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Enumeration of Independent Sets in Benzenoid Chains

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Abstract

The Merrifield-Simmons index of a graph G is defined as the summation of the number $i(G,k)$ of k-independent sets in G. It has applications in structural chemistry such as correlation with the thermodynamic properties of hydrocarbons. For this reason, enumeration of $i(G,k)$ of molecular graphs comes into prominence. In this paper, a method based on the transfer matrix technique is presented for enumerating $i(G,k)$ in benzenoid chains. As a consequence, for all $k \geq 0$, each $i(G,k)$ in arbitrary benzenoid chains is obtained via an appropriate product of three transfer matrices with dimension $5(k+1) \times 5(k+1)$ and a vector. In addition, we present two algorithms to make easier application of the method so that the applicability remains the same when the k value increases.

1 Introduction

Let G be a graph with vertex set V and edge set E. A set consisting of all adjacent vertices to a vertex v is called the neighborhood set of v, and it is denoted by $N_G(v)$. The union of the sets $N_G(v)$ and $\{v\}$ forms the closed neighborhood $N_G[v]$. If all vertices in a subset $S \subseteq V$ are pairwise nonadjacent, then S is called an independent set. An independent set with k vertices is called a k-independent set. The number of possible independent sets in G with k vertices is called the number of k-independent sets of G and it is denoted by $i(G,k)$. In connection with k-independent sets, the Merrifield-Simmons index is defined as

$$\sigma(G) = \sum_{k\geq 0} i(G,k)$$

where $i(G,0) = 1$ and it is trivial that $i(G,1) = |V|$.

The Merrifield-Simmons index has an important role in mathematical chemistry as it is used to predict thermodynamic properties of corresponding molecules by using molecular graphs, for a detailed survey, see [7, 8, 16].

Hexagonal systems are molecular graphs of benzenoid hydrocarbons so that they are also called benzenoid systems. A benzenoid system is a 2-connected planar graph in which each finite region is a regular hexagon. In a benzenoid system, a vertex that is contained by three hexagons is called the internal vertex. A benzenoid system without any internal vertex is called catacondensed benzenoid system, [3]. If every hexagon is adjacent to at most two hexagons in a catacondensed benzenoid system, then it is called a benzenoid chain. Benzenoid chains are one of the prominent subclasses of catacondensed benzenoid systems and a great deal of mathematical and chemical studies are carried out on them. Some topological indices of benzenoid chains were studied in [4, 6, 10, 12, 15]. Extremal properties of hexagonal chains were studied in [9, 18–20].

The transfer matrix method has been used on several enumeration problems in combinatorial and chemical graph theory, [13, 14]. Enumeration of independent sets in various molecular structures has been the topic of several studies. In [1, 2, 17], the numbers of independent sets of small size in various fullerene graphs are computed. In [5], explicit formulae are presented for the number of independent sets of certain types of chain hexagonal cacti. Moreover, a method is presented for calculating the Merrifield-Simmons index of any benzenoid chains in [11]. However, for every $k \geq 0$, $i(G,k)$ values were not computed, separately. In this paper, we familiarize the k-independence vector at an edge of a hexagon of a given benzenoid chain and we use the transfer matrix technique to construct a method for enumerating $i(G,k)$ values in arbitrary benzenoid chains. The method is based on an appropriate multiplication of three transfer matrices with dimension $5(k+1) \times 5(k+1)$ and a vector with dimension $5(k+1) \times 1$, where $k \geq 0$. Furthermore, in Section 3, we design two algorithms to facilitate the application of the method as k values increase.

Two significant recurrence relations for computing the number of k-independent sets in a graph G are given as follows:

$$i(S\cup H,k)=i(S,k)i(H,0)+i(S,k-1)i(H,1)+\cdots+i(S,1)i(H,k-1)+i(S,0)i(H,k), \quad (1)$$

where $G=S\cup H$ and S,H are two connected components of G. Moreover,

$$i(G,k)=i(G-uz,k)-i(G-N_G[u]-N_G[z],k-2), e=uz\in G. \quad (2)$$

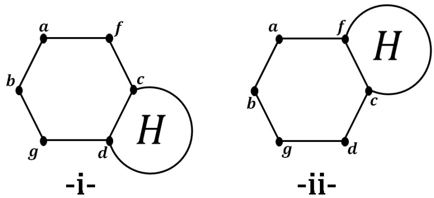

Figure 1. Benzenoid chain structures used in the next theorems

In Fig. 1, we show two isomorphic graphs with different vertex labels for the future use.

2 Enumeration of *k*-independent sets in benzenoid chains

Let us now introduce the k-independence vector of G at a given edge to compute $i(G,k)$ of G.

Definition 2.1. *Let $G=(V,E)$ be a graph and $e=uz\in E$. The k-independence vector of G at $e=uz$ is as shown below:*

$$i_{uz}(G,k)=\begin{pmatrix} i(G,k)\\ i(G,k-1)\\ \vdots\\ i(G,0)\\ i(G-N_G[u],k)\\ i(G-N_G[u],k-1)\\ \vdots\\ i(G-N_G[u],0)\\ i(G-N_G[z],k)\\ i(G-N_G[z],k-1)\\ \vdots\\ i(G-N_G[z],0)\\ i(G-u,k)\\ i(G-u,k-1)\\ \vdots\\ i(G-u,0)\\ i(G-z,k)\\ i(G-z,k-1)\\ \vdots\\ i(G-z,0) \end{pmatrix}.$$

