly, for every $k \le \frac{n}{2}$ we have $\frac{n}{2} - k \ge 0$ and thus

$$\begin{aligned} & \left|\tfrac{n}{2} - k + \tfrac{1}{4}\right| < \left|\tfrac{n}{2} - k + \tfrac{3}{4}\right| \\ \Longrightarrow\ & \left|-\left(\tfrac{n}{2} - \tfrac{1}{4} - (n-k)\right)\right| < \left|\tfrac{n}{2} - \tfrac{1}{4} - (k-1)\right| \\ \Longrightarrow\ & n-k \prec k-1 \end{aligned} \tag{31}$$

Equations (25) and (26) can now be proven by induction following the order given by $\prec$. The base case corresponds to the first element of the sequences given by Eq. (28), and thus is treated separately for even and odd n.

- *Base case for even n*

  Evaluating Eq. (9a) at $k = \frac{n}{2}$ gives

$$F_{\frac{n}{2},n}(t) = \frac{-1}{-1+zt} F_{\frac{n}{2}-1,n}(t) = \tau(-1) F_{\frac{n}{2}-1,n}(t) = A_{\frac{n}{2}} F_{\frac{n}{2}-1,n}(t). \tag{32}$$

- *Base case for odd n*

  Evaluating Eq. (9a) at $k = \frac{n}{2} + \frac{1}{2}$ gives

$$F_{\frac{n}{2}-\frac{1}{2},n}(t) = \frac{1}{1+zt} F_{\frac{n}{2}+\frac{1}{2},n}(t) = -\tau(1) F_{\frac{n}{2}+\frac{1}{2},n}(t) = A_{\frac{n}{2}-\frac{1}{2}} F_{\frac{n}{2}+\frac{1}{2},n}(t). \tag{33}$$

The proof of the inductive step is separated into two cases: $A_k \to A_{n-k}$ with $1 \leq k < \frac{n}{2}$, and $A_{n-k} \to A_{k-1}$ with $1 \leq k \leq \frac{n}{2}$. Note that because of Eqs. (30) and (31), we have $k \prec n-k \prec k-1$.

- *Inductive step 1: $A_k \to A_{n-k}$*

  Assume that Eqs. (25a) and (26a) are true for some $1 \leq k < \frac{n}{2}$. Then, substituting $F_{k,n}(t) = A_k F_{n-k,n}(t)$ to Eq. (9a) gives upon solution

$$\begin{aligned} F_{n-k,n}(t) &= \frac{-1}{zt - A_k} F_{k-1,n}(t) \\ &= \tau(-A_k) F_{k-1,n}(t) \\ &= \tau^{n-2k+1}\left((-1)^{n+1}\right) F_{k-1,n}(t) \\ &= A_{n-k} F_{k-1,n}(t). \end{aligned} \tag{34}$$

- *Inductive step 2: $A_{n-k} \to A_{k-1}$*

  Assume that Eqs. (25b) and (26b) are true for some $1 \leq k \leq \frac{n}{2}$. Then, by substituting k for $n-k+1$ in Eq. (9a) and further by substituting $F_{n-k,n}(t) = A_{n-k} F_{k-1,n}(t)$

to the resulting equation, we obtain

$$\begin{aligned} F_{k-1,n}(t) &= \frac{1}{A_{n-k}+zt} F_{n-k+1,n}(t) \\ &= -\tau(A_{n-k}) F_{n-k+1,n}(t) \\ &= -\tau^{n-2(k-1)}\left((-1)^{n+1}\right) F_{n-k+1,n}(t) \\ &= A_{k-1} F_{n-k+1,n}(t). \end{aligned} \tag{35}$$

This shows that Eqs. (25) and (26) are correct for all relevant values of k. □

Theorem 4. *The generating function of the Zhang-Zhang polynomials of $Z(m,n)$ with arbitrary n is given by*

$$\sum_{m=0}^{\infty} ZZ(Z(m,n),z)t^m = \frac{-1}{\tau^n\left((-1)^{n+1}\right)+t}. \tag{36}$$

