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Zhang-Zhang Polynomials of Phenylenes and Benzenoid Graphs

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Abstract

The aim of this paper is to study some variations of the Zhang-Zhang polynomial for phenylenes, which can be obtained as special cases of the multivariable Zhang-Zhang polynomial. Firstly, we prove the equality between the first Zhang-Zhang polynomial of a phenylene and the generalized Zhang-Zhang polynomial of some benzenoid graph, which enables us to prove also the equality between the first Zhang-Zhang polynomial and the generalized cube polynomial of the resonance graph. Next, some results on the roots of the second Zhang-Zhang polynomial of phenylenes are provided and another expression for this polynomial is established. Finally, we give structural interpretation for (partial) derivatives of different Zhang-Zhang polynomials.

1 Introduction

Kekulé and Clar structures of polycyclic conjugated molecules are investigated in mathematical chemistry because they can provide some insights into the π-electron structure of the mentioned chemical compounds [9, 10, 16]. Based on the Clar's aromatic sextet theory [9], the concept of

Clar covers was introduced in [33] for benzenoid graphs. More precisely, a *Clar cover* is a spanning subgraph whose connected components are only hexagons (representing aromatic sextets) and edges (representing double bonds). The well-known *Clar number* of a benzenoid graph is then defined as the maximum possible number of hexagons among all Clar covers of the given graph. In the same paper [33], H. Zhang and F. Zhang introduced also the so-called *Clar covering polynomial*, which is nowadays usually referred to as the *Zhang-Zhang polynomial* (shortly *ZZ polynomial*). For a benzenoid graph G, this polynomial is defined in the following way:

$$ZZ(G;x) = \sum_{a \geq 0} z(G;a)\, x^a,$$

where $z(G;a)$ is the number of Clar covers of G with exactly a hexagons. It is worth noting that this polynomial contains information about the Clar number of G (the degree of the polynomial), the number of Kekulé structures of G (the constant term), and the first Herndon number. For some recent investigations related to the Clar number and the ZZ polynomial see [13] and [18–22, 28, 29], respectively. Moreover, chemical applicability of the ZZ polynomial was discussed in [12].

In order to increase the sensibility of the standard Zhang-Zhang polynomial and to give an explicit information on π-electron cyclic conjugation within 10-membered rings, the generalized Zhang-Zhang polynomial (GZZ polynomial) of two variables has been introduced for benzenoid graphs [36]. It counts generalized Clar covers, which can contain also 10-cycles (representing two adjacent hexagons). Similarly, the multivariable Zhang-Zhang polynomial (shortly MZZ polynomial) of three variables has been introduced [24] for phenylenes, which are conjugated systems composed of 6-membered rings and 4-membered rings. The corresponding Clar covers for this polynomial are composed of 4-cycles (quadrilaterals), 6-cycles (hexagons), 8-cycles, and edges. Note that π-electron properties of these molecules are of great interest for theoretical chemistry [14, 15, 17]. It is also worth mentioning that some techniques for computing GZZ and MZZ polynomials were reported in [11, 24] and applications of the GZZ polynomial in chemistry were investigated in [11, 23].

In this paper, we investigate the relation between a special case of the MZZ polynomial, named as the first ZZ polynomial, of a phenylene and the GZZ polynomial of some benzenoid graph, which is described in Section 5. Before that, we introduce some basic concepts of graph theory in Section 2, formally define GZZ and MZZ polynomials in Section 3, and put forward three special cases of the MZZ polynomial in Section 4.

Then, in Section 6, the equality between the first ZZ polynomial of a phenylene and the generalized cube polynomial of its resonance graph is proved. Note that resonance graphs are used to model interactions among different Kekulé structures [30] and that the relation between the (generalized) Zhang-Zhang polynomial of a molecular graph and the (generalized) cube polynomial of its resonance graph was investigated in the past for other families of graphs [1, 25, 26, 32, 36]. For some recent research on resonance graphs see [3, 5, 6, 8, 27].

Moreover, we provide some results on the roots of the second ZZ polynomial and find another expression of this polynomial in Sections 7 and 8, respectively. Finally, in Section 9, we give structural interpretation for partial derivatives of GZZ and MZZ polynomials.

2 Preliminaries

The aim of this section is to state some basic definitions, which are mostly taken from [24]. If G is a graph, we denote by $V(G)$ the set of vertices and by $E(G)$ the set of edges of G. As usual, the *degree* of a vertex $v \in V(G)$ is the number of vertices adjacent to v. For any $k \geq 3$, a cycle of length k in G will be denoted as C_k and referred to as a *k-cycle* of G. Moreover, for $n \geq 1$ let P_n be the *path* on n vertices and K_n the *complete graph* on n vertices. If H is a subgraph of a graph G, then by $G - H$ we denote the graph obtained from G by deleting all the vertices of H.

Suppose G is a plane graph. Two distinct faces of G are *adjacent* if they share a common edge. The set of edges lying on some face f of G will be denoted by $E(f)$. Moreover, the subgraph induced by the edges in $E(f)$ is known as the *boundary* of f. A *hexagon* of G is an inner face of G whose boundary is a 6-cycle C_6. Analogously, a *quadrilateral* of G is an

inner face of G whose boundary is a 4-cycle C_4. In addition, the vertices of G belonging to the outer face are called *boundary* vertices and all the other vertices of G are *interior* vertices. Similarly, the edges lying on the outer face will be called *boundary* edges. An *outerplane graph* is a plane graph in which any vertex is a boundary vertex.

Throughout this paper, a *benzenoid graph* is a bipartite 2-connected plane graph in which all interior vertices have degree 3, all boundary vertices have degree 2 or 3, and all inner faces are hexagons (note that in some literature these graphs are called *fusenes* [7]). It is also worth mentioning that a benzenoid graph may not be a subgraph of the regular hexagonal lattice. Therefore, a benzenoid graph that can be embedded into the regular hexagonal lattice will be called a *hexagonal system*. Furthermore, a *catacondensed benzenoid graph* is a benzenoid graph which does not contain any interior vertices.

Let B be a catacondensed benzenoid graph. If we add a quadrilateral between any two adjacent hexagons of B, then the obtained graph is called a *phenylene*. In Figure 1 we can see a catacondensed benzenoid graph B and the corresponding phenylene G.

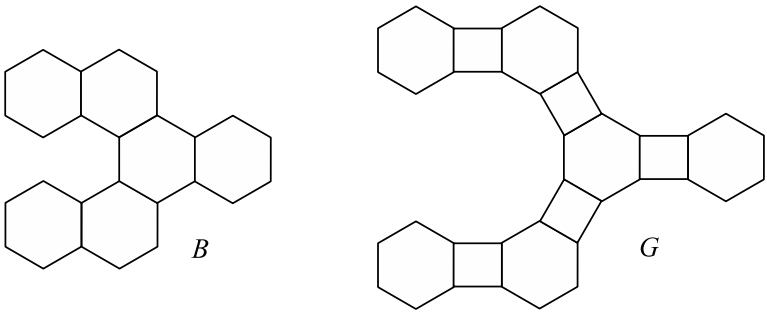

Figure 1. A benzenoid graph B and the corresponding phenylene G.

