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Zhang–Zhang Polynomials of Regular 5-tier Benzenoid Strips

Henryk A. Witek*[a], Johanna Langner[a], Grzegorz Moś[b], Chien-Pin Chou[a]

[a] *Department of Applied Chemistry and Institute of Molecular Science, National Chiao Tung University, Hsinchu 30010, Taiwan*

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

*hwitek@mail.nctu.edu.tw

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Abstract

Formal derivations of closed-form expressions for Clar covering polynomials (*aka* Zhang–Zhang polynomials or ZZ polynomials) of twelve classes of regular 5-tier benzenoid strips are presented. The derived formulas, together with the results reported previously in the literature, complete the full collection of ZZ polynomial formulas for the regular 5-tier benzenoid strips.

1. Introduction

The regular 5-tier benzenoids constitute an important class of benzenoid structures [1,2]. This class consists of 27 families of structures, which are schematically depicted in Figure 1. The common characteristic of all benzenoids belonging to this class are: i) they can be constructed by merging five strips of 1-tier benzenoids (i.e., polyacenes), ii) two adjacent strips differ at each end by $\pm\frac{1}{2}$ hexagon unit, and iii) the terminal strips have the same length n. The families 1–16 are structurally related with the lower and upper terminal strips being located exactly above each other. Similarly, the families 17–26 are structurally related with the lower and upper terminal strips being shifted with respect to each other by one hexagon unit. The last family, $M(5,n)$, with the horizontal shift of two hexagon units between the lower and upper strip, is unique and is not directly related to any of the other families.

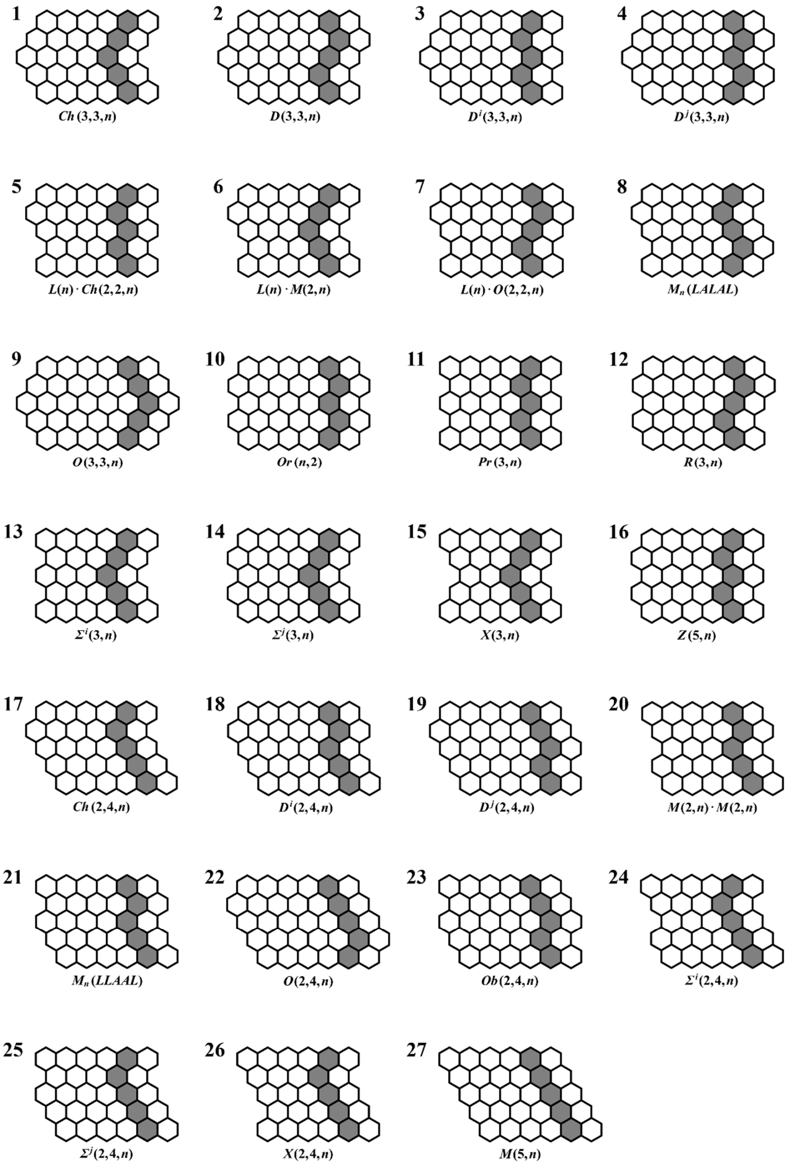


Figure 1. 27 families of regular 5-tier benzenoid strips. The shaded hexagons represent schematically a segment of a width $\boldsymbol{n-5}$.

The regular 5-tier benzenoids have been extensively studied [1–6], with particular attention to the structural relations between the families and to the closed form formulas for their number of Kekulé structures (i.e., the zeroth-order Clar covers). For some of the families, closed-form formulas for higher-order Clar covers [7] were also reported [8–12] in the form of an appropriate Clar covering polynomial (*aka* the Zhang–Zhang polynomial or the ZZ polynomial) [13–16].

