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Matching Polynomials and Independence Polynomials of Benzenoid Chains

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Abstract

Benzenoid chains, also known as hexagonal chains, are a class of organic compounds that consist of an arrangement of hexagonal rings fused together. In this article, we first present reduction formulas to compute the matching polynomial and independence polynomial of any benzenoid chain by utilizing the transfer matrix technique. Subsequently, computational formulas for the Hosoya index and Merrifield-Simmons index of benzenoid chains are derived. Furthermore, the expected values of the Hosoya index and Merrifield-Simmons index for random benzenoid chains are also obtained.

1 Introduction

Let $G = (V(G), E(G))$ be a graph with vertex set $V(G)$ and edge set $E(G)$. A matching in a graph is a set of edges in which no two edges share a common vertex. The size of a matching refers to the number of edges it contains. The matching (generating) polynomial of a graph is a polynomial that counts the number of matchings of different sizes in the

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graph [6, 13]. For a graph G, it is defined as

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

where $m_k(G)$ denotes the number of matchings of size k in graph G.

An independent set in a graph is a set of vertices in which no two vertices are adjacent. Similar as matching polynomial, the independence polynomial [9] counts the number of independent sets of different sizes in the graph G, it is defined as

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

where $i_k(G)$ denotes the number of independent sets in G with k vertices.

It is well known that the matchings and independent sets, along with their associated polynomials, are fundamental in graph theory and have far-reaching implications in diverse fields. They provide powerful tools for analyzing graph structures, optimizing real-world problems, and understanding the fundamental properties of complex systems. Clearly, if the matching (independence) polynomial of a graph can be expressed concisely, the coefficients of the polynomial can be examined to fully determine the distribution of matchings (independent sets) on the graph. Hence, studying the computation of the matching polynomial and independence polynomial of a graph holds significant importance.

The Hosoya index [10], also known as z-index, is particularly useful in the study of molecular structure-activity relationships and chemical similarity analysis [20]. The Hosoya index of a graph G is defined as

$$z(G) = \sum_{k\geq 0} m_k(G).$$

Obviously, the Hosoya index of a graph G can be obtained from the matching polynomial $\psi(G;x)$ by setting $x = 1$, i.e., $z(G) = \psi(G;1)$. The Merrifield-Simmons index, also known as σ-index, was introduced by R. E. Merrifield and H. E. Simmons [14]. The Merrifield-Simmons index of a graph G is defined as

$$\sigma(G) = \sum_{k\geq 0} i_k(G).$$

And the Merrifield-Simmons index of a graph G can be also obtained by the way of that $\sigma(G) = \phi(G;1)$. Both the Merrifield-Simmons index and Hosoay index provide valuable insights into the structure and properties of graphs and chemical compounds, and have garnered significant attention from numerous scholars [1,3,5,11,15,21].

Benzenoid systems are a class of organic compounds characterized by a cyclic structure consisting of six carbon atoms arranged in a hexagonal shape. These systems have been widely studied due to their unique electronic and structural properties, making them important in various fields such as organic chemistry, drug design, and materials science. A benzenoid (hexagonal) chain refers to a linear arrangement of benzene rings connected in a chain-like fashion. Each benzenoid chain B_h with h hexagons can be obtained from a benzenoid chain B_{h-1} by attaching it to a new hexagon. Hence, a benzenoid chain can be constructed inductively. The number of hexagons in a benzenoid chain is called the length. There are three ways for attaching a hexagon $C_6^{(h)}$ to a benzenoid chain B_{h-1} with $h-1$ hexagons $C_6^{(1)}, C_6^{(2)}, \ldots, C_6^{(h-1)}$. Let l be a direct line from the center of $C_6^{(h-2)}$ to $C_6^{(h-1)}$. If $C_6^{(h)}$ is on the line l, it is called α-type fusing. If $C_6^{(h)}$ is on the left-hand of line l, it is called β-type fusing. If $C_6^{(h)}$ is on the right-hand of line l, it is called γ-type fusing. Any benzenoid chain B_h, $h \geq 3$, can be obtained from B_2 by selecting a θ-type fusion at each step to obtain, where $\theta \in \{\alpha, \beta, \gamma\}$. Let $B(\theta_3, \theta_4, \ldots, \theta_h)$ be a benzenoid chain with h hexagons obtained from B_2 by θ_3-type, θ_4-type, $\ldots$,θ_h-type fusing, successively. Then $B(\alpha, \alpha, \ldots, \alpha)$ is called a linear chain, $B(\beta, \beta, \ldots, \beta)$ or $B(\gamma, \gamma, \ldots, \gamma)$ is called a helicene chain, $B(\beta, \gamma, \beta, \gamma, \cdots)$ or $B(\gamma, \beta, \gamma, \beta, \cdots)$ is called a zig-zag chain. A benzenoid chain $B(\gamma, \alpha, \beta, \gamma, \gamma, \alpha, \beta, \beta, \gamma, \beta)$ is shown in Figure 1. In addition, it can be seen that, for $i \in \{3, 4, \ldots, h\}$,

$$B(\theta_3, \theta_4, \ldots, \theta_h) \cong B(\theta_3', \theta_4', \ldots, \theta_h') \text{ when } \theta_i' = \begin{cases} \alpha, & \text{if } \theta_i = \alpha; \\ \beta, & \text{if } \theta_i = \gamma; \\ \gamma, & \text{if } \theta_i = \beta. \end{cases}$$

A random benzenoid chain $B_h(p_1, p_2, p_3)$ with h hexagons is a benzenoid chain obtained by stepwise addition of terminal hexagons. At each step t, $t \in \{3, 4, \ldots, h\}$, a random selection is made from one of the three possible constructions:

(i) $B(\theta_3, \theta_4, \ldots, \theta_{t-1}) \to B(\theta_3, \theta_4, \ldots, \theta_{t-1}, \alpha)$ with probability p_1;

(ii) $B(\theta_3, \theta_4, \ldots, \theta_{t-1}) \to B(\theta_3, \theta_4, \ldots, \theta_{t-1}, \beta)$ with probability p_2;

(iii) $B(\theta_3, \theta_4, \ldots, \theta_{t-1}) \to B(\theta_3, \theta_4, \ldots, \theta_{t-1}, \gamma)$ with probability $p_3 = 1 - p_1 - p_2$.

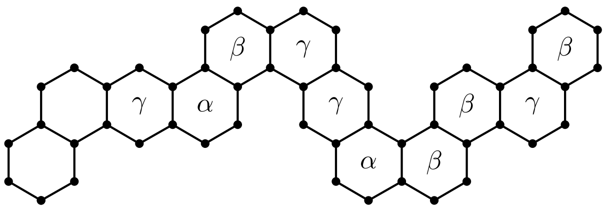

Figure 1. A benzenoid chain $B(\gamma, \alpha, \beta, \gamma, \gamma, \alpha, \beta, \beta, \gamma, \beta)$.

Up to now, researchers have conducted extensive investigations into the enumeration and extremal problems related to various topological invariants on benzenoid chains. Gutman [8] obtained the extremal benzenoid chains with respect to Hosoya index, perfect matchings, Merrifield-Simmons index, Wiener index and largest graph eigenvalue. Bermudo, Higuita and Rada [2] gave bounds for the domination number in benzenoid chains. The benzenoid chains with the first three maximal Mostar indices and the first three minimal Mostar indices have been obtained in [22] and [23] respectively. The explicit analytical expressions of the expected values and variances for the Sombor index of benzenoid chains were obtained in [25]. Li and Yan [12] enumerated the number of spanning trees with a Kekulé structure in the linear benzenoid chains. Extremal benzenoid chains concerning k-matchings and k-independent sets were determined in [24]. Cruz et al. [4] gave a method based on some transfer matrices to compute the Hosoya index of catacondensed benzenoid systems in 2017, and Oz and Cangul [18] computed the Merrifield-Simmons indices of benzenoid chains and double benzenoid chains. Furthermore, based on transfer matrix technique, Oz and Cangul [16, 17] have studied the computation of k-matchings and k-independent sets in benzenoid chains. Inspired by the findings of the aforementioned literature, in this paper, we approach the counting of matchings and independent sets on benzenoid chains from the perspective of graph polynomials.

2 Preliminaries

All graphs considered in this paper are simple and finite. The vertex set and edge set of a graph G are denoted by $V(G)$ and $E(G)$ respectively. The neighbor set $N(v)$ of v in G is the set of vertices that are adjacent to v. The closed neighborhood of a vertex v, denoted as $N[v]$, is the set that includes v and all its neighbors. If S is a vertex set of G, then by $G - S$ refers to the graph obtained by removing all vertices in S and all the edges incident to those vertices from G. Specifically, if $v \in V(G)$, then $G - v$ is the graph obtained by deleting the vertex v along with its incident edges from G. Analogously, for $\{u, v\} \subseteq V(G)$, $G - u - v$ denotes the graph obtained by removing both vertices u and v, as well as their incident edges. Furthermore, if $uv \in E(G)$, then $G - uv$, then $G - uv$ represents the subgraph of G obtained by deleting the edge uv, while preserving all other vertices. A path consisting of n vertices is represented by P_n while a cycle with n vertices is denoted as C_n.

The following two lemmas serve as useful tools in the computation of matching polynomials and independence polynomials.

Lemma 2.1 ([13]).

(i) *Let G be a graph and $uv \in E(G)$. Then* $\psi(G;x) = \psi(G - uv;x) +$

$x\psi(G-\{u,v\})$;

(ii) *Let $G = G_1 \cup G_2 \cup \cdots \cup G_k$ be a graph consisting of k components $G_1, G_2, \ldots, G_k$. Then $\psi(G;x) = \psi(G_1;x)\psi(G_2;x)\cdots\psi(G_k;x)$.*

Lemma 2.2 ([9]).