Any subgraph of a benzenoid graph will be called a *generalized benzenoid graph* [11, 33]. Moreover, a *generalized phenylene* is an outerplane bipartite graph in which no two distinct quadrilaterals are adjacent [24]. We can easily see that every 4-cycle of a generalized phenylene is the boundary of some quadrilateral, every 6-cycle is the boundary of some

hexagon, and in the interior of every 8-cycle there is either one inner face or one quadrilateral and one hexagon (with exactly one common edge).

A subset of edges M of a graph G is called a *perfect matching* of G if every vertex of G is an end vertex of exactly one edge from M. In chemistry, perfect matchings are also called *Kekulé structures*.

3 GZZ and MZZ polynomials

Firstly, we state some definitions from [36]. A spanning subgraph C of a generalized benzenoid graph G is a *generalized Clar cover* of G if every connected component of C is a 6-cycle C_6 (a hexagon), a 10-cycle C_{10}, or an edge K_2. On the right hand side of Figure 3 we can see a benzenoid graph with a generalized Clar cover containing one 10-cycle, two hexagons, and eight edges (the bold edges in the figure represent connected components of this generalized Clar cover). Additionally, any edge that belongs to a connected component K_2 of C will be called an *isolated edge* of C.

Suppose that G is a generalized benzenoid graph. The *generalized Zhang-Zhang polynomial* (or shortly *GZZ polynomial*) of G, denoted as $GZZ(G; x, z)$, is defined in the following way:

$$GZZ(G; x, z) = \sum_{a \geq 0, b \geq 0} gz(G; a, b)\, x^a z^b,$$

where $gz(G; a, b)$ represents the number of generalized Clar covers of G that contain exactly a hexagons and b 10-cycles. If G has no vertices, we consider the empty set as the unique generalized Clar cover of G, and therefore set $GZZ(G; x, z) = 1$. We should mention that in [36] the variables x and y were used, but for some technical reasons we prefer x and z in this paper (see Section 5). Moreover, it is obvious that the number $GZZ(G; 0, 0) = gz(G; 0, 0)$ equals the number of perfect matchings of G.

In addition, for any generalized benzenoid graph G we can define the *Zhang-Zhang polynomial* of G, denoted by $ZZ(G; x)$, as $ZZ(G; x) = GZZ(G; x, 0)$. Note that in such definitions we always interpret 0^0 as 1.

To present equivalent definition of the GZZ polynomial, let G be a generalized benzenoid graph with a perfect matching and let $\mathbb{GC}(G)$ be

the set of all generalized Clar covers of G. Moreover, for any $C \in \mathbb{GC}(G)$ let $h(C)$ be the number of hexagons of C and $t(C)$ the number of 10-cycles of C. Obviously, the GZZ polynomial can be written as

$$GZZ(G; x, z) = \sum_{C \in \mathbb{GC}(G)} x^{h(C)} z^{t(C)}.$$

The next concepts are taken from [24]. A spanning subgraph C of a generalized phenylene G is a *(4,6,8)-Clar cover* of G if every connected component of C is a 4-cycle C_4 (a quadrilateral), a 6-cycle C_6 (a hexagon), an 8-cycle C_8, or an edge K_2. On the left hand side of Figure 3 we can see a phenylene with a (4,6,8)-Clar cover composed of one 8-cycle, one hexagon, one quadrilateral, and six edges (the bold edges in the figure represent connected components of this (4,6,8)-Clar cover). Moreover, any edge that belongs to a connected component K_2 of C will be called an *isolated edge* of C.

Let G be a generalized phenylene. The *multivariable Zhang-Zhang polynomial* (or shortly *MZZ polynomial*) of G, denoted as $MZZ(G; x, y, z)$, is defined in the following way:

$$MZZ(G; x, y, z) = \sum_{a \geq 0, b \geq 0, c \geq 0} mz(G; a, b, c)\, x^a y^b z^c,$$

where $mz(G; a, b, c)$ represents the number of (4,6,8)-Clar covers of G that contain exactly a quadrilaterals, b hexagons, and c 8-cycles. Similarly as before, if G has no vertices, we define $MZZ(G; x, y, z) = 1$.

It is easy to observe that the number of perfect matchings of G is exactly $mz(G; 0, 0, 0)$, which is equal to $MZZ(G; 0, 0, 0)$. Moreover, if G is a phenylene, then the set of all hexagons of G is always a (4,6,8)-Clar cover of G, so the MZZ polynomial of a phenylene with $h(G)$ hexagons always contains the term $y^{h(G)}$.

Suppose that G is a generalized phenylene with a perfect matching and let $\mathbb{CC}(G)$ be the set of all (4,6,8)-Clar covers of G. In addition, for any $C \in \mathbb{CC}(G)$ let $q(C)$ be the number of quadrilaterals of C, $h(C)$ the number of hexagons of C, and $o(C)$ as the number of 8-cycles of C. It is

easy to see that the MZZ polynomial can be written as

$$MZZ(G;x,y,z) = \sum_{C \in \mathbb{CC}(G)} x^{q(C)} y^{h(C)} z^{o(C)}.$$

4 Special cases of the MZZ polynomial

In this section, we consider three special cases of the MZZ polynomial and in this way obtain three new polynomials (with one or two variables) for phenylenes.

Firstly, for any generalized phenylene G, we define the *first Zhang-Zhang polynomial* of G, denoted as $ZZ_1(G;x,z)$, in the following way:

$$ZZ_1(G;x,z) = MZZ(G;x,x,z).$$

The difference between the MZZ polynomial and the first ZZ polynomial is in the fact that ZZ_1 does not distinguish between hexagons and quadrilaterals of G. Therefore, this polynomial can be written as

$$ZZ_1(G;x,z) = \sum_{C \in \mathbb{CC}(G)} x^{q(C)+h(C)} z^{o(C)}.$$

Next, we define the *second Zhang-Zhang polynomial* of a generalized phenylene G, denoted by $ZZ_2(G;x)$, as

$$ZZ_2(G;x) = MZZ(G;x,x,0) = ZZ_1(G;x,0).$$

Obviously, this polynomial counts so called $(4,6)$-Clar covers of G and does not distinguish between different inner faces (hexagons and quadrilaterals) of G. More precisely, a $(4,6,8)$-Clar cover without 8-cycles is called a *(4,6)-Clar cover* of G. If we denote by $\mathbb{CC}_2(G)$ the set of all $(4,6)$-Clar covers of G, then the second ZZ polynomial can be also written as

