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

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ABSTRACT

Gutman et al. gave some relations for computing the Hosoya indices of two special benzenoid systems R_n and P_n. In this paper, we compute the Hosoya index and Merrifield-Simmons index of R_n and 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 R_n and 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 [8]. It is denoted

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by $Z(G)$ and is defined as $Z(G) = \sum_{k=0}^{r} p(G,k)$, 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 $n(G,1) = n$. 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 [10]. In fact, the Merrifield-Simmons index was introduced in 1982 by Prodinger and Tichy as just Fibonacci number of a graph [11]. Moreover, Ivan Gutman first named Merrifield-Simmons index in [6].

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, 18, 19]. In recent years, numerous papers have been published on the Hosoya index and the Merrifield-Simmons index of various molecular structures, some of them are listed in [2, 5, 9, 16-18, 20, 21].

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, 2, 6, 7, 12-15, 21]. Let us denote two types of pericondensed benzenoid systems in Figure 1 and Figure 2 by R_n and P_n.

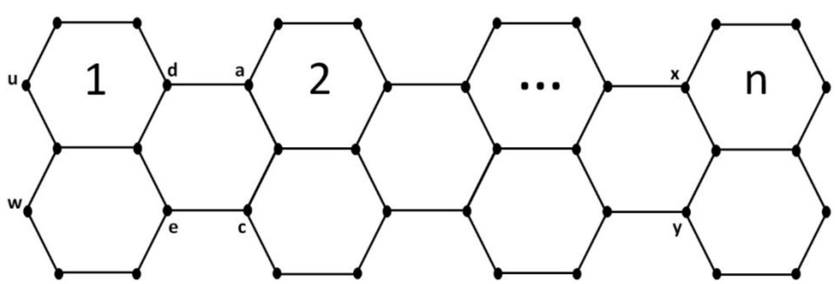

Figure 1. Benzenoid system R_n.

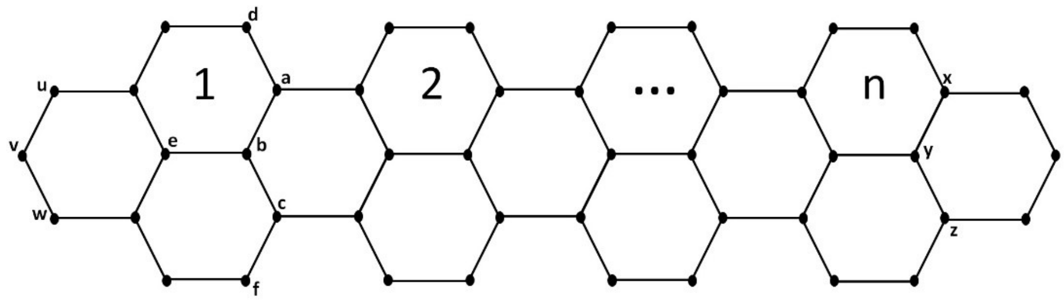

Figure 2. Benzenoid system P_n.

Gutman et al. gave relations for computing the Hosoya indices of the benzenoid systems R_n and P_n in [5]. In the next section, we compute the Hosoya index and the Merrifield-Simmons index of benzenoid systems R_n and P_n by means of introducing four vectors for each value.

2. COMPUTING THE HOSOYA INDEX OF BENZENOID SYSTEMS R_n AND P_n

The most used recurrence relations to compute the Hosoya and the Merrifield-Simmons indices of a graph G are as follows, see [18]:

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

$Z(G) = Z(G - ab) + Z(G - a - b)$, for an edge $e = ab$ of G, (1b)

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

$\sigma(G) = \sigma(G - ab) - \sigma(G - (N_G[a] - N_G[b]))$, for an edge $e = ab$ of G. (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, similar to the vector introduced at an edge of G by Cruz et al. in [2].

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 Figure 3) is defined as

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

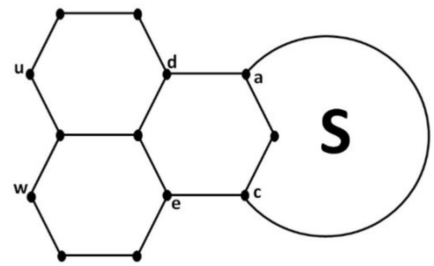

Figure 3. Graph G used in Theorems 2.1 and 3.1.

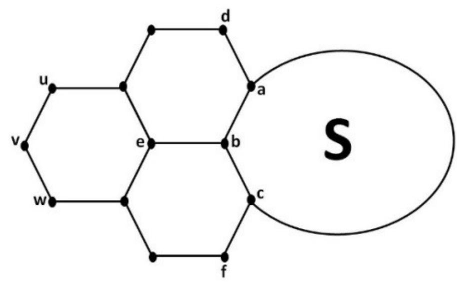

Figure 4. Graph G used in Theorems 2.3 and 3.3.

