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Maximal matching polynomials of phenylene and benzenoid chains

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Abstract. A matching in a graph refers to a collection of edges where no two edges share common endpoints. A maximal matching (MM) of a graph is defined as a matching such that it is impossible to add any more edges to it within the graph to form a larger matching. The maximal matching polynomial (MMP) of a graph is the generating polynomial for the number of MMs of each size. In this article, through the employment of the transfer matrix technique, we first present formulas for calculating the MMPs of phenylene and benzenoid chains. Subsequently, computational formulas for the number of MMs of phenylene and benzenoid chains are derived. Moreover, we determine the expected values of the number of MMs for random phenylene and benzenoid chains.

1. Introduction

Let $G = (V(G), E(G))$ be a graph with vertex set $V(G)$ and edge set $E(G)$. A matching is a set of edges in a graph such that no two edges in the set share a common vertex. A maximum matching is a matching that contains the largest possible number of edges among all possible matchings in a given graph. In other words, it is a matching that meets the maximum cardinality. The number of edges in any maximum matching of a graph G is known as the matching number of G, and denoted by $\mu(G)$. When each vertex in a graph G has an edge of the matching incident to it, the matching is called perfect. Perfect matching, also known as Kekulé structure, holds significant importance in chemistry. It is evident that perfect matchings are also maximum matchings. A maximal matching (MM) is a matching that cannot be enlarged by adding any more edges from the graph while still maintaining the property of being a matching. That is, if we try to add any other edge to a maximal matching, it will result in two edges sharing a common vertex, which violates the definition of a matching. Clearly, every maximum matching is a maximal matching, but not every maximal matching is a maximum matching. The cardinality of any smallest MM in G is the saturation number of G, and denoted by $s(G)$.

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Let $\mathcal{K}$ be the set of all MMs in graph G. The maximal matching polynomial (MMP) of a graph was introduced by Došlić and Zubac [5] in 2016. For a graph G, it is defined as

$$Z(G;x) = \sum_{K\in\mathcal{K}} x^{|K|} = \sum_{k=s(G)}^{\mu(G)} z_k(G)x^k,$$

where $z_k(G)$ denotes the number of MMs of size k in graph G. The total number of MMs of a graph G is defined as $\zeta(G) = |\mathcal{K}| = \sum_{k=s(G)}^{\mu(G)} z_k(G)$.

The roots of the maximal matching polynomial $Z(G;x)$ are referred to as the maximal matching roots of graph G. Since the maximal matching polynomial inherently lacks a constant term, it immediately follows that 0 is a root for all such polynomials. Notably, the multiplicity of the root 0 corresponds exactly to the saturation number of the graph. Furthermore, the evaluation of $Z(G;1)$ yields the total number of maximal matchings in G, i.e., $Z(G;1) = \zeta(G)$. Meanwhile, $Z(G;-1)$ gives the difference between the number of MMs of even size and the number of MMs of odd size within the graph.

Phenylenes are chemical compounds comprising carbon atoms that form both 6-membered hexagons and 4-membered squares. Each square is adjacent to two non-overlapping hexagons, and hexagons are not directly adjacent to each other. Benzenoid systems, in the context related to phenylenes, refer to the catacondensed benzenoid systems obtained by eliminating the squares from phenylenes, known as the hexagonal squeeze. There is a one-to-one correspondence between phenylenes and their hexagonal squeezes, with both having the same number of hexagons. Additionally, a phenylene with h hexagons has $h-1$ squares, while the catacondensed benzenoid system, being the result of the squeeze, consists only of hexagons and has a structure that is related to but distinct from the original phenylene.

Phenylene chains, a subset of phenylenes, consist of a linear, alternating sequence of 6-membered (hexagonal) and 4-membered (square) rings. Phenylene chains can be constructed inductively. Given a phenylene chain PC_{k-1} with $k-1$ hexagons $H^{(1)}, H^{(2)}, \ldots, H^{(k-1)}$, we can form PC_k by adding a hexagon $H^{(k)}$ using two new edges. When attaching a hexagon $H^{(k)}$ to PC_{k-1}, there are three attachment methods. Let ℓ be a straight line passing through the centers of $H^{(k-2)}$ and $H^{(k-1)}$. If the center of $H^{(k)}$ lies on ℓ, then it's an α-type attachment. If its center is on the left of ℓ, then it's a β-type attachment, and if its center is on the right of ℓ, then it's a γ-type attachment. Starting from a phenylene chain PC_2 of length 2, any PC_k, $k \geq 3$, can be created through successive ϑ-type ($\vartheta \in \{\alpha, \beta, \gamma\}$) attachments. Let $PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h}$ denote a phenylene chain with h hexagons obtained from PC_2 by ϑ_3-type, ϑ_4-type, ..., ϑ_h-type attachments, successively. The number of hexagons in a phenylene chain is usually referred to as its length. For example, a phenylene chain of length 12 is shown in Figure 1.

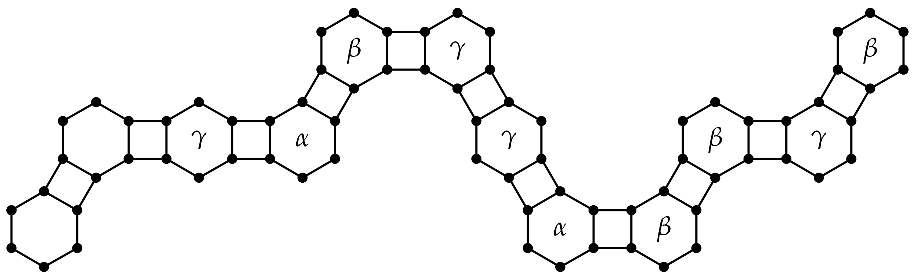

Figure 1: Phenylene chain $PC_{\gamma,\alpha,\beta,\gamma,\gamma,\alpha,\beta,\beta,\gamma,\beta}$.

Benzenoid chains are a fundamental part of catacondensed benzenoid systems. In a benzenoid chain, each hexagon is adjacent to at most two other hexagons. We can also build benzenoid chains inductively. Starting from a benzenoid chain BC_{k-1} with $k-1$ hexagons $H^{(1)}, H^{(2)}, \ldots, H^{(k-1)}$, we can obtain BC_k by adding an additional hexagon $H^{(k)}$. Similar to phenylene chains, when adding a new hexagon $H^{(k)}$ to BC_{k-1}, based on a straight line ℓ that goes through the centers of $H^{(k-2)}$ and $H^{(k-1)}$, there are three fusion types: α-type (when the center of $H^{(k)}$ lies on ℓ), β-type (when the center of $H^{(k)}$ on the left of ℓ), and γ-type (when the center of $H^{(k)}$ on the right of ℓ). We can generate a benzenoid chain $BC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h}$ containing h hexagons by performing the ϑ_3-type, ϑ_4-type, ..., ϑ_h-type attaching operations in sequence, starting from the benzenoid chain BC_2, $\vartheta_i \in \{\alpha, \beta, \gamma\}$ and $i \in \{3, 4, \ldots, h\}$. The length of a benzenoid chain refers to the number of hexagons it contains. A benzenoid chain of length 12 is illustrated in Figure 2.

A random phenylene chain $PC_h(p_1, p_2, p_3)$ composed of h hexagons is constructed via the successive addition of terminal hexagons. At each step k, $k \in \{3, 4, \ldots, h\}$, a random choice is made from three distinct construction approaches when attaching the subsequent hexagon:

(i) $PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_{k-1}} \to PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_{k-1},\alpha}$ with probability p_1;
(ii) $PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_{k-1}} \to PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_{k-1},\beta}$ with probability p_2;
(iii) $PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_{k-1}} \to PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_{k-1},\gamma}$ with probability $p_3 = 1 - p_1 - p_2$.

Meanwhile, a random benzenoid chain $BC_h(p_1, p_2, p_3)$ can be defined in a similar manner.

As fundamental aromatic hydrocarbons in mathematical chemistry, phenylene and benzenoid chains have seen substantial research progress in the study of substructure-based parameters in recent years, with their matchings and independent sets being a focus of investigation [1, 2, 4, 6, 7, 9].

In their pioneering work [5], Došlić and Zubac provided robust evidence demonstrating that MMs offer an effective framework for modeling diverse chemical and technical problems. They calculated the number of MMs in several graph classes constructed through the linear or cyclic assembly of basic components and determined the number of MMs in the join and corona products of specific graph classes. Building on this foundation, Došlić and Short [3] extended their research to consider the calculation of MMs in certain special benzenoid and polyspiro chains. More recently, Shi and Deng [8] further delved into the problem of counting MMs on benzenoid chains. Notwithstanding these advancements, significant knowledge gaps remain. The distribution of MMs of all sizes within phenylenes and benzenoid systems remains poorly understood, and a comprehensive, in-depth investigation of MMPs for these systems is still lacking. In this study, we seek to address these deficiencies by undertaking a systematic exploration of the MMPs of phenylene and benzenoid chains. We will introduce innovative computational methods for MMPs, derive the number of MMs in phenylene and benzenoid chains, and calculate the expected values of the number of MMs for random phenylene and benzenoid chains.