$$ZZ_2(G;x) = \sum_{C \in \mathbb{CC}_2(G)} x^{q(C)+h(C)}.$$

Finally, it could be also interesting to consider a polynomial which

counts $(4,6)$-Clar covers and distinguishes between hexagons and quadrilaterals. Therefore, the *third Zhang-Zhang polynomial* of G, denoted as $ZZ_3(G;x,y)$, is defined by

$$ZZ_3(G;x,y) = MZZ(G;x,y,0).$$

It is obvious that $ZZ_2(G;x) = ZZ_3(G;x,x)$ and that the third ZZ polynomial can be calculated as

$$ZZ_3(G;x,y) = \sum_{C \in \mathbb{CC}_2(G)} x^{q(C)} y^{h(C)}.$$

5 Relation between the first ZZ polynomial and the GZZ polynomial

In this section, we show that the first ZZ polynomial of a phenylene G, which has two variables and represents a special case of the MZZ polynomial, is equal to the GZZ polynomial of some particular benzenoid graph obtained from G.

Firstly, we introduce the following transformation to obtain the benzenoid graph from a given phenylene. Let G be a phenylene with hexagons $h_1, \ldots, h_n$ and quadrilaterals $q_1, \ldots, q_{n-1}$. Obviously, every quadrilateral of G contains exactly two boundary edges of G. For any $i \in \{1, \ldots, n-1\}$, choose one of the two boundary edges of G that also belong to the face q_i and denote the chosen edge by e_i. Then, subdivide edge e_i exactly two times for all $i \in \{1, \ldots, n-1\}$. With other words, replace the path on two vertices in G that contains the edge e_i by the path on four vertices. Obviously, the obtained graph is a catacondensed benzenoid graph and we will denote it as $B(G)$, see Figure 2. Moreover, we need some additional notation:

- For any inner face f of G denote by $B(f)$ the corresponding inner face (hexagon) of $B(G)$.
- For any edge $e \in E(G) \setminus \{e_1, \ldots, e_{n-1}\}$ denote by $B(e)$ the corresponding edge of $B(G)$.

- For any $i \in \{1, \ldots, n-1\}$, denote by $B(e_i)$ the path on four vertices in $B(G)$ that is obtained from the edge e_i.

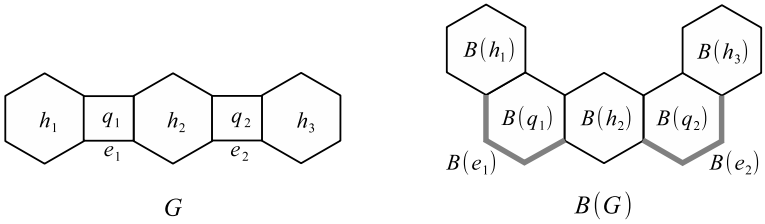

Figure 2. A phenylene G and the corresponding benzenoid graph $B(G)$.

Finally, if G is a phenylene, f a hexagon of G, and f' a quadrilateral of G such that f and f' are adjacent, then ff' denotes the unique 8-cycle of G induced by f and f'. Similarly, if B is a benzenoid graph and h, h' two adjacent hexagons of B, then by hh' we denote the unique 10-cycle of B induced by h and h'.

We are now ready for the following lemma.

Lemma 1. *Let G be a phenylene and $B(G)$ the corresponding benzenoid graph. Then there exists a bijection f between the set $\mathbb{CC}(G)$ and the set $\mathbb{GC}(B(G))$ such that any $(4,6,8)$-Clar cover of G with a quadrilaterals, b hexagons, and c 8-cycles is mapped to the generalized Clar cover of $B(G)$ with $a+b$ hexagons and c 10-cycles.*

Proof. Define the function $f : \mathbb{CC}(G) \to \mathbb{GC}(B(G))$ as described below. Let C be a $(4,6,8)$-Clar cover of G with a quadrilaterals, b hexagons, and c 8-cycles. Define the generalized Clar cover $f(C)$ of $B(G)$ as follows:

(*i*) If quadrilateral q_i belongs to C, where $i \in \{1, \ldots, n-1\}$, then include hexagon $B(q_i)$ in $f(C)$.

(*ii*) If hexagon h_i belongs to C, where $i \in \{1, \ldots, n\}$, then include hexagon $B(h_i)$ in $f(C)$.

(*iii*) If the 8-cycle $h_i q_j$ belongs to C, where $i \in \{1, \ldots, n\}$ and j is from $\{1, \ldots, n-1\}$, then include the 10-cycle $B(h_i)B(q_j)$ in $f(C)$.

(*iv*) If an edge $e \in E(G) \setminus \{e_1, \ldots, e_{n-1}\}$ is an isolated edge of C, then include the edge $B(e)$ in $f(C)$ as an isolated edge.

(*v*) If edge e_i is an isolated edge of C, where $i \in \{1, \ldots, n-1\}$, then include the two terminal edges of the path $B(e_i)$ in $f(C)$ as isolated edges.

(*vi*) If edge e_i is not an isolated edge of C and e_i also does not belong to some 4-cycle or 8-cycle from C, where $i \in \{1, \ldots, n-1\}$, then include the middle edge of the path $B(e_i)$ in $f(C)$ as an isolated edge.

It is easy to check that $f(C)$ is a generalized Clar cover of the benzenoid graph $B(G)$. Obviously, $f(C)$ contains $a + b$ hexagons and c cycles of length 10, see Figure 3 for an example.

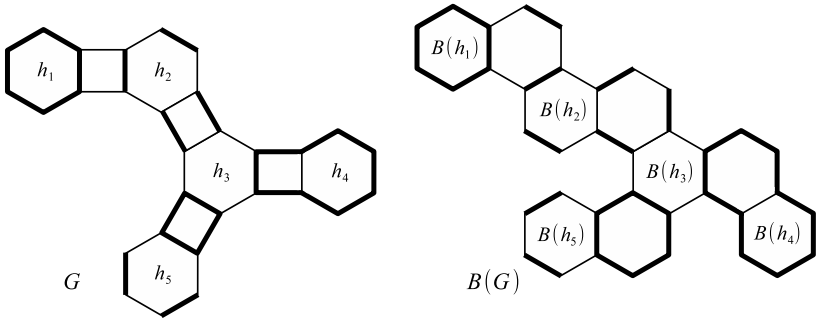

Figure 3. A (4,6,8)-Clar cover of a phenylene G and the corresponding generalized Clar cover of $B(G)$.

