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Computing the Merrifield-Simmons Index of Double Benzenoid Chains

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Abstract:	In this paper, we introduce the Merrifield-Simmons vector defined at a path of corresponding double hexagonal (benzenoid) chain. By utilizing this vector, we present reduction formulae to compute the Merrifield-Simmons index $\sigma(\mathcal{H})$ of the corresponding double hexagonal (benzenoid) chain $\mathcal{H}$. As the result, we compute $\sigma(\mathcal{H})$ of $\mathcal{H}$ by means of a product of some of obtained six matrices and a vector with entries in $\mathbb{N}$. Subsequently, we introduce the simple Merrifield-Simmons vector defined at an edge of given graph G. By using simple Merrifield-Simmons vector we present reduction formulae to compute the $\sigma(G)$ where G represents any hexagonal (benzenoid) chain.
Response to Reviewers:	Dear Editor and Dear Reviewers, We added a word file with the name "Responses for the Reviewers' Remarks". Our responses to your valuable remarks are available in there. Best Regards

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Responses for the Reviewers Remarks

First of all, we are grateful for the valuable comments of reviewers which improved our manuscript a lot. Therefore, we thank to two reviewers. Please find our responses to reviewers' remarks below:

First Reviewer's Remark: *There is no reference in the paper mentioning the problem of computing the Merrifield-Simmons index of hexagonal chains. Was this problem considered by other authors? If it was, a reference should be added. Otherwise, the authors of JAMC-D-21-01768 should consider this problem which should be simpler than the double hexagonal chains. Can they apply their technique to solve the problem over hexagonal chains?*

Authors' Response: The problem of computing the Merrifield-Simmons index of any hexagonal chain was not considered by other authors exactly. There is a study related to this problem but not the exact solution of this problem. Even so, we added the paper as a reference at the beginning of Section 3. We considered this problem thanks to the remark of the reviewer. Then, we added a new section as a new Section 3. In Section 3, we presented reduction formulae to compute the Merrifield-Simmons index of hexagonal chains by introducing the simple Merrifield-Simmons vector similarly to the technique that is applied in Section 2. As the result, we can get the Merrifield-Simmons index of any hexagonal chain using a proper product of some of obtained three matrices and a vector that are called Q, P, R, and (3,1,1,2,2)^T.

Second Reviewer's Remark: *The research method is feasible and the result is correct. I recommend the publication of this paper in the Journal of Applied Mathematics and Computing.*

Authors' Response: Thanks a lot for the positive comment. Here, there is nothing to do.

- If any part of these clarifications is not sufficient, we are ready to do further changes.

Best Regards…

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Computing the Merrifield-Simmons Index of Double Benzenoid Chains

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Abstract In this paper, we introduce the Merrifield-Simmons vector defined at a path of corresponding double hexagonal (benzenoid) chain. By utilizing this vector, we present reduction formulae to compute the Merrifield-Simmons index $\sigma(\mathcal{H})$ of the corresponding double hexagonal (benzenoid) chain $\mathcal{H}$. As the result, we compute $\sigma(\mathcal{H})$ of $\mathcal{H}$ by means of a product of some of obtained six matrices and a vector with entries in $\mathbb{N}$. Subsequently, we introduce the simple Merrifield-Simmons vector defined at an edge of given graph G. By using simple Merrifield-Simmons vector we present reduction formulae to compute the $\sigma(G)$ where G represents any hexagonal (benzenoid) chain.

Keywords Double benzenoid chains · double hexagonal chains · hexagonal chains · topological index · Merrifield-Simmons index

Mathematics Subject Classification (2000) 05C09 · 05C92 · 05C50

1 Introduction

Let $G = (V, E)$ be a graph with vertex set $V(G)$ and edge set $E(G)$. The neighborhood set of a vertex v contains all neighbor vertices of v and it is denoted by $N_G(v)$. Closed neighborhood set of v is a set containing all neighbor vertices of v together with v itself and it is denoted by $N_G[v] = N_G(v) \cup \{v\}$. If any two vertices in a subset of $V(G)$ are not adjacent, then the subset is called an independent set in G. The number of possible independent sets in G

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with k vertices is denoted by $n(G,k)$. By definition, $n(G,0)=1$ for all graphs, and it is clear that $n(G,1)$ is equal to the number of vertices of G.

On the purpose of determining molecular structure via finite set topology, R. E. Merrifield and H. E. Simmons elaborated a mathematical theory in 1970s and 1980s. In this context, they published a series of papers and a book, see [12–15,21,16]. Despite the theory was not improved further, one point attracted attention. This point was the number of open sets of the finite topology, that Merrifield and Simmons directly recognized to correspond to the number of independent sets of vertices of the graph corresponding to that topology. Thus, this number started to be used as a topological index that. The symbol σ was used for this index in [12] and Ivan Gutman was the first researcher to use the name Merrifield-Simmons index [8], for more details see elaborated survey [23].

The Merrifield-Simmons index of G is defined as

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

where $n(G,t)\neq 0$ whereas $n(G,t+1)=0$.

Topological indices are significant in chemical graph theory and they have many applications in quantitative structure-activity relationships (QSARs). The Merrifield-Simmons index is one of the best known topological indices in mathematical chemistry. It has an important practical role as a molecular descriptor and it is comprehensively studied to determine physico-chemical properties of molecular structures; for more details, see [7,23]. In the past few decades, many properties of the Merrifield-Simmons index have been studied on various molecular graph structures, some of them can be found in [2,4, 9–11,17,19,22,24].

Hexagonal systems are natural graph forms of benzenoid hydrocarbons that play a significant role in theoretical chemistry. A hexagonal (benzenoid) system is a finite $2-$connected graph without any cut vertex whose interior regions are mutually congruent regular hexagons. In a hexagonal system, if there is at least one vertex belonging to three hexagons, then the hexagonal system is called pericondensed, and catacondensed otherwise. A hexagonal system that there is no hexagon adjacent to more than two hexagons is called a hexagonal chain. An $n-$tuple hexagonal chain is formed by n condensed identical hexagonal chains, [5,18]. When n is equal to 2, then it is called a double hexagonal (benzenoid) chain, [6,7]. A double hexagonal (benzenoid) chain is a type of pericondensed hexagonal system and it is derived from a naphthalene by stepwise fusion of a new naphthalene, for more studies about double hexagonal (benzenoid) chains, see [1,5,18–20].

Let us consider the naphthalene structure in the form that interior edges are horizontal. In this aspect, there are two naphthalene fusion types as follows, see Fig. 1:

$$\alpha - type : y \equiv a,\ z \equiv b,\ t \equiv c,\ \ q \equiv d$$

$$\beta - type : x \equiv b,\ y \equiv c,\ z \equiv d,\ t \equiv e.$$

At every step, fusion type is determined by θ, where $\theta \in \{\alpha, \beta\}$.

Let us denote a double hexagonal (benzenoid) chain by $\mathcal{H}(\theta_1, \theta_2, \cdots, \theta_n)$ where $\theta_1, \theta_2, \cdots, \theta_n \in \{\alpha, \beta\}$ are fusion types, respectively. It is easy to observe that $\mathcal{H}(\theta_1, \theta_2, \cdots, \theta_n)$ consists of $n+1$ naphthalene and $2n+2$ regular hexagons. If for all i, $\theta_i = \theta_{i+1}$ in $\mathcal{H}(\theta_1, \theta_2, \cdots, \theta_n)$, then $\mathcal{H}(\theta_1, \theta_2, \cdots, \theta_n)$ is called double linear hexagonal (benzenoid) chain that we denote by $L_{2\times n}$, see Fig. 2.

