Computing Hosoya and Merrifield-Simmons Indices of Two Special Benzenoid Systems

Mert Sinan OZ *and Ismail Naci CANGUL†

Faculty of Engineering and Natural Sciences, Department of Mathematics, Bursa Technical University, 16320 Bursa, Turkey

Faculty of Arts and Science, Department of Mathematics, Bursa Uludag University, 16059 Bursa, Turkey

28th July 2021

Abstract

Gutman et al. gave some relations for computing the Hosoya indices of two special benzenoid systems $\mathcal{R}_n$ and $\mathcal{P}_n$. In this paper, we compute the Hosoya index and Merrifield-Simmons index of $\mathcal{R}_n$ and $\mathcal{P}_n$ by means of introducing four vectors for each benzenoid system and index. As a result, we compute the Hosoya index and the Merrifield-Simmons index of $\mathcal{R}_n$ and $\mathcal{P}_n$ by means of a product of a certain matrix of degree n and a certain vector.

1 Introduction

Let $G = (V, E)$ be a finite simple graph with n vertices and m edges. A matching in G is a set of independent edges such that no two edges have a common vertex. A matching containing k mutually independent edges is called a $k-$matching. Maximum possible value of k in G is called the $k-$matching number and it is denoted by $p(G, k)$. By definition $p(G, 0) = 1$. The Hosoya index (Z index) of G was defined by Hosoya in [7]. It is denoted by $Z(G)$ and is defined as

$$Z(G) = \sum_{k=0}^{r} p(G, k)$$

*sinan.oz@btu.edu.tr

†cangul@uludag.edu.tr

AMS 2010 Subject Classification Number: 05C09, 05C92

Keywords: Benzenoid systems, hexagonal systems, Hosoya index, Merrifield-Simmons index

where $p(G, r) \neq 0$ whereas $p(G, r + 1) = 0$.

A set containing all neighbor vertices of a vertex v is called the neighborhood set of v and we denote it by $N_G(v)$. Closed neighborhood set of v is a set containing all neighbor vertices of v with v itself and we denote it by $N_G[v]$. Clearly, $N_G[v] = N_G(v) \cup \{v\}$. If any two vertices in a subset of $V(G)$ are not adjacent, then the subset is called an independent vertex set of G. We denote the number of possible independent vertex sets in G with k vertices by $n(G, k)$. By definition, $n(G, 0) = 1$ for all graphs and it is clear that $n(G, 1) = m$. The Merrifield-Simmons index of G is denoted by $\sigma(G)$ and it is defined as

$$\sigma(G) = \sum_{k=0}^{r} n(G, k)$$

where $n(G, r) \neq 0$ whereas $n(G, r + 1) = 0$ in [9].

The Hosoya index and the Merrifield-Simmons index are two best known topological invariants that play an important role in chemical graph theory. They are intensively used and studied as molecular descriptors for determining some physico-chemical properties of corresponding molecules in mathematical chemistry, see for detailed survey [3, 16]. In recent years, numerous papers have been published on the Hosoya index and Merrifield-Simmons index of various molecular structures, some of them are listed in [2, 5, 8, 14–17].

Benzenoid systems are represented as finite $2-$ connected graphs where the closed regions are regular hexagons. In a benzenoid system, a vertex can belong to at most three hexagons and a vertex that belongs to three hexagons is called an internal vertex of the corresponding benzenoid system. A benzenoid system with no internal vertex is called catacondensed benzenoid system. Conversely, if a benzenoid system has at least one internal vertex, then it is called pericondensed benzenoid system, see for more details [4]. Some studies on benzenoid (hexagonal) systems can be found in [1, 6, 10–13]. Let us denote two types of pericondensed benzenoid systems in Fig. 1 and Fig. 2 by $\mathcal{R}_n$ and $\mathcal{P}_n$.

