MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **71** (2014) 741-764

ISSN 0340 - 6253

ZZDecomposer: A Graphical Toolkit for Analyzing the Zhang-Zhang Polynomials of Benzenoid Structures

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(Received July 24, 2013)

Abstract

We report a specialized, proof-oriented, graphical computer environment (referred to as ZZDecomposer) capable of performing interactive decompositions of the Zhang-Zhang polynomials for arbitrary benzenoid structures and enabling one in this way to conduct formal proofs of the derived formulas. The functionality and capabilities of the presented program are illustrated on a series of carefully selected examples. The introduced tool, described in detail in the body of the current paper, is subsequently applied for performing formal proofs for some of the heuristically discovered formulas presented in our previous work [*MATCH Commun. Math. Comput. Chem.* **68** (2012) 3–30; *ibidem*, **68** (2012) 31–64]. ZZDecomposer is freely available for download from http://qcl.ac.nctu.edu.tw/zzdecomposer for two platforms, Windows and Linux.

1. Introduction

Main practical problems associated with formal derivation of Zhang-Zhang (ZZ) polynomials[1-11] for a given subfamily of benzenoid structures are: (*i*) analysis of a large number of possible decomposition pathways, (*ii*) discovery of the optimal decomposition pathway yielding convenient recurrence formulas, and (*iii*) bookkeeping and accounting for numerous intermediate structures appearing during a given decomposition process. Performing all these tasks in a standard, pencil-and-paper approach is formidable, allowing one for a successful execution of such a process but in the simplest and most obvious cases. The complexity associated with discovering the optimal decomposition pathway is one of the main obstacles responsible for the fact that the closed-form ZZ polynomial formulas are known only for a limited class of benzenoid compounds.[1-3, 5-11] The specialized, proof-oriented, graphical computer environment (ZZDecomposer) introduced in the current paper has been designed in order to combine and fully automatize the three abovementioned tasks needed for deriving and proving closed-form ZZ polynomial formulas. We hope that ZZDecomposer, which we make freely available to the community of graph theorists and mathematically-oriented chemists upon a request from the authors, will soon be used to derive many missing formulas in the theory of ZZ polynomial for the remaining important classes of pericondensed benzenoid systems.

2. Benzenoid structures, polyhexes, and ZZ polynomials

Benzenoid structures are aromatic chemical compounds composed of fused benzene rings. Their chemical and physical properties are to a large extent controlled by the delocalized cloud of π electrons sandwiching these otherwise planar structures.[12] Historically, the most important role in theoretical description of a delocalized system of π electrons was played by the well-known Kekulé structures.[13, 14] The concept of Kekulé structures was particularly important for the development of quantum chemical methods in 1970s and 1980s, especially those based on Hückel theory.[15] Modern computational chemistry seldom uses the concept of Kekulé structures as the density functional theory (DFT)[16] based approaches usually offer much better quantitative agreement with experiment than simple Hückel theory. Nevertheless, Kekulé structures are still often used for interpretational purposes [17-21] and qualitative analysis of benzenoid structures, especially for systems which escape the

possibility of DFT treatment due to their prohibitively large size. The computation of the number of conceivable Kekulé structures for various benzenoid structures received considerable attention, both from the community of chemists and graph theorists.[14]

From a graph-theoretical point of view, Kekulé structures can be considered as perfect matchings for the planar hexagonal graph (polyhex) defined by the network of C–C bonds in a given benzenoid structure.[14] In practice, a Kekulé structure is obtained by covering the graph of a benzenoid structure C_nH_m by $n/2$ disjoint edge-covering bars. Clar extended the concept of Kekulé structures to something that we call now Clar covers.[22] A Clar cover is obtained by covering a given polyhex with two types of objects: (*i*) a bar covering two adjacent vertices (usually referred to by chemists as a double bond) and (*ii*) a circle covering six adjacent hexagon vertices (usually referred to by chemists as an aromatic sextet). Clar covers retain the characteristics of a perfect matching: each vertex is covered only once by either a bar or a circle. Few properties of the resulting Clar covers are immediately clear. (*i*) There exists a maximal number $0 \leq Cl \leq n/6$ of aromatic sextets that can be placed in a given polyhex; this number is usually referred to as the Clar number. (*ii*) The number c_0 of Clar covers without aromatic sextets is equal to the number of Kekulé structures. (*iii*) Two aromatic sextets cannot be placed in adjacent hexagons. (*iv*) The number of double bonds in a Clar cover with k aromatic sextets is $(n - 6k)/2$. The bookkeeping for the numbers c_k of Clar covers with k aromatic sextets for a given benzenoid structure S can be conveniently performed using a combinatorial polynomial

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

known from the names of its creators as the Zhang-Zhang polynomial or the ZZ polynomial. [1-4] The ZZ polynomials possess a number of inviting properties that makes their evaluation easy and straightforward.[5] An algorithm and computer program for computing the ZZ polynomial for an arbitrary catacondensed benzenoid structure up to approximately 10000 carbon atoms and for an arbitrary pericondensed benzenoid structure up to approximately 500 carbon atoms was given by as in a recent publication. [10]

3. ZZDecomposer: a proof-oriented, graphical environment for determination of ZZ polynomials

ZZDecomposer is an interactive computer environment designed for convenient and semi-automatized derivation of closed-form ZZ polynomials for general classes of benzenoid compounds. ZZDecomposer has been written in C++ programming language with the Qt UI framework[23]. It is distributed free of charge at http://qcl.ac.nctu.edu.tw/zzdecomposer. ZZDecomposer can be considered as a collection of four independent research tools.