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 Figure 3). Then

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

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:

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

$$\begin{aligned} Z(G-u) &= Z(G-u-ad-ce) + Z(G-u-ad-c-e) \\ &\quad + Z(G-u-a-d-ce) + Z(G-u-a-d-c-e) \\ &= 70Z(S) + 34Z(S-c) + 36Z(S-a) + 16Z(S-a-c) \end{aligned}$$

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

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

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

Let us present a natural result of the previous theorem.

Corollary 2.2. Let R_n be a benzenoid system with n naphthalene as shown in Figure 1. Then

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

Proof. By Theorem 2.1, we know that $Z_{uw}(G) = X \cdot Z_{ac}(S)$. If we apply Theorem 2.1 to R_n $n-1$ times, then we get $Z_{uw}(R_n) = X^{n-1}\cdot Z_{xy}(S')$, 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, $Z_{uw}(R_n) = X^{n-1}\cdot[148,70,70,30]^T$. ■

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 Figure 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 2.3. 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 Figure 4). Then

$$Z_{uvw}(G) = A \cdot Z_{abc}(S), \text{ where } A = \begin{bmatrix} 107 & 63 & 55 & 63 & 34 & 34 & 37 & 21 \\ 52 & 32 & 24 & 31 & 16 & 15 & 19 & 10 \\ 45 & 26 & 25 & 26 & 15 & 15 & 15 & 9 \\ 52 & 31 & 24 & 32 & 15 & 16 & 19 & 10 \\ 31 & 19 & 15 & 18 & 10 & 9 & 11 & 6 \\ 31 & 18 & 15 & 19 & 9 & 10 & 11 & 6 \\ 21 & 13 & 9 & 13 & 6 & 6 & 8 & 4 \\ 21 & 13 & 9 & 13 & 6 & 6 & 8 & 4 \end{bmatrix}.$$

Proof. By Definition 2.2, we have to compute $Z(G), Z(G-u), Z(G-v), \ldots, Z(G-u-v-w)$ 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:

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

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

$$\begin{aligned} Z(G-v) &= Z\binom{G-v-cf}{be-ad} + Z\binom{G-v-cf}{-be-a-d} \\ &\quad + Z\binom{G-v-cf}{-b-e-ad} + Z\binom{G-v-cf}{-b-e-a-d} \end{aligned}$$

$$+Z\binom{G-v-c}{-f-be-ad}+Z\binom{G-v-c}{-f-be-a-d}$$
$$+Z\binom{G-v-c}{-f-b-e-ad}+Z\binom{G-v-c}{-f-b-e-a-d}$$
$$=45Z(S)+26Z(S-a)+25Z(S-b)+15Z(S-a-b)$$
$$+26Z(S-c)+15Z(S-a-c)+15Z(S-b-c)+9Z\binom{S-a}{b-c}$$
$$=(45,26,25,26,15,15,15,9)\cdot Z_{abc}(S),$$

$$Z(G-w)=Z\binom{G-w-cf}{be-ad}+Z\binom{G-w-cf}{-be-a-d}$$
$$+Z\binom{G-w-cf}{-b-e-ad}+Z\binom{G-w-cf}{-b-e-a-d}$$
$$+Z\binom{G-w-c}{-f-be-ad}+Z\binom{G-w-c}{-f-be-a-d}$$
$$+Z\binom{G-w-c}{-f-b-e-ad}+Z\binom{G-w-c}{-f-b-e-a-d}$$
$$=52Z(S)+31Z(S-a)+24Z(S-b)+15Z(S-a-b)$$
$$+32Z(S-c)+19Z(S-a-c)+16Z(S-b-c)+10Z\binom{S-a}{b-c}$$
$$=(52,31,24,32,15,16,19,10)\cdot Z_{abc}(S),$$

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

$$Z(G-v-w)=Z\binom{G-v-w}{-cf-be-ad}+Z\binom{G-v-w-cf}{-be-a-d}$$
$$+Z\binom{G-v-w-cf}{-b-e-ad}+Z\binom{G-v-w-cf}{-b-e-a-d}$$
$$+Z\binom{G-v-w-c}{-f-be-ad}+Z\binom{G-v-w-c}{-f-be-a-d}$$
$$+Z\binom{G-v-w-c}{-f-b-e-ad}+Z\binom{G-v-w-c}{-f-b-e-a-d}$$

$$= 31Z(S) + 18Z(S-a) + 15Z(S-b) + 9Z(S-a-b)$$
$$+19Z(S-c) + 11Z(S-a-c) + 10Z(S-b-c) + 6Z\binom{S-a}{b-c}$$
$$= (31,18,15,19,9,10,11,6) \cdot Z_{abc}(S),$$