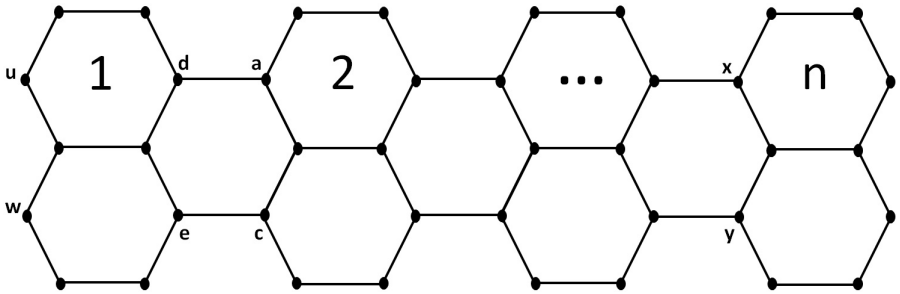


Figure 1: Benzenoid system $\mathcal{R}_n$

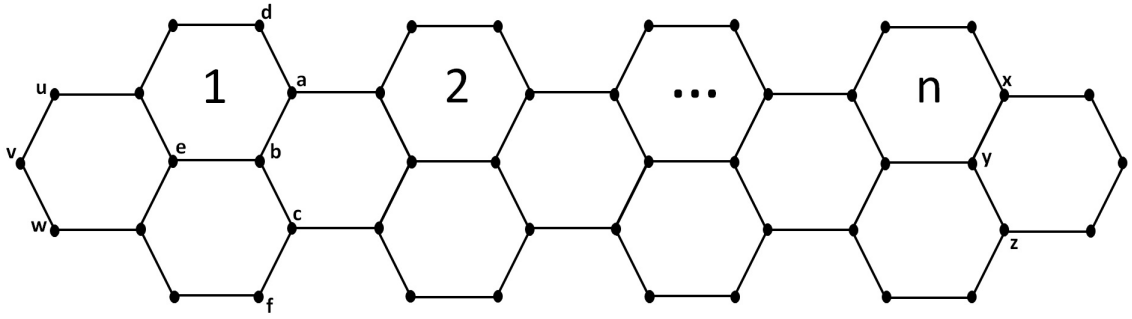


Figure 2: Benzenoid system $\mathcal{P}_n$

Gutman et al. gave relations for computing the Hosoya indices of the benzenoid systems $\mathcal{R}_n$ and $\mathcal{P}_n$ in [5]. In the next section, we compute the Hosoya index and Merrifield-Simmons index of benzenoid systems $\mathcal{R}_n$ and $\mathcal{P}_n$ by means of introducing four vectors for each value.

2 Computing the Hosoya index of benzenoid systems $\mathcal{R}_n$ and $\mathcal{P}_n$

The most used recurrence relations to compute the Hosoya and Merrifield-Simmons indices of a graph G are as follows, see [16]:

$$Z(G) = \prod_{i=1}^{k} Z(G_i), \text{ where } G_1, G_2, \cdots, G_k \text{ are connected components of } G. \tag{1a}$$

$$Z(G) = Z(G - ab) + Z(G - a - b), \text{ for an edge } e = ab \text{ of } G. \tag{1b}$$

$$\sigma(G) = \prod_{i=1}^{k} \sigma(G_i), \text{ where } G_1, G_2, \cdots, G_k \text{ are connected components of } G. \tag{1c}$$

$$\sigma(G) = \sigma(G - ab) - \sigma(G - (N_G[a] \cup N_G[b])), \text{ for an edge } e = ab \text{ of } G. \tag{1d}$$

In the next definition, we introduce the Hosoya vector of a graph G at the path P_3 by means of two terminal vertices.

Definition 2.1. *Let G be a graph. The Hosoya vector of G at the path P_3 with the terminal vertices u and w (see Fig. 3) is defined as*

$$Z_{uw}(G) = [Z(G), Z(G - u), Z(G - w), Z(G - u - w)]^T.$$

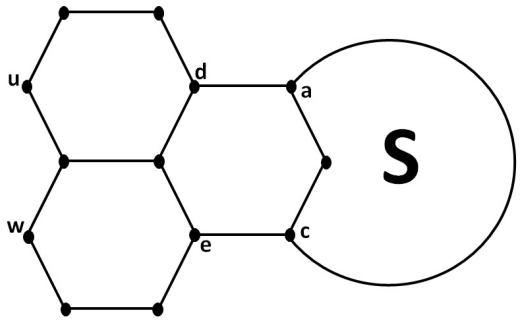


Figure 3: Graph G used in Thms. 2.1 and 3.1

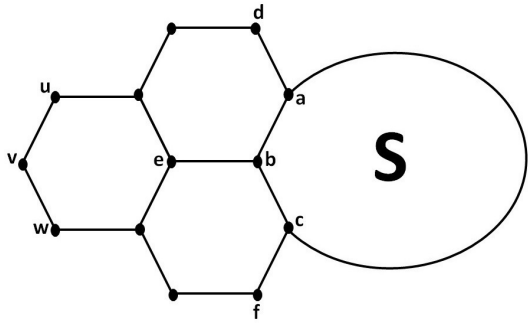


Figure 4: Graph G used in Thms. 2.2 and 3.2

Theorem 2.1. *Let G be a graph derived from the edge-coalescence of a graph S and a pericondensed hexagonal system with three hexagons at the path P_3 with the terminal vertices a and c of S (see Fig. 3). Then*

$$Z_{uw}(G) = X \cdot Z_{ac}(S)$$

where $X = \begin{bmatrix} 148 & 70 & 70 & 30 \\ 30 & 36 & 34 & 16 \\ 30 & 34 & 36 & 16 \\ 30 & 16 & 16 & 8 \end{bmatrix}$.