1. **Interactive graphical builder** allows for a convenient mouse-based definition of the molecular graph of a given structure using a sequence of simple mouse operations performed on the underlying honeycomb-like graphene sheet. The created molecular graph representation can be used by the other modules of ZZDecomposer or can be exported to a file in the Chemical Markup Language (CML)[24-28] format or in the XYZ format.
2. **Depth-mode ZZDecomposer** has been created for studying various decomposition pathways of a given benzenoid S in order to discover an optimal decomposition, which yields a recurrence relation (possibly non-homogeneous) allowing for determination of the ZZ polynomial of S. The decomposition pathways are represented in a form of a rooted tree with the root corresponding to the structure S and with the leaves corresponding to various easy-to-identify substructures of S. The depth of the tree is interactively controlled by the user with the option to reverse unfavorable decomposition steps. This tool, particularly suitable for studying decomposition pathways of simple, high-symmetry structures, is probably the most useful component of the reported by us new software.
3. **Width-mode ZZDecomposer** is similar to the discussed above depth-mode ZZDecomposer, with the main difference concerning the representation of the decomposition pathway. In the depth-mode, the decomposition pathway is represented in a form of a rooted tree with all the intermediate substructures explicitly displayed, which often results in very large, difficult-to-embrace graphs. In the width-mode, the user has only an access to the tree leaves at a given decomposition level, which makes the representation more compact. The leaves are stored in a graphical library; the user can decide which of the leaves will be decomposed in the next step of the decomposition

process. After performing such a single step, the parent substructure is removed from the library, replaced by the children substructures. In addition, the user can combine identical and isomorphic substructures originating from different decomposition branches; this option is particularly useful, allowing for substantial compression of the representation. (The number of isomorphic substructures produced by different branches can be truly surprising!) The decomposition can be reverted, allowing users for reversing unfavorable decomposition paths leading to dead-end recesses. The bookkeeping of the resulting substructures is additionally facilitated by the possibility of identifying some of the resulting substructures as known fragments and moving them to the separate graphical library of identified graphs. This tool is particularly suitable for discovering not obvious decomposition paths requiring many intermediate steps before obtaining appropriate recurrence relation.

4. **ZZCalculator** is an interface to the previously reported program [10] for brute force computation of ZZ polynomials for an arbitrary benzenoid. It can be useful for fast determination of the ZZ polynomials for isostructural members of some series in order to verify the correctness of closed-form formulas discovered with other reported here tools. It is a desktop replacement of the online ZZCalculator tool provided by us at http://qcl.ac.nctu.edu.tw/zzpolynomial.

The graphical builder and the ZZCalculator are easy-to-use modules and do not require particular explanations or usage directions. For the remaining tools, depth-mode and width-mode ZZDecomposers, the user may benefit from additional discussion. We explain the functions of the depth-mode ZZDecomposer on three, self-explanatory examples presented and in **Figures 1**, **2**, and **3**. A single example illustrating the usage of the width-mode ZZDecomposer is presented in **Figure 4**. Similar approach as shown here for parallelograms $M(m,n)$ (**Figure 3**) and for the $O(2,2,6)$ hexagon (**Figure 4**) is used in the next Section and in the sequel to this paper [29] to prove formally a number of heuristically derived formulas from our previous publications [10, 11].

A number of technical issues should be addressed in order to facilitate the ZZDecomposer usage.

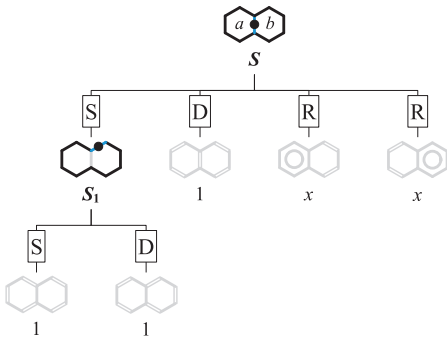

Figure 1. Total decomposition of naphthalene generates five distinct Clar covers of this molecule and demonstrates that its ZZ polynomial is equal to $3 + 2x$.

(i) Structure labels (**A1**, **A2**, **A3**, etc.) are automatically generated by the ZZDecomposer for each node of the decomposition tree. One can replace these automatic labels with user-defined labels by double-clicking on the label text. Labels are defined in the HTML text standard, so for example the label S_2 is obtained by typing `<i>S</i><sub>2</sub>`.)

(ii) It is possible to reverse the decomposition process by clicking on inactive bonds of the parent substructures in the depth-mode and by the undo button in the width-mode.

(iii) Each of the paths in the depth-mode decomposition tree is labeled using the following symbols: S for single bond covering, D for double bond (bar) covering, R for aromatic sextets (circle = ring) covering, and F for fragmentation associated with disconnecting the molecular graph during decomposition.

(iv) For larger and more complicated structures, the action of ZZCalculator may take a longer moment. Therefore, the brute-force calculation of the ZZ polynomials is performed at the background. User submits the job using the start button and the results appears on the screen once the computation process is finished; in the meantime other functions of the ZZDecomposer are still available. For smaller and medium-size structures, the computations are instantaneous; for larger structures, the user can terminate the computational process using the cancel button.

(v) When isomorphic or identical substructures are combined by the width-mode ZZDecomposer, the program ensures that the resulting single structure has a correct coefficient. Note that the program does not attempt to verify if the

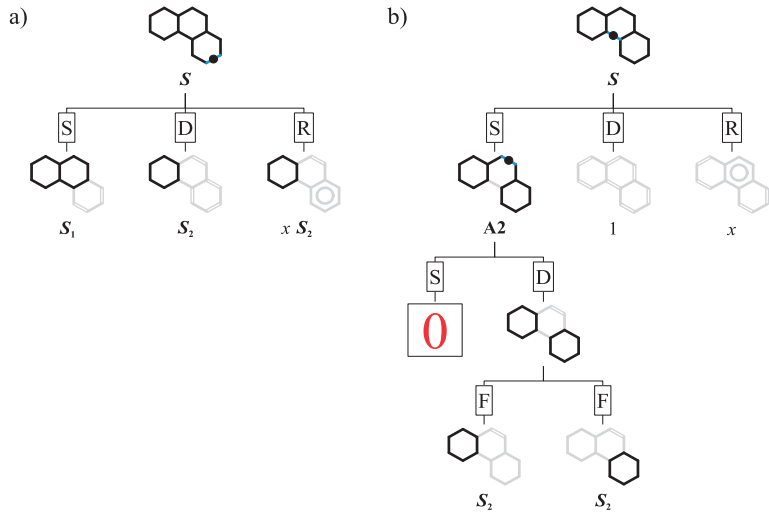

Figure 2. Two possible partial decompositions of phenanthrene yield two equivalent formulas for its ZZ polynomial, a) $ZZ(S,x) = ZZ(S_1,x) + (1+x)ZZ(S_2,x)$ and b) $ZZ(S,x) = 1 + x + ZZ(S_2,x)^2$, in terms of ZZ polynomials of smaller, well-defined substructures, benzene (S_2) and naphthalene (S_1).

combined structures are indeed isomorphic (which constitutes by itself a very interesting and not fully understood puzzle),[30, 31] so the user should be particularly careful while performing this operation.