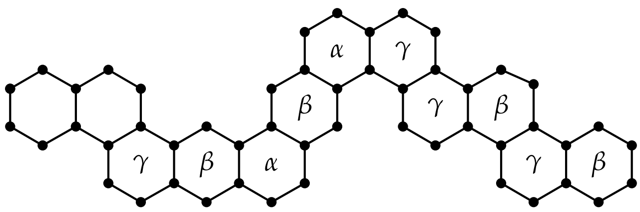

Figure 2: Benzenoid chain $BC_{\gamma,\beta,\alpha,\beta,\alpha,\gamma,\gamma,\beta,\gamma,\beta}$.

2. Prelimiminaries

Throughout this study, all the graphs we are concerned with are finite and simple. For a graph G, we use $V(G)$ to represent its vertex set and $E(G)$ for its edge set. Given a vertex $v \in V(G)$ in a graph G, the neighborhood $N_G(v)$ consists of those vertices that are connected to v by an edge. The degree $d_G(v)$ of a vertex $v \in V(G)$ is calculated as the number of vertices in its neighborhood $N_G(v)$, that is, $d_G(v) = |N_G(v)|$. The closed neighborhood $N_G[v]$ of a vertex v includes v itself and all the vertices adjacent to it. When X is a subset of the vertex set of graph G, the symbol $G - X$ refers to the graph that is obtained by removing all the vertices in X and the edges incident to them from G. In particular, if $v \in V(G)$, then $G - v$ is the graph formed by taking away the vertex v and its incident edges from G. Similarly, for $\{u, v\} \subseteq V(G)$, $G - u - v$ represents the graph after removing both vertices u and v along with their incident edges. Additionally, if

$uv \in E(G)$, then $G - uv$ is the subgraph of G which is created by removing the edge uv while leaving all other vertices unchanged. We denote a path having n vertices as P_n, and a cycle with n vertices as C_n.

The following properties can be obtained through the definition of maximal matching polynomial and some local structural analysis.

Proposition 2.1. (i) *If $uv \in E(G)$ and $d_G(u) = 1$, then*

$$Z(G;x) = xZ(G-u-v;x) + x\sum_{w\in N_G(v)\setminus\{u\}} Z(G-u-v-w;x).$$

(ii) *If $puvw$ is a path of length 3 in G, where $d_G(u) = d_G(v) = 2$, $d_G(p) \geq 2$ and $d_G(w) \geq 2$, then*

$$\begin{aligned}Z(G;x) =& xZ(G-u-v;x) + x^2 Z(G-N_G[u]-N_G[v];x)\\ &+ x^2\sum_{s\in N_G(w)\setminus\{p,v\}} Z(G-N_G[u]-w-s;x) + x^2\sum_{t\in N_G(p)\setminus\{w,u\}} Z(G-N_G[v]-p-t;x).\end{aligned}$$

(iii) *If uvw is a path of length 2 in G, where $d_G(v) = 2$, $d_G(u) \geq 2$, $d_G(w) \geq 2$ and $vw \notin E(G)$, then*

$$Z(G;x) = xZ(G-u-v;x) + xZ(G-v-w;x) + x^2\sum_{\substack{s\in N_G(u)\setminus\{v\},\\ t\in N_G(w)\setminus\{v\}}} Z(G-u-w-s-t;x).$$

(iv) *If G is a graph with t components $R_1, R_2, \ldots, R_t$, then $Z(G;x) = \prod_{i=1}^{t} Z(R_i;x)$.*

Proof. (i) Every maximal matching (MM) of G either contains the edge uv or does not. Those containing it are counted by the first term on the *r.h.s.* of the equation. If the edge uv is not contained in a MM, then vertex v must be covered. Leaving it uncovered would contradict the maximality of the considered matching, since it could be extended by adding the edge uv. Hence, v must be covered by some other edge vw, where $w \in N_G(v) \setminus \{u\}$. Such matchings are counted by the second term in the *r.h.s.* of the equation.

(ii) When the edge uv is included in a MM of G, the remaining edges of this MM create a valid MM in the subgraph $G - u - v$. If pu and vw are both part of a MM of G, then the rest edges of the MM form a MM in the subgraph $G - N_G(u) - N_G(v)$. Given that pu is in a MM of G, while uv and vw are not in the MM of G, there must be a vertex $s \in N_G(w) \setminus \{p, v\}$ such that ws is included in the MM of G. As a result, the remaining edges form a MM in the subgraph $G - N_G[u] - w - s$. Likewise, when vw is in a MM of G, and uv and pu are absent from the MM of G, there exists a vertex $t \in N_G(p) \setminus \{w, u\}$ with the edge pt included in the MM of G, and the remaining edges form a MM in the subgraph $G - N_G[v] - p - t$. For the first scenario, the size of the remaining edges in the MM is one less than the original MM. However, for the last three scenarios, the size of the remaining edges in the MM is two less than the initial one. This explains why the factors x and x^2 are used in these different cases.

(iii) When uv (or vw) is in a MM of G, the remaining edges form a MM in $G - u - v$ ($G - v - w$). If uv and vw are not in a MM of G, there are vertices $s \in N_G(u) \setminus \{v\}$ and $t \in N_G(w) \setminus \{v\}$ with us and wt in the MM of G, and the remaining edges form a MM in $G - u - w - s - t$. The size of the remaining edges in the MM is one less than the original in the first two cases and two less in the last, explaining the use of factors x and x^2.

(iv) It can be directly obtained according to the definition of the maximal matching polynomial. □

Proposition 2.2. (i) *If $uv \in E(G)$ and $d_G(u) = 1$, then*

$$\zeta(G) = \zeta(G-u-v) + \sum_{w\in N_G(v)\setminus\{u\}} \zeta(G-u-v-w).$$

(ii) *If $puvw$ is a path of length 3 in G, where $d_G(u) = d_G(v) = 2$, $d_G(p) \geq 2$ and $d_G(w) \geq 2$, then*

$$\begin{aligned}\zeta(G) =& \zeta(G-u-v) + \zeta(G-N_G[u]-N_G[v]) + \sum_{s\in N_G(w)\setminus\{p,v\}} \zeta(G-N_G[u]-w-s)\\ &+ \sum_{t\in N_G(p)\setminus\{w,u\}} \zeta(G-N_G[v]-p-t).\end{aligned}$$

(iii) *If uvw is a path of length* 2 *in G, where* $d_G(v) = 2$, $d_G(u) \geq 2$, $d_G(w) \geq 2$ *and* $vw \notin E(G)$, *then*

$$\zeta(G) = \zeta(G-u-v) + \zeta(G-v-w) + \sum_{\substack{s \in N_G(u)\setminus\{v\},\\ t\in N_G(w)\setminus\{v\}}} \zeta(G-u-w-s-t).$$

(iv) *If G is a graph with t components* $R_1, R_2, \ldots, R_t$, *then* $\zeta(G) = \prod_{i=1}^{t} \zeta(R_i)$.

Proof. Given that $\zeta(G) = Z(G;1)$, the conclusion is an immediate consequence of Proposition 2.1. □

According to the definition of the MMP, Propositions 2.1 and 2.2, we can get the following two results.

Proposition 2.3. $Z(C_n;x) = xZ(P_{n-2};x) + x^2Z(P_{n-4};x) + 2x^2Z(P_{n-5};x) = 2xZ(P_{n-2};x) + x^2Z(P_{n-5};x) = xZ(C_{n-2};x) + xZ(C_{n-3};x)$ *for* $n > 6$, *and* $Z(P_n;x) = xZ(P_{n-2};x) + xZ(P_{n-3};x)$, *with initial conditions* $Z(P_1;x) = 1$, $Z(P_2;x) = x$, $Z(P_3;x) = 2x$, $Z(C_3;x) = 3x$, $Z(C_4;x) = 2x^2$, $Z(C_5;x) = 5x^2$ *and* $Z(C_6;x) = 2x^3 + 3x^2$.

Proposition 2.4. $\zeta(C_n) = \zeta(P_{n-2}) + \zeta(P_{n-4}) + 2\zeta(P_{n-5}) = 2\zeta(P_{n-2}) + \zeta(P_{n-5}) = \zeta(C_{n-2}) + \zeta(C_{n-3})$ *for* $n > 6$, *and* $\zeta(P_n) = \zeta(P_{n-2}) + \zeta(P_{n-3})$, *with initial conditions* $\zeta(P_1) = 1$, $\zeta(P_2) = 1$, $\zeta(P_3) = 2$, $\zeta(C_3) = 3$, $\zeta(C_4) = 2$, $\zeta(C_5) = 5$ *and* $\zeta(C_6) = 5$.

3. The maximal matching polynomial of phenylene chains

In this section, we study the enumeration of maximal matching polynomials (MMPs) for phenylene chains. To this end, we first introduce a polynomial vector of a graph with a given edge.