(i) *Let G be a graph and $u \in V(G)$. Then $\phi(G;x) = \phi(G-u;x) + x\phi(G-N[u];x)$;*

(ii) *Let $G = G_1 \cup G_2 \cup \cdots \cup G_k$ be a graph consisting of k components $G_1, G_2, \ldots, G_k$. Then $\phi(G;x) = \phi(G_1;x)\phi(G_2;x)\cdots\phi(G_k;x)$.*

For path P_n and cycle C_n, the matching polynomials and independence polynomials can be written respectively as

$$\psi(P_n;x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \binom{n-k}{k} x^k, \ \psi(C_n;x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{n}{n-k}\binom{n-k}{k} x^k$$

and

$$\phi(P_n;x) = \sum_{k=0}^{\lfloor \frac{n+1}{2} \rfloor} \binom{n+1-k}{k} x^k, \ \phi(C_n;x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{n}{n-k}\binom{n-k}{k} x^k.$$

In particular, we have

(i) $\psi(P_1;x) = 1$, $\psi(P_2;x) = 1+x$, $\psi(P_3;x) = 1+2x$, $\psi(P_4;x) = 1 + 3x + x^2$, $\psi(P_5;x) = 1+4x+3x^2$ and $\psi(C_6;x) = 1+6x+9x^2+2x^3$;

(ii) $\phi(P_1;x) = 1+x$, $\phi(P_2;x) = 1+2x$, $\phi(P_3;x) = 1+3x+x^2$, $\phi(P_4;x) = 1+4x+3x^2$, $\phi(P_5;x) = 1+5x+6x^2+x^3$ and $\phi(C_6;x) = 1+6x+9x^2+2x^3$.

3 Matching polynomials of benzenoid chains

In order to compute the matching polynomial of benzenoid chains, we introduce a column polynomial vector that relates the matching polynomial

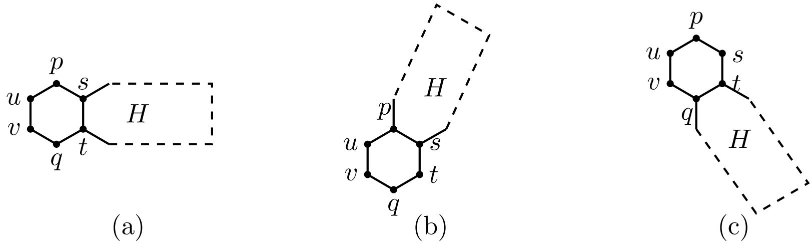

Figure 2. The graphs used in Lemmas 3.1–3.3, and Lemmas 4.1–4.3.

at an edge $uv \in E(G)$ in the following manner:

$$\psi_{uv}(G;x) = (\psi(G;x), \psi(G-u;x), \psi(G-v;x), \psi(G-u-v;x))^{\mathrm{T}}.$$

Lemma 3.1. *Let G be a graph obtained from the edge-coalescence of H and a hexagon $C_6 = uvqtsp$ at edge st, see* Figure 2(a). *Then we have $\psi_{uv}(G;x) = \mathbf{A}(x)\psi_{st}(H;x)$, where*

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

Proof. By the definition of the column vector $\psi_{uv}(G;x)$ at a given edge uv, we just need to consider the values $\psi(G;x)$, $\psi(G-u;x)$, $\psi(G-v;x)$ and $\psi(G-u-v;x)$. Note that $\psi(P_1;x) = 1$, $\psi(P_2;x) = 1+x$, $\psi(P_3;x) = 1+2x$ and $\psi(P_4;x) = 1+3x+x^2$. Then by using Lemma 2.1 we have

$$\begin{aligned}\psi(G;x) =& \psi(G-ps;x) + x\psi(G-p-s;x) \\ =& \psi(G-ps-tq;x) + x\psi(G-ps-t-q;x) \\ & + x\psi(G-p-s-tq;x) + x^2\psi(G-p-s-t-q;x) \\ =& \psi(P_4;x)\psi(H;x) + x\psi(P_3;x)\psi(H-t;x) \\ & + x\psi(P_3;x)\psi(H-s;x) + x^2\psi(P_2;x)\psi(H-s-t;x) \\ =& (1+3x+x^2)\psi(H;x) + (x+2x^2)\psi(H-t;x) \\ & + (x+2x^2)\psi(H-s;x) + (x^2+x^3)\psi(H-s-t;x)\end{aligned}$$

$$=(1+3x+x^2, x+2x^2, x+2x^2, x^2+x^3)\psi_{st}(H;x),$$

$$\begin{aligned}\psi(G-u;x) =&\psi(G-u-ps;x)+x\psi(G-u-p-s;x)\\ =&\psi(G-u-ps-tq;x)+x\psi(G-u-ps-t-q;x)\\ &+x\psi(G-u-p-s-tq;x)+x^2\psi(G-\{u,p,s,t,q\};x)\\ =&\psi(P_1;x)\psi(P_2;x)\psi(H;x)+x\psi(P_1;x)^2\psi(H-t;x)\\ &+x\psi(P_2;x)\psi(H-s;x)+x^2\psi(P_1;x)\psi(H-s-t;x)\\ =&(1+x)\psi(H;x)+(x+x^2)\psi(H-s;x)\\ &+x\psi(H-t;x)+x^2\psi(H-s-t;x)\\ =&(1+x, x+x^2, x, x^2)\psi_{st}(H;x),\end{aligned}$$

$$\begin{aligned}\psi(G-v;x) =&\psi(G-v-ps;x)+x\psi(G-v-p-s;x)\\ =&\psi(G-v-ps-tq;x)+x\psi(G-v-ps-t-q;x)\\ &+x\psi(G-v-p-s-tq;x)+x^2\psi(G-\{v,p,s,t,q\};x)\\ =&\psi(P_1;x)\psi(P_2;x)\psi(H;x)+x\psi(P_2;x)\psi(H-t;x)\\ &+x\psi(P_1;x)^2\psi(H-s;x)+x^2\psi(P_1;x)\psi(H-s-t;x)\\ =&(1+x)\psi(H;x)+x\psi(H-s;x)+(x+x^2)\psi(H-t;x)\\ &+x^2\psi(H-s-t;x)\\ =&(1+x, x, x+x^2, x^2)\psi_{st}(H;x),\end{aligned}$$

$$\begin{aligned}\psi(G-u-v;x) =&\psi(G-u-v-ps;x)+x\psi(G-u-v-p-s;x)\\ =&\psi(G-u-v-ps-tq;x)\\ &+x\psi(G-u-v-ps-t-q;x)\\ &+x\psi(G-u-v-p-s-tq;x)\\ &+x^2\psi(G-u-v-p-s-t-q;x)\\ =&\psi(P_1;x)^2\psi(H;x)+x\psi(P_1;x)\psi(H-t;x)\\ &+x\psi(P_1;x)\psi(H-s;x)+x^2\psi(H-s-t;x)\\ =&\psi(H;x)+x\psi(H-s;x)+x\psi(H-t;x)\end{aligned}$$

$$
\begin{aligned}
&+ x^2\psi(H-s-t;x)\\
=&(1,x,x,x^2)\psi_{st}(H;x).
\end{aligned}
$$

Thus, we get $\psi_{uv}(G;x) = \mathbf{A}(x)\psi_{st}(H;x)$. ∎

Lemma 3.2. *Let G be a graph obtained from the edge-coalescence of H and a hexagon $C_6 = uvqtsp$ at edge ps, see* Figure 2(b). *Then $\psi_{uv}(G;x) = \mathbf{B}(x)\psi_{ps}(H;x)$, where*

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

Proof. By the use of Lemma 2.1 one can obtain that

$$
\begin{aligned}
\psi(G;x) =&(1+3x+x^2)\psi(H;x) + (x+2x^2)\psi(H-s;x)\\
&+ (x+2x^2)\psi(H-p;x) + (x^2+x^3)\psi(H-p-s;x)\\
=&(1+3x+x^2, x+2x^2, x+2x^2, x^2+x^3)\psi_{ps}(H;x),
\end{aligned}
$$

$$
\begin{aligned}
\psi(G-u;x) =&(1+2x)\psi(H;x) + (x+x^2)\psi(H-s;x),\\
=&(1+2x, 0, x+x^2, 0)\psi_{ps}(H;x),
\end{aligned}
$$

$$
\begin{aligned}
\psi(G-v;x) =&(1+x)\psi(H;x) + (x+x^2)\psi(H-p;x)\\
&+ x\psi(H-s;x) + x^2\psi(H-p-s;x)\\
=&(1+x, x+x^2, x, x^2)\psi_{ps}(H;x)
\end{aligned}
$$

and

$$
\begin{aligned}
\psi(G-u-v;x) =&(1+x)\psi(H;x) + x\psi(H-s;x)\\
=&(1+x, 0, x, 0)\psi_{ps}(H;x).
\end{aligned}
$$

Hence, we get $\psi_{uv}(G;x) = \mathbf{B}(x)\psi_{ps}(H;x)$. ∎

Lemma 3.3. *Let G be a graph obtained from the edge-coalescence of H and a hexagon $C_6 = uvqtsp$ at edge tq, see* Figure 2(c). *Then $\psi_{uv}(G;x) = \mathbf{C}(x)\psi_{tq}(H;x)$, where*

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

Proof. Similarly, by the use of Lemma 2.1 we have

$$\begin{aligned} \psi(G;x) =&(1+3x+x^2)\psi(H;x) + (x+2x^2)\psi(H-t;x) \\ &+ (x+2x^2)\psi(H-q;x) + (x^2+x^3)\psi(H-t-q;x) \\ =&(1+3x+x^2, x+2x^2, x+2x^2, x^2+x^3)\psi_{tq}(H;x), \end{aligned}$$

$$\begin{aligned} \psi(G-u;x) =&(1+x)\psi(H;x) + x\psi(H-t;x) + (x+x^2)\psi(H-q;x) \\ &+ x^2\psi(H-t-q;x) \\ =&(1+x, x, x+x^2, x^2)\psi_{tq}(H;x), \end{aligned}$$

$$\begin{aligned} \psi(G-v;x) =&(1+2x)\psi(H;x) + (x+x^2)\psi(H-t;x) \\ =&(1+2x, x+x^2, 0, 0)\psi_{tq}(H;x), \end{aligned}$$

$$\begin{aligned} \psi(G-u-v;x) =&(1+x)\psi(H;x) + x\psi(H-t;x) \\ =&(1+x, x, 0, 0)\psi_{tq}(H;x). \end{aligned}$$

Thus, the desired result $\psi_{uv}(G;x) = \mathbf{C}(x)\psi_{tq}(H;x)$ is obtained. ■

By Lemmas 3.1, 3.2 and 3.3, one can get the following conclusion.