(vi) Note that the combination of isomorphic structures necessarily wipes out the information about the pattern of already determined single, double and aromatic bonds in each parent structure. Fortunately, the information is only removed from the graphical interface; the program still remembers the individual components, which can be accessed using the undo button.

(vii) If a leaf produced by the width-mode ZZDecomposer is completely decomposed (i.e., has the ZZ polynomial equal to 1), it does not appear as an entry in the graphical library but rather contributes to the free term coefficients shown in the right bottom frame.

(viii) Graphical representation of the decompositions can be always conveniently saved as a SVG file produced by ZZDecomposer, yielding camera-ready illustrations for the resulting research papers.

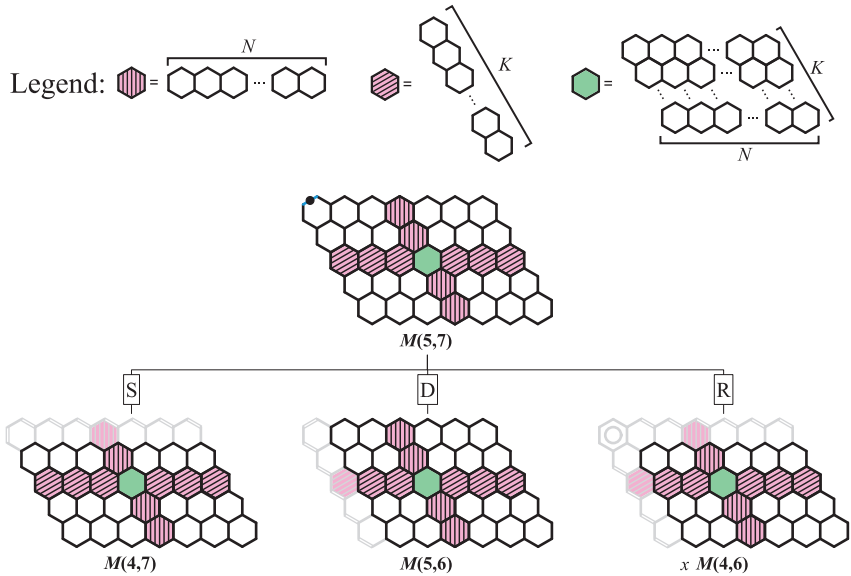

Figure 3. A convenient graph decomposition of parallelogram $M(5,7)$ yields a homogeneous recursive formula for its ZZ polynomial in terms of ZZ polynomials of smaller parallelograms, $M(4,7)$, $M(5,6)$, and $M(4,6)$. A generalization to the parallelogram $M(m,n)$ using the color scheme is straightforward.

(ix) ZZDecomposer can be only used to discover facts about particular members of a given class of structures. Generalizations to arbitrary values of indices should be performed by the user independently on the base of the discovered regularities. Analogous extrapolation approaches were used to derive other topological indices. [32, 33]

4. Application of the ZZDecomposer graphical toolkit for formal derivation of ZZ polynomials for four classes of benzenoid systems

Below, we give formal derivations of the ZZ polynomials for four well-known families of benzenoid structures: multiple-segment polyacene chains $L(m,n)$, zigzag-edge coronoids $ZC(n,m,l)$, fenestrenes $F(n,m)$, and parallelograms $M(m,n)$. All these derivations—in more or less satisfactory or formal ways— have been already presented in the literature.

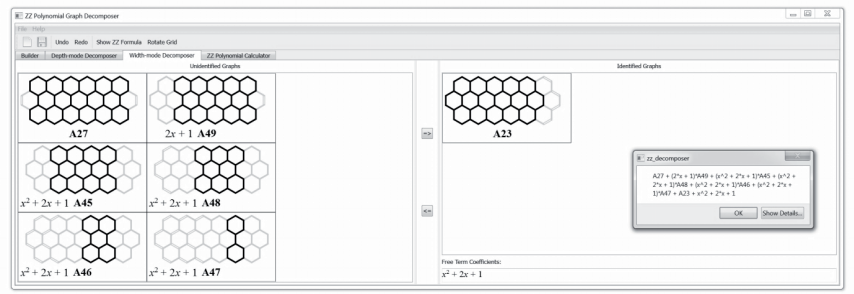

Figure 4. Recursive decomposition of the hexagon $O(2,2,6)$ using the width-mode ZZDecomposer reveals that its ZZ polynomial can be expressed in terms of ZZ polynomials of the hexagon $O(2,2,5)$ and the prolate rectangles $Pr(k,2)$ with $k = 0, 1, \ldots, 6$.

Formal proofs for the remaining general classes of benzenoid structures, for which heuristically derived ZZ polynomials were offered by us previously,[10, 11] are treated in the sequel to this article. [29] The development of ZZDecomposer helped us to discover and formally prove the form of ZZ polynomials also for other families of pericondensed benzenoids, which will be treated individually in separate publications due to the complexity of the underlying theory. First two of these publications, giving a general, closed-form formula for chevrons $Ch(k,m,n)$ and generalized chevrons $Ch(k,m,n_1,n_2)$ [34] and for prolate rectangles $Pr(m,n)$ and generalized prolate structures $Pr([m_1,m_2,\ldots,m_n],n)$ [35] accompany this paper. The remaining classes, including multiple zigzag chains $Z(m,n)$, ribbons $Rb(k,m,n)$ and generalized ribbons $Rb(m_1,n_1,m_2,n_2)$ [36], and oblate rectangles $Or(m,n)$, require somewhat more involved theory and will be published shortly. In our opinion, the most difficult structures are hexagon benzenoids $O(k,m,n)$, for which all our attack attempts remained in vain.

a) Multiple segment polyacenes $L(m,n)$

Formal derivation of the ZZ polynomial for a multiple segment polyacene $L(m,n)$ (Eq. (12) of [11]) is a relatively complex task. The recurrence relation for $L(m,n)$ is obtained by combining a number of decomposition relations and cancelling the undesired terms corresponding to the auxiliary structures $La(m,n-1)$ and $La(m,n-2)$. The first recurrence relation is obtained by the decomposition of $L(m,n)$ shown in **Figure 5a** and reads