Definition 3.1. *Let G be a graph such that* $\{pu, uv, vw\} \subseteq E(G)$ *and* $d_G(u) = d_G(v) = 2$. *The vector* $Z_{uv}(G;x)$ *that is associated with the MMPs in G corresponding to the edge uv is given by* $Z_{uv}(G;x) = (Z(G;x), Z(G-u;x), Z(G-v;x), Z(G-u-v;x), Z(G-p-u;x), Z(G-v-w;x), Z(G-N_G[u];x), Z(G-N_G[v];x))^{\mathrm{T}}$.

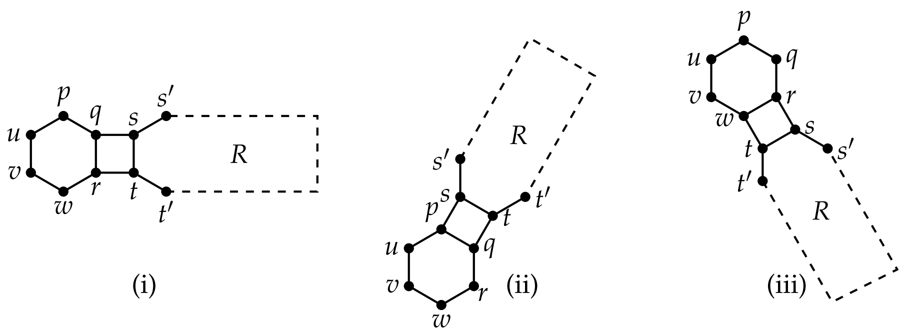

Figure 3: The graphs employed in Lemmas 3.1–3.3.

Lemma 3.1. *Let G be a graph constructed from a hexagon uvwrqpu and a graph R by adding two new edges qs and rt, where* $\{st, ss', tt'\} \subseteq E(R)$ *and* $d_R(s) = d_R(t) = 2$, *as shown in* Figure 3(i). *Then we have* $Z_{uv}(G;x) = \mathbf{A}(x)Z_{st}(R;x)$, *where*

$$\mathbf{A}(x) = \begin{pmatrix} 2x^3+x^2 & 2x^3 & 2x^3 & x^4+3x^3 & x^3 & x^3 & x^4 & x^4 \\ 2x^2 & x^2 & x^3 & 2x^3 & 0 & x^3 & 0 & x^3 \\ 2x^2 & x^3 & x^2 & 2x^3 & x^3 & 0 & x^3 & 0 \\ x^2+x & x^2 & x^2 & x^2 & 0 & 0 & 0 & 0 \\ x^2 & x^2 & 0 & x^3+x^2 & x^2 & 0 & x^3 & x^3 \\ x^2 & 0 & x^2 & x^3+x^2 & 0 & x^2 & x^3 & x^3 \\ x & x^2 & 0 & 2x^2 & x^2 & 0 & x^2 & 0 \\ x & 0 & x^2 & 2x^2 & 0 & x^2 & 0 & x^2 \end{pmatrix}.$$

Proof. For the sake of convenience, let $G_1 = G - u - v$, $G_1' = G_1 - p - q$, $G_1'' = G_1 - p - q - s$, $G_2 = G - N_G[u] - N_G[v]$, $G_3 = G - N_G[u] - N_G[w]$ and $G_4 = G - N_G[v] - N_G[p]$. Applying Proposition 2.1, one can first show that

$$\begin{aligned}Z(G-u-v;x) =& Z(G_1;x) = xZ(G_1';x) + xZ(G_1'';x) + xZ(G_1 - p - q - r;x)\\ =& x^2Z(G_1' - w - r;x) + x^2Z(G_1' - w - r - t;x)\\ &+ x^2Z(G_1'' - w - r;x) + x^2Z(G_1'' - w - r - t;x) + xZ(R;x)\\ =& x^2Z(R;x) + x^2Z(R-t;x) + x^2Z(R-s;x) + x^2Z(R-s-t;x) + xZ(R;x)\\ =& (x^2+x)Z(R;x) + x^2Z(R-s;x) + x^2Z(R-t;x) + x^2Z(R-s-t;x)\\ =& (x^2+x, x^2, x^2, x^2, 0, 0, 0, 0)Z_{st}(R;x),\end{aligned}$$

$$\begin{aligned}Z(G - N_G[u] - N_G[v];x) =& Z(G_2;x) = xZ(G_2 - q - r;x) + x^2Z(G_2 - N_G[q] - N_G[r];x)\\ &+ x^2Z(G_2 - N_G[q] - N_G[t];x) + x^2Z(G_2 - N_G[r] - N_G[s];x)\\ =& xZ(R;x) + x^2Z(R-s-t;x) + x^2Z(R - N_R[s];x) + x^2Z(R - N_R[t];x),\end{aligned}$$

$$\begin{aligned}Z(G_3;x) =& xZ(G_3 - q - s;x) + xZ(G_3 - q - s - t;x) + xZ(G_3 - q - s - s';x)\\ =& xZ(R-s;x) + xZ(R-s-t;x) + xZ(R-s-s';x),\end{aligned}$$

$$\begin{aligned}Z(G_4;x) =& xZ(G_4 - r - t;x) + xZ(G_4 - r - t - s;x) + xZ(G_4 - r - t - t';x)\\ =& xZ(R-t;x) + xZ(R-s-t;x) + xZ(R-t-t';x).\end{aligned}$$

Then, by continuing to use Proposition 2.1, we have

$$\begin{aligned}Z(G;x) =& xZ(G_1;x) + x^2Z(G_2;x) + x^2Z(G_3;x) + x^2Z(G_4;x)\\ =& (x^3+x^2)Z(R;x) + x^3Z(R-s;x) + x^3Z(R-t;x) + x^3Z(R-s-t;x)\\ &+ x^3Z(R;x) + x^4Z(R-s-t;x) + x^4Z(R-N_R[s];x) + x^4Z(R-N_R[t];x)\\ &+ x^3Z(R-s;x) + x^3Z(R-s-t;x) + x^3Z(R-s-s';x)\\ &+ x^3Z(R-t;x) + x^3Z(R-s-t;x) + x^3Z(R-t-t';x)\\ =& (2x^3+x^2)Z(R;x) + 2x^3Z(R-s;x) + 2x^3Z(R-t;x) + (x^4+3x^3)Z(R-s-t;x)\\ &+ x^3Z(R-s-s';x) + x^3Z(R-t-t';x) + x^4Z(R-N_R[s];x) + x^4Z(R-N_R[t];x)\\ =& (2x^3+x^2, 2x^3, 2x^3, x^4+3x^3, x^3, x^3, x^4, x^4)Z_{st}(R;x).\end{aligned}$$

Additionally, leveraging Proposition 2.1 enables us to derive the following equations.

$$\begin{aligned}Z(G-u-v-w;x) =& xZ(G-u-v-w-p-q;x) + xZ(G-u-v-w-p-q-s;x)\\ &+ xZ(G-u-v-w-p-q-r;x)\\ =& x^2Z(R-t;x) + x^2Z(R-s-t;x) + x^2Z(R-t-t';x) + x^2Z(R-s-t;x)\\ &+ x^2Z(R-N_R[t];x) + xZ(R;x),\end{aligned}$$

$$\begin{aligned}Z(G-u-v-w-r;x) =& xZ(G-u-v-w-r-p-q;x) + xZ(G-u-v-w-r-p-q-s;x)\\ =& xZ(R;x) + xZ(R-s;x),\end{aligned}$$

$$
\begin{aligned}
Z(G-u;x) =& xZ(G-u-v-w;x)+xZ(G-u-v-w-r;x)\\
=& x^3Z(R-t;x)+x^3Z(R-s-t;x)+x^3Z(R-t-t';x)+x^3Z(R-s-t;x)\\
&+x^3Z(R-N_R[t];x)+x^2Z(R;x)+x^2Z(R;x)+x^2Z(R-s;x)\\
=& 2x^2Z(R;x)+x^2Z(R-s;x)+x^3Z(R-t;x)+2x^2Z(R-s-t;x)\\
&+x^3Z(R-t-t';x)+x^3Z(R-N_R[t];x)\\
=& (2x^2,x^2,x^3,2x^3,0,x^3,0,x^3)Z_{st}(R;x),
\end{aligned}
$$

$$
\begin{aligned}
Z(G-v;x) =& xZ(G-v-u-p;x)+xZ(G-v-u-p-q;x)\\
=& 2x^2Z(R;x)+x^3Z(R-s;x)+x^2Z(R-t;x)+2x^2Z(R-s-t;x)\\
&+x^3Z(R-s-s';x)+x^3Z(R-N_R[s];x)\\
=& (2x^2,x^3,x^2,2x^3,x^3,0,x^3,0)Z_{st}(R;x),
\end{aligned}
$$

$$
\begin{aligned}
Z(G-u-p;x) =& xZ(G-u-p-v-w;x)+xZ(G-u-p-v-w-r;x)\\
=& x^2Z(R;x)+x^2Z(R-s;x)+(x^3+x^2)Z(R-s-t;x)+x^2Z(R-s-s';x)\\
&+x^3Z(R-N_R[s];x)+x^3Z(R-N_R[t];x)\\
=& (x^2,x^2,0,x^3+x^2,x^2,0,x^3,x^3)Z_{st}(R;x),
\end{aligned}
$$