Theorem 3.1. *Let $B(\theta_3, \theta_4, \ldots, \theta_h)$ be a benzenoid chain with h hexagons. Then the matching polynomial of $B(\theta_3, \theta_4, \ldots, \theta_h)$ is given by*

$$\psi(B(\theta_3, \theta_4, \ldots, \theta_h); x) = \mathbf{x}^{\mathrm{T}}\mathbf{M}_2(x)\mathbf{M}_3(x)\cdots\mathbf{M}_{h-1}(x)\mathbf{y},$$

where $\mathbf{x} = (1+3x+x^2, x+2x^2, x+2x^2, x^2+x^3)^{\mathrm{T}}$, $\mathbf{y} = (1+6x+9x^2+2x^3, 1+4x+3x^2, 1+4x+3x^2, 1+3x+x^2)^{\mathrm{T}}$ *and*

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

Proof. For a benzenoid chain $B(\theta_3, \theta_4, \ldots, \theta_h)$ consisting of an arrangement of hexagons $C_6^{(1)}, C_6^{(2)}, \ldots, C_6^{(h)}$ consecutively, we denote the common edge shared by $C_6^{(i)}$ and $C_6^{(i+1)}$ by u_iv_i , $i \in \{1, 2, \ldots, h-1\}$, and denote the unique parallel edge of u_1v_1 on $C_6^{(1)}$ by u_0v_0. Let $G_i = C_6^{(i)} \cup C_6^{(i+1)} \cup \cdots C_6^{(h)}$ be the vertex induced sub-chain of $B(\theta_3, \theta_4, \ldots, \theta_h)$. Then by Lemma 3.1 we have $\psi_{u_0v_0}(B(\theta_3, \theta_4, \ldots, \theta_h); x) = \mathbf{A}(x)\psi_{u_1v_1}(G_2; x)$. By the use of Lemmas 3.1, 3.2 and 3.3, we have $\psi_{u_1v_1}(G_2; x) = \mathbf{M}_2(x)\psi_{u_2v_2}(G_3; x)$, where $\mathbf{M}_2(x) = \mathbf{A}(x)$ if $\theta_3 = \alpha$; $\mathbf{M}_2(x) = \mathbf{B}(x)$ if $\theta_3 = \beta$; $\mathbf{M}_2(x) = \mathbf{C}(x)$ if $\theta_3 = \gamma$. It can be verified that for any edge uv of a hexagon C_6 we have $\psi_{uv}(C_6) = (1+6x+9x^2+2x^3, 1+4x+3x^2, 1+4x+3x^2, 1+3x+x^2)^{\mathrm{T}} = \mathbf{y}$. Iteratively, we can get that

$$\psi_{u_0v_0}(B(\theta_3, \theta_4, \ldots, \theta_h); x) = \mathbf{A}(x)\mathbf{M}_2(x)\mathbf{M}_3(x) \cdots \mathbf{M}_{h-1}(x)\mathbf{y}.$$

Thus, we have $\psi(B(\theta_3, \theta_4, \ldots, \theta_h); x) = \mathbf{x}^{\mathrm{T}}\mathbf{M}_2(x)\mathbf{M}_3(x) \cdots \mathbf{M}_{h-1}(x)\mathbf{y}$, where $\mathbf{x} = (1+3x+x^2, x+2x^2, x+2x^2, x^2+x^3)^{\mathrm{T}}$, $\mathbf{y} = (1+6x+9x^2+2x^3, 1+4x+3x^2, 1+4x+3x^2, 1+3x+x^2)^{\mathrm{T}}$ and

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

Therefore, the proof is concluded. ■

Theorem 3.1 demonstrates that the matching polynomial of any benzenoid chain can be derived by an appropriate multiplication of three 4×4 matrices with two terminal vectors. For example, by applying Theorem 3.1 one can get the matching polynomial of the benzenoid chain

$G = B(\gamma, \alpha, \beta, \gamma, \gamma, \alpha, \beta, \beta, \gamma, \beta)$ as described in Figure 1. That is

$$\begin{aligned}\psi(G; x) =& \mathbf{x}^{\mathrm{T}}\mathbf{C}(x)\mathbf{A}(x)\mathbf{B}(x)\mathbf{C}(x)\mathbf{C}(x)\mathbf{A}(x)\mathbf{B}(x)\mathbf{B}(x)\mathbf{C}(x)\mathbf{B}(x)\mathbf{y} \\ =& 308x^{25} + 27369x^{24} + 861258x^{23} + 13491411x^{22} + 123662031x^{21} \\ &+ 731312365x^{20} + 2977863580x^{19} + 8741059239x^{18} \\ &+ 19127948257x^{17} + 32000273261x^{16} + 41717398775x^{15} \\ &+ 42998766072x^{14} + 35422384953x^{13} + 23505158443x^{12} \\ &+ 12627604944x^{11} + 5506294323x^{10} + 1948857056x^{9} \\ &+ 558325960x^{8} + 128704790x^{7} + 23635364x^{6} + 3404687x^{5} \\ &+ 375772x^{4} + 30634x^{3} + 1736x^{2} + 61x + 1.\end{aligned}$$

By considering isomorphisms, it can be readily verified that there are precisely 10 benzenoid chains of length 5 and 25 benzenoid chains of length 6. By applying Theorem 3.1, the matching polynomials of all the benzenoid chains of length 5 and benzenoid chains of length 6 are listed in Appendix.

Since the Hosoya index of a graph G can be obtained by $z(G) = \psi(G; 1)$, then from Theorem 3.1 we have

Theorem 3.2. *Let $B(\theta_3, \theta_4, \ldots, \theta_h)$ be a benzenoid chain with h hexagons. Then the Hosoya index of $B(\theta_3, \theta_4, \ldots, \theta_h)$ is given by*

$$z(B(\theta_3, \theta_4, \ldots, \theta_h)) = \mathbf{u}^{\mathrm{T}}\mathbf{M}_2\mathbf{M}_3 \cdots \mathbf{M}_{h-1}\mathbf{w},$$

where $\mathbf{u} = (5, 3, 3, 2)^{\mathrm{T}}$, $\mathbf{w} = (18, 8, 8, 5)^{\mathrm{T}}$, $\mathbf{M}_i = \begin{cases} \mathbf{A}, & \text{if } \theta_{i+1} = \alpha; \\ \mathbf{B}, & \text{if } \theta_{i+1} = \beta; \\ \mathbf{C}, & \text{if } \theta_{i+1} = \gamma \end{cases}$ *and*

$$\mathbf{A} = \begin{pmatrix} 5 & 3 & 3 & 2 \\ 2 & 2 & 1 & 1 \\ 2 & 1 & 2 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}, \mathbf{B} = \begin{pmatrix} 5 & 3 & 3 & 2 \\ 3 & 0 & 2 & 0 \\ 2 & 2 & 1 & 1 \\ 2 & 0 & 1 & 0 \end{pmatrix}, \mathbf{C} = \begin{pmatrix} 5 & 3 & 3 & 2 \\ 2 & 1 & 2 & 1 \\ 3 & 2 & 0 & 0 \\ 2 & 1 & 0 & 0 \end{pmatrix}.$$

By applying Theorem 3.2, the Hosoya indices for all benzenoid chains of length 5 and benzenoid chains of length 6 can be obtained directly, and they are listed in Table 1 and Table 2, respectively.

Corollary 3.1. *For a linear chain L_h with $h \geq 3$ hexagons, we have* $z(L_h) = \mathbf{u}^{\mathrm{T}}\mathbf{A}^{h-2}\mathbf{w}$.

Corollary 3.2. *For a helicene chain H_h with $h \geq 3$ hexagons, we have* $z(H_h) = \mathbf{u}^{\mathrm{T}}\mathbf{B}^{h-2}\mathbf{w} = \mathbf{u}^{\mathrm{T}}\mathbf{C}^{h-2}\mathbf{w}$.

Corollary 3.3. *For a zig-zag chain Z_h with $h \geq 3$ hexagons, we have*

$$z(Z_h) = \begin{cases} \mathbf{u}^{\mathrm{T}}(\mathbf{BC})^{\frac{h-2}{2}}\mathbf{w} & \text{if } h \text{ is even,} \\ \mathbf{u}^{\mathrm{T}}(\mathbf{BC})^{\frac{h-3}{2}}\mathbf{Bw} & \text{if } h \text{ is odd.} \end{cases}$$

Now, we give the expected value of Hosoya index of a random benzenoid chain.