Now, it remains to show that f is a bijection. To prove that f is injective, take two distinct $(4, 6, 8)$-Clar covers of G and denote them by C and C'. Then, C and C' must differ in some hexagon, quadrilateral, 8-cycle, or edge. Therefore, by definition of function f, generalized Clar covers $f(C)$ and $f(C')$ can not be the same. Consequently, function f is injective.

On the other hand, to show that f is surjective, take some generalized Clar cover C_1 of $B(G)$. Define the $(4, 6, 8)$-Clar cover C of G as follows:

(*i*) If hexagon $B(q_i)$ belongs to C_1, where $i \in \{1, \ldots, n-1\}$, then include quadrilateral q_i in C.

(*ii*) If hexagon $B(h_i)$ belongs to C_1, where $i \in \{1, \ldots, n\}$, then include hexagon h_i in C.

(*iii*) It is easy to see that every 10-cycle of $B(G)$ is composed of one hexagon $B(h_i)$, where $i \in \{1, \ldots, n\}$, and one hexagon $B(q_j)$, where $j \in \{1, \ldots, n-1\}$. If this 10-cycle belongs to C_1, then include the 8-cycle $h_i q_j$ in C.

(*iv*) If an edge $B(e)$, where $e \in E(G) \setminus \{e_1, \ldots, e_{n-1}\}$, is an isolated edge of C_1, then include the edge e in C as an isolated edge.

(*v*) Let $i \in \{1, \ldots, n-1\}$. We can easily check that the terminal edges of the path on four vertices $B(e_i)$ are either both isolated edges of C_1 or neither of them is an isolated edge of C_1. If these two terminal edges are isolated edges of C_1, then include the edge e_i in C as an isolated edge.

It is straightforward to prove that C is a $(4, 6, 8)$-Clar cover of G and that $f(C) = C_1$. Therefore, f is surjective and we are done. ■

The main result of this section can now be stated. It relates the first ZZ polynomial of a phenylene G to the GZZ polynomial of $B(G)$.

Theorem 1. *If G is a phenylene and $B(G)$ the corresponding benzenoid graph, then*

$$ZZ_1(G; x, z) = GZZ(B(G); x, z).$$

Proof. Let $f : \mathbb{CC}(G) \to \mathbb{GC}(B(G))$ be the bijection from Lemma 1. Then by the same lemma we obtain

$$\begin{aligned} ZZ_1(G; x, z) &= \sum_{C \in \mathbb{CC}(G)} x^{q(C)+h(C)} z^{o(C)} \\ &= \sum_{C \in \mathbb{CC}(G)} x^{h(f(C))} z^{t(f(C))} \\ &= \sum_{C_1 \in \mathbb{GC}(B(G))} x^{h(C_1)} z^{t(C_1)} \\ &= GZZ(B(G); x, z), \end{aligned}$$

which completes the proof. ■

This result also explains why the computation of the MZZ polynomial for a linear phenylene chain is much more difficult than calculating the (generalized) ZZ polynomial of a linear benzenoid chain, which was observed in [24]. In fact, every quadrilateral of a phenylene G is replaced by an angular hexagon in $B(G)$ and consequently, from a linear phenylene chain we obtain a benzenoid chain with many angular hexagons. For more information and corresponding definitions see [24].

As a special case of the stated theorem, we also obtain the next corollary, which claims that the second ZZ polynomial of a phenylene G coincides with the ZZ polynomial of $B(G)$.

Corollary 1. *If G is a phenylene and $B(G)$ the corresponding benzenoid graph, then*

$$ZZ_2(G;x) = ZZ(B(G);x).$$

Proof. We already know that $ZZ_2(G;x) = ZZ_1(G;x,0)$ and $ZZ(B(G);x) = GZZ(B(G);x,0)$. Hence, the result follows by Theorem 1. ■

6 Relation between the first ZZ polynomial and the generalized cube polynomial

The aim of this section is to prove that the first ZZ polynomial of a phenylene G is equal to the generalized cube polynomial of the resonance graph of G. In order to do this, we should firstly introduce several concepts.

An *even ring system* is a simple bipartite 2-connected plane graph with all interior vertices of degree 3 and all boundary vertices of degree 2 or 3. Obviously, an even ring system whose inner faces are only hexagons is a benzenoid graph. Moreover, an even ring system is *catacondensed* if it does not contain interior vertices; in such a case we shortly call it CERS. It is easy to see that any catacondensed benzenoid graph and any phenylene is a CERS. See [4, 5] for more information on these graphs.

Let G be a plane bipartite graph with a perfect matching. The *resonance graph* $R(G)$ is the graph whose vertices are the perfect matchings of G, and two perfect matchings M_1, M_2 are adjacent whenever their symmetric difference $M_1 \oplus M_2$ forms exactly one cycle that is the boundary

of some inner face f of G, i.e. $M_1 \oplus M_2 = E(f)$. For a survey paper on resonance graphs see [30].

If G is a CERS with an inner face f and the outer face f_0, then a connected component of the graph induced by the edges in $E(f) \cap E(f_0)$ is called a *boundary segment*. The following transformation was considered in [4, 5].

Transformation 1. *Let G be a CERS and P a boundary segment of G. A CERS G' is obtained from G by subdividing edges of P an even number of times or reversely, smoothing an even number of vertices of P.*

Moreover, the authors of [4,5] proposed the next definition. Let G and H be two CERS. Then G is *evenly homeomorphic* to H if it is possible to successively apply Transformation 1 on G and H to obtain graphs G' and H', respectively, such that G' and H' are isomorphic. The following results was proved in [4].

Theorem 2. *[4] Let G and H be two CERS. If G and H are evenly homeomorphic, then the resonance graph $R(G)$ is isomorphic to the resonance graph $R(H)$.*

We can now show that the resonance graph of a phenylene G is isomorphic to the resonance graph of the corresponding benzenoid graph $B(G)$ defined in the previous section.

Proposition 1. *If G is a phenylene and $B(G)$ the corresponding benzenoid graph, then the resonance graphs $R(G)$ and $R(B(G))$ are isomorphic.*

Proof. Obviously, catacondensed benzenoid graph $B(G)$ can be obtained from a phenylene G by applying Transformation 1. Therefore, G and $B(G)$ are evenly homeomorphic CERS and hence, by Theorem 2 the resonance graphs $R(G)$ and $R(B(G))$ are isomorphic. ■

Some additional definitions are needed to present the main theorem of the section.

The *Cartesian product* of graphs $G_1, G_2, \ldots, G_m$, denoted as $\Box_{i=1}^{m} G_i = G_1 \Box G_2 \Box \cdots \Box G_m$, where $m \geq 1$, is a graph with the vertex set $\prod_{i=1}^{m} V(G_i)$

such that two vertices $a = (a_1, a_2, \ldots, a_m)$, $b = (b_1, b_2, \ldots, b_m)$ are adjacent if there exists exactly one $j \in \{1, \ldots, m\}$ such that $a_j b_j \in E(G_j)$ and $a_i = b_i$ for every $i \in \{1, \ldots, m\} \setminus \{j\}$.