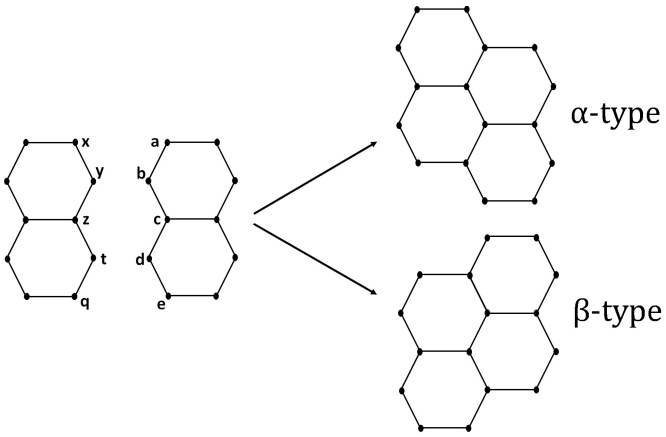


Fig. 1: Naphthalene fusion types in double hexagonal (benzenoid) chains

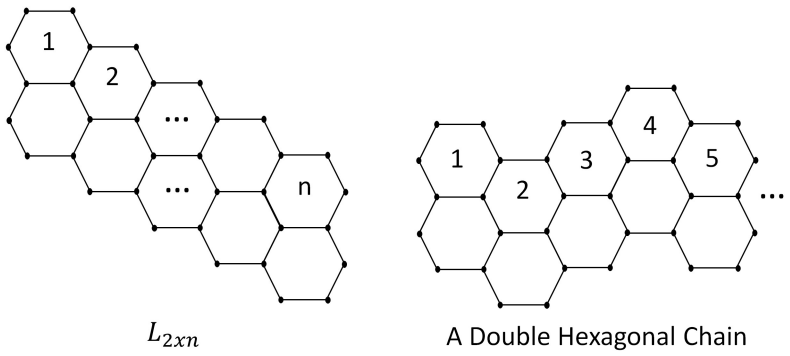


Fig. 2: A double linear hexagonal (benzenoid) chain $L_{2\times n} = \mathcal{H}(\alpha, \alpha, \cdots, \alpha)$ and a double hexagonal (benzenoid) chain $\mathcal{H}(\alpha, \beta, \beta, \alpha, \cdots)$

The Merrifield-Simmons index of some certain types of hexagonal systems were studied in [9,17]. However, a practical way for computing the Merrifield-Simmons index of any double hexagonal (benzenoid) chain does not exist. In this paper, we focus on this problem and we introduce the Merrifield-Simmons vector at a path with some vertices of the corresponding double hexagonal (benzenoid) chain. Afterwards, by using this vector and some recurrence formulae, we present reduction formulae to compute the Merrifield-Simmons index of the double hexagonal (benzenoid) chain by means of a multiplication of some of the obtained six matrices and a vector with entries in $\mathbb{N}$.

2 Computing the Merrifield-Simmons index of double benzenoid chains

Let us recall two practical recurrence relations to compute the Merrifield-Simmons index of a graph G for future use which can be found in [7]:

$$\sigma(G) = \prod_{i=1}^{k} \sigma(G_i) \tag{1}$$

where $G_1,\ G_2,\ \cdots,\ G_k$ are connected components of G.

$$\sigma(G) = \sigma(G - ab) - \sigma(G - (N_G[a] \cup N_G[b])) \tag{2}$$

for an edge $e = ab$ of G.

In the next definition, we introduce the Merrifield-Simmons vector of a graph G at the path that contains the vertices a, b and c.

Definition 1 Let G be a graph and a, b, c be three vertices of a path in G. We denote the Merrifield-Simmons vector of G at the path P_n that contains the vertices a, b and c by $\sigma_{abc}(G)$ and define it by

$$\sigma_{abc}(G) = \begin{bmatrix} \sigma(G) \\ \sigma(G - N_G[a]) \\ \sigma(G - N_G[b]) \\ \sigma(G - N_G[c]) \\ \sigma(G - N_G[b] - N_G[c]) \\ \sigma(G - N_G[b] - N_G[a]) \\ \sigma(G - N_G[a] - N_G[b] - N_G[c]) \\ \sigma(G - c) \\ \sigma(G - b) \\ \sigma(G - a) \\ \sigma(G - b - c) \\ \sigma(G - b - a) \\ \sigma(G - N_G[a] - c) \\ \sigma(G - N_G[c] - a) \\ \sigma(G - N_G[b] - c) \\ \sigma(G - N_G[b] - a) \\ \sigma(G - N_G[c] - b) \\ \sigma(G - N_G[a] - b) \end{bmatrix}.$$

Let us show two graphs that is illustrated in different aspects in Fig. 3 and Fig. 4 to make the following theorems and corollaries clear.

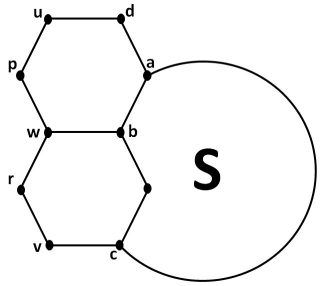


Fig. 3: Graph $G = \mathcal{H}(\alpha, \theta_1, \cdots, \theta_n)$ used in Thms. 1, 2 and 3

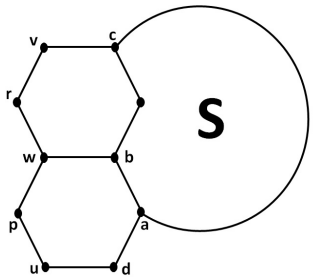


Fig. 4: Graph $G = \mathcal{H}(\beta, \theta_1, \cdots, \theta_n)$ used in Cors. 1, 2 and 3

Theorem 1 *Let $G = \mathcal{H}(\alpha, \theta_1, \cdots, \theta_n)$ be a graph derived from the edge-coalescence of the double hexagonal (benzenoid) chain graph $S = \mathcal{H}(\theta_1, \theta_2, \cdots, \theta_n)$ and a naphthalene at the path P_4 between the vertices a and c of S (see Fig. 3). Then*

$$\sigma_{uwv}(G) = A \cdot \sigma_{abc}(S)$$

where $A =$

$$\begin{pmatrix}
21 & -8 & -6 & -8 & 3 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
5 & 0 & -2 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -2 & 0 & 0 & 0 & 0 & 1 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -3 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & -3 & 0 & -3 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
13 & -5 & -3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
15 & -6 & 0 & -5 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
16 & -8 & -4 & -6 & 2 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
10 & -4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
12 & -6 & 0 & -4 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
3 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & -3 & 0 & -2 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -2 & 0 & 0 & 0 & 0 & 1 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 5 & 0 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 \\
3 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}.$$

Proof By the definition of Merrifield-Simmons vector $\sigma_{uwv}(G)$ at the path P_5 with contained vertices u, w and v, we have to focus on the values $\sigma(G)$, $\sigma(G - N_G[u])$, $\sigma(G - N_G[w])$, $\sigma(G - N_G[v])$, $\cdots$, $\sigma(G - N_G[v] - w)$ and $\sigma(G - N_G[u] - w)$. We compute them by deleting some independent edges from G and by using the recurrence relations 1 and 2 for every value as follows:
$\sigma(G) = \sigma(G - cv - bw - ad) - \sigma(G - cv - bw - N_G[a] - N_G[d])$

$$- \sigma(G - cv - N_G[b] - N_G[w]) - \sigma(G - bw - ad - N_G[c] - N_G[v])$$

$$
\begin{aligned}
&+ \sigma(G - bw - N_G[c] - N_G[v] - N_G[a] - N_G[d]) \\
&+ \sigma(G - N_G[c] - N_G[d] - N_G[b] - N_G[w]) \\
&= \sigma(P_6)\sigma(S) - \sigma(P_4)\sigma(S - N_G[a]) \\
&- \sigma(P_1)\sigma(P_2)\sigma(S - N_G[b]) \\
&- \sigma(P_4)\sigma(S - N_G[c]) \\
&+ \sigma(P_2)\sigma(S - N_G[a] - N_G[b] - N_G[c]) \\
&+ \sigma(P_2)\sigma(S - N_G[b] - N_G[c]) \\
&= (21, -8, -6, -8, 3, 0, 3, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \cdot \sigma_{abc}(S),
\end{aligned}
$$

$$
\begin{aligned}
\sigma(G - N_G[u]) &= \sigma(G - N_G[u] - cv - bw) \\
&- \sigma(G - N_G[u] - cv - N_G[b] - N_G[w]) \\
&- \sigma(G - N_G[u] - N_G[c] - N_G[v] - bw) \\
&+ \sigma(G - N_G[u] - N_G[c] - N_G[v] - N_G[b] - N_G[w]) \\
&= \sigma(P_3)\sigma(S) - \sigma(P_1)\sigma(S - N_G[b]) - \sigma(P_1)\sigma(S - N_G[c]) \\
&+ \sigma(S - N_G[b]) - N_G[c]) \\
&= (5, 0, -2, -2, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \cdot \sigma_{abc}(S),
\end{aligned}
$$