Proof. By Definition 2.1, we need to compute $Z(G), Z(G-u), Z(G-w)$ and $Z(G-u-w)$ to obtain $Z_{uw}(G)$. We compute these values by deleting independent edges ad and ce from G and using the recurrence relations 1a and 1b as follows:

$$
\begin{aligned}
Z(G) &= Z(G-ad-ce)+Z(G-ad-c-e)\\
&\quad +Z(G-a-d-ce)+Z(G-a-d-c-e)\\
&= 148Z(S)+70Z(S-c)+70Z(S-a)+30Z(S-a-c)\\
&= (148,70,70,30)\cdot Z_{ac}(S),\\
Z(G-u) &= Z(G-u-ad-ce)+Z(G-u-ad-c-e)\\
&\quad +Z(G-u-a-d-ce)+Z(G-u-a-d-c-e)\\
&= 30Z(S)+34Z(S-c)+36Z(S-a)+16Z(S-a-c)\\
&= (30,36,34,16)\cdot Z_{ac}(S),\\
Z(G-w) &= Z(G-w-ad-ce)+Z(G-w-ad-c-e)\\
&\quad +Z(G-w-a-d-ce)+Z(G-w-a-d-c-e)\\
&= 30Z(S)+36Z(S-c)+34Z(S-a)+16Z(S-a-c)\\
&= (30,34,36,16)\cdot Z_{ac}(S),\\
Z(G-u-w) &= Z(G-u-w-ad-ce)+Z(G-u-w-ad-c-e)\\
&\quad +Z(G-u-w-a-d-ce)+Z(G-u-w-a-d-c-e)\\
&= 30Z(S)+16Z(S-c)+16Z(S-a)+8Z(S-a-c)\\
&= (30,16,16,8)\cdot Z_{ac}(S).
\end{aligned}
$$

As the result, we have $Z_{uw}(G) = X \cdot Z_{ac}(S)$ where $X = \begin{bmatrix} 148 & 70 & 70 & 30 \\ 30 & 36 & 34 & 16 \\ 30 & 34 & 36 & 16 \\ 30 & 16 & 16 & 8 \end{bmatrix}$. □

Let us present a natural result of the previous theorem.

Corollary 2.1. *Let $\mathcal{R}_n$ be a benzenoid system with n naphthalene as shown in Fig 1. Then*

$$Z_{uw}(\mathcal{R}_n) = X^{n-1} \cdot [148,70,70,30]^T.$$

Proof. By Thm. 2.1, we know that $Z_{uw}(G) = X \cdot Z_{ac}(S)$. If we apply Thm. 2.1 to $\mathcal{R}_n$ $n-1$ times, then we get $Z_{uw}(\mathcal{R}_n) = X^{n-1} \cdot Z_{xy}(S')$, where S' is a fused pair of two hexagons (naphthalene).

Since S' is naphthalene, it is clear that $Z_{xy}(S') = [148, 70, 70, 30]^T$. As the result, $Z_{uw}(\mathcal{R}_n) = X^{n-1} \cdot [148, 70, 70, 30]^T$. □

In the next definition, we introduce the Hosoya vector of graph G at the path P_3 by means of all three vertices of the path.

Definition 2.2. *Let G be a graph. The vector at the path P_3 of G with vertices u, v and w (see Fig 4) is*

$$Z_{uvw}(G) = \begin{bmatrix} Z(G) \\ Z(G-u) \\ Z(G-v) \\ Z(G-w) \\ Z(G-u-v) \\ Z(G-v-w) \\ Z(G-u-w) \\ Z(G-u-v-w) \end{bmatrix}.$$

Theorem 2.2. *Let G be a graph derived from the edge-coalescence of a graph S and a pericondensed hexagonal system with three hexagons at the path P_3 with the vertices a, b and c of S (see Fig. 4). Then*

$$Z_{uvw}(G) = A \cdot Z_{abc}(S)$$

where $A = \begin{bmatrix} 107 & 63 & 55 & 63 & 34 & 34 & 37 & 21 \\ 52 & 32 & 24 & 31 & 16 & 15 & 19 & 10 \\ 45 & 26 & 25 & 15 & 26 & 15 & 15 & 9 \\ 52 & 31 & 24 & 32 & 15 & 16 & 19 & 10 \\ 31 & 19 & 15 & 18 & 10 & 9 & 11 & 6 \\ 31 & 18 & 15 & 19 & 9 & 10 & 11 & 6 \\ 21 & 13 & 9 & 13 & 6 & 6 & 8 & 4 \\ 21 & 13 & 9 & 13 & 6 & 6 & 8 & 4 \end{bmatrix}$.