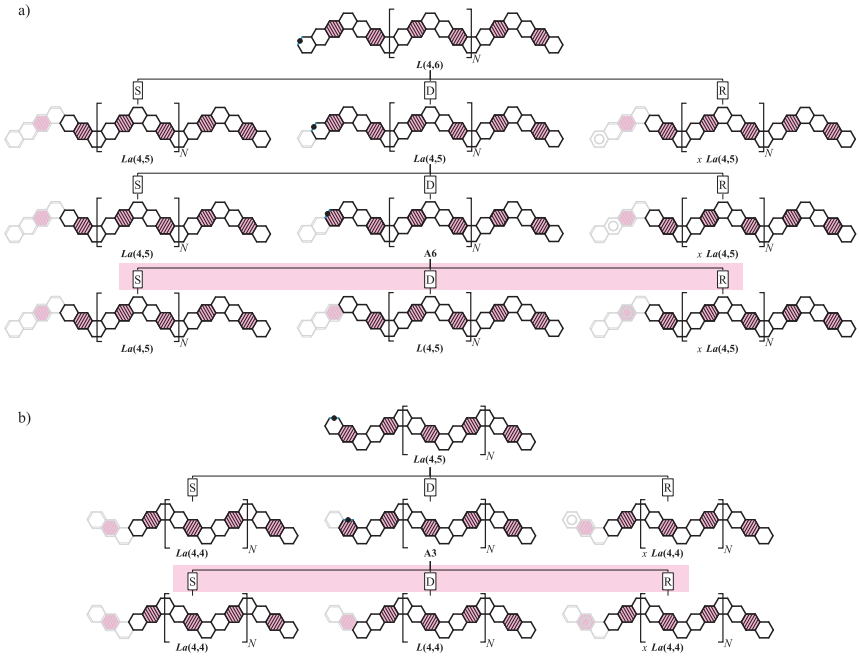

Figure 5. Two graph decompositions needed to obtain a recursive equation for the ZZ polynomial of a multiple segment polyacene $L(4,6)$. The first decomposition (a) expresses the ZZ polynomial of $L(4,6)$ as a function of the ZZ polynomials of $L(4,5)$ and an auxiliary structure $La(4,5)$. The second decomposition (b) suggests how to determine the ZZ polynomial of the auxiliary structures $La(4,5)$ and $La(4,4)$ in a recursive manner. The color scheme generalizes the decomposition to an arbitrary length structure $L(m,n)$.

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

The second recurrence relation is obtained by the decomposition of $La(m,n)$; it is shown in **Figure 5b** and reads

$$\mathrm{ZZ}\big(La(m,n),x\big) = \mathrm{ZZ}\big(L(m,n-1),x\big)+(m-2)\cdot(1+x)\cdot\mathrm{ZZ}\big(La(m,n-1),x\big) \tag{3}$$

Both generalizations may seem not obvious at first, but careful analysis of the color scheme for both decomposition schemes in **Figure 5** reveals that the number of segments (n) is practically irrelevant here provided that $n \geq 3$. The length of the single segment (m)

determines the number of intermediate steps in both decompositions in **Figure 5**, effectively entering Eqs. (2) and (3) in a form of multiplicative factors $(m-1)$ and $(m-2)$, respectively.

The general case recurrence is obtained by multiplying a version of Eq. (2)

$$ZZ\big(L(m,n-1),x\big)=ZZ\big(L(m,n-2),x\big)+(m-1)\cdot(1+x)\cdot ZZ\big(La(m,n-2),x\big) \tag{4}$$

by $(2-m)$ and adding Eq. (3) multiplied by $(m-1)$ to yield

$$(m-1)\cdot ZZ\big(La(m,n-1),x\big)=ZZ\big(L(m,n-2),x\big)+(m-2)\cdot ZZ\big(L(m,n-1),x\big) \tag{5}$$

Substituting this result into Eq. (2) produces the final recurrence formula

$$ZZ\big(L(m,n),x\big)=\big((m-1)+(m-2)x\big)\cdot ZZ\big(L(m,n-1),x\big)+(1+x)\cdot ZZ\big(L(m,n-2),x\big) \tag{6}$$

identical to Eq. (9) of [11] and to the equation in **Lemma 5** of [3] on p. 168. The solution to this recurrence relation

$$\begin{aligned} ZZ\big(L(m,n),x\big)=&\frac{1}{2}\left(x+2+\frac{(2-m)x^2+(5-m)x+4}{\sqrt{k}}\right)\left(\frac{(m-1)+(m-2)x+\sqrt{k}}{2}\right)^n \\ &+\frac{1}{2}\left(x+2-\frac{(2-m)x^2+(5-m)x+4}{\sqrt{k}}\right)\left(\frac{(m-1)+(m-2)x-\sqrt{k}}{2}\right)^n \end{aligned} \tag{7}$$

where $k=(m^2+4)(1+x)^2-2m(1+x)(2x+1)+1$, was given previously as Eq. (12) of [11]. An equivalent but less transparent result (Eq. (4.12) of [1]) was obtained by Zhang and Zhang. Note that our derivation is valid only for $n\geq 3$ and $m\geq 3$, but the final formula (i.e., Eq. (7)) is valid without these restrictions as can be easily verified. The case with $m=1$ reduces to benzene $L(1)$ with ZZ polynomial of $2+x$. The case with $m=2$ reduces to a single armchair chain $N(n+1)$ (see Eq. (12) of [10]). The case with $n=1$ reduces to a polyacene $L(m)$ (see Eq. (8) of [10]), and the case with $n=2$ is trivially given by

$$ZZ\big(L(m,2),x\big)=ZZ\big(L(m-1),x\big)^2+1+x \tag{8}$$

as demonstrated earlier by Zhang and Zhang [1] and clearly obvious from **Figure 6**. All the special cases analyzed here are consistent with Eq. (7). Note that the amount of effort associated with this particular structure is considerably larger than with the heuristic analysis given by us previously in [11]. Note finally that the multiple segment polyacene $L(m,n)$ can be formally expressed as a variable-length, multiple segment polyacene $ZZ(L([r_1,r_2,\ldots,r_n]),x)$ with $r_1 = r_2 = \cdots = r_n = m$, which were studied earlier by Zhang and Zhang [1, 7] and Guo, Deng, and Chen [1, 7] without offering a closed-form expression for its ZZ polynomial.