Theorem 2.1. *Let $G = (V, E)$ be a graph obtained by fusing a graph H and a hexagon with the edge cd in common (see Fig. 1 (i)). Then*

$$i_{ab}(G, k) = M_1 \cdot i_{cd}(H, k)$$

where M_1 is a transfer matrix with dimension $5(k+1) \times 5(k+1)$ as follows:

$$\left(\begin{array}{cccccc:cccccc:cccccc:ccccccc:ccccccc}
1 & 4 & 3 & 0 & \cdots & 0 & 0 & 0 & -1 & -2 & \cdots & 0 & 0 & 0 & -1 & -2 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 4 & 3 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & & & & & & & & \\
0 & \cdots & 0 & 1 & 4 & 3 & 0 & \cdots & 0 & 0 & -1 & -2 & 0 & \cdots & 0 & 0 & -1 & -2 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 1 & 4 & 3 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 1 & 4 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
\hdashline
1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & & & & & & & & \\
0 & \cdots & 0 & 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
\hdashline
1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & & & & & & & & \\
0 & \cdots & 0 & 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
\hdashline
1 & 3 & 2 & 0 & \cdots & 0 & 0 & 0 & -1 & -2 & \cdots & 0 & 0 & 0 & -1 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 3 & 2 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & & & & & & & & \\
0 & \cdots & 1 & 3 & 2 & 0 & 0 & \cdots & 0 & 0 & -1 & -2 & 0 & \cdots & 0 & 0 & -1 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 1 & 3 & 2 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 1 & 3 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
\hdashline
1 & 3 & 2 & 0 & \cdots & 0 & 0 & 0 & -1 & -1 & \cdots & 0 & 0 & 0 & -1 & -2 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 3 & 2 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & & & & & & & & \\
0 & \cdots & 1 & 3 & 2 & 0 & 0 & \cdots & 0 & 0 & -1 & -1 & 0 & \cdots & 0 & 0 & -1 & -2 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 1 & 3 & 2 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 1 & 3 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0
\end{array}\right).$$

Proof. By the definition of the k-independence vector at the edge ab of G, firstly let us aim to get the values $i(G, k), i(G - N_G[a], k)$, $i(G - N_G[b], k), i(G - a, k)$ and $i(G - b, k)$ as a product of a vector and $i_{cd}(H, k)$. To achieve this purpose, let us delete suitable combinations of edges cf and dg from each corresponding subgraph. Thus, we can get desired equations by using the recurrence relations 1 and 2 as follows:

$$
\begin{aligned}
i(G,k) =\; & i(G-cf-dg,k) - i(G-cf-N_G[d]-N_G[g],k-2) - i(G-N_G[c]-N_G[f],k-2)\\
=\; & i(P_4\cup H,k) - i(P_2\cup(H-N_G[d]),k-2) - i(P_2\cup(H-N_G[c]),k-2)\\
=\; & i(H,k)+4i(H,k-1)+3i(H,k-2)-i(H-N_G[d],k-2)-2i(H-N_G[d],k-3)\\
-\; & i(H-N_G[c],k-2)-2i(H-N_G[c],k-3)\\
=\; & (1,4,3,0,\cdots,0,0,0,-1,-2,0,\cdots,0,0,0,-1,-2,0,\cdots,0,0,\cdots,0,0,\cdots,0)\cdot i_{cd}(H,k),\\
i(G-N_G[a],k) =\; & i(G-N_G[a]-dg,k) - i(G-N_G[a]-N_G[d]-N_G[g],k-2)\\
=\; & i(P_1\cup H,k) - i(H-N_G[d],k-2)\\
=\; & i(H,k)+i(H,k-1)-i(H-N_G[d],k-2)\\
=\; & (1,1,0,0,\cdots,0,0,\cdots,0,0,0,-1,0,\cdots,0,0,\cdots,0,0,\cdots,0)\cdot i_{cd}(H,k),\\
i(G-N_G[b],k) =\; & i(G-N_G[b]-cf,k) - i(G-N_G[b]-N_G[c]-N_G[f],k-2)\\
=\; & i(P_1\cup H,k) - i(H-N_G[c],k-2)\\
=\; & i(H,k)+i(H,k-1)-i(H-N_G[c],k-2)\\
=\; & (1,1,0,0,\cdots,0,0,0,-1,0,\cdots,0,0,\cdots,0,0,\cdots,0,0,\cdots,0)\cdot i_{cd}(H,k),\\
i(G-a,k) =\; & i(G-a-cf-dg,k) - i(G-a-cf-N_G[d]-N_G[g],k-2)\\
-\; & i(G-a-N_G[c]-N_G[f],k-2)\\
=\; & i(P_1\cup P_2\cup H,k) - i(P_1\cup(H-N_G[d]),k-2) - i(P_2\cup(H-N_G[c]),k-2)\\
=\; & i(H,k)+3i(H,k-1)+2i(H,k-2)-i(H-N_G[d],k-2)-i(H-N_G[d],k-3)\\
-\; & i(H-N_G[c],k-2)-2i(H-N_G[c],k-3)\\
=\; & (1,3,2,0,\cdots,0,0,0,-1,-2,0,\cdots,0,0,0,-1,-1,0,\cdots,0,0,\cdots,0,0,\cdots,0)\cdot i_{cd}(H,k),\\
i(G-b,k) =\; & i(G-b-cf-dg,k) - i(G-b-cf-N_G[d]-N_G[g],k-2)\\
-\; & i(G-b-N_G[c]-N_G[f],k-2)\\
=\; & i(P_1\cup P_2\cup H,k) - i(P_2\cup(H-N_G[d]),k-2) - i(P_1\cup(H-N_G[c]),k-2)\\
=\; & i(H,k)+3i(H,k-1)+2i(H,k-2)-i(H-N_G[d],k-2)-2i(H-N_G[d],k-3)\\
-\; & i(H-N_G[c],k-2)-i(H-N_G[c],k-3)\\
=\; & (1,3,2,0,\cdots,0,0,0,-1,-1,0,\cdots,0,0,0,-1,-2,0,\cdots,0,0,\cdots,0,0,\cdots,0)\cdot i_{cd}(H,k).
\end{aligned}
$$