Proof. By Definition 2.2, we have to compute $Z(G), Z(G-u), Z(G-v), \cdots, Z(G-u-v-w)$ to get $Z_{uvw}(G)$. This time, we delete independent edges cf, be and ad from G and using the recurrence relations 1a, 1b, we compute these values as follows:

$$
\begin{aligned}
Z(G) &= Z(G-cf-be-ad)+Z(G-cf-be-a-d)\\
&+Z(G-cf-b-e-ad)+Z(G-cf-b-e-a-d)\\
&+Z(G-c-f-be-ad)+Z(G-c-f-be-a-d)\\
&+Z(G-c-f-b-e-ad)+Z(G-c-f-b-e-a-d)\\
&=107Z(S)+63Z(S-a)+55Z(S-b)+34Z(S-a-b)\\
&+63Z(S-c)+37Z(S-a-c)+34Z(S-b-c)+21Z(S-a-b-c)\\
&=(107,63,55,63,34,34,37,21)\cdot Z_{abc}(S),\\
Z(G-u) &= Z(G-u-cf-be-ad)+Z(G-u-cf-be-a-d)\\
&+Z(G-u-cf-b-e-ad)+Z(G-u-cf-b-e-a-d)\\
&+Z(G-u-c-f-be-ad)+Z(G-u-c-f-be-a-d)\\
&+Z(G-u-c-f-b-e-ad)+Z(G-u-c-f-b-e-a-d)\\
&=52Z(S)+32Z(S-a)+24Z(S-b)+16Z(S-a-b)
\end{aligned}
$$

$$
\begin{aligned}
&+31Z(S-c)+19Z(S-a-c)+15Z(S-b-c)\\
&+10Z(S-a-b-c)\\
&=(52,32,24,31,16,15,19,10)\cdot Z_{abc}(S),\\
Z(G-v)\quad &=Z(G-v-cf-be-ad)+Z(G-v-cf-be-a-d)\\
&+Z(G-v-cf-b-e-ad)+Z(G-v-cf-b-e-a-d)\\
&+Z(G-v-c-f-be-ad)+Z(G-v-c-f-be-a-d)\\
&+Z(G-v-c-f-b-e-ad)+Z(G-v-c-f-b-e-a-d)\\
&=45Z(S)+26Z(S-a)+25Z(S-b)+15Z(S-a-b)\\
&+26Z(S-c)+15Z(S-a-c)+15Z(S-b-c)+9Z(S-a-b-c)\\
&=(45,26,25,15,26,15,15,9)\cdot Z_{abc}(S),\\
Z(G-w)\quad &=Z(G-w-cf-be-ad)+Z(G-w-cf-be-a-d)\\
&+Z(G-w-cf-b-e-ad)+Z(G-w-cf-b-e-a-d)\\
&+Z(G-w-c-f-be-ad)+Z(G-w-c-f-be-a-d)\\
&+Z(G-w-c-f-b-e-ad)+Z(G-w-c-f-b-e-a-d)\\
&=52Z(S)+31Z(S-a)+24Z(S-b)\\
&+15Z(S-a-b)+32Z(S-c)\\
&+19Z(S-a-c)+16Z(S-b-c)+10Z(S-a-b-c)\\
&=(52,31,24,32,15,16,19,10)\cdot Z_{abc}(S),\\
Z\begin{pmatrix} G-u\\ -v\end{pmatrix}\quad &=Z(G-u-v-cf-be-ad)+Z(G-u-v-cf-be-a-d)\\
&+Z(G-u-v-cf-b-e-ad)\\
&+Z(G-u-v-cf-b-e-a-d)
\end{aligned}
$$

$$
\begin{aligned}
&+Z(G-u-v-c-f-be-ad)\\
&+Z(G-u-v-c-f-be-a-d)\\
&+Z(G-u-v-c-f-b-e-ad)\\
&+Z(G-u-v-c-f-b-e-a-d)\\
&=31Z(S)+19Z(S-a)+15Z(S-b)+10Z(S-a-b)\\
&+18Z(S-c)+11Z(S-a-c)+9Z(S-b-c)+6Z(S-a-b-c)\\
&=(31,19,15,18,10,9,11,6)\cdot Z_{abc}(S),\\
Z(G-v-w) &= Z(G-v-w-cf-be-ad)+Z(G-v-w-cf-be-a-d)\\
&+Z(G-v-w-cf-b-e-ad)\\
&+Z(G-v-w-cf-b-e-a-d)\\
&+Z(G-v-w-c-f-be-ad)\\
&+Z(G-v-w-c-f-be-a-d)\\
&+Z(G-v-w-c-f-b-e-ad)\\
&+Z(G-v-w-c-f-b-e-a-d)\\
&=31Z(S)+18Z(S-a)+15Z(S-b)+9Z(S-a-b)\\
&+19Z(S-c)+6Z(S-a-c)+10Z(S-b-c)+6Z(S-a-b-c)\\
&=(31,18,15,19,9,10,11,6)\cdot Z_{abc}(S),\\
Z(G-u-w) &= Z(G-u-w-cf-be-ad)\\
&+Z(G-u-w-cf-be-a-d)\\
&+Z(G-u-w-cf-b-e-ad)\\
&+Z(G-u-w-cf-b-e-a-d)
\end{aligned}
$$