The closed form expression for the ZZ polynomial of an arbitrary multiple segment polyacene $L(m,n)$, given by Eq. (7), has a multiplicative structure. It is rather cumbersome to extract from it the number of Clar covers with exactly k aromatic sextets. It would be advantageous to obtain an additive analog of Eq. (7), where the ZZ polynomial of $L(m,n)$ is given as a power series in powers of x or $1+x$. Such a simple additive formula for $L(2,n-1) = N(n)$ was given by us previously (Eq. (12) of [10])

$$\mathrm{ZZ}\left(N\left(n\right),x\right) = \sum_{k=0}^{n} \binom{n-k+1}{k} \left(1+x\right)^{k} \tag{9}$$

Note that Eq. (9) is a special case ($m = 2$) of the recursion formula given earlier by Zhang and Zhang (Eq. (4.9) of [1]). Note also that the closed form solution to this recursion offered by Zhang and Zhang (Eq. (4.12) of [1] with $m = 2$) has much more complex form than the solution offered here; both solutions are consistent. Note finally that Eq. (9) is almost

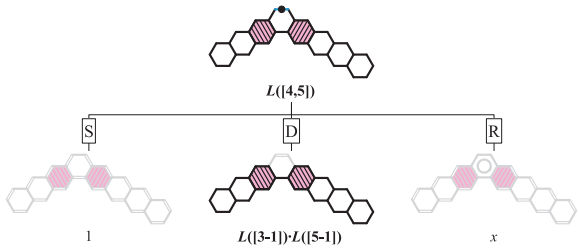

Figure 6. One-step decomposition of a "hockey stick" composed of two fused polyacenes, $L(n)$ and $L(m)$, shows that its ZZ polynomial is given by $ZZ(L(m-1),x)\cdot ZZ(L(n-1),x)+1+x$, as demonstrated earlier by Zhang and Zhang.[1] Note that this structure is formally equivalent to a tripod $T(m,1,n)$. [11, 12]

identical to one of the equations in **Example 2** of [3] on p.167; the difference in the upper summation index is irrelevant here owing to the properties of binomial coefficients. The simplicity of Eq. (9) suggests that it should be possible to cast Eq. (7) in analogous simple additive form for the general case of $L(m,n)$; unfortunately, this has not been achieved to date. The preliminary analysis performed for $L(3,n)$ shows that for $n \geq 1$ the ZZ polynomial for this structure can be written in the following additive form

$$ZZ\left(L\left(3,n\right),x\right)=\sum_{k=0}^{n}\left[\sum_{j=0}^{k}\binom{n-k+2}{j}\binom{n-j}{k-j}\right]\left(1+x\right)^{k} \tag{10}$$

It is possible to evaluate the inner sum in terms of Gaussian hypergeometric functions, which for $n \geq 2$ casts Eq. (10) in the following form

$$ZZ\left(L\left(3,n\right),x\right)=\sum_{k=0}^{n}\binom{n}{k}\,{}_2F_1\left[\begin{matrix}-k,-n+k-2\\-n\end{matrix};-1\right]\left(1+x\right)^{k} \tag{11}$$

analogous to Eq. (9) corresponding to $L(2,n-1)$. Further explicit summation of this series is unlikely as the summations over products of hypergeometric functions has not been yet well studied.[37] It is also unlikely to transform Eq. (11) into elementary functions as for the given set of indices of ${}_2F_1$ such a transformation is unknown. [38] It is possible, however, to transform the hypergeometric function in Eq. (11) into a Jacobi polynomial $P_l^{(\alpha,\beta)}(y)$, which casts Eq. (11) into the following transparent form

$$ZZ\left(L\left(3,n\right),x\right)=\sum_{k=0}^{n}P_k^{(-2,-n-1)}\left(-3\right)\cdot\left(1+x\right)^{k} \tag{12}$$

The value of -3 appearing as the argument of the Jacobi polynomial coincides with the value of $-m$; this seems to be too fortunate to be purely accidental, suggesting that the coefficients of a similar equation for $L(m,n)$ may be expressed in terms of $P_k^{(\alpha,\beta)}(-m)$. The relevant formula remains to be discovered. Note finally that the set of Jacobi polynomials in Eq. (12) are well defined even if they do not form a set of orthogonal polynomials as the appropriate weight function $(1-y)^{-2}(1+y)^{-n-1}$ is not integrable over the interval $[-1,1]$. [37]

Another important aspect of the preliminary analysis performed here for $L(3,n)$ is the following discovery. It is possible to represent the ZZ polynomials of the $L(3,n)$ structures in an infinite matrix representation given by

$$\begin{bmatrix} \mathrm{ZZ}\left(L(3,-1),x\right) \\ \mathrm{ZZ}\left(L(3,0),x\right) \\ \mathrm{ZZ}\left(L(3,1),x\right) \\ \mathrm{ZZ}\left(L(3,2),x\right) \\ \mathrm{ZZ}\left(L(3,3),x\right) \\ \mathrm{ZZ}\left(L(3,4),x\right) \\ \mathrm{ZZ}\left(L(3,5),x\right) \\ \mathrm{ZZ}\left(L(3,6),x\right) \\ \vdots \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ z & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 3z & 1 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 4z^2 & 5z & 1 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 4z^3 & 12z^2 & 7z & 1 & 0 & 0 & 0 & \cdots \\ 0 & 4z^4 & 20z^3 & 24z^2 & 9z & 1 & 0 & 0 & \cdots \\ 0 & 4z^5 & 28z^4 & 56z^3 & 40z^2 & 11z & 1 & 0 & \cdots \\ 0 & 4z^6 & 36z^5 & 104z^4 & 120z^3 & 60z^2 & 13z & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ \vdots \end{bmatrix} \tag{13}$$

where z is a shorthand notation for $(1+x)$. The lower triangular matrix (call it M) is easily identified as a Riordan array [39-42] with the generating function for the m^{th} column given by

$$GF\left(w,m\right) = \frac{\left(1+zw\right)^m w^{m-1}}{\left(1-zw\right)^{m-1}} \tag{14}$$