$$
\begin{aligned}
\sigma(G - N_G[w]) &= \sigma(G - N_G[w] - cv - ad) \\
&- \sigma(G - N_G[w] - cv - N_G[a] - N_G[d]) \\
&- \sigma(G - N_G[w] - N_G[c] - N_G[v] - ad) \\
&+ \sigma(G - N_G[w] - N_G[c] - N_G[v] - N_G[a] - N_G[d]) \\
&= \sigma(P_1)\sigma(P_2)\sigma(S - b) - \sigma(P_1)\sigma(S - N_G[a]) \\
&- \sigma(P_2)\sigma(S - N_G[c] - b) \\
&+ \sigma(S - N_G[a]) - N_G[b] - N_G[c]) \\
&= (0, -2, 0, 0, 0, 0, 1, 0, 6, 0, 0, 0, 0, 0, 0, 0, -3, 0) \cdot \sigma_{abc}(S),
\end{aligned}
$$

$$
\sigma(G - N_G[v]) = \sigma(G - N_G[v] - bw - ad)
$$

$$
\begin{aligned}
&- \sigma(G - N_G[v] - bw - N_G[a] - N_G[d]) \\
&- \sigma(G - N_G[v] - N_G[b] - N_G[w]) \\
&= \sigma(P_4)\sigma(S - c) - \sigma(P_2)\sigma(S - N_G[a] - c) \\
&- \sigma(P_2)\sigma(S - N_G[b] - c) \\
&= (0,0,0,0,0,0,0,8,0,0,0,0,-3,0,-3,0,0,0)\cdot\sigma_{abc}(S),
\end{aligned}
$$

$$
\begin{aligned}
\sigma\begin{pmatrix} G - N_G[w] \\ -N_G[v] \end{pmatrix} &= \sigma(G - N_G[w] - N_G[v] - ad) \\
&- \sigma(G - N_G[w] - N_G[v] - N_G[a] - N_G[d]) \\
&= \sigma(P_2)\sigma(S - b - c) - \sigma(S - N_G[a] - c) \\
&= (0,0,0,0,0,0,0,0,0,0,3,0,-1,0,0,0,0,0)\cdot\sigma_{abc}(S),
\end{aligned}
$$

$$
\begin{aligned}
\sigma\begin{pmatrix} G - N_G[w] \\ -N_G[u] \end{pmatrix} &= \sigma(G - N_G[w] - N_G[u] - cv) \\
&- \sigma(G - N_G[w] - N_G[v] - N_G[c] - N_G[v]) \\
&= \sigma(P_1)\sigma(S - b) - \sigma(S - N_G[c] - b) \\
&= (0,0,0,0,0,0,0,0,2,0,0,0,0,0,0,0,-1,0)\cdot\sigma_{abc}(S),
\end{aligned}
$$

$$
\begin{aligned}
\sigma\begin{pmatrix} G - N_G[u] \\ -N_G[w] \\ -N_G[v] \end{pmatrix} &= \sigma(S - b - c) \\
&= (0,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0)\cdot\sigma_{abc}(S),
\end{aligned}
$$

$$
\begin{aligned}
\sigma(G - v) &= \sigma(G - v - bw - ad) \\
&- \sigma(G - v - bw - N_G[a] - N_G[d]) \\
&- \sigma(G - v - N_G[b] - N_G[w]) \\
&= \sigma(P_5)\sigma(S) - \sigma(P_3)\sigma(S - N_G[a]) - \sigma(P_2)\sigma(S - N_G[b]) \\
&= (13,-5,-3,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0)\cdot\sigma_{abc}(S), \\
\sigma(G - w) &= \sigma(G - w - ad - cv) - \sigma(G - w - ad - N_G[c] - N_G[v]) \\
&- \sigma(G - w - N_G[a] - N_G[d] - cv)
\end{aligned}
$$

$$
\begin{aligned}
&+ \sigma(G - w - N_G[a] - N_G[d] - N_G[c] - N_G[v]) \\
&= \sigma(P_2)\sigma(P_3)\sigma(S) - \sigma(P_3)\sigma(S - N_G[c]) \\
&- \sigma(P_1)\sigma(P_2)\sigma(S - N_G[a]) \\
&+ \sigma(P_1)\sigma(S - N_G[a] - N_G[b] - N_G[c]) \\
&= (15, -6, 0, -5, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \cdot \sigma_{abc}(S), \\
\sigma(G - u) &= \sigma(G - u - cv - bw - ad) \\
&- \sigma(G - u - cv - bw - N_G[a] - N_G[d]) \\
&- \sigma(G - u - cv - N_G[b] - N_G[w]) \\
&- \sigma(G - u - bw - ad - N_G[c] - N_G[v]) \\
&+ \sigma(G - u - N_G[c] - N_G[v] - N_G[a] - N_G[d] - bw) \\
&+ \sigma(G - u - N_G[c] - N_G[v] - N_G[b] - N_G[w]) \\
&= \sigma(P_1)\sigma(P_4)\sigma(S) - \sigma(P_4)\sigma(S - N_G[a]) \\
&- \sigma(P_1)\sigma(P_1)\sigma(S - N_G[b]) - \sigma(P_1)\sigma(P_2)\sigma(S - N_G[c]) \\
&+ \sigma(P_2)\sigma(S - N_G[a] - N_G[b] - N_G[c]) \\
&+ \sigma(P_1)\sigma(S - N_G[b] - N_G[c]) \\
&= (16, -8, -4, -6, 2, 0, 3, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \cdot \sigma_{abc}(S), \\
\sigma(G - w - v) &= \sigma(G - w - v - ad) - \sigma(G - w - v - N_G[a] - N_G[d]) \\
&= \sigma(P_1)\sigma(P_3)\sigma(S) - \sigma(P_1)\sigma(P_1)\sigma(S - N_G[a]) \\
&= (10, -4, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \cdot \sigma_{abc}(S), \\
\sigma(G - w - u) &= \sigma(G - w - u - cv - ad) \\
&- \sigma(G - w - u - cv - N_G[a] - N_G[d]) \\
&- \sigma(G - w - u - N_G[c] - N_G[v] - ad) \\
&+ \sigma(G - w - u - N_G[c] - N_G[v] - N_G[a] - N_G[d]) \\
&= \sigma(P_1)\sigma(P_1)\sigma(P_2)\sigma(S) - \sigma(P_1)\sigma(P_2)\sigma(S - N_G[a])
\end{aligned}
$$

$$
\begin{aligned}
&\quad - \sigma(P_1)\sigma(P_1)\sigma(S - N_G[c]) \\
&\quad + \sigma(P_1)\sigma(S - N_G[a] - N_G[b] - N_G[c]) \\
&\quad = (12, -6, 0, -4, 0, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \cdot \sigma_{abc}(S), \\
\sigma\begin{pmatrix} G - N_G[u] \\ -v \end{pmatrix} &= \sigma(G - N_G[u] - v - bw) \\
&\quad - \sigma(G - N_G[u] - v - N_G[b] - N_G[w]) \\
&\quad = \sigma(P_2)\sigma(S) - \sigma(S - N_G[b]) \\
&\quad = (3, 0, -1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \cdot \sigma_{abc}(S), \\
\sigma\begin{pmatrix} G - N_G[v] \\ -u \end{pmatrix} &= \sigma(G - N_G[v] - u - bw - ad) \\
&\quad - \sigma(G - N_G[v] - u - bw - N_G[a] - N_G[d]) \\
&\quad - \sigma(G - N_G[v] - u - N_G[b] - N_G[w]) \\
&\quad = \sigma(P_1)\sigma(P_2)\sigma(S - c) - \sigma(P_2)\sigma(S - N_G[a] - c) \\
&\quad - \sigma(P_1)\sigma(S - N_G[b] - c) \\
&\quad = (0, 0, 0, 0, 0, 0, 0, 6, 0, 0, 0, 0, -3, 0, -2, 0, 0, 0) \cdot \sigma_{abc}(S), \\
\sigma\begin{pmatrix} G - N_G[w] \\ -v \end{pmatrix} &= \sigma(G - N_G[w] - v - ad) \\
&\quad - \sigma(G - N_G[w] - v - N_G[a] - N_G[d]) \\
&\quad = \sigma(P_2)\sigma(S - b) - \sigma(S - N_G[a]) \\
&\quad = (0, -1, 0, 0, 0, 0, 0, 0, 3, 0, 0, 0, 0, 0, 0, 0, 0, 0) \cdot \sigma_{abc}(S), \\
\sigma\begin{pmatrix} G - N_G[w] \\ -u \end{pmatrix} &= \sigma(G - N_G[w] - u - cv - ad) \\
&\quad - \sigma(G - N_G[w] - u - cv - N_G[a] - N_G[d]) \\
&\quad - \sigma(G - N_G[w] - u - N_G[c] - N_G[v] - ad) \\
&\quad + \sigma(G - N_G[w] - u - N_G[c] - N_G[v] - N_G[a] - N_G[d]) \\
&\quad = \sigma(P_1)\sigma(P_1)\sigma(S - b) - \sigma(P_1)\sigma(S - N_G[a])
\end{aligned}
$$