Let G be a graph and $m \geq 1$ an integer. By G^m we denote the Cartesian product of m copies of G, i.e. $G^m = \Box_{i=1}^m G$. Moreover, let $G^0 = P_1$. The *hypercube* Q_k of dimension $k \geq 0$ is then defined as P_2^k. Moreover, the *cube polynomial* of a graph G, which was introduced in [2], is calculated in the following way:

$$C(G; x) = \sum_{k \geq 0} \alpha_k(G) x^k,$$

where $\alpha_k(H)$ denotes the number of induced subgraphs of G that are isomorphic to the k-dimensional hypercube.

A subgraph H of a graph G is *induced* if for any two vertices u, v from H, u and v are adjacent in H if and only if they are adjacent in G. Moreover, a subgraph H of a graph G is *convex* in G if every shortest path in G between any two vertices of H lies entirely in H. Obviously, any convex subgraph of G is also an induced subgraph of G.

Next, for any $k, l \geq 0$ we define $Q_{k,l} = P_2^k \Box P_3^l$. It is easy to see that $Q_{k,0}$ is the k-dimensional hypercube and therefore, graphs $Q_{k,l}$ generalize hypercubes. In order to count these graphs, a new polynomial of two variables was introduced in [36]. More precisely, the *generalized cube polynomial* of a graph G is defined as

$$GC(G; x, z) = \sum_{k \geq 0, l \geq 0} \alpha_{k,l}(H) x^k z^l,$$

where $\alpha_{k,l}(H)$ represents the number of convex subgraphs of H that are isomorphic to the graph $Q_{k,l}$. Note that in [36] the variables x and y were used for this polynomial, but here we use x and z such that the notation coincides with the first ZZ polynomial.

The next result follows by Theorem 4.1 from [36]. Note that in the mentioned paper this theorem was proved only for benzenoid graphs that can be embedded into the regular hexagonal lattice. However, the same proof works for all benzenoid graphs.

Theorem 3. *[36] If G is a benzenoid graph with a perfect matching, then the GZZ polynomial of G equals the generalized cube polynomial of its resonance graph $R(G)$, i.e.*

$$GZZ(G; x, z) = GC(R(G); x, z).$$

Finally, we can formulate the main theorem of the section.

Theorem 4. *If G is a phenylene, then the first ZZ polynomial of G equals the generalized cube polynomial of its resonance graph $R(G)$, i.e.*

$$ZZ_1(G; x, z) = GC(R(G); x, z).$$

Proof. Let $B(G)$ be the corresponding benzenoid graph for phenylene G. Then, by Theorem 1 it follows that the first ZZ polynomial of G equals the GZZ polynomial of $B(G)$, so $ZZ_1(G; x, z) = GZZ(B(G); x, z)$. However, because of Theorem 3, the GZZ polynomial of $B(G)$ is equal to the generalized cube polynomial of the resonance graph of $B(G)$, i.e. $GZZ(B(G); x, z) = GC(R(B(G)); x, z)$. Finally, by Proposition 1 we know that the resonance graphs $R(G)$ and $R(B(G))$ are isomorphic and therefore, they have the same generalized cube polynomial, which means $GC(R(B(G)); x, z) = GC(R(G); x, z)$. From the stated equalities we can now conclude that $ZZ_1(G; x, z) = GC(R(G); x, z)$. ■

Let G be a phenylene shown in Figure 2. The MZZ polynomial of G was already obtained in [24]: $MZZ(G; x, y, z) = y^3 + 2xy + 6y^2 + 4yz + 4x + 14y + 8z + 12$. Therefore, the first ZZ polynomial of G equals

$$ZZ_1(G; x, z) = MZZ(G; x, x, z) = x^3 + 8x^2 + 4xz + 18x + 8z + 12.$$

On the other hand, the resonance graph $R(G)$ is shown in Figure 4 and it can be easily checked that $GC(R(G); x, z) = ZZ_1(G; x, z)$. Note also that to obtain graph $R(G)$ one can apply the algorithms presented in [4, 6].

To show another example, let G be a phenylene from Figure 3. This graph has 92 perfect matchings, so it is more difficult to draw the corresponding resonance graph. However, the MZZ polynomial of G was cal-

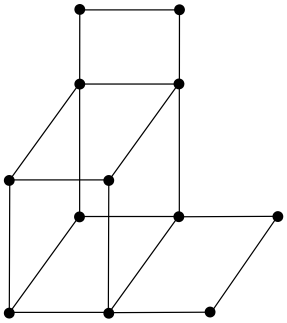

Figure 4. Resonance graph $R(G)$ of a phenylene from Figure 2.

culated in [24] by using some techniques developed there. Consequently, by using the mentioned result we can obtain the first ZZ polynomial of G, which is by Theorem 4 equal to the generalized cube polynomial of $R(G)$. The two polynomials are:

$$\begin{aligned} ZZ_1(G;x,z) &= GC(R(G);x,z) = x^5 + 22x^4 + 26x^3z + 12x^2z^2 \\ &+ 2xz^3 + 114x^3 + 137x^2z + 50xz^2 + 5z^3 + 248x^2 \\ &+ 236xz + 50z^2 + 246x + 133z + 92. \end{aligned}$$

To obtain a similar connection also for the second ZZ polynomial and the cube polynomial, we firstly need two additional propositions.

Proposition 2. *Let G be a benzenoid graph or a phenylene. If H is a subgraph of the resonance $R(G)$ such that H is isomorphic the hypercube Q_n, where $n \geq 0$, then H is a convex subgraph of $R(G)$.*

Proof. We already now that for any phenylene G the resonance graph $R(G)$ is isomorphic to the resonance graph $R(B(G))$, where $B(G)$ is the corresponding benzenoid graph defined in the previous section. Therefore, in the rest of the proof we assume that G is a benzenoid graph.

Let H be a subgraph of $R(G)$ isomorphic to the n-dimensional hypercube Q_n. In addition, assume that $n \geq 1$ (if $n = 0$, the result follows trivially) and choose some vertex M of H. Obviously, M has exactly n incident edges in H which determine some hexagons $h_1, \ldots, h_n$ of G. In the

same way as in the proof of Lemma 4.5 from [1] it can be shown that these hexagons, together with the remaining edges of perfect matching M, form some Clar cover C of G with exactly n hexagons. Moreover, any vertex of H (which is clearly also a perfect matching of G) can be obtained by selecting some perfect matching for every hexagon h_i, $i \in \{1, \ldots, n\}$, and adding all isolated edges of C.