Proof. Eq. (9b) together with Eq. (25b) evaluated at $k=1$ gives

$$\left(A_{n-1}+zt-\frac{1}{t}\right) F_{0,n}(t) = -\frac{1}{t^2}, \tag{37}$$

which, by applying Eq. (26b), solves to

$$\begin{aligned} \frac{-1}{F_{0,n}(t)-\frac{1}{t}} &= t-\frac{1}{A_{n-1}+zt} \\ \frac{-1}{F_{0,n}(t)-\frac{1}{t}} &= t+\tau(A_{n-1}) \\ F_{0,n}(t)-\frac{1}{t} &= \frac{-1}{\tau^n\left((-1)^{n+1}\right)+t}, \end{aligned} \tag{38}$$

which proves Eq. (36) owing to the definition of $F_{k,n}(t)$ in Eq. (5). □

Corollary 5. *Combination of* Lemma 3 *and* Theorem 4 *yields a formula for the generating functions for the Zhang-Zhang polynomials of $Z_k(m,n)$ with an arbitrary value of n and $0<k<n$ given by*

$$\sum_{m=0}^{\infty} ZZ(Z_k(m,n),z)t^m = F_k(t)-\frac{1}{t} = \left(\frac{-1}{\tau^n\left((-1)^{n+1}\right)+t}+\frac{1}{t}\right)\prod_{l=j}^{n-1} A_{c_l}-\frac{1}{t}, \tag{39}$$

where A_{c_l} are defined by Eqs. (26), and j is determined by requiring $k=c_j$ in Eq. (29).

Example 6. The explicit form of the generating functions for Zhang-Zhang polynomials ZZ$(Z(m,n),z)$ of multiple zigzag chains can be found using Eq. (36). The case of $n=1$, agreeing with the derived formulas, has been already used in the motivating Example 1. For $n=2$ we have

$$\begin{aligned}\sum_{m=0}^{\infty} \mathrm{ZZ}(Z(m,2),z)t^m &= \frac{-1}{\tau^2\left(-1\right)+t} \\ &= \frac{-1}{\frac{-1}{\frac{-1}{-1+zt}+zt}+t}.\end{aligned} \tag{40}$$

This generating function for the ZZ polynomials of $Z(m,2)$ zigzag chains is consistent with the recurrence relation for these polynomials given by Eq. (48) of [11]. This case will be further examined in Example 9.

Example 7. The explicit form of generating functions for the sequence of Zhang–Zhang polynomials $\mathrm{ZZ}(Z_k(m,n),z)$, $k=0,\ldots,n$, can be found using Eqs. (36) and (39). For example, for $n=5$ we have

