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Zhang–Zhang Polynomials of Various Classes of Benzenoid Systems

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Abstract

The Zhang–Zhang(ZZ) polynomials (*aka* Clar covering polynomial) for several subclasses of catacondensed and pericondensed benzenoid systems have been computed using an automatic computer code developed in our group and described in [C.-P. Chou and H.A. Witek, MATCH Commun. Math. Comput. Chem., submitted]. General closed-form expressions for several series of catacondensed benzenoids and for the prolate rectangular pericondensed benzenoids have been obtained. The presented results suggest that general closed-form expressions for the ZZ polynomials of many classes of pericondensed benzenoid systems can be discovered by analysis of structural similarities between the ZZ polynomials of their subclasses. Methods and techniques of finding such similarities are outlined.

1. Introduction

In the preceding paper[1] (hereafter referred to as **I**) we have reported a computer program developed in our group to determine the Zhang–Zhang (ZZ) polynomials of benzenoid systems. The ZZ polynomial[2-14] is a combinatorial polynomial representing in a very convenient way all the conceivable resonance structures that can be written for a given aromatic system. It has a finite order equal to the Clar number *Cl*, i.e., the maximal number of aromatic Clar sextets that can be accommodated inside a given benzenoid structure. The ZZ polynomial of some benzenoid system *B* can be expressed as

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

where x is a dummy variable used to differentiate between various classes of resonance structures and c_k denotes the number of Clar covers in a given class possessing exactly k aromatic Clar sextets[15]. The term Clar cover of order k was first introduced by Zhang and Zhang[2-5] to denote a permissible resonance structure of some benzenoid system *B* built of n sp^2-hybridized carbon atoms, which is characterized by k aromatic Clar sextets and $n/2-3k$ localized double bonds. The knowledge of the ZZ polynomial yields immediately a number of important topological invariants characterizing the structure *B*; c_0 is equal to the number of its Kekulé structures and c_{Cl} is equal to the number of its Clar structures. The importance of the ZZ polynomial representations stems from the possibility of its fast evaluation owing to convenient recursive properties it obeys (for details see **I**). Our program is capable to evaluate the ZZ polynomials for dense, pericondensed benzenoids containing up to 500 carbon atoms. For catacondensed and quasi-linear pericondensed benzenoids, the limiting number of carbon atoms is much larger and may exceed 10000. For even larger structures, one needs to execute our program in parallel mode, which makes the maximal number of atoms in the system under consideration dependent on the number of employed processors.

The theory of ZZ polynomials was reviewed in the preceding publication **I** together with simple examples enabling a novice in the field deeper understanding of the main underlying concepts. We have also discussed the recursive properties of ZZ polynomials, which were extensively used to develop our program. We concluded the preceding publication **I** by reviewing a number of general combinatorial techniques, which can be used for finding the ZZ polynomials for various classes of benzenoid structures. In this study, we apply the developed techniques for finding the explicit, closed-form of the ZZ polynomial for certain subfamilies of benzenoid structures. Our main aim is to show that the developed program can be a useful theoretical tool for this purpose. Our study closely follows the thorough and monumental account of benzenoid structures given by Cyvin and Gutman[16]. We show that our approach is capable of finding closed-form expressions for the ZZ polynomials for many benzenoid systems in analogy to the closed-form expressions for the numbers of Kekulé structures compiled by Cyvin and Gutman[16]. We do not attempt to make the current study complete; the given here ZZ polynomials are computed only for certain subclasses of benzenoids systems obtained by fixing some of the indices. Only in few cases, we are able to give most general formulas. More complete studies focusing on each family of benzenoids and giving the most general forms of the ZZ polynomial will be published subsequently. Note that the compact form of the presented here results strongly indicates that this goal can be achieved, even if its realization may require considerable effort.

2. Catacondensed benzenoid systems

a. Multiple segment linear hexagonal chain $L(m,n)$, $m \geq 3$

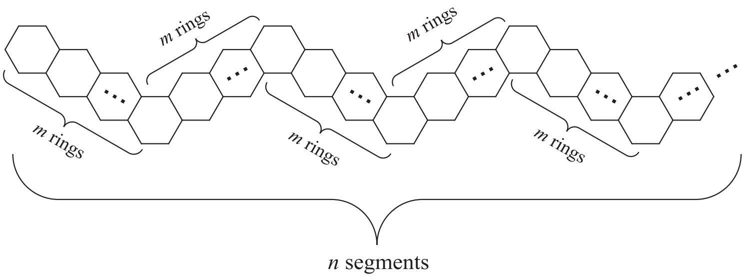

Figure 1. Multiple segment linear hexagonal chain $L(m,n)$

We attempt to find the ZZ polynomial of multiple segment linear hexagonal chains $L(m,n)$, shown in Figure 1, by fixing first the value of m and generalizing later the resulting family of ZZ polynomials to some non-fixed value of m. The simplest structure in this family, with m = 2, has been already discussed in **I**. Note that the case m = 2 reduces to a single armchair chain $N(n)$ of length n obeying the recurrence relation

$$\mathrm{ZZ}(N(n),x) = \mathrm{ZZ}(N(n-1),x) + (x+1)\cdot \mathrm{ZZ}(N(n-2),x) \tag{1}$$

and having the ZZ polynomial given explicitly by

$$\mathrm{ZZ}\left(N(n),x\right)=\mathrm{ZZ}(L(2,n-1),x)=\frac{1}{2}\left(1+\frac{2x+3}{\sqrt{4x+5}}\right)\left(\frac{1+\sqrt{4x+5}}{2}\right)^{n}+\frac{1}{2}\left(1-\frac{2x+3}{\sqrt{4x+5}}\right)\left(\frac{1-\sqrt{4x+5}}{2}\right)^{n}. \tag{2}$$

When $m = 3$, the ZZ polynomials of the shortest few $L(3,n)$ structures are given by

$$\begin{cases} \mathrm{ZZ}\left(L(3,0),x\right)=2+x \\ \mathrm{ZZ}\left(L(3,1),x\right)=4+3x \\ \mathrm{ZZ}\left(L(3,2),x\right)=10+13x+4x^{2} \\ \mathrm{ZZ}\left(L(3,3),x\right)=24+43x+24x^{2}+4x^{3} \\ \mathrm{ZZ}\left(L(3,4),x\right)=58+133x+108x^{2}+36x^{3}+4x^{4} \\ \mathrm{ZZ}\left(L(3,5),x\right)=140+391x+416x^{2}+208x^{3}+48x^{4}+4x^{5}. \end{cases} \tag{3}$$

From Eq. (3), it is clear that the ZZ polynomials of the $L(3,n)$ series obey a recurrence relation given by

$$ZZ(L(3,n),x)=(x+2)\cdot ZZ(L(3,n-1),x)+(x+1)\cdot ZZ(L(3,n-2),x). \tag{4}$$

The recurrence can be easily solved using MAPLE[17], giving the following closed-form formula for the ZZ polynomial of $L(3,n)$

$$\mathrm{ZZ}(L(3,n),x)=\frac{1}{2}\left(x+2+\frac{(-x^{2}+2x+4)}{\sqrt{x^{2}+8x+8}}\right)\left(\frac{(x+2)+\sqrt{x^{2}+8x+8}}{2}\right)^{n}+\frac{1}{2}\left(x+2-\frac{(-x^{2}+2x+4)}{\sqrt{x^{2}+8x+8}}\right)\left(\frac{(x+2)-\sqrt{x^{2}+8x+8}}{2}\right)^{n}. \tag{5}$$

When $m = 4$, the ZZ polynomial for the shortest few $L(4,n)$ are given by

$$\begin{cases} \mathrm{ZZ}\left(L(4,1),x\right)=5+4x \\ \mathrm{ZZ}\left(L(4,2),x\right)=17+25x+9x^{2} \\ \mathrm{ZZ}\left(L(4,3),x\right)=56+118x+81x^{2}+18x^{3} \\ \mathrm{ZZ}\left(L(4,4),x\right)=185+508x+513x^{2}+225x^{3}+36x^{4} \\ \mathrm{ZZ}\left(L(4,5),x\right)=611+2068x+2754x^{2}+1800x^{3}+576x^{4}+72x^{5}. \end{cases} \tag{6}$$

The corresponding recurrence relation is found to be

$$ZZ(L(4,n),x) = (2x+3)\cdot ZZ(L(4,n-1),x) + (x+1)\cdot ZZ(L(4,n-2),x). \quad (7)$$

By solving the recurrence relation, one gets the closed form of the ZZ polynomial for the $L(4,n)$ series that can be written as

$$\begin{aligned} ZZ(L(4,n),x) = & \frac{1}{2}\left(x+2+\frac{(-2x^2+x+4)}{\sqrt{4x^2+16x+13}} \right)\left(\frac{(2x+3)+\sqrt{4x^2+16x+13}}{2} \right)^n \\ & +\frac{1}{2}\left(x+2-\frac{(-2x^2+x+4)}{\sqrt{4x^2+16x+13}} \right)\left(\frac{(2x+3)-\sqrt{4x^2+16x+13}}{2} \right)^n . \end{aligned} \quad (8)$$

An analysis of the recursion formulas for the $L(m,n)$ series shows that in the general case the recurrence relation for the ZZ polynomials of $L(m,n)$ can be expressed as

$$ZZ(L(m,n),x) = \left[(m-2)x+(m-1)\right]\cdot ZZ(L(m,n-1),x) + (x+1)\cdot ZZ(L(m,n-2),x). \quad (9)$$

Using standard techniques for solving recurrence formula as described in **I** with initial conditions

$$ZZ\left(L(m,1),x\right) = 1+m(1+x) \quad (10)$$

$$ZZ\left(L(m,2),x\right) = (1+m^2)+(1-2m+2m^2)x+(m-1)^2x^2 \quad (11)$$

yields the closed formula of the Zhang–Zhang polynomial for $L(m,n)$ in the following form

$$\begin{aligned} ZZ(L(m,n),x) = & \frac{1}{2}\left((x+2)+\frac{(2-m)x^2+(5-m)x+4}{\sqrt{k}} \right)\left(\frac{(m-1)+(m-2)x+\sqrt{k}}{2} \right)^n \\ & +\frac{1}{2}\left((x+2)-\frac{(2-m)x^2+(5-m)x+4}{\sqrt{k}} \right)\left(\frac{(m-1)+(m-2)x-\sqrt{k}}{2} \right)^n , \end{aligned} \quad (12)$$

where $k = (x+1)^2m^2 - 2(x+1)(2x+1)m + 4x^2 + 8x + 5$. This formula can be also obtained by extrapolating the series given by the Eqs. (2), (5), and (8), but probably a large number of terms would be required to discover all the underlying regularities. Note that by setting $x = 0$, Eq. (12) reduces to the formula for calculating number of Kekulé structure reported in [18].