Then, by using the five obtained equations, it is deducable that the k value decreases only for $i(G,k-1)$, $\cdots$, $i(G,0)$, $i(G-N_G[a],k-1),\cdots$, $i(G-N_G[a],0)$, $i(G-N_G[b],k-1),\cdots,i(G-N_G[b],0), i(G-a,k-1),\cdots,i(G-a,0)$ and $i(G-b,k-1),\cdots,i(G-b,0)$. Hence $i_{ab}(G,k)$ is obtained as the product of $i_{cd}(H,k)$ and a $5(k+1)\times 5(k+1)$ dimensional matrix whose the first, $(k+2)$-th, $(2k+3)$-th , $(3k+4)$-th and $(4k+5)$-th rows are the vectors as follows, respectively:

$(1,4,3,0,\cdots,0,0,0,-1,-2,0,\cdots,0,0,0,-1,-2,0,\cdots,0,0,\cdots,0,0,\cdots,0)$,
$(1,1,0,0,\cdots,0,0,\cdots,0,0,0,-1,0,\cdots,0,0,\cdots,0,0,\cdots,0)$,
$(1,1,0,0,\cdots,0,0,0,-1,0,\cdots,0,0,\cdots,0,0,\cdots,0,0,\cdots,0)$,
$(1,3,2,0,\cdots,0,0,0,-1,-2,0,\cdots,0,0,0,-1,-1,0,\cdots,0,0,\cdots,0,0,\cdots,0)$,

$(1,3,2,0,\cdots,0,0,0,-1,-1,0,\cdots,0,0,0,-1,-2,0,\cdots,0,0,\cdots,0,0,\cdots,0)$.

The remaining rows of the matrix excluding the first, $(k+2)$-th, $(2k+3)$-th, $(3k+4)$-th and $(4k+5)$-th rows, are determined in the echelon form in every 25 submatrices by depending on these rows since just k value decreases in the equations of $i(G,k-1)$, $\cdots$, $i(G,0)$, $i(G-N_G[a],k-1),\cdots$, $i(G-N_G[a],0)$, $i(G-N_G[b],k-1),\cdots,i(G-N_G[b],0),i(G-a,k-1),\cdots,i(G-a,0)$ and $i(G-b,k-1),\cdots,i(G-b,0)$. In conclusion, it is reached that $i_{ab}(G,k)=M_1\cdot i_{cd}(H,k)$ where M_1 is the given matrix above with dimension $5(k+1)\times 5(k+1)$. ■

As a natural result of Theorem 2.1, in the case of S is isomorphic to path graph P_2, it is obtained that

$$i_{ab}(G,k)=M_1\cdot\left[\begin{array}{ccccccccccccccccccccccc} 0 & \cdots & 0 & 2 & 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 1 & 1 & 0 & \cdots & 0 & 1 & 1 \end{array}\right]^T.$$

Theorem 2.2. *Let $G=(V,E)$ be a graph obtained by fusing a graph H and a hexagon with the edge fc in common (see Fig. 1 (ii)). Then*

$$i_{ab}(G,k)=M_2\cdot i_{fc}(H,k)$$

where M_2 is a transfer matrix with dimension $5(k+1)\times 5(k+1)$ as follows:

$$\left(\begin{array}{cccccc|cccccc|cccccc|ccccccc|ccccccc}
1 & 4 & 3 & 0 & \cdots & 0 & 0 & 0 & -1 & -2 & \cdots & 0 & 0 & 0 & -1 & -2 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 4 & 3 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & & & & & & & & \\
0 & \cdots & 0 & 1 & 4 & 3 & 0 & \cdots & 0 & 0 & -1 & -2 & 0 & \cdots & 0 & 0 & -1 & -2 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 1 & 4 & 3 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 1 & 4 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 1 & 2 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 1 & 2 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & & & & & & & & \\
0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 1 & 2 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 2 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
\hline
1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & & & & & & & & \\
0 & \cdots & 0 & 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
\hline
1 & 3 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 3 & 1 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & & & & & & & & \\
0 & \cdots & 1 & 3 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -1 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 1 & 3 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 1 & 3 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
\hline
1 & 3 & 2 & 0 & \cdots & 0 & 0 & 0 & -1 & -2 & \cdots & 0 & 0 & 0 & -1 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 3 & 2 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & & & & & & & & \\
0 & \cdots & 1 & 3 & 2 & 0 & 0 & \cdots & 0 & 0 & -1 & -2 & 0 & \cdots & 0 & 0 & -1 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 1 & 3 & 2 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 1 & 3 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0
\end{array}\right).$$