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

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

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

Corollary 2.4. Let P_n be a benzenoid system with n naphthalene as shown in Figure 2. Then

$$Z_{uvw}(P_n) = A^n \cdot [18,8,8,8,5,5,3,3]^T.$$

Proof. By Theorem 2.3, we know that $Z_{uvw}(G) = A \cdot Z_{abc}(S)$. We apply Theorem 2.3 to P_n n times, then we get $Z_{uvw}(P_n) = A^n \cdot Z_{xyz}(S')$, where S' is a hexagon (benzene). Since S' is a hexagon (benzene), it is clear that $Z_{xyz}(S') = [18,8,8,8,5,5,3,3]^T$. As the result, we achieve $Z_{uvw}(P_n) = A^n \cdot [18,8,8,8,5,5,3,3]^T$. ■

3. Computing the Merrifield–Simmons Index of Benzenoid Systems R_n and 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 (see Figure 3) 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 pericondensed hexagonal system with three hexagons at the path P_3 with the terminal vertices a and c of S (see Figure 3). Then

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

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:

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

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

$$\begin{aligned}\sigma(G - N_G[w]) &= \sigma(G - N_G[w] - ad - ce) - \sigma\begin{pmatrix} G - N_G[w] - ad \\ -N_G[c] - N_G[e] \end{pmatrix} \\ &\quad - \sigma\begin{pmatrix} G - N_G[w] - N_G[a] \\ -N_G[d] - ce \end{pmatrix} + \sigma\begin{pmatrix} G - N_G[w] - N_G[a] \\ -N_G[d] - N_G[c] - N_G[e] \end{pmatrix}\end{aligned}$$

$$= 34\sigma(S) - 8\sigma(S - N_G[c]) - 9\sigma(S - N_G[a]) + 3\sigma\binom{S - N_G[a]}{-N_G[c]}$$
$$= (34, -9, -8, 3) \cdot \sigma_{ac}(S),$$

$$\sigma\binom{G - N_G[u]}{-N_G[w]} = \sigma\binom{G - N_G[u] - N_G[w]}{-ad - ce} - \sigma\binom{G - N_G[u] - N_G[w]}{-ad - N_G[c] - N_G[e]}$$
$$-\sigma\binom{G - N_G[u] - N_G[w]}{-N_G[a] - N_G[d] - ce} + \sigma\binom{G - N_G[u] - N_G[w] - N_G[a]}{-N_G[d] - N_G[c] - N_G[e]}$$
$$= 13\sigma(S) - 3\sigma(S - N_G[c]) - 3\sigma(S - N_G[a]) + \sigma\binom{S - N_G[a]}{-N_G[c]}$$
$$= (13, -3, -3, 1) \cdot \sigma_{ac}(S).$$

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

Corollary 3.2. Let R_n be a benzenoid system with n naphthalene as shown in Figure 1. Then
$$\sigma_{uw}(R_n) = Y^{n-1} \cdot [114, 34, 34, 13]^T.$$

Proof. By Theorem 3.1, we know that $\sigma_{uw}(G) = Y \cdot \sigma_{ac}(S)$. We apply Theorem 3.1 to R_n $n-1$ times to get $\sigma_{uw}(R_n) = Y^{n-1} \cdot \sigma_{xy}(S')$, 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, $\sigma_{uw}(R_n) = Y^{n-1} \cdot [114, 34, 34, 13]^T$. ■

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 (see Figure 4) is defined as
$$\sigma_{uvw}(G) = \begin{bmatrix} \sigma(G) \\ \sigma(G - N_G[u]) \\ \sigma(G - N_G[v]) \\ \sigma(G - N_G[w]) \\ \sigma(G - N_G[u] - N_G[w]) \end{bmatrix}.$$

Theorem 3.3. Let G be a graph derived from the edge-coalescence of the 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 Figure 4). Then

$$\sigma_{uvw}(G) = B \cdot \sigma_{abc}(S), \text{ where } B = \begin{bmatrix} 134 & -49 & -45 & -49 & 18 \\ 42 & -14 & -18 & -15 & 5 \\ 34 & -13 & -9 & -13 & 5 \\ 42 & -15 & -18 & -14 & 5 \\ 18 & -6 & -9 & -6 & 2 \end{bmatrix}.$$