$$
\begin{aligned}
& +Z(G-u-w-c-f-be-ad) \\
& +Z(G-u-w-c-f-be-a-d) \\
& +Z(G-u-w-c-f-b-e-ad) \\
& +Z(G-u-w-c-f-b-e-a-d) \\
& = 21Z(S)+13Z(S-a)+9Z(S-b)+6Z(S-a-b) \\
& +13Z(S-c)+8Z(S-a-c)+6Z(S-b-c) \\
& +4Z(S-a-b-c) \\
& = (21,13,9,13,6,6,8,4)\cdot Z_{abc}(S),
\end{aligned}
$$

$$
\begin{aligned}
Z(G-u-v-w) &= Z(G-u-v-w-cf-be-ad) \\
& +Z(G-u-v-w-cf-be-a-d) \\
& +Z(G-u-v-w-cf-b-e-ad) \\
& +Z(G-u-v-w-cf-b-e-a-d) \\
& +Z(G-u-v-w-c-f-be-ad) \\
& +Z(G-u-v-w-c-f-be-a-d) \\
& +Z(G-u-v-w-c-f-b-e-ad) \\
& +Z(G-u-v-w-c-f-b-e-a-d) \\
& = 21Z(S)+13Z(S-a)+9Z(S-b)+6Z(S-a-b) \\
& +13Z(S-c)+8Z(S-a-c)+6Z(S-b-c) \\
& +4Z(S-a-b-c) \\
& = (21,13,9,13,6,6,8,4)\cdot Z_{abc}(S).
\end{aligned}
$$

As the result, we have $Z_{uvw}(G) = A \cdot Z_{abc}(S)$ where A is as given in Theorem. □

Corollary 2.2. *Let $\mathcal{P}_n$ be a benzenoid system with n naphthalene as shown in Fig 2. Then*

$$Z_{uvw}(\mathcal{P}_n) = A^n \cdot [18, 13, 13, 13, 5, 5, 3, 3]^T .$$

Proof. By Thm. 2.2, we know that $Z_{uvw}(G) = A \cdot Z_{abc}(S)$. We apply Thm. 2.2 to $\mathcal{P}_n$ n times, then we get $Z_{uvw}(\mathcal{P}_n) = A^n \cdot Z_{xyz}(S')$, where S' is a hexagon (benzene). Since S' is a hexagon (benzene), it is clear that $Z_{xyz}(S') = [18, 13, 13, 13, 5, 5, 3, 3]^T$. As the result, $Z_{uvw}(\mathcal{P}_n) = A^n \cdot [18, 13, 13, 13, 5, 5, 3, 3]^T$. □

3 Computing the Merrifield-Simmons index of benzenoid systems $\mathcal{R}_n$ and $\mathcal{P}_n$

In the next definition, we introduce the Merrifield-Simmons vector of graph G at the path P_3 by means of terminal two vertices.

Definition 3.1. *Let G be a graph. The Merrifield-Simmons vector of a graph G at the path P_3 with terminal vertices u and w is defined as*

$$\sigma_{uw}(G) = [\sigma(G), \sigma(G - N_G[u]), \sigma(G - N_G[w]), \sigma(G - N_G[u] - N_G[w])]^T .$$

Theorem 3.1. *Let G be a graph derived from the edge-coalescence of the graph S and a a pericondensed hexagonal system with three hexagons at the path P_3 with the terminal vertices a and c of S (See Fig. 3). Then*

$$\sigma_{uw}(G) = Y \cdot \sigma_{ac}(S)$$

, where $Y = \begin{bmatrix} 114 & -34 & -34 & 13 \\ 21 & -8 & -9 & 3 \\ 34 & -9 & -8 & 3 \\ 13 & -3 & -3 & 1 \end{bmatrix}$.