b. Hammer *H*(*n*)

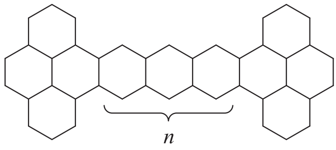

Figure 2. Hammer-like benzenoid $H(n)$

The hammer-like $H(n)$ structures, shown in Figure 2 and at page 100 of [16], can be obtained by terminating the ends of a linear polyacene of length n with two pyrene fragments. In principle, $H(n)$ is not a catacondensed benzenoid due to the presence of pericondensed terminal groups, but we treat it in this section as the varying fragment is catacondensed. The ZZ polynomials of the shortest ten structures of this type are given by

$$\begin{cases} \mathrm{ZZ}(H(0),x) = 35+70x+47x^2+12x^3+x^4 \\ \mathrm{ZZ}(H(1),x) = 60+145x+132x^2+57x^3+12x^4+x^5 \\ \mathrm{ZZ}(H(2),x) = 85+220x+217x^2+102x^3+23x^4+2x^5 \\ \mathrm{ZZ}(H(3),x) = 110+295x+302x^2+147x^3+34x^4+3x^5 \\ \mathrm{ZZ}(H(4),x) = 135+370x+387x^2+192x^3+45x^4+4x^5 \\ \mathrm{ZZ}(H(5),x) = 160+445x+472x^2+237x^3+56x^4+5x^5 \\ \mathrm{ZZ}(H(6),x) = 185+520x+557x^2+282x^3+67x^4+6x^5 \\ \mathrm{ZZ}(H(7),x) = 210+595x+642x^2+327x^3+78x^4+7x^5 \\ \mathrm{ZZ}(H(8),x) = 235+670x+727x^2+372x^3+89x^4+8x^5 \\ \mathrm{ZZ}(H(9),x) = 260+745x+812x^2+417x^3+100x^4+9x^5. \end{cases} \tag{13}$$

This series has a constant order and can be expressed in a closed-form as

$$\begin{aligned} \mathrm{ZZ}(H(n),x) &= 5(5n+7)+5(15n+14)x+(85n+47)x^2+3(15n+4)x^3+(11n+1)x^4+nx^5 \\ &= 1+(8+n)(1+x)+(17+6n)(1+x)^2+(8+11n)(1+x)^3+(1+6n)(1+x)^4 \\ &\quad +n(1+x)^5. \end{aligned} \tag{14}$$

The first term, $25n+35$, agrees with the number of Kekulé formulas given by Cyvin and Gutman[16]. Furthermore, using the obvious, natural decomposition of this structure into the pyrene and polyacene fragments, as suggested by Zhang and Zhang[2], yields the same ZZ polynomial in somewhat more natural form given by

$$\mathrm{ZZ}\big(H(n),x\big)=(x^2+5x+5)^2(1+n(1+x))+2(x+1)(x^2+5x+5), \tag{15}$$

where x^2+5x+5 is easily identified as the ZZ polynomial of phenantrene.

c. Starphenes *St*(*n*,*m*,*l*)

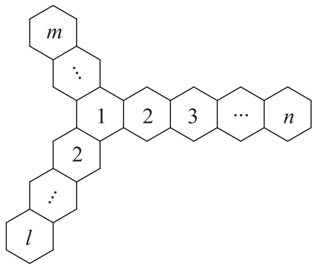

Figure 3. Starphene *St*(*n*,*m*,*l*) structure

A starphene *St*(*n*,*m*,*l*), shown in Figure 3, can be considered as a structure obtained by fusing three linear polyacenes of length *n*, *m*, and *l*, respectively. It is easy to see that an application of **Property 2** of **I** to the central hexagon immediately yields the ZZ polynomial of *St*(*n*,*m*,*l*) given by

$$\mathrm{ZZ}\big(St(n,m,l),x\big)=\mathrm{ZZ}\big(L(n-1),x\big)\cdot\mathrm{ZZ}\big(L(m-1),x\big)\cdot\mathrm{ZZ}\big(L(l-1),x\big)+1+x$$

with $\mathrm{ZZ}\big(L(k),x\big)$ given by Eq. (10). In starphenes, the first decomposition step leading to this nice recursive form is clear, but for many other structures, mostly of pericondensed nature, the first step (or steps) is not immediately obvious. Therefore, we re-derive this formula using an alternative approach similar in spirit to those discussed in **I**. We believe that this analysis can be helpful for more complicated systems, even if here it may look here like overcomplicating a simple issue. The ZZ polynomials for the smallest few *St*(*n*,*m*,*l*) structures are given by

$$\begin{cases} ZZ(St(2,2,2),x) = 9+13x+6x^2+x^3 \\ ZZ(St(2,2,3),x) = 13+21x+11x^2+2x^3 \\ ZZ(St(2,3,3),x) = 19+34x+20x^2+4x^3 \\ ZZ(St(3,3,3),x) = 28+55x+36x^2+8x^3 \\ ZZ(St(2,2,4),x) = 17+29x+16x^2+3x^3 \\ ZZ(St(2,3,4),x) = 25+47x+29x^2+6x^3 \\ ZZ(St(3,3,4),x) = 37+76x+52x^2+12x^3 \\ ZZ(St(2,4,4),x) = 33+65x+42x^2+9x^3 \\ ZZ(St(3,4,4),x) = 49+105x+75x^2+18x^3 \\ ZZ(St(4,4,4),x) = 65+145x+108x^2+27x^3 \end{cases} \tag{16}$$

Obviously, the ZZ polynomials of starphenes have the order not greater than 3 and can be expressed in the following form

$$\mathrm{ZZ}\big(St(n,m,l),x\big) = \sum_{k=0}^{3} f_k(n,m,l)x^k \tag{17}$$

with the yet unknown functions $f_k(n,m,l)$. A better insight in the unknown functions $f_k(n,m,l)$ can be obtained from the analysis of the ZZ polynomials for starphenes with two indices fixed. It is easy to find that the ZZ polynomials for the $St(2,2,l)$ series have a closed form given by

$$\mathrm{ZZ}\big(St(2,2,l),x\big) = 1+4l+(8l-3)x+(5l-4)x^2+(l-1)x^3, \tag{18}$$

which suggest that the unknown function $f_k(n,m,l)$ are functions of indices n, m, and l of degree 0 or 1. The associated multinomial basis $\{1,n\}\times\{1,m\}\times\{1,l\}$ consists of eight terms. Clear permutational symmetry of the unknown functions

$$f_k(n,m,l) = f_k(n,l,m) = f_k(m,n,l) = f_k(m,l,n) = f_k(l,m,n) = f_k(l,n,m)$$

allows one to reduce the size of the basis to only four fully-symmetric terms $\{\ 1,\ l+m+n,\ lm + ln + mn,\ lmn\ \}$ corresponding to the fully-symmetric irreducible representation of the symmetric group S_3, casting Eq. (17) in the following matrix form

$$ZZ\left(St(n,m,l),x\right)=\begin{pmatrix}1\\x\\x^2\\x^3\end{pmatrix}^T\begin{pmatrix}a_{0,0,0,0} & a_{0,1,0,0} & a_{0,1,1,0} & a_{0,1,1,1}\\a_{1,0,0,0} & a_{1,1,0,0} & a_{1,1,1,0} & a_{1,1,1,1}\\a_{2,0,0,0} & a_{2,1,0,0} & a_{2,1,1,0} & a_{2,1,1,1}\\a_{3,0,0,0} & a_{3,1,0,0} & a_{3,1,1,0} & a_{3,1,1,1}\end{pmatrix}\begin{pmatrix}1\\l+m+n\\lm+ln+mn\\lmn\end{pmatrix}. \tag{19}$$

Substituting the ZZ polynomials listed in Eq. (16) into this linear equations and solving the (possibly overdetermined) linear problem gives the general formula for the ZZ polynomial of *St*(*n*,*m*,*l*) as

$$ZZ\left(St(n,m,l),x\right)=\begin{pmatrix}1\\x\\x^2\\x^3\end{pmatrix}^T\begin{pmatrix}1 & 0 & 0 & 1\\1 & 0 & -1 & 3\\0 & 1 & -2 & 3\\-1 & 1 & -1 & 1\end{pmatrix}\begin{pmatrix}1\\l+m+n\\lm+ln+mn\\lmn\end{pmatrix}. \tag{20}$$

Using slightly different bases for solving the linear problem simplifies Eq. (20) even further giving the following general formula of ZZ polynomials of starphenes

$$ZZ\left(St(n,m,l),x\right)=\begin{pmatrix}1\\1+x\\(1+x)^2\\(1+x)^3\end{pmatrix}^T\begin{pmatrix}1 & 0 & 0 & 0\\1 & 1 & 0 & 0\\0 & 0 & 1 & 0\\0 & 0 & 0 & 1\end{pmatrix}\begin{pmatrix}1\\L+M+N\\LM+LN+MN\\LMN\end{pmatrix}, \tag{21}$$

where $N = n - 1$, $M = m - 1$, and $L = l - 1$, which can be expressed readily in the familiar form

$$ZZ\left(St(n,m,l),x\right)=1+x+\left(N(1+x)+1\right)\left(M(1+x)+1\right)\left(L(1+x)+1\right) \tag{22}$$

given earlier by Zhang and Zhang[2]. By setting $x = 0$ in Eq. (22), one obtains the number of Kekulé structures reported previously[19, 20]. Note that the regularity observed here is general; the basis constructed from the powers of $1 + x$ gives usually much shorter expansions then the basis of monomials x^k and solves the set of linear equations giving smaller numerical coefficients. Similar observation is true for the basis of indices, where a homogeneous shift by an integer may lead to great simplification of the final formulas.

d. Tripod *T*(*n*,*m*,*l*)