Proof. We need to compute $i(G,k), i(G-N_G[a],k)$, $i(G-N_G[b],k), i(G-a,k)$ and $i(G-b,k)$ by deleting appropriate combinations of edges dc and fa to get the subgraph S apart from the hexagon. Afterwards, we utilize the recurrence relations 1 and 2 as the following:

$$\begin{aligned}
i(G,k) &= i(G-fa-cd,k)-i(G-fa-N_G[c]-N_G[d],k-2)-i(G-N_G[f]-N_G[a],k-2)\\
&= i(P_4\cup H,k)-i(P_2\cup(H-N_G[c]),k-2)-i(P_2\cup(H-N_G[f]),k-2)\\
&= i(H,k)+4i(H,k-1)+3i(H,k-2)-i(H-N_G[c],k-2)-2i(H-N_G[c],k-3)\\
&- i(H-N_G[f],k-2)-2i(H-N_G[f],k-3)\\
&= (1,4,3,0,\cdots,0,0,0,-1,-2,0,\cdots,0,0,0,-1,-2,0,\cdots,0,0,\cdots,0,0,\cdots,0)\cdot i_{fc}(H,k),\\
i(G-N_G[a],k) &= i(G-N_G[a]-cd,k)-i(G-N_G[a]-N_G[c]-N_G[d],k-2)\\
&= i(P_2\cup(H-f),k)-i(H-N_G[c],k-2)\\
&= i(H-f,k)+2i(H-f,k-1)-i(H-N_G[c],k-2)\\
&= (0,\cdots,0,0,\cdots,0,0,0,-1,0,\cdots,0,1,2,0,\cdots,0,0,\cdots,0)\cdot i_{fc}(H,k),\\
i(G-N_G[b],k) &= i(G-N_G[b]-cd,k)-i(G-N_G[b]-N_G[c]-N_G[d],k-2)\\
&= i(P_1\cup H,k)-i(H-N_G[c],k-2)\\
&= i(H,k)+i(H,k-1)-i(H-N_G[c],k-2)\\
&= (1,1,0,0,\cdots,0,0,\cdots,0,0,0,-1,0,\cdots,0,0,\cdots,0,0,\cdots,0)\cdot i_{fc}(H,k),\\
i(G-a,k) &= i(G-a-cd,k)-i(G-a-N_G[c]-N_G[d],k-2)\\
&= i(P_3\cup H,k)-i(P_1\cup(H-N_G[c]),k-2)\\
&= i(H,k)+3i(H,k-1)+i(H,k-2)-i(H-N_G[c],k-2)-i(H-N_G[c],k-3)\\
&= (1,3,1,0,\cdots,0,0,\cdots,0,0,0,-1,-1,0,\cdots,0,0,\cdots,0,0,\cdots,0)\cdot i_{fc}(H,k),\\
i(G-b,k) &= i(G-b-fa-cd,k)-i(G-b-fa-N_G[c]-N_G[d],k-2)-i(G-b-N_G[f]-N_G[a],k-2)\\
&= i(P_1\cup P_2\cup H,k)-i(P_1\cup(H-N_G[c]),k-2)-i(P_2\cup(H-N_G[f]),k-2)\\
&= i(H,k)+3i(H,k-1)+2i(H,k-2)-i(H-N_G[c],k-2)-i(H-N_G[c],k-3)\\
&- i(H-N_G[f],k-2)-2i(H-N_G[f],k-3)\\
&= (1,3,2,0,\cdots,0,0,0,-1,-2,0,\cdots,0,0,0,-1,-1,0,\cdots,0,0,\cdots,0,0,\cdots,0)\cdot i_{fc}(H,k).
\end{aligned}$$

From the five equations obtained above, other required equations in which only k value decreases for $i(G,k-1),\cdots,i(G,0)$, $i(G-N_G[a],k-1),\cdots,i(G-N_G[a],0)$, $i(G-N_G[b],k-1),\cdots,i(G-N_G[b],0), i(G-a,k-1),\cdots,i(G-a,0)$ and $i(G-b,k-1),\cdots,i(G-b,0)$ are obtained in the form of a product of a vector and $i_{fc}(H,k)$. Consequently, $i_{ab}(G,k)$ is reached as the product of $i_{fc}(H,k)$ and $5(k+1)\times 5(k+1)$ dimensional matrix whose the first, $(k+2)$-th, $(2k+3)$-th, $(3k+4)$-th and $(4k+5)$-th rows are the vectors as given below, respectively:

$(1,4,3,0,\cdots,0,0,0,-1,-2,0,\cdots,0,0,0,-1,-2,0,\cdots,0,0,\cdots,0,0,\cdots,0)$,

$(0,\cdots,0,0,\cdots,0,0,0,-1,0,\cdots,0,1,2,0,\cdots,0,0,\cdots,0)$,

$(1,1,0,0,\cdots,0,0,\cdots,0,0,0,-1,0,\cdots,0,0,\cdots,0,0,\cdots,0)$,

$(1, 3, 1, 0, \cdots, 0, 0, \cdots, 0, 0, 0, -1, -1, 0, \cdots, 0, 0, \cdots, 0, 0, \cdots, 0),$

$(1, 3, 2, 0, \cdots, 0, 0, 0, -1, -2, 0, \cdots, 0, 0, 0, -1, -1, 0, \cdots, 0, 0, \cdots, 0, 0, \cdots, 0).$

Since only k value decreases for other equations, the rest of the rows of the matrix exist in the echelon form in each of the 25 submatrices by depending on the stated rows above. Let us call the above matrix by M_2. Then we get the result as $i_{ab}(G, k) = M_2 \cdot i_{fc}(H, k)$.