In this paper we present a review of available results on the ZZ polynomials of the regular 5-tier benzenoids together with a derivation of closed-form ZZ polynomials for the remaining classes of regular 5-tier benzenoids, which are not available in the literature. The formal derivations are obtained using the graphical computer environment called ZZDecomposer developed recently in our group [17]. ZZDecomposer is a collection of formal programming tools that can be used for: i) easy and convenient construction of a graph representing a given benzenoid structure, ii) brute force computation of the ZZ polynomial of such a graph, iii) construction of a graph decomposition tree allowing for formal derivation of the ZZ polynomial of such a graph based on the recursive properties of ZZ polynomials, iv) construction and management of a library of ZZ polynomials of subgraphs of a given graph, v) saving the produced results in a ready-to-publish vector format. All the described here functionalities of the ZZDecomposer environment make it an indispensable tool in the research of ZZ polynomials, allowing one to conduct formal proofs of theorems and finding closed-form formulas related to ZZ polynomials. ZZDecomposer has been extensively used [10–12,17–19] to augment the rich collection of results pertaining to the general theory of ZZ polynomials [20–30].

The concept of the Clar covering polynomial (*aka* the Zhang–Zhang polynomial or the ZZ polynomial) was introduced by Zhang and Zhang [13–16] in order to facilitate the enumeration of Clar covers [7] of benzenoid structures. A Clar cover of a benzenoid structure S can be defined from two different perspectives. From the chemical point of view, a Clar cover is a resonance structure of S, in which every carbon atom is involved in either a double π bond or in an aromatic π sextet. From the graph-theoretical point of view, a Clar cover of S (perceived as a 2-connected subgraph of a hexagonal lattice) is a spanning subgraph of S such that every component of it is either a hexagon or an edge. The ZZ polynomial of a benzenoid structure S has the following form

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

where the Clar number Cl denotes the maximal number of aromatic sextets that can be accommodated inside a given benzenoid S and the coefficients c_k denote the number of Clar covers of order k (i.e., Clar covers containing exactly k aromatic sextets) conceivable for a given benzenoid S. The combinatorial polynomial in the dummy variable x given by Eq. (1) can be thought of as a generating function for the sequence of the numbers of Clar covers $(c_0, c_1, c_2, \dots, c_{Cl})$ conceivable for a given benzenoid S. Zhang and Zhang demonstrated [13–16] that the ZZ polynomials possess a number of recursive properties, which makes their determination more convenient and straightforward than the determination of only some selected coefficients c_k. The recursive properties of the ZZ polynomials were used to propose computer algorithms [17,25,31] aiming at automatized determination of the ZZ polynomials and resulted in computer software (ZZCalculator and ZZDecomposer) capable of computing the ZZ polynomials for a large class of benzenoid structures [8,25,26] and deriving a number of formal results in the theory of ZZ polynomials [9–12,17–19]. Recent demonstration [32,33] of the equivalence between the ZZ polynomials and the cube polynomials extended the field of applicability of the developed theoretical tools also to the theory of cube polynomials.

2. Review of previous results

The closed-form ZZ polynomial formulas for some of the classes of regular 5-tier benzenoid strips (for the complete list of all classes see Figure 1) were reported previously in the literature. The exposition below collects known results and gives compact representations of the available formulas that may prove useful for deriving the general theory of ZZ polynomials.

The ZZ polynomial for the parallelogram $M(5,n)$ is a special case of the ZZ polynomials of general parallelograms $M(m,n)$ derived by Gutman and Borovićanin [11,17,22,26]. We have

$$ZZ(M(m,n),x) \quad = \quad {}_2F_1\left[{-m,-n \atop 1}; 1+x\right] \quad = \quad \sum_{k=0}^{\min(m,n)} \binom{m}{k}\binom{n}{k}(1+x)^k . \tag{2}$$

The ZZ polynomial for the prolate rectangle $Pr(3,n)$ is a special case of the ZZ polynomial of a general prolate rectangle $Pr(m,n)$ derived by Zhang and Zhang [12,16]. We have

$$ZZ(Pr(m,n),x) \quad = \quad \big(1+n(1+x)\big)^m . \tag{3}$$

The ZZ polynomials for the chevrons $Ch(3,3,n)$ and $Ch(2,4,n)$ are special cases of the ZZ polynomial of a general chevron $Ch(k,m,n)$ derived by Chou and Witek [11]. We have

$$ZZ(Ch(3,3,n),x) = \sum_{k=0}^{5}\left[\binom{5}{k}\binom{n}{k} + 4\binom{3}{k-2}\binom{n+1}{k} + \binom{1}{k-4}\binom{n+2}{k}\right](1+x)^k, \quad (4)$$

$$ZZ(Ch(4,2,n),x) = \sum_{k=0}^{5}\left[\binom{5}{k}\binom{n}{k} + 3\binom{3}{k-2}\binom{n+1}{k}\right](1+x)^k. \quad (5)$$

The ZZ polynomial of the goblet $X(3,n)$ vanishes owing to the concealed non-Kekuléan character [6,34] of this structure

$$ZZ(X(3,n),x) = 0. \quad (6)$$

The form of the ZZ polynomials for oblate streamers $\Sigma^j(3,n)$ and $\Sigma^j(2,4,n)$ and the structures $M(2,n)\cdot M(2,n)$ were not reported explicitly before, but the formulas are a direct consequence of Theorem 7 of [11], which states that the ZZ polynomial of two fused parallelograms is equal to the product of the ZZ polynomials of both parallelograms. We have

$$\left.\begin{array}{r} ZZ(\Sigma^j(3,n),x) \\ ZZ(M(2,n)\cdot M(2,n),x) \end{array}\right\} = ZZ(M(2,n),x)\cdot ZZ(M(2,n),x) \quad (7)$$

$$= \sum_{k=0}^{4}\left[\binom{4}{k}\binom{n}{k} + 4\binom{2}{k-2}\binom{n+1}{k} + \binom{0}{k-4}\binom{n+2}{k}\right](1+x)^k$$

and

$$ZZ(\Sigma^j(2,4,n),x) = ZZ(M(1,n),x)\cdot ZZ(M(3,n),x) \quad (8)$$

$$= \sum_{k=0}^{4}\left[\binom{4}{k}\binom{n}{k} + 3\binom{2}{k-2}\binom{n+1}{k}\right](1+x)^k.$$