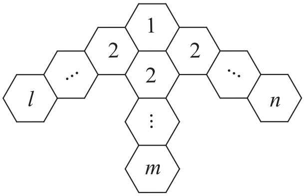

Figure 4. Tripod structure *T*(*n*,*m*,*l*)

The next system is a tripod-like system *T* with three indices *n*, *m*, *l*. Again, this system is pericondensed rather than catacondensed, but we study it here as the varying fragments are catacondensed. When *n* or *l* = 1, tripod is non-Kekuléan and the ZZ polynomial vanishes. When *n* = *l* = 1, tripod reduces to a linear polyacene *L*(*m*). When *m* = 1, the ZZ polynomial is given by a simple formula

$$\mathrm{ZZ}\big(T(n,1,l),x\big)=(x+1)+\mathrm{ZZ}\big(L(n-1),x\big)\mathrm{ZZ}\big(L(l-1),x\big). \tag{23}$$

The ZZ polynomials of *T*(*n*,*m*,*l*) for *n*, *m*, *l* = 2 and 3 are given by

$$\begin{cases} \mathrm{ZZ}(T(2,2,2),x)=6+6x+x^2 \\ \mathrm{ZZ}(T(2,2,3),x)=9+11x+3x^2 \\ \mathrm{ZZ}(T(2,3,2),x)=11+16x+7x^2+x^3 \\ \mathrm{ZZ}(T(2,3,3),x)=16+26x+13x^2+2x^3 \\ \mathrm{ZZ}(T(3,2,2),x)=9+11x+3x^2 \\ \mathrm{ZZ}(T(3,2,3),x)=14+21x+9x^2+x^3 \\ \mathrm{ZZ}(T(3,3,2),x)=16+26x+13x^2+2x^3 \\ \mathrm{ZZ}(T(3,3,3),x)=24+44x+26x^2+5x^3 \end{cases} \tag{24}$$

The technique used for finding the formula for starphene can be applied here after some modification. The coefficients of the ZZ polynomial of this system are found to be maximally linear functions of the indices *n*, *m*, and *l* in close analogy to starphene. However, instead of having 3 interchangeable indecies like in starphene, only two indices, *n* and *l*, are related by permutational symmetry. Thus, eight terms in the $\{1,n\}\times\{1,m\}\times\{1,l\}$ basis reduce to six terms

{1, *m*, *l* + *n*, *lm* + *mn*, *ln*, *lmn*}. After solving the linear equations, one gets the formula for tripod *T*(*n*, *m*, *l*) as

$$\mathrm{ZZ}\big(T(n,m,l),x\big)=\begin{pmatrix}1\\x\\x^2\\x^3\end{pmatrix}^T\begin{pmatrix}0&1&-1&0&0&1\\2&2&-3&-1&-1&3\\5&2&-2&-2&-2&3\\2&1&0&-1&-1&1\end{pmatrix}\begin{pmatrix}1\\m\\l+n\\lm+mn\\nl\\lmn\end{pmatrix},\tag{25}$$

or alternatively in the (1+*x*) basis as

$$\mathrm{ZZ}\big(T(n,m,l),x\big)=\begin{pmatrix}1\\1+x\\(1+x)^2\\(1+x)^3\end{pmatrix}^T\begin{pmatrix}1&0&0&0&0&0\\-2&1&1&0&0&0\\-1&-1&-2&1&1&0\\2&1&0&-1&-1&1\end{pmatrix}\begin{pmatrix}1\\m\\l+n\\lm+mn\\nl\\lmn\end{pmatrix}.\tag{26}$$

Decomposition of this system in a conventional way gives the formula of tripod *T*(*n*,*m*,*l*) as

$$\begin{aligned}\mathrm{ZZ}\big(T(n,m,l),x\big)&=\Big(\mathrm{ZZ}\big(L(m-2),x\big)\cdot\mathrm{ZZ}\big(L(n-1),x\big)\cdot\mathrm{ZZ}\big(L(l-1),x\big)\Big)\\&\quad+(1+x)\Big(\mathrm{ZZ}\big(L(m-2),x\big)+\mathrm{ZZ}\big(L(n-2),x\big)\cdot\mathrm{ZZ}\big(L(l-2),x\big)\Big),\end{aligned}\tag{27}$$

where *L*(*n*) is a linear polyacene with length *n*.

e. Zigzag-edge coronoids *ZC*(*n*, *m*, *l*)

The zigzag-edge coronoids *ZC*(*n*,*m*,*l*), shown in Figure 5, can be considered as a structure obtained by fusing six segments of linear polyacenes into a closed loop. To find a closed form of the ZZ polynomial for this family of benzenoid structures, we first consider its certain subfamily obtained by fixing *n* = *m* = 3. The ZZ polynomials of the smallest few *ZC*(3,3,*l*) structures are given by

$$\begin{cases} \mathrm{ZZ}\left(ZC(3,3,3),x\right) = 200+594x+699x^2+408x^3+123x^4+18x^5+x^6 \\ \mathrm{ZZ}\left(ZC(3,3,4),x\right) = 365+1184x+1537x^2+1008x^3+349x^4+60x^5+4x^6 \\ \mathrm{ZZ}\left(ZC(3,3,5),x\right) = 580+1974x+2695x^2+1868x^3+687x^4+126x^5+9x^6 \\ \mathrm{ZZ}\left(ZC(3,3,6),x\right) = 845+2964x+4173x^2+2988x^3+1137x^4+216x^5+16x^6 \\ \mathrm{ZZ}\left(ZC(3,3,7),x\right) = 1160+4154x+5971x^2+4368x^3+1699x^4+330x^5+25x^6 \\ \mathrm{ZZ}\left(ZC(3,3,8),x\right) = 1525+5544x+8089x^2+6008x^3+2373x^4+468x^5+36x^6 \\ \mathrm{ZZ}\left(ZC(3,3,9),x\right) = 1940+7134x+10527x^2+7908x^3+3159x^4+630x^5+49x^6 \\ \mathrm{ZZ}\left(ZC(3,3,10),x\right) = 2405+8924x+13285x^2+10068x^3+4057x^4+816x^5+64x^6. \end{cases} \quad (28)$$

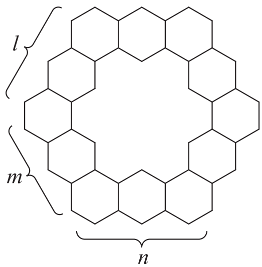

Figure 5. Zigzag-edge coronoid *ZC*(*n*,*m*,*l*)

It is easy to find that this constant-order series can be written in a closed form as

$$\begin{aligned} \mathrm{ZZ}\left(ZC(3,3,l),x\right) = {} & 5(5l^2-2l+1)+2(5l-4)(10l-3)x \\ & +(160l^2-282l+105)x^2+2(65l^2-155l+84)x^3 \\ & +(56l^2-166l+117)x^4+6(l-2)(2l-3)x^5+(l-2)^2x^6. \end{aligned} \quad (29)$$

Eq. (29) suggests that the coefficients of the ZZ polynomial for *ZC*(*m*,*n*,*l*) are maximally quadratic functions of the indices. The full index basis contains 27 functions: $\{1,n,n^2\}\times\{1,m,m^2\}\times\{1,l,l^2\}$,but permutational symmetry allows for reducing it to only 10 their fully-symmetric linear combinations. Following the same train of arguments as for starphenes in the previous section, the general formula of the ZZ polynomial for zigzag-edge coronoids *ZC*(*m*,*n*,*l*) can be expressed in the symmetry-adapted basis of multinomials as

$$
\mathrm{ZZ}\big(ZC(n,m,l),x\big)=
\begin{pmatrix} 1 \\ x+1 \\ (x+1)^2 \\ (x+1)^3 \\ (x+1)^4 \\ (x+1)^5 \\ (x+1)^6 \end{pmatrix}^T
\begin{pmatrix}
1+2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
6 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
9 & 8 & 4 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
2 & 6 & 10 & 8 & 2 & 2 & 0 & 0 & 0 & 0 \\
0 & 0 & 2 & 12 & 1 & 2 & 4 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 2 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}
\begin{pmatrix} 1 \\ L+M+N \\ LM+LN+MN \\ LMN \\ L^2+M^2+N^2 \\ L^2(M+N)+M^2(L+N)+N^2(L+M) \\ LMN(L+M+N) \\ L^2M^2+L^2N^2+M^2N^2 \\ LMN(LM+LN+MN) \\ L^2M^2N^2 \end{pmatrix}, \tag{30}
$$

where $N = (n-2)$, $M = (m-2)$, and $L = (l-2)$.

The sparse matrix representation of Eq. (30) is quite robust for actual calculations, but it may be advantageous to cast Eq. (30) in a simpler form. It is quite straightforward to identify that the blue, green, and red entries in Eq. (30) define the expansion of the following simple three functions in our basis

$$
\begin{cases}
(Ns+1)^2(Ms+1)^2(Ls+1)^2, \\
2s(Ns+1)(Ms+1)(Ls+1)\big[(Ns+1)+(Ms+1)+(Ls+1)\big], \\
s^2\big[(Ns+1)+(Ms+1)+(Ls+1)\big]^2,
\end{cases} \tag{31}
$$

where $s = x + 1$. This identification helps to cast Eq. (30) in much simpler form

$$
\begin{aligned}
\mathrm{ZZ}\big(ZC(n,m,l),x\big) &= \big[(Ns+1)(Ms+1)(Ls+1)+(Ns+1)s+(Ms+1)s+(Ls+1)s\big]^2 \\
&\quad +2s^3+2,
\end{aligned} \tag{32}
$$

where $N = (n-2)$, $M = (m-2)$, $L = (l-2)$, and $s = x + 1$.