Theorem 3.3. *The expected value of the Hosoya index of a random benzenoid chain $B_h(p_1, p_2, p_3)$, $p_3 = 1 - p_1 - p_2$, is given by*

$$\mathbb{E}(z(B_h(p_1, p_2, p_3))) = \mathbf{u}^{\mathrm{T}}\mathbf{S}^{h-2}\mathbf{w},$$

where $\mathbf{u} = (5, 3, 3, 2)^{\mathrm{T}}$, $\mathbf{w} = (18, 8, 8, 5)^{\mathrm{T}}$ *and*

$$\mathbf{S} = \begin{pmatrix} 5 & 3 & 3 & 2 \\ 2 + p_2 & 3p_1 + p_2 - 1 & 2 - p_1 & 1 - p_2 \\ 3 - p_1 - p_2 & 2 - p_1 & 2p_1 + p_2 & p_1 + p_2 \\ 2 - p_1 & 1 - p_2 & p_1 + p_2 & p_1 \end{pmatrix}.$$

Proof. Let

$$\begin{aligned} \mathbf{S} =& p_1\mathbf{A} + p_2\mathbf{B} + p_3\mathbf{C} \\ =& \begin{pmatrix} 5 & 3 & 3 & 2 \\ 2 + p_2 & 3p_1 + p_2 - 1 & 2 - p_1 & 1 - p_2 \\ 3 - p_1 - p_2 & 2 - p_1 & 2p_1 + p_2 & p_1 + p_2 \\ 2 - p_1 & 1 - p_2 & p_1 + p_2 & p_1 \end{pmatrix}. \end{aligned}$$

Then by the law of total expectation [7, 19] and Theorem 3.2, we have

$$\begin{aligned}
\mathbb{E}(z(B(\theta_3,\theta_4,\ldots,\theta_h))) =&\mathbb{E}(\mathbf{u}^{\mathrm{T}}\mathbf{M}_2\mathbf{M}_3\cdots\mathbf{M}_{h-1}\mathbf{w})\\
=&p_1\mathbb{E}(\mathbf{u}^{\mathrm{T}}\mathbf{M}_2\cdots\mathbf{M}_{h-2}\mathbf{A}\mathbf{w}|\theta_h=\alpha)\\
&+p_2\mathbb{E}(\mathbf{u}^{\mathrm{T}}\mathbf{M}_2\cdots\mathbf{M}_{h-2}\mathbf{B}\mathbf{w}|\theta_h=\beta)\\
&+p_3\mathbb{E}(\mathbf{u}^{\mathrm{T}}\mathbf{M}_2\mathbf{M}_3\cdots\mathbf{M}_{h-2}\mathbf{C}\mathbf{w}|\theta_h=\gamma)\\
=&\mathbb{E}(\mathbf{u}^{\mathrm{T}}\mathbf{M}_2\mathbf{M}_3\cdots\mathbf{M}_{h-2}(p_1\mathbf{A}+p_2\mathbf{B}+p_3\mathbf{C})\mathbf{w})\\
=&\mathbb{E}(\mathbf{u}^{\mathrm{T}}\mathbf{M}_2\mathbf{M}_3\cdots\mathbf{M}_{h-2}\mathbf{S}\mathbf{w})\\
=&p_1\mathbb{E}(\mathbf{u}^{\mathrm{T}}\mathbf{M}_2\cdots\mathbf{M}_{h-3}\mathbf{A}\mathbf{S}\mathbf{w}|\theta_{h-1}=\alpha)\\
&+p_2\mathbb{E}(\mathbf{u}^{\mathrm{T}}\mathbf{M}_2\cdots\mathbf{M}_{h-3}\mathbf{B}\mathbf{S}\mathbf{w}|\theta_{h-1}=\beta)\\
&+p_3\mathbb{E}(\mathbf{u}^{\mathrm{T}}\mathbf{M}_2\mathbf{M}_3\cdots\mathbf{M}_{h-3}\mathbf{C}\mathbf{S}\mathbf{w}|\theta_{h-1}=\gamma)\\
=&\cdots\\
=&p_1\mathbb{E}(\mathbf{u}^{\mathrm{T}}\mathbf{A}\mathbf{S}^{h-3}\mathbf{w}|\theta_3=\alpha)\\
&+p_2\mathbb{E}(\mathbf{u}^{\mathrm{T}}\mathbf{B}\mathbf{S}^{h-3}\mathbf{w}|\theta_3=\beta)\\
&+p_3\mathbb{E}(\mathbf{u}^{\mathrm{T}}\mathbf{C}\mathbf{S}^{h-3}\mathbf{w}|\theta_3=\gamma)\\
=&\mathbf{u}^{\mathrm{T}}(p_1\mathbf{A}+p_2\mathbf{B}+p_3\mathbf{C})\mathbf{S}^{h-3}\mathbf{w}=\mathbf{u}^{\mathrm{T}}\mathbf{S}^{h-2}\mathbf{w}.
\end{aligned}$$

Therefore, we complete the proof. ■

4 Independence polynomials of benzenoid chains

To derive the reduced formula for computing the independence polynomial of benzenoid chains, we need a column polynomial vector relating the independence polynomial at an edge $uv \in E(G)$ as follows:

$$\phi_{uv}(G;x) = (\phi(G;x), \phi(G-u;x), \phi(G-v;x), \phi(G-u-v;x))^{\mathrm{T}}.$$

Lemma 4.1. *Let G be a graph obtained from the edge-coalescence of H and a hexagon $C_6 = uvqtsp$ at edge st, see* Figure 2(a). *Then we have*

$\phi_{uv}(G;x) = \mathbf{P}(x)\phi_{st}(H;x)$, *where*

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

Proof. By the definition of the column vector $\phi_{uv}(G;x)$ at a given edge uv, we just need to consider the values $\phi(G;x)$, $\phi(G-u;x)$, $\phi(G-v;x)$ and $\phi(G-u-v;x)$. Bearing in mind that $\phi(P_1;x) = 1+x$ and $\phi(P_2;x) = 1+2x$, by using Lemma 2.2 we deduce that

$$\begin{aligned}
\phi(G;x) =& \phi(G-p;x) + x\phi(G-N[p];x) \\
=& \phi(G-p-q;x) + x\phi(G-p-N[q];x) \\
& + x\phi(G-N[p]-q;x) + x^2\phi(G-N[p]-N[q];x) \\
=& \phi(P_2;x)\phi(H;x) + x\phi(P_1;x)\phi(H-t;x) \\
& + x\phi(P_1;x)\phi(H-s;x) + x^2\phi(P_1;x)\phi(H-s-t;x) \\
=& (1+2x)\phi(H;x) + (x+x^2)\phi(H-s;x) \\
& + (x+x^2)\phi(H-t;x) + x^2\phi(H-s-t;x) \\
=& (1+2x, x+x^2, x+x^2, x^2)\phi_{st}(H;x),
\end{aligned}$$

$$\begin{aligned}
\phi(G-u;x) =& \phi(G-u-p;x) + x\phi(G-u-N[p];x) \\
=& \phi(G-u-p-q;x) + x\phi(G-u-p-N[q];x) \\
& + x\phi(G-u-N[p]-q;x) \\
& + x^2\phi(G-u-N[p]-N[q];x) \\
=& \phi(P_1;x)\phi(H;x) + x\phi(H-t;x) \\
& + x\phi(P_1;x)\phi(H-s;x) + x^2\phi(H-s-t;x) \\
=& (1+x)\phi(H;x) + (x+x^2)\phi(H-s;x) \\
& + x\phi(H-t;x) + x^2\phi(H-s-t;x) \\
=& (1+x, x+x^2, x, x^2)\phi_{st}(H;x),
\end{aligned}$$

$$\begin{aligned}\phi(G-v;x) =&\phi(G-v-p;x)+x\phi(G-v-N[p];x)\\ =&\phi(G-v-p-q;x)+x\phi(G-v-p-N[q];x)\\ &+x\phi(G-v-N[p]-q;x)+x^2\phi(G-v-N[p]-N[q];x)\\ =&\phi(P_1;x)\phi(H;x)+x\phi(P_1;x)\phi(H-t;x)\\ &+x\phi(H-s;x)+x^2\phi(H-s-t;x)\\ =&(1+x)\phi(H;x)+x\phi(H-s;x)\\ &+(x+x^2)\phi(H-t;x)+x^2\phi(H-s-t;x)\\ =&(1+x,x,x+x^2,x^2)\phi_{st}(H;x)\end{aligned}$$

and

$$\begin{aligned}\phi(G-u-v;x) =&\phi(G-u-v-p;x)+x\phi(G-u-v-N[p];x)\\ =&\phi(G-u-v-p-q;x)+x\phi(G-u-v-p-N[q];x)\\ &+x\phi(G-u-v-N[p]-q;x)\\ &+x^2\phi(G-u-v-N[p]-N[q];x)\\ =&\phi(H;x)+x\phi(H-s;x)+x\phi(H-t;x)\\ &+x^2\phi(H-s-t;x)\\ =&(1,x,x,x^2)\phi_{st}(H;x).\end{aligned}$$

Combining the above four equations, we get $\phi_{uv}(G;x) = \mathbf{P}(x)\phi_{st}(H;x)$. ■

Lemma 4.2. *Let G be a graph obtained from the edge-coalescence of H and a hexagon $C_6 = uvqtsp$ at edge ps, see* Figure 2(b). *Then $\phi_{uv}(G;x) = \mathbf{Q}(x)\phi_{ps}(H;x)$, where*

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

Proof. By utilizing Lemma 2.2 we have

$$\begin{aligned}\phi(G;x) =&(1+2x)\phi(H;x) + x\phi(H-p;x) + x\phi(H-s;x)\\ &+ x^2\phi(H-p-s;x)\\ =&(1+2x, x+x^2, x+x^2, x^2)\phi_{ps}(H;x),\end{aligned}$$

$$\begin{aligned}\phi(G-u;x) =&(1+2x)\phi(H;x) + (x+x^2)\phi(H-s;x)\\ =&(1+2x, 0, x+x^2, 0)\phi_{ps}(H;x),\end{aligned}$$

$$\begin{aligned}\phi(G-v;x) =&(1+x)\phi(H;x) + (x+x^2)\phi(H-p;x)\\ &+ x\phi(H-s;x) + x^2\phi(H-p-s;x)\\ =&(1+x, x+x^2, x, x^2)\phi_{ps}(H;x),\end{aligned}$$

and

$$\begin{aligned}\phi(G-u-v;x) =&(1+x)\phi(H;x) + x\phi(H-s;x)\\ =&(1+x, 0, x, 0)\phi_{ps}(H;x).\end{aligned}$$