Similarly, the explicit forms of the ZZ polynomials for the structures $L(n)\cdot O(2,2,n)$ and $L(n)\cdot Ch(2,2,n)$ have never been reported before but the formulas follow directly from Theorem 2 of [12], which states that the ZZ polynomial of a parallelogram fused with another benzenoid is equal to the product of the ZZ polynomials of both fragments. We have

$$ZZ(L(n)\cdot O(2,2,n),x) = ZZ(M(1,n),x)\cdot ZZ(O(2,2,n),x) \quad (9)$$

$$= \sum_{k=0}^{5}\left[\binom{5}{k}\binom{n}{k} + \left\{6\binom{3}{k-2} - \binom{2}{k-2}\right\}\binom{n+1}{k} + \left\{3\binom{1}{k-4} + \binom{1}{k-3}\right\}\binom{n+2}{k}\right](1+x)^k,$$

$$ZZ(L(n)\cdot Ch(2,2,n),x) = ZZ(M(1,n),x)\cdot ZZ(Ch(2,2,n),x) \quad (10)$$

$$= \sum_{k=0}^{4}\left[\binom{4}{k}\binom{n}{k} + \left\{5\binom{2}{k-2} - \binom{1}{k-2}\right\}\binom{n+1}{k} + \left\{\binom{0}{k-4} + \binom{1}{k-3}\right\}\binom{n+2}{k}\right](1+x)^k.$$

ZZ polynomials for a number of a few other families of regular 5-tier benzenoid strips (zigzag chain $Z(5,n)$, oblate rectangle $Or(n,2)$, intermediate rectangle $R(3,n)$, oblate pentagon $D^j(3,n)$, and hexagon $O(3,3,n)$) were obtained before in more or less explicit form using standard decomposition techniques. These results are summarized below. The lengthy formulas for the ZZ polynomial of $Z(5,n)$ discovered by us previously and given by Eq. (45) of [8] and by Eqs. (34) and (35) of [10] can be rewritten in a compact form as follows

$$ZZ(Z(5,n),x) = \sum_{k=0}^{5}\left[\binom{5}{k}\binom{n}{k} + \left\{7\binom{3}{k-2} - \binom{2}{k-2}\right\}\binom{n+1}{k} + \right. \\ \left. + \left\{7\binom{1}{k-4} + \binom{0}{k-3}\right\}\binom{n+2}{k} + \binom{0}{k-5}\binom{n+3}{k}\right](1+x)^k . \tag{11}$$

Similarly, the lengthy formulas for $Or(n,2)$ (Eq. (58) of [8] and Eq. (46) of [10]), $O(3,3,n)$ (Eq. (37) of [8] and Eqs. (70) and (71) of [10]), $R(3,n)$ (Eq. (45) of [10]), and $D^j(3,n)$ (Eq. (69) of [10]) can be rewritten in a compact, isostructural and more explicit form as follows

$$ZZ(Or(n,2),x) = \sum_{k=0}^{7}\left[\binom{7}{k}\binom{n}{k} + \left\{10\binom{5}{k-2} - \binom{4}{k-2}\right\}\binom{n+1}{k} + \binom{0}{k-7}\binom{n+4}{k} + \right. \\ + \left\{20\binom{3}{k-4} + \binom{1}{k-3} - \binom{1}{k-5}\right\}\binom{n+2}{k} + \\ \left. + \left\{10\binom{1}{k-6} + \binom{0}{k-5} + \binom{1}{k-5}\right\}\binom{n+3}{k}\right](1+x)^k , \tag{12}$$

$$ZZ(O(3,3,n),x) = \sum_{k=0}^{9}\left[\binom{9}{k}\binom{n}{k} + \left\{10\binom{7}{k-2} - \binom{6}{k-2}\right\}\binom{n+1}{k} + \binom{2}{k-7}\binom{n+4}{k} + \right. \\ + \left\{20\binom{5}{k-4} + \binom{3}{k-3} - \binom{3}{k-5}\right\}\binom{n+2}{k} + \\ \left. + \left\{10\binom{3}{k-6} + \binom{2}{k-5} + \binom{3}{k-5}\right\}\binom{n+3}{k}\right](1+x)^k , \tag{13}$$

$$ZZ(R(3,n),x) = \sum_{k=0}^{6}\left[\binom{6}{k}\binom{n}{k} + \left\{8\binom{4}{k-2} - \binom{3}{k-2}\right\}\binom{n+1}{k} + \left\{10\binom{2}{k-4} + \right.\right. \\ \left.\left. + \binom{1}{k-3}\right\}\binom{n+2}{k} + \left\{\binom{0}{k-6} + \binom{1}{k-5}\right\}\binom{n+3}{k}\right](1+x)^k , \tag{14}$$

$$ZZ\left(D^j(3,n),x\right) = \sum_{k=0}^{8}\left[\binom{8}{k}\binom{n}{k} + \left\{10\binom{6}{k-2} - \binom{5}{k-2}\right\}\binom{n+1}{k} + \binom{1}{k-7}\binom{n+4}{k} + \right. \\ + \left\{20\binom{4}{k-4} + \binom{2}{k-3} - \binom{2}{k-5}\right\}\binom{n+2}{k} + \\ \left. + \left\{10\binom{2}{k-6} + \binom{1}{k-5} + \binom{2}{k-5}\right\}\binom{n+3}{k}\right](1+x)^k . \tag{15}$$

The ZZ polynomials for the remaining 12 families of regular 5-tier benzenoid strips have never been reported before. The main goal of the current work is to fill this gap.