Note that the $ZC(n, m, l)$ system is a cyclo-polyphenacene with number of segments $t = 6$. The formula of the ZZ polynomial for cyclo-polyphenacenes has been reported by Guo, Deng, and Chen[21] with number of segments $t \geq 2$; however, no closed-form formula was provided. Besides, the formula provided in [21] is erroneous; its corrected version is given in [22].

f. Fenestrene *F*(*n*,*m*)

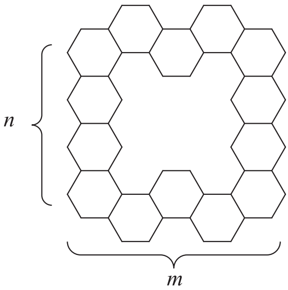

Figure 6. Fenestrene structure *F*(*n*,*m*)

The next system studied here is the fenestrene structure abbreviated as *F*(*n*,*m*) and shown in Figure 6. We consider here only the structures with the index *m* odd. From the analysis of the ZZ polynomials of *F*(*n*,*m*) with *n* = 3,4,5,6,7,8, and 9 and *m* = 5,7,9,11, and 13, we find that the general formula are given by

$$\mathrm{ZZ}\left(F(n,m),x\right)=\left(\left(L_{n-2}-2\right)N_{m-2}+2N_{m-1}\right)^{2}+2N_{m}N_{m-2}-2N_{m-1}{}^{2}+2, \tag{33}$$

where $L_n = \mathrm{ZZ}(L(n), x) = 1+(1+x)n$ and $N_n = \mathrm{ZZ}\left(N(n),x\right)=\sum_{k=0}^{n}\binom{n+1-k}{k}(1+x)^{k}$, are the ZZ polynomials of the zigzag and armchair single chains, respectively.

3. Pericondensed benzenoid systems

a. Hexagons *O*(*m*,*k*,*n*) with *m* = 1, 2, and 3

The hexagonal-shaped graphene flakes *O*(*m*,*k*,*n*), *aka* hexagons, fully characterized by giving a set of 3 indices (*m*,*k*,*n*), constitute one of the most important classes of benzenoid structures.

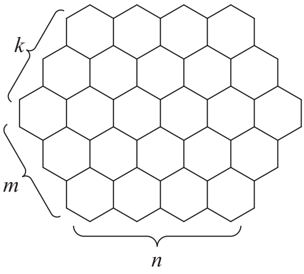

Figure 7. Hexagon $O(m,k,n)$

Here, we will analyze a subfamily of these structures obtained by first setting $m = k$ and then fixing the value of m to 1, 2, and 3. When $m = 1$, the $O(m,m,n)$ subfamily reduces to linear polyacenes $L(n)$ of length n with the ZZ polynomial given by Eq. (10). When $m = 2$, the ZZ polynomials for the shortest few $O(2,2,n)$ structures are given by

$$\begin{cases} ZZ\left(O(2,2,1),x\right) = 6 + 6x + x^2 \\ ZZ\left(O(2,2,2),x\right) = 20 + 32x + 15x^2 + 2x^3 \\ ZZ\left(O(2,2,3),x\right) = 50 + 100x + 66x^2 + 16x^3 + x^4 \\ ZZ\left(O(2,2,4),x\right) = 105 + 240x + 190x^2 + 60x^3 + 6x^4 \\ ZZ\left(O(2,2,5),x\right) = 196 + 490x + 435x^2 + 160x^3 + 20x^4 \\ ZZ\left(O(2,2,6),x\right) = 336 + 896x + 861x^2 + 350x^3 + 50x^4 \\ ZZ\left(O(2,2,7),x\right) = 540 + 1512x + 1540x^2 + 672x^3 + 105x^4 \\ ZZ\left(O(2,2,8),x\right) = 825 + 2400x + 2556x^2 + 1176x^3 + 196x^4 \\ ZZ\left(O(2,2,9),x\right) = 1210 + 3630x + 4005x^2 + 1920x^3 + 336x^4. \end{cases} \tag{34}$$

This series has a constant order. It is easy to find a closed formula for it given by

$$\begin{aligned} ZZ\left(O(2,2,n),x\right) &= 1 + 4n(1+x) + \frac{1}{2}n(7n-5)(1+x)^2 \\ &\quad + 2\binom{n}{2}\binom{n-1}{1}(1+x)^3 + \frac{1}{3}\binom{n}{2}\binom{n-1}{2}(1+x)^4. \end{aligned} \tag{35}$$

When $m = 3$, the ZZ polynomial for the few shortest $O(3,3,n)$ are given by

$$\begin{cases} ZZ\left(O(3,3,1),x\right) = 20+30x+12x^2+x^3 \\ ZZ\left(O(3,3,2),x\right) = 175+450x+425x^2+180x^3+33x^4+2x^5 \\ ZZ\left(O(3,3,3),x\right) = 980+3308x+4458x^2+3065x^3+1140x^4+225x^5+22x^6+x^7 \\ ZZ\left(O(3,3,4),x\right) = 4116+16468x+27293x^2+24262x^3+12521x^4+3796x^5+653x^6+58x^7+2x^8 \\ ZZ\left(O(3,3,5),x\right) = 14112+63522x+120848x^2+126518x^3+79506x^4+30681x^5+7132x^6+933x^7+58x^8+x^9 \\ ZZ\left(O(3,3,6),x\right) = 41580+204180x+429030x^2+503664x^3+361690x^4+163380x^5+45885x^6+7588x^7+648x^8 \\ \qquad +20x^9 \\ ZZ\left(O(3,3,7),x\right) = 108900+571890x+1295700x^2+1656270x^3+1310568x^4+661962x^5+211820x^6+40950x^7+4260x^8 \\ \qquad +175x^9 \\ ZZ\left(O(3,3,8),x\right) = 259545+1437876x+3456486x^2+4719660x^3+4021290x^4+2208360x^5+777630x^6+168084x^7 \\ \qquad +20010x^8+980x^9 \\ ZZ\left(O(3,3,9),x\right) = 572572+3313596x+8355996x^2+12027279x^3+10863732x^4+6367482x^5+2412816x^6+567126x^7 \\ \qquad +74484x^8+4116x^9. \end{cases} \tag{36}$$

Again this series has constant order. A closed formula for it can be found as

$$\begin{aligned} ZZ\left(O(3,3,n),x\right) = {} & 1+9n(1+x)+\frac{9}{2}(5n-3)n(1+x)^2 \\ & +\frac{1}{6}\left(149(n-1)^2+49(n-1)+6\right)n(1+x)^3+\frac{1}{3}\binom{n}{2}(n-1)(86n-103)(1+x)^4 \\ & +\frac{1}{3}\binom{n}{2}(n-1)\left(28(n-2)^2+23(n-2)+6\right)(1+x)^5 \\ & +\frac{1}{60}\binom{n}{3}\left(316(n-2)^3+432(n-2)^2+137(n-2)+15\right)(x+1)^6 \\ & +\frac{1}{420}\binom{n}{3}\left(236(n-2)^4+104(n-2)^3-119(n-2)^2+79(n-2)+120\right)(x+1)^7 \\ & +\frac{1}{840}\binom{n}{4}\left(105(n-2)^4+2(n-2)^3-81(n-2)^2+94(n-2)+120\right)(x+1)^8 \\ & +\frac{1}{40}\binom{n-2}{3}\binom{n-1}{3}\binom{n}{3}(x+1)^9. \end{aligned} \tag{37}$$

Note that the formulas for calculating the number of Kekulé structure derived from Eqs. (35) and (37) can be found as $\frac{1}{3}\binom{n+2}{2}\binom{n+3}{2}$ and $\frac{1}{40}\binom{n+3}{3}\binom{n+4}{3}\binom{n+5}{3}$, respectively, which agree with the formula given previously[16, 23-25].

We believe that further analysis of the presented here ZZ polynomials for the $O(m,m,n)$ series of hexagon structures may cast them in a simpler form that will be easy to generalize for any value of m. We further expect that a more extensive study of the ZZ polynomial series for the hexagon benzenoid structures will yield a closed-form expression for the ZZ polynomial of any $O(m,k,n)$ benzenoid structure in close analogy to the corresponding formula for the number of Kekulé structures. We are planning to perform such a study devoted to thorough analysis of the ZZ polynomials of the $O(m,k,n)$ structures in near future. The results presented here are a mere indication that this task can be accomplished, though relative complexity of the ZZ polynomials for the $O(2,2,n)$ and $O(3,3,n)$ subfamilies of structures suggests rather high degree of difficulties to be encountered in such a study unless serious simplifications of presented here formulas can be discovered.

b. Chevron $Ch(k,m,n)$

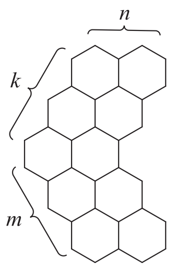

Figure 8. Chevron $Ch(k,m,n)$

The next important class of regular benzenoid structures are chevron-shaped structures (*aka* chevrons) defined by a set of three indices as $Ch(k,m,n)$, shown in Figure 8. Here, we analyze a subfamily of these structures obtained by setting $k = m$ and further fixing the value of k to 1, 2, and 3. When $k = 1$, the $Ch(1,1,n)$ structures reduce to linear polyacenes with the ZZ polynomial given by Eq. (10). When $k = 2$, the ZZ polynomials for the shortest few $Ch(2,2,n)$ structures are given by

$$\begin{cases} \mathrm{ZZ}\big(Ch(2,2,1),x\big) = 5 + 5x + 1x^2 \\ \mathrm{ZZ}\big(Ch(2,2,2),x\big) = 14 + 21x + 9x^2 + 1x^3 \\ \mathrm{ZZ}\big(Ch(2,2,3),x\big) = 30 + 54x + 30x^2 + 5x^3 \\ \mathrm{ZZ}\big(Ch(2,2,4),x\big) = 55 + 110x + 70x^2 + 14x^3 \\ \mathrm{ZZ}\big(Ch(2,2,5),x\big) = 91 + 195x + 135x^2 + 30x^3 \\ \mathrm{ZZ}\big(Ch(2,2,6),x\big) = 140 + 315x + 231x^2 + 55x^3 \\ \mathrm{ZZ}\big(Ch(2,2,7),x\big) = 204 + 476x + 364x^2 + 91x^3 \\ \mathrm{ZZ}\big(Ch(2,2,8),x\big) = 285 + 684x + 540x^2 + 140x^3 \\ \mathrm{ZZ}\big(Ch(2,2,9),x\big) = 385 + 945x + 765x^2 + 204x^3 \\ \mathrm{ZZ}\big(Ch(2,2,10),x\big) = 506 + 1265x + 1045x^2 + 285x^3. \end{cases} \quad (38)$$

