ZZ Polynomials of Regular m-tier Benzenoid Strips as Extended Strict Order Polynomials of Associated Posets Part 3. Compilation of Results for m = 1 - 6

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Abstract

We report closed-form formulas for the ZZ polynomials of all *m*-tier regular strips with m = 1-6 and an arbitrary length *n*. The ZZ polynomials were calculated fully automatically using the equivalence between the ZZ polynomial ZZ(S, x) of a regular benzenoid strip S and the extended strict order polynomial $E_S^{\circ}(n, 1 + x)$ of the corresponding poset S, demonstrated formally in Part 1 of this series and the corresponding algorithm introduced in Part 2. The results for m = 1-5 reproduce the previous, laboriously-derived collection of formulas, while the results for m = 6, constituting about 70% of the presented compilation, are new. The applied algorithm can be employed just as well for larger regular strips; the scope of the present tabulation is limited by the sheer amount of conceivable regular strips with 7 and more tiers.

1 Introduction

In the papers preceding the presented here compilation of ZZ polynomials, we have demonstrated that the ZZ polynomial of a regular *m*-tier strip S, ZZ(S, x), can be computed as the extended strict order polynomial $E^{\circ}_{\mathcal{S}}(n, 1+x)$ of the corresponding poset \mathcal{S} [32,33] and we have given a guide demonstrating how to carry out such computations in practice [34]. The current publication is concerned with an application of the designed machinery to the determination of the ZZ polynomials of all *m*-tier regular strips with m = 1-6 and arbitrary length n. The results for the m-tier regular strips with $m = 1, 2, 3, \ldots, 5$ have been published previously [19,41,42,50], but we re-derive them here using the new algorithm for the sake of completeness of the present tabulation and to facilitate comparisons between strips with a different number of tiers. The new, binomial-like presentation of these formulas provides also a unified framework for understanding and explaining the "quantum numbers" a_1 and a_2 appearing in the previous tabulation [42]. The results for the 6-tier regular strips—constituting the major part (*circa* 70%) of the compiled here results—are new and—with a few exceptions—have never been reported before. The only reason preventing us from extending the presented compilation to larger regular strips is the bulky volume of such a collection, originating both from an abundance of regular strips for larger widths m and from the relatively complex formulas of their ZZ polynomials.

Regular *m*-tier strips constitute an important subclass of benzenoids; their detailed characterization can be found in [15]. Topological invariants of regular *m*-tier strips are well known for small values of *m*; their most compact representation is given the ZZ polynomial, $ZZ(\mathbf{S}, x)$ [44,45,48,50,51], which comprises the following information: (*i*) the number of Kekulé structures of \mathbf{S} can be computed as $\mathcal{K}(\mathbf{S}) = ZZ(\mathbf{S}, 0)$ [13,15–17, 37,43], (*ii*) the total number of Clar covers of \mathbf{S} , as $\mathcal{C}(\mathbf{S}) = ZZ(\mathbf{S}, 1)$ [33, 34, 41, 42], (*iii*) the Clar number of \mathbf{S} , $Cl(\mathbf{S})$, as the degree of $ZZ(\mathbf{S}, x)$ [2], (*iv*) the number of Clar formulas of \mathbf{S} , as the leading coefficient of $ZZ(\mathbf{S}, x)$ [46], (*v*) the first Herndon number of \mathbf{S} , as the coefficient in $ZZ(\mathbf{S}, x)$ at *x*, and (*vi*) the number of Clar covers with *k* aromatic sextets, as he coefficient in $ZZ(\mathbf{S}, x)$ at x^k . Closed-form ZZ polynomial formulas for numerous classes of elementary benzenoids have been obtained using various methods: elementary considerations [4, 18, 45, 48, 50, 51], analysis of recurrence relations [12, 19, 21], generalization of ZZ polynomials for sequences of isostructural benzenoids [7, 8], application of ZZDecomposer [6, 9–11, 22–26, 35, 38–40, 53, 54], transfer matrix approach [49], connectivity graph technique [27], interface theory of benzenoids [28,30,31], and now, the equivalence with the extended strict order polynomial [32–34] and other polynomials [3, 29, 47, 52]. It is important to stress that the presented here results are valid for an arbitrary length n of the studied regular m-tier strips, and can be, for example, used to study the asymptotic transition from the molecular to graphene-like bulk regime [5, 36].

2 Results

The ZZ polynomials for the regular 1–3, 4, 5, and 6-tier benzenoid strips are given in Tables 1, 2, 3 and 4, respectively. The presented tables can be thought of as an extension of the compilation of the formulas for $\mathcal{K}(\mathbf{S})$ presented in Chapter 10 of [15] for strips \mathbf{S} with m = 1-5 and in Chapter 13 of [15] (see also partially [14, 20]) for strips \mathbf{S} with m = 6. The table entry for each strip \mathbf{S} consists of: a sequence of m - 1 fragment shapes



which uniquely define the shape of S by specifying the transition from each row to the next, a symbol for S (if previously established), a depiction of S with a gray row of hexagons schematically symbolizing a sequence of n-3 such rows, the Hasse diagram of the poset S associated with S, and the ZZ polynomial of S computed as $E_{S}^{\circ}(n, z)$ using the variable z = 1 + x. In the electronic PDF version of the manuscript, a clickable comment on the right side of each table row contains a Maple [1] formula of ZZ(S, x), which can be copied and pasted directly into Maple. The ZZ polynomial formulas are kept unevaluated to highlight the correspondence with the general form of the extended strict order polynomial given by

$$\mathbf{E}_{\mathcal{S}}^{\circ}(n,z) = \sum_{w \in \mathcal{L}(\mathcal{S})} \sum_{k=0}^{|\mathcal{S}|} \binom{|\mathcal{S}| - \operatorname{fix}_{\mathcal{S}}(w)}{k - \operatorname{fix}_{\mathcal{S}}(w)} \binom{n + \operatorname{des}(w)}{k} z^{k}, \tag{1}$$

where the detailed meaning of: a poset S and its cardinality |S|, the Jordan-Hölder set $\mathcal{L}(S)$ of linear extensions w of S, the number of descents des(w) in w, and the number of fixed elements fix_S(w) in w is explained in our earlier work [32–34].

	Structur	е		ZZ polynomial
[]	L(n)	8	o	$\sum_{k=0}^{1} \left(\binom{1}{k} \binom{n}{k} \right) z^k$
[R]	M(2,n)	8	o P	$\sum_{k=0}^{2} \left(\binom{2}{k} \binom{n}{k} \right) z^k$
[R, R]	M(3,n)		~~~~	$\sum_{k=0}^{3} \left(\binom{3}{k} \binom{n}{k} \right) z^{k}$
[N, W]	Pr(2, n)	88	0 0	$\sum_{k=0}^{2} \left(\binom{2}{k} \binom{n}{k} + \binom{0}{k-2} \binom{n+1}{k} \right) z^{k}$
[R, L]	Ch(2,2,n)		~	$\sum_{k=0}^{3} \left(\binom{3}{k} \binom{n}{k} + \binom{1}{k-2} \binom{n+1}{k} \right) z^{k}$
[W, N]	O(2, 2, n)		Ŷ	$\sum_{k=0}^{4} \left(\binom{4}{k} \binom{n}{k} + \binom{2}{k-2} \binom{n+1}{k} \right) z^k$

Table 1. ZZ polynomials of all regular 1-, 2-, and 3-tier benzenoid strips.

Table 2. ZZ polynomials of all regular 4-tier benzenoid strips

	Structur	e		ZZ polynomial
[R, R, R]	M(4,n)		0,000	$\sum_{k=0}^4 \left(\binom{4}{k} \binom{n}{k} \right) z^k$
[N, R, W]	X(2,3,n)		0 0	$\sum_{k=0}^{2} \left(\binom{2}{k} \binom{n}{k} + \binom{0}{k-2} \binom{n+1}{k} \right) z^{k}$
[N, W, R]	$\Sigma(2,3,n)$		° °	$\sum_{k=0}^{3} \left(\binom{3}{k} \binom{n}{k} + 2\binom{1}{k-2} \binom{n+1}{k} \right) z^{k}$
[R, R, L]	Ch(3,2,n)		~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	$\sum_{k=0}^{4} \left(\binom{4}{k} \binom{n}{k} + 2\binom{2}{k-2} \binom{n+1}{k} \right) z^{k}$
[R, L, R]	Z(4,n)		~~	$\sum_{k=0}^{4} \left(\binom{4}{k} \binom{n}{k} + 3\binom{2}{k-2} \binom{n+1}{k} + \binom{0}{k-4} \binom{n+2}{k} \right) z^{k}$
[W, N, R]	D(2,3,n)		Ŷ	$\sum_{k=0}^{5} \left(\binom{5}{k} \binom{n}{k} + 3\binom{3}{k-2} \binom{n+1}{k} + \binom{1}{k-4} \binom{n+2}{k} \right) z^{k}$
[W, R, N]	O(2,3,n)		\checkmark	$\sum_{k=0}^{6} \left(\binom{6}{k} \binom{n}{k} + 3\binom{4}{k-2} \binom{n+1}{k} + \binom{2}{k-4} \binom{n+2}{k} \right) z^{k}$