3. New results

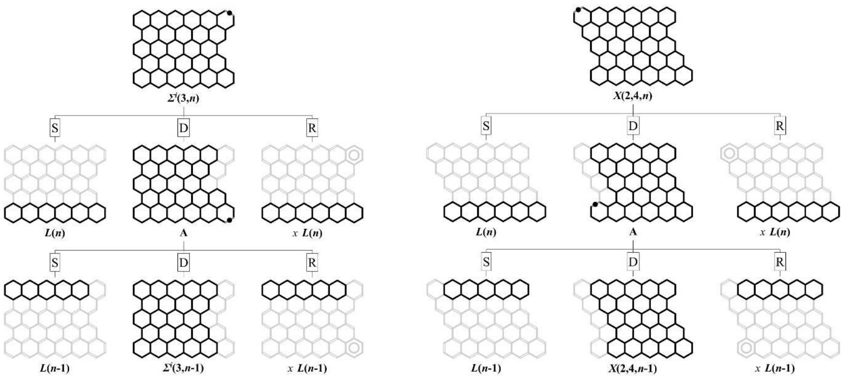
The ZZ polynomials for further four families of the regular 5-tier benzenoid strips can be expressed in a compact form owing to their essentially disconnected character. The ZZ polynomials of prolate streamers $\Sigma^i(3,n)$ and goblets $X(2,4,n)$ are given by

$$\left.\begin{array}{r} ZZ\big(\Sigma^i(3,n),x\big) \\ ZZ\big(X(2,4,n),x\big) \end{array}\right\} \;=\; \big(1+n(1+x)\big)^2 \tag{16}$$

and the ZZ polynomials of prolate streamers $\Sigma^i(2,4,n)$ and the structures $L(n)\cdot M(2,n)$ are given by

$$\left.\begin{array}{r} ZZ\big(\Sigma^i(2,4,n),x\big) \\ ZZ\big(L(n)\cdot M(2,n),x\big) \end{array}\right\} \;=\; \left(1+2n(1+x)+\binom{n}{2}(1+x)^2\right)\cdot\big(1+n(1+x)\big)\,. \tag{17}$$

Formal demonstration of these facts is based on the recurrence relations that can be obtained from graph decompositions of these structures performed with the ZZDecomposer program [17]. For the prolate streamers $\Sigma^i(3,n)$ and goblets $X(2,4,n)$, the recursive decomposition pathways given by



yield the same recurrence relation

$$ZZ(W(n),x) = ZZ(W(n-1),x) + (1+x)[ZZ(L(n),x) + ZZ(L(n-1),x)]\;, \tag{18}$$

where $W(n)$ denotes either of the $\Sigma^i(3,n)$ and $X(2,4,n)$ structures and $L(n)$ denotes a polyacene of length n with a ZZ polynomial given by [13]

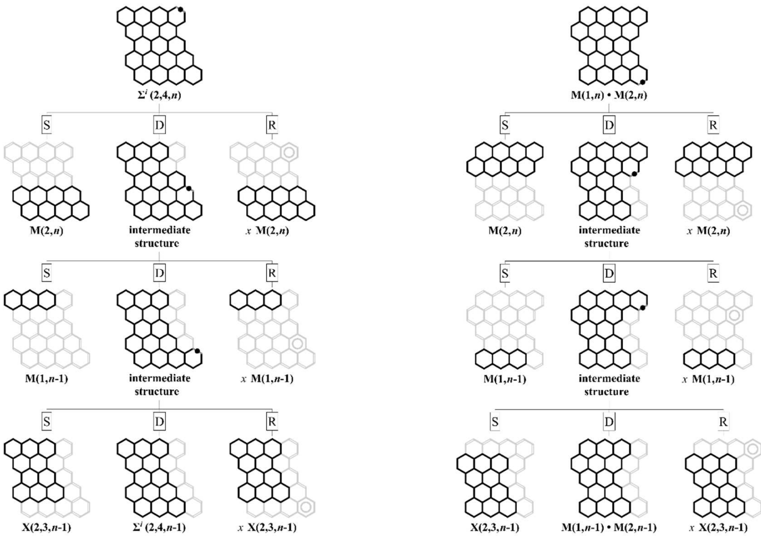
$$ZZ(L(n),x) = ZZ(M(1,n),x) = 1+n(1+x)\,. \tag{19}$$

The recurrence relation (18) can be telescopically folded to

$$ZZ(W(n),x) \quad = \quad ZZ(W(0),x) + (1+x)\left[\sum_{j=1}^{n} ZZ(L(j),x) + \sum_{j=0}^{n-1} ZZ(L(j),x)\right]. \qquad (20)$$

Initialization with the boundary conditions $ZZ(W(0),x) = ZZ(X(2,4,0),x) = ZZ\left(\Sigma^i(3,0),x\right) = 1$ yields the formula given by Eq. (16).