A closed-form formula of for this constant-order series can be found as

$$\begin{aligned} \mathrm{ZZ}\big(Ch(2,2,n),x\big) = {} & \frac{1}{3}\binom{n+2}{2}(2n+3) + \binom{n+1}{2}(2n+3)x \\ & + \binom{n+1}{2}(2n-1)x^2 + \frac{1}{3}\binom{n}{2}(2n-1)x^3 \end{aligned} \quad (39)$$

This formula can be further simplified by factorizing the powers of $x+1$ giving

$$\mathrm{ZZ}\big(Ch(2,2,n),x\big) = 1 + 3n(1+x) + \binom{2n}{2}(1+x)^2 + \frac{1}{4}\binom{2n}{3}(1+x)^3. \quad (40)$$

For $k = m = 3$, the ZZ polynomial of the shortest few $Ch(3,3,n)$ are given by

$$\begin{cases} \mathrm{ZZ}\big(Ch(3,3,1),x\big) = 10 + 13x + 4x^2 \\ \mathrm{ZZ}\big(Ch(3,3,2),x\big) = 46 + 94x + 64x^2 + 16x^3 + 1x^4 \\ \mathrm{ZZ}\big(Ch(3,3,3),x\big) = 146 + 370x + 340x^2 + 136x^3 + 22x^4 + 1x^5 \\ \mathrm{ZZ}\big(Ch(3,3,4),x\big) = 371 + 1070x + 1160x^2 + 580x^3 + 130x^4 + 10x^5 \\ \mathrm{ZZ}\big(Ch(3,3,5),x\big) = 812 + 2555x + 3080x^2 + 1760x^3 + 470x^4 + 46x^5 \\ \mathrm{ZZ}\big(Ch(3,3,6),x\big) = 1596 + 5348x + 6944x^2 + 4340x^3 + 1295x^4 + 146x^5 \\ \mathrm{ZZ}\big(Ch(3,3,7),x\big) = 2892 + 10164x + 13944x^2 + 9296x^3 + 2996x^4 + 371x^5 \\ \mathrm{ZZ}\big(Ch(3,3,8),x\big) = 4917 + 17940x + 25680x^2 + 17976x^3 + 6132x^4 + 812x^5 \\ \mathrm{ZZ}\big(Ch(3,3,9),x\big) = 7942 + 29865x + 44220x^2 + 32160x^3 + 11460x^4 + 1596x^5 \\ \mathrm{ZZ}\big(Ch(3,3,10),x\big) = 12298 + 47410x + 72160x^2 + 54120x^3 + 19965x^4 + 2892x^5. \end{cases} \quad (41)$$

Again, a closed-form formula of the ZZ polynomial for $Ch(3,3,n)$ is easy to be found as

$$\begin{aligned}ZZ\left(Ch(3,3,n),x\right) &= \frac{1}{10}\binom{n+3}{3}(3n^2+12n+10)+\frac{1}{2}\binom{n+2}{3}(3n^2+12n+11)x \\ &+\binom{n+2}{3}(3n^2+3n-2)x^2+\binom{n+1}{3}(3n^2+3n-2)x^3 \\ &+\frac{1}{2}\binom{n+1}{3}(3n^2-6n+2)x^4+\frac{1}{10}\binom{n}{3}(3n^2-6n+1)x^5.\end{aligned} \tag{42}$$

Similar factorization like for *Ch*(2,2,*n*) yields more compact formula given by

$$\begin{aligned}ZZ\left(Ch(3,3,n),x\right) &= 1+5n(1+x)+n(7n-3)(1+x)^2+\frac{2}{3}\binom{n}{2}(11n-4)(1+x)^3 \\ &+\frac{1}{6}\binom{n}{2}(9n^2-17n+4)(1+x)^4+\frac{1}{10}\binom{n}{3}(3n^2-6n+1)(1+x)^5.\end{aligned} \tag{43}$$

Note that the first term in Eq. (42), the formula for calculating the number of Kekulé structure, agrees the formula for reported previously[23, 26].

The presented here ZZ polynomials for chevron structures have simpler structure than those for the studied here hegagons and in principle it should be easier to find a general, three-index closed-form formula for the ZZ polynomials of *Ch*(*k*,*m*,*n*). We are planning to study this class of structures in one of our subsequent papers.

c. Multiple zigzag chains *Z*(*m*,*n*)

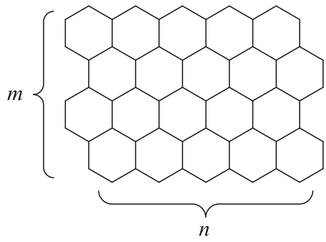

Figure 9. Multiple zigzag chains *Z*(*m*,*n*)

Multiple zigzag chains *Z*(*m*,*n*), shown in Figure 9, constitute next basic class of pericondensed benzenoid structures. This family of structures is fully characterized by giving two indices, n corresponding to the length of the zigzag-like edge and m giving the length of the armchair-like edge. When $m = 1$, the $Z(1,n)$ class reduces to linear polyacenes with the ZZ polynomials given by Eq. (10). When $m = 2$, the $Z(2,n)$ class reduces to parallelograms $M(2,n)$ with the ZZ polynomials given by Eq. (14) of **I**. When $m = 3$, the $Z(3,n)$ class reduces to chevron structures $Ch(2,2,n)$ with the ZZ polynomials given by Eq. (40). The ZZ polynomials of the shortest few $Z(4,n)$, $Z(5,n)$, and $Z(6,n)$ structures are given in Table I. It is immediately clear that the order of these polynomials is equal to m. Closed-form formulas for these series can be easily found as

$$\begin{aligned} \mathrm{ZZ}\left(Z(4,n),x\right) &= 1+4n(1+x)+\frac{3}{2}n(3n-1)(1+x)^2+\frac{1}{3}(n-1)n(5n-1)(1+x)^3 \\ &\quad +\frac{1}{24}(n-1)n(5n^2-5n+2)(1+x)^4, \end{aligned} \tag{44}$$

$$\begin{aligned} \mathrm{ZZ}\left(Z(5,n),x\right) &= 1+5n(1+x)+2n(4n-1)(1+x)^2+\frac{1}{2}n(10n^2-9n+1)(1+x)^3 \\ &\quad +\frac{1}{6}(n-1)n(2n-1)(4n-1)(1+x)^4 \\ &\quad +\frac{1}{30}(n-1)n(2n-1)(2n^2-2n+1)(1+x)^5, \end{aligned} \tag{45}$$

$$\begin{aligned} \mathrm{ZZ}\left(Z(6,n),x\right) &= 1+6n(1+x)+\frac{5}{2}n(5n-1)(1+x)^2+\frac{2}{3}n(17n^2-12n+1)(1+x)^3 \\ &\quad +\frac{1}{8}(n-1)n(3n-1)(13n-2)(1+x)^4 \\ &\quad +\frac{1}{60}(n-1)n(61n^3-79n^2+36n-4)(1+x)^5 \\ &\quad +\frac{1}{720}(n-1)n(61n^4-122n^3+113n^2-52n+12)(1+x)^6. \end{aligned} \tag{46}$$

Note that the formulas for calculating the number of Kekulé structure obtained by transforming Eqs. (44), (45), and (46) to the x basis agree with the formulas reported previously[16, 24, 25, 27].

Low-order coefficients of these series have simple form that can be readily generalized for any value of m. The free coefficient is always equal to 1, the coefficient multiplying

$(x+1)$ is equal to *mn*, and the coefficient multiplying $(x+1)^2$ is equal to $\binom{n(m-1)}{2}$. However, coefficients accompanying higher-order terms have more complicated structure that cannot be easily generalized for any value of *m*. Work along this line is in progress in our group and we hope to be able to present a closed-form ZZ polynomial for multiple zigzag chain *Z*(*m*,*n*) in one of our next studies.

Another possible path of finding a closed-form expression for the ZZ polynomials of the multiple zigzag chain *Z*(*m*,*n*) structures can be pursued by fixing the value of *n* and obtaining a general one-dimensional formulas as functions of the index *m*. When *n* = 1, the *Z*(*m*,1) structures reduce to a single armchair chain system *N*(*m*) with 2 hexagons in each segment. The closed-form of the ZZ polynomial for this system was given in Eqs. (11) and (12) of **I**. When *n* = 2, the ZZ polynomials for the shortest few *Z*(*m*,2) structures are given by

$$\begin{cases} \mathrm{ZZ}\left(Z(0,2),x\right)=1 \\ \mathrm{ZZ}\left(Z(1,2),x\right)=3+2x \\ \mathrm{ZZ}\left(Z(2,2),x\right)=6+6x+x^2 \\ \mathrm{ZZ}\left(Z(3,2),x\right)=14+21x+9x^2+x^3 \\ \mathrm{ZZ}\left(Z(4,2),x\right)=31+60x+39x^2+10x^3+x^4 \\ \mathrm{ZZ}\left(Z(5,2),x\right)=70+168x+149x^2+61x^3+12x^4+x^5 \\ \mathrm{ZZ}\left(Z(6,2),x\right)=157+448x+500x^2+280x^3+85x^4+14x^5+x^6 \\ \mathrm{ZZ}\left(Z(7,2),x\right)=353+1169x+1575x^2+1122x^3+463x^4 \\ \qquad\qquad +114x^5+16x^6+x^7 \\ \mathrm{ZZ}\left(Z(8,2),x\right)=793+2988x+4712x^2+4072x^3+2130x^4 \\ \qquad\qquad +704x^5+147x^6+18x^7+x^8 \\ \mathrm{ZZ}\left(Z(9,2),x\right)=1782+7529x+13603x^2+13825x^3+8772x^4 \\ \qquad\qquad +3651x^5+1014x^6+184x^7+20x^8+x^9 \\ \mathrm{ZZ}\left(Z(10,2),x\right)=4004+18746x+38169x^2+44596x^3+33289x^4 \\ \qquad\qquad +16746x^5+5823x^6+1400x^7+225x^8+22x^9+x^{10}. \end{cases} \tag{47}$$

The order of the ZZ polynomials in this series shows constant linear progression suggesting that the members of the series may be connected via some recursion formula in analogy to the recurrence formula of the *Z*(*m*,1) structures, which was given by Eq. (10) of **I**. It is indeed quite easy to find such a recurrence given by

$$\mathrm{ZZ}\big(Z(m,2),x\big)=(2+x)\,\mathrm{ZZ}\big(Z(m-1,2),x\big)+(1+x)\,\mathrm{ZZ}\big(Z(m-2,2),x\big)$$
$$-(1+x)^2\,\mathrm{ZZ}\big(Z(m-3,2),x\big), \tag{48}$$

This recurrence relation is a third-order linear homogeneous recurrence relation with constant coefficients, which can be readily used for computing the ZZ polynomial of the *Z*(*m*,2) structures in a recursive fashion taking the following initial values as a starting point: $\mathrm{ZZ}(Z(0,2),x)=1$, $\mathrm{ZZ}(Z(-1,2),x)=1$, and $\mathrm{ZZ}(Z(-2,2),x)=0$. In principle, it is possible to solve this recurrence using MAPLE, however the resulting explicit formula involves summation over quite complicated roots of the characteristic polynomial, which in practice is more cumbersome than using the recurrence relation.