Thus we get $\phi_{uv}(G;x) = \mathbf{Q}(x)\phi_{ps}(H;x)$. ■

Lemma 4.3. *Let G be a graph obtained from the edge-coalescence of H and a hexagon $C_6 = uvqtsp$ at edge tq, see* Figure 2(c). *Then $\phi_{uv}(G;x) = \mathbf{R}(x)\phi_{tq}(H;x)$, where*

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

Proof. By employing Lemma 2.2 we have the following four equations.

$$\begin{aligned}\phi(G;x) =&(1+2x)\phi(H;x) + (x+x^2)\phi(H-t;x)\\ &+ (x+x^2)\phi(H-q;x) + x^2\phi(H-q-t;x)\end{aligned}$$

$$=(1+2x, x+x^2, x+x^2, x^2)\phi_{tq}(H;x),$$

$$\begin{aligned}\phi(G-u;x) =&(1+x)\phi(H;x)+x\phi(H-t;x)\\ &+(x+x^2)\phi(H-q;x)+x^2\phi(H-t-q;x),\\ =&(1+x, x, x+x^2, x^2)\phi_{tq}(H;x),\end{aligned}$$

$$\begin{aligned}\phi(G-v;x) =&(1+2x)\phi(H;x)+(x+x^2)\phi(H-t;x)\\ =&(1+2x, x+x^2, 0, 0)\phi_{tq}(H;x),\end{aligned}$$

$$\begin{aligned}\phi(G-u-v;x) =&(1+x)\phi(H;x)+x\phi(H-t;x)\\ =&(1+x, x, 0, 0)\phi_{tq}(H;x).\end{aligned}$$

Hence, we get $\phi_{uv}(G;x)=\mathbf{R}(x)\phi_{tq}(H;x)$. ■

Using a method similar to Theorem 3.1, by Lemmas 4.1, 4.2 and 4.3, one can get the following conclusion.

Theorem 4.1. *Let $B(\theta_3, \theta_4, \ldots, \theta_h)$ be a benzenoid chain with h hexagons. Then the independence polynomial of $B(\theta_3, \theta_4, \ldots, \theta_h)$ is given by*

$$\phi(B(\theta_3, \theta_4, \ldots, \theta_h);x)=\mathbf{f}^{\mathrm{T}}\mathbf{M}_2(x)\mathbf{M}_3(x)\cdots\mathbf{M}_{h-1}(x)\mathbf{h},$$

where $\mathbf{f}=(1+2x, x+x^2, x+x^2, x^2)^{\mathrm{T}}$, $\mathbf{h}=(1+6x+9x^2+2x^3, 1+5x+6x^2+x^3, 1+5x+6x^2+x^3, 1+4x+3x^2)^{\mathrm{T}}$ *and*

$$\mathbf{M}_i(x)=\begin{cases}\mathbf{P}(x) & \text{if } \theta_{i+1}=\alpha,\\ \mathbf{Q}(x) & \text{if } \theta_{i+1}=\beta,\\ \mathbf{R}(x) & \text{if } \theta_{i+1}=\gamma.\end{cases}$$

Theorem 4.1 shows that the independence polynomial of any benzenoid chain can be derived by multiplying particular 4×4 matrices and two terminal vectors. As an example, for the benzenoid chain $G=B(\gamma, \alpha, \beta, \gamma, \gamma, \alpha, \beta, \beta, \gamma, \beta)$ illustrated in Figure 1, applying Theorem 4.1

one can get easily that

$$\begin{aligned}\phi(G;x) =&\mathbf{f}^{\mathrm{T}}\mathbf{R}(x)\mathbf{P}(x)\mathbf{Q}(x)\mathbf{R}(x)\mathbf{R}(x)\mathbf{P}(x)\mathbf{Q}(x)\mathbf{Q}(x)\mathbf{R}(x)\mathbf{Q}(x)\mathbf{h}\\ =&2x^{25}+149x^{24}+4716x^{23}+84219x^{22}+944939x^{21}+7113921x^{20}\\ &+37612865x^{19}+144452239x^{18}+413698802x^{17}+902406309x^{16}\\ &+1525202659x^{15}+2025080563x^{14}+2135176098x^{13}\\ &+1802245211x^{12}+1224596278x^{11}+671898432x^{10}\\ &+297831095x^{9}+106415501x^{8}+30479416x^{7}+6931079x^{6}\\ &+1232582x^{5}+167478x^{4}+16766x^{3}+1164x^{2}+50x+1.\end{aligned}$$

For all the benzenoid chains with 5 hexagons and benzenoid chains with 6 hexagons, the independence polynomials are listed in Appendix.

Since the Merrifield-Simmons index of a graph G can be obtained by $\sigma(G)=\phi(G;1)$, then from Theorem 4.1 we have

Theorem 4.2. *Let $B(\theta_3,\theta_4,\ldots,\theta_h)$ be a benznoid chain with h hexagons. Then the Merrifield-Simmons index of $B(\theta_3,\theta_4,\ldots,\theta_h)$ is given by*

$$\sigma(B(\theta_3,\theta_4,\ldots,\theta_h))=\mathbf{s}^{\mathrm{T}}\mathbf{M}_2\mathbf{M}_3\cdots\mathbf{M}_{h-1}\mathbf{t},$$

where $\mathbf{s}=(3,2,2,1)^{\mathrm{T}}$, $\mathbf{t}=(18,13,13,8)^{\mathrm{T}}$, $\mathbf{M}_i=\begin{cases}\mathbf{P}, & \textit{if } \theta_{i+1}=\alpha;\\ \mathbf{Q}, & \textit{if } \theta_{i+1}=\beta;\\ \mathbf{R}, & \textit{if } \theta_{i+1}=\gamma\end{cases}$ *and*

$$\mathbf{P}=\begin{pmatrix}3&2&2&1\\2&2&1&1\\2&1&2&1\\1&1&1&1\end{pmatrix},\mathbf{Q}=\begin{pmatrix}3&2&2&1\\3&0&2&0\\2&2&1&1\\2&0&1&0\end{pmatrix},\mathbf{R}=\begin{pmatrix}3&2&2&1\\2&1&2&1\\3&2&0&0\\2&1&0&0\end{pmatrix}.$$

Applying Theorem 4.2, the Merrifield-Simmons indices of benzenoid chains with h hexagons are listed in Table 1 and Table 2 for $h=5$ and $h=6$, respectively.

The explicit closed formula for the Merrifield-Simmons index of linear chain L_h is in the following.

Corollary 4.1. *For a linear chain L_h with $h \geq 3$ hexagons, we have $\sigma(L_h) = \mathbf{s}^{\mathrm{T}}\mathbf{P}^{h-2}\mathbf{t} = \frac{33+5\sqrt{33}}{22}\left(\frac{7+\sqrt{33}}{2}\right)^h + \frac{33-5\sqrt{33}}{22}\left(\frac{7-\sqrt{33}}{2}\right)^h$.*

Proof. We can diagonalize matrix $\mathbf{P}$ as

$$\mathbf{U}^{-1}\mathbf{P}\mathbf{U} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{7-\sqrt{33}}{2} & 0 \\ 0 & 0 & 0 & \frac{7+\sqrt{33}}{2} \end{pmatrix},$$

where

$$\mathbf{U} = \begin{pmatrix} 1 & 0 & \frac{3\left(5\sqrt{33}-29\right)}{7\sqrt{33}-39} & \frac{3\left(5\sqrt{33}+29\right)}{7\sqrt{33}+39} \\ -1 & -1 & \frac{11\sqrt{33}-63}{7\sqrt{33}-39} & \frac{11\sqrt{33}+63}{7\sqrt{33}+39} \\ -1 & 1 & \frac{11\sqrt{33}-63}{7\sqrt{33}-39} & \frac{11\sqrt{33}+63}{7\sqrt{33}+39} \\ 1 & 0 & 1 & 1 \end{pmatrix}$$

and

$$\mathbf{U}^{-1} = \begin{pmatrix} \frac{1}{4} & -\frac{1}{4} & -\frac{1}{4} & \frac{1}{4} \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ \frac{-5\sqrt{33}-11}{88} & \frac{1}{8} - \frac{1}{8\sqrt{33}} & \frac{1}{8} - \frac{1}{8\sqrt{33}} & \frac{3}{8} + \frac{13}{8\sqrt{33}} \\ \frac{5\sqrt{33}-11}{88} & \frac{\sqrt{33}+33}{264} & \frac{\sqrt{33}+33}{264} & \frac{3}{8} - \frac{13}{8\sqrt{33}} \end{pmatrix}.$$

Then,

$$\mathbf{P}^{h-2} = \mathbf{U} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \left(\frac{7-\sqrt{33}}{2}\right)^{h-2} & 0 \\ 0 & 0 & 0 & \left(\frac{\sqrt{33}+7}{2}\right)^{h-2} \end{pmatrix} \mathbf{U}^{-1}.$$

Thus, by Theorem 4.2 we get $\sigma(L_h) = \mathbf{s}^{\mathrm{T}}\mathbf{P}^{h-2}\mathbf{t} = \frac{33+5\sqrt{33}}{22}\left(\frac{7+\sqrt{33}}{2}\right)^h + \frac{33-5\sqrt{33}}{22}\left(\frac{7-\sqrt{33}}{2}\right)^h$. ■

Corollary 4.2. *For a helicene chain H_h with $h \geq 3$ hexagons, we have $\sigma(H_h) = \mathbf{s}^{\mathrm{T}}\mathbf{Q}^{h-2}\mathbf{t} = \mathbf{s}^{\mathrm{T}}\mathbf{R}^{h-2}\mathbf{t}$.*

Corollary 4.3. *For a zig-zag chain Z_h with $h \geq 3$ hexagons, we have*

$$\sigma(Z_h) = \begin{cases} \mathbf{s}^{\mathrm{T}}(\mathbf{QR})^{\frac{h-2}{2}}\mathbf{t} & \textit{if } h \textit{ is even,} \\ \mathbf{s}^{\mathrm{T}}(\mathbf{QR})^{\frac{h-3}{2}}\mathbf{Qt} & \textit{if } h \textit{ is odd.} \end{cases}$$

In the following, we give the expected value of Merrifield-Simmons index for a random benzenoid chain.