Similarly, for the prolate streamers $\Sigma^i(2,4,n)$ and the structures $L(n) \cdot M(2,n)$, the decomposition paths given by



yield the same recurrence relation

$$ZZ(W(n),x) = ZZ(W(n-1),x) + (1+x)[ZZ(M(2,n),x) + ZZ(L(n-1),x) + ZZ(X(2,3,n-1),x)]\,, \qquad (21)$$

where $W(n)$ denotes either $\Sigma^i(2,4,n)$ or $L(n) \cdot M(2,n)$, $ZZ(L(n),x)$ is given by Eq. (19), and the ZZ polynomials of the parallelogram $M(2,n)$ [17,22,25] and the goblet $X(2,3,n)$ [19] are given by

$$ZZ(M(2,n),x) = 1 + 2n(1+x) + \binom{n}{2}(1+x)^2\,, \qquad (22)$$

$$ZZ(X(2,3,n),x) = \big(1 + n(1+x)\big)^2\,. \qquad (23)$$

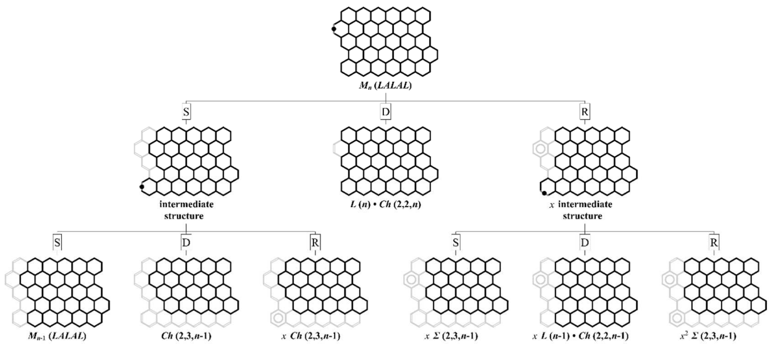
The recurrence relation (21) can be telescopically folded to

$$ZZ(W(n),x) = ZZ(W(0),x) + (1+x)\left[\sum_{j=1}^{n} ZZ(M(2,j),x) + \sum_{j=0}^{n-1}\big(ZZ(L(j),x) + ZZ(X(2,3,j),x)\big)\right]. \quad (24)$$

Initialization with the boundary conditions $ZZ(W(0),x) = ZZ\big(\Sigma^{i}(2,4,0),x\big) = ZZ(L(0)\cdot M(2,0),x) = 1$ yields the formula given by Eq. (17).

Multiple chain $\boldsymbol{M_n(LALAL)}$

The ZZ polynomial for the multiple chain $M_n(LALAL)$ can be derived using the following decomposition graph for this structure:



This decomposition yields the following recurrence relation

$$\begin{aligned} ZZ(M_n(LALAL),x) &= ZZ(M_{n-1}(LALAL),x) + ZZ(L(n)\cdot Ch(2,2,n),x) \\ &+ (1+x)\cdot ZZ(Ch(2,3,n-1),x) + x(1+x)\cdot ZZ(\Sigma(2,3,n-1),x) \\ &+ x\cdot ZZ(L(n-1)\cdot Ch(2,2,n-1),x)\ , \end{aligned} \quad (25)$$

which can be telescopically folded to

$$\begin{aligned} ZZ(M_n(LALAL),x) &= ZZ(M_0(LALAL),x) + \sum_{k=1}^{n} ZZ(L(k)\cdot Ch(2,2,k),x) \\ &+ (1+x)\sum_{k=0}^{n-1}[x\cdot ZZ(\Sigma(2,3,k),x) + ZZ(Ch(2,3,k),x)] \\ &+ x\sum_{k=0}^{n-1} ZZ(L(k)\cdot Ch(2,2,k),x)\ . \end{aligned} \quad (26)$$

Initialization of this formula with $ZZ(M_0(LALAL),x) = 1$ and substitution of $ZZ(L(n)\cdot Ch(2,2,n),x)$ given by Eq. (10), and the ZZ polynomials of the streamer $\Sigma(2,3,n)$ and the chevron $Ch(2,3,n)$ derived in [19] and [11,19], respectively, and given explicitly by

$$ZZ(\Sigma(2,3,n),x) = \sum_{k=0}^{3}\left[\binom{3}{k}\binom{n}{k} + 2\binom{1}{k-2}\binom{n+1}{k}\right](1+x)^k, \tag{27}$$

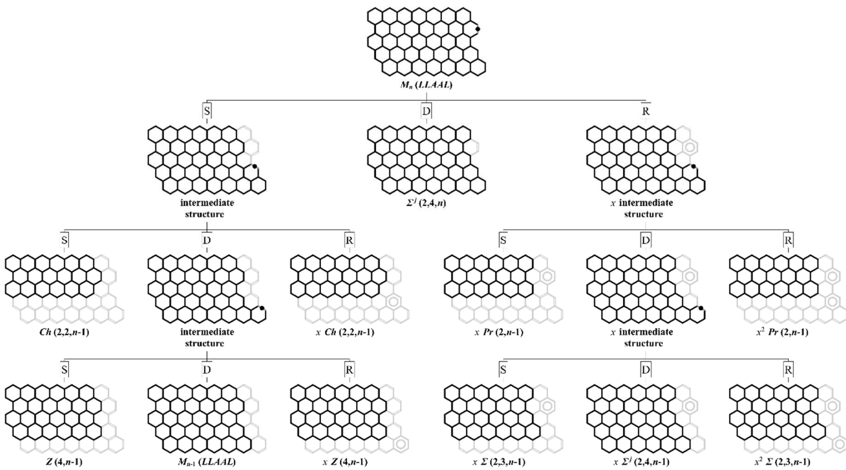
$$ZZ(Ch(2,3,n),x) = \sum_{k=0}^{4}\left[\binom{4}{k}\binom{n}{k} + 2\binom{2}{k-2}\binom{n+1}{k}\right](1+x)^k \tag{28}$$

gives after evaluation the following formula

$$\begin{aligned} ZZ(M_n(LALAL),x) \;&=\; \sum_{k=0}^{5}\Bigg[\binom{5}{k}\binom{n}{k} + \left\{6\binom{3}{k-2} - \binom{2}{k-2}\right\}\binom{n+1}{k} \\ &\quad + \left\{4\binom{1}{k-4} + \binom{1}{k-3}\right\}\binom{n+2}{k}\Bigg](1+x)^k . \end{aligned} \tag{29}$$