Similar analysis performed for the *Z*(*m*,3), *Z*(*m*,4), and *Z*(*m*,5) subfamilies (See Table II) reveals that also these families can be generated recursively by the following recurrence relations

$$\mathrm{ZZ}\big(Z(m,3),x\big)=(x+2)\,\mathrm{ZZ}\big(Z(m-1,3),x\big)+(x+3)(x+1)\,\mathrm{ZZ}\big(Z(m-2,3),x\big)$$
$$-(x+1)^2\,\mathrm{ZZ}\big(Z(m-3,3),x\big)-(x+1)^3\,\mathrm{ZZ}\big(Z(m-4,3),x\big), \tag{49}$$

$$\mathrm{ZZ}\big(Z(m,4),x\big)=(2x+3)\,\mathrm{ZZ}\big(Z(m-1,4),x\big)+(x+3)(x+1)\,\mathrm{ZZ}\big(Z(m-2,4),x\big)$$
$$-(x+4)(x+1)^2\,\mathrm{ZZ}\big(Z(m-3,4),x\big)-(x+1)^3\,\mathrm{ZZ}\big(Z(m-4,4),x\big) \tag{50}$$
$$+(x+1)^4\,\mathrm{ZZ}\big(Z(m-5,4),x\big),$$

$$\mathrm{ZZ}\big(Z(m,5),x\big)=(2x+3)\,\mathrm{ZZ}\big(Z(m-1,5),x\big)+(3x+6)(x+1)\,\mathrm{ZZ}\big(Z(m-2,5),x\big)$$
$$-(x+4)(x+1)^2\,\mathrm{ZZ}\big(Z(m-3,5),x\big)-(x+5)(x+1)^3\,\mathrm{ZZ}\big(Z(m-4,5),x\big) \tag{51}$$
$$+(x+1)^4\,\mathrm{ZZ}\big(Z(m-5,5),x\big)+(x+1)^5\,\mathrm{ZZ}\big(Z(m-6,5),x\big),$$

with appropriate number of initial terms equal to 4, 5, and 6, respectively. An analysis of these formulas yields a general recurrence relation formula for the *Z*(*m*,*n*) structures that can be expressed as

Table I. The ZZ polynomial of multiple zigzag chains $Z(m,n)$ for n = 1–10 and m = 4, 5, and 6.

	m=4	m = 5	m = 6
$n=1$	$8+10x+3x^2$	$13+20x+9x^2+x^3$	$21+38x+22x^2+4x^3$
$n=2$	$31+60x+39x^2+10x^3+x^4$	$70+168x+149x^2+61x^3+12x^4+1x^5$	$157+448x+500x^2+280x^3+85x^4+14x^5+x^6$
$n=3$	$85+200x+168x^2+60x^3+8x^4$	$246+720x+814x^2+446x^3+120x^4+13x^5$	$707+2470x+3500x^2+2584x^3+1057x^4+230x^5+21x^6$
$n=4$	$190+500x+480x^2+200x^3+31x^4$	$671+2200x+2830x^2+1790x^3+560x^4+70x^5$	$2353+9226x+14855x^2+12600x^3+5960x^4+1498x^5+157x^6$
$n=5$	$371+1050x+1095x^2+500x^3+85x^4$	$1547+5460x+7615x^2+5255x^3+1800x^4+246x^5$	$6405+27062x+47215x^2+43600x^3+22520x^4+6184x^5+707x^6$
$n=6$	$658+1960x+2163x^2+1050x^3+190x^4$	$3164+11760x+17339x^2+12691x^3+4620x^4+671x^5$	$15106+67256x+124012x^2+121324x^3+66500x^4+19390x^5+2353x^6$
$n=7$	$1086+3360x+3864x^2+1960x^3+371x^4$	$5916+22848x+35084x^2+26796x^3+10192x^4+1547x^5$	$31998+148092x+284340x^2+290080x^3+165970x^4+50540x^5+6405x^6$
$n=8$	$1695+5400x+6408x^2+3360x^3+658x^4$	$10317+41040x+65004x^2+51276x^3+20160x^4+3164x^5$	$62349+297300x+588750x^2+620064x^3+366492x^4+115332x^5+15106x^6$
$n=9$	$2530+8250x+10035x^2+5400x^3+1086x^4$	$17017+69300x+112485x^2+91005x^3+36720x^4+5916x^5$	$113641+554862x+1125960x^2+1215900x^3+737220x^4+238056x^5+31998x^6$
$n=10$	$3641+12100x+15015x^2+8250x^3+1695x^4$	$26818+111320x+184305x^2+152185x^3+62700x^4+10317x^5$	$196119+976184x+2020480x^2+2226400x^3+1377915x^4+454278x^5+62349x^6$

Table II. The ZZ polynomial of multiple zigzag chains $Z(m,n)$ for m = 1–10 and n = 3, 4, and 5.

	n=3	n = 4	n = 5
$m=1$	$4+3x$	$5+4x$	$6+5x$
$m=2$	$10+12x+3x^2$	$15+20x+6x^2$	$21+30x+10x^2$
$m=3$	$30+54x+30x^2+5x^3$	$55+110x+70x^2+14x^3$	$91+195x+135x^2+30x^3$
$m=4$	$85+200x+168x^2+60x^3+8x^4$	$190+500x+480x^2+200x^3+31x^4$	$371+1050x+1095x^2+500x^3+85x^4$
$m=5$	$246+720x+814x^2+446x^3+120x^4+13x^5$	$671+2200x+2830x^2+1790x^3+560x^4+70x^5$	$1547+5460x+7615x^2+5255x^3+1800x^4+246x^5$
$m=6$	$707+2470x+3500x^2+2584x^3+1057x^4+230x^5$ $+21x^6$	$2353+9226x+14855x^2+12600x^3+5960x^4+1498x^5$ $+157x^6$	$6405+27062x+47215x^2+43600x^3+22520x^4+6184x^5$ $+707x^6$
$m=7$	$2037+8277x+14103x^2+13099x^3+7201x^4$ $+2361x^5+431x^6+34x^7$	$8272+37763x+73029x^2+77685x^3+49215x^4$ $+18627x^5+3913x^6+353x^7$	$26585+130858x+274092x^2+317015x^3+218960x^4$ $+90459x^5+20733x^6+2037x^7$
$m=8$	$5864+27162x+54047x^2+60480x^3+41790x^4$ $+18354x^5+5033x^6+792x^7+55x^8$	$29056+151344x+341579x^2+436902x^3+347020x^4$ $+175656x^5+55469x^6+10014x^7+793x^8$	$110254+619506x+1514051x^2+2103864x^3+1819830x^4$ $+1004568x^5+346016x^6+68076x^7+5864x^8$
$m=9$	$16886+87825x+199851x^2+261645x^3+217817x^4$ $+120031x^5+43975x^6+10373x^7+1435x^8+89x^9$	$102091+597487x+1541441x^2+2303323x^3+2199963x^4$ $+1395141x^5+588497x^6+159511x^7+25253x^8+1782x^9$	$457379+2888678x+8068606x^2+13090532x^3+13605311x^4$ $+9402058x^5+4324173x^6+1277511x^7+220197x^8+16886x^9$
$m=10$	$48620+280536x+718455x^2+1077148x^3+1049335x^4$ $+696066x^5+319466x^6+100516x^7+20817x^8+2570x^9$ $+144x^{10}$	$358671+2329998x+6762915x^2+11560164x^3$ $+12901440x^4+9835254x^5+5194053x^6+1879020x^7$ $+446274x^8+62920x^9+4004x^{10}$	$1897214+13304180x+41804631x^2+77553400x^3$ $+94123337x^4+78141678x^5+44974435x^6+17732716x^7$ $+4587330x^8+703592x^9+48620x^{10}$

$$\mathrm{ZZ}\big(Z(m,n),x\big)=\sum_{k=0}^{n}(-1)^{\left\lfloor \frac{k}{2}\right\rfloor}(x+1)^{k}\left((x+1)\binom{\left\lfloor \frac{k+n}{2}\right\rfloor}{k+1}+\binom{\left\lfloor \frac{k+n}{2}\right\rfloor}{k}\right)\cdot \mathrm{ZZ}\big(Z(m-k-1,n),x\big), \tag{52}$$

where $\lfloor r \rfloor$ denotes the floor function. Note that by setting $x = 0$ in Eq. (52), it reduces to the general recursion relation formula for calculating the number of Kekulé structure, which has been reported in several publications[27-29]. Formula (52) can be used to generate the ZZ polynomial for the structure *Z*(*m*,*n*) provided that the ZZ polynomials for the initial $n+1$ members of this subfamily are known: $\mathrm{ZZ}(Z(-2,n),x)$, $\mathrm{ZZ}(Z(-1,n),x)$,…, $\mathrm{ZZ}(Z(n-1,n),x)$, where the following values can be assumed for the first few artificial members of this series: $\mathrm{ZZ}(Z(0,n),x)=1$, $\mathrm{ZZ}(Z(-1,n),x)=1$, and $\mathrm{ZZ}(Z(-2,n),x)=0$. Note that for practical calculations with large *n* this recurrence formula is not very useful, because the determination of the ZZ polynomial for the first *n* + 1 members of this family may constitute a considerable computational problem. In our opinion the first of the presented here possible paths of finding the closed-form expression for the ZZ polynomials of the *Z*(*m*,*n*) structures, with the fixed value of *m* rather than with the fixed value of *n*, is more promising for accomplishing this task.