Theorem 4.3. *The expected value of the Merrifield-Simmons index of a random benzenoid chain $B_h(p_1, p_2, p_3)$, $p_3 = 1 - p_1 - p_2$, is given by*

$$\mathbb{E}(\sigma(B_h(p_1, p_2, p_3))) = \mathbf{s}^{\mathrm{T}}\mathbf{W}^{h-2}\mathbf{t},$$

where $\mathbf{s} = (3, 2, 2, 1)^{\mathrm{T}}$, $\mathbf{t} = (18, 13, 13, 8)^{\mathrm{T}}$ *and*

$$\mathbf{W} = \begin{pmatrix} 3 & 2 & 2 & 1 \\ 2 + p_2 & 1 - p_1 + p_2 & 2 - p_1 & 1 - p_2 \\ 3 - p_1 - p_2 & 2 - p_1 & 2p_1 + p_2 & p_1 + p_2 \\ 2 - p_1 & 1 - p_2 & p_1 + p_2 & p_1 \end{pmatrix}.$$

Proof. Let

$$\begin{aligned} \mathbf{W} =& p_1\mathbf{P} + p_2\mathbf{Q} + p_3\mathbf{R} \\ =& \begin{pmatrix} 3 & 2 & 2 & 1 \\ 2 + p_2 & 1 - p_1 + p_2 & 2 - p_1 & 1 - p_2 \\ 3 - p_1 - p_2 & 2 - p_1 & 2p_1 + p_2 & p_1 + p_2 \\ 2 - p_1 & 1 - p_2 & p_1 + p_2 & p_1 \end{pmatrix}. \end{aligned}$$

Then by the law of total expectation [7, 19] and Theorem 4.2, we have

$$\begin{aligned} \mathbb{E}(\sigma(B(\theta_3, \theta_4, \ldots, \theta_h))) =& \mathbb{E}(\mathbf{s}^{\mathrm{T}}\mathbf{M}_2\mathbf{M}_3 \cdots \mathbf{M}_{h-1}\mathbf{t}) \\ =& p_1\mathbb{E}(\mathbf{s}^{\mathrm{T}}\mathbf{M}_2 \cdots \mathbf{M}_{h-2}\mathbf{Pt}|\theta_h = \alpha) \\ & + p_2\mathbb{E}(\mathbf{s}^{\mathrm{T}}\mathbf{M}_2 \cdots \mathbf{M}_{h-2}\mathbf{Qt}|\theta_h = \beta) \\ & + p_3\mathbb{E}(\mathbf{s}^{\mathrm{T}}\mathbf{M}_2\mathbf{M}_3 \cdots \mathbf{M}_{h-2}\mathbf{Rt}|\theta_h = \gamma) \\ =& \mathbb{E}(\mathbf{s}^{\mathrm{T}}\mathbf{M}_2\mathbf{M}_3 \cdots \mathbf{M}_{h-2}(p_1\mathbf{P} + p_2\mathbf{Q} + p_3\mathbf{R})\mathbf{t}) \end{aligned}$$

$$
\begin{aligned}
&=\mathbb{E}(\mathbf{s}^{\mathrm{T}}\mathbf{M}_2\mathbf{M}_3\cdots\mathbf{M}_{h-2}\mathbf{W}\mathbf{t})\\
&=p_1\mathbb{E}(\mathbf{s}^{\mathrm{T}}\mathbf{M}_2\cdots\mathbf{M}_{h-3}\mathbf{P}\mathbf{W}\mathbf{t}|\theta_{h-1}=\alpha)\\
&\quad+p_2\mathbb{E}(\mathbf{s}^{\mathrm{T}}\mathbf{M}_2\cdots\mathbf{M}_{h-3}\mathbf{Q}\mathbf{W}\mathbf{t}|\theta_{h-1}=\beta)\\
&\quad+p_3\mathbb{E}(\mathbf{s}^{\mathrm{T}}\mathbf{M}_2\mathbf{M}_3\cdots\mathbf{M}_{h-3}\mathbf{R}\mathbf{W}\mathbf{t}|\theta_{h-1}=\gamma)\\
&=\cdots\\
&=p_1\mathbb{E}(\mathbf{s}^{\mathrm{T}}\mathbf{P}\mathbf{W}^{h-3}\mathbf{t}|\theta_3=\alpha)\\
&\quad+p_2\mathbb{E}(\mathbf{s}^{\mathrm{T}}\mathbf{Q}\mathbf{W}^{h-3}\mathbf{t}|\theta_3=\beta)\\
&\quad+p_3\mathbb{E}(\mathbf{s}^{\mathrm{T}}\mathbf{R}\mathbf{W}^{h-3}\mathbf{t}|\theta_3=\gamma)\\
&=\mathbf{s}^{\mathrm{T}}(p_1\mathbf{P}+p_2\mathbf{Q}+p_3\mathbf{R})\mathbf{W}^{h-3}\mathbf{t}=\mathbf{s}^{\mathrm{T}}\mathbf{W}^{h-2}\mathbf{t}.
\end{aligned}
$$

Therefore, we complete the proof. ■

5 Conclusion

In this paper, we have effectively obtained reduction formulas for the matching polynomial and independence polynomial of benzenoid chains through the utilization of the transfer matrix technique. These formulas have facilitated the computation of the Hosoya index and Merrifield-Simmons index for benzenoid chains with h hexagons, and have also enabled the derivation of explicit formulas for the expected values of these indices in random benzenoid chains. Moreover, the techniques developed in this study can be naturally extended to compute matching polynomials and independence polynomials for catacondensed benzenoid systems and k-polygonal chains, such as polyomino chains, pentagonal chains, heptagonal chains, and octagonal chains.

Appendix

1. The matching polynomials of benzenoid chains with 5 hexagons.

   $\psi(B(\alpha,\alpha,\alpha);x) = 6x^{11} + 281x^{10} + 2706x^9 + 10407x^8 + 20314x^7 + 22653x^6 + 15382x^5 + 6557x^4 + 1758x^3 + 287x^2 + 26x + 1;$

$\psi(B(\alpha,\alpha,\beta);x) = 9x^{11} + 330x^{10} + 2945x^9 + 10922x^8 + 20872x^7 + 22976x^6 + 15483x^5 + 6573x^4 + 1759x^3 + 287x^2 + 26x + 1;$

$\psi(B(\alpha,\beta,\alpha);x) = 10x^{11} + 337x^{10} + 2978x^9 + 10971x^8 + 20903x^7 + 22985x^6 + 15484x^5 + 6573x^4 + 1759x^3 + 287x^2 + 26x + 1;$

$\psi(B(\alpha,\beta,\beta);x) = 11x^{11} + 364x^{10} + 3134x^9 + 11344x^8 + 21338x^7 + 23253x^6 + 15573x^5 + 6588x^4 + 1760x^3 + 287x^2 + 26x + 1;$

$\psi(B(\alpha,\beta,\gamma);x) = 11x^{11} + 366x^{10} + 3154x^9 + 11407x^8 + 21417x^7 + 23297x^6 + 15584x^5 + 6589x^4 + 1760x^3 + 287x^2 + 26x + 1;$

$\psi(B(\beta,\alpha,\beta);x) = 12x^{11} + 379x^{10} + 3184x^9 + 11437x^8 + 21430x^7 + 23299x^6 + 15584x^5 + 6589x^4 + 1760x^3 + 287x^2 + 26x + 1;$

$\psi(B(\beta,\alpha,\gamma);x) = 12x^{11} + 380x^{10} + 3190x^9 + 11448x^8 + 21436x^7 + 23300x^6 + 15584x^5 + 6589x^4 + 1760x^3 + 287x^2 + 26x + 1;$

$\psi(B(\beta,\beta,\beta);x) = 13x^{11} + 400x^{10} + 3320x^9 + 11762x^8 + 21803x^7 + 23530x^6 + 15663x^5 + 6603x^4 + 1761x^3 + 287x^2 + 26x + 1;$

$\psi(B(\beta,\beta,\gamma);x) = 13x^{11} + 400x^{10} + 3327x^9 + 11797x^8 + 21859x^7 + 23566x^6 + 15673x^5 + 6604x^4 + 1761x^3 + 287x^2 + 26x + 1;$

$\psi(B(\beta,\gamma,\beta);x) = 13x^{11} + 402x^{10} + 3347x^9 + 11860x^8 + 21938x^7 + 23610x^6 + 15684x^5 + 6605x^4 + 1761x^3 + 287x^2 + 26x + 1.$

2. The matching polynomials of benzenoid chains with 6 hexagons.

$\psi(B(\alpha,\alpha,\alpha,\alpha);x) = 7x^{13} + 469x^{12} + 6374x^{11} + 34836x^{10} + 98213x^9 + 161973x^8 + 167919x^7 + 114157x^6 + 52024x^5 + 15962x^4 + 3247x^3 + 419x^2 + 31x + 1;$

$\psi(B(\alpha,\alpha,\alpha,\beta);x) = 11x^{13} + 571x^{12} + 7099x^{11} + 37185x^{10} + 102270x^9 + 166003x^8 + 170315x^7 + 115019x^6 + 52207x^5 + 15983x^4 + 3248x^3 + 419x^2 + 31x + 1;$