Multiple chain $M_n(LLAAL)$

The ZZ polynomial for the multiple chain $M_n(LLAAL)$ can be derived using the following decomposition graph for this structure:



This decomposition yields the following recurrence relation

$$\begin{aligned} ZZ(M_n(LLAAL),x) \;&=\; ZZ(M_{n-1}(LLAAL),x) + ZZ\big(\Sigma^j(2,4,n),x\big) + x\cdot ZZ\big(\Sigma^j(2,4,n-1),x\big) \\ &+\; (1+x)\cdot[ZZ(Ch(2,2,n-1),x) + ZZ(Z(4,n-1),x)] \\ &+\; x(1+x)\cdot[ZZ(\Sigma(2,3,n-1),x) + ZZ(Pr(2,n-1),x)] \;, \end{aligned} \tag{30}$$

which can be telescopically folded to

$$
\begin{aligned}
ZZ(M_n(LLAAL),x) &= ZZ(M_0(LLAAL),x) + \sum_{k=1}^{n} ZZ\big(\Sigma^j(2{,}4,k),x\big) + x\sum_{k=0}^{n-1} ZZ\big(\Sigma^j(2{,}4,k),x\big) \\
&+ (1+x)\sum_{k=0}^{n-1}[ZZ(Ch(2{,}2,k),x) + ZZ(Z(4,k),x)] \\
&+ x(1+x)\sum_{k=0}^{n-1}[ZZ(\Sigma(2{,}3,k),x) + ZZ(Pr(2,k),x)]\;. \qquad (31)
\end{aligned}
$$

Initialization of this formula with $ZZ(M_0(LLAAL),x) = 1$ and substitution of $ZZ\big(\Sigma^j(2{,}4,n),x\big)$ given by Eq. (8), $ZZ(\Sigma(2{,}3,n),x)$ given by Eq. (27), and the ZZ polynomials of the prolate rectangle $Pr(2,n)$ [10,16,19], the chevron $Ch(2{,}2,n)$ [8,10,11,19], and the multiple zigzag chain $Z(4,n)$ [8,10,19] given explicitly by

$$ZZ(Pr(2,n),x) = \sum_{k=0}^{2}\left[\binom{2}{k}\binom{n}{k} + \binom{0}{k-2}\binom{n+1}{k}\right](1+x)^k \qquad (32)$$

$$ZZ(Ch(2{,}2,n),x) = \sum_{k=0}^{3}\left[\binom{3}{k}\binom{n}{k} + \binom{1}{k-2}\binom{n+1}{k}\right](1+x)^k \qquad (33)$$

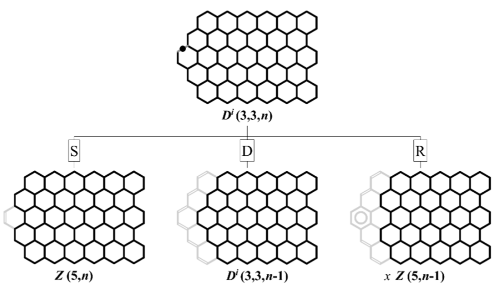
$$ZZ(Z(4,n),x) = \sum_{k=0}^{4}\left[\binom{4}{k}\binom{n}{k} + 3\binom{2}{k-2}\binom{n+1}{k} + \binom{0}{k-4}\binom{n+2}{k}\right](1+x)^k \qquad (34)$$

gives after evaluation the following formula

$$ZZ(M_n(LLAAL),x) = \sum_{k=0}^{5}\left[\binom{5}{k}\binom{n}{k} + 5\binom{3}{k-2}\binom{n+1}{k} + 3\binom{1}{k-4}\binom{n+2}{k}\right](1+x)^k\;. \qquad (35)$$

Prolate pentagon $D^i(3,3,n)$

The ZZ polynomial for the prolate pentagon $D^i(3{,}3,n)$ can be derived using the following decomposition graph for this structure:



This decomposition yields the following recurrence relation

$$ZZ\big(D^i(3,3,n),x\big) \quad = \quad ZZ\big(D^i(3,3,n-1),x\big) + ZZ(Z(5,n),x) + x \cdot ZZ(Z(5,n-1),x)\,, \qquad (36)$$

which can be telescopically folded to

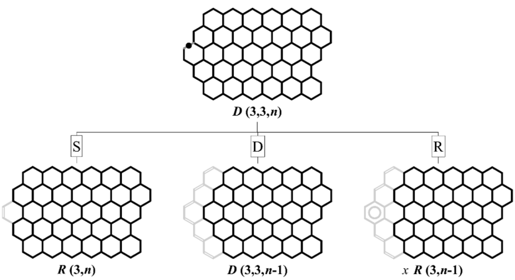
$$ZZ\big(D^i(3,3,n),x\big) \quad = \quad ZZ\big(D^i(3,3,0),x\big) + \sum_{k=1}^{n} ZZ(Z(5,k),x) + x\sum_{k=0}^{n-1} ZZ(Z(5,k),x)\,. \qquad (37)$$

Initialization of this formula with $ZZ\big(D^i(3,3,0),x\big) = 1$ and substitution of $ZZ(Z(5,n),x)$ given by Eq. (11) gives after evaluation the following formula

$$ZZ\big(D^i(3,3,n),x\big) = \sum_{k=0}^{6}\Bigg[\binom{6}{k}\binom{n}{k} + \left\{7\binom{4}{k-2} - \binom{3}{k-2}\right\}\binom{n+1}{k} + \\ + \left\{7\binom{2}{k-4} + \binom{1}{k-3}\right\}\binom{n+2}{k} + \binom{1}{k-5}\binom{n+3}{k}\Bigg](1+x)^k\,. \qquad (38)$$