Obviously, by the above discussion it follows that the vertices of H, which are perfect matchings of G, can differ only in the edges of hexagons that belong to C. Therefore, in resonance graph $R(G)$ any vertex of H should have exactly n neighbours from H. On the other hand, since H is isomorphic to Q_n, any vertex of H has degree n in H. Therefore, H is an induced subgraph of $R(G)$.

Now, suppose that M and M' are two distinct vertices of H. As we already observed, M and M' can differ only in the edges of some hexagons that belong to C. Therefore, any shortest path between M and M' in $R(G)$ goes through vertices of H. Since H is also an induced subgraph of $R(G)$, any shortest path between M and M' in $R(G)$ lies entirely in H. This means that H is a convex subgraph in $R(G)$. ■

Proposition 3. *Let G be a benzenoid graph or a phenylene and let $R(G)$ be its resonance graph. Then the cube polynomial of $R(G)$ can be obtained from the generalized cube polynomial in the following way:*

$$C(R(G); x) = GC(R(G); x, 0).$$

Proof. By Proposition 2, any induced hypercube of $R(G)$ is also a convex subgraph of $R(G)$. Therefore, the number $\alpha_{k,0}(R(G))$, which represents the number of convex subgraphs of $R(G)$ that are isomorphic to the graph $Q_{k,0} = Q_k$, is equal to the number of induced subgraphs of $R(G)$ isomorphic to Q_k for any $k \geq 0$. This means $\alpha_{k,0}(R(G)) = \alpha_k(R(G))$ for any $k \geq 0$. Consequently, by the definition of the (generalized) cube polynomial we obtain $C(R(G); x) = GC(R(G); x, 0)$. ■

The following corollary of Theorem 4 can now be stated.

Corollary 2. *If G is a phenylene, then the second ZZ polynomial of G equals the cube polynomial of its resonance graph $R(G)$, i.e.*

$$ZZ_2(G;x) = C(R(G);x).$$

Proof. We know that the second ZZ polynomial of G can be expressed by the first ZZ polynomial as follows: $ZZ_2(G;x) = ZZ_1(G;x,0)$. On the other hand, by Proposition 3 the cube polynomial of $R(G)$ is a special case of the generalized cube polynomial of $R(G)$, i.e. $C(R(G);x) = GC(R(G);x,0)$. Therefore, the desired result follows by Theorem 4. ■

Remark. *Note that Corollary 2 also follows by Theorem 1.5 from [25], where this equality was proved in a more general way.*

7 Roots of the second ZZ polynomial

The authors of [32] obtained some results related to the roots of the ZZ polynomial of hexagonal systems (it can be checked that they hold for all benzenoid graphs). Therefore, in this section we present analogous results for the second ZZ polynomial of phenylenes. Firstly, we state the definition of a median graph and some results on the roots of the cube polynomial of such graphs.

Let G be a connected graph. A *median* of a triple of vertices u, v, w of G is a vertex z that lies on a shortest u,v-path, on a shortest u,w-path and on a shortest v,w-path (note that z can be one of the vertices u, v, w). If every triple of vertices in G has a unique median, then G is called a *median graph*. The following results were proved in [2].

Theorem 5. *[2] If G is a median graph, then the cube polynomial $C(G;x)$ has no roots in $[-1,\infty)$. In addition, if G is a nontrivial median graph, then $C(G;x)$ has a real root in the interval $[-2,-1)$.*

Theorem 6. *[2] Let G be a median graph. If a rational number r is a root of the cube polynomial $C(G;x)$, then $r = -\frac{t+1}{t}$ for some integer $t \geq 1$.*

A bipartite graph G is called *elementary* if G is connected and every edge belongs to some perfect matching of G (see [30] for more informa-

tion). Obviously, every phenylene G has exactly two perfect matchings that contain only boundary edges of G. Therefore, every boundary edge of G belongs to some perfect matching. On the other hand, if e is not a boundary edge of G, then it is easy to see that there exists a perfect matching M of G such that M contains e and some boundary edges of G. Hence, every phenylene is a plane elementary bipartite graph.

It is well known that the resonance graph of a plane elementary bipartite graph is a median graph [31]. Therefore, the resonance graph $R(G)$ of a phenylene G is a nontrivial median graph. Consequently, by using Corollary 2 together with Theorems 5 and 6, we obtain the following results.

Corollary 3. *If G is a phenylene, then $ZZ_2(G;x)$ has no roots in $[-1,\infty)$, but it has a real root in the interval $[-2,-1)$.*

Corollary 4. *Let G be a phenylene. If a rational number r is a root of $ZZ_2(G;x)$, then $r=-\frac{t+1}{t}$ for some integer $t\geq 1$.*

8 Another expression for the second ZZ polynomial

In [34] it was shown that the ZZ polynomial of a hexagonal system can be expressed in another way. In particular, so called proper sextets of a hexagonal system were used for this purpose. Here we show a similar result for the second ZZ polynomial of phenylenes, but since the graphs considered in [34] are always subgraphs of the regular hexagonal lattice, the results stated there can not be directly applied to achieve our goal. Firstly, we state some standard definitions which are used to adopt the concept of a proper sextet to phenylenes.

Let G be a phenylene and M a perfect matching of G. A cycle C of G is called *M-alternating* if the edges of C appear alternately in M and in $E(G)\setminus M$. Furthermore, assume that the vertices of a phenylene G are colored black and white such that adjacent vertices receive different colors (we call such coloring a *proper coloring*). An M-alternating cycle C of G is *proper* if every edge of C belonging to M goes from white to black vertex

along the clockwise orientation of C. In addition, we say that a proper M-alternating cycle C of G is a *minimum proper M-alternating cycle* if there is no other proper M-alternating cycle C' of G such that the interior of C' is contained in the interior of C. Finally, an inner face f of G is *proper M-resonant* if the boundary of f is a proper M-alternating cycle.

For any integer $k \geq 0$ denote by $a(G;k)$ the number of perfect matchings M of G with exactly k proper M-resonant inner faces. The following theorem can now be stated.

Theorem 7. *If G is a phenylene whose vertices are properly colored black and white, then the second ZZ polynomial of G can be expressed as*

$$ZZ_2(G;x) = \sum_{k\geq 0} a(G;k)(x+1)^k.$$

Proof. We follow similar reasoning as in the proof of Theorem 2 from [34]. Let C be a $(4,6)$-Clar cover of G. Define the perfect matching M of G in the following way:

(i) For every hexagon h of C include in M three edges of h such that h becomes proper M-resonant inner face.

(ii) For every quadrilateral q of C include in M two edges of q such that q becomes proper M-resonant inner face.

(iii) Additionally, include in M all isolated edges of C.