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:

$$\begin{aligned}\sigma(G) &= \sigma(G - cf - be - ad) - \sigma(G - cf - be - N_G[a] - N_G[d]) \\ &\quad - \sigma(G - cf - N_G[b] - N_G[e]) - \sigma(G - N_G[c] - N_G[f] - ad) \\ &\quad + \sigma(G - N_G[c] - N_G[f] - N_G[a] - N_G[d]) \\ &= 134\sigma(S) - 49\sigma(S - N_G[a]) - 45\sigma(S - N_G[b]) - 49\sigma(S - N_G[c]) \\ &\quad + 18\sigma(S - N_G[a] - N_G[c]) \\ &= (134, -49, -45, -49, 18) \cdot \sigma_{abc}(S),\end{aligned}$$

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

$$\begin{aligned}\sigma(G - N_G[v]) &= \sigma(G - N_G[v] - cf - be - ad) - \sigma\begin{pmatrix} G - N_G[v] - cf \\ -be - N_G[a] - N_G[d] \end{pmatrix} \\ &\quad - \sigma\begin{pmatrix} G - N_G[v] - cf \\ -N_G[b] - N_G[e] \end{pmatrix} - \sigma\begin{pmatrix} G - N_G[v] - N_G[c] \\ -N_G[f] - ad \end{pmatrix} \\ &\quad + \sigma\begin{pmatrix} G - N_G[v] - N_G[c] \\ -N_G[f] - N_G[a] - N_G[d] \end{pmatrix} \\ &= 34\sigma(S) - 13\sigma(S - N_G[a]) - 9\sigma(S - N_G[b]) \\ &\quad - 13\sigma(S - N_G[c]) + 5\sigma(S - N_G[a] - N_G[c]) \\ &= (34, -13, -9, -13, 5) \cdot \sigma_{abc}(S),\end{aligned}$$

$$\sigma(G-N_G[w]) = \sigma(G-N_G[w]-cf-be-ad) - \sigma\binom{G-N_G[w]-cf}{-be-N_G[a]-N_G[d]}$$

$$-\sigma\binom{G-N_G[w]-cf}{-N_G[b]-N_G[e]} - \sigma\binom{G-N_G[w]-N_G[c]}{-N_G[f]-ad}$$

$$+\sigma\binom{G-N_G[w]-N_G[c]}{-N_G[f]-N_G[a]-N_G[d]}$$

$$= 42\sigma(S) - 15\sigma(S-N_G[a]) - 18\sigma(S-N_G[b])$$
$$-14\sigma(S-N_G[c]) + 5\sigma(S-N_G[a]-N_G[c])$$
$$= (42,-15,-18,-14,5)\cdot\sigma_{abc}(S),$$

$$\sigma\binom{G-N_G[u]}{-N_G[w]} = \sigma\binom{G-N_G[u]-N_G[w]}{-cf-be-ad} - \sigma\binom{G-N_G[u]-N_G[w]-cf}{-be-N_G[a]-N_G[d]}$$

$$-\sigma\binom{G-N_G[u]-N_G[w]}{-cf-N_G[b]-N_G[e]} - \sigma\binom{G-N_G[u]-N_G[w]}{-N_G[c]-N_G[f]-ad}$$

$$+\sigma\binom{G-N_G[u]-N_G[w]-N_G[c]}{-N_G[f]-N_G[a]-N_G[d]}$$
$$= 18\sigma(S) - 6\sigma(S-N_G[a]) - 9\sigma(S-N_G[b])$$
$$-6\sigma(S-N_G[c]) + 2\sigma(S-N_G[a]-N_G[c])$$
$$= (18,-6,-9,-6,2)\cdot\sigma_{abc}(S).$$

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

Corollary 3.4. Let P_n be a benzenoid system with n naphthalene as shown in Figure 2. Then $\sigma_{uvw}(P_n)\ =\ B^n\cdot[18,5,5,5,2]^{\,T}$.

Proof. By Theorem 3.3, we know that $\sigma_{uvw}(G) = B\cdot\sigma_{abc}(S)$. We apply Theorem 3.3 to P_n n times to get $\sigma_{uvw}(P_n) = B^n\cdot\sigma_{xyz}(S')$, where S' is a hexagon (benzene). Since S' is a hexagon (benzene), it is clear that $\sigma_{xy}\ (S') = [18,5,5,5,2]^T$. Consequently, $\sigma_{uvw}(P_n) = B^n\cdot[18,5,5,5,2]^{\,T}$. ■

As a consequence, we achieve the formulae of R_n and P_n that depend on the number of naphthalene to compute the Hosoya index and Merrifield-Simmons index in Corollaries 2.2 2.4 3.2 and 3.4. We believe that the methods given here for the two indices can be extended to other topological graph indices.

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