Intermediate pentagon $D(3,3,n)$

The ZZ polynomial for the intermediate pentagon $D(3,3,n)$ can be derived using the following decomposition graph for this structure:



This decomposition yields the following recurrence relation

$$ZZ(D(3,3,n),x) \quad = \quad ZZ(D(3,3,n-1),x) + ZZ(R(3,n),x) + x \cdot ZZ(R(3,n-1),x)\,, \qquad (39)$$

which can be telescopically folded to

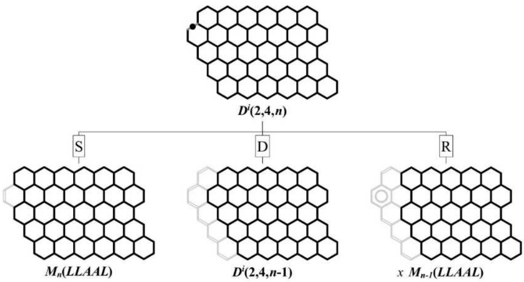
$$ZZ(D(3,3,n),x) \quad = \quad ZZ(D(3,3,0),x) + \sum_{k=1}^{n} ZZ(R(3,k),x) + x\sum_{k=0}^{n-1} ZZ(R(3,k),x)\,. \qquad (40)$$

Initialization of this formula with $ZZ(D(3,3,0),x) = 1$ and substitution of $ZZ(R(3,n),x)$ given by Eq. (14) gives after evaluation the following formula

$$ZZ(D(3,3,n),x) = \sum_{k=0}^{7} \Bigg[\binom{7}{k}\binom{n}{k} + \left\{ 8\binom{5}{k-2} - \binom{4}{k-2} \right\} \binom{n+1}{k} + \\ + \left\{ 10\binom{3}{k-4} + \binom{2}{k-3} \right\} \binom{n+2}{k} + \left\{ \binom{1}{k-6} + \binom{2}{k-5} \right\} \binom{n+3}{k} \Bigg] (1+x)^k \,. \tag{41}$$

Prolate pentagon $\boldsymbol{D^i(2,4,n)}$

The ZZ polynomial for the prolate pentagon $D^i(2,4,n)$ can be derived using the following decomposition graph for this structure:



This decomposition yields the following recurrence relation

$$\begin{aligned} ZZ\big(D^i(2,4,n),x\big) &= ZZ\big(D^i(2,4,n-1),x\big) + ZZ(M_n(LLAAL),x) \\ &+ x \cdot ZZ(M_{n-1}(LLAAL),x)\,, \end{aligned} \tag{42}$$

which can be telescopically folded to

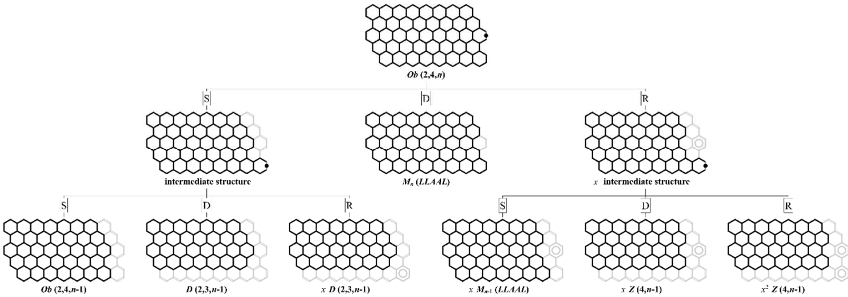
$$\begin{aligned} ZZ\big(D^i(2,4,n),x\big) &= ZZ\big(D^i(2,4,0),x\big) + \sum_{k=1}^{n} ZZ(M_k(LLAAL),x) \\ &+ x\sum_{k=0}^{n-1} ZZ(M_k(LLAAL),x)\,. \end{aligned} \tag{43}$$

Initialization of this formula with $ZZ\big(D^i(2,4,0),x\big) = 1$ and substitution of $ZZ(M_n(LLAAL),x)$ given by Eq. (35) gives after evaluation the following formula

$$ZZ\big(D^i(2,4,n),x\big) = \sum_{k=0}^{6} \left[\binom{6}{k}\binom{n}{k} + 5\binom{4}{k-2}\binom{n+1}{k} + 3\binom{2}{k-4}\binom{n+2}{k} \right] (1+x)^k \,. \tag{44}$$

Hexagon without two corners $Ob(2,4,n)$

The ZZ polynomial for the hexagon without two corners $Ob(2,4,n)$ can be derived using the following decomposition graph for this structure:



This decomposition yields the following recurrence relation

$$\begin{aligned} ZZ(Ob(2,4,n),x) \;&=\; ZZ(Ob(2,4,n-1),x) + ZZ(M_n(LLAAL),x) \\ &+\; x \cdot ZZ(M_{n-1}(LLAAL),x) + (1+x)\cdot ZZ(D(2,3,n-1),x) \\ &+\; x(1+x)\cdot ZZ(Z(4,n-1),x)\ , \end{aligned} \tag{45}$$

which can be telescopically folded to

$$ZZ(Ob(2,4,n),x) = ZZ(Ob(2,4,0),x) + (1+x)\sum_{k=0}^{n-1} ZZ(D(2,3,k),x) \tag{46}$$

$$+x\sum_{k=0}^{n-1} ZZ(M_k(LLAAL),x) + \sum_{k=1}^{n} ZZ(M_k(LLAAL),x) + x(1+x)\sum_{k=0}^{n-1} ZZ(Z(4,k),x)\ .$$