∎

Theorem 2.3. *Let $G = (V, E)$ be a graph obtained by fusing a graph H and a hexagon with the edge cd in common (see Fig. 1). Then*

$$i_{bg}(G, k) = M_3 \cdot i_{cd}(H, k)$$

where M_3 is a transfer matrix with dimension $5(k+1) \times 5(k+1)$ as follows:

$$\left(\begin{array}{cccccc|cccccc|cccccc|ccccccc|ccccccc}
1 & 4 & 3 & 0 & \cdots & 0 & 0 & 0 & -1 & -2 & \cdots & 0 & 0 & 0 & -1 & -2 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 4 & 3 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & & & & & & & & \\
0 & \cdots & 0 & 1 & 4 & 3 & 0 & \cdots & 0 & 0 & -1 & -2 & 0 & \cdots & 0 & 0 & -1 & -2 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 1 & 4 & 3 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 1 & 4 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
\hline
1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & & & & & & & & \\
0 & \cdots & 0 & 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 1 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 & 2 & 0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 2 & 0 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & & & & & & & & \\
0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 2 & 0 \\
0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 2 \\
0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 1 \\
\hline
1 & 3 & 2 & 0 & \cdots & 0 & 0 & 0 & -1 & -1 & \cdots & 0 & 0 & 0 & -1 & -2 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 3 & 2 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & & & & & & & & \\
0 & \cdots & 1 & 3 & 2 & 0 & 0 & \cdots & 0 & 0 & -1 & -1 & 0 & \cdots & 0 & 0 & -1 & -2 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 1 & 3 & 2 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 1 & 3 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
\hline
1 & 3 & 1 & 0 & \cdots & 0 & 0 & 0 & -1 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & 1 & 3 & 1 & \cdots & 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
 & & & & & & & & & & & & \vdots & & & & & & & & & & & & & & & & & & & \\
0 & \cdots & 1 & 3 & 1 & 0 & 0 & \cdots & 0 & 0 & -1 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 1 & 3 & 1 & 0 & \cdots & 0 & 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 1 & 3 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\
0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0
\end{array}\right).$$

Proof. First of all, three of the values required for the proof have already been determined in the proof of Theorem 2.1 as presented below:

$i(G, k) = (1, 4, 3, 0, \cdots, 0, 0, 0, -1, -2, 0, \cdots, 0, 0, 0, -1, -2, 0, \cdots, 0, 0, \cdots, 0, 0, \cdots, 0) \cdot i_{cd}(H, k),$

$i(G - N_G[b], k) = (1, 1, 0, 0, \cdots, 0, 0, 0, -1, 0, \cdots, 0, 0, \cdots, 0, 0, \cdots, 0, 0, \cdots, 0) \cdot i_{cd}(H, k),$

$i(G - b, k) = (1, 3, 2, 0, \cdots, 0, 0, 0, -1, -1, 0, \cdots, 0, 0, 0, -1, -2, 0, \cdots, 0, 0, \cdots, 0, 0, \cdots, 0) \cdot i_{cd}(H, k).$

Hence, we need to compute just $i(G - N_G[g], k)$ and $i(G - g, k)$ by deleting the edge cf. Then by utilizing the recurrence relations 1 and 2 we get equations as below:

$$\begin{aligned}
i(G - N_G[g], k) &= i(G - N_G[g] - cf, k) - i(G - N_G[g] - N_G[c] - N_G[f], k-2) \\
&= i(P_2 \cup (H - d), k) - i((H - N_G[c]), k-2) \\
&= i(H - d, k) + 2i(H - d, k-1) - i(H - N_G[c], k-2) \\
&= (0, \cdots, 0, 0, 0, -1, 0, \cdots, 0, 0, \cdots, 0, 0, \cdots, 0, 1, 2, 0, \cdots, 0) \cdot i_{cd}(H, k), \\
i(G - g, k) &= i(G - g - cf, k) - i(G - g - N_G[c] - N_G[f], k-2) \\
&= i(P_3 \cup H, k) - i(P_1 \cup (H - N_G[c]), k-2) \\
&= i(H, k) + 3(H, k-1) + i(H, k-2) - i(H - N_G[c], k-2) - i(H - N_G[c], k-3) \\
&= (1, 3, 1, 0, \cdots, 0, 0, 0, -1, -1, 0, \cdots, 0, 0, \cdots, 0, 0, \cdots, 0, 0, \cdots, 0) \cdot i_{cd}(H, k).
\end{aligned}$$

It is deducable that only the k value decreases for the rest of the entries of the vector $i_{bg}(G, k)$, each of these values can be achieved as a product of $i_{cd}(H, k)$ and a $5(k+1) \times 1$ dimensional vector by using the equations above. Then it is clear that $i_{bg}(G, k)$ can be written as $M_3 \cdot i_{cd}(H, k)$ where M_3 is a $5(k+1) \times 5(k+1)$ dimensional matrix whose the first, $(k+2)$-th, $(2k+3)$-th, $(3k+4)$-th and $(4k+5)$-th rows are the following vectors, respectively, and remaining rows are in the echelon form in each of the 25 submatrices:
$(1, 4, 3, 0, \cdots, 0, 0, 0, -1, -2, 0, \cdots, 0, 0, 0, -1, -2, 0, \cdots, 0, 0, \cdots, 0, 0, \cdots, 0)$,
$(1, 1, 0, 0, \cdots, 0, 0, 0, -1, 0, \cdots, 0, 0, \cdots, 0, 0, \cdots, 0, 0, \cdots, 0)$,
$(0, \cdots, 0, 0, 0, -1, 0, \cdots, 0, 0, \cdots, 0, 0, \cdots, 0, 1, 2, 0, \cdots, 0)$,
$(1, 3, 2, 0, \cdots, 0, 0, 0, -1, -1, 0, \cdots, 0, 0, 0, -1, -2, 0, \cdots, 0, 0, \cdots, 0, 0, \cdots, 0)$,
$(1, 3, 1, 0, \cdots, 0, 0, 0, -1, -1, 0, \cdots, 0, 0, \cdots, 0, 0, \cdots, 0, 0, \cdots, 0)$.
Consequently, this completes the proof. ■