$$
\begin{aligned}
Z(G-v-w;x) =& xZ(G-v-w-u-p;x)+xZ(G-v-w-u-p-q;x)\\
=& x^2Z(R;x)+x^2Z(R-t;x)+(x^3+x^2)Z(R-s-t;x)+x^2Z(R-t-t';x)\\
&+x^3Z(R-N_R[s];x)+x^3Z(R-N_R[t];x)\\
=& (x^2,0,x^2,x^3+x^2,0,x^2,x^3,x^3)Z_{st}(R;x),
\end{aligned}
$$

$$
\begin{aligned}
Z(G-N_G[u];x) =& x^2Z(R-s;x)+x^2Z(R-s-t;x)+x^2Z(R-s-s';x)+xZ(R;x)\\
&+x^2Z(R-s-t;x)+x^2Z(R-N_R[s];x)\\
=& (x,x^2,0,2x^2,x^2,0,x^2,0)Z_{st}(R;x),
\end{aligned}
$$

$$
\begin{aligned}
Z(G-N_G[v];x) =& x^2Z(R-t;x)+x^2Z(R-s-t;x)+x^2Z(R-t-t';x)+xZ(R;x)\\
&+x^2Z(R-s-t;x)+x^2Z(R-N_R[t];x)\\
=& (x,0,x^2,2x^2,0,x^2,0,x^2)Z_{st}(R;x).
\end{aligned}
$$

Thus, the desired result $Z_{uv}(G;x)=\mathbf{A}(x)Z_{st}(R;x)$ follows. □

Lemma 3.2. *Let G be a graph constructed from a hexagon uvwrqpu and a graph R by adding two new edges ps and qt, where $\{st, ss', tt'\}\subseteq E(R)$ and $d_R(s)=d_R(t)=2$, as shown in* Figure 3(ii). *Then we have $Z_{uv}(G;x)=\mathbf{B}(x)Z_{st}(R;x)$, where*

$$
\mathbf{B}(x)=\begin{pmatrix}
2x^3+x^2 & 2x^3 & 2x^3 & x^4+3x^3 & x^3 & x^3 & x^4 & x^4\\
2x^2 & x^3 & 0 & 3x^3 & x^3 & 0 & 2x^3 & x^3\\
2x^2 & x^2 & x^3 & 2x^3 & 0 & x^3 & 0 & x^3\\
x^2 & x^2 & 0 & x^3+x^2 & x^2 & 0 & x^3 & x^3\\
x^2 & 0 & 2x^2 & x^2 & 0 & x^2 & 0 & 0\\
x^2+x & x^2 & x^2 & x^2 & 0 & 0 & 0 & 0\\
x & 0 & x^2 & x^2 & 0 & x^2 & 0 & 0\\
x & x^2 & 0 & 2x^2 & x^2 & 0 & x^2 & 0
\end{pmatrix}.
$$

Proof. Similar to the way of proving Lemma 3.1, applying Proposition 2.1, it can be deduced that

$$\begin{aligned}Z(G;x) =& xZ(G-v-w;x)+x^2Z(G-N_G[v]-N_G[w];x)\\&+x^2Z(G-N_G[v]-N_G[r];x)+x^2Z(G-N_G[u]-N_G[w];x)\\=&(2x^3+x^2)Z(R;x)+2x^3Z(R-s;x)+2x^3Z(R-t;x)+(x^4+3x^3)Z(R-s-t;x)\\&+x^3Z(R-s-s';x)+x^3Z(R-t-t';x)+x^4Z(R-N_R[s];x)+x^4Z(R-N_R[t];x)\\=&(2x^3+x^2,2x^3,2x^3,x^4+3x^3,x^3,x^3,x^4,x^4)Z_{st}(R;x),\end{aligned}$$

$$\begin{aligned}Z(G-u;x) =& xZ(G-u-v-w;x)+xZ(G-u-v-w-r;x)\\=&xZ(G-N_G[v];x)+xZ(G-N_G[v]-N_G[w];x)\\=&x^2Z(R;x)+x^3Z(R-s;x)+2x^3Z(R-s-t;x)+x^3Z(R-s-s';x)+x^3Z(R-N_R[s];x)\\&+x^2Z(R;x)+x^3Z(R-s-t;x)+x^3Z(R-N_R[s];x)+x^3Z(R-N_R[t];x)\\=&2x^2Z(R;x)+x^3Z(R-s;x)+3x^3Z(R-s-t;x)+x^3Z(R-s-s';x)\\&+2x^3Z(R-N_R[s];x)+x^3Z(R-N_R[t];x)\\=&(2x^2,x^3,0,3x^3,x^3,0,2x^3,x^3)Z_{st}(R;x),\end{aligned}$$

$$\begin{aligned}Z(G-v;x) =& xZ(G-v-w-r;x)+xZ(G-v-w-r-q;x)\\=&2x^2Z(R;x)+x^2Z(R-s;x)+x^3Z(R-t;x)+2x^2Z(R-s-t;x)\\&+x^3Z(R-t-t';x)+x^3Z(R-N_R[t];x)\\=&(2x^2,x^2,x^3,2x^3,0,x^3,0,x^3)Z_{st}(R;x),\end{aligned}$$

$$\begin{aligned}Z(G-u-v;x) =& xZ(G-u-v-w-r;x)+xZ(G-u-v-w-r-q;x)\\=&x^2Z(R;x)+x^2Z(R-s;x)+(x^3+x^2)Z(R-s-t;x)\\&+x^2Z(R-s-s';x)+x^3Z(R-N_R[s];x)+x^3Z(R-N_R[t];x)\\=&(x^2,x^2,0,x^3+x^2,x^2,0,x^3,x^3)Z_{st}(R;x),\end{aligned}$$

$$\begin{aligned}Z(G-u-p;x) =& xZ(G-u-p-v-w;x)+xZ(G-u-p-v-w-r;x)\\=&x^2Z(R;x)+2x^2Z(R-t;x)+x^2Z(R-s-t;x)+x^2Z(R-t-t';x)\\=&(x^2,0,2x^2,x^2,0,x^2,0,0)Z_{st}(R;x),\end{aligned}$$

$$\begin{aligned}Z(G-v-w;x) =& xZ(G-v-w-u-p;x)+xZ(G-v-w-u-p-s;x)\\&+xZ(G-v-w-u-p-q;x)\\=&(x^2+x)Z(R;x)+x^2Z(R-s;x)+x^2Z(R-t;x)+x^2Z(R-s-t;x)\\=&(x^2+x,x^2,x^2,x^2,0,0,0,0)Z_{st}(R;x),\end{aligned}$$

$$\begin{aligned}Z(G-N_G[u];x) =& xZ(G-N_G[u]-w-r;x)+xZ(G-N_G[u]-w-r-q;x)\\=&x^2Z(G-N_G[u]-w-r-q-t;x)+x^2Z(G-N_G[u]-w-r-q-t-s;x)\\&+x^2Z(G-N_G[u]-w-r-q-t-t';x)+xZ(R;x)\\=&x^2Z(R-t;x)+x^2Z(R-s-t;x)+x^2Z(R-t-t';x)+xZ(R;x)\\=&(x,0,x^2,x^2,0,x^2,0,0)Z_{st}(R;x),\end{aligned}$$

$$
\begin{aligned}
Z(G-N_G[v];x) =& xZ(G-N_G[v]-r-q;x)+xZ(G-N_G[v]-r-q-t;x)\\
&+xZ(G-N_G[v]-r-q-p;x)\\
=& x^2Z(G-N_G[v]-r-q-p-s;x)+x^2Z(G-N_G[v]-r-q-p-s-t;x)\\
&+x^2Z(G-N_G[v]-r-q-p-s-s';x)+x^2Z(G-N_G[v]-r-q-t-p-s;x)\\
&+x^2Z(G-N_G[v]-r-q-t-p-s-s';x)+xZ(R;x)\\
=& xZ(R;x)+x^2Z(R-s;x)+2x^2Z(R-s-t;x)\\
&+x^2Z(R-s-s';x)+x^2Z(R-N_R[s];x)\\
=& (x,x^2,0,2x^2,x^2,0,x^2,0)Z_{st}(R;x).
\end{aligned}
$$