$$
\begin{aligned}
&- \sigma(P_1)\sigma(S - N_G[c] - b)\\
&+ \sigma(S - N_G[a] - N_G[b] - N_G[c])\\
&= (0,-2,0,0,0,0,1,0,4,0,0,0,0,0,0,0,-2,0)\cdot\sigma_{abc}(S),\\
\sigma(G - N_G[v] - w) &= \sigma(G - N_G[v] - w - ad)\\
&- \sigma(G - N_G[v] - w - N_G[a] - N_G[d])\\
&= \sigma(P_3)\sigma(S - c) - \sigma(P_1)\sigma(S - N_G[a] - c)\\
&= (0,0,0,0,0,0,0,5,0,0,0,0,-2,0,0,0,0,0)\cdot\sigma_{abc}(S),\\
\sigma(G - N_G[u] - w) &= \sigma(G - N_G[u] - w - cv)\\
&- \sigma(G - N_G[u] - w - N_G[c] - N_G[v])\\
&= \sigma(P_2)\sigma(S) - \sigma(S - N_G[c])\\
&= (3,0,0,-1,0,0,0,0,0,0,0,0,0,0,0,0,0,0)\cdot\sigma_{abc}(S).
\end{aligned}
$$

As the result, we get $\sigma_{uwv}(G) = A \cdot \sigma_{abc}(S)$.

Theorem 2 *Let $G = \mathcal{H}(\alpha, \theta_1, \cdots, \theta_n)$ be a graph derived from the edge-coalescence of the double hexagonal (benzenoid) chain graph $S = \mathcal{H}(\theta_1, \theta_2, \cdots, \theta_n)$ and a naphthalene at the path P_4 between the vertices a and c of S (see Fig. 3). Then*

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

where $B =$

$$\begin{pmatrix}
21 & -8 & -6 & -8 & 3 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
5 & 0 & -2 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
6 & -3 & 0 & -2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
5 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
3 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
16 & -6 & -6 & -8 & 3 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
15 & -5 & -6 & -6 & 3 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
16 & -8 & -4 & -6 & 2 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
12 & -4 & -6 & -6 & 3 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
10 & -5 & -4 & -4 & 2 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
4 & 0 & -2 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
4 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
4 & -2 & 0 & -2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
6 & -3 & 0 & -2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
3 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
5 & 0 & -2 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}.$$

Proof To compute $\sigma_{upr}(G)$ at the path P_4 with contained vertices u, p and r, we need to calculate the values $\sigma(G), \sigma(G - N_G[u]), \sigma(G - N_G[p]), \sigma(G -$

$N_G[r]), \cdots, \sigma(G-N_G[r]-p)$ and $\sigma(G-N_G[u]-p)$. Some of these values have been found in the proof of Thm. 1, so we skip them in the proof. We compute the rest of these values by deleting some independent edges from G and by using the recurrence relations 1 and 2 for every value as follows:

$$\begin{aligned}
\sigma(G-N_G[p]) &= \sigma(G-N_G[p]-cv-ad)\\
&\quad-\sigma(G-N_G[p]-cv-N_G[a]-N_G[d])\\
&\quad-\sigma(G-N_G[p]-N_G[c]-N_G[v]-ad)\\
&\quad+\sigma(G-N_G[p]-N_G[c]-N_G[v]-N_G[a]-N_G[d])\\
&= \sigma(P_1)\sigma(P_2)\sigma(S)-\sigma(P_2)\sigma(S-N_G[a])\\
&\quad-\sigma(P_1)\sigma(S-N_G[c])+\sigma(S-N_G[a]-N_G[b]-N_G[c])\\
&= (6,-3,0,-2,0,0,1,0,0,0,0,0,0,0,0,0,0,0)\cdot\sigma_{abc}(S),\\
\sigma(G-N_G[r]) &= \sigma(G-N_G[r]-ad)-\sigma(G-N_G[r]-N_G[a]-N_G[d])\\
&= \sigma(P_3)\sigma(S)-\sigma(P_1)\sigma(S-N_G[a])\\
&= (5,-2,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0)\cdot\sigma_{abc}(S),\\
\sigma(G-N_G[p]-N_G[r]) &= \sigma(G-N_G[p]-N_G[r]-ad)\\
&\quad-\sigma(G-N_G[p]-N_G[r]-N_G[a]-N_G[d])\\
&= \sigma(P_1)\sigma(S)-\sigma(S-N_G[a])\\
&= (2,-1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0)\cdot\sigma_{abc}(S),\\
\sigma(G-N_G[p]-N_G[u]) &= \sigma(G-N_G[p]-N_G[u]-cv)\\
&\quad-\sigma(G-N_G[p]-N_G[u]-N_G[c]-N_G[v])\\
&= \sigma(P_2)\sigma(S)-\sigma(S-N_G[c])\\
&= (3,0,0,-1,0,0,0,0,0,0,0,0,0,0,0,0,0,0)\cdot\sigma_{abc}(S),\\
\sigma\begin{pmatrix}G-N_G[u]\\-N_G[p]-N_G[r]\end{pmatrix} &= \sigma(S)\\
&= (1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0)\cdot\sigma_{abc}(S),\\
\sigma(G-r) &= \sigma(G-r-cv-bw-ad)
\end{aligned}$$

$$
\begin{aligned}
&- \sigma(G - r - cv - bw - N_G[a] - N_G[d]) \\
&- \sigma(G - r - cv - N_G[b] - N_G[w]) \\
&- \sigma(G - r - N_G[c] - N_G[v] - bw - ad) \\
&+ \sigma(G - r - N_G[c] - N_G[v] - bw - N_G[a] - N_G[d]) \\
&+ \sigma(G - r - N_G[c] - N_G[v] - N_G[b] - N_G[w]) \\
&= \sigma(P_1)\sigma(P_4)\sigma(S) - \sigma(P_1)\sigma(P_2)\sigma(S - N_G[a]) \\
&- \sigma(P_1)\sigma(P_2)\sigma(S - N_G[b]) - \sigma(P_4)\sigma(S - N_G[c]) \\
&+ \sigma(P_2)\sigma(S - N_G[a] - N_G[b] - N_G[c]) \\
&+ \sigma(P_2)\sigma(S - N_G[b] - N_G[c]) \\
&= (16, -6, -6, -8, 3, 0, 3, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \cdot \sigma_{abc}(S),
\end{aligned}
$$

$$
\begin{aligned}
\sigma(G - p) &= \sigma(G - p - cv - bw - ad) \\
&- \sigma(G - p - cv - bw - N_G[a] - N_G[d]) \\
&- \sigma(G - p - N_G[c] - N_G[v] - N_G[b] - N_G[w]) \\
&- \sigma(G - p - N_G[c] - N_G[v] - bw - ad) \\
&+ \sigma(G - p - N_G[c] - N_G[v] - bw - N_G[a] - N_G[d]) \\
&+ \sigma(G - p - N_G[c] - N_G[v] - N_G[b] - N_G[w]) \\
&= \sigma(P_2)\sigma(P_3)\sigma(S) - \sigma(P_3)\sigma(S - N_G[a]) \\
&- \sigma(P_1)\sigma(P_2)\sigma(S - N_G[b]) - \sigma(P_1)\sigma(P_2)\sigma(S - N_G[c]) \\
&+ \sigma(P_1)\sigma(S - N_G[a] - N_G[b] - N_G[c]) \\
&+ \sigma(P_2)\sigma(S - N_G[b] - N_G[c]) \\
&= (15, -5, -6, -6, 3, 0, 2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \cdot \sigma_{abc}(S),
\end{aligned}
$$

$$
\begin{aligned}
\sigma(G - p - r) &= \sigma(G - p - r - cv - bw - ad) \\
&- \sigma(G - p - r - cv - bw - N_G[a] - N_G[d]) \\
&- \sigma(G - p - r - cv - N_G[b] - N_G[w])
\end{aligned}
$$

$$
\begin{aligned}
&- \sigma(G-p-r-N_G[c]-N_G[v]-bw-ad)\\
&+ \sigma(G-p-r-N_G[c]-N_G[v]-bw-N_G[a]-N_G[d])\\
&+ \sigma(G-p-r-N_G[c]-N_G[v]-N_G[b]-N_G[w])\\
&= \sigma(P_1)\sigma(P_1)\sigma(P_2)\sigma(S)-\sigma(P_1)\sigma(P_1)\sigma(S-N_G[a])\\
&- \sigma(P_1)\sigma(P_2)\sigma(S-N_G[b])-\sigma(P_1)\sigma(P_2)\sigma(S-N_G[c])\\
&+ \sigma(P_1)\sigma(S-N_G[a]-N_G[b]-N_G[c])\\
&+ \sigma(P_2)\sigma(S-N_G[b]-N_G[c])\\
&= (12,-4,-6,-6,3,0,2,0,0,0,0,0,0,0,0,0,0)\cdot\sigma_{abc}(S),
\end{aligned}
$$