d. Ribbon *Rb*(*m*,*m*,*n*) with *n* = 2, *m* ≥ *n*

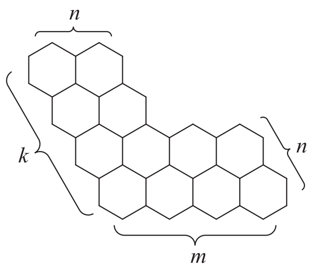

Figure 10. Ribbon *Rb*(*k*,*m*,*n*)

The next important class of benzenoids is the family of ribbon-like structures *Rb*(*k*,*m*,*n*) defined in Figure 10. Here, we restrict our attention to a subclass of these structures obtained by setting $k = m$ and further restricting *n* to 2 and 3. The ZZ polynomials of the shortest few *Rb*(*m*,*m*,2) structures are given by

$$\begin{cases} \mathrm{ZZ}(Rb(2,2,2),x) = 6+6x+x^2 \\ \mathrm{ZZ}(Rb(3,3,2),x) = 19+29x+12x^2+x^3 \\ \mathrm{ZZ}(Rb(4,4,2),x) = 53+106x+69x^2+16x^3+x^4 \\ \mathrm{ZZ}(Rb(5,5,2),x) = 126+297x+244x^2+81x^3+9x^4 \\ \mathrm{ZZ}(Rb(6,6,2),x) = 262+686x+645x^2+256x^3+36x^4 \\ \mathrm{ZZ}(Rb(7,7,2),x) = 491+1381x+1416x^2+625x^3+100x^4 \\ \mathrm{ZZ}(Rb(8,8,2),x) = 849+2514x+2737x^2+1296x^3+225x^4 \\ \mathrm{ZZ}(Rb(9,9,2),x) = 1378+4241x+4824x^2+2401x^3+441x^4 \\ \mathrm{ZZ}(Rb(10,10,2),x) = 2126+6742x+7929x^2+4096x^3+784x^4. \end{cases} \tag{53}$$

Since the order of the ZZ polynomials in this series is constant, a closed formula of the ZZ polynomial for it can be found by

$$\begin{aligned} \mathrm{ZZ}\left(Rb(m,m,2),x\right) &= 1+2(m-2)(1+x)+(5m^2-17m+15)(1+x)^2 \\ &\quad+\binom{m-2}{1}^2(2m-5)(1+x)^3+\binom{m-2}{2}^2(1+x)^4. \end{aligned} \tag{54}$$

For $n = 3$, the ZZ polynomials of the shortest few $Rb(m,m,3)$ structures are given by

$$\begin{cases} \mathrm{ZZ}(Rb(3,3,3),x) = 20+30x+12x^2+x^3 \\ \mathrm{ZZ}(Rb(4,4,3),x) = 69+139x+90x^2+20x^3+x^4 \\ \mathrm{ZZ}(Rb(5,5,3),x) = 226+573x+520x^2+201x^3+30x^4+x^5 \\ \mathrm{ZZ}(Rb(6,6,3),x) = 662+1986x+2265x^2+1220x^3+312x^4+33x^5+x^6 \\ \mathrm{ZZ}(Rb(7,7,3),x) = 1716+5806x+7716x^2+5085x^3+1720x^4+276x^5+16x^6 \\ \mathrm{ZZ}(Rb(8,8,3),x) = 3985+14715x+21742x^2+16336x^3+6525x^4+1300x^5+100x^6 \\ \mathrm{ZZ}(Rb(9,9,3),x) = 8434+33249x+53040x^2+43645x^3+19446x^4+4425x^5+400x^6 \\ \mathrm{ZZ}(Rb(10,10,3),x) = 16526+68518x+115785x^2+101816x^3+49000x^4+12201x^5+1225x^6. \end{cases} \tag{55}$$

Again, the order of the ZZ polynomials in this series is constant and a closed-form for the series can be expressed as

$$\begin{aligned} \mathrm{ZZ}\left(Rb(m,m,3),x\right) &= 1+3(2m-3)(1+x)+3(4m^2-19m+24)(1+x)^2 \\ &\quad+\frac{1}{3}(28m^3-246m^2+731m-732)(1+x)^3 \\ &\quad+\frac{1}{4}\binom{m-3}{1}^2(13m^2-96m+180)(1+x)^4 \\ &\quad+\binom{m-3}{2}^2(2m-9)(1+x)^5+\binom{m-3}{3}^2(1+x)^6. \end{aligned} \tag{56}$$

Note that the formula for calculating the number of Kekulé structure agrees with the formula given previously[16, 30].

The resulting formulas display quite high degree of internal symmetry suggesting that extending this study to other, more general ribbon structures can yield a general formula applicable to computing the ZZ polynomial of any $Rb(k,m,n)$ ribbon-like benzenoid structure. Needless to say, we are planning to perform this task in the near future.

e. Oblate rectangle *Or*(*m*,*n*)

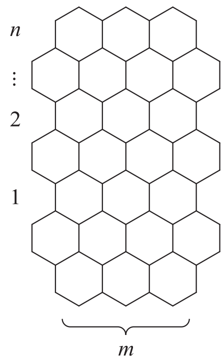

Figure 11. Oblate rectangle $Or(m,n)$

Next important family of pericondensed benzenoid structures is the class of oblate rectangular benzenoids $Or(m,n)$ shown in Figure 11. This case with $m = 1$ was studied previously by Gutman, Furtula, and Balaban[7], who offered a closed form solution obtained as a solution to the discovered recurrence relation. When $n = 0$, this class reduces again to polyacenes $L(m)$ with the ZZ polynomials given by Eq. (10) and when $n = 1$, it reduces to the hexagon $O(2, 2, m)$ structures with the ZZ polynomials given by Eq. (35). When $n = 2$, the ZZ polynomials of the shortest few $Or(m,2)$ structures are given by

$$
\begin{cases}
ZZ(Or(1,2),x) = 18 + 28x + 12x^2 + x^3 \\
ZZ(Or(2,2),x) = 136 + 354x + 344x^2 + 154x^3 + 31x^4 + 2x^5 \\
ZZ(Or(3,2),x) = 650 + 2166x + 2894x^2 + 1990x^3 + 754x^4 + 158x^5 + 18x^6 + x^7 \\
ZZ(Or(4,2),x) = 2331 + 9002x + 14334x^2 + 12170x^3 + 5950x^4 + 1686x^5 + 262x^6 + 18x^7 \\
ZZ(Or(5,2),x) = 6860 + 29232x + 52066x^2 + 50225x^3 + 28370x^4 \\
\qquad +9424x^5 + 1722x^6 + 136x^7 \\
ZZ(Or(6,2),x) = 17472 + 79884x + 153832x^2 + 161756x^3 + 100415x^4 \\
\qquad +36904x^5 + 7476x^6 + 650x^7 \\
ZZ(Or(7,2),x) = 39852 + 192108x + 391860x^2 + 438564x^3 + 291116x^4 \\
\qquad +114828x^5 + 25004x^6 + 2331x^7 \\
ZZ(Or(8,2),x) = 83325 + 418572x + 892428x^2 + 1047180x^3 + 730884x^4 \\
\qquad +303828x^5 + 69804x^6 + 6860x^7 \\
ZZ(Or(9,2),x) = 162382 + 843084x + 1861728x^2 + 2267265x^3 + 1645500x^4 \\
\qquad +712392x^5 + 170604x^6 + 17472x^7 \\
ZZ(Or(10,2),x) = 298584 + 1592734x + 3618912x^2 + 4541350x^3 + 3400815x^4 \\
\qquad +1520838x^5 + 376464x^6 + 39852x^7
\end{cases}
\tag{57}
$$

This series has a constant order and it is possible to find its closed-form formula, which is given by

$$
\begin{aligned}
ZZ\left(Or(m,2),x\right) = 1 + 7m(1+x) + 3\binom{m}{1}(5m-2)(1+x)^2 \\
+\frac{1}{3}\binom{m}{1}(41m^2 - 51m + 13)(1+x)^3 \\
+\frac{1}{6}\binom{m}{2}(75m^2 - 103m + 32)(1+x)^4 \\
+\frac{1}{30}\binom{m}{2}(89m^3 - 251m^2 + 214m - 76)(1+x)^5 \\
+\frac{1}{20}\binom{m}{3}(3m-4)(7m^2 - 8m + 5)(1+x)^6 \\
+\frac{1}{20}\binom{m}{3}(m-1)^2(m^2 - 2m + 2)(1+x)^7 .
\end{aligned}
\tag{58}
$$

Again, similarly to other pericondensed structures studied earlier, this closed-form expression has a familiar form with the free coefficient equal to 1 and with the coefficient multiplying the $(1+x)^k$ term being a polynomial in *n* of degree *k*. Note that the formula for calculating the number of Kekulé structures obtained from Eq. (58) by setting $x = 0$ is identical to the formula reported previously[23].

f. Prolate rectangle *Pr*(*m*,*n*)

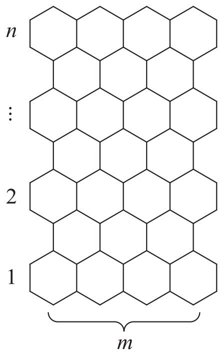

Figure 12. Prolate rectangle *Pr*(*m*,*n*)

The next class of benzenoids studied here comprises the prolate rectangular structures *Pr*(*m*,*n*) shown in Figure 12. This class of structures is quite special as it has an essentially disconnected character and can be treated as a parallel arrangement of *n* linear polyacenes of length *m*. Consequently, we are able to find the ZZ polynomials of this class of structures for a general case. To do so, we proceed as follows. When $m = 1$, the studied family of structures reduces to poly-phenylenes of length *n* and the ZZ polynomial given by

$$ZZ(Pr(1,n),x) = (2+x)^n. \tag{59}$$

When $m = 2$, the ZZ polynomials of the shortest few *Pr*(2,*n*) structures have the obvious closed form given by

$$\left.\begin{array}{l} ZZ(Pr(2,1),x) = (3+2x) \\ ZZ(Pr(2,2),x) = (3+2x)^2 \\ ZZ(Pr(2,3),x) = (3+2x)^3 \\ ZZ(Pr(2,4),x) = (3+2x)^4 \\ ZZ(Pr(2,5),x) = (3+2x)^5 \end{array}\right\} \Rightarrow ZZ(Pr(2,n),x) = (3+2x)^n. \tag{60}$$