Therefore, the proof is complete. □

Lemma 3.3. *Let G be a graph constructed from a hexagon $uvwrqpu$ and a graph R by adding two new edges rs and wt, where $\{st,ss',tt'\}\subseteq E(R)$ and $d_R(s)=d_R(t)=2$, as shown in* Figure 3(iii)*. Then we have $Z_{uv}(G;x)=\mathbf{C}(x)Z_{st}(R;x)$, where*

$$
\mathbf{C}(x)=\begin{pmatrix}
2x^3+x^2 & 2x^3 & 2x^3 & x^4+3x^3 & x^3 & x^3 & x^4 & x^4\\
2x^2 & x^3 & x^2 & 2x^3 & x^3 & 0 & x^3 & 0\\
2x^2 & 0 & x^3 & 3x^3 & 0 & x^3 & x^3 & 2x^3\\
x^2 & 0 & x^2 & x^3+x^2 & 0 & x^2 & x^3 & x^3\\
x^2+x & x^2 & x^2 & x^2 & 0 & 0 & 0 & 0\\
x^2 & 2x^2 & 0 & x^2 & x^2 & 0 & 0 & 0\\
x & 0 & x^2 & 2x^2 & 0 & x^2 & 0 & x^2\\
x & x^2 & 0 & x^2 & x^2 & 0 & 0 & 0
\end{pmatrix}.
$$

Proof. Using an analysis approach comparable to that employed in the proof procedures of Lemma 3.2, the result can be derived, so we omit the detailed proof here. □

Theorem 3.1. *Let $PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h}$ be a phenylene chain of length h, $h\geq 3$. The MMP of $PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h}$ is given by*

$$Z(PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h};x)=\mathbf{t}^{\mathrm{T}}\mathbf{\Gamma}_2(x)\mathbf{\Gamma}_3(x)\cdots\mathbf{\Gamma}_{h-1}(x)\mathbf{u},$$

where $\mathbf{t}=(2x^3+x^2,2x^3,2x^3,x^4+3x^3,x^3,x^3,x^4,x^4)^{\mathrm{T}}$, $\mathbf{u}=(2x^3+3x^2,3x^2,3x^2,x^2+x,x^2+x,x^2+x,2x,2x)^{\mathrm{T}}$,

$$
\mathbf{\Gamma}_i(x)=\begin{cases}
\mathbf{A}(x) & \text{if } \vartheta_{i+1}=\alpha,\\
\mathbf{B}(x) & \text{if } \vartheta_{i+1}=\beta,\\
\mathbf{C}(x) & \text{if } \vartheta_{i+1}=\gamma,
\end{cases}
$$

$i\in\{2,3,\ldots,h-1\}$, $\mathbf{A}(x)$, $\mathbf{B}(x)$ and $\mathbf{C}(x)$ are illustrated in Lemmas 3.1-3.3, respectively.

Proof. Let $PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h}$ be a phenylene chain with h hexagons, denoted as $H^{(1)}$, $H^{(2)}$, $\cdots$, $H^{(h-1)}$, $H^{(h)}$, and $h-1$ squares, denoted as $S^{(1)}$, $S^{(2)}$, $\cdots$, $S^{(h-1)}$. The hexagons and squares in this chain are arranged alternately in the sequence $H^{(1)}S^{(1)}H^{(2)}S^{(2)}\cdots H^{(h-1)}S^{(h-1)}H^{(h)}$. For $i=1,2,\ldots,h-1$, we denote the common edge between $S^{(i)}$ and $H^{(i+1)}$ by s_it_i. Additionally, we denote the unique edge in $E(H^{(1)})\backslash E(S^{(1)})$ that is parallel to s_1t_1 as s_0t_0. Define $R_i=H^{(i)}\cup S^{(i)}\cup H^{(i+1)}\cup S^{(i+1)}\cup\cdots S^{(h-1)}\cup H^{(h)}$ as the vertex-induced sub-chain of $PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h}$. According to Lemma 3.1, we obtain the relationship $Z_{s_0t_0}(PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h};x)=\mathbf{A}(x)Z_{s_1t_1}(R_2;x)$. By applying Lemmas 3.1, 3.2 and 3.3, we further derive that $Z_{s_1t_1}(R_2;x)=\mathbf{\Gamma}_2(x)Z_{s_2t_2}(R_3;x)$, where $\mathbf{\Gamma}_2(x)=\mathbf{A}(x)$ when $\vartheta_3=\alpha$; $\mathbf{\Gamma}_2(x)=\mathbf{B}(x)$ when $\vartheta_3=\beta$; $\mathbf{\Gamma}_2(x)=\mathbf{C}(x)$ when $\vartheta_3=\gamma$. By repeatedly applying the above-derived relationships and observing that for the edge $s_{h-1}t_{h-1}$ which is the common edge between $S^{(h-1)}$ and $H^{(h)}$, we can eventually obtain that

$$Z_{s_0t_0}(PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h};x)=\mathbf{A}(x)\mathbf{\Gamma}_2(x)\mathbf{\Gamma}_3(x)\cdots\mathbf{\Gamma}_{h-1}(x)Z_{s_{h-1}t_{h-1}}(H^{(h)};x).$$

It is not difficult to get that $Z_{s_{h-1}t_{h-1}}(H^{(h)};x) = (2x^3+3x^2, x^3+3x^2, x^3+3x^2, 3x^2, x^2+x, x, x^2+x)^{\mathrm{T}}$. Consequently, we can express $Z(PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h};x)$ in the form $\mathbf{p}^{\mathrm{T}}\mathbf{\Gamma}_2(x)\cdots\mathbf{\Gamma}_{h-1}(x)\mathbf{q}$, where $\mathbf{p} = (0, x^2, x^2, x^2, x^2, x^2)^{\mathrm{T}}$, $\mathbf{q} = (2x^3+3x^2, x^3+3x^2, x^3+3x^2, 3x^2, x^2+x, x, x^2+x)^{\mathrm{T}}$ and $\mathbf{\Gamma}_i(x) = \mathbf{A}(x)$ if $\vartheta_{i+1} = \alpha$, $\mathbf{\Gamma}_i(x) = \mathbf{B}(x)$ if $\vartheta_{i+1} = \beta$, $\mathbf{\Gamma}_i(x) = \mathbf{C}(x)$ if $\vartheta_{i+1} = \gamma$. This completes the proof. $\square$

In the following example, we present a straightforward illustration of using Theorem 3.1 to compute the MMP of a phenylene chain.

Example 3.1. *For the phenylene chain $G = PC_{\gamma,\alpha,\beta,\gamma,\gamma,\alpha,\beta,\beta,\gamma,\beta}$ depicted in Figure 1, applying Theorem 3.1 we have* $Z(G;x) = \mathbf{p}^{\mathrm{T}}\mathbf{C}(x)\mathbf{A}(x)\mathbf{B}(x)\mathbf{C}(x)\mathbf{C}(x)\mathbf{A}(x)\mathbf{B}(x)\mathbf{B}(x)\mathbf{C}(x)\mathbf{B}(x)\mathbf{q} = 60178x^{36} + 4049284x^{35} + 97476333x^{34} + 1078339460x^{33} + 5963904444x^{32} + 17096955574x^{31} + 25698414099x^{30} + 20173385234x^{29} + 8159205034x^{28} + 1664405310x^{27} + 165424772x^{26} + 7375210x^{25} + 115684x^{24}$. *Therefore, the distribution of all the MMs on the phenylene chain $PC_{\gamma,\alpha,\beta,\gamma,\gamma,\alpha,\beta,\beta,\gamma,\beta}$ has been completely characterized.*

The following conclusion gives a computational formula for the number of MMs in a phenylene chain.

Theorem 3.2. *Let $PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h}$ be a phenylene chain of length h, $h \geq 3$. The number of MMs of $PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h}$ is*

$$\zeta(PC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h}) = \mathbf{v}^{\mathrm{T}}\mathbf{\Gamma}_2\mathbf{\Gamma}_3\cdots\mathbf{\Gamma}_{h-1}\mathbf{w},$$

where $\mathbf{v} = (3,2,2,4,1,1,1,1)^{\mathrm{T}}$, $\mathbf{w} = (5,3,3,2,2,2,2,2)^{\mathrm{T}}$, $\mathbf{\Gamma}_i = \begin{cases} \mathbf{A} & \text{if } \vartheta_{i+1} = \alpha, \\ \mathbf{B} & \text{if } \vartheta_{i+1} = \beta, \; i \in \{2,3,\ldots,h-1\}, \\ \mathbf{C} & \text{if } \vartheta_{i+1} = \gamma, \end{cases}$ *and*

$$\mathbf{A} = \begin{pmatrix} 3&2&2&4&1&1&1&1\\ 2&1&1&2&0&1&0&1\\ 2&1&1&2&1&0&1&0\\ 2&1&1&1&0&0&0&0\\ 1&1&0&2&1&0&1&1\\ 1&0&1&2&0&1&1&1\\ 1&1&0&2&1&0&1&0\\ 1&0&1&2&0&1&0&1 \end{pmatrix}, \mathbf{B} = \begin{pmatrix} 3&2&2&4&1&1&1&1\\ 2&1&0&3&1&0&2&1\\ 2&1&1&2&0&1&0&1\\ 1&1&0&2&1&0&1&1\\ 1&0&2&1&0&1&0&0\\ 2&1&1&1&0&0&0&0\\ 1&0&1&1&0&1&0&0\\ 1&1&0&2&1&0&1&0 \end{pmatrix}, \mathbf{C} = \begin{pmatrix} 3&2&2&4&1&1&1&1\\ 2&1&1&2&1&0&1&0\\ 2&0&1&3&0&1&1&2\\ 1&0&1&2&0&1&1&1\\ 2&1&1&1&0&0&0&0\\ 1&2&0&1&1&0&0&0\\ 1&0&1&2&0&1&0&1\\ 1&1&0&1&1&0&0&0 \end{pmatrix}.$$

Proof. Given that for a graph G, $\zeta(G) = Z(G;1)$, the result can be straightforwardly derived from Theorem 3.1 when substituting $x = 1$. $\square$

From Theorem 3.2, we can get the expected value of the number of MMs for a random phenylene chain.