$$
\begin{aligned}
\sigma(G-p-u) &= \sigma(G-p-u-cv-bw-ad)\\
&- \sigma(G-p-u-cv-bw-N_G[a]-N_G[d])\\
&- \sigma(G-p-u-cv-N_G[b]-N_G[w])\\
&- \sigma(G-p-u-N_G[c]-N_G[v]-bw-ad)\\
&+ \sigma(G-p-u-N_G[c]-N_G[v]-bw-N_G[a]-N_G[d])\\
&+ \sigma(G-p-u-N_G[c]-N_G[v]-N_G[b]-N_G[w])\\
&= \sigma(P_1)\sigma(P_3)\sigma(S)-\sigma(P_3)\sigma(S-N_G[a])\\
&- \sigma(P_1)\sigma(P_1)\sigma(S-N_G[b])-\sigma(P_1)\sigma(P_1)\sigma(S-N_G[c])\\
&+ \sigma(P_1)\sigma(S-N_G[a]-N_G[b]-N_G[c])\\
&+ \sigma(P_1)\sigma(S-N_G[b]-N_G[c])\\
&= (10,-5,-4,-4,2,0,2,0,0,0,0,0,0,0,0,0,0)\cdot\sigma_{abc}(S),
\end{aligned}
$$

$$
\begin{aligned}
\sigma(G-N_G[u]-r) &= \sigma(G-N_G[u]-r-cv-bw)\\
&- \sigma(G-N_G[u]-r-cv-N_G[b]-N_G[w])\\
&- \sigma(G-N_G[u]-r-N_G[c]-N_G[v]-bw)\\
&+ \sigma(G-N_G[u]-r-N_G[c]-N_G[v]-N_G[b]-N_G[w])\\
&= \sigma(P_1)\sigma(P_1)\sigma(S)-\sigma(P_1)\sigma(S-N_G[b])
\end{aligned}
$$

$$
\begin{aligned}
&\quad - \sigma(P_1)\sigma(S - N_G[c]) + \sigma(S - N_G[b] - N_G[c]) \\
&\quad = (4, 0, -2, -2, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \cdot \sigma_{abc}(S), \\
\sigma(G - N_G[r] - u) &= \sigma(G - N_G[r] - u - ad) \\
&\quad - \sigma(G - N_G[r] - u - N_G[a] - N_G[d]) \\
&\quad = \sigma(P_1)\sigma(P_1)\sigma(S) - \sigma(P_1)\sigma(S - N_G[a]) \\
&\quad = (4, -2, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \cdot \sigma_{abc}(S), \\
\sigma(G - N_G[p] - r) &= \sigma(G - N_G[p] - r - cv - ad) \\
&\quad - \sigma(G - N_G[p] - r - cv - N_G[a] - N_G[d]) \\
&\quad - \sigma(G - N_G[p] - r - N_G[c] - N_G[v] - ad) \\
&\quad + \sigma(G - N_G[p] - r - N_G[c] - N_G[v] - N_G[a] - N_G[d]) \\
&\quad = \sigma(P_1)\sigma(P_1)\sigma(S) - \sigma(P_1)\sigma(S - N_G[a]) \\
&\quad - \sigma(P_1)\sigma(S - N_G[c]) + \sigma(S - N_G[a] - N_G[b] - N_G[c]) \\
&\quad = (4, -2, 0, -2, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \cdot \sigma_{abc}(S), \\
\sigma(G - N_G[p] - u) &= \sigma(G - N_G[p] - u - cv - ad) \\
&\quad - \sigma(G - N_G[p] - u - cv - N_G[a] - N_G[d]) \\
&\quad - \sigma(G - N_G[p] - u - N_G[c] - N_G[v] - ad) \\
&\quad + \sigma(G - N_G[p] - u - N_G[c] - N_G[v] - N_G[a] - N_G[d]) \\
&\quad = \sigma(P_1)\sigma(P_2)\sigma(S) - \sigma(P_2)\sigma(S - N_G[a]) \\
&\quad - \sigma(P_1)\sigma(S - N_G[c]) + \sigma(S - N_G[a] - N_G[b] - N_G[c]) \\
&\quad = (6, -3, 0, -2, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \cdot \sigma_{abc}(S), \\
\sigma(G - N_G[r] - p) &= \sigma(G - N_G[r] - p - ad) \\
&\quad - \sigma(G - N_G[r] - p - N_G[a] - N_G[d]) \\
&\quad = \sigma(P_2)\sigma(S) - \sigma(S - N_G[a]) \\
&\quad = (3, -1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \cdot \sigma_{abc}(S),
\end{aligned}
$$

$$\sigma(G - N_G[u] - p) = \sigma(G - N_G[u])$$

$$= (5, 0, -2, -2, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0) \cdot \sigma_{abc}(S).$$

As the consequence, we conclude that $\sigma_{upr}(G) = B \cdot \sigma_{abc}(S)$.

Theorem 3 *Let $G = \mathcal{H}(\alpha, \theta_1, \cdots, \theta_n)$ be a graph derived from the edge-coalescence of the double hexagonal (benzenoid) chain graph $S = \mathcal{H}(\theta_1, \theta_2, \cdots, \theta_n)$ and a naphthalene at the path P_4 between the vertices a and c of S (see Fig. 3). Then*

$$\sigma_{prv}(G) = C \cdot \sigma_{abc}(S)$$

where $C =$

$$\begin{pmatrix}
21 & -8 & -6 & -8 & 3 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
6 & -3 & 0 & -2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
5 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & -3 & 0 & -3 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 5 & 0 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 \\
2 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
13 & -5 & -3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
16 & -6 & -6 & -8 & 3 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
15 & -5 & -6 & -6 & 3 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
8 & -3 & -3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
12 & -4 & -6 & -6 & 3 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
4 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & -2 & 0 & -3 & 0 & 0 & 0 \\
5 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
3 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & -3 & 0 & -3 & 0 & 0 & 0 \\
4 & -2 & 0 & -2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}.$$

Proof Rows of the vector $\sigma_{prv}(G)$ at the path P_4 with contained vertices p, r and v consists of the values $\sigma(G), \sigma(G - N_G[p]), \sigma(G - N_G[r]), \sigma(G - N_G[v]), \cdots, \sigma(G - N_G[v] - r)$ and $\sigma(G - N_G[p] - r)$. Some of these values have already been found in the proofs of Thms. 1 and 2, so we compute the rest of these values by deleting some independent edges from G and by using the recurrence relations 1 and 2 for every value as follows:

$$\sigma(G - N_G[r] - N_G[v]) = \sigma(G - N_G[r] - N_G[v] - ad)$$

$$- \sigma(G - N_G[r] - N_G[v] - N_G[a] - N_G[d])$$

$$= \sigma(P_3)\sigma(S - c) - \sigma(P_1)\sigma(S - N_G[a] - c)$$

$$= (0, 0, 0, 0, 0, 0, 0, 5, 0, 0, 0, 0, -2, 0, 0, 0, 0, 0) \cdot \sigma_{abc}(S),$$

$$\sigma \begin{pmatrix} G - N_G[p] \\ -N_G[r] - N_G[v] \end{pmatrix} = \sigma(G - N_G[p] - N_G[r] - N_G[v] - ad)$$

$$- \sigma(G - N_G[p] - N_G[r] - N_G[v] - N_G[a] - N_G[d])$$

$$= \sigma(P_1)\sigma(S-c) - \sigma(S - N_G[a] - c)$$

$$= (0,0,0,0,0,0,0,2,0,0,0,0,-1,0,0,0,0,0) \cdot \sigma_{abc}(S),$$

$$\sigma(G-r-v) = \sigma(G-r-v-bw-ad)$$

$$- \sigma(G-r-v-bw-N_G[a]-N_G[d])$$

$$- \sigma(G-r-v-N_G[b]-N_G[w])$$

$$= \sigma(P_4)\sigma(S) - \sigma(P_2)\sigma(S-N_G[a]) - \sigma(P_2)\sigma(S-N_G[b])$$

$$= (8,-3,-3,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0) \cdot \sigma_{abc}(S),$$