$$\begin{aligned}
\sum_{m=0}^{\infty} \mathrm{ZZ}(Z_0(m,5),z)t^m &= \frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{1+zt}+zt}+zt}+zt}+zt}+t} \\
&= \frac{-t^5z^5-t^4z^4+4t^3z^3+3t^2z^2-3tz-1}{t^6z^5+t^5z^4-t^4z^4-4t^4z^3-t^3z^3-3t^3z^2+3t^2z^2+3t^2z+2tz+t-1}, \\
\sum_{m=0}^{\infty} \mathrm{ZZ}(Z_1(m,5),z)t^m &= \frac{1}{\frac{-1}{\frac{-1}{1+zt}+zt}+zt}\,\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{1+zt}+zt}+zt}+zt}\left(\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{1+zt}+zt}+zt}+zt}+zt}+t}+\frac{1}{t}\right)\text{-}\frac{1}{t} \\
&= \frac{\left(-t^5z^5-t^4z^4+4t^3z^3+3t^2z^2-3tz-1\right)+t^3z^4+t^2z^3-2tz^2-z}{t^6z^5+t^5z^4-t^4z^4-4t^4z^3-t^3z^3-3t^3z^2+3t^2z^2+3t^2z+2tz+t-1}, \\
\sum_{m=0}^{\infty} \mathrm{ZZ}(Z_2(m,5),z)t^m &= \frac{1}{1+zt}\,\frac{-1}{\frac{-1}{1+zt}+zt}\,\frac{1}{\frac{-1}{\frac{-1}{1+zt}+zt}+zt}\,\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{1+zt}+zt}+zt}+zt}\left(\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{1+zt}+zt}+zt}+zt}+zt}+t}+\frac{1}{t}\right)\text{-}\frac{1}{t} \\
&= \frac{\left(-t^5z^5-t^4z^4+4t^3z^3+3t^2z^2-3tz-1\right)+t^3z^4+t^2z^3-3tz^2-2z}{t^6z^5+t^5z^4-t^4z^4-4t^4z^3-t^3z^3-3t^3z^2+3t^2z^2+3t^2z+2tz+t-1}, \\
\sum_{m=0}^{\infty} \mathrm{ZZ}(Z_3(m,5),z)t^m &= \frac{-1}{\frac{-1}{1+zt}+zt}\,\frac{1}{\frac{-1}{\frac{-1}{1+zt}+zt}+zt}\,\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{1+zt}+zt}+zt}+zt}\left(\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{1+zt}+zt}+zt}+zt}+zt}+t}+\frac{1}{t}\right)\text{-}\frac{1}{t} \\
&= \frac{\left(-t^5z^5-t^4z^4+4t^3z^3+3t^2z^2-3tz-1\right)+t^3z^4+t^2z^3-3tz^2-3z}{t^6z^5+t^5z^4-t^4z^4-4t^4z^3-t^3z^3-3t^3z^2+3t^2z^2+3t^2z+2tz+t-1},
\end{aligned} \tag{41}$$

$$\begin{aligned}
\sum_{m=0}^{\infty} \mathrm{ZZ}(Z_4(m,5),z)t^m &= \frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{1+zt}+zt}+zt}+zt}\left(\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{1+zt}+zt}+zt}+zt}+zt}+t}+\frac{1}{t}\right)-\frac{1}{t} \\
&= \frac{\left(-t^5z^5-t^4z^4+4t^3z^3+3t^2z^2-3tz-1\right)+t^3z^4+2t^2z^3-2tz^2-4z}{t^6z^5+t^5z^4-t^4z^4-4t^4z^3-t^3z^3-3t^3z^2+3t^2z^2+3t^2z+2tz+t-1},
\end{aligned} \tag{42}$$

$$\begin{aligned}
\sum_{m=0}^{\infty} \mathrm{ZZ}(Z_5(m,5),z)t^m &= \frac{1}{t}\,\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{\frac{-1}{1+zt}+zt}+zt}+zt}+zt}+t}-\frac{1}{t} \\
&= \frac{\left(-t^5z^5-t^4z^4+4t^3z^3+3t^2z^2-3tz-1\right)-t^4z^5+5t^2z^3-5z}{t^6z^5+t^5z^4-t^4z^4-4t^4z^3-t^3z^3-3t^3z^2+3t^2z^2+3t^2z+2tz+t-1}.
\end{aligned} \tag{43}$$

Expansion of these formulas in a power series in the variable t and retaining the expansion coefficient of t^m produces the Zhang-Zhang polynomials for the generalized multiple zigzag chain $Z_k(m,5)$. The Zhang-Zhang polynomials for the generalized multiple zigzag chain $Z_k(m,n)$ can be obtained analogously. The Zhang-Zhang polynomials for the multiple zigzag chain $Z(m,n)$ are of particular importance for the general theory of Zhang-Zhang polynomials of benzenoid structures. For this reason, in the next section we derive explicit closed-form formulas for these structures for arbitrary values of the indices n and m.