(Note the clear connection with the OEIS sequence A186827 with $z=-1$. [43]) Using the standard notation for Riordan arrays, $M = \left(f(w), g(w)\right)$ with $f(w) = 1+zw$ and $g(w) = \frac{w(1+zw)}{(1-zw)}$, and easily identifying the generating function for the unit vector as $A(w) = \frac{1}{1-w}$, we can use the fundamental theorem of Riordan arrays [37] giving us the generating function for the ZZ polynomials of $L(3,n)$ in the following compact form

$$GF\left(w\right) = g\left(w\right) A\left(f\left(w\right)\right) = \frac{1}{\frac{1}{1+zw} - \frac{w}{1-zw}} \tag{15}$$

It is clear that this generating function could be obtained directly from the recurrence relation given in Eq. (6) for $m=3$ but then the connection to the theory of Riordan arrays would be missed that way. The somewhat unanticipated and exciting interrelations between the theory of ZZ polynomials, the theory of Riordan arrays, and the theory of hypergeometric functions and Jacobi polynomials, not pursued in detail in this study, definitely warrant further research.

It has been mentioned that it is possible to solve the recurrence relation for $L(m,n)$ given by Eq. (6) with the initial conditions given by Eqs. (10) and (11) of [11] in terms of an appropriate generating function

$$GF(t,x)=\sum_{n=0}^{\infty}\mathrm{ZZ}\left(L(m,n),x\right)\cdot t^{n} \tag{16}$$

Indeed, the function $GF(t,x)$ computed using standard methods with MAPLE [44] reads

$$GF(t,x)=\frac{\left(1+(1+x)t\right)^{2}}{1-\left((m-2)\cdot(1+x)+1\right)\cdot t-(1+x)\cdot t^{2}} \tag{17}$$

This function is a convenient starting point for obtaining a closed form expression for $ZZ(L(m,n),x)$ alternative to Eq. (7). A series expansion of a simple rational function $(at^2+bt+c)^{-1}$, where a, b, and c are arbitrary non-zero parameters is given by

$$\begin{aligned}
\frac{1}{at^{2}+bt+c}&=\sum_{n=0}^{\infty}\frac{-4a\cdot(2at+b)^{2n}}{\left(b^{2}-4ac\right)^{n+1}}=\sum_{n=0}^{\infty}\sum_{l=0}^{2n}\frac{-2\binom{2n}{l}(2a)^{l+1}t^{l}b^{2n-l}}{\left(b^{2}-4ac\right)^{n+1}}\\
&=\sum_{n=0}^{\infty}\sum_{l=0}^{\infty}\frac{-2\binom{2l+2\frac{n+1}{2}}{n}(2a)^{n+1}\,b^{2l+2\frac{n+1}{2}-n}}{\left(b^{2}-4ac\right)^{l+1+\frac{n+1}{2}}}t^{n}\\
&=\sum_{n=0}^{\infty}\sum_{l=0}^{\infty}\frac{-2\binom{2l+2n}{2n}(2a)^{2n+1}b^{2l}}{\left(b^{2}-4ac\right)^{l+1+n}}t^{2n}+\sum_{n=0}^{\infty}\sum_{l=0}^{\infty}\frac{-2\binom{2l+2n+2}{2n+1}(2a)^{2n+2}\,b^{2l+1}}{\left(b^{2}-4ac\right)^{l+2+n}}t^{2n+1}\\
&=\sum_{n=0}^{\infty}\frac{(-1)^{n}\cdot a^{n}}{c^{n+1}}\,{}_2F_1\left[\begin{matrix}-n,n+1\\ \frac{1}{2}\end{matrix};\frac{b^{2}}{4ac}\right]t^{2n}+\sum_{n=0}^{\infty}\frac{(-1)^{n+1}\cdot(n+1)\cdot ba^{n}}{c^{n+2}}\,{}_2F_1\left[\begin{matrix}-n,n+2\\ \frac{3}{2}\end{matrix};\frac{b^{2}}{4ac}\right]t^{2n+1}
\end{aligned} \tag{18}$$

Both hypergeometric functions with the definite sets of parameters can be identified (see p. 467 of [38]) as Chebyshev polynomials U_n of the second type [45]; this identification is not surprising as the generating function for Chebyshev polynomials displays close structural similarity with the function analyzed here. Upon this identification our expansion becomes

$$\frac{1}{at^2+bt+c}=\frac{1}{c}\sum_{n=0}^{\infty}(-1)^n\left(\frac{a}{c}\right)^{\frac{n}{2}}U_n\left(\frac{b}{\sqrt{4ac}}\right)t^n \tag{19}$$

Now, setting $c=1$, $a=-(1+x)$, and $b=-(m-2)(1+x)-1$, we obtain a series expansion for $GF(t,x)$ in the following form

$$GF(t,x)=1+\sum_{n=1}^{\infty}(-i)^n\sqrt{1+x}^n\left[U_n(y)+2i\sqrt{1+x}U_{n-1}(y)-(1+x)U_{n-2}(y)\right]t^n \tag{20}$$

where y is a shorthand notation for $\frac{i}{2}\left((m-2)\sqrt{1+x}+\frac{1}{\sqrt{1+x}}\right)$. Comparison of Eqs. (16) and (20) reveals that the ZZ polynomial for a general multiple-segment polyacene $L(m,n)$ is given by a linear combination of three Chebyshev polynomials of the second kind

$$\begin{aligned}ZZ\left(L(m,n),x\right)=&(-i)^n\sqrt{1+x}^nU_n\left(\frac{i}{2}\left((m-2)\sqrt{1+x}+\frac{1}{\sqrt{1+x}}\right)\right)\\&+2(-i)^{n-1}\sqrt{1+x}^{n+1}U_{n-1}\left(\frac{i}{2}\left((m-2)\sqrt{1+x}+\frac{1}{\sqrt{1+x}}\right)\right)\\&+(-i)^{n-2}\sqrt{1+x}^{n+2}U_{n-2}\left(\frac{i}{2}\left((m-2)\sqrt{1+x}+\frac{1}{\sqrt{1+x}}\right)\right)\end{aligned} \tag{21}$$

This expression is equivalent to Eq. (7). Further simplification of this expression and possibly expressing it in basis of powers of $1+x$ is not attempted here.