Str	ructure		ZZ polynomial
$\begin{bmatrix} \mathtt{R}, \mathtt{R}, \mathtt{R}, \mathtt{R} \end{bmatrix}$ $_{M(5,n)}$		or or or o	$\sum_{k=0}^{5} \left(\binom{5}{k} \binom{n}{k} \right) z^k$
$\begin{bmatrix} [\mathtt{N}, \mathtt{R}, \mathtt{R}, \mathtt{W}] \\ X(2,4,n) \end{bmatrix}$	888	o o	$\sum_{k=1}^{2} \left(\binom{2}{k} \binom{n}{k} + \binom{0}{k} \binom{n+1}{k} \right) z^{k}$
$\begin{bmatrix} \mathbb{N}, \mathbb{R}, \mathbb{L}, \mathbb{W} \end{bmatrix}$ $\Sigma^{i}(3,n)$		o o	$=\sum_{k=0}^{\infty} \left(\left(k \right) \left(k \right) + \left(k - 2 \right) \left(k \right) \right)^{2}$
$\begin{bmatrix} \texttt{N},\texttt{R},\texttt{W},\texttt{R} \end{bmatrix} \\ \Sigma^i(2,4,n)$		° °	$\sum_{k=1}^{3} \left(\binom{3}{k} \binom{n}{k} + 2\binom{1}{k} \binom{n+1}{k} \right) z^{k}$
$\begin{bmatrix} \texttt{N},\texttt{R},\texttt{W},\texttt{L} \end{bmatrix}$ $L(n) \cdot M(2,n)$		° °	$\sum_{k=0}^{2} \left($
$\begin{bmatrix} \mathtt{N}, \mathtt{W}, \mathtt{R}, \mathtt{R} \end{bmatrix}$ $\Sigma^{j}(2, 4, n)$		° ,000	$\sum_{k=0}^{4} \left(\binom{4}{k} \binom{n}{k} + 3\binom{2}{k-2} \binom{n+1}{k} \right) z^k$
$egin{array}{c} [{\tt R},{\tt R},{\tt R},{\tt L}] \ Ch(4,2,n) \end{array}$		0000	$\sum_{k=0}^{5} \left({5 \choose k} {n \choose k} + 3 {3 \choose k-2} {n+1 \choose k} \right) z^k$
$\begin{bmatrix} \texttt{R},\texttt{N},\texttt{W},\texttt{R} \end{bmatrix} \\ M(2,n)^2$		~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	$\frac{4}{\sum} \left(\binom{4}{n} + 4\binom{2}{2} \binom{n+1}{2} + \binom{0}{2} \binom{n+2}{2} \right) z^k$
$\begin{bmatrix} \mathtt{R}, \mathtt{N}, \mathtt{W}, \mathtt{L} \end{bmatrix} \\ \Sigma^{j}(3, n)$		~ ~	$\sum_{k=0}^{2} \left(\frac{1}{k} + \frac{1}{k} +$
$\begin{bmatrix} \mathtt{R}, \mathtt{R}, \mathtt{L}, \mathtt{L} \end{bmatrix}$ $Ch(3,3,n)$		~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	$\sum_{k=0}^{5} \left(\binom{5}{k} \binom{n}{k} + 4\binom{3}{k-2} \binom{n+1}{k} + \binom{1}{k-4} \binom{n+2}{k} \right) z^{k}$
$egin{array}{c} [{ t R},{ t R},{ t L},{ t R}] \ M_n(LAALL) \end{array}$		~~~~	$\sum_{k=0}^{5} \left({5 \choose k} {n \choose k} + 5 {3 \choose k-2} {n+1 \choose k} + 3 {1 \choose k-4} {n+2 \choose k} \right) z^k$
$\begin{bmatrix} \texttt{W},\texttt{N},\texttt{R},\texttt{R} \end{bmatrix} \\ D^i(2,4,n)$		\$~°°	$\sum_{k=0}^{6} \left(\binom{6}{k} \binom{n}{k} + 5\binom{4}{k-2} \binom{n+1}{k} + 3\binom{2}{k-4} \binom{n+2}{k} \right) z^{k}$
$\begin{bmatrix} [\texttt{N},\texttt{W},\texttt{N},\texttt{W}] \\ Pr(3,n) \end{bmatrix}$			$\sum_{k=0}^{3} \left(\binom{3}{k} \binom{n}{k} + \binom{3}{k-2} + \binom{0}{k-3} \binom{n+1}{k} + \binom{0}{k-3} \binom{n+2}{k} z^k \right)$
$\begin{bmatrix} \mathbf{R}, \mathbf{L}, \mathbf{N}, \mathbf{W} \end{bmatrix}$ $L(n) \cdot Ch(2,2,n)$		~ °	$ \sum_{k=0}^{4} \left(\binom{4}{k} \binom{n}{k} + \binom{4}{\binom{2}{k-2}} + \binom{1}{\binom{1}{k-3}} \binom{n+1}{k} + \binom{1}{\binom{1}{k-4}} + \binom{0}{\binom{n+2}{k}} z^k \right) z^k $
$\begin{bmatrix} \texttt{W},\texttt{N},\texttt{N},\texttt{W} \end{bmatrix}$ $L(n) \cdot O(2,2,n)$		\$ •	$ \sum_{k=0}^{5} \left({5 \choose k} {n \choose k} + \left(5 {3 \choose k-2} + {2 \choose k-3} \right) {n+1 \choose k} + \left({2 \choose k-3} + 2 {1 \choose k-4} \right) {n+2 \choose k} z^{k} $
$\begin{bmatrix} \mathtt{R}, \mathtt{L}, \mathtt{L}, \mathtt{R} \end{bmatrix}$ $M_n(LALAL)$		~~~	$ \begin{vmatrix} \sum_{k=0}^{5} \left({5 \choose k} {n \choose k} + \left(5 {n \choose k-2} + {2 \choose k-3} \right) {n+1 \choose k} \\ + \left({2 \choose k-3} + 3 {1 \choose k-4} \right) {n+2 \choose k} z^k \end{vmatrix} $