In this way, we obtain the function α from the set of all $(4,6)$-Clar covers of G, denoted as $\mathbb{CC}_2(G)$, to the set of all perfect matchings of G, which will be denoted as $\mathcal{M}(G)$. If we again use the notation stated above, this function maps any Clar cover C to the perfect matching M, which means $\alpha(C) = M$.

Moreover, for any perfect matching M of G we define the set $\mathcal{C}(M) = \{C \in \mathbb{CC}_2(G) \mid \alpha(C) = M\}$. Consequently, the set of all $(4,6)$-Clar covers of G can be partitioned as $\mathbb{CC}_2(G) = \bigcup_{M\in\mathcal{M}(G)} \mathcal{C}(M)$.

Let M be a perfect matching of G and suppose that G has exactly $p(M)$ proper M-resonant inner faces, where $p(M) \geq 0$. Obviously, if we want to

construct all $(4,6)$-Clar covers from the set $\mathcal{C}(M)$, we have two options for any proper M-resonant inner face: we can include in C the corresponding inner face or two/three isolated edges of M. Thus, the number of $(4,6)$-Clar covers from $\mathcal{C}(M)$ with exactly j quadrilaterals or hexagons is equal to $\binom{p(M)}{j}$ for any $j \in \{0,1,\ldots,p(M)\}$. Therefore, we obtain

$$\sum_{C\in\mathcal{C}(M)} x^{q(C)+h(C)} = \sum_{j=0}^{p(M)} \binom{p(M)}{j} x^j = (x+1)^{p(M)}.$$

Finally, one can get

$$\begin{aligned} ZZ_2(G;x) &= \sum_{C\in\mathbb{CC}_2(G)} x^{q(C)+h(C)} = \sum_{M\in\mathcal{M}(G)} \left(\sum_{C\in\mathcal{C}(M)} x^{q(C)+h(C)} \right) \\ &= \sum_{M\in\mathcal{M}(G)} (x+1)^{p(M)} = \sum_{k\geq 0} a(G;k)(x+1)^k, \end{aligned}$$

which is the desired result. ■

Let G be a phenylene from Figure 2. In Section 6 we obtained the first ZZ polynomial of G: $ZZ_1(G;x,z) = MZZ(G;x,x,z) = x^3 + 8x^2 + 4xz + 18x + 8z + 12$. Therefore, the second ZZ polynomial equals $ZZ_2(G;x) = x^3 + 8x^2 + 18x + 12$, which can be rewritten as

$$ZZ_2(G;x) = (x+1)^3 + 5(x+1)^2 + 5(x+1) + 1.$$

This tells us, for example, that in whichever way we properly color the vertices of G with two colors, G has five perfect matchings M with exactly two proper M-resonant inner faces.

By using Theorem 7 together with Taylor's theorem for the second ZZ polynomial at $x = -1$, we obtain the next corollary, which connects the numbers $a(G;k)$ with partial derivatives of the second ZZ polynomial.

Corollary 5. *If G is a phenylene whose vertices are properly colored black and white, then for any integer $k \geq 0$ it holds*

$$a(G;k) = \frac{ZZ_2^{(k)}(G;-1)}{k!}.$$

Denote by $h(G)$ the number of hexagons of a phenylene G. The following proposition can be stated.

Proposition 4. *If G is a phenylene whose vertices are properly colored black and white, then $a(G;0) = 1$, $a(G;h(G)) = 1$. Moreover, if $h(G) \geq 2$, then $a(G;k) > 0$ for any $k \in \{1, \ldots, h(G) - 1\}$.*

Proof. Obviously, the degree of the second ZZ polynomial is $h(G)$ and there exists exactly one $(4,6)$-Clar cover C of G that contains $h(G)$ cycles (in fact, these cycles are all 6-cycles representing the hexagons of G). Therefore, there is only one perfect matching M_0 of G with exactly $h(G)$ proper M_0-resonant inner faces. Note that M_0 can be obtained from C be selecting three edges in every hexagon such that all the hexagons are proper M_0-resonant. This means that $a(G;h(G)) = 1$.

On the other hand, by Corollary 10 from [35] we know that there exists exactly one perfect matching M_1 of G with no proper M_1-alternating cycle (note that M_1 is one of the two perfect matchings that contain only boundary edges of G). Obviously, this means that G does not have any proper M_1-resonant inner face. Suppose that there exists some other perfect matching M_2 of G such that G does not have any proper M_2-resonant inner face. Therefore, there should exist a minimum proper M_2-alternating cycle D of G which is not the boundary of some inner face. Thus, by Lemma 3 from [35] it follows that the edges in the interior of D incident with the vertices of D are not contained in any perfect matching of G. However, this is a contradiction because we already know from Section 7 that G is elementary. Consequently, M_1 is the only perfect matching of G such that there is no proper M_1-resonant inner face. Hence, $a(G;0) = 1$.

For the last part of the proof we will use similar reasoning as in the proof of Lemma 1 from [34]. Suppose that $k \in \{1, \ldots, h(G) - 1\}$, take any k hexagons of G, and let H be the subgraph of G induced by these hexagons. Let $H_1 = G - H$ be the graph obtained from G by deleting all the vertices of H. Obviously, H_1 has a perfect matching. Moreover, by Corollary 10 from [35] there exists exactly one perfect matching M' of H_1 such that H_1 does not contain any proper M'-alternating cycle, which also means that H_1 does not contain any proper M'-resonant inner face. On

the other hand, let M'' be the perfect matching of H with exactly k proper M-resonant hexagons. Obviously, $\overline{M} = M' \cup M''$ is a perfect matching of G and the number of proper $\overline{M}$-resonant inner faces of G is exactly k. Therefore, $a(G;k) > 0$. ■

By Corollary 5 and Proposition 4 we also obtain a simple consequence, which gives us the value of the second ZZ polynomial at $x = -1$.

Corollary 6. *If G is a phenylene, then $ZZ_2(G;-1) = 1$.*

9 Partial derivatives of MZZ and GZZ polynomials

In this section, we investigate how the partial derivatives of MZZ and GZZ polynomials are related to the corresponding polynomials of subgraphs. Note that the derivatives of the ZZ polynomial of hexagonal systems were studied in [32].

Let G be a generalized phenylene. A set R of 4-cycles (quadrilaterals), 6-cycles (hexagons), and 8-cycles of G is called a $(4,6,8)$-*resonant set* of G if there exists some $(4,6,8)$-Clar cover C of G such that every element of R represents some connected component of C. The set of all $(4,6,8)$-resonant sets of G which contain exactly a quadrilaterals, b hexagons, and c 8-cycles will be denoted as $\mathcal{R}(G;a,b,c)$.