3 Zhang–Zhang polynomials of multiple zigzag chains $Z(m,n)$

Closed-form, compact expressions for the ZZ polynomials of the $Z(m,n)$ structures can be obtained by formal expansion of the generating functions $F_{0,n}(t)-\frac{1}{t}$ in power series in the variable t. We obtain the following formulas *via* the standard binomial expansion of the generating functions

$$F_{0,0}(t) - \frac{1}{t} = (1-t)^{-1} = \sum_{k=0}^{\infty} \binom{-1}{k} (-1)^k t^k, \tag{44}$$

$$F_{0,1}(t) - \frac{1}{t} = \left((1+zt)^{-1} - t\right)^{-1} \tag{45}$$

$$= \sum_{k=0}^{\infty} \binom{-1}{k} (-1)^k t^k (1+zt)^{1+k}$$

$$= \sum_{k=0}^{\infty} \binom{-1}{k} (-1)^k t^k \sum_{j=0}^{\infty} \binom{1+k}{j} z^j t^j$$

$$= \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} \binom{-1}{k} \binom{1+k}{j} (-1)^k z^j t^{k+j}, \tag{46}$$

$$F_{0,2}(t) - \frac{1}{t} = \left(\left((1-zt)^{-1} + zt\right)^{-1} - t\right)^{-1}$$

$$= \sum_{k=0}^{\infty} \binom{-1}{k} (-1)^k t^k \left((1-zt)^{-1} + zt\right)^{1+k}$$

$$= \sum_{k=0}^{\infty} \binom{-1}{k} (-1)^k t^k \sum_{j=0}^{\infty} \binom{1+k}{j} z^j t^j (1-zt)^{-1-k+j}$$

$$= \sum_{k=0}^{\infty} \binom{-1}{k} (-1)^k t^k \sum_{j=0}^{\infty} \binom{1+k}{j} z^j t^j \sum_{l=0}^{\infty} \binom{-1-k+j}{l} (-1)^l t^l z^l$$

$$= \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} \sum_{l=0}^{\infty} \binom{-1}{k} \binom{1+k}{j} \binom{-1-k+j}{l} (-1)^{k+l} z^{j+l} t^{k+j+l}. \tag{47}$$

These expansions can be further put in more transparent form using the fact that $\binom{-1}{k} = (-1)^k$ and introducing a unified notation for the summation indices. We have

$$F_{0,0}(t) - \frac{1}{t} = \sum_{k_0=0}^{\infty} t^{k_0}, \tag{48}$$

$$F_{0,1}(t) - \frac{1}{t} = \sum_{k_0=0}^{\infty} \sum_{k_1=0}^{\infty} \binom{1+k_0}{k_1} z^{k_1} t^{k_0+k_1}, \tag{49}$$

$$F_{0,2}(t) - \frac{1}{t} = \sum_{k_0=0}^{\infty} \sum_{k_1=0}^{\infty} \sum_{k_2=0}^{\infty} \binom{1+k_0}{k_1} \binom{-1-k_0+k_1}{k_2} (-1)^{k_2} z^{k_1+k_2} t^{k_0+k_1+k_2}. \tag{50}$$

It is not difficult to see that an analogous expansion applied to $F_{0,n}(t)$ yields

$$F_{0,n}(t) - \frac{1}{t} =$$
$$= \sum_{k_0=0}^{\infty} \cdots \sum_{k_n=0}^{\infty} \prod_{j=0}^{n-1} \binom{(-1)^j \left(1 + \sum_{i=0}^{j} (-1)^i k_i\right)}{k_{j+1}} (-1)^{k_2+k_4+\cdots+k_{2\lfloor \frac{n}{2} \rfloor}} (tz)^{k_1+\cdots+k_n} t^{k_0}. \quad (51)$$