Table 3. ZZ polynomials of regular 5-tier benzenoid strips

abie 3 (continueu). 44 potynomiais of regular 5-tier penzenout starps ZZ polynomial	$\sum_{k=0}^{6} \left(\binom{6}{k} \binom{n}{k} + 6\binom{4}{k-2} \binom{n+1}{k} + 6\binom{2}{k-4} \binom{n+2}{k} + \binom{0}{k-6} \binom{n+3}{k} \right) z^{k}$	$\sum_{k=0}^{7} \left(\binom{7}{k} \binom{n}{k} + 6\binom{5}{k-2} \binom{n+1}{k} + 6\binom{3}{k-4} \binom{n+2}{k} + \binom{1}{k-6} \binom{n+3}{k-6} \binom{n+3}{k} \right) z^{k}$	$\sum_{k=0}^{8} \left(\binom{8}{k} \binom{n}{k} + 6\binom{6}{k-2} \binom{n+1}{k} + 6\binom{4}{k-4} \binom{n+2}{k} + \binom{2}{k-6} \binom{n+3}{k} \right) z^{k}$	$\sum_{k=0}^{5} \left(\binom{5}{k} \binom{n}{k} + \left(6\binom{3}{k-2} + \binom{2}{k-3} \right) \binom{n+1}{k} + \left(\binom{2}{k-3} + 5\binom{1}{k-4} + \binom{0}{k-5} \right) \binom{n+2}{k} + \binom{0}{k-5} \binom{n+3}{k} z^k$	$\sum_{k=0}^{6} \left(\binom{6}{k} \binom{n}{k} + \left(6\binom{4}{k-2} + \binom{3}{k-3} \right) \binom{n+1}{k} + \left(\binom{3}{k-3} + 5\binom{2}{k-4} + \binom{1}{k-5} \right) \binom{n+2}{k} + \binom{1}{k-5} \binom{n+3}{k} z^k$	$\sum_{k=0}^{6} \left(\binom{6}{k} \binom{n}{k} + \left(7\binom{4}{k-2} + \binom{3}{k-3} \right) \binom{n+1}{k} + \left(\binom{3}{k-3} + 8\binom{2}{k-4} + \binom{1}{k-5} \right) \binom{n+2}{k} + \binom{1}{\binom{k-5}{k-5}} + \binom{1}{\binom{k-5}{k-5}} \binom{n+3}{k} \frac{3}{k} + \binom{n}{k} n$	$\sum_{k=0}^{7} \left(\binom{7}{k} \binom{n}{k} + \left(7\binom{5}{k-2} + \binom{4}{k-3} \right) \binom{n+1}{k} + \left(\binom{4}{k-3} + 8\binom{3}{k-4} + \binom{2}{k-5} \right) \binom{n+2}{k} + \binom{2}{\binom{k-5}{k-5}} + \binom{2}{\binom{k-5}{k-5}} \binom{n+3}{k} \frac{3}{k} \frac{3}{k} + \binom{3}{k} \binom{n}{k} \frac{3}{k} \binom{n}{k} \frac{3}{k} \binom{n}{k} \frac{3}{k} \binom{n}{k} n$	$\sum_{k=0}^{7} \left({\binom{7}{k}} {\binom{7}{k}} + \left(9 {\binom{5}{k-2}} + {\binom{4}{k-3}} \right) {\binom{n+1}{k}} + \left({\binom{4}{k-3}} + 17 {\binom{3}{k-4}} + 2 {\binom{2}{k-5}} \right) {\binom{n+2}{k}} \\ + \left(2 {\binom{2}{k-5}} + 7 {\binom{1}{k-6}} + {\binom{0}{k-7}} {\binom{n+3}{k-7}} + {\binom{0}{k-7}} {\binom{n+3}{k-7}} + {\binom{0}{k-7}} {\binom{n+4}{k-7}} \right) z^k$	$\sum_{k=0}^{8} \left(\binom{8}{k} \binom{n}{k} + \left(9\binom{6}{k-2} + \binom{5}{k-3} \binom{n+1}{k} + \left(\binom{5}{k-3} + 17\binom{4}{k-4} + 2\binom{3}{k-5} \binom{n+2}{k} \binom{n+2}{k} + \binom{1}{k-1} \binom{n+4}{k} + \binom{1}{k} \binom{n+4}{k} \binom$	$\sum_{k=0}^{9} \left(\binom{9}{k} \binom{n}{k} + \left(9\binom{7}{k-2} + \binom{6}{k-3} \binom{n+1}{k} + \binom{6}{k-3} + 17\binom{6}{k-4} + 2\binom{4}{k-4} + \binom{1}{k} \binom{n+2}{k} + \binom{1}{k} \binom{n+3}{k} + \binom{2}{k}\binom{n+4}{k-1}\binom{n+4}{k} \binom{n+4}{k} \binom{n+4}$
r	\sim	\checkmark	\checkmark	<i>\$</i> ₽₽	Ś	Ş	Ś	\Rightarrow	\diamondsuit	\diamond
ucture										
Stı	$\begin{bmatrix} \mathbf{R}, \mathbf{W}, \mathbf{N}, \mathbf{R} \end{bmatrix}$ Ob(2, 4, n)	$\begin{bmatrix} W, R, N, R \end{bmatrix}$	$\begin{bmatrix} W, R, R, N \end{bmatrix} \\ O(2, 4, n)$	$\begin{bmatrix} \mathbf{R}, \mathbf{L}, \mathbf{R}, \mathbf{L} \end{bmatrix}_{Z(5,n)}$	$\begin{bmatrix} \mathbf{R}, \mathbf{W}, \mathbf{N}, \mathbf{L} \end{bmatrix}$ $D^i(3,n)$	$\begin{bmatrix} W,N,R,L \end{bmatrix}_{R(3,n)}$	$\begin{bmatrix} W, R, N, L \end{bmatrix}_{D(3,n)}$	$\begin{bmatrix} W,N,W,N \end{bmatrix}$ Or(n,2)	$egin{array}{c} [{\sf W},{\sf R},{\sf L},{\sf N}]\ D^j(3,n) \end{array}$	$\begin{bmatrix} W,W,N,N \end{bmatrix} \\ O(3,3,n)$

St	ructure	1 poigi		ZZ polynomial
$\begin{bmatrix} \mathtt{R}, \mathtt{R}, \mathtt{R}, \mathtt{R}, \mathtt{R} \end{bmatrix}$ $M(6,n)$		000	s or the	$\sum\limits_{k=0}^6 \left({6 \choose k} {n \choose k} \right) z^k$
$\begin{bmatrix} \mathtt{N}, \mathtt{R}, \mathtt{R}, \mathtt{R}, \mathtt{W} \end{bmatrix}_{X(2,5,n)}$	8888	•	0	2
[N, R, R, L, W]	8888	•	٥	$\sum_{k=0}^{2} \left(\binom{2}{k} \binom{n}{k} + \binom{0}{k-2} \binom{n+1}{k} \right) z^{k}$
[N, R, L, R, W]	8888	•	٥	
[R, N, R, R, W]	888	_م ه	٥	
[R, N, R, L, W]		مہ	٥	$\int_{-\infty}^{3} \left(\binom{3}{l} \binom{n}{l} + 2\binom{1}{l} \binom{n+1}{l} \right) z^{k}$
[R, N, L, R, W]		مہ	٥	$\sum_{k=0}^{2} \left(\left(\frac{k}{k} \right) \left(\frac{k}{k} \right)^{k} + \left(\frac{k}{k-2} \right)^{k} \right)^{k}$
[R, N, L, L, W]		مح	٥	
[R, R, N, R, W]		o o o	o	$\sum_{k=1}^{4} \left(\binom{4}{k} \binom{n}{k} + 3\binom{2}{k} \binom{n+1}{k} \right) z^{k}$
[R, R, N, L, W]		000	o	$\sum_{k=0}^{2^{n}} \left(\left(k\right) \left(k\right) + \left(k-2\right) \left(k\right) \right)^{2^{n}}$
[R, R, R, N, W]		0,000	0	$\sum_{k=0}^{5} \left(\binom{5}{k} \binom{n}{k} + 4\binom{3}{k-2} \binom{n+1}{k} \right) z^k$
$\begin{bmatrix} \mathtt{R}, \mathtt{R}, \mathtt{R}, \mathtt{R}, \mathtt{L} \end{bmatrix}$ $Ch(5,2,n)$		000	∽	$\sum_{k=0}^{6} \left(\binom{6}{k} \binom{n}{k} + 4\binom{4}{k-2} \binom{n+1}{k} \right) z^k$
[R, N, R, W, R]		_م م	_م م	
[R, N, R, W, L]		<i>م</i> و	مرم	$\int_{k=0}^{4} \left(\binom{4}{k} \binom{n}{k} + 4\binom{2}{k-2} \binom{n+1}{k} + \binom{0}{k-4} \binom{n+2}{k} \right) z^{k}$
[R, N, L, W, R]		_م م	r	
[R, R, N, W, R]		o o o	_م م	$\sum_{n=1}^{5} \left(\binom{5}{n} \binom{n}{n} + 6\binom{3}{n} \binom{n+1}{n} + 3\binom{1}{n} \binom{n+2}{n} \right) z^{k}$
[R, R, N, W, L]		000	ممه	$\sum_{k=0}^{2} \left(\frac{k}{k} + \frac{k}{k} +$
$\begin{bmatrix} \mathtt{R}, \mathtt{R}, \mathtt{R}, \mathtt{L}, \mathtt{L} \end{bmatrix}$ $Ch(4,3,n)$		0,000	d d d	$\sum_{k=0}^{6} \left({\binom{6}{k} \binom{n}{k} + 6\binom{4}{k-2} \binom{n+1}{k} + 3\binom{2}{k-4} \binom{n+2}{k}} \right) z^k$
$egin{array}{l} [extbf{R}, extbf{R}, extbf{R}, extbf{L}, extbf{R}]\ M_n(LAALLL) \end{array}$		o o o	\checkmark	$ \sum_{k=0}^{6} \left(\binom{6}{k} \binom{n}{k} + 7\binom{4}{k-2} \binom{n+1}{k} + 6\binom{2}{k-4} \binom{n+2}{k} \right) z^{k} $
[R, R, R, W, N]		000	\diamond	$ \sum_{k=0}^{7} \left(\binom{7}{k} \binom{n}{k} + 7\binom{5}{k-2} \binom{n+1}{k} + 6\binom{3}{k-4} \binom{n+2}{k} \right) z^{k} $