b) Zigzag-edge coronoids $ZC(n,m,l)$

The derivation of the ZZ polynomial for a general zigzag-edge coronoid $ZC(n,m,l)$ is schematically represented in **Error! Reference source not found.**. The ZZ polynomial of a general zigzag-edge coronoid $ZC(n,m,l)$ can be expressed *via* the ZZ polynomials of variable-length multiple segment polyacenes as

$$\begin{aligned}ZZ\left(ZC(n,m,l),x\right)=&(1+x)\cdot ZZ\left(L([n-1,m,l,n-1]),x\right)\\&+ZZ\left(L([l-1,n,m,l,n,m-1]),x\right)+2\end{aligned} \tag{22}$$

The recursive formula for the ZZ polynomials of variable-length multiple segment polyacenes was given previously by Zhang and Zhang (Eq. (4.6) of [1] with initial conditions $ZZ(L([r_1]),x) = ZZ(L(r_1),x)$ and $ZZ(L([r_1,r_2]),x)$ given in the caption to **Figure 6**; see also p. 352 of [7]) as

$$\begin{aligned} ZZ\left(L\left(\left[r_1,r_2,\ldots,r_t\right]\right),x\right) = &\left[\left(r_t-1\right)\left(1+x\right)+1-\frac{r_t-1}{r_{t-1}-1}\left(1+x\right)\right]ZZ\left(L\left(\left[r_1,r_2,\ldots,r_{t-1}\right]\right),x\right) \\ &+\frac{r_t-1}{r_{t-1}-1}\left(1+x\right)ZZ\left(L\left(\left[r_1,r_2,\ldots,r_{t-2}\right]\right),x\right) \end{aligned} \tag{23}$$

Note that this equation is a generalization of Eq. (6) to multiple segment polyacenes with variable length. Direct repeated application of this recursive formula to Eq. (23) allows one to express it as a sixth-order polynomial in x with quite lengthy coefficients being functions of n, m, and l only identical with Eq. (31) of [11], which can be transformed to a highly compact form

$$\begin{aligned} ZZ\left(ZC\left(n,m,l\right),x\right) = &2+\left(1+x\right)^3 \\ &+\Big[ZZ\left(L\left(n-2\right),x\right)\cdot ZZ\left(L\left(m-2\right),x\right)\cdot ZZ\left(L\left(l-2\right),x\right) \\ &+\left(1+x\right)\left(ZZ\left(L\left(n-2\right),x\right)+ZZ\left(L\left(m-2\right),x\right)+ZZ\left(L\left(l-2\right),x\right)\right)\Big]^2 \end{aligned} \tag{24}$$

exploiting the invariance of $ZZ(ZC(n,m,l),x)$ under the permutations of the indices n, m, and l as explained in [11]. This equation is identical to Eq. (33) of [11] and is consistent with the corrected version [9] of the formula derived by Guo, Deng, and Chen [7] for cyclo-polyphenacenes with six segments. Note that for zigzag-edge coronoids $ZC(n,m,l)$, it would be relatively difficult to discover the final highly-symmetric formula given by Eq. (24) directly from the recursive decomposition properties of ZZ polynomials. In this sense, the previously performed analysis of finite members of this class of benzenoids was helpful not only to discover the closed form of their ZZ polynomials but also to put this form in structurally simplest form.

c) Fenestrenes $F(n,m)$

The derivation of the closed formula for a general fenestrene $F(n,m)$ is schematically represented in **Figure 8**. The formula of the ZZ polynomial of a general fenestrene $F(n,m)$ can be expressed by

$$\begin{aligned} ZZ\left(F(n,m),x\right) &= (1+x)\cdot ZZ\left(L\left(\left[\underbrace{2,\ldots,2}_{\frac{m-1}{2}-2},n,\underbrace{2,\ldots,2}_{m-1},n,\underbrace{2,\ldots,2}_{\frac{m-1}{2}-2}\right]\right),x\right) \\ &+ZZ\left(L\left(\left[\underbrace{2,\ldots,2}_{\frac{m-1}{2}-1},n,\underbrace{2,\ldots,2}_{m-1},n,\underbrace{2,\ldots,2}_{\frac{m-1}{2}-1}\right]\right),x\right)+2 \end{aligned} \tag{25}$$

Repeated application of Eq. (23) allows us to express this formula in the form given by Eq. (28) of [11]

$$\begin{aligned} ZZ\left(F(n,m),x\right) &= \left[\left(ZZ\left(L(n-2),x\right)-2\right)\cdot ZZ\left(N(m-2),x\right)+2\cdot ZZ\left(N(m-1),x\right)\right]^2 \\ &+2\cdot ZZ\left(N(m),x\right)\cdot ZZ\left(N(m-2),x\right)-2\cdot ZZ\left(N(m-1),x\right)^2+2 \end{aligned} \tag{26}$$

Use of the width mode of the ZZDecomposer allows us to find an alternative formula for the ZZ polynomial of fenestrenes $F(n,m)$. Repeated decomposition of $F(n,m)$ with respect to the edges connecting the armchair and zigzag single chains produces four distinct disconnected fragments, as shown in **Figure 9** for $F(5,7)$. The decomposition again is general (after accounting for the color scheme) and yields the following closed-form formula for the ZZ polynomial of $F(n,m)$

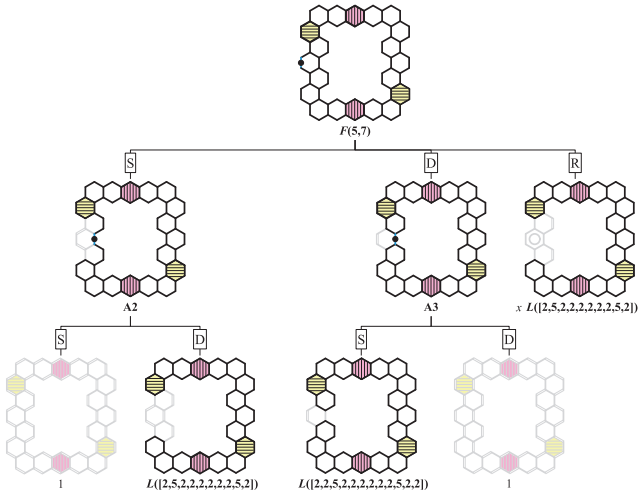

Figure 7. Graph decomposition of a fenestrene $F(5,7)$ suggests how the ZZ polynomial of a general structure $F(n,m)$ can be expressed in terms of ZZ polynomials of $L\left(\left[\underbrace{2,\ldots,2}_{\frac{m-1}{2}-2},n,\underbrace{2,2,\ldots,2}_{m-1},n,\underbrace{2,\ldots,2}_{\frac{m-1}{2}-2}\right]\right)$ and $L\left(\left[\underbrace{2,\ldots,2}_{\frac{m-1}{2}-1},n,\underbrace{2,2,\ldots,2}_{m-1},n,\underbrace{2,\ldots,2}_{\frac{m-1}{2}-1}\right]\right)$ given by Eq. (23).