$\psi(B(\alpha,\alpha,\beta,\beta);x) = 14x^{13} + 641x^{12} + 7660x^{11} + 39093x^{10} + 105624x^9 + 169383x^8 + 172366x^7 + 115778x^6 + 52374x^5 + 16003x^4 + 3249x^3 + 419x^2 + 31x + 1;$

$\psi(B(\alpha,\beta,\alpha,\alpha);x) = 13x^{13} + 591x^{12} + 7223x^{11} + 37498x^{10} + 102640x^9 + 166234x^8 + 170394x^7 + 115033x^6 + 52208x^5 + 15983x^4 + 3248x^3 + 419x^2 + 31x + 1;$

$\psi(B(\alpha,\beta,\alpha,\beta);x) = 17x^{13} + 693x^{12} + 7948x^{11} + 39847x^{10} + 106697x^9 + 170264x^8 + 172790x^7 + 115895x^6 + 52391x^5 + 16004x^4 + 3249x^3 + 419x^2 + 31x + 1;$

$\psi(B(\alpha,\beta,\alpha,\gamma);x) = 17x^{13} + 695x^{12} + 7968x^{11} + 39910x^{10} + 106776x^9 + 170308x^8 + 172801x^7 + 115896x^6 + 52391x^5 + 16004x^4 + 3249x^3 + 419x^2 + 31x + 1;$

$\psi(B(\alpha,\beta,\beta,\alpha);x) = 15x^{13} + 653x^{12} + 7744x^{11} + 39324x^{10} + 105914x^9 + 169574x^8 + 172435x^7 + 115791x^6 + 52375x^5 + 16003x^4 + 3249x^3 + 419x^2 + 31x + 1;$

$\psi(B(\alpha,\beta,\beta,\gamma);x) = 18x^{13} + 728x^{12} + 8313x^{11} + 41300x^{10} + 109536x^9 + 173336x^8 + 174742x^7 + 116638x^6 + 52557x^5 + 16024x^4 + 3250x^3 + 419x^2 + 31x + 1;$

$\psi(B(\alpha,\beta,\gamma,\alpha);x) = 15x^{13} + 657x^{12} + 7800x^{11} + 39596x^{10} + 106478x^9 + 170163x^8 + 172767x^7 + 115893x^6 + 52391x^5 + 16004x^4 + 3249x^3 + 419x^2 + 31x + 1;$

$\psi(B(\alpha,\beta,\gamma,\beta);x) = 18x^{13} + 732x^{12} + 8369x^{11} + 41572x^{10} + 110100x^9 + 173925x^8 + 175074x^7 + 116740x^6 + 52573x^5 + 16025x^4 + 3250x^3 + 419x^2 + 31x + 1;$

$\psi(B(\beta,\alpha,\alpha,\beta);x) = 16x^{13} + 684x^{12} + 7870x^{11} + 39626x^{10} + 106419x^9 + 170079x^8 + 172722x^7 + 115882x^6 + 52390x^5 + 16004x^4 + 3249x^3 + 419x^2 + 31x + 1;$

$\psi(B(\beta,\alpha,\alpha,\gamma);x) = 16x^{13} + 685x^{12} + 7876x^{11} + 39637x^{10} + 106425x^9 + 170080x^8 + 172722x^7 + 115882x^6 + 52390x^5 + 16004x^4 + 3249x^3 + 419x^2 + 31x + 1;$

$\psi(B(\beta,\alpha,\beta,\gamma);x) = 19x^{13} + 757x^{12} + 8480x^{11} + 41773x^{10} + 110288x^9 + 174017x^8 + 175096x^7 + 116742x^6 + 52573x^5 + 16025x^4 + 3250x^3 + 419x^2 + 31x + 1;$

$\psi(B(\beta,\alpha,\gamma,\beta);x) = 19x^{13} + 759x^{12} + 8500x^{11} + 41836x^{10} + 110367x^9 + 174061x^8 + 175107x^7 + 116743x^6 + 52573x^5 + 16025x^4 + 3250x^3 + 419x^2 + 31x + 1;$

$\psi(B(\beta,\alpha,\gamma,\gamma);x) = 19x^{13} + 755x^{12} + 8444x^{11} + 41580x^{10} + 109835x^9 + 173496x^8 + 174783x^7 + 116642x^6 + 52557x^5 + 16024x^4 + 3250x^3 + 419x^2 + 31x + 1;$

$\psi(B(\beta,\beta,\alpha,\beta);x) = 19x^{13} + 755x^{12} + 8437x^{11} + 41545x^{10} + 109779x^{9} + 173460x^{8} + 174773x^{7} + 116641x^{6} + 52557x^{5} + 16024x^{4} + 3250x^{3} + 419x^{2} + 31x + 1;$

$\psi(B(\beta,\beta,\beta,\alpha);x) = 18x^{13} + 729x^{12} + 8306x^{11} + 41207x^{10} + 109242x^{9} + 172945x^{8} + 174485x^{7} + 116550x^{6} + 52542x^{5} + 16023x^{4} + 3250x^{3} + 419x^{2} + 31x + 1;$

$\psi(B(\beta,\beta,\beta,\beta);x) = 21x^{13} + 805x^{12} + 8868x^{11} + 43090x^{10} + 112570x^{9} + 176316x^{8} + 176535x^{7} + 117309x^{6} + 52709x^{5} + 16043x^{4} + 3251x^{3} + 419x^{2} + 31x + 1;$

$\psi(B(\beta,\beta,\beta,\gamma);x) = 21x^{13} + 807x^{12} + 8897x^{11} + 43241x^{10} + 112932x^{9} + 176745x^{8} + 176802x^{7} + 117398x^{6} + 52724x^{5} + 16044x^{4} + 3251x^{3} + 419x^{2} + 31x + 1;$

$\psi(B(\beta,\beta,\gamma,\alpha);x) = 18x^{13} + 729x^{12} + 8320x^{11} + 41333x^{10} + 109585x^{9} + 173367x^{8} + 174751x^{7} + 116639x^{6} + 52557x^{5} + 16024x^{4} + 3250x^{3} + 419x^{2} + 31x + 1;$

$\psi(B(\beta,\beta,\gamma,\beta);x) = 21x^{13} + 807x^{12} + 8911x^{11} + 43367x^{10} + 113275x^{9} + 177167x^{8} + 177068x^{7} + 117487x^{6} + 52739x^{5} + 16045x^{4} + 3251x^{3} + 419x^{2} + 31x + 1;$

$\psi(B(\beta,\beta,\gamma,\gamma);x) = 21x^{13} + 805x^{12} + 8868x^{11} + 43139x^{10} + 112766x^{9} + 176610x^{8} + 176745x^{7} + 117386x^{6} + 52723x^{5} + 16044x^{4} + 3251x^{3} + 419x^{2} + 31x + 1;$

$\psi(B(\beta,\gamma,\alpha,\alpha);x) = 14x^{13} + 644x^{12} + 7709x^{11} + 39332x^{10} + 106139x^{9} + 169941x^{8} + 172689x^{7} + 115879x^{6} + 52390x^{5} + 16004x^{4} + 3249x^{3} + 419x^{2} + 31x + 1;$

$\psi(B(\beta,\gamma,\beta,\gamma);x) = 21x^{13} + 811x^{12} + 8967x^{11} + 43623x^{10} + 113807x^{9} + 177732x^{8} + 177392x^{7} + 117588x^{6} + 52755x^{5} + 16046x^{4} + 3251x^{3} + 419x^{2} + 31x + 1;$

$\psi(B(\beta,\gamma,\gamma,\beta);x) = 21x^{13} + 807x^{12} + 8911x^{11} + 43351x^{10} + 113243x^{9} + 177143x^{8} + 177060x^{7} + 117486x^{6} + 52739x^{5} + 16045x^{4} + 3251x^{3} + 419x^{2} + 31x + 1.$

3. The independence polynomials of benzenoid chains with 5 hexagons.

$\phi(B(\alpha,\alpha,\alpha);x) = 2x^{11} + 81x^{10} + 730x^{9} + 2921x^{8} + 6356x^{7} + 8210x^{6} + 6570x^{5} + 3322x^{4} + 1058x^{3} + 205x^{2} + 22x + 1;$

$\phi(B(\alpha,\alpha,\beta);x) = 2x^{11}+69x^{10}+662x^9+2786x^8+6234x^7+8155x^6+6558x^5+3321x^4+1058x^3+205x^2+22x+1;$

$\phi(B(\alpha,\beta,\alpha);x) = 2x^{11}+65x^{10}+650x^9+2773x^8+6228x^7+8154x^6+6558x^5+3321x^4+1058x^3+205x^2+22x+1;$

$\phi(B(\alpha,\beta,\beta);x) = 2x^{11}+61x^{10}+614x^9+2684x^8+6136x^7+8108x^6+6547x^5+3320x^4+1058x^3+205x^2+22x+1;$

$\phi(B(\alpha,\beta,\gamma);x) = 2x^{11}+61x^{10}+606x^9+2660x^8+6114x^7+8100x^6+6546x^5+3320x^4+1058x^3+205x^2+22x+1;$

$\phi(B(\beta,\alpha,\beta);x) = 2x^{11}+61x^{10}+602x^9+2656x^8+6113x^7+8100x^6+6546x^5+3320x^4+1058x^3+205x^2+22x+1;$

$\phi(B(\beta,\alpha,\gamma);x) = 2x^{11}+61x^{10}+598x^9+2652x^8+6112x^7+8100x^6+6546x^5+3320x^4+1058x^3+205x^2+22x+1;$

$\phi(B(\beta,\beta,\beta);x) = 2x^{11}+57x^{10}+570x^9+2583x^8+6038x^7+8061x^6+6536x^5+3319x^4+1058x^3+205x^2+22x+1;$