Theorem 3.3. *The expected value of the number of MMs of a random phenylene chain $PC_h(p_1,p_2,p_3)$ is*

$$\mathbb{E}(\zeta(PC_h(p_1,p_2,p_3))) = \mathbf{v}^{\mathrm{T}}\mathbf{P}^{h-2}\mathbf{w},$$

where $\mathbf{v} = (3,2,2,4,1,1,1,1)^{\mathrm{T}}$, $\mathbf{w} = (5,3,3,2,2,2,2,2)^{\mathrm{T}}$, $\mathbf{P} = p_1\mathbf{A} + p_2\mathbf{B} + p_3\mathbf{C}$, and the matrices $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{C}$ are depicted in Theorem 3.2.

Proof. By making use of the law of total expectation along with Theorem 3.2, one can get the desired result. $\square$

4. The maximal matching polynomial of benzenoid chains

In this section, we consider the computation of MMPs for benzenoid chains.

Definition 4.1. *Let G be a graph such that $\{pu, uv, vw\} \subseteq E(G)$ and $d_G(u) = d_G(v) = 2$. The vector $\widetilde{Z}_{uv}(G;x)$ corresponding to the edge uv is given by* $\widetilde{Z}_{uv}(G;x) = (Z(G;x), Z(G-u;x), Z(G-v;x), Z(G-u-v;x), Z(G-p-u;x), Z(G-v-w;x), Z(G-N_G[u];x), Z(G-N_G[v];x), Z(G-N_G[u]-N_G[v];x))^{\mathrm{T}}$.

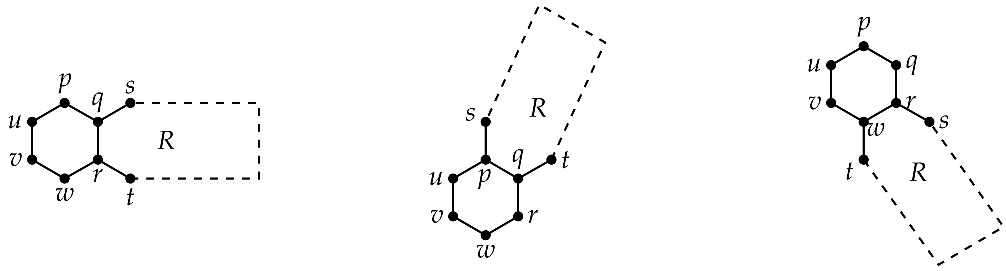

Figure 4: The graphs employed in Lemmas 4.1–4.3.

Lemma 4.1. *Let G be a graph created through the edge-merging of a hexagon uvwrqpu and a graph R at the edge qr, where* $\{sq, qr, rt\} \subseteq E(R)$ *and* $d_R(q) = d_R(r) = 2$*, as shown in* Figure 4(i)*. Then* $\widetilde{Z}_{uv}(G;x) = \mathbf{X}(x)\widetilde{Z}_{qr}(R;x)$*, where*

$$\mathbf{X}(x) = \begin{pmatrix} x^2 & x^2 & x^2 & x^3+x^2 & 0 & 0 & x^3 & x^3 & x^3 \\ 0 & x^2 & 0 & 2x^2 & x^2 & 0 & x^2 & 0 & 0 \\ 0 & 0 & x^2 & 2x^2 & 0 & x^2 & 0 & x^2 & 0 \\ 0 & 0 & 0 & x^2+x & 0 & 0 & x^2 & x^2 & x^2 \\ x & 0 & x & 0 & 0 & 0 & 0 & 0 & 0 \\ x & x & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & x & x & 0 & x & 0 & 0 & 0 \\ 0 & x & 0 & x & x & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Proof. Based on the definition of the column vector $\widetilde{Z}_{uv}(G;x)$ for a specified edge $uv \in E(G)$, it suffices for us to take into account the values of the nine components associated with this vector separately. Note that $Z(P_1;x) = 1$ and $Z(P_2;x) = x$. Using Proposition 2.1, we have

$$\begin{aligned} Z(G-u-v;x) =& xZ(G-u-v-p-q;x) + xZ(G-u-v-p-q-s;x) \\ &+ xZ(G-u-v-p-q-r;x) \\ =& x^2Z(G-u-v-p-q-w-r;x) + x^2Z(G-u-v-p-q-w-r-t;x) \\ &+ x^2Z(G-u-v-p-q-s-w-r;x) \\ &+ x^2Z(G-u-v-p-q-s-w-r-t;x) + xZ(G-u-v-p-q-r;x) \\ =& x^2Z(R-q-r;x) + x^2Z(R-N_R[q];x) + x^2Z(R-N_R[r];x) \\ &+ x^2Z(R-N_R[q]-N_R[r];x) + xZ(R-q-r;x) \\ =& (0,0,0,x^2+x,0,0,x^2,x^2,x^2)\widetilde{Z}_{qr}(R;x). \end{aligned}$$

Then, applying Proposition 2.1, we can get

$$\begin{aligned} Z(G;x) =& xZ(G-u-v;x) + x^2Z(G-N_G[u]-N_G[v];x) \\ &+ x^2Z(G-N_G[u]-N_G[w];x) + x^2Z(G-N_G[v]-N_G[p];x) \\ =& xZ(G-u-v;x) + x^2Z(R;x) + x^2Z(R-r;x) + x^2Z(R-q;x) \\ =& x^3Z(R-q-r;x) + x^3Z(R-N_R[q];x) + x^3Z(R-N_R[r];x) + x^3Z(R-N_R[q]-N_R[r];x) \\ &+ x^2Z(R-q-r;x) + x^2Z(R;x) + x^2Z(R-r;x) + x^2Z(R-q;x) \\ =& (x^2,x^2,x^2,x^3+x^2,0,0,x^3,x^3,x^3)\widetilde{Z}_{qr}(R;x). \end{aligned}$$

Subsequently, through repeated application of Proposition 2.1(i) and Proposition 2.1(iv), we can obtain the following equations.

$$\begin{aligned}Z(G-u;x) =& xZ(G-u-v-w;x)+xZ(G-u-v-w-r;x)\\ =& x^2Z(G-u-v-w-p-q;x)+x^2Z(G-u-v-w-p-q-s;x)\\ &+x^2Z(G-u-v-w-p-q-r;x)+x^2Z(G-u-v-w-r-p-q;x)\\ &+x^2Z(G-u-v-w-r-p-q-s;x)\\ =& x^2Z(R-q;x)+2x^2Z(R-q-r;x)+x^2Z(R-s-q;x)+x^2Z(R-N_R[q];x)\\ =& (0,x^2,0,2x^2,x^2,0,x^2,0,0)\widetilde{Z}_{qr}(R;x),\end{aligned}$$

$$\begin{aligned}Z(G-v;x) =& xZ(G-v-u-p;x)+xZ(G-v-u-p-q;x)\\ =& x^2Z(G-v-u-p-w-r;x)+x^2Z(G-v-u-p-w-r-q;x)\\ &+x^2Z(G-v-u-p-w-r-t;x)+x^2Z(G-v-u-p-q-w-r;x)\\ &+x^2Z(G-v-u-p-q-w-r-t;x)\\ =& x^2Z(R-r;x)+2x^2Z(R-q-r;x)+x^2Z(R-r-t;x)+x^2Z(R-N_R[r];x)\\ =& (0,0,x^2,2x^2,0,x^2,0,x^2,0)\widetilde{Z}_{qr}(R;x),\end{aligned}$$

$$\begin{aligned}Z(G-p-u;x) =& xZ(G-p-u-v-w;x)+xZ(G-p-u-v-w-r;x)\\ =& xZ(R;x)+xZ(R-r;x)\\ =& (x,0,x,0,0,0,0,0,0)\widetilde{Z}_{qr}(R;x),\end{aligned}$$

$$\begin{aligned}Z(G-v-w;x) =& xZ(G-v-w-u-p;x)+xZ(G-v-w-u-p-q;x)\\ =& xZ(R;x)+xZ(R-q;x)\\ =& (x,x,0,0,0,0,0,0,0)\widetilde{Z}_{qr}(R;x),\end{aligned}$$

$$\begin{aligned}Z(G-N_G[u];x) =& xZ(G-N_G[u]-w-r;x)+xZ(G-N_G[u]-w-r-q;x)\\ &+xZ(G-N_G[u]-w-r-t;x)\\ =& xZ(R-r;x)+xZ(R-q-r;x)+xZ(R-r-t;x)\\ =& (0,0,x,x,0,x,0,0,0)\widetilde{Z}_{qr}(R;x),\end{aligned}$$