$$\sigma(G-N_G[p]-v) = \sigma(G-N_G[p]-v-ad)$$

$$- \sigma(G-N_G[p]-v-N_G[a]-N_G[d])$$

$$= \sigma(P_1)\sigma(P_1)\sigma(S) - \sigma(P_1)\sigma(S-N_G[a])$$

$$= (4,-2,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0) \cdot \sigma_{abc}(S),$$

$$\sigma(G-N_G[v]-p) = \sigma(G-N_G[v]-p-bw-ad)$$

$$- \sigma(G-N_G[v]-p-bw-N_G[a]-N_G[d])$$

$$- \sigma(G-N_G[v]-p-N_G[b]-N_G[w])$$

$$= \sigma(P_1)\sigma(P_2)\sigma(S-c) - \sigma(P_1)\sigma(S-N_G[a]-c)$$

$$- \sigma(P_2)\sigma(S-N_G[b]-c)$$

$$= (0,0,0,0,0,0,0,6,0,0,0,0,-2,0,-3,0,0,0) \cdot \sigma_{abc}(S),$$

$$\sigma(G-N_G[r]-v) = \sigma(G-N_G[r]-v-ad)$$

$$- \sigma(G-N_G[r]-v-N_G[a]-N_G[d])$$

$$= \sigma(P_3)\sigma(S) - \sigma(P_1)\sigma(S-N_G[a])$$

$$= (5,-2,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0) \cdot \sigma_{abc}(S),$$

$$\sigma(G-N_G[v]-r) = \sigma(G-N_G[v])$$

$$= (0,0,0,0,0,0,0,8,0,0,0,0,-3,0,-3,0,0,0) \cdot \sigma_{abc}(S).$$

It follows that $\sigma_{prv}(G) = C \cdot \sigma_{abc}(S)$.

Corollary 1 *Let $G = \mathcal{H}(\beta, \theta_1, \cdots, \theta_n)$ be a graph derived from the edge-coalescence of the double hexagonal (benzenoid) chain $S = \mathcal{H}(\theta_1, \theta_2, \cdots, \theta_n)$ and a naphthalene at the path with three edges between the vertices c and a of S (see Fig. 4). Then*

$$\sigma_{vwu}(G) = D \cdot \sigma_{cba}(S)$$

where $D =$

$$\begin{pmatrix}
21 & -8 & -6 & -8 & 0 & 3 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & -3 & 0 & -3 & 0 & 0 \\
0 & 0 & 0 & -2 & 0 & 0 & 1 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -3 \\
5 & -2 & -2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
16 & -6 & -4 & -8 & 0 & 2 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
15 & -5 & 0 & -6 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
13 & 0 & -3 & -5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
12 & -4 & 0 & -6 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
10 & 0 & 0 & -4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & -3 & 0 & -2 & 0 & 0 \\
3 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & -2 & 0 & 0 & 1 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
3 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0
\end{pmatrix}.$$

Proof By Defn. 1, it is clear that the rows of the vector $\sigma_{vwu}(G)$ have been computed in the Thms. 1, 2 and 3. Hence, we conclude that $\sigma_{vwu}(G) = D \cdot \sigma_{cba}(S)$.

Corollary 2 *Let $G = \mathcal{H}(\beta, \theta_1, \cdots, \theta_n)$ be a graph derived from the edge-coalescence of the double hexagonal (benzenoid) chain $S = \mathcal{H}(\theta_1, \theta_2, \cdots, \theta_n)$ and a naphthalene at the path with three edges between the vertices c and a of S (see Fig. 4). Then*

$$\sigma_{rpu}(G) = E \cdot \sigma_{cba}(S)$$

where $E =$

$$\begin{pmatrix}
21 & -8 & -6 & -8 & 0 & 3 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
5 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
6 & -2 & 0 & -3 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
5 & -2 & -2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
3 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
2 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
16 & -6 & -4 & -8 & 0 & 2 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
15 & -6 & -6 & -5 & 0 & 3 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
16 & -8 & -6 & -6 & 0 & 3 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
10 & -4 & -4 & -5 & 0 & 2 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
12 & -6 & -6 & -4 & 0 & 3 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
4 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
4 & -2 & -2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
6 & -2 & 0 & -3 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
4 & -2 & 0 & -2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
5 & -2 & -2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
3 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}.$$

Proof Since the rows of vector $\sigma_{rpu}(G)$ have been computed in Thms. 1, 2 and 3, we get $\sigma_{rpu}(G) = E \cdot \sigma_{cba}(S)$.

To make more clear what has happened so far, let us explain things with an example. It can be observed that if there is a double linear hexagonal (benzenoid) chain $L_{2\times n} = \mathcal{H}(\alpha, \alpha, \cdots, \alpha)$ instead of a naphthalene in Theorem 1, then $\sigma_{uwv}(G) = A \cdot B^{n-1} \cdot \sigma_{abc}(S)$ is obtained by induction. Congruently, if there is a double linear hexagonal (benzenoid) chain $L_{2\times n} = \mathcal{H}(\beta, \beta, \cdots, \beta)$ instead of a naphthalene in Corollary 1, then the equality $\sigma_{uwv}(G) = D \cdot E^{n-1} \cdot \sigma_{cba}(S)$ is achieved by induction.

Corollary 3 *Let $G = \mathcal{H}(\beta, \theta_1, \cdots, \theta_n)$ be a graph derived from the edge-coalescence of the double hexagonal (benzenoid) chain $S = \mathcal{H}(\theta_1, \theta_2, \cdots, \theta_n)$ and a naphthalene at the path with three edges between the vertices c and a of S (see Fig. 4). Then*

$$\sigma_{vrp}(G) = F \cdot \sigma_{cba}(S)$$

where $F =$

$$\begin{pmatrix}
21 & -8 & -6 & -8 & 0 & 3 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & -3 & 0 & -3 & 0 & 0 \\
5 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
6 & -2 & 0 & -3 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
2 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 5 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
15 & -6 & -6 & -5 & 0 & 3 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
16 & -8 & -6 & -6 & 0 & 3 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
13 & 0 & -3 & -5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
12 & -6 & -6 & -4 & 0 & 3 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
8 & 0 & -3 & -3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & -2 & 0 & -3 & 0 & 0 \\
4 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
3 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
5 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
4 & -2 & 0 & -2 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & -3 & 0 & -3 & 0 & 0
\end{pmatrix}.$$

Proof Analogously with the previous corollaries, the vector $\sigma_{vrp}(G)$ consists of some rows computed in Thms. 1, 2 and 3 in a new order. As the consequence, we achieve $\sigma_{vrp}(G) = F \cdot \sigma_{cba}(S)$.

Example 1 Let $\mathcal{H}(\alpha, \beta, \beta, \alpha)$ be a double hexagonal (benzenoid) chain as shown in Fig. 5:

Then let us compute the Merrifield-Simmons index of $\mathcal{H}(\alpha, \beta, \beta, \alpha)$ by means of the Merrifield-Simmons vector at the path P_5 containing vertices u, w and v.

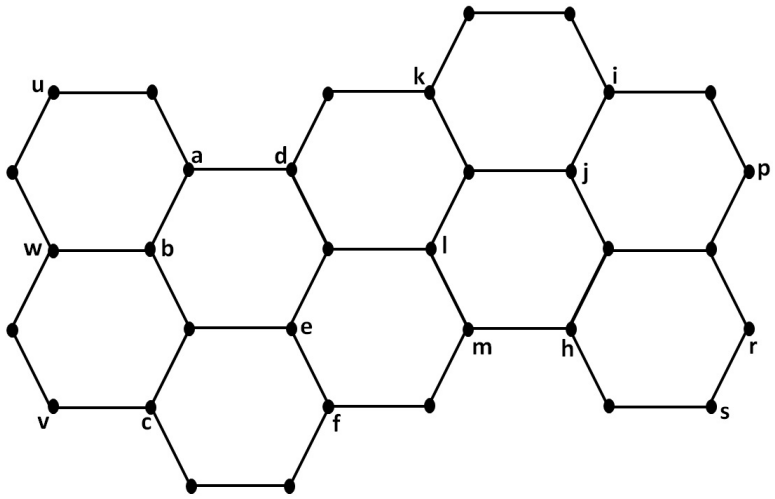


Fig. 5: A double hexagonal (benzenoid) chain $\mathcal{H}(\alpha, \beta, \beta, \alpha)$

An appropriate product of some of the matrices A, B, C, D, E, F and the vector $(8, 3, 2, 3, 1, 2, 1, 5, 6, 5, 4, 3, 2, 2, 1, 2, 2, 3)^T$, that is equal to $\sigma_{prs}(P_4)$, the Merrifield-Simmons index of $\mathcal{H}(\alpha, \beta, \beta, \alpha)$ can be computed as follows:

$$\begin{aligned}\sigma_{uwv}(\mathcal{H}(\alpha, \beta, \beta, \alpha)) = A \cdot \sigma_{abc}(S^I) &= A \cdot F \cdot \sigma_{def}(S^{II}) \\ &= A \cdot F \cdot E \cdot \sigma_{klm}(S^{III}) \\ &= A \cdot F \cdot E \cdot C \cdot \sigma_{ijh}(S^{IV}) \\ &= A \cdot F \cdot E \cdot C \cdot B \cdot \sigma_{prs}(P_4)\end{aligned}$$

$\sigma_{uwv}(\mathcal{H}(\alpha, \beta, \beta, \alpha)) = A \cdot F \cdot E \cdot C \cdot B \cdot (8, 3, 2, 3, 1, 2, 1, 5, 6, 5, 4, 3, 2, 2, 1, 2, 2, 3)^T$.