Table 4. ZZ polynomials of regular 6-tier benzenoid strips

ontinued). ZZ polynomials of regular 6-tier benzenoid strips	ZZ polynomial	$\sum_{i=0}^{k} \left(\binom{3}{k}\binom{n}{k} + \left(3\binom{1}{k-2} \right) + \binom{0}{k-3} \right) \binom{n+1}{k} + \binom{0}{k-3}\binom{n+2}{k} z^k$	$\sum_{n=1}^{n} \left(\left(\left\{ 1, \left\{ n \right\} \right\} + \left\{ \left\{ 1, $	$= \left(\left(k \right) \left(k \right) \left(k \right) + \left(\frac{1}{k} \left(k - 2 \right) + \left(k - 3 \right) \right) \left(k \right) + \left(\left(k - 3 \right) + \left(k - 4 \right) \right) \left(k \right) \right) = \left(k - 2 \right) \right)$	$\sum_{k=1}^{n} \left(\left[\left\{ A_{k} \right\} \left(n \right] + \left\{ f_{k} \right\} + \left\{$	$= \left(\left(k \right) \left(k \right) \left(k \right) \left(k \right) \left(k - 2 \right) \left(k - 3 \right) \left(k \right) \left(k \right) \left(k - 3 \right) \left(k - 3 \right) \left(k - 4 \right) \right) \left(k - 1 \right) \right) = \left(k - 2 \right) \left(k - 3 \right) \right) = \left(k - 3 \right) \right) = \left(k - 3 \right) \left(k $	$\sum_{i=0}^{k-1} \left(\binom{5}{k} \binom{n}{k} + \left(5\binom{3}{k-2} + \binom{2}{k-3} \right) \binom{n+1}{k} + \left(\binom{2}{k-3} + 2\binom{1}{k-4} \binom{n+2}{k} \right) z^k$	$\sum_{i=1}^{n} \left(\left\{ 5 \right\} \left(n \right) + \left\{ 6 \left\{ -3 - 3 \right\} + 2 \left\{ -2 - 3 \right\} \right) + \left\{ -2 \left\{ -2 - 3 \right\} + 4 \left\{ -1 - 3 \right\} \right\} \right\} = 2^{n} k^{2}$	$\int \left(\sqrt{k} \sqrt{k} + \sqrt{k} \sqrt{k} + \sqrt{k} + 2 \sqrt{k} + \sqrt{k} \sqrt{k} \sqrt{k} \sqrt{k} + \sqrt{k} \sqrt{k} \sqrt{k} \sqrt{k} \sqrt{k} \sqrt{k} \sqrt{k} \sqrt{k}$	$\sum_{i=0}^{i} \left(\binom{6}{k} \binom{n}{k} + \left(7\binom{4}{k-2} \right) + 2\binom{3}{k-3} \right) \binom{n+1}{k} + \left(2\binom{3}{k-3} + 7\binom{2}{k-4} \right) \binom{n+2}{k} z^k$	$\sum_{i=0}^{i} \left(\binom{6}{k} \binom{n}{k} + 8\binom{4}{k-2} \binom{n+1}{k} + 9\binom{2}{k-4} \binom{n+2}{k} + \binom{0}{k-6} \binom{n+3}{k-6} z^k \right) z^k$	$\sum_{i=0}^{n} \left(\binom{7}{k} + 9\binom{5}{k-2} \binom{n+1}{k} + 14\binom{3}{k-4} \binom{n+2}{k} + 4\binom{1}{k-6} \binom{n+3}{k} \right) z^{k}$	$\sum_{c=0}^{t} \left(\binom{8}{k} \binom{n}{k} + 9\binom{6}{k-2} \binom{n+1}{k} + 14\binom{4}{k-4} \binom{n+2}{k} + 4\binom{2}{k-6} \binom{n+3}{k} \right) z^k$	$\sum_{n=0}^{1} \left({\binom{5}{k}} {\binom{n}{k}} + \left(7 {\binom{3}{k-2}} \right) + 2 {\binom{2}{k-3}} \right) {\binom{n+1}{k}} + \left(2 {\binom{2}{k-3}} + 6 {\binom{1}{k-4}} + {\binom{0}{k-5}} \right) {\binom{n+2}{k}} + {\binom{0}{k-5}} {\binom{n+3}{k}} z = 2 $
Table 4		0 0	°	°	0 0 0 0	ه مره	°	° °	~ ~	La construction	d a d a d a d a d a d a d a d a d a d a	d de la como		مہ م
	icture													
	Stru	[N, R, W, N, W]	[R, L, N, R, W]	[R, L, N, L, W]	[R, N, W, N, W]	$[\mathrm{N}, \mathrm{W}, \mathrm{R}, \mathrm{N}, \mathrm{W}]$	[W, N, N, R, W]	[R, R, L, N, W]	[R, L, L, N, W]	$egin{bmatrix} { m [R, L, L, L, R]} \ M_n(LALLAL) \end{cases}$	$egin{bmatrix} { m [R,R,L,R,R]} \ M_n^{(LLAALL)} \end{cases}$	[R, R, W, N, R]	$[\mathbf{R},\mathbf{R},\mathbf{W},\mathbf{R},\mathbf{N}]$	[R, L, N, W, R]

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ZZ polynomiae or regulation of the polynomiae of the polynomial	$\sum_{k=0}^{5} \left(\binom{5}{k} \binom{n}{k} + \left(7\binom{3}{k-2} + 2\binom{2}{k-3} \right) \binom{n+1}{k} + \left(2\binom{2}{k-3} + 6\binom{1}{k-4} + \binom{0}{k-5} \right) \binom{n+2}{k} + \binom{0}{k-5} \binom{n+3}{k-5} z^k$	$\sum_{k=0}^{5} \left(\binom{5}{k} \binom{n}{k} + \left(7\binom{3}{k-2} + 3\binom{2}{k-3} \right) \binom{n+1}{k} + \left(3\binom{2}{k-3} + 7\binom{1}{k-4} + 2\binom{0}{k-5} \right) \binom{n+2}{k} + 2\binom{0}{k-5} \binom{n+3}{k} 2^k$	$\sum_{k=0}^{6} \left(\binom{6}{k} \binom{n}{k} + \binom{4}{k-2} + 2\binom{3}{k-3} \binom{n+1}{k} + \binom{2\binom{3}{k-3}}{2\binom{k-3}{k-3}} + 10\binom{2}{k-4} + \binom{1}{\binom{k-5}{k-5}} \binom{1}{\binom{k-5}{k-5}} + \binom{0}{\binom{k-5}{k-5}} \binom{n+3}{\binom{k-5}{k-5}} \frac{2^{k-3}}{\binom{k-5}{k-5}} \binom{n+3}{k} \binom{n+3}{k-5} \binom{n+3}{k} \binom{n+3}{k-5} \binom{n+3}{k} \binom{n+3}{k-5} $	$\left \sum_{k=0}^{6} \left(\binom{6}{k} \binom{n}{k} + \left(9\binom{4}{k-2} + 2\binom{3}{k-3} \binom{n+1}{k} + \left(2\binom{3}{k-3} + 11\binom{2}{k-4} + 2\binom{1}{k-5} + \binom{0}{k-6} \binom{n+3}{k} + 2\binom{1}{k} \binom{n+2}{k} + 2\binom{1}{k-6} \binom{n+3}{k} \binom{n+3}{k} \binom{n+3}{k} + 2\binom{1}{k} \binom{n+3}{k} n$	$\sum_{i=1}^{n} \left(f(i) f(n) + f(i) + f(i) + f(i) + f(i) + f(i) + f(i) + i + f(i) + i + i + i + i + i + i + i + i + i +$	$= \sum_{k=0}^{\infty} \left(\left(k \right) \left(k \right) + \left(O\left(k-2\right) + O\left(k-3\right) \right) \left(k \right) + \left(O\left(k-3\right) + O\left(k-4\right) + 2\left(k-5\right) \right) \left(k \right) + \left(2\left(k-5\right) + \left(k-6\right) \right) \left(k \right) \right) = 0$	$\left \sum_{k=0}^{6} \left(\binom{6}{k} \binom{n}{k} + \left(9\binom{4}{k-2} + 2\binom{3}{k-3} \binom{n+1}{k} + \left(2\binom{3}{k-3} + 13\binom{2}{k-4} + 3\binom{1}{k-5} + 3\binom{1}{k-5} + 2\binom{0}{k-6} \binom{n+3}{k-5} + 2\binom{1}{k-6} \binom{n+3}{k-5} + 2\binom{1}{k-5} + 2\binom{1}{k-5} \binom{n+3}{k-5} + 2\binom{1}{k-5} \binom{n+3}{k-5} \binom{n+3}{k-5} + 2\binom{1}{k-5} \binom{n+3}{k-5} n$	$\left \sum_{k=0}^{6} \left(\binom{6}{k} \binom{n}{k} + \left(9\binom{4}{k-2} + 3\binom{3}{k-3} \binom{n+1}{k} + \binom{3}{k-3} + 14\binom{2}{k-4} + 4\binom{1}{k-4} + 4\binom{1}{k} \binom{n+2}{k} + \binom{1}{4\binom{1}{k-5}} + 2\binom{0}{\binom{n+3}{k-3}} \frac{n+3}{k} \right) \right ^{n+3} \right = \frac{1}{k} \left(\binom{6}{k} \binom{n}{k} + \binom{6}{k-5} \binom{n+3}{k-5} \binom{n+3}$	$\left \sum_{k=0}^{7} \left(\binom{7}{k} \binom{n}{k} + \left(9\binom{5}{k-2} + 3\binom{4}{k-3} \binom{n+1}{k} + \left(3\binom{4}{k-3} + 13\binom{3}{k-4} + 2\binom{2}{k-5} + 2\binom{1}{k-5} + 2\binom{1}{k-6} \binom{n+3}{k} \frac{n+2}{k-5} + 2\binom{1}{k-6} \binom{n+3}{k-2} + 2\binom{2}{k-5} + 2\binom{2}{k-5} \frac{n+3}{k-5} + 2\binom{2}{k-5} \binom{n+3}{k-5} \frac{n+3}{k-5} + 2\binom{2}{k-5} \binom{n+3}{k-5} \frac{n+3}{k-5} + 2\binom{2}{k-5} \binom{n+3}{k-5} \binom{n+3}{k-5} \binom{n+3}{k-5} \frac{n+3}{k-5} + 2\binom{2}{k-5} \binom{n+3}{k-5} n$	$\left \sum_{k=0}^{7} \left(\binom{7}{k} \binom{n}{k} + \left(9\binom{5}{k-2} + 2\binom{4}{k-3} \binom{n+1}{k} + \left(2\binom{4}{k-3} + 13\binom{3}{k-4} + 3\binom{2}{k-5} + 3\binom{2}{k-5} + 2\binom{1}{k-6} \binom{n+3}{k} \frac{n+3}{k} \right) \right) \frac{1}{k} \right = \frac{1}{k} \left(\sum_{k=0}^{7} \binom{n}{k-5} + 2\binom{1}{k-5} \binom{n+3}{k-5} + 2\binom{1}{k-5} \binom{n+3}{k-5} + 2\binom{1}{k-5} \binom{n+3}{k-5} \frac{1}{k-5} \binom{n+3}{k-5} + 2\binom{1}{k-5} \binom{n+3}{k-5} \binom{n+3}$	$\sum_{k=0}^{7} \left(\binom{7}{k}\binom{n}{k} + \left(10\binom{5}{k-2} + 3\binom{4}{k-3} \right)\binom{n+1}{k} + \left(3\binom{4}{k-3} + 19\binom{3}{k-4} + 4\binom{2}{k-5} \right)\binom{n+2}{k} + \left(4\binom{2}{k-5} + 5\binom{1}{k-6} \binom{n+3}{k} \right) \frac{n+3}{k} = \frac{1}{k} + 1$
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ucture											
Str	$[\mathrm{R},\mathrm{L},\mathrm{N},\mathrm{W},\mathrm{L}]$	$[\mathrm{R},\mathrm{L},\mathrm{R},\mathrm{N},\mathrm{W}]$	$[\mathrm{R},\mathrm{R},\mathrm{L},\mathrm{L},\mathrm{R}]$ $M_n(LALALL)$	[R, N, W, W, N]	[R, W, N, N, W]	[W, N, R, N, W]	$[\mathbf{R}, \mathbf{R}, \mathbf{L}, \mathbf{R}, \mathbf{L}]$ $M_n(LAAALL)$	$\left[\mathrm{R}, \mathrm{L}, \mathrm{R}, \mathrm{R}, \mathrm{L} ight] _{M_{n}(LALAAL)}$	[W, R, N, N, W]	[R, R, W, N, L]	$\left[\mathrm{R},\mathrm{L},\mathrm{L},\mathrm{W},\mathrm{N}\right]$