$$\begin{aligned}Z(G-N_G[v];x) =& xZ(G-N_G[v]-p-q;x)+xZ(G-N_G[v]-p-q-r;x)\\ &+xZ(G-N_G[v]-p-q-s;x)\\ =& xZ(R-q;x)+xZ(R-q-r;x)+xZ(R-q-s;x)\\ =& (0,x,0,x,x,0,0,0,0)\widetilde{Z}_{qr}(R;x),\end{aligned}$$

$$Z(G-N_G[u]-N_G[v];x)=Z(R;x)=(1,0,0,0,0,0,0,0,0)\widetilde{Z}_{qr}(R;x).$$

Combining all the equations presented above, we arrive at the desired result. □

Lemma 4.2. *Let G be a graph created through the edge-merging of a hexagon $uvwrqpu$ and a graph R at the edge pq, where $\{sp,pq,qt\}\subseteq E(R)$ and $d_R(p)=d_R(q)=2$, as shown in* Figure 4(ii)*. Then $\widetilde{Z}_{uv}(G;x)=\mathbf{Y}(x)\widetilde{Z}_{pq}(R;x)$,* *where*

$$\mathbf{Y}(x)=\begin{pmatrix} x^2 & x^2 & x^2 & x^3+x^2 & 0 & 0 & x^3 & x^3 & x^3 \\ x & 0 & x^2 & x^2 & 0 & x^2 & 0 & 0 & 0 \\ 0 & x^2 & 0 & 2x^2 & x^2 & 0 & x^2 & 0 & 0 \\ x & 0 & x & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & x & 0 & x^2 & 0 & 0 & 0 & x^2 & 0 \\ 0 & 0 & 0 & x^2+x & 0 & 0 & x^2 & x^2 & x^2 \\ 0 & x & 0 & x & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & x & x & 0 & x & 0 & 0 & 0 \\ 0 & 0 & 0 & x & 0 & 0 & 0 & x & 0 \end{pmatrix}.$$

Proof. Analogously to the proof of Lemma 4.1, applying Proposition 2.1, it can be derived that

$$\begin{aligned} Z(G;x) =& xZ(G-v-w;x)+x^2Z(G-N_G[v]-N_G[w];x) \\ &+x^2Z(G-N_G[v]-N_G[r];x)+x^2Z(G-N_G[w]-N_G[u];x) \\ =& xZ(G-v-w;x)+x^2Z(R;x)+x^2Z(R-q;x)+x^2Z(R-p;x) \\ =& (x^3+x^2)Z(R-p-q;x)+x^3Z(R-N_R[p];x)+x^3Z(R-N_R[q];x) \\ &+x^3Z(R-N_R[p]-N_R[q];x)+x^2Z(R;x)+x^2Z(R-r;x)+x^2Z(R-q;x) \\ =& (x^2,x^2,x^2,x^3+x^2,0,0,x^3,x^3,x^3)\widetilde{Z}_{pq}(R;x), \end{aligned}$$

$$\begin{aligned} Z(G-u;x) =& xZ(G-u-v-w;x)+xZ(G-u-v-w-r;x) \\ =& x^2Z(G-u-v-w-r-q;x)+x^2Z(G-u-v-r-q-p;x) \\ &+x^2Z(G-u-v-w-r-q-t;x)+xZ(R;x) \\ =& xZ(R;x)+x^2Z(R-q;x)+x^2Z(R-p-q;x)+x^2Z(R-q-t;x) \\ =& (x,0,x^2,x^2,0,x^2,0,0,0)\widetilde{Z}_{pq}(R;x), \end{aligned}$$

$$\begin{aligned} Z(G-v;x) =& xZ(G-v-u-p;x)+xZ(G-v-u-p-s;x)+xZ(G-v-u-p-q;x) \\ =& x^2Z(G-v-u-p-w-r;x)+x^2Z(G-v-u-p-w-r-q;x) \\ &+x^2Z(G-v-u-p-s-w-r;x)+x^2Z(G-v-u-p-s-w-r-q;x) \\ &+xZ(P_2;x)Z(R-p-q;x) \\ =& x^2Z(R-p;x)+2x^2Z(R-p-q;x)+x^2Z(R-s-p;x)+x^2Z(R-N_R[p];x) \\ =& (0,x^2,0,2x^2,x^2,0,x^2,0,0)\widetilde{Z}_{pq}(R;x), \end{aligned}$$

$$\begin{aligned} Z(G-u-v;x) =& xZ(G-u-v-w-r;x)+xZ(G-u-v-w-r-q;x) \\ =& xZ(R;x)+xZ(R-q;x) \\ =& (x,0,x,0,0,0,0,0,0)\widetilde{Z}_{pq}(R;x), \end{aligned}$$

$$\begin{aligned} Z(G-p-u;x) =& xZ(G-p-u-v-w;x)+xZ(G-p-u-v-w-r;x) \\ =& x^2Z(G-p-u-v-w-r-q;x)+x^2Z(G-p-u-v-w-r-q-t;x) \\ &+xZ(G-p-u-v-w-r;x) \\ =& x^2Z(R-p-q;x)+x^2Z(R-N_R[q];x)+xZ(R-p;x) \\ =& (0,x,0,x^2,0,0,0,x^2,0)\widetilde{Z}_{pq}(R;x), \end{aligned}$$

$$\begin{aligned}Z(G-v-w;x) =& xZ(G-v-w-u-p;x)+xZ(G-v-w-u-p-s;x)\\&+xZ(G-v-w-u-p-q;x)\\=&x^2Z(G-v-w-u-p-r-q;x)+x^2Z(G-v-w-u-p-r-q-t;x)\\&+x^2Z(G-v-w-u-p-s-r-q;x)\\&+x^2Z(G-v-w-u-p-s-r-q-t;x)+xZ(G-v-w-u-p-q;x)\\=&(x^2+x)Z(R-p-q;x)+x^2Z(R-N_R[p];x)+x^2Z(R-N_R[q];x)\\&+x^2Z(R-N_R[p]-N_R[q];x)\\=&(0,0,0,x^2+x,0,0,x^2,x^2,x^2)\widetilde{Z}_{pq}(R;x),\end{aligned}$$

$$\begin{aligned}Z(G-N_G[u];x) =& xZ(G-N_G[u]-w-r;x)+xZ(G-N_G[u]-w-r-q;x)\\=&xZ(R-p;x)+xZ(R-p-q;x)\\=&(0,x,0,x,0,0,0,0,0)\widetilde{Z}_{pq}(R;x),\end{aligned}$$

$$\begin{aligned}Z(G-N_G[v];x) =& xZ(G-N_G[v]-r-q;x)+xZ(G-N_G[v]-r-q-p;x)\\&+xZ(G-N_G[v]-r-q-t;x)\\=&xZ(R-q;x)+xZ(R-p-q;x)+xZ(R-q-t;x)\\=&(0,0,x,x,0,x,0,0,0)\widetilde{Z}_{pq}(R;x),\end{aligned}$$

$$\begin{aligned}Z(G-N_G[u]-N_G[v];x) =& xZ(G-N_G[u]-N_G[v]-r-q;x)+xZ(G-N_G[u]-N_G[v]-r-q-t;x)\\=&xZ(R-p-q;x)+xZ(R-N_R[q];x)\\=&(0,0,0,x,0,0,0,x,0)\widetilde{Z}_{pq}(R;x).\end{aligned}$$

Hence, the proof is complete. □

Lemma 4.3. *Let G be a graph created through the edge-merging of a hexagon $uvwrqpu$ and a graph R at the edge rw, where $\{sr, rw, wt\} \subseteq E(R)$ and $d_R(r) = d_R(w) = 2$, as shown in* Figure 4(iii). *Then $\widetilde{Z}_{uv}(G;x) = \mathbf{Z}(x)\widetilde{Z}_{rw}(R;x)$, where*

$$\mathbf{Z}(x)=\begin{pmatrix} x^2 & x^2 & x^2 & x^3+x^2 & 0 & 0 & x^3 & x^3 & x^3\\ 0 & 0 & x^2 & 2x^2 & 0 & x^2 & 0 & x^2 & 0\\ x & x^2 & 0 & x^2 & x^2 & 0 & 0 & 0 & 0\\ x & x & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & x^2+x & 0 & 0 & x^2 & x^2 & x^2\\ 0 & 0 & x & x^2 & 0 & 0 & x^2 & 0 & 0\\ 0 & x & 0 & x & x & 0 & 0 & 0 & 0\\ 0 & 0 & x & x & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & x & 0 & 0 & x & 0 & 0 \end{pmatrix}.$$

Proof. By adopting an analysis method analogous to that in the proof of Lemma 4.2, the result is derivable, and we hence omit the details. □