$\phi(B(\beta,\beta,\gamma);x) = 2x^{11}+57x^{10}+570x^9+2571x^8+6022x^7+8054x^6+6535x^5+3319x^4+1058x^3+205x^2+22x+1;$

$\phi(B(\beta,\gamma,\beta);x) = 2x^{11}+57x^{10}+562x^9+2547x^8+6000x^7+8046x^6+6534x^5+3319x^4+1058x^3+205x^2+22x+1.$

4. The independence polynomials of benzenoid chains with 6 hexagons.

$\phi(B(\alpha,\alpha,\alpha,\alpha);x) = 2x^{13}+109x^{12}+1306x^{11}+7058x^{10}+21342x^9+39803x^8+48162x^7+38860x^6+21182x^5+7795x^4+1902x^3+294x^2+26x+1;$

$\phi(B(\alpha,\alpha,\alpha,\beta);x) = 2x^{13}+93x^{12}+1162x^{11}+6582x^{10}+20566x^9+39109x^8+47806x^7+38756x^6+21166x^5+7794x^4+1902x^3+294x^2+26x+1;$

$\phi(B(\alpha,\alpha,\beta,\beta);x) = 2x^{13}+81x^{12}+1058x^{11}+6231x^{10}+19971x^9+38553x^8+47507x^7+38664x^6+21151x^5+7793x^4+1902x^3+294x^2+26x+1;$

$\phi(B(\alpha,\beta,\alpha,\alpha);x) = 2x^{13}+85x^{12}+1122x^{11}+6504x^{10}+20490x^9+39070x^8+47796x^7+38755x^6+21166x^5+7794x^4+1902x^3+294x^2+26x+1;$

$\phi(B(\alpha,\beta,\alpha,\beta);x) = 2x^{13} + 77x^{12} + 1010x^{11} + 6074x^{10} + 19744x^9 + 38385x^8 + 47441x^7 + 38651x^6 + 21150x^5 + 7793x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\alpha,\beta,\alpha,\gamma);x) = 2x^{13} + 77x^{12} + 1002x^{11} + 6050x^{10} + 19722x^9 + 38377x^8 + 47440x^7 + 38651x^6 + 21150x^5 + 7793x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\alpha,\beta,\beta,\alpha);x) = 2x^{13} + 77x^{12} + 1034x^{11} + 6178x^{10} + 19914x^9 + 38521x^8 + 47498x^7 + 38663x^6 + 21151x^5 + 7793x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\alpha,\beta,\beta,\gamma);x) = 2x^{13} + 73x^{12} + 958x^{11} + 5837x^{10} + 19260x^9 + 37882x^8 + 47154x^7 + 38560x^6 + 21135x^5 + 7792x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\alpha,\beta,\gamma,\alpha);x) = 2x^{13} + 77x^{12} + 1018x^{11} + 6098x^{10} + 19766x^9 + 38393x^8 + 47442x^7 + 38651x^6 + 21150x^5 + 7793x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\alpha,\beta,\gamma,\beta);x) = 2x^{13} + 73x^{12} + 942x^{11} + 5757x^{10} + 19112x^9 + 37754x^8 + 47098x^7 + 38548x^6 + 21134x^5 + 7792x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\beta,\alpha,\alpha,\beta);x) = 2x^{13} + 81x^{12} + 1034x^{11} + 6123x^{10} + 19797x^9 + 38416x^8 + 47450x^7 + 38652x^6 + 21150x^5 + 7793x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\beta,\alpha,\alpha,\gamma);x) = 2x^{13} + 81x^{12} + 1030x^{11} + 6119x^{10} + 19796x^9 + 38416x^8 + 47450x^7 + 38652x^6 + 21150x^5 + 7793x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\beta,\alpha,\beta,\gamma);x) = 2x^{13} + 73x^{12} + 942x^{11} + 5745x^{10} + 19096x^9 + 37747x^8 + 47097x^7 + 38548x^6 + 21134x^5 + 7792x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\beta,\alpha,\gamma,\beta);x) = 2x^{13} + 73x^{12} + 934x^{11} + 5721x^{10} + 19074x^9 + 37739x^8 + 47096x^7 + 38548x^6 + 21134x^5 + 7792x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\beta,\alpha,\gamma,\gamma);x) = 2x^{13} + 73x^{12} + 946x^{11} + 5789x^{10} + 19209x^9 + 37861x^8 + 47151x^7 + 38560x^6 + 21135x^5 + 7792x^4 + 1902x^3 + 294x^2 +$

$26x + 1;$

$\phi(B(\beta,\beta,\alpha,\beta);x) = 2x^{13} + 73x^{12} + 946x^{11} + 5801x^{10} + 19225x^9 + 37868x^8 + 47152x^7 + 38560x^6 + 21135x^5 + 7792x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\beta,\beta,\beta,\alpha);x) = 2x^{13} + 73x^{12} + 954x^{11} + 5849x^{10} + 19327x^9 + 37966x^8 + 47199x^7 + 38571x^6 + 21136x^5 + 7792x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\beta,\beta,\beta,\beta);x) = 2x^{13} + 69x^{12} + 890x^{11} + 5552x^{10} + 18764x^9 + 37419x^8 + 46901x^7 + 38479x^6 + 21121x^5 + 7791x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\beta,\beta,\beta,\gamma);x) = 2x^{13} + 69x^{12} + 886x^{11} + 5520x^{10} + 18679x^9 + 37328x^8 + 46855x^7 + 38468x^6 + 21120x^5 + 7791x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\beta,\beta,\gamma,\alpha);x) = 2x^{13} + 73x^{12} + 954x^{11} + 5825x^{10} + 19247x^9 + 37876x^8 + 47153x^7 + 38560x^6 + 21135x^5 + 7792x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\beta,\beta,\gamma,\beta);x) = 2x^{13} + 69x^{12} + 886x^{11} + 5496x^{10} + 18599x^9 + 37238x^8 + 46809x^7 + 38457x^6 + 21119x^5 + 7791x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\beta,\beta,\gamma,\gamma);x) = 2x^{13} + 69x^{12} + 890x^{11} + 5552x^{10} + 18728x^9 + 37359x^8 + 46864x^7 + 38469x^6 + 21120x^5 + 7791x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\beta,\gamma,\alpha,\alpha);x) = 2x^{13} + 81x^{12} + 1046x^{11} + 6163x^{10} + 19836x^9 + 38431x^8 + 47452x^7 + 38652x^6 + 21150x^5 + 7793x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\beta,\gamma,\beta,\gamma);x) = 2x^{13} + 69x^{12} + 874x^{11} + 5428x^{10} + 18464x^9 + 37116x^8 + 46754x^7 + 38445x^6 + 21118x^5 + 7791x^4 + 1902x^3 + 294x^2 + 26x + 1;$

$\phi(B(\beta,\gamma,\gamma,\beta);x) = 2x^{13} + 69x^{12} + 890x^{11} + 5508x^{10} + 18612x^9 + 37244x^8 + 46810x^7 + 38457x^6 + 21119x^5 + 7791x^4 + 1902x^3 + 294x^2 + 26x + 1.$

Table 1. The z-index and σ-index of benzenoid chains with 5 hexagons.

Benzenoid chain	z-index	σ-index	Benzenoid chain	z-index	σ-index
$B(\alpha,\alpha,\alpha)$	80378	29478	$B(\beta,\alpha,\beta)$	83988	28686
$B(\alpha,\alpha,\beta)$	82183	29073	$B(\beta,\alpha,\gamma)$	84013	28677
$B(\alpha,\beta,\alpha)$	82314	29037	$B(\beta,\beta,\beta)$	85169	28452
$B(\alpha,\beta,\beta)$	83679	28758	$B(\beta,\beta,\gamma)$	85314	28416
$B(\alpha,\beta,\gamma)$	83899	28695	$B(\beta,\gamma,\beta)$	85534	28353

Table 2. The z-index and σ-index of benzenoid chains with 6 hexagons.

Benzenoid chain	z-index	σ-index	Benzenoid chain	z-index	σ-index
$B(\alpha,\alpha,\alpha,\alpha)$	655632	187842	$B(\beta,\alpha,\gamma,\beta)$	699691	180336
$B(\alpha,\alpha,\alpha,\beta)$	670362	185259	$B(\beta,\alpha,\gamma,\gamma)$	697836	180741
$B(\alpha,\alpha,\beta,\beta)$	682636	183234	$B(\beta,\beta,\alpha,\beta)$	697691	180777
$B(\alpha,\beta,\alpha,\alpha)$	671516	185007	$B(\beta,\beta,\beta,\alpha)$	695748	181092
$B(\alpha,\beta,\alpha,\beta)$	686246	182550	$B(\beta,\beta,\beta,\beta)$	707968	179211
$B(\alpha,\beta,\alpha,\gamma)$	686466	182487	$B(\beta,\beta,\beta,\gamma)$	709313	178941
$B(\alpha,\beta,\beta,\alpha)$	683528	183054	$B(\beta,\beta,\gamma,\alpha)$	697024	180840
$B(\alpha,\beta,\beta,\gamma)$	696893	180876	$B(\beta,\beta,\gamma,\beta)$	710589	178689
$B(\alpha,\beta,\gamma,\alpha)$	685464	182613	$B(\beta,\beta,\gamma,\gamma)$	708809	179067
$B(\alpha,\beta,\gamma,\beta)$	698829	180435	$B(\beta,\gamma,\alpha,\alpha)$	684441	182829
$B(\beta,\alpha,\alpha,\beta)$	685392	182721	$B(\beta,\gamma,\beta,\gamma)$	712444	178284
$B(\beta,\alpha,\alpha,\gamma)$	685417	182712	$B(\beta,\gamma,\gamma,\beta)$	710508	178725
$B(\beta,\alpha,\beta,\gamma)$	699471	180399			

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