In order to make these expansions useful for the purpose of determination of the ZZ polynomials of the $Z(m,n)$ structures, we apply the following sum rotation identity

$$\sum_{k_0=0}^{\infty} \cdots \sum_{k_n=0}^{\infty} c_{k_0,\ldots,k_n} t^{k_0+\cdots+k_n} = \sum_{l_0=0}^{\infty} \left[\sum_{l_1=0}^{l_0} \sum_{l_2=0}^{l_1} \cdots \sum_{l_n=0}^{l_{n-1}} c_{l_0-l_1, l_1-l_2, \ldots, l_{n-1}-l_n, l_n} \right] t^{l_0}, \quad (52)$$

being the immediate $(n+1)$-dimensional generalization of the well-known [24] 2-dimensional case

$$\sum_{k_0=0}^{\infty} \sum_{k_1=0}^{\infty} c_{k_0,k_1} t^{k_0+k_1} = \sum_{l_0=0}^{\infty} \left[\sum_{l_1=0}^{l_0} c_{l_0-l_1,l_1} \right] t^{l_0}. \quad (53)$$

The change of indices

$$k_i \to \begin{cases} l_i - l_{i+1} & \text{when } i = 0, \ldots, n-1 \\ l_i & \text{when } i = n \end{cases} \quad (54)$$

implied by the sum rotation identity immediately gives

$$k_0 + \cdots + k_n \;\to\; l_0 \quad (55a)$$
$$k_1 + \cdots + k_n \;\to\; l_1 \quad (55b)$$
$$1 + 2k_0 - \sum_{i=0}^{j} k_i \;\to\; 1 + l_0 - 2l_1 + l_{j+1} \quad (55c)$$
$$k_2 + k_4 + \cdots + k_{2\lfloor \frac{n}{2} \rfloor} \to l_2 - l_3 + l_4 - l_5 + \cdots + (-1)^n l_n. \quad (55d)$$

Since

$$(-1)^{k_2+k_4+\cdots+k_{2\lfloor \frac{n}{2} \rfloor}} \to (-1)^{l_2-l_3+l_4-l_5+\cdots+(-1)^n l_n} = \prod_{j=2}^{n} (-1)^{l_j} \quad (56)$$

we can express after some rearrangements $F_{0,n}(t) - \frac{1}{t}$ in the following form

$$F_{0,n}(t) - \frac{1}{t} =$$
$$= \sum_{m=0}^{\infty} t^m \left\{ \sum_{l_1=0}^{m} z^{l_1} \left[\sum_{l_2=0}^{l_1} \cdots \sum_{l_n=0}^{l_{n-1}} \prod_{j=2}^{n+1} (-1)^{l_j} \binom{(-1)^j \left(1 + m + 2\sum_{i=1}^{j-2} (-1)^i l_i\right) - l_{j-1}}{l_{j-1} - l_j} \right] \right\}, \quad (57)$$

where we have replaced l_0 by m and introduced an auxiliary index $l_{n+1} = 0$. A comparison of Eq. (57) with Eq. (5) gives the expression for the ZZ polynomial of a structure $Z(m,n)$ in the following form

$$\mathrm{ZZ}(Z(m,n),x) = \sum_{l_1=0}^{m} d_{l_1}(1+x)^{l_1}, \tag{58}$$

where z was replaced by $1+x$ and the coefficient d_{l_1} is given explicitly by

$$d_{l_1} = \sum_{l_2=0}^{l_1} \cdots \sum_{l_n=0}^{l_{n-1}} \prod_{j=2}^{n+1} (-1)^{l_j} \binom{(-1)^j \left(1+m+2\sum_{i=1}^{j-2}(-1)^i l_i\right) - l_{j-1}}{l_{j-1}-l_j}. \tag{59}$$

Example 8. In the case $n = 1$, we obtain directly from Eqs. (58) and (59)

$$\mathrm{ZZ}(Z(m,1),x) = \sum_{l_1=0}^{m} \binom{1+m-l_1}{l_1} (1+x)^{l_1}, \tag{60}$$

which is identical to the expression for $\mathrm{ZZ}(Z(m,1),x)$ given by Eq. (12) of [8].