Hence, $\sigma_{uwv}(\mathcal{H}(\alpha, \beta, \beta, \alpha)) = (5967989, 1555736, 1253034, 1733170, 526867, 485079, 204036, 4234819, 4714955, 4412253, 3508652, 3644298, 1076343, 1253777, 726167, 767955, 1206303, 1070657)^T$ where $S^I, S^{II}, S^{III}, S^{IV}$ are corresponding subgraphs in $\mathcal{H}(\alpha, \beta, \beta, \alpha)$. As the result, we obtain the Merrifield-Simmons index as $\sigma(\mathcal{H}(\alpha, \beta, \beta, \alpha)) = 5967989$.

In conclusion, we can compute the Merrifield-Simmons index of any double hexagonal (benzenoid) chain via an appropiate product of some of the matrices A, B, C, D, E, F and the vector $(8, 3, 2, 3, 1, 2, 1, 5, 6, 5, 4, 3, 2, 2, 1, 2, 2, 3)^T$ by utilizing the Merrifield-Simmons vector together with Thms. 1, 2, 3, Cors. 1, 2 and 3.

3 Computing the Merrifield-Simmons index of hexagonal (benzenoid) chains

In [3], explicit expressions for the expected value of the Merrifield-Simmons index of a random hexagon chain were obtained. However, there is no practical way for computing $\sigma(G)$ where G represents any hexagonal chain. In this section, in parallel with the technique we applied in Sec. 2 we present reduction formulae to compute the Merrifield-Simmons index of hexagonal (benzenoid) chains by using the equations 1 and 2. As a beginning, let us introduce a vector at the edge ab that we call the simple Merrifield-Simmons vector in the next definition.

Definition 2 Let G be a graph and ab be an edge of G. The simple Merrifield-Simmons vector of G at the edge ab is defined as

$$\sigma_{ab}(G) = \begin{bmatrix} \sigma(G) \\ \sigma(G - N_G[a]) \\ \sigma(G - N_G[b]) \\ \sigma(G - a) \\ \sigma(G - b) \end{bmatrix}.$$

In a hexagonal chain, hexagons appear in three types that are shown below.

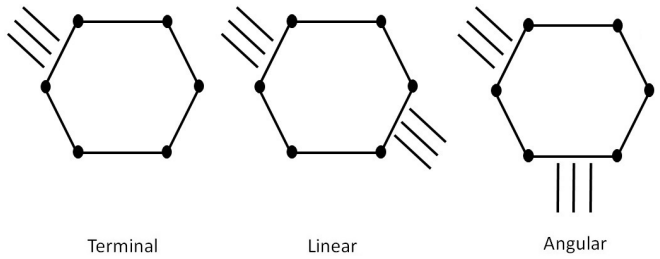


Fig. 6: Hexagon existence types in hexagonal chains

In Figs. 7 and 8, we show two graph structures where a hexagon has two different edge fusions with graph S to clarify the following theorems.

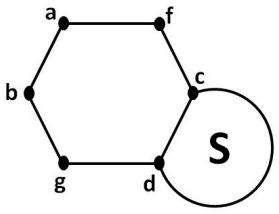


Fig. 7: Graph used in Thms. 4 and 6

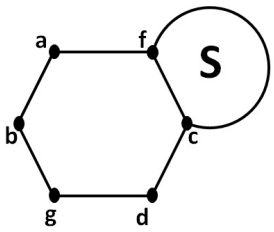


Fig. 8: Graph used in Thm. 5

Theorem 4 *Let $G = (V, E)$ be a graph derived from the edge-coalescence of the graph S and a hexagon at the edge cd of S (See Fig. 7). Then*

$$\sigma_{ab}(G) = Q \cdot \sigma_{cd}(S),$$

where $Q = \begin{bmatrix} 8 & -3 & -3 & 0 & 0 \\ 2 & 0 & -1 & 0 & 0 \\ 2 & -1 & 0 & 0 & 0 \\ 6 & -3 & -2 & 0 & 0 \\ 6 & -2 & -3 & 0 & 0 \end{bmatrix}$.

Proof Let P_n be path graph with n vertices. First of all, we calculate the Merrifield-Simmons indices of $G, G - N_G[a], G - N_G[b], G - a$ and $G - b$ by deleting some edges according to our need. Subsequently, we use the recurrence formulae 1 and 2 that are given at the beginning of the Sec. 2 as follows:

$$\begin{aligned}
\sigma(G) &= \sigma(G - cf) - \sigma(G - (N_G[c] \cup N_G[f])) \\
&= \sigma(G - cf) - \sigma(P_2 \cup (S - N_G[c])) \\
&= \sigma(G - cf - dg) - \sigma(G - cf - (N_G[d] \cup N_G[g])) \\
&\quad -\sigma(P_2 \cup (S - N_G[c])) \\
&= \sigma(P_4 \cup S) - \sigma(P_2 \cup (S - N_G[d])) - \sigma(P_2 \cup (S - N_G[c])) \\
&= 8\sigma(S) - 3\sigma(S - N_G[c]) - 3\sigma(S - N_G[d]) \\
&= (8, -3, -3, 0, 0) \cdot \sigma_{cd}(S), \\
\sigma(G - N_G[a]) &= \sigma(G - N_G[a] - dg) - \sigma(G - N_G[a] - (N_G[d] \cup N_G[g])) \\
&= \sigma(P_1 \cup S) - \sigma(S - N_G[d]) \\
&= 2\sigma(S) - \sigma(S - N_G[d]) \\
&= (2, 0, -1, 0, 0) \cdot \sigma_{cd}(S), \\
\sigma(G - N_G[b]) &= \sigma(G - N_G[b] - cf) - \sigma(G - N_G[b] - (N_G[c] \cup N_G[f])) \\
&= \sigma(P_1 \cup S) - \sigma(S - N_G[c]) \\
&= 2\sigma(S) - \sigma(S - N_G[c]) \\
&= (2, -1, 0, 0, 0) \cdot \sigma_{cd}(S), \\
\sigma(G - a) &= \sigma(G - a - cf) - \sigma(G - a - (N_G[c] \cup N_G[f])) \\
&= \sigma(G - a - cf) - \sigma(P_2 \cup (S - N_G[c]))
\end{aligned}$$

$$= \sigma(G-a-cf-dg) - \sigma(G-a-cf-(N_G[d]\cup N_G[g]))$$

$$-\sigma(P_2 \cup (S-N_G[c]))$$

$$= \sigma(P_1)\sigma(P_2)\sigma(S) - \sigma(P_1)\sigma(S-N_G[d]) - \sigma(P_2)\sigma(S-N_G[c])$$

$$= 2\cdot 3\sigma(S) - 3\sigma(S-N_G[c]) - 2\sigma(S-N_G[d])$$

$$= (6,-3,-2,0,0)\cdot\sigma_{cd}(S),$$

$$\sigma(G-b) = \sigma(G-b-cf) - \sigma(G-b-(N_G[c]\cup N_G[f]))$$

$$= \sigma(G-b-cf) - \sigma(P_1 \cup (S-N_G[c]))$$

$$= \sigma(G-b-cf-dg) - \sigma(G-b-cf-(N_G[d]\cup N_G[g]))$$

$$-\sigma(P_1 \cup (S-N_G[c]))$$

$$= \sigma(P_1)\sigma(P_2)\sigma(S) - \sigma(P_2)\sigma(S-N_G[d]) - \sigma(P_1)\sigma(S-N_G[c])$$

$$= 2\cdot 3\sigma(S) - 2\sigma(S-N_G[c]) - 3\sigma(S-N_G[d])$$

$$= (6,-2,-3,0,0)\cdot\sigma_{cd}(S).$$

As the result, we get $\sigma_{ab}(G) = Q\cdot\sigma_{cd}(S)$ where $Q = \begin{bmatrix} 8 & -3 & -3 & 0 & 0 \\ 2 & 0 & -1 & 0 & 0 \\ 2 & -1 & 0 & 0 & 0 \\ 6 & -3 & -2 & 0 & 0 \\ 6 & -2 & -3 & 0 & 0 \end{bmatrix}$.