Moreover, we denote by $\mathcal{Q}(G)$ the set of all $(4,6,8)$-resonant sets of G that contain exactly one quadrilateral and no hexagons or 8-cycles, this means $\mathcal{Q}(G) = \mathcal{R}(G;1,0,0)$. Similarly, let $\mathcal{H}(G)$ the set of all $(4,6,8)$-resonant sets that contain only one hexagon of G (and no quadrilaterals or 8-cycles) and let $\mathcal{O}(G)$ be the set of all $(4,6,8)$-resonant sets that contain only one 8-cycle (and no quadrilaterals or hexagons). The first theorem can now be stated. Note that in this section whenever the index set in the summation is empty, we define the corresponding sum to be zero.

Theorem 8. *If G is a generalized phenylene, then the partial derivatives of the MZZ polynomial of G can be computed as*

$$\begin{aligned}
\frac{\partial}{\partial x} MZZ(G;x,y,z) &= \sum_{q\in\mathcal{Q}(G)} MZZ(G-q;x,y,z),\\
\frac{\partial}{\partial y} MZZ(G;x,y,z) &= \sum_{h\in\mathcal{H}(G)} MZZ(G-h;x,y,z),\\
\frac{\partial}{\partial z} MZZ(G;x,y,z) &= \sum_{o\in\mathcal{O}(G)} MZZ(G-o;x,y,z).
\end{aligned}$$

Proof. We present only the proof for the first equality, since the other two can be shown in a similar way. To prove the result, we will follow similar reasoning as in the proof of Theorem 4.1 from [32].

Let us count the number of order pairs (C,q), where C is a $(4,6,8)$-Clar cover of G with a quadrilaterals, b hexagons, c 8-cycles and q is some quadrilateral of C. Obviously, if C is fixed, then the number of pairs (C,q) is exactly a. Therefore, the total number of such pairs in G equals $a\cdot mz(G;a,b,c)$.

On the other hand, if q is fixed, the number of pairs (C,q) is equal to the number of $(4,6,8)$-Clar covers of $G-q$ with $a-1$ quadrilaterals, b hexagons, and c 8-cycles. Consequently, the number of pairs (C,q) is exactly $\sum_{q\in\mathcal{Q}(G)} mz(G-q;a-1,b,c)$.

Denote $MZZ(G;x,y,z)$ simply as $MZZ(G)$. We can now obtain

$$\begin{aligned}
\frac{\partial}{\partial x} MZZ(G) &= \frac{\partial}{\partial x}\left(\sum_{a\geq 0,b\geq 0,c\geq 0} mz(G;a,b,c)\, x^a y^b z^c\right)\\
&= \sum_{a\geq 0,b\geq 0,c\geq 0} a\cdot mz(G;a,b,c)\, x^{a-1} y^b z^c\\
&= \sum_{a\geq 1,b\geq 0,c\geq 0}\left(\sum_{q\in\mathcal{Q}(G)} mz(G-q;a-1,b,c)\right) x^{a-1} y^b z^c\\
&= \sum_{a\geq 1,b\geq 0,c\geq 0}\left(\sum_{q\in\mathcal{Q}(G)} mz(G-q;a-1,b,c)\, x^{a-1} y^b z^c\right)
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{q\in\mathcal{Q}(G)} \left(\sum_{a\geq 1, b\geq 0, c\geq 0} mz(G-q; a-1, b, c)\, x^{a-1} y^b z^c \right) \\
&= \sum_{q\in\mathcal{Q}(G)} \left(\sum_{a'\geq 0, b\geq 0, c\geq 0} mz(G-q; a', b, c)\, x^{a'} y^b z^c \right) \\
&= \sum_{q\in\mathcal{Q}(G)} MZZ(G-q; x, y, z),
\end{aligned}
$$

which completes the proof. ■

By applying Theorem 8 several times, we can obtain the following corollary.

Corollary 7. *If G is a generalized phenylene and $i, j, k \geq 0$ some integers, then the corresponding higher order partial derivative of the MZZ polynomial of G can be computed as*

$$\frac{\partial^{i+j+k}}{\partial x^i \partial y^j \partial z^k} MZZ(G; x, y, z) = \sum_{H\in\mathcal{R}(G;i,j,k)} MZZ(G-H; x, y, z).$$

Note also that similar formulas can be obtained for the first, second, and third ZZ polynomial. Firstly, denote by $\mathcal{R}_1(G; a, b)$ the set of all $(4, 6, 8)$-resonant sets of G with a quadrilaterals or hexagons and b 8-cycles.

Proposition 5. *If G is a generalized phenylene and $i, j \geq 0$ some integers, then the corresponding higher order partial derivative of the first ZZ polynomial of G can be computed as*

$$\frac{\partial^{i+j}}{\partial x^i \partial z^j} ZZ_1(G; x, z) = \sum_{H\in\mathcal{R}_1(G;i,j)} ZZ_1(G-H; x, z).$$

Next, denote by $\mathcal{R}_2(G; a)$ the set of all $(4, 6, 8)$-resonant sets of G with a quadrilaterals or hexagons and no 8-cycles.

Proposition 6. *If G is a generalized phenylene and $i \geq 0$ some integer, then the corresponding higher derivative of the second ZZ polynomial of*

G can be computed as

$$ZZ_2^{(i)}(G;x) = \sum_{H \in \mathcal{R}_2(G;i)} ZZ_2(G-H;x).$$

Finally, let $\mathcal{R}_3(G;a,b)$ be the set of all $(4,6,8)$-resonant sets of G with a quadrilaterals, b hexagons, and no 8-cycles.

Proposition 7. *If G is a generalized phenylene and $i,j \geq 0$ some integers, then the corresponding higher order partial derivative of the third ZZ polynomial of G can be computed as*

$$\frac{\partial^{i+j}}{\partial x^i \partial y^j} ZZ_3(G;x,y) = \sum_{H \in \mathcal{R}_3(G;i,j)} ZZ_3(G-H;x,y).$$

In the last part of the section, we consider also partial derivatives of the GZZ polynomial. Let G be a generalized benzenoid graph. A set R of 6-cycles (hexagons) and 10-cycles of G is called a *generalized resonant set* of G if there exists some generalized Clar cover C of G such that every element of R represents some connected component of C. The set of all generalized resonant sets of G which contain exactly a hexagons and b 10-cycles will be denoted as $\mathcal{GR}(G;a,b)$. The following theorem can be proved similarly as Theorem 8.

Theorem 9. *If G is a generalized benzenoid graph and $i,j \geq 0$ some integers, then the corresponding higher order partial derivative of the GZZ polynomial of G can be computed as*

$$\frac{\partial^{i+j}}{\partial x^i \partial z^j} GZZ(G;x,z) = \sum_{H \in \mathcal{GR}(G;i,j)} GZZ(G-H;x,z).$$

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