Example 9. For $n = 2$, we obtain from Eqs. (58) and (59)

$$\begin{aligned} \mathrm{ZZ}(Z(m,2),x) &= \sum_{l_1=0}^{m} \sum_{l_2=0}^{l_1} \prod_{j=2}^{3} (-1)^{l_j} \binom{(-1)^j \left(1+m+2\sum_{i=1}^{j-2}(-1)^i l_i\right) - l_{j-1}}{l_{j-1}-l_j} (1+x)^{l_1} \\ &= \sum_{l_1=0}^{m} \sum_{l_2=0}^{l_1} (-1)^{l_2} \binom{1+m-l_1}{l_1-l_2} \binom{-1-m+2l_1-l_2}{l_2} (1+x)^{l_1} \end{aligned} \tag{61}$$

Explicitly evaluating this formula at $m = 1, 2, \ldots$ yields exactly the polynomials $\mathrm{ZZ}(Z(m,2),x)$ previously given by Eqs. (47) in [11]. We would not be surprised if the inner sum could be evaluated to a more compact form. A similar remark seems to be appropriate for the multiple sums appearing in the functional form of the coefficient d_{l_1} in Eq. (59). We communicate this anticipated simplification to stimulate other researchers to attempt this task.

The Zhang-Zhang polynomials for multiple zigzag chains $Z(m,n)$ obtained from Eqs. (58) and (59) also agree with the ones given in Table I of [11] for $m = 3, 4, 5$. However, the closed form reported here is structurally very different from the form of previously reported Zhang-Zhang polynomials for $m = 4, \ldots, 9$ and arbitrary n [11, 15] in that it has n nested summations. This makes it difficult to directly compare these formulas and suggests that it may be possible to further simplify Eq. (59). We are planning to investigate this possibility in near future.

4 Application to Kekulé structures of multiple zigzag chains $Z(m, n)$

The obtained results have an immediate application to the theory of Kekulé structures of multiple zigzag chains $Z(m, n)$. The number of Kekulé structures of $Z(m, n)$ is equal to the coefficient c_0 in the ZZ polynomial corresponding to a given multiple zigzag chain $Z(m, n)$. It is easy to notice that $c_0 = \mathrm{ZZ}(Z(m, n), 0)$, so the generating function for the number of Kekulé structures in multiple zigzag chains $Z(m, n)$, analogous to that one in Eq. (5), is again given by Eq. (36), but this time with the linear fractional transformation $\tau(a)$ defined by

$$\tau(a) = -\frac{1}{a+t}, \tag{62}$$

which is simply the original linear fractional transformation $\tau(a)$ defined by Eq. (21) evaluated at $x = 0$ (i.e., $z = 1$). Accordingly, the number of Kekulé structures for a multiple zigzag chain $Z(m, n)$ is given by a modified version of Eq. (58) evaluated at $x = 0$ and expressed explicitly by

$$c_0 = \sum_{l_1=0}^{m} d_{l_1}, \tag{63}$$

with the coefficients d_{l_1} given by Eq. (59). Computing this sum in a more compact form has not been achieved and remains one of the challenges of the general theory of Kekulé structures.

He *et al.* [23] derived a different way to obtain the Kekulé structure count for single zigzag chains $Z(m, 1)$, which, surprisingly, also makes use of continued fractions. Specifically, the number of Kekulé structures can be expressed using the linear fractional transformation

$$\tau_3(a) = -\frac{1}{a+3}, \tag{64}$$

which happens to be the linear fractional transformation given by Eq. (62) evaluated at $t = 3$, and is given by

$$\mathrm{ZZ}(Z(m,1),1) = \prod_{k=0}^{\left\lfloor \frac{m-1}{2} \right\rfloor} \left(t_k + \tau_3^k(0)\right), \tag{65}$$

where

$$t_k = \begin{cases} 3 & \text{for } k < \left\lfloor \frac{m-1}{2} \right\rfloor \\ 3 & \text{for } k = \left\lfloor \frac{m-1}{2} \right\rfloor \text{ and } m \text{ even} \\ 2 & \text{for } k = \left\lfloor \frac{m-1}{2} \right\rfloor \text{ and } m \text{ odd.} \end{cases}$$