3 Algorithms

In Section 2, we presented the theoretical part of our method used to compute the k-independent sets in benzenoid chains. This method is based on three transfer matrices and a vector that we called M_1, M_2, M_3 and $i_{cd}(P_2, k)$, respectively. However, when the k value increases, computation is getting difficult because of the dimensions of the transfer matrices and the vector. Therefore, in this section we present two algorithms that are designed in MATLAB to easily get M_1, M_2, M_3 and $i_{cd}(P_2, k)$ for all $k \geq 0$. In the first algorithm, based on the input that is k value, for a path graph P_2 with the edge cd,

$i_{cd}(P_2, k)$ is obtained as follows:

$$i_{cd}(P_2,k) = \begin{bmatrix} 0 & \cdots & 0 & 2 & 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 1 & 1 & 0 & \cdots & 0 & 1 & 1 \end{bmatrix}^T.$$

Let us present Algorithm 1 below:

Algorithm 1: Algorithm to obtain $i_{cd}(P_2, k)$ where cd is the edge of P_2.

Input: Enter the value of k.
Result: $i_{cd}(P_2, k)$.
$V = zeros(1, 5 * k + 5);$
$V(k) = 2;$
$V(k + 1) = 1;$
$V(2 * k + 2) = 1;$
$V(3 * k + 3) = 1;$
$V(4 * k + 3) = 1;$
$V(4 * k + 4) = 1;$
$V(5 * k + 4) = 1;$
$V(5 * k + 5) = 1;$
$V1 = transpose(V);$

In the Algorithm 2, based on the input k value, we get the transfer matrices M_1, M_2, M_3 by adding a couple of steps at the beginning before the step "$M(1, :) = T1;$" as follows:

For the transfer matrix M_1, it is needed to add the steps consequtively as follows: $T1 = zeros(1, 5*k+5);$ $T1(1) = 1;$ $T1(2) = 4;$ $T1(3) = 3;$ $T1(k+4) = -1;$ $T1(k+5) = -2;$ $T1(2 * k + 5) = -1;$ $T1(2 * k + 6) = -2;$ $T2 = zeros(1, 5 * k + 5);$ $T2(1) = 1;$ $T2(2) = 1;$ $T2(2 * k + 5) = -1;$ $T3 = zeros(1, 5 * k + 5);$ $T3(1) = 1;$ $T3(2) = 1;$ $T3(k+4) = -1;$ $T4 = zeros(1, 5*k+5);$ $T4(1) = 1;$ $T4(2) = 3;$ $T4(3) = 2;$ $T4(k+4) = -1;$ $T4(k + 5) = -2;$ $T4(2 * k + 5) = -1;$ $T4(2 * k + 6) = -1;$ $T5 = zeros(1, 5 * k + 5);$ $T5(1) = 1;$ $T5(2) = 3;$ $T5(3) = 2;$ $T5(k + 4) = -1;$ $T5(k + 5) = -1;$ $T5(2 * k + 5) = -1;$ $T5(2 * k + 6) = -2;$

For the transfer matrix M_2, it is needed to add the steps consequtively as follows: $T1 = zeros(1, 5*k+5);$ $T1(1) = 1;$ $T1(2) = 4;$ $T1(3) = 3;$ $T1(k+4) = -1;$ $T1(k+5) = -2;$ $T1(2 * k + 5) = -1;$ $T1(2 * k + 6) = -2;$ $T2 = zeros(1, 5 * k + 5);$ $T2(2 * k + 5) = -1;$ $T2(3 * k + 4) = 1;$ $T2(3 * k + 5) = 2;$ $T3 = zeros(1, 5 * k + 5);$ $T3(1) = 1;$ $T3(2) = 1;$ $T3(2 * k + 5) = -1;$ $T4 = zeros(1, 5 * k + 5);$ $T4(1) = 1;$ $T4(2) = 3;$ $T4(3) = 1;$ $T4(2*k+5) = -1;$ $T4(2*k+6) = -1;$ $T5 = zeros(1, 5*k+5);$ $T5(1) = 1;$ $T5(2) = 3;$ $T5(3) = 2;$ $T5(k+4) = -1;$ $T5(k+5) = -2;$ $T5(2*k+5) = -1;$ $T5(2*k+6) = -1;$

For the transfer matrix M_3, it is needed to add the steps consequtively as follows: $T1 = zeros(1, 5*k+5);$ $T1(1) = 1;$ $T1(2) = 4;$ $T1(3) = 3;$ $T1(k+4) = -1;$ $T1(k+5) = -2;$ $T1(2 * k + 5) = -1;$ $T1(2 * k + 6) = -2;$ $T2 = zeros(1, 5 * k + 5);$ $T2(1) = 1;$ $T2(2) = 1;$ $T2(k+4) = -1;$ $T3 = zeros(1, 5*k+5);$ $T3(k+4) = -1;$ $T3(4*k+5) = 1;$ $T3(4 * k + 6) = 2;$ $T4 = zeros(1, 5 * k + 5);$ $T4(1) = 1;$ $T4(2) = 3;$ $T4(3) =$

2; $T4(k+4) = -1$; $T4(k+5) = -1$; $T4(2*k+5) = -1$; $T4(2*k+6) = -2$; $T5 = zeros(1, 5*k+5)$; $T5(1) = 1$; $T5(2) = 3$; $T5(3) = 1$; $T5(k+4) = -1$; $T5(k+5) = -1$;

Now, let us present the Algorithm 2, which runs according to the inputs above:

Algorithm 2: Algorithm to obtain the transfer matrices M_1, M_2, M_3 according to k.

```
Input: Enter the value of k.
Result: M1, M2 and M3.
M = zeros(5*k+5, 5*k+5);
"According to the transfer matrix desired to be obtained, the steps given before the algorithm will be entered in
  this part ";
M(1,:) = T1;
M(k+2,:) = T2;
M(2*k+3,:) = T3;
M(3*k+4,:) = T4;
M(4*k+5,:) = T5;
for from i = 1 to k+1 do
    for from j = i to k do
        M(i+1, j+1) = M(i, j);
        M(i+1, j+k+2) = M(i, j+k+1);
        M(i+1, j+2*k+3) = M(i, j+2*k+2);
        M(i+1, j+3*k+4) = M(i, j+3*k+3);
        M(i+1, j+4*k+5) = M(i, j+4*k+4);
    end
end
for from i = k+2 to 2*k+1 do
    for from j = 1 to k do
        M(i+1, j+1) = M(i, j);
        M(i+1, j+k+2) = M(i, j+k+1);
        M(i+1, j+2*k+3) = M(i, j+2*k+2);
        M(i+1, j+3*k+4) = M(i, j+3*k+3);
        M(i+1, j+4*k+5) = M(i, j+4*k+4);
    end
end
for from i = 2*k+3 to 3*k+2 do
    for from j = 1 to k do
        M(i+1, j+1) = M(i, j);
        M(i+1, j+k+2) = M(i, j+k+1);
        M(i+1, j+2*k+3) = M(i, j+2*k+2);
        M(i+1, j+3*k+4) = M(i, j+3*k+3);
        M(i+1, j+4*k+5) = M(i, j+4*k+4);
    end
end
for from i = 3*k+4 to 4*k+3 do
    for from j = 1 to k do
        M(i+1, j+1) = M(i, j);
        M(i+1, j+k+2) = M(i, j+k+1);
        M(i+1, j+2*k+3) = M(i, j+2*k+2);
        M(i+1, j+3*k+4) = M(i, j+3*k+3);
        M(i+1, j+4*k+5) = M(i, j+4*k+4);
    end
end
for from i = 4*k+5 to 5*k+4 do
    for from j = 1 to k do
        M(i+1, j+1) = M(i, j);
        M(i+1, j+k+2) = M(i, j+k+1);
        M(i+1, j+2*k+3) = M(i, j+2*k+2);
        M(i+1, j+3*k+4) = M(i, j+3*k+3);
        M(i+1, j+4*k+5) = M(i, j+4*k+4);
    end
end
```

Example 3.1. *Let G be a benzenoid chain with 11 hexagons as shown in Fig. 2.*

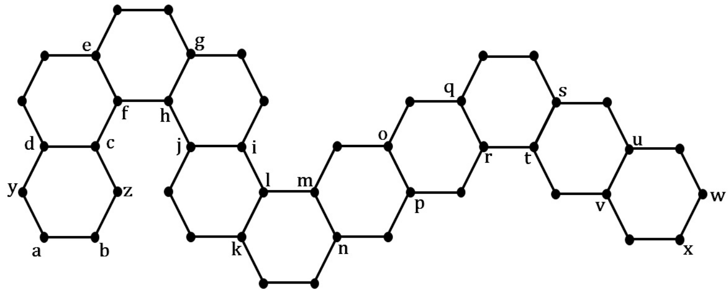

Figure 2. Benzenoid chain with 11 hexagons

For all $k \geq 0$, $i(G,k)$ of G can be computed by means of the vector $i_{ab}(G,k)$ and Thms. 2.1, 2.2, 2.3 as follows:

$$
\begin{aligned}
i_{ab}(G,k) &= M_1 \cdot i_{dc}(S^I,k),\\
&= M_1 \cdot M_3 \cdot i_{ef}(S^{II},k),\\
&= M_1 \cdot M_3 \cdot M_3 \cdot i_{gh}(S^{III},k),\\
&= M_1 \cdot M_3 \cdot M_3 \cdot M_3 \cdot i_{ij}(S^{IV},k),\\
&= M_1 \cdot M_3 \cdot M_3 \cdot M_3 \cdot M_2 \cdot i_{lk}(S^{V},k),\\
&= M_1 \cdot M_3 \cdot M_3 \cdot M_3 \cdot M_2 \cdot M_2 \cdot i_{mn}(S^{VI},k),\\
&= M_1 \cdot M_3 \cdot M_3 \cdot M_3 \cdot M_2 \cdot M_2 \cdot M_1 \cdot i_{op}(S^{VII},k),\\
&= M_1 \cdot M_3 \cdot M_3 \cdot M_3 \cdot M_2 \cdot M_2 \cdot M_1 \cdot M_1 \cdot i_{qr}(S^{VIII},k),\\
&= M_1 \cdot M_3 \cdot M_3 \cdot M_3 \cdot M_2 \cdot M_2 \cdot M_1 \cdot M_1 \cdot M_3 \cdot i_{st}(S^{IX},k),\\
&= M_1 \cdot M_3 \cdot M_3 \cdot M_3 \cdot M_2 \cdot M_2 \cdot M_1 \cdot M_1 \cdot M_3 \cdot M_1 \cdot i_{uv}(S^{X},k),\\
&= M_1 \cdot M_3 \cdot M_3 \cdot M_3 \cdot M_2 \cdot M_2 \cdot M_1 \cdot M_1 \cdot M_3 \cdot M_1 \cdot M_1 \cdot i_{wx}(P_2,k),
\end{aligned}
$$

where $S^I, S^{II}, \cdots, S^X$ are corresponding subgraphs.