Proof. By Definition 3.1, we compute $\sigma(G), \sigma(G-N_G[u]), \sigma(G-N_G[w]), \sigma(G-N_G[u]-N_G[w])$ by deleting independent edges ad and ce from G and using the recurrence relations 1c, 1d as follows:

$$
\begin{aligned}
\sigma(G) &= \sigma(G - ad - ce) - \sigma(G - ad - N_G[c] - N_G[e]) \\
&\quad -\sigma(G - N_G[a] - N_G[d] - ce) \\
&\quad +\sigma(G - N_G[a] - N_G[d] - N_G[c] - N_G[e]) \\
&= 114\sigma(S) - 34\sigma(S - N_G[c]) - 34\sigma(S - N_G[a]) \\
&\quad +13\sigma(S - N_G[a] - N_G[c]) \\
&= (114, -34, -34, 13) \cdot \sigma_{ac}(S), \\
\sigma(G - N_G[u]) &= \sigma(G - N_G[u] - ad - ce) \\
&\quad -\sigma(G - N_G[u] - ad - N_G[c] - N_G[e]) \\
&\quad -\sigma(G - N_G[u] - N_G[a] - N_G[d] - ce) \\
&\quad +\sigma(G - N_G[u] - N_G[a] - N_G[d] - N_G[c] - N_G[e]) \\
&= 21\sigma(S) - 9\sigma(S - N_G[c]) - 8\sigma(S - N_G[a]) \\
&\quad +3\sigma(S - N_G[a] - N_G[c]) \\
&= (21, -8, -9, 3) \cdot \sigma_{ac}(S), \\
\sigma(G - N_G[w]) &= \sigma(G - N_G[w] - ad - ce) \\
&\quad -\sigma(G - N_G[w] - ad - N_G[c] - N_G[e]) \\
&\quad -\sigma(G - N_G[w] - N_G[a] - N_G[d] - ce) \\
&\quad +\sigma(G - N_G[w] - N_G[a] - N_G[d] - N_G[c] - N_G[e]) \\
&= 34\sigma(S) - 8\sigma(S - N_G[c]) - 9\sigma(S - N_G[a]) \\
&\quad +3\sigma(S - N_G[a] - N_G[c]) \\
&= (34, -9, -8, 3) \cdot \sigma_{ac}(S), \\
\sigma\begin{pmatrix} G - N_G[u] \\ -N_G[w] \end{pmatrix} &= \sigma(G - N_G[u] - N_G[w] - ad - ce)
\end{aligned}
$$

$$-\sigma(G - N_G[u] - N_G[w] - ad - N_G[c] - N_G[e])$$

$$-\sigma(G - N_G[u] - N_G[w] - N_G[a] - N_G[d] - ce)$$

$$+\sigma(G - N_G[u] - N_G[w] - N_G[a] - N_G[d] - N_G[c] - N_G[e])$$

$$= 13\sigma(S) - 3\sigma(S - N_G[c]) - 3\sigma(S - N_G[a])$$

$$+\sigma(S - N_G[a] - N_G[c])$$

$$= (13, -3, -3, 1) \cdot \sigma_{ac}(S).$$

As the result, we have $\sigma_{uw}(G) = Y \cdot \sigma_{ac}(S),$ where $Y = \begin{bmatrix} 114 & -34 & -34 & 13 \\ 21 & -8 & -9 & 3 \\ 34 & -9 & -8 & 3 \\ 13 & -3 & -3 & 1 \end{bmatrix}$. □

Corollary 3.1. *Let $\mathcal{R}_n$ be a benzenoid system with n naphthalene as shown in Fig 1. Then*

$$\sigma_{uw}(\mathcal{R}_n) = Y^{n-1} \cdot [114, 34, 34, 13]^T.$$

Proof. By Thm. 3.1, we know that $\sigma_{uw}(G) = Y \cdot Z_{ac}(S)$. We apply Thm. 3.1 to $\mathcal{R}_n$ $n-1$ times to get $\sigma_{uw}(\mathcal{R}_n) = Y^{n-1} \cdot \sigma_{xy}(S')$ where S' is a fused pair of two hexagons (naphthalene). Since S' is naphthalene, it is clear that $\sigma_{xy}(S') = [114, 34, 34, 13]^T$. As the result, $\sigma_{uw}(\mathcal{R}_n) = Y^{n-1} \cdot [114, 34, 34, 13]^T$. □

In the next definition, we introduce the Merrifield-Simmons vector of a graph G at the path P_3 by means of all three vertices of the path.

Definition 3.2. *Let G be a graph. The Merrifield-Simmons vector of G at the path P_3 with vertices u, v and w is defined as*

$$\sigma_{uvw}(G) = [\sigma(G), \sigma(G - N_G[u]), \sigma(G - N_G[v]), \sigma(G - N_G[w]), \sigma(G - N_G[u] - N_G[w])]^T.$$

Theorem 3.2. *Let G be a graph derived from the edge-coalescence of a graph S and a pericondensed hexagonal system with three hexagons at the path P_3 with the vertices a, b and c of S (see Fig. 4). Then*

$$\sigma_{uvw}(G) = B \cdot \sigma_{abc}(S)$$

where $B = \begin{bmatrix} 111 & -49 & -45 & -49 & 18 \\ 42 & -14 & -18 & -15 & 5 \\ 34 & -13 & -9 & -13 & 5 \\ 42 & -15 & -18 & -14 & 5 \\ 18 & -6 & -9 & -6 & 2 \end{bmatrix}$.