Table 4 (continued). ZZ polynomials of regular 6-tier benzenoid strips

4 (continued). ZZ polynomials of regular 6-tier benzenoid strips ZZ polynomial	$\sum_{k=0}^{8} \left(\binom{8}{k} \binom{n}{k} + 10\binom{6}{k-2} \binom{n+1}{k} + 20\binom{4}{k-4} \binom{n+2}{k} + 10\binom{2}{k-6} \binom{n+3}{k} + \binom{0}{k-8} \binom{n+4}{k} \binom{n+4}{k} z^k \right) z^k$	$\sum_{k=0}^{9} \left(\binom{9}{k} \binom{n}{k} + 10\binom{7}{k-2} \binom{n+1}{k} + 20\binom{5}{k-4} \binom{n+2}{k} + 10\binom{3}{k-6} \binom{n+3}{k} + \binom{1}{k-8} \binom{n+4}{k} \binom{n+4}{k} \right) z^k$	$\sum_{k=0}^{10} \left(\binom{10}{k} \binom{n}{k} + 10\binom{8}{k-2}\binom{n+1}{k} + 20\binom{6}{k-4}\binom{6}{k-4} \binom{4}{k-6}\binom{4}{k-6}\binom{4}{k}\binom{n+3}{k} + \binom{2}{k-8}\binom{n+4}{k-8}\binom{n+4}{k} \right) z^k$	$\sum_{k=0}^{6} \left(\binom{6}{k} \binom{n}{k} + \left(10\binom{4}{k-2} + 4\binom{3}{k-3} \binom{n+1}{k} + \left(4\binom{3}{k-3} + 18\binom{2}{k-4} + 8\binom{1}{k-5} + \binom{0}{k-5} \binom{n+2}{k} \binom{n+4}{k} \right) z^k + \left(8\binom{1}{k-5} + 6\binom{0}{k-6} \binom{n+3}{k} + \binom{0}{k-6} \binom{n+4}{k} z^k \right) z^k$	$\sum_{k=0}^{7} \left({\binom{7}{k}} {\binom{7}{k}} + \left({11\binom{5}{k-2} + 2\binom{4}{k-3}} \right) {\binom{n+1}{k}} + \left({2\binom{4}{k-3}} + 22\binom{3}{k-4} + 4\binom{2}{k-5} \right) {\binom{n+2}{k}} + \left({4\binom{2}{k-5}} + 8\binom{4}{k-6} + \binom{0}{\binom{n+3}{k}} \right) {\binom{n+3}{k}} + \binom{0}{\binom{n+3}{k}} {\binom{n+3}{k}} {\binom{n+3}{k}} + \binom{0}{\binom{n+3}{k}} {\binom{n+3}{k}} {\binom$	$\sum_{k=0}^{7} \left(\binom{7}{k} \binom{n}{k} + \left(11\binom{5}{k-2} + 3\binom{4}{k-3} \binom{n+1}{k} + \left(3\binom{4}{k-3} + 24\binom{3}{k-4} + 7\binom{2}{k-5} \binom{n}{k} \binom{n+2}{k} \right) + \left(2\binom{4}{k-5} + 10\binom{1}{k-6} + 2\binom{0}{k-7} \binom{n+3}{k} + 2\binom{0}{k-7} \binom{n+4}{k} \right) z^k$	$\sum_{k=0}^{8} \binom{\binom{8}{k}}{\binom{k}{k}} + \left(11\binom{6}{k-2} + 2\binom{5}{k-3}\binom{n+1}{k} + \left(2\binom{5}{k-3} + 22\binom{4}{k-4} + 4\binom{3}{k-5}\binom{n+2}{\binom{k}{k-5}}\binom{n+2}{\binom{k}{k}} + \left(4\binom{3}{k-5} + 8\binom{2}{k-6} + \binom{1}{\binom{n+1}{k}}\binom{n+3}{\binom{k}{k}} + \binom{1}{\binom{k}{k}}\binom{n+3}{\binom{k}{k}} + \binom{1}{\binom{k}{k}}\binom{n+3}{\binom{k}{k}}\binom{n+3}{\binom{k}{k}}\binom{n+3}{\binom{k}{k}} + \binom{1}{\binom{k}{k}}\binom{n+3}}\binom{n+3}{\binom{k}{k}}\binom{n+3}\binom{n+3}{\binom{k}{k}}\binom{n+3}{\binom{k}{k}}n$	$\sum_{k=0}^{8} \left(\binom{8}{k} \binom{n}{k} + \left(11\binom{6}{k-2} + 3\binom{5}{k-3} \right) \binom{n+1}{k} + \left(3\binom{5}{k-3} + 24\binom{4}{k-4} + 7\binom{3}{k-5} \right) \binom{n+2}{k} + \left(7\binom{3}{k-5} + 10\binom{2}{k-6} + 2\binom{1}{k-7} \binom{n+3}{k} + 2\binom{1}{k-7} \binom{n+4}{k} \right) z^k$
Table	کر کر	<u></u>	${\checkmark}$	ŝ	\$	Ş	Ŕ	Ś
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Stri	$[\mathbf{R}, \mathbf{W}, \mathbf{R}, \mathbf{N}, \mathbf{R}]$	$\left[R,W,R,R,N\right]$	$\begin{bmatrix} W,R,R,R,N \end{bmatrix}_{O(2,5,n)}$	$egin{array}{c} [{ m R},{ m L},{ m R},{ m L},{ m R} \ { m Z}^{(6,n)} \end{array}$	[R, R, L, W, N]	[R, L, W, N, L]	[R, R, W, L, N]	$[\mathbf{R},\mathbf{W},\mathbf{R},\mathbf{N},\mathbf{L}]$