Eq. (65) can be explicitly written as

$$\mathrm{ZZ}(Z(m,1),1) = \underbrace{3\left(3-\tfrac{1}{3}\right)\left(3-\frac{1}{3-\frac{1}{3}}\right)\cdots\left(3-\cfrac{1}{3-\ddots-\cfrac{1}{3-\frac{1}{3}}}\right)\left(t_{\left\lfloor\frac{m-1}{2}\right\rfloor}-\cfrac{1}{3-\cfrac{1}{3-\ddots-\cfrac{1}{3-\frac{1}{3}}}}\right)}_{\left\lfloor\frac{m+1}{2}\right\rfloor \text{ factors}}.$$

This shows that, for single zigzag chains $Z(m,1)$, the Kekulé structure counts $\mathrm{ZZ}(Z(m,1),1)$ and their generating function

$$\sum_{m=0}^{\infty} \mathrm{ZZ}(Z(m,1),1)t^m = \frac{-1}{\tau(1)+t} = \frac{-1}{\frac{-1}{1+t}+t}, \tag{66}$$

can both be written in form of highly regular continued fractions, suggesting a much deeper connection between resonance structures of zigzag chains and continued fraction expressions. It might be worth to investigate whether the coefficients d_{l_1} in Eq. (59) can be formulated as some continued fraction.

Note further that, since the Kekulé structure counts $\mathrm{ZZ}(Z(m,1),1)$ are given by the Fibonacci numbers [25], Eq. (65) produces exactly the $(m+2)^{\mathrm{nd}}$ Fibonacci number.

5 Conclusion

Generating functions of the Zhang-Zhang polynomials of multiple zigzag chains $Z(m,n)$ and generalized multiple zigzag chains $Z_k(m,n)$ have been derived for arbitrary values of m and k. The generating functions for the Zhang-Zhang polynomials of $Z(m,n)$ can be expressed in the form of highly regular finite continued fractions,

$$\begin{aligned} \sum_{m=0}^{\infty} \mathrm{ZZ}(Z(m,n),z)t^m &= \left[0; -t, (-1)^2 zt, (-1)^3 zt, \ldots, (-1)^n zt, 1+(-1)^{n+1} zt\right] \\ &= -\left(\tau^n\left((-1)^{n+1}\right)+t\right)^{-1}, \end{aligned} \tag{67}$$

where $\tau(a) = -(a + zt)^{-1}$, while the generating functions for the Zhang-Zhang polynomials of $Z_k(m,n)$ are products of such continued fractions. For the particularly important case of the multiple zigzag chains $Z(m,n)$, the generating functions have been expanded to yield a closed form for the Zhang-Zhang polynomials of multiple zigzag chains $Z(m,n)$ that is valid for arbitrary values of m and n.

References

[1] H. P. Zhang, F. J. Zhang, The Clar covering polynomial of hexagonal systems I, *Discr. Appl. Math.* **69** (1996) 147–167.

[2] F. J. Zhang, H. P. Zhang, Y. T. Liu, The Clar covering polynomial of hexagonal systems II, *Chin. J. Chem.* **14** (1996) 321–325.

[3] H. P. Zhang, The Clar covering polynomial of hexagonal systems with an application to chromatic polynomials, *Discr. Math.* **172** (1997) 163–173.

[4] H. P. Zhang, F. J. Zhang, The Clar covering polynomial of hexagonal systems III, *Discr. Math.* **212** (2000) 261–269.

[5] T. F. Yen, Resonance topology of polynuclear aromatic hydrocarbons, *Theor. Chim. Acta* **20** (1971) 399–404.