Proof. By Definition 3.2, we compute $\sigma(G), \sigma(G-N_G[u]), \sigma(G-N_G[v]), \sigma(G-N_G[w]), \sigma(G-N_G[u]-N_G[w])$ by deleting independent edges cf, be and ad from G and using the recurrence relations 1c, 1d as follows:

$$\begin{aligned}
\sigma(G) &= \sigma(G-cf-be-ad)-\sigma(G-cf-N_G[a]-N_G[d])\\
&\quad -\sigma(G-cf-N_G[b]-N_G[e])-\sigma(G-N_G[c]-N_G[f]-ad)\\
&\quad +\sigma(G-N_G[c]-N_G[f]-N_G[a]-N_G[d])\\
&= 111\sigma(S)-49\sigma(S-N_G[a])-45\sigma(S-N_G[b])\\
&\quad -49\sigma(S-N_G[c])+18\sigma(S-N_G[a]-N_G[c])\\
&= (111,-49,-45,-49,18)\cdot\sigma_{abc}(S),\\
\sigma(G-N_G[u]) &= \sigma(G-N_G[u]-cf-be-ad)\\
&\quad -\sigma(G-N_G[u]-cf-be-N_G[a]-N_G[d])\\
&\quad -\sigma(G-N_G[u]-cf-N_G[b]-N_G[e])\\
&\quad -\sigma(G-N_G[u]-N_G[c]-N_G[f]-ad)\\
&\quad +\sigma(G-N_G[u]-N_G[c]-N_G[f]-N_G[a]-N_G[d])\\
&= 42\sigma(S)-14\sigma(S-N_G[a])-18\sigma(S-N_G[b])\\
&\quad -15\sigma(S-N_G[c])+5\sigma(S-N_G[a]-N_G[c])\\
&= (42,-14,-18,-15,5)\cdot\sigma_{abc}(S),\\
\sigma(G-N_G[v]) &= \sigma(G-N_G[v]-cf-be-ad)\\
&\quad -\sigma(G-N_G[v]-cf-be-N_G[a]-N_G[d])\\
&\quad -\sigma(G-N_G[v]-cf-N_G[b]-N_G[e])\\
&\quad -\sigma(G-N_G[v]-N_G[c]-N_G[f]-ad)\\
&\quad +\sigma(G-N_G[v]-N_G[c]-N_G[f]-N_G[a]-N_G[d])
\end{aligned}$$

$$
\begin{aligned}
&= 34\sigma(S) - 13\sigma(S - N_G[a]) - 9\sigma(S - N_G[b]) \\
&-13\sigma(S - N_G[c]) + 5\sigma(S - N_G[a] - N_G[c]) \\
&= (34, -13, -9, -13, 5) \cdot \sigma_{abc}(S), \\
\sigma(G - N_G[w]) \quad &= \sigma(G - N_G[w] - cf - be - ad) \\
&-\sigma(G - N_G[w] - cf - be - N_G[a] - N_G[d]) \\
&-\sigma(G - N_G[w] - cf - N_G[b] - N_G[e]) \\
&-\sigma(G - N_G[w] - N_G[c] - N_G[f] - ad) \\
&+\sigma(G - N_G[w] - N_G[c] - N_G[f] - N_G[a] - N_G[d]) \\
&= 42\sigma(S) - 15\sigma(S - N_G[a]) - 18\sigma(S - N_G[b]) \\
&-14\sigma(S - N_G[c]) + 5\sigma(S - N_G[a] - N_G[c]) \\
&= (42, -15, -18, -14, 5) \cdot \sigma_{abc}(S), \\
\sigma\begin{pmatrix} G - N_G[u] \\ -N_G[w] \end{pmatrix} \quad &= \sigma(G - N_G[u] - N_G[w] - cf - be - ad) \\
&-\sigma(G - N_G[u] - N_G[w] - cf - be - N_G[a] - N_G[d]) \\
&-\sigma(G - N_G[u] - N_G[w] - cf - N_G[b] - N_G[e]) \\
&-\sigma(G - N_G[u] - N_G[w] - N_G[c] - N_G[f] - ad) \\
&+\sigma(G - N_G[u] - N_G[w] - N_G[c] - N_G[f] - N_G[a] - N_G[d]) \\
&= 18\sigma(S) - 6\sigma(S - N_G[a]) - 9\sigma(S - N_G[b]) \\
&-6\sigma(S - N_G[c]) + 2\sigma(S - N_G[a] - N_G[c]) \\
&= (18, -6, -9, -6, 2) \cdot \sigma_{abc}(S).
\end{aligned}
$$