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ŭ	ructure		LL polynomial
$\left[\mathbf{R},\mathbf{L},\mathbf{W},\mathbf{L},\mathbf{N}\right]$		Ş	$\sum_{k=0}^{8} \left(\binom{3}{k} \binom{n}{k} + \left(12\binom{6}{k-2} + 3\binom{5}{k-3} \binom{n+1}{k} + \left(3\binom{5}{k-3} + 30\binom{4}{k-3} + 7\binom{3}{k-5} \right)\binom{n+2}{k} \right) \right. \\ \left. + \left(7\binom{2}{k-5} + 16\binom{2}{k-6} + 2\binom{1}{k-1} \binom{n+3}{k} + \left(2\binom{1}{k-7} + \binom{0}{k-3} \binom{n+4}{k} \right) 2^k \right) \right]$
[R, W, L, L, N]		A	$\sum_{k=0}^{9} \left(\binom{9}{k} \binom{n}{k} + \left(12\binom{7}{k-2} + 3\binom{6}{k-3} \right) \binom{n+1}{k} + \left(3\binom{6}{k-3} + 30\binom{6}{k-4} + 7\binom{4}{k-5} \right) \binom{n+2}{k} + \left(7\binom{4}{k-5} + 16\binom{3}{k-6} + 2\binom{2}{k-7} \right) \binom{n+3}{k} + \left(2\binom{2}{k-5} + 16\binom{3}{k-6} + 2\binom{2}{k-7} \right) \binom{n+3}{k} + \binom{2}{k-7} + \binom{2}{k-3} \binom{n+4}{k} \binom{n+4}{k-7} \binom{n+4}{k} \binom{n+4}{k} $
$\left[\mathrm{R},\mathrm{L},\mathrm{W},\mathrm{N},\mathrm{R}\right]$		$\langle \rangle$	$\sum_{k=0}^{7} \left(\binom{7}{k} \binom{n}{k} + \left(11\binom{5}{k-2} + 4\binom{4}{k-3} \binom{1}{k} \binom{n+1}{k} + \left(4\binom{4}{k-3} + 24\binom{3}{k-5} + \binom{1}{k-6} \binom{1}{k} \binom{n+2}{k} \right) \binom{n+2}{k} + \left(9\binom{2}{k-5} + 11\binom{1}{k-6} + \binom{0}{k-7} \binom{n+3}{k} \binom{1}{k} + \binom{1}{k-6} \binom{1}{k} \binom{n+4}{k} \binom{1}{k} $
$\left[\mathrm{R},\mathrm{L},\mathrm{R},\mathrm{W},\mathrm{N}\right]$		¢,	$ \sum_{k=0}^{7} \left(\binom{7}{k} \binom{n}{k} + \left(12\binom{5}{k-2} + 4\binom{4}{k-3} \right) \binom{n+1}{k} + \left(4\binom{4}{k-3} + 28\binom{3}{k-6} + 11\binom{2}{k-5} + \binom{1}{k-6} \right) \binom{n+2}{k} \\ + \left(11\binom{2}{k-5} + 14\binom{1}{k-6} + 2\binom{0}{k-7} \right) \binom{n+3}{k} + \left(\binom{1}{k-6} + 2\binom{0}{k-7} \right) \binom{n+4}{k} 2^k $
$\left[\mathrm{R},\mathrm{W},\mathrm{L},\mathrm{N},\mathrm{R}\right]$		A	$ \sum_{k=0}^{8} \left(\binom{8}{k} \binom{n}{k} + \left(12\binom{6}{k-2} + 4\binom{5}{k-3} \right) \binom{n+1}{k} + \left(4\binom{5}{k-3} + 31\binom{4}{k-3} + 10\binom{3}{k-6} + \binom{2}{k-6} \right) \binom{n+2}{k} \\ + \left(10\binom{3}{k-5} + 19\binom{2}{k-6} + 2\binom{1}{k-1} \binom{2}{k-6} + 2\binom{1}{k-1} + \binom{6}{k-6} + 2\binom{1}{k-1} + \binom{6}{k-6} \binom{n+4}{k} \right) 2^k $
$\left[R,L,W,R,N\right]$		\sim	$\sum_{k=0}^{8} \left(\binom{8}{k} \binom{n}{k} + \left(13\binom{6}{k-2} + 4\binom{5}{k-3} \right) \binom{n+1}{k} + \left(4\binom{5}{k-3} + 35\binom{4}{k-3} + 12\binom{2}{k-6} + \binom{2}{k-6} \right) \binom{n+2}{k} \\ + \left(12\binom{2}{k-5} + 22\binom{2}{k-6} + 3\binom{1}{k-7} \binom{n+3}{k} + \binom{2}{k-6} + 3\binom{1}{k-7} + \binom{6}{k-8} \binom{n+4}{k} \binom{n+4}{k} \right) \binom{n+4}{k} 2^k$
[W, N, R, W, N]		$\overset{\bullet}{\checkmark}$	$\sum_{k=0}^{8} \binom{\binom{8}{k}\binom{n}{k} + \left(14\binom{6}{k-2} + 4\binom{5}{k-3}\binom{n+1}{k} + \left(4\binom{5}{k-3} + 42\binom{4}{k-3} + 14\binom{2}{k-6} + \binom{2}{k}\binom{n+2}{k} + \left(14\binom{3}{k-5} + 31\binom{2}{k-6} + 6\binom{1}{k-7}\binom{n+3}{k-6} + \binom{2}{k-6} + 6\binom{1}{k-7} + 2\binom{0}{k}\binom{n}{k}\binom{n+4}{k}\binom{2}{k} z^k$

ζ.	-	Table 4	4 (continued). ZZ polynomials of regular 6-tier benzenoid strips $\frac{\pi}{27}$
St	ructure		ZZ polynomial
[R, W, N, W, N]		Ş	$\begin{split} &\sum_{k=0}^{8} \left(\binom{3}{k} \binom{n}{k} + \left(14\binom{6}{k-2} \right) + 4\binom{5}{k-3} \binom{n+1}{k} + \left(4\binom{5}{k-3} \right) + 44\binom{4}{k-4} + 16\binom{3}{k-5} + \binom{2}{k-6} \binom{n+2}{k} \\ &+ \left(16\binom{3}{k-5} + 37\binom{2}{k-6} + 11\binom{1}{k-7} + \binom{0}{k-8} \binom{n+3}{k} + \binom{2}{k-6} + 11\binom{1}{k-7} + 6\binom{0}{k-8} \binom{n+4}{k} \right) \\ &+ \binom{0}{k-8} \binom{n+5}{k} 2^k \end{split}$
[R, W, R, L, N]		Ŕ	$\begin{split} & \sum_{k=0}^{9} \left(\binom{9}{k}, \binom{7}{k} + \left(14\binom{7}{k-2} + 4\binom{6}{k-3} \right) \binom{n+1}{k} + \left(4\binom{6}{k-3} + 44\binom{5}{k-4} + 16\binom{4}{k-5} + \binom{3}{k-6} \right) \binom{n+2}{k} \\ & + \left(16\binom{4}{k-5} + 37\binom{3}{k-6} + 11\binom{2}{k-7} + \binom{1}{k-8} \right) \binom{n+3}{k} + \left(\binom{3}{k-6} + 11\binom{2}{k-7} + 6\binom{1}{k-7} \right) \binom{n+4}{k} \end{split}$
[R, W, L, R, N]		Ş	$\begin{split} & \sum_{k=0}^{9} \left(\binom{9}{k} \binom{n}{k} + \left(15\binom{7}{k-2} + 4\binom{6}{k-3} \right) \binom{n+1}{k} + \left(4\binom{6}{k-3} + 53\binom{5}{k-4} + 17\binom{4}{k-5} + \binom{3}{k-6} \right) \binom{n+2}{k} \\ & + \left(17\binom{4}{k-5} + 54\binom{3}{k-6} + 13\binom{2}{k-7} + \binom{1}{k-8} \right) \binom{n+3}{k} + \left(\binom{3}{k-6} + 13\binom{2}{k-7} + \binom{3}{k-6} \right) \binom{n+4}{k} \\ & + \left(\binom{1}{k-8} + \binom{0}{k-8} \right) \binom{n+4}{k} 2^k \end{split}$
[W, R, N, W, N]		\$	$\begin{split} & \sum_{k=0}^{9} \left(\binom{9}{k}, \binom{7}{k} + \left(16\binom{7}{k-2} + 4\binom{6}{k-3} \right) \binom{n+1}{k} + \left(4\binom{6}{k-3} + 61\binom{5}{k-4} + 19\binom{4}{k-5} + \binom{3}{k-6} \right) \binom{n+2}{k} \\ & + \left(19\binom{4}{k-5} + 67\binom{3}{k-6} + 18\binom{2}{k-7} + \binom{1}{k-8} \right) \binom{n+3}{k} + \left(\binom{3}{k-6} + 18\binom{2}{k-7} + 17\binom{1}{k-9} + 2\binom{0}{k-9} \right) \binom{n+4}{k} \\ & + \left(\binom{1}{k-8} + 2\binom{0}{k-9} \right) \binom{n+5}{k} 2^k \end{split}$
[R, W, W, N]		$\langle \langle \rangle$	$\begin{split} & \sum_{k=0}^{10} \left(\binom{100}{k} \left(\binom{5}{k} \right) + \left(15\binom{8}{k-2} \right) + 4\binom{7}{k-3} \right) \binom{n+1}{k} + \left(4\binom{7}{k-3} \right) + 53\binom{6}{k-4} + 17\binom{5}{k-5} + \binom{4}{k-6} \right) \binom{n+2}{k} \\ & + \left(17\binom{5}{k-5} + 54\binom{4}{k-6} + 13\binom{3}{k-7} + \binom{2}{k-8} \right) \binom{n+3}{k} + \left(\binom{4}{k-6} + 13\binom{3}{k-7} + 13\binom{2}{k-9} + \binom{1}{k-9} \right) \binom{n+4}{k} \\ & + \left(\binom{2}{k-8} + \binom{1}{k-9} \right) \binom{n+5}{k} 2 \end{split}$