Similarly for m = 3, the ZZ polynomials of the shortest few $Pr(3,n)$ structures are given by

$$\left.\begin{array}{l} \mathrm{ZZ}(Pr(3,1),x)=(4+3x) \\ \mathrm{ZZ}(Pr(3,2),x)=(4+3x)^2 \\ \mathrm{ZZ}(Pr(3,3),x)=(4+3x)^3 \\ \mathrm{ZZ}(Pr(3,4),x)=(4+3x)^4 \\ \mathrm{ZZ}(Pr(3,5),x)=(4+3x)^5 \end{array}\right\} \Rightarrow \mathrm{ZZ}(Pr(3,n),x)=(4+3x)^n. \qquad (61)$$

It is immediately clear that the general form of the ZZ polynomial for the $Pr(m,n)$ structure is given by

$$\mathrm{ZZ}(Pr(m,n),x)=(1+m(1+x))^n \qquad (62)$$

Note that the formula of calculating the number of Kekulé structures given by Yen[31] for $Pr(m,n)$ can be recovered by simply setting $x = 0$ in Eq. (62). In addition, Eq. (62) can be further extended to a general prolate rectangle-like structure, in which the length of each polyacene chain is not the same. Assuming that such a structure is given by parallel arrangement of m polyacenes of length m_1, m_2, …, m_n, respectively, the corresponding ZZ polynomial is given by

$$\mathrm{ZZ}\left(Pr([m_1,m_2,...,m_n],n),x\right)=\prod_{k=1}^{n}\left(1+m_k(x+1)\right). \qquad (63)$$

This formula is probably the most important single result obtained in this study.

g. Zigzag-edge coronoid fused with starphene *ZCS*(*n*,*m*,*l*)

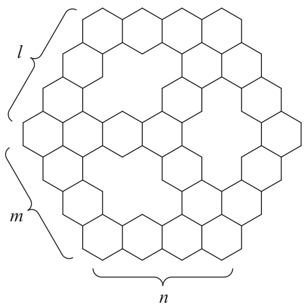

Figure 13. Zigzag-edge coronoid fused with starphene $ZCS(n,m,l)$

The last system considered in this work is a composite benzenoid obtained by fusing a zigzag-edge coronoid *ZC*(*n*,*m*,*l*) with a starphene *St*(*n*,*m*,*l*). This system, abbreviated as *ZCS*(*n*,*m*,*l*), is shown in Figure 13. The ZZ polynomials for *n*, *m*, *l* = 4 and 5 are given by

$$\begin{cases} \mathrm{ZZ}\big(ZCS(4,4,4),x\big) = 21574 + 113245x + 263802x^2 + 356338x^3 + 306449x^4 \\ \qquad\qquad + 173571x^5 + 64679x^6 + 15295x^7 + 2085x^8 + 125x^9 \\ \mathrm{ZZ}\big(ZCS(4,4,5),x\big) = 49533 + 279405x + 698997x^2 + 1014780x^3 + 939847x^4 \\ \qquad\qquad + 574906x^5 + 232060x^6 + 59588x^7 + 8833x^8 + 576x^9 \\ \mathrm{ZZ}\big(ZCS(4,5,5),x\big) = 114980 + 691009x + 1842394x^2 + 2854591x^3 + 2828177x^4 \\ \qquad\qquad + 1856201x^5 + 806597x^6 + 223725x^7 + 35941x^8 + 2548x^9 \\ \mathrm{ZZ}\big(ZCS(5,5,5),x\big) = 268916 + 1709693x + 4826193x^2 + 7929355x^3 + 8348930x^4 \\ \qquad\qquad + 5838936x^5 + 2711559x^6 + 806211x^7 + 139260x^8 + 10648x^9. \end{cases} \tag{64}$$

The resulting ZZ polynomials have a constant order equal to 9. Moreover, from the analysis of the ZZ polynomials for the *ZCS*(4,4,*l*) series, it is possible to find that the ZZ polynomial coefficients depend on the index *l* up to the third power. The same technique, which was used earlier for the starphene, coronoid, and tripod systems, can be applied here again with the basis $\{1,n,n^2,n^3\}\times\{1,m,m^2,m^3\}\times\{1,l,l^2,l^3\}$. The resulting 64-dimensional basis can be seriously reduced by the permutational symmetry adaptation, giving a fully-symmetric basis with only 20 functions. Thus, the resulting coefficient matrix has the dimension 10 by 20. The ZZ polynomial of *ZCS*(*n*,*m*,*l*) can be thus expressed as

$$\mathrm{ZZ}\big(ZCS(n,m,l),x\big) = \begin{pmatrix} 1 \\ s \\ s^2 \\ s^3 \\ s^4 \\ s^5 \\ s^6 \\ s^7 \\ s^8 \\ s^9 \end{pmatrix}^T \begin{pmatrix} 15 & 36 & 30 & 5 & 8 & 36 & -42 & 21 & -6 & 1 \\ 0 & 19 & 34 & 2 & -27 & 27 & 20 & -27 & 11 & -2 \\ 0 & 0 & 27 & 41 & -13 & -57 & 54 & -1 & -10 & 3 \\ 0 & 0 & 0 & 47 & 74 & -48 & -82 & 84 & -18 & 1 \\ 0 & 0 & 7 & 15 & -9 & -16 & 12 & 5 & -5 & 1 \\ 0 & 0 & 0 & 13 & 23 & -18 & -21 & 17 & -2 & -1 \\ 0 & 0 & 0 & 0 & 31 & 50 & -47 & -21 & 22 & -4 \\ 0 & 0 & 0 & 0 & 9 & 15 & -15 & -3 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 27 & 32 & -34 & 0 & 3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 27 & 19 & -21 & 3 \\ 0 & 0 & 0 & 2 & 3 & -1 & -2 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 4 & 4 & -3 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 10 & 8 & -7 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 3 & 2 & -2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 9 & 4 & -4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9 & 2 & -2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}^T \begin{pmatrix} 1 \\ N+M+L \\ LM+LN+MN \\ NML \\ N^2+M^2+L^2 \\ N^2(L+M)+M^2(L+N)+L^2(N+M) \\ NML(N+M+L) \\ L^2M^2+L^2N^2+M^2N^2 \\ NML(NM+ML+LN) \\ N^2M^2L^2 \\ N^3+M^3+L^3 \\ N^3(L+M)+M^3(L+N)+L^3(N+M) \\ NML(N^2+M^2+L^2) \\ N^3(L^2+M^2)+M^3(L^2+N^2)+L^3(N^2+M^2) \\ NML(N^2(L+M)+M^2(L+N)+L^2(N+M)) \\ N^2M^2L^2(N+M+L) \\ L^3M^3+L^3N^3+M^3N^3 \\ NML(L^2M^2+N^2L^2+M^2N^2) \\ N^2M^2L^2(NM+ML+LN) \\ N^3M^3L^3 \end{pmatrix}, \tag{65}$$

where $s = (1+x)$, $N = n - 2$, $M = m - 2$, and $L = l - 2$. Any attempts to cast this matrix equations into a simple functional form, as successfully performed for zigzag-edge coronene *ZC(n,m,l)*, fail; the simplest expression we could obtain reads

$$\begin{aligned}
ZZ\left(ZCS(n,m,l),x\right) = &\left(W+(s-s^2)V\right)^2(s+W)+W^2 3s^2(s-1) \\
&+WV(1-2s-s^3+7s^4-4s^5+V) \\
&+W(5+6s+6s^2+2s^3+3s^4+3s^5+4s^6) \\
&+V^2\left((s+s^5)(1+V)-3s^2+s^3+2s^4-3s^6+s^7\right) \\
&+Vs(-1+10s+s^2-4s^3+s^4-2s^5+3s^6-2s^7) \\
&-VUs(2+s+2s^3+s^4+s^5)+WU(-2-2s^3+s^4) \\
&+U(1+3s+5s^2+2s^3-s^4+s^5-s^6+s^7) \\
&+(5s+9s^2+6s^3+5s^4+3s^5-s^6+s^9),
\end{aligned} \tag{66}$$

where $W = (Ns+1)(Ms+1)(Ls+1)$, $V = (Ns+1)+(Ms+1)+(Ls+1)$, and $U = (Ns+1)(Ms+1)+(Ms+1)(Ls+1) + (Ns+1)(Ls+1)$. Relatively high degree of complexity of this equation motivated us to look for the ZZ polynomial by recursive decomposition of the *ZCS(n,m,l)* structure, which yielded even more complicated equation containing 39 addends.

4. Conclusion

We illustrate the capabilities of the developed automatic computer program for determination of the Zhang–Zhang (ZZ) polynomials by computing of the ZZ polynomials for several subclasses of catacondensed and pericondensed benzenoid systems. For all the studied here catacondensed benzenoids and for one class of pericondensed benzenoids—prolate rectangular structures *Pr*(*m*,*n*)—we were able to obtain closed-form expressions applicable to any member of a given class. For the remaining pericondensed benzenoid systems, we are able to determine the ZZ polynomials only for certain subfamilies of a given class. From the presented results, it is clear how to generalize our results to the remaining subfamilies. We notice after Zhang and Zhang that the ZZ polynomials for most of the pericondensed structures have very similar form, provided that the ZZ polynomial is expressed as a sum of powers of $(1+x)$. The results presented in this manuscript suggest that general closed-form expressions for the ZZ polynomials of many classes of pericondensed benzenoid systems can be discovered by a somewhat tedious analysis of structural similarities between the ZZ polynomials of their subclasses. Methods and techniques of finding such similarities are outlined. We plan to investigate these similarities in a series of subsequent papers, which hopefully will reveal a general closed-form expression of the ZZ polynomial for each class.

It is important to stress here that the results presented in this manuscript are not *sensu stricto* proofs of these properties, but should be rather treated as conjectures. However, the resulting formulas have been verified against a large number of ZZ polynomials for structures not comprised in the search sets, confirming their transferability. We believe that these tests guarantee that the expressions for the ZZ polynomials given here are valid in general. For those interested in strict demonstration of the presented here formulas, we stress that the presented formulas usually suggest a certain way of decomposing the original structures using the recursive properties of the ZZ polynomials described in **I**, which can be used for a regular proof.

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