$$\begin{aligned} ZZ\left(F\left(n,m\right),x\right) &= \left[ZZ\left(L\left(n-2\right),x\right)\cdot ZZ\left(N\left(m-2\right),x\right)\right]^2 \\ &+2\cdot\left(1+x\right)^2\left[\left(ZZ\left(N\left(m-3\right),x\right)\right)^2+ZZ\left(N\left(m-2\right),x\right)\cdot ZZ\left(N\left(m-4\right),x\right)\right] \\ &+4\cdot\left(1+x\right)\cdot ZZ\left(L\left(n-2\right),x\right)\cdot ZZ\left(N\left(m-2\right),x\right)\cdot ZZ\left(N\left(m-3\right),x\right)+2 \end{aligned} \tag{27}$$

consistent with our previous result (Eq. (26) of the current paper and Eq. (28) of [11]). Note finally that both the classes of the zigzag coronoids $ZC(n,m,l)$ and fenestrenes $F(n,m)$ analyzed in the last two subsections are special cases of cyclic polyphenacenes studied earlier by Guo, Deng, and Chen[7, 9] and therefore their ZZ polynomials can in principle be computed in terms of variable-length multiple segment polyacenes $L([r_1,r_2,\ldots,r_t])$ introduced by Zhang and Zhang [1] but such calculations may prove to be quite cumbersome and lengthy in practice.

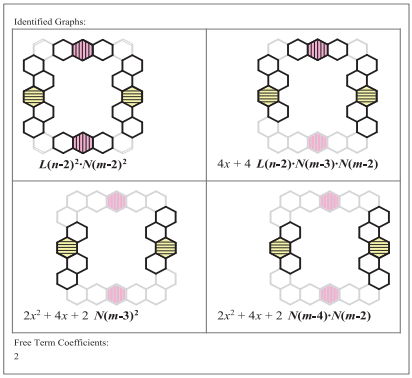

Figure 8. Width-mode decomposition of $F(m,n)$ with respect to the hexagons located at the corners shows how to express its ZZ polynomial in terms of ZZ polynomials of polyacenes and single armchair chains.

d) Parallelograms $M(m,n)$

Recursive decomposition of a parallelogram $M(m,n)$ shown in **Figure 3** yields a recursion formula

$$ZZ\left(M\left(m,n\right),x\right)=ZZ\left(M\left(m-1,n\right),x\right)+ZZ\left(M\left(m,n-1\right),x\right)+x\cdot ZZ\left(M\left(m-1,n-1\right),x\right) \quad (28)$$

obtained earlier by Gutman and Borovićanin (Eq. (8) of [6]). Solution to the recursion [6, 10] yields the ZZ polynomial of the parallelogram $M(m,n)$ given in particularly simple form

$$ZZ\left(M\left(m,n\right),x\right)=\sum_{i=0}^{\min(m,n)}\binom{m}{i}\binom{n}{i}\left(x+1\right)^{i} \quad (29)$$

This equation is new and can be considered as a particularly compact and elegant form of the ZZ polynomial formula for a parallelogram $M(m,n)$ replacing the formulas previously given by Gutman and Borovićanin (Eq. (16) of [6]) and by us (Eqs. (18) and (19) of [10]). Note that the summation in Eq. (29) can be actually evaluated, which casts Eq. (29) in a hypergeometrical form; for details, see Eq. (5) of [34].

5. Conclusion

An interactive, graphical computer environment (ZZDecomposer) designed to perform derivations of ZZ polynomials for various classes of benzenoid hydrocarbons is presented and discussed. The main objective of introducing ZZDecomposer is to provide the community of graph theoreticians and discrete chemists with a research tool capable of discovering closed-form formulas of ZZ polynomials and proving their correctness. Various practical aspects associated with proficient application of ZZDecomposer for solving real problems are discussed on a series of carefully selected examples. The program is distributed free of charge (http://qcl.ac.nctu.edu.tw/zzdecomposer) for two platforms: Windows and Linux.

The final section of the current study gives applications of ZZDecomposer for formal rederivations of the ZZ polynomials for some well-known families of benzenoid structures: multiple-segment polyacene chains $L(m,n)$, zigzag-edge coronoids $ZC(n,m,l)$, fenestrenes $F(n,m)$, and parallelograms $M(m,n)$. Some aspects of the presented results (additive form of the ZZ polynomials for $L(3,n)$, connection of the ZZ polynomials of the $L(3,n)$ structures to the theory of hypergeometric functions and Riordan arrays, obtaining closed forms of ZZ polynomials *via* formal series expansions of generating functions, new and simpler formulas for the ZZ polynomials of fenestrenes $F(n,m)$ and parallelograms $M(n,m)$) are completely new and signalize novel research directions in the theory of ZZ polynomials. The work initiated here is continued in the sequels to this paper focusing on: (*i*) formal derivations of ZZ polynomials for the remaining seven families of benzenoid structures derived by us in a heuristic fashion, [29] (*ii*) formal derivation of ZZ polynomials for chevrons $Ch(k,m,n)$ and generalized chevrons $Ch(k,m,n_1,n_2)$[34] and (*iii*) formal derivation of ZZ polynomials for prolate rectangles $Pr(m,n)$ and generalized prolate structures $Pr([m_1,m_2,\dots,m_n],n)$ [35].

Acknowledgment: National Science Council of Taiwan (grant NSC 99-2113-M-009-011-MY3 and 102-2113-M-009-015-MY3) and Ministry of Education (MOE-ATU project) are acknowledged for financial support.

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