Str	ucture		ZZ polynomial
[W, R, R, L, N]		¢,	$\begin{split} & \sum_{k=0}^{10} \left(\binom{10}{k} \binom{n}{k} + \left(16\binom{8}{k-2} + 4\binom{7}{k-3} \right) \binom{n+1}{k} + \left(4\binom{7}{k-3} + 61\binom{6}{k-4} + 19\binom{5}{k-5} + \binom{4}{k-6} \right) \binom{n+2}{k} \\ & + \left(19\binom{5}{k-5} + 67\binom{4}{k-6} + 18\binom{3}{k-7} + \binom{2}{k-8} \right) \binom{n+3}{k} + \left(\binom{4}{k-6} + 18\binom{3}{k-7} + \binom{2}{k-8} \right) \binom{n+3}{k} \\ & + \left(\binom{2}{k-8} + 2\binom{1}{k-9} \right) \binom{n+5}{k} \binom{2}{k} \end{split}$
[W, R, L, R, N]		\diamond	$\begin{split} & \prod_{k=0}^{10} \left(\binom{10}{k} + \left(18\binom{8}{k-5} + 4\binom{7}{k-3} \right) \binom{n+1}{k} + \left(4\binom{7}{k-3} + 84\binom{6}{k-4} + 24\binom{5}{k-5} + \binom{4}{k-6} \right) \binom{n+2}{k} \\ & + \left(24\binom{5}{k-5} + 128\binom{4}{k-6} + 36\binom{3}{k-7} + 2\binom{2}{k-8} \right) \binom{n+3}{k} + \left(\binom{4}{k-6} + 36\binom{3}{k-7} + 6\binom{2}{k-8} \right) \binom{n+3}{k} \\ & + \left(14\binom{1}{k-9} + \binom{0}{k-10} \right) \binom{n+4}{k} + \left(2\binom{2}{k-8} + 14\binom{1}{k-9} + 6\binom{0}{k-10} \right) \binom{n+5}{k} + \binom{0}{k} \binom{n+6}{k} \binom{n+6}{k} 2k \end{split}$
[W, R, W, N, N]		\bigotimes	$\begin{split} &\sum_{k=0}^{11} \left(\binom{11}{k} \binom{n}{k} + \left(18\binom{8}{k-2} \right) + 4\binom{8}{k-3} \right) \binom{n+1}{k} + \left(4\binom{8}{k-3} + 84\binom{7}{k-4} + 24\binom{6}{k-5} + \binom{5}{k-6} \right) \binom{n+2}{k} \\ &+ \left(24\binom{6}{k-5} + 128\binom{5}{k-6} + 36\binom{4}{k-7} + 2\binom{3}{k-8} \right) \binom{n+3}{k} + \left(\binom{5}{k-6} + 36\binom{4}{k-7} + 61\binom{8}{k-8} \right) \\ &+ \left(14\binom{2}{k-9} + \binom{1}{k-10} \right) \binom{n+4}{k} + \left(2\binom{3}{k-8} + 14\binom{2}{k-9} + 6\binom{1}{k-10} \right) \binom{n+5}{k} + \binom{1}{k} \binom{n+6}{k} + \binom{n+6}{k} \binom{n+6}{k} $
$\begin{bmatrix} \textbf{W}, \textbf{W}, \textbf{R}, \textbf{N}, \textbf{N} \end{bmatrix}$ $O(3, 4, n)$		${\checkmark}$	$\begin{split} &\sum_{k=0}^{12} \left(\binom{12}{k} \binom{n}{k} + \left(18\binom{10}{k-2} + 4\binom{9}{k-2} \right) \binom{n+1}{k} + \left(4\binom{9}{k-3} + 84\binom{8}{k-4} + 24\binom{7}{k-5} + \binom{6}{k-6} \right) \binom{n+2}{k} \\ &+ \left(24\binom{7}{k-5} + 128\binom{6}{k-6} + 36\binom{5}{k-7} + 2\binom{4}{k-8} \right) \binom{n+3}{k} + \left(\binom{6}{k-6} + 36\binom{5}{k-7} + 61\binom{4}{k-8} \right) \\ &+ \left(14\binom{3}{k-9} + \binom{2}{k-9} + \binom{2}{k-10} \right) \binom{n+4}{k} + \left(2\binom{4}{k-8} + 14\binom{3}{k-9} + 6\binom{2}{k-10} \right) \binom{n+5}{k} \binom{n+5}{k} + \binom{2}{k} \binom{n+6}{k} \\ \end{split}{}$

Table 4 (continued). ZZ polynomials of regular 6-tier benzenoid strips

3 Discussion

The ZZ polynomials presented in Tables 1–4 correspond to KekulÄ©an strips, i.e., strips for which at least one Clar cover can be constructed. For every Kekuléan strip S, there exists an associated poset S that can be used to determine the extended strict order polynomial $E_{S}^{\circ}(n, 1 + x)$, which in turn is equal to the ZZ polynomial of S, ZZ(S, x). However, starting from m = 5, each family of regular m-tier benzenoid strips contains also some non-Kekuléan strips. It is easy to identify these structures using interface theory of benzenoids [30,31] as those which possess a row with fewer than n - 1 hexagons (which corresponds to an interface with a negative order). Simple geometrical considerations show that there exists exactly one such structure, the goblet X(3,3,n) (see p. 169 of [15]), for m = 5 and three such structures for m = 6: the goblet X(3,4,n) (see p. 232 of [15]). The ZZ polynomials—and thus, the numbers of Clar covers—of these four structures are identically equal to 0. For non-Kekuléan structures S, no associated poset S can be constructed, as it would be required by the interface theory of benzenoids that S contains a negative number of elements associated with the short row(s) of S, which is absurd.

The collection presented in Tables 1–4 might be also of interest for a mathematician looking for a closed-form formula of the extended strict order polynomial $E_{\mathcal{S}}^{\circ}(n, z)$ for some particular poset \mathcal{S} . Note that in this sense, the presented catalog of formulas is not complete. The regular *m*-tier benzenoid strips always generate a poset that is an induced subposet of the lattice $\mathbf{m} \times \mathbf{m}$, with some further restrictions. For a poset \mathcal{S} which does not belong to this category, Eq. (1) still computes a valid extended strict order polynomial, but no regular *m*-tier strip can be associated with it and consequently such a formula is missing from our tables. For small \mathcal{S} with $|\mathcal{S}| \leq 3$, all possible posets are included in our collection. (Note that a poset \mathcal{S} and its order dual \mathcal{S}' share the same extended strict order polynomial, $E_{\mathcal{S}}^{\circ}(n, z) = E_{\mathcal{S}'}^{\circ}(n, z)$.) However, for larger posets, only a small portion belong to the studied here category of $\mathbf{m} \times \mathbf{m}$ subposets; for $|\mathcal{S}| = 4$, we tabulate the extended strict order polynomials of only 62% of conceivable posets, and for $|\mathcal{S}| = 5$, only of 25% of conceivable posets. The remaining posets are yet to be studied.

A short reflection suggests how one could possibly generalize the presented here technique to non-regular *m*-tier strips. In the extended strict order polynomial $E^{\circ}_{\mathcal{S}}(n, z)$ defined by Eq. (1), it is assumed that vertices in every column of the Hasse diagram of \mathcal{S}

are assigned numbers between 1 and n and that such an assignment is order-preserving, i.e., that if two elements t_j and t_k , being in a relation $t_j <_{\mathcal{S}} t_k$ in the poset \mathcal{S} , are assigned the numbers λ_j and λ_k , respectively, then $\lambda_j < \lambda_k$. A detailed analysis of such order-preserving assignments led us to the discovery of the formula for $E^{\circ}_{\mathcal{S}}(n,z)$ given by Eq. (1). In order to generalize this approach to non-regular strips, one needs to allow for the flexibility associated with the fact that each row of the non-regular *m*-tier strip might have a distinct length $n_i = \mu_i - \nu_i$ defined by the pair of numbers $[\nu_i, \mu_i]$, where the sequence $\nu_1, \nu_2, \ldots, \nu_m$ describes the shape of the left rim of the non-regular *m*-tier strip S, and the sequence $\mu_1, \mu_2, \ldots, \mu_m$, its right rim. Then, the map $\phi : t_j \mapsto \lambda_j$ should be orderpreserving in S and the number λ_j should satisfy $\nu_i \leq \lambda_j \leq \mu_i$, where the element $t_j \in S$ is located in the interface *i* of S. Detailed construction of the sequences $\nu_1, \nu_2, \ldots, \nu_m$ and $\mu_1, \mu_2, \ldots, \mu_m$, which should simultaneously encompass the information about the shape of S and the order of interfaces in S, remains to be elucidated. The suggested here line of development might produce an useful viable algorithm for finding ZZ(S, x), but we seriously doubt if the corresponding formula for $E^{\circ}_{\mathcal{S}}(n, z)$ can be expressed in some general, structured, closed form.