Hence desired k value can be chosen in the last equation above to get $i_{ab}(G,k)$. Since the vector $i_{ab}(G,k)$ contains the numbers of all k-independent sets in G up to the k value including k value, all of these are obtained. Let us choose $k = 25$ as follows:

$$i_{ab}(G,25) \;=\; M_1 \cdot M_3 \cdot M_3 \cdot M_3 \cdot M_2 \cdot M_2 \cdot M_1 \cdot M_1 \cdot M_3 \cdot M_1 \cdot M_1 \cdot i_{wx}(P_2,25),$$

By using this equation together with Algorithms 1 and 2, the result is obtained as follows:

$i_{ab}(G, 25)$	$= [0$	0	2	145	4268	68002
662662	4240055	18729664	59359916	139073582	246477981	336273579
357809386	299711119	198824106	104766545	43837794	14510552	3768649
757403	115209	12802	979	46	1	0
0	0	1	73	1960	29072	267747
1626798	6828646	20539053	45535285	76028515	97152079	96128659
74239291	44953503	21366091	7950163	2299484	510343	85075
10289	851	43	1	0	0	0
1	67	1981	30694	284616	1718068	7138367
21247946	46673132	77340774	98256520	96812984	74552134	45058462
21391547	7954496	2299974	510376	85076	10289	851
43	1	0	0	1	72	2308
38930	394915	2613257	11901018	38820863	93538297	170449466
239121500	261680727	225471828	153870603	83400454	35887631	12211068
3258306	672328	104920	11951	936	45	1
0	0	1	78	2287	37308	378046
2521987	11591297	38111970	92400450	169137207	238017059	260996402
225158985	153765644	83374998	35883298	12210578	3258273	672327
104920	11951	936	45	$1]^T$.		

As a consequence, the entries starting from the first entry to the twenty-sixth entry give the following values, respectively:

$i(G, 25) = 0$, $i(G, 24) = 0$, $i(G, 23) = 2$, $i(G, 22) = 145$, $i(G, 21) = 4268$, $i(G, 20) = 68002$, $i(G, 19) = 662662$, $i(G, 18) = 4240055$, $i(G, 17) = 18729664$,$i(G, 16) = 59359916$, $i(G, 15) = 139073582$, $i(G, 14) = 246477981$, $i(G, 13) = 336273579$, $i(G, 12) = 357809386$, $i(G, 11) = 299711119$, $i(G, 10) = 198824106$, $i(G, 9) = 104766545$, $i(G, 8) = 43837794$, $i(G, 7) = 14510552$, $i(G, 6) = 3768649$, $i(G, 5) = 757403$, $i(G, 4) = 115209$, $i(G, 3) = 12802$, $i(G, 2) = 979$, $i(G, 1) = 46$ *and* $i(G, 0) = 1$.

In addition, for $k = 25$*, the first and second entries of* $i_{ab}(G, 25)$ *are equal to zero and it means that the maximum* k *value is* 23 *for nonzero* $i(G, k)$*. Therefore, by the definition of the Merrifield-Simmons index, the summation of* $i(G, 23), i(G, 22), \cdots, i(G, 1)$ *and* $i(G, 0)$ *gives the Merrifield-Simmons index of* G*. Hence, by summing the first,* $\cdots$*, twenty-sixth entries of* $i_{ab}(G, 25)$*, the Merrifield-Simmons index of* G *is achieved as* 1829004447*. Note that, since* $i(G, 24) = 0$*, the selection* $k = 23$ *in* $i_{ab}(G, k)$ *will actually be sufficient for computing the Merrifield-Simmons index of* G*.*

Alternatively, for all $k \geq 0$*, the same* $i(G, k)$ *values can be obtained by using the following vectors and equations:*

$$i_{ya}(G,25) = M_2 \cdot M_3 \cdot M_3 \cdot M_3 \cdot M_2 \cdot M_2 \cdot M_1 \cdot M_1 \cdot M_3 \cdot M_1 \cdot M_1 \cdot i_{wx}(P_2,25),$$

$$i_{bz}(G,25) = M_3 \cdot M_3 \cdot M_3 \cdot M_3 \cdot M_2 \cdot M_2 \cdot M_1 \cdot M_1 \cdot M_3 \cdot M_1 \cdot M_1 \cdot i_{wx}(P_2,25).$$

The difference between the equations of the vectors $i_{ab}(G,25)$*,* $i_{ya}(G,25)$ *and* $i_{bz}(G,25)$ *is just the* M_1*,* M_2*,* M_3 *matrices obtained due to the reduction difference in the first step.*

Finally, $i(G,k)$ *values can also be computed by using the* k*-independence vector of* G *at the edge* xw *as follows:*

$$i_{xw}(G,25) = M_1 \cdot M_1 \cdot M_2 \cdot M_1 \cdot M_1 \cdot M_3 \cdot M_3 \cdot M_2 \cdot M_2 \cdot M_2 \cdot M_1 \cdot i_{ba}(P_2,25).$$

In conclusion, for all $k \geq 0$, $i(G,k)$ can be computed by using the k-independence vector and Thms. 2.1, 2.2, 2.3 for arbitrary benzenoid chains. Furthermore, for the maximum $k \geq 0$ such that $i(G,k) \neq 0$, since the sum of the rows of $i_{ab}(G,k)$ between the first and $(k+1)$-th corresponds to the Merrifield-Simmons index of G, this value is obtained by using the method. Similarly, the sum of the rows of $i_{ab}(G,k)$ between $k+2$ and $2k+2$, $2k+3$ and $3k+3$, $3k+4$ and $4k+4$, $4k+5$ and $5k+5$ corresponds to the Merrifield-Simmons indices of $G - N_G[a]$, $G - N_G[b]$, $G - a$, $G - b$, respectively. Hence, all of these values are achieved by utilizing the method.

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