Theorem 4.1. *Let $BC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h}$ be a benzenoid chain of length h, $h \geq 3$. The MMP of $BC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h}$ is given by*

$$Z(BC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h};x) = \mathbf{p}^{\mathrm{T}}\mathbf{\Gamma}_2(x)\mathbf{\Gamma}_3(x)\cdots\mathbf{\Gamma}_{h-1}(x)\mathbf{q},$$

where $\mathbf{p} = (x^2, x^2, x^2, x^3 + x^2, 0, 0, x^3, x^3, x^3)^{\mathrm{T}}$, $\mathbf{q} = (2x^3 + 3x^2, 3x^2, 3x^2, x^2 + x, x^2 + x, x^2 + x, 2x, 2x, x)^{\mathrm{T}}$,

$$\mathbf{\Gamma}_i(x) = \begin{cases} \mathbf{X}(x) & \text{if } \vartheta_{i+1} = \alpha, \\ \mathbf{Y}(x) & \text{if } \vartheta_{i+1} = \beta, \\ \mathbf{Z}(x) & \text{if } \vartheta_{i+1} = \gamma, \end{cases}$$

$i \in \{2, 3, \ldots, h-1\}$, $\mathbf{X}(x)$, $\mathbf{Y}(x)$ *and* $\mathbf{Z}(x)$ *are illustrated in Lemmas 4.1-4.3, respectively.*

Proof. Analogously to the proof of Theorem 3.1, the result can be derived by applying Lemmas 4.1 – 4.3. □

Example 4.1. *Let* $G = BC_{\gamma,\beta,\alpha,\beta,\alpha,\gamma,\gamma,\beta,\gamma,\beta}$ *be the benzenoid chain illustrated in Figure 2. Applying Theorem 4.1 we have* $Z(G;x) = \mathbf{p}^{\mathrm{T}}\mathbf{Z}(x)\mathbf{Y}(x)\mathbf{X}(x)\mathbf{Y}(x)\mathbf{X}(x)\mathbf{Z}(x)\mathbf{Z}(x)\mathbf{Y}(x)\mathbf{Z}(x)\mathbf{Y}(x)\mathbf{q} = 311x^{25} + 19810x^{24} + 345671x^{23} + 2128523x^{22} + 5012994x^{21} + 4573866x^{20} + 1499171x^{19} + 156329x^{18} + 3732x^{17}$. *Therefore, the number of MMs of all possible sizes on the benzenoid chain* $BC_{\gamma,\beta,\alpha,\beta,\alpha,\gamma,\gamma,\beta,\gamma,\beta}$ *has been fully characterized.*

The following conclusion gives a computational formula for the number of MMs in a benzenoid chain.

Theorem 4.2. *Let* $BC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h}$ *be a benzenoid chain of length h,* $h \geq 3$. *The number of MMs of* $BC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h}$ *is*

$$\zeta(BC_{\vartheta_3,\vartheta_4,\ldots,\vartheta_h}) = \mathbf{r}^{\mathrm{T}}\mathbf{\Gamma}_2\mathbf{\Gamma}_3\cdots\mathbf{\Gamma}_{h-1}\mathbf{s},$$

where $\mathbf{r} = (1,1,1,2,0,0,1,1,1)^{\mathrm{T}}$, $\mathbf{s} = (5,3,3,2,2,2,2,2,1)^{\mathrm{T}}$, $\mathbf{\Gamma}_i = \begin{cases} \mathbf{X} & \text{if } \vartheta_{i+1} = \alpha, \\ \mathbf{Y} & \text{if } \vartheta_{i+1} = \beta, \\ \mathbf{Z} & \text{if } \vartheta_{i+1} = \gamma, \end{cases}$ $i \in \{2, 3, \ldots, h-1\}$, *and*

$$\mathbf{X} = \begin{pmatrix} 1&1&1&2&0&0&1&1&1 \\ 0&1&0&2&1&0&1&0&0 \\ 0&0&1&2&0&1&0&1&0 \\ 0&0&0&2&0&0&1&1&1 \\ 1&0&1&0&0&0&0&0&0 \\ 1&1&0&0&0&0&0&0&0 \\ 0&0&1&1&0&1&0&0&0 \\ 0&1&0&1&1&0&0&0&0 \\ 1&0&0&0&0&0&0&0&0 \end{pmatrix}, \mathbf{Y} = \begin{pmatrix} 1&1&1&2&0&0&1&1&1 \\ 1&0&1&1&0&1&0&0&0 \\ 0&1&0&2&1&0&1&0&0 \\ 1&0&1&0&0&0&0&0&0 \\ 0&1&0&1&0&0&0&1&0 \\ 0&0&0&2&0&0&1&1&1 \\ 0&1&0&1&0&0&0&0&0 \\ 0&0&1&1&0&1&0&0&0 \\ 0&0&0&1&0&0&0&1&0 \end{pmatrix}, \mathbf{Z} = \begin{pmatrix} 1&1&1&2&0&0&1&1&1 \\ 0&0&1&2&0&1&0&1&0 \\ 1&1&0&1&1&0&0&0&0 \\ 1&1&0&0&0&0&0&0&0 \\ 0&0&0&2&0&0&1&1&1 \\ 0&0&1&1&0&0&1&0&0 \\ 0&1&0&1&1&0&0&0&0 \\ 0&0&1&1&0&0&0&0&0 \\ 0&0&0&1&0&0&1&0&0 \end{pmatrix}.$$

Proof. Since $\zeta(G)$ is equal to $Z(G;1)$ for any graph G, one can directly obtain the number of MMs in a benzenoid chain by plugging $x = 1$ into Theorem 4.1. □

Remark 4.1. *Shi and Deng [8] also obtained a method for calculating the number of MMs in benzenoid chains by adopting technical means different from those in our paper.*

Based on Theorem 4.2 and the law of total expectation, we are able to derive the expected value of MMs for a random benzenoid chain.

Theorem 4.3. *The expected value of the number of MMs of a random benzenoid chain* $BC_h(p_1, p_2, p_3)$ *is*

$$\mathbb{E}(\zeta(BC_h(p_1, p_2, p_3))) = \mathbf{r}^{\mathrm{T}}\mathbf{Q}^{h-2}\mathbf{s},$$

where $\mathbf{r} = (1,1,1,2,0,0,1,1,1)^{\mathrm{T}}$, $\mathbf{s} = (5,3,3,2,2,2,2,2,1)^{\mathrm{T}}$, $\mathbf{Q} = p_1\mathbf{X} + p_2\mathbf{Y} + p_3\mathbf{Z}$, *and the matrices* $\mathbf{X}$, $\mathbf{Y}$ *and* $\mathbf{Z}$ *are depicted in Theorem 4.2.*

5. Conclusion

In this study, we successfully derived formulas for calculating the MMPs of phenylene chains and benzenoid chains separately. These formulas not only allow us to precisely determine the number of maximal matchings, the number of perfect matchings, the matching number, and the saturation number for any phenylene and benzenoid chain with length h, but also provide a powerful tool for in-depth analysis of their matching-related properties. Additionally, we obtained explicit expressions for the expected values of the number of maximal matchings in random phenylene and benzenoid chains, shedding new light on the probabilistic characteristics of these molecular structures. Furthermore, the methodology proposed in this paper for solving the MMPs of phenylene and benzenoid chains demonstrates remarkable versatility. It can be effectively extended to count the maximal matchings of various other significant chemical molecular graphs. Examples of such graphs include general phenylenes and catacondensed benzenoid systems (with full-hexagons), double benzenoid chains, polyphenylene chains, spiro chains, and primitive coronoid systems, among others.

Upon meticulous, comprehensive examination of the maximal matching polynomials for short-length phenylene and benzenoid chains, one observes that unlike benzenoid chains (which exhibit variable saturation numbers), all phenylene chains of the same length share an identical saturation number. In fact, this consistency can be formally verified via mathematical induction to show $s(PC_h) = 2h$ for any phenylene chain PC_h of length h: the base cases hold ($s(PC_1) = 2$, $s(PC_2) = 4$, $s(PC_3) = 6$, $s(PC_4) = 8$, $s(PC_5) = 10$, $s(PC_6) = 12$), and for the inductive step, any maximal matching K of PC_{h-1} (satisfying $|K| = 2(h-1)$) can be extended to a maximal matching K' of PC_h by adding two edges from the newly attached hexagon.

In the end, the following conjectures can be put forward for further research.

Conjecture 5.1. *Among all phenylene chains with length of $h \geq 4$, the linear phenylene chain $PC_{\alpha,\alpha,\ldots,\alpha}$ achieves the maximum number of MMs, while the helicene phenylene chain $PC_{\beta,\beta,\ldots,\beta}$ reaches the minimum number of MMs.*

Conjecture 5.2 ([3]). *Among all benzenoid chains with length of $h \geq 4$, the helicene benzenoid chain $BC_{\beta,\beta,\ldots,\beta}$ possesses the minimum number of MMs.*

Remark 5.1. *In [3], Došlić and Short proved that the linear benzenoid chain $PC_{\alpha,\alpha,\ldots,\alpha}$ attains the maximum number of MMs among all benzenoid chains of length $h \geq 4$.*

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