4 Conclusion

We have presented a compilation of ZZ polynomials of regular *m*-tier strips of an arbitrary length *n* for m = 1-6. For each regular strip S, its ZZ polynomial ZZ(S, x) has been computed as the extended strict order polynomial $E_{\mathcal{S}}^{\circ}(n, z)$ of a poset S associated with S. The presented collection of formulas could be derived owing to the equivalence between the ZZ polynomials and extended strict order polynomials recently discovered by us [33]. A detailed explanation of techniques and methods needed to evaluate the extended strict order polynomial $E_{\mathcal{S}}^{\circ}(n, z)$ defined by Eq. (1) is given in [34]. The presented tabulation can be easily extended to regular *m*-tier strips with m > 6.

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References

- M. 16., Maplesoft, a division of Waterloo Maple Inc., Waterloo, Ontario. Maple is a trademark of Waterloo Maple Inc.
- [2] N. Bašić, I. Estélyi, R. Skrekovski, N. Tratnik, On the Clar number of benzenoid graphs, MATCH Commun. Math. Comput. Chem. 80 (2018) 173–188.
- [3] M. Berlič, N. Tratnik, P. Žigert Pleteršek, Equivalence of Zhang–Zhang polynomial and cube polynomial for spherical benzenoid systems, *MATCH Commun. Math. Comput. Chem.* **73** (2015) 443–456.
- [4] 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.
- [5] C.-P. Chou, H. A. Witek, S. Irle, When finite becomes infinite: convergence properties of vibrational spectra of oligomer chains, J. Mol. Model. 24 (2018) #244.
- [6] 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.
- [7] 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.
- [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, Closed-form formulas for the Zhang–Zhang polynomials of benzenoid structures: Chevrons and generalized chevrons, *MATCH Commun. Math. Comput. Chem.* 72 (2014) 105–124.
- [10] 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.
- [11] 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.
- [12] 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.
- [13] S. J. Cyvin, B. N. Cyvin, I. Gutman, Number of Kekulé structures of five-tier strips, Z. Naturforsch. 40a (1985) 1253–1261.

- [14] S. J. Cyvin, I. Gutman, Kekulé structures and their symmetry properties, *Comput. Math. Appl.* **12B** (1986) 859–876.
- [15] S. J. Cyvin, I. Gutman, Kekulé Structures in Benzenoid Hydrocarbons, Springer, Berlin, 1988.
- [16] S. J. Cyvin, The number of Kekulé structures of hexagon-shaped benzenoids and members of other related classes, *Monatsh. Chem.* 117 (1986) 33–45.
- [17] M. Gordon, W. H. T. Davison, Theory of resonance topology of fully aromatic hydrocarbons. 1, J. Chem. Phys. 20 (1952) 428–435.
- [18] Q. Z. Guo, H. Y. Deng, D. D. Chen, Zhang-Zhang polynomials of cyclo-polyphenacenes, J. Math. Chem. 46 (2009) 347–362.
- [19] I. Gutman, B. Borovićanin, Zhang–Zhang polynomial of multiple linear hexagonal chains, Z. Naturforsch. 61a (2006) 73–77.
- [20] I. Gutman, S. J. Cyvin, Topological properties of benzenoid systems. XXXV. Number of Kekulé structures of multiple–chain aromatics, *Monatsh. Chem.* 118 (1987) 541– 552.
- [21] 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.
- [22] B. H. He, C. P. Chou, J. Langner, H. A. Witek, Zhang-Zhang polynomials of ribbons, Symmetry 12 (2020) #2060.
- [23] B. H. He, J. Langner, H. A. Witek, Hexagonal flakes as fused parallelograms: A determinantal formula for Zhang-Zhang polynomials of the O(2, m, n) benzenoids, J. Chin. Chem. Soc. 68 (2021) 1231–1242.
- [24] B. H. He, H. A. Witek, Clar theory for hexagonal benzenoids with corner defects, MATCH Commun. Math. Comput. Chem. 86 (2021) 121–140.
- [25] B. H. He, H. A. Witek, Enumeration of Clar covers of parallelogram chains, *Discr. Appl. Math.* **302** (2021) 221–233.
- [26] B. H. He, H. A. Witek, J. Langner, R. Podeszwa, Can the John-Sachs theorem be extended to Clar covers?, *MATCH Commun. Math. Comput. Chem.* 86 (2021) 141–163.
- [27] J. Langner, H. A. Witek, Connectivity graphs for single zigzag chains and their application for computing ZZ polynomials, *Croat. Chem. Acta* **90** (2017) 391–400.
- [28] J. Langner, H. A. Witek, Algorithm for generating generalized resonance structures of single zigzag chains based on Interface Theory, J. Math. Chem. 56 (2018) 1393–1406.

- [29] J. Langner, H. A. Witek, Equivalence between Clar covering polynomials of single zigzag chains and tiling polynomials of 2×n rectangles, *Discr. Appl. Math.* 243 (2018) 297–303.
- [30] J. Langner, H. A. Witek, Interface theory of benzenoids, MATCH Commun. Math. Comput. Chem. 84 (2020) 143–176.
- [31] J. Langner, H. A. Witek, Interface theory of benzenoids: Basic applications, MATCH Commun. Math. Comput. Chem. 84 (2020) 177–215.
- [32] J. Langner, H. A. Witek, Extended strict order polynomial of a poset and fixed elements of linear extensions, Australas. J. Comb. 81 (2021) 187–207.
- [33] J. Langner, H. A. Witek, ZZ polynomials of regular *m*-tier benzenoid strips as extended strict order polynomials of associated posets. Part 1. Proof of equivalence, *MATCH Commun. Math. Comput. Chem.* 87 (2022) 585–620.
- [34] J. Langner, H. A. Witek, ZZ polynomials of regular *m*-tier benzenoid strips as extended strict order polynomials of associated posets. Part 2. Guide to practical computation, *MATCH Commun. Math. Comput. Chem.* 88 (2022) 109–130.
- [35] J. Langner, H. A. Witek, G. Moś, Zhang–Zhang polynomials of multiple zigzag chains, MATCH Commun. Math. Comput. Chem. 80 (2018) 245–265.
- [36] W. F. Li, M. Andrzejak, H. A. Witek, Evolution of physical properties of conjugated systems, *Phys. Status Solidi B* 249 (2012) 306–316.
- [37] N. Ohkami, H. Hosoya, Topological dependency of the aromatic sextets in polycyclic benzenoid hydrocarbons. Recursive relations of the sextet polynomial, *Theor. Chim. Acta* 64 (1983) 153–170.
- [38] H. A. Witek, J. S. Kang, ZZ polynomials for isomers of (5,6)-fullerenes C_n with n = 20 50, Symmetry 12 (2020) #1483.
- [39] H. A. Witek, J. Langner, Clar covers of overlapping benzenoids: Case of two identically-oriented parallelograms, *Symmetry* **12** (2020) #1599.
- [40] H. A. Witek, J. Langner, R. Podeszwa, Closed-form formulas for Zhang-Zhang polynomials of hexagonal graphene flakes O(k, m, n) with k, m = 1 - 7 and arbitrary n, MATCH Commun. Math. Comput. Chem. 86 (2021) 165–194.
- [41] 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.
- [42] 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.
- [43] T. F. Yen, Resonance topology of polynuclear aromatic hydrocarbons, *Theor. Chim. Acta* 20 (1971) 399–404.

- [44] F. J. Zhang, H. P. Zhang, Y. T. Liu, The Clar covering polynomial of hexagonal systems II, *Chin. J. Chem.* 14 (1996) 321–325.
- [45] H. P. Zhang, The Clar covering polynomial of S,T–isomers, MATCH Commun. Math. Comput. Chem. 29 (1993) 189–197.
- [46] H. P. Zhang, The Clar formulas of regular t-tier strip benzenoid systems, Syst. Sci. Math. Sci. 8 (1995) 327–337.
- [47] H. P. Zhang, W. C. Shiu, P. K. Sun, A relation between Clar covering polynomial and cube polynomial, MATCH Commun. Math. Comput. Chem. 70 (2013) 477–492.
- [48] H. P. Zhang, The Clar covering polynomial of hexagonal systems with an application to chromatic polynomials, *Discr. Math.* **172** (1997) 163–173.
- [49] 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.
- [50] H. P. Zhang, F. J. Zhang, The Clar covering polynomial of hexagonal systems I, Discr. Appl. Math. 69 (1996) 147–167.
- [51] H. P. Zhang, F. J. Zhang, The Clar covering polynomial of hexagonal systems III, Discr. Math. 212 (2000) 261–269.
- [52] P. Žigert Pleteršek, Equivalence of the generalized Zhang–Zhang polynomial and the generalized cube polynomial, MATCH Commun. Math. Comput. Chem. 80 (2018) 215–226.
- [53] ZZDecomposer, https://bitbucket.org/peggydbc1217/zzdecomposer_hsi/downloads/
- [54] ZZDecomposer, https://bitbucket.org/solccp/zzdecomposer_binary/downloads/