It is clear that when S is isomorphic to P_2, we have $\sigma_{ab}(G) = Q\cdot(3,1,1,2,2)^T$ by Thm. 4. Moreover, if G be a graph obtained from the edge-coalescence of the graph S and a linear hexagonal chain with k hexagons at the edge cd of S, then it can be derived that $\sigma_{ab}(G) = Q^k\cdot\sigma_{cd}(S)$ by Thm. 4 and in the case of S is isomorphic to P_2 for this G, then $\sigma_{ab}(G) = Q^k\cdot(3,1,1,2,2)^T$.

Theorem 5 *Let $G=(V,E)$ be a graph derived from the edge-coalescence of the graph S and a hexagon at the edge fc of S (See Fig. 8). Then*

$$\sigma_{ab}(G) = P\cdot\sigma_{fc}(S),$$

where $P = \begin{bmatrix} 8 & -3 & -3 & 0 & 0 \\ 0 & 0 & -1 & 3 & 0 \\ 2 & 0 & -1 & 0 & 0 \\ 5 & 0 & -2 & 0 & 0 \\ 6 & -3 & -2 & 0 & 0 \end{bmatrix}$.

Proof Since we have $\sigma(G)$, $\sigma(G-N_G[b])$ and $\sigma(G-b)$ by the proof of Thm. 4, it can be observable that $\sigma(G) = (8,-3,-3,0,0)\cdot\sigma_{fc}(S)$, $\sigma(G-N_G[b]) =$

$(2,0,-1,0,0)\cdot\sigma_{fc}(S)$ and $\sigma(G-b)=(6,-3,-2,0,0)\cdot\sigma_{fc}(S)$. Therefore we only deal with the calculation of $\sigma(G-N_G[a])$ and $\sigma(G-a)$ by deleting the some certain edges. Later on, we use the recurrence formulae that are given at the beginning of the Sec. 2 as follows:

$$\begin{aligned}\sigma(G-N_G[a]) &= \sigma(G-N_G[a]-cd)-\sigma(G-N_G[a]-(N_G[c]\cup N_G[d]))\\ &= \sigma(P_2\cup(S-f))-\sigma(S-N_G[c])\\ &= \sigma(P_2)\sigma(S-f)-\sigma(S-N_G[c])\\ &= -\sigma(S-N_G[c])+3\sigma(S-f)\\ &= (0,0,-1,3,0)\cdot\sigma_{fc}(S),\\ \sigma(G-a) &= \sigma(G-a-cd)-\sigma(G-a-(N_G[c]\cup N_G[d]))\\ &= \sigma(P_3\cup S)-\sigma(P_1\cup(S-N_G[c]))\\ &= \sigma(P_3)\sigma(S)-\sigma(P_1)\sigma(S-N_G[c])\\ &= 5\sigma(S)-2\sigma(S-N_G[c])\\ &= (5,0,-2,0,0)\cdot\sigma_{fc}(S),\end{aligned}$$

Consequently, we get $\sigma_{ab}(G)=P\cdot\sigma_{fc}(S)$ where $P=\begin{bmatrix}8&-3&-3&0&0\\0&0&-1&3&0\\2&0&-1&0&0\\5&0&-2&0&0\\6&-3&-2&0&0\end{bmatrix}$.

Theorem 6 *Let $G=(V,E)$ be a graph derived from the edge-coalescence of the graph S and a hexagon at the edge cd of S (See Fig. 7). Then*

$$\sigma_{bg}(G)=R\cdot\sigma_{cd}(S),$$

where $R=\begin{bmatrix}8&-3&-3&0&0\\2&-1&0&0&0\\0&-1&0&0&3\\6&-2&-3&0&0\\5&-2&0&0&0\end{bmatrix}$.

Proof Similarly to the proof of Thm. 5, we have $\sigma(G)$, $\sigma(G-N_G[b])$ and $\sigma(G-b)$ by the proof of Thm. 4. Thus, it can be seen that $\sigma(G)=(8,-3,-3,0,0)\cdot\sigma_{cd}(S)$, $\sigma(G-N_G[b])=(2,-1,0,0,0)\cdot\sigma_{cd}(S)$ and $\sigma(G-b)=(6,-2,-3,0,0)\cdot\sigma_{cd}(S)$. Moreover, by the proof of Thm. 5, it can be observable that $\sigma(G-N_G[g])=(0,-1,0,0,3)\cdot\sigma_{cd}(S)$ and $\sigma(G-g)=(5,-2,0,0,0)\cdot\sigma_{cd}(S)$ by noticing the similarity of graphs in Figs. 7 and 8 and by utilizing the definition of the simple Merrifield-Simmons vector at the edge *cd*.

As the consequence, we get $\sigma_{bg}(G) = R \cdot \sigma_{cd}(S)$ where $R = \begin{bmatrix} 8 & -3 & -3 & 0 & 0 \\ 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 3 \\ 6 & -2 & -3 & 0 & 0 \\ 5 & -2 & 0 & 0 & 0 \end{bmatrix}$.

Example 2 Let G be a hexagonal (benzenoid) chain as shown in Fig. 9:

Then let us compute the Merrifield-Simmons index of G by utilizing the simple Merrifield-Simmons vector at the edge ab.

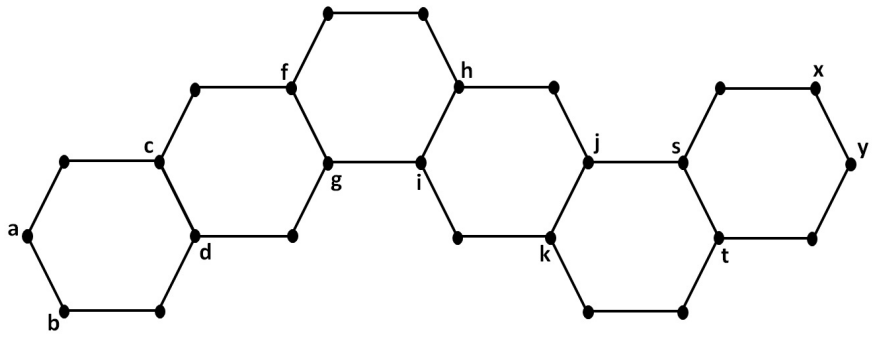


Fig. 9: A hexagonal (benzenoid) chain G

The Merrifield-Simmons index of G can be computed by taking an appropriate product of the matrices Q, P, R and the vector $(3,1,1,2,2)^T$, that is equal to $\sigma_{xy}(P_2)$ as follows:

$$\begin{aligned}
\sigma_{ab}(G) = Q \cdot \sigma_{cd}(S^I) &= Q \cdot Q \cdot \sigma_{fg}(S^{II}) \\
&= Q \cdot Q \cdot R \cdot \sigma_{hi}(S^{III}) \\
&= Q \cdot Q \cdot R \cdot Q \cdot \sigma_{jk}(S^{IV}) \\
&= Q \cdot Q \cdot R \cdot Q \cdot P \cdot \sigma_{st}(S^{V}) \\
&= Q \cdot Q \cdot R \cdot Q \cdot P \cdot Q \cdot \sigma_{xy}(P_2) \\
&= Q \cdot Q \cdot R \cdot Q \cdot P \cdot Q \cdot (3,1,1,2,2)^T \\
&= Q^2 \cdot R \cdot Q \cdot P \cdot Q \cdot (3,1,1,2,2)^T. \\
&= (182487, 49465, 49600, 133022, 132887)^T,
\end{aligned}$$

where S^I, S^{II}, S^{III}, S^{IV} and S^V are corresponding subgraphs in G. Consequently, we achieve the Merrifield-Simmons index of G as $\sigma(G) = 182487$.

As the result, we can compute the Merrifield-Simmons index of any hexagonal (benzenoid) chain by means of a proper product of some of the matrices Q, P, R and the vector $(3, 1, 1, 2, 2)^T$ by using the simple Merrifield-Simmons vector together with Thms. 4, 5 and 6.

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