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Two Examples for the Application of the ZZDecomposer: Zigzag-Edge Coronoids and Fenestrenes

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Abstract

In our recent paper [*MATCH Commun. Math. Comput. Chem.* **71** (2013) 741-764] some formulas and figures were misprinted. In this paper, we correct these problems giving formal derivations of Zhang-Zhang (ZZ) polynomials for two classes of benzenoid systems, zigzag-edge coronoids and fenestrenes.

1 Introduction

Zhang–Zhang (ZZ) polynomials, [1-5] sometimes referred to as Clar cover polynomials, are combinatorial polynomials used to enumerate conceivable Clar covers of benzenoid structures. Determination of ZZ polynomials for various classes of benzenoids is an intensively developing discipline of chemical graph theory.[6-12] In our recent paper [9], formal derivations of ZZ polynomials for various families of benzenoids were presented. However, due to inattentive typesetting and an editorial oversight, one of the figures (showing recursive decomposition of zigzag-edge coronoid) was missing, which made part of the text incomprehensible and resulted in wrong ordering of the following figures. Therefore, in this paper, we formally coherent derivation of the ZZ polynomials of two families of benzenoid structures: zigzag-edge coronoids $ZC(n,m,l)$and fenestrenes $F(n,m)$. In addition, we take here the liberty to correct two mistakes in the citation list; the references 32 and 33 of [9] are now correctly given as references 12 and 13.

2 ZZ polynomials of 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 **Figure 1**. $ZZ(ZC(n,m,l))$ can be expressed *via* the ZZ polynomials of variable-length multiple segment polyacenes as

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

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 $ZZ(L([r_1,r_2]),x)$; see also p. 352 of [15]) as

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

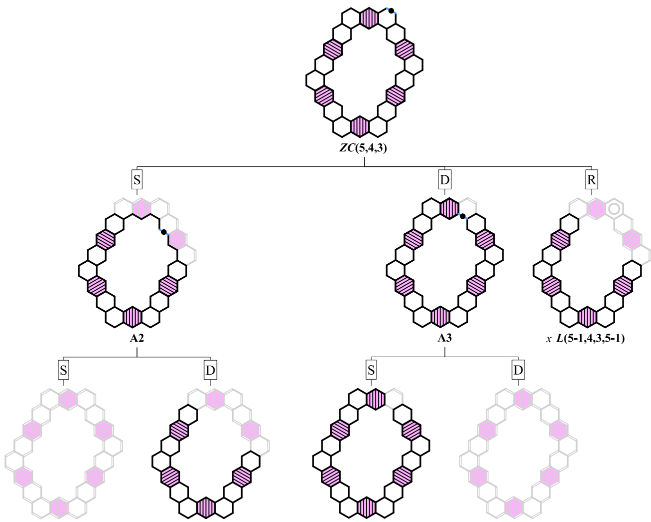

Figure 1. Graph decomposition of a zigzag-edge coronoid $ZC(5,4,3)$ suggests how the ZZ polynomial of a general structure $ZC(n,m,l)$ can be expressed in terms of ZZ polynomials of variable-length, multiple segment polyacenes $L([n-1,m,l,n-1])$ and $L([l-1,n,m,l,n,m-1])$, studied earlier by Zhang and Zhang.[1]

Note that this equation is a generalization of Eq. (6) of [9] to multiple segment polyacenes with variable length. Direct repeated application of this recursive formula to Eq. (2) 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 [8], which can be transformed to a highly compact form

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

exploiting the invariance of $ZZ(ZC(n,m,l),x)$ under the permutations of the indices n, m, and l as explained in [8]. This equation is identical to Eq. (33) of [8] and is consistent with the corrected version [16] of the formula derived by Guo, Deng, and Chen [15] 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. (3) 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.