[6] E. Clar, *The Aromatic Sextet*, Wiley, London, 1972.

[7] I. Gutman, B. Furtula, A. T. Balaban, Algorithm for simultaneous calculation of Kekulé and Clar structure counts, and Clar number of benzenoid molecules, *Polycyc. Arom. Comp.* **26** (2006) 17–35.

[8] C. P. Chou, H. A. Witek, An algorithm and FORTRAN program for automatic computation of the Zhang–Zhang polynomial of benzenoids, *MATCH Commun. Math. Comput. Chem* **68** (2012) 3–30.

[9] C. P. Chou, H. A. Witek, ZZDecomposer: A graphical toolkit for analyzing the Zhang–Zhang polynomials of benzenoid structures, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 741–764.

[10] H. P. Zhang, N. D. Ji, H. Y. Yao, Transfer–matrix calculation of the Clar covering polynomial of hexagonal systems, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 379–392.

[11] C. P. Chou, Y. T. Li, H. A. Witek, Zhang–Zhang polynomials of various classes of benzenoid systems, *MATCH Commun. Math. Comput. Chem.* **68** (2012) 31–64.

[12] Q. Z. Guo, H. Y. Deng, D. D. Chen, Zhang–Zhang polynomials of cyclo-polyphenacenes, *J. Math. Chem.* **46** (2009) 347–362.

[13] C. P. Chou, H. A. Witek, Comment on "Zhang–Zhang polynomials of cyclo-polyphenacenes" by Q. Guo, H. Deng, and D. Chen, *J. Math. Chem.* **50** (2012) 1031–1033.

[14] C. P. Chou, H. A. Witek, Two examples for the application of the ZZDecomposer: Zigzag–edge coronoids and fenestrenes, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 421–426.

[15] C. P. Chou, H. A. Witek, Determination of Zhang–Zhang polynomials for various classes of benzenoid systems: Non–heuristic approach, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 75–104.

[16] M. Randić, Resonance energy of very large benzenoid hydrocarbons, *Int. J. Quantum Chem.* **17** (1980) 549–586.

[17] I. Gutman, B. Borovićanin, Zhang–Zhang polynomial of multiple linear hexagonal chains, *Z. Naturforsch.* **61a** (2006) 73–77.

[18] C. P. Chou, H. A. Witek, Closed–form formulas for the Zhang–Zhang polynomials of benzenoid structures: Chevrons and generalized chevrons, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 105–124.

[19] C.-P. Chou, J.-S. Kang, H. A. Witek, Closed–form formulas for the Zhang–Zhang polynomials of benzenoid structures: Prolate rectangles and their generalizations, *Discr. Appl. Math.* **198** (2016) 101–108.

[20] D. D. Chen, H. Y. Deng, Q. Z. Guo, Zhang–Zhang polynomials of a class of pericondensed benzenoid graphs, *MATCH Commun. Math. Comput. Chem.* **63** (2010) 401–410.

[21] H. A. Witek, G. Moś, C. P. Chou, Zhang–Zhang polynomials of regular 3- and 4-tier benzenoid strips, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 427–442.

[22] H. A. Witek, J. Langner, G. Moś, C. P. Chou, Zhang–Zhang polynomials of regular 5-tier benzenoid strips, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 487–504.

[23] W. J. He, W. C. He, S. L. Xie, Algebraic expressions for Kekulé structure counts of nonbranched cata-condensed benzenoid, *Discr. Appl. Math.* **35** (1992) 91–106.

[24] E. Hansen, *A Table of Series and Products*, Prentice Hall, Englewood Cliffs, 1975, pp. 14–14.

[25] A. T. Balaban, I. Tomescu, Chemical graphs. XLI. Numbers of conjugated circuits and Kekulé structures for zigzag catafusenes a nd (J, K)–hexes; generalized fibonacci numbers, *MATCH Commun. Math. Comput. Chem.* **17** (1985) 91–120.