As the result, we have $\sigma_{uvw}(G) = B \cdot \sigma_{abc}(S)$ where B is as given in Theorem. □

Corollary 3.2. *Let $\mathcal{P}_n$ be a benzenoid system with n naphthalene as shown in Fig. 2. Then*

$$\sigma_{uvw}(\mathcal{P}_n) = B^n \cdot [18, 5, 5, 5, 2]^T .$$

Proof. By Thm. 3.2, we know that $\sigma_{uvw}(G) = B \cdot Z_{abc}(S)$. We apply Thm. 3.2 to $\mathcal{P}_n$ n times to get $\sigma_{uvw}(\mathcal{P}_n) = B^n \cdot \sigma_{xyz}(S')$ where S' is a hexagon (benzene). Since S' is a hexagon, it is clear that $\sigma_{xyz}(S') = [18, 5, 5, 5, 2]^T$. Consequently, $\sigma_{uvw}(\mathcal{P}_n) = B^n \cdot [18, 5, 5, 5, 2]^T$. □

As the consequence, we achieve the formulae of $\mathcal{R}_n$ and $\mathcal{P}_n$ that depend on the number of naphthalene to compute the Hosoya index and Merrifield-Simmons index in Cors. 2.1 2.2 3.1 and 3.2. We believe that the methods given here for the two indices can be extended to other topological graph indices.

References

[1] M. Alishahi, S. H. Shalmaee, On the edge eccentric and modified edge eccentric connectivity indices of linear benzenoid chains and double hexagonal chains, Journal of Molecular Structure, **1204**, 127446 (2020)

[2] R. Cruz, C. A. Marín, J. Rada, Computing the Hosoya Index of Catacondensed Hexagonal Systems, MATCH Commun. Math. Comput. Chem., **77**, 749-764 (2017)

[3] I. Gutman, O. E. Polansky, Mathematical Concepts in Organic Chemistry, Springer, Berlin, Germany (1986)

[4] I. Gutman, S. J. Cyvin, Introduction to the Theory of Benzenoid Hydrocarbons, Springer-Verlag, Berlin, Germany (1989)

[5] I. Gutman, N. Kolaković , A. Graovac, D. Babić, A method for calculation of the Hosoya index of polymers, Studies in physical and theoretical chemistry, **63**, 141-154 (1989)

[6] I. Gutman, Extremal hexagonal chains, Journal of Mathematical Chemistry, **12**, 197-210 (1993)

[7] H. Hosoya, Topological index. A newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons, Bull. Chem. Soc. Jpn., **44**, 2332-2339 (1971)

[8] G. Huang, M. Kuang, H. Deng, The expected values of Hosoya index and Merrifield-Simmons index in a random polyphenylene chain, Journal of Combinatorial Optimization, **32**, 550-562 (2016)

[9] R. E. Merrifield, H. E. Simmons, Topological Methods in Chemistry, Wiley, New York (1989)

[10] J. Rada, Vertex-degree-based topological indices of hexagonal systems with equal number of edges, Applied Mathematics and Computation, **296**, 270-276 (2017)

[11] J. Rada, R. Cruz, I. Gutman, Vertex-degree-based topological indices of catacondensed hexagonal systems, Chemical Physics Letters, **572**, 154-157 (2013)

[12] H. Ren, F. Zhang, Double hexagonal chains with minimal total $\pi-$ electron energy, J. Math. Chem., **42 (4)**, 1041-1056 (2007)

[13] H. Ren, F. Zhang, Extremal double hexagonal chains with respect to $k-$ matchings and $k-$ independent sets, Discrete Appl. Math., **155 (17)**, 2269-2281 (2007)

[14] H. Ren, F. Zhang, Double hexagonal chains with maximal Hosoya index and minimal Merrifield-Simmons index, Journal of Mathematical Chemistry **42 (4)** (2007) 679-690.

[15] W. C. Shiu, Extremal Hosoya index and Merrifield-Simmons index of hexagonal spiders, Discrete Applied Mathematics, **156(15)** (2008), 2978-2985.

[16] S. Wagner, I. Gutman, Maxima and Minima of the Hosoya Index and Merrifield-Simmons, Acta Appl. Math. **112** (2010) 323-346.

[17] W. Wei, S. Li, Extremal phenylene chains with respect to the coefficients sum of the permanental polynomial, the spectral radius, the Hosoya index and the Merrifield-Simmons index, Discrete Applied Mathematics **271** (2019), 205-217.