3 ZZ polynomials of fenestrenes *F*(*n*,*m*)

The derivation of the closed formula for a general fenestrene $F(n,m)$ is schematically represented in **Figure 2**. The formula of the ZZ polynomial of a general fenestrene $F(n,m)$ can be expressed by

$$\begin{aligned} ZZ\left(F(n,m),x\right) = (1+x)\cdot ZZ\left(L\left(\left[\underbrace{2,\ldots,2}_{\frac{m-1}{2}-2},n,\underbrace{2,\ldots,2}_{m-1},n,\underbrace{2,\ldots,2}_{\frac{m-1}{2}-2}\right]\right),x\right) \\ + ZZ\left(L\left(\left[\underbrace{2,\ldots,2}_{\frac{m-1}{2}-1},n,\underbrace{2,\ldots,2}_{m-1},n,\underbrace{2,\ldots,2}_{\frac{m-1}{2}-1}\right]\right),x\right) + 2 \end{aligned} \tag{4}$$

Repeated application of Eq. (2) allows us to express this formula in the form given by Eq. (28) of [8]

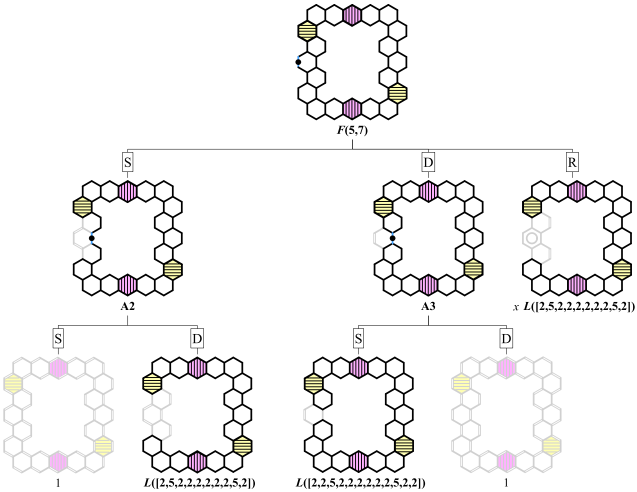

Figure 2. Graph decomposition of a fenestrene $F(5,7)$ suggests how the ZZ polynomial of a general structure $F(n,m)$ can be expressed in terms of ZZ polynomials of $L\left(\left[\underbrace{2,\ldots,2}_{\frac{m-1}{2}-2},n,\underbrace{2,2,\ldots,2}_{m-1},n,\underbrace{2,\ldots,2}_{\frac{m-1}{2}-2}\right]\right)$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

$$ZZ(F(n,m),x)=\left[\left(ZZ(L(n-2),x)-2\right)\cdot ZZ(N(m-2),x)+2\cdot ZZ(N(m-1),x)\right]^2 \\ +2\cdot ZZ(N(m),x)\cdot ZZ(N(m-2),x)-2\cdot ZZ(N(m-1),x)^2+2 \tag{5}$$

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 3** 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 $F(n,m)$

$$\mathrm{ZZ}(F(n,m),x)=\left[\mathrm{ZZ}(L(n-2),x)\cdot \mathrm{ZZ}(N(m-2),x)\right]^2 \\ +2\cdot(1+x)^2\left[\left(\mathrm{ZZ}(N(m-3),x)\right)^2+\mathrm{ZZ}(N(m-2),x)\cdot \mathrm{ZZ}(N(m-4),x)\right] \\ +4\cdot(1+x)\cdot \mathrm{ZZ}(L(n-2),x)\cdot \mathrm{ZZ}(N(m-2),x)\cdot \mathrm{ZZ}(N(m-3),x)+2 \tag{6}$$

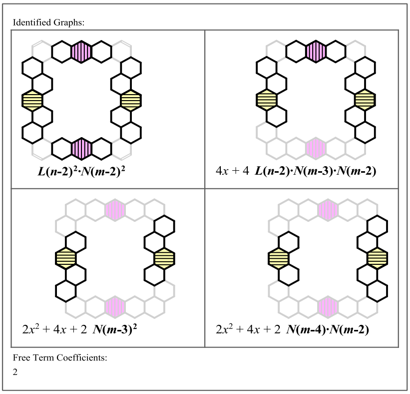

Figure 3. Width-mode decomposition of $F(m,n)$ with respect to the hexagons located at the corners shows how to express its ZZ polynomial in terms of ZZ polynomials of polyacenes and single armchair chains.

consistent with our previous result (Eq. (5) of the current paper and Eq. (28) of [8]). 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[15, 16] and therefore their ZZ polynomials can in principle be computed in terms of variable-length multiple segment polyacenes $L([r_1, r_2, \dots, r_t])$ introduced by Zhang and Zhang [1] but such calculations may prove to be quite cumbersome and lengthy in practice.

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