Initialization of this formula with $ZZ(Ob(2,4,0),x) = 1$ and substitution of $ZZ(M_n(LLAAL),x)$ given by Eq. (35), $ZZ(Z(4,n),x)$ given by Eq. (34), and the ZZ polynomial of the pentagon $D(2,3,n)$ derived in [10,19] and explicitly given by

$$ZZ(D(2,3,n),x) = \sum_{k=0}^{5}\left[\binom{5}{k}\binom{n}{k} + 3\binom{3}{k-2}\binom{n+1}{k} + \binom{1}{k-4}\binom{n+2}{k}\right](1+x)^k \tag{47}$$

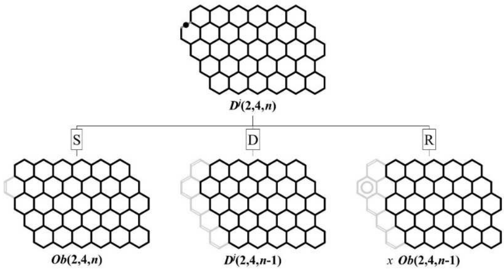
gives after evaluation the following formula

$$ZZ(Ob(2,4,n),x) = \tag{48}$$

$$= \sum_{k=0}^{6}\left[\binom{6}{k}\binom{n}{k} + 6\binom{4}{k-2}\binom{n+1}{k} + 6\binom{2}{k-4}\binom{n+2}{k} + \binom{0}{k-6}\binom{n+3}{k}\right](1+x)^k\ .$$

Hexagon without two corners $\boldsymbol{D^j(2,4,n)}$

The ZZ polynomial for the hexagon without two corners $D^j(2,4,n)$ can be derived using the following decomposition graph for this structure:



This decomposition yields the following recurrence relation

$$ZZ\big(D^j(2,4,n),x\big) = ZZ\big(D^j(2,4,n-1),x\big) + ZZ(Ob(2,4,n),x) + x\,ZZ(Ob(2,4,n-1),x)\,, \quad (49)$$

which can be telescopically folded to

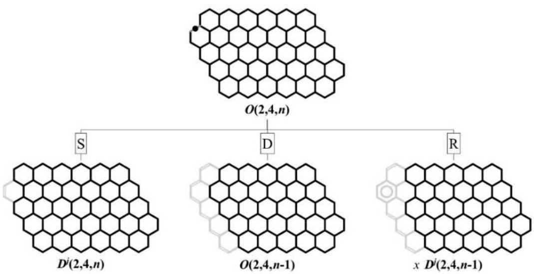
$$ZZ\big(D^j(2,4,n),x\big) = ZZ\big(D^j(2,4,0),x\big) + \sum_{k=1}^{n} ZZ(Ob(2,4,k),x) + x\sum_{k=0}^{n-1} ZZ(Ob(2,4,k),x)\,. \quad (50)$$

Initialization of this formula with $ZZ\big(D^j(2,4,0),x\big) = 1$ and substitution of $ZZ(Ob(2,4,n),x)$ given by Eq. (48) gives after evaluation the following formula

$$ZZ\big(D^j(2,4,n),x\big) = \quad (51)$$
$$= \sum_{k=0}^{7}\left[\binom{7}{k}\binom{n}{k} + 6\binom{5}{k-2}\binom{n+1}{k} + 6\binom{3}{k-4}\binom{n+2}{k} + \binom{1}{k-6}\binom{n+3}{k}\right](1+x)^k\,.$$

Hexagon $\boldsymbol{O(2,4,n)}$

Finally, the ZZ polynomial for the hexagon $O(2,4,n)$ can be derived using the following decomposition graph for this structure:



This decomposition yields the following recurrence relation

$$ZZ(O(2,4,n),x) = ZZ(O(2,4,n-1),x) + ZZ\big(D^j(2,4,n),x\big) + x\,ZZ\big(D^j(2,4,n-1),x\big)\,, \quad (52)$$

which can be telescopically folded to

$$ZZ(O(2,4,n),x) = ZZ(O(2,4,0),x) + \sum_{k=1}^{n} ZZ\big(D^j(2,4,k),x\big) + x \sum_{k=0}^{n-1} ZZ\big(D^j(2,4,k),x\big)\,. \quad (53)$$

Initialization of this formula with $ZZ(O(2,4,0),x) = 1$ and substitution of $ZZ\big(D^j(2,4,n),x\big)$ given by Eq. (51) gives after evaluation the following formula

$$ZZ(O(2,4,n),x) = \quad (54)$$

$$= \sum_{k=0}^{8} \left[\binom{8}{k}\binom{n}{k} + 6\binom{6}{k-2}\binom{n+1}{k} + 6\binom{4}{k-4}\binom{n+2}{k} + \binom{2}{k-6}\binom{n+3}{k}\right](1+x)^k\,.$$

4. Conclusion

We have presented here compact formulas for the ZZ polynomials of 27 classes of regular 5-tier benzenoid strips. The ZZ polynomials of 9 classes were reported earlier in the literature [6,8,10,11,12,16,17,22,25,34] and are given here only for completeness. For some of these classes, we were able to cast the previously derived formulas into a structurally simpler form. The ZZ polynomials for further 6 classes have never been reported before in explicit form but their formulas follow directly from known and previously reported theorems pertaining to the general theory of ZZ polynomials [11,12]. The ZZ polynomial formulas for the final 12 classes of regular 5-tier benzenoid strips are new. They are derived here using standard decomposition techniques based on the recurrence properties of ZZ polynomials with the help of the graphical computer environment called ZZDecomposer developed recently in our group [10,17]. The new 12 formulas derived in this study complete the full collection of ZZ polynomial formulas for the regular 5-tier benzenoid strips. This collection constitutes a natural extension to the formulas of the number of Kekulé structures reported earlier by Cyvin, Cyvin, and Gutman [2,6].

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