

Computing the Number of Matchings in Catacondensed Benzenoid Systems

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Abstract

The Hosoya index of G is defined as the total number of independent edge sets (number of k -matchings $p(G, k)$) in G . The Hosoya index is one of the most important topological indices in the field of mathematical chemistry because of its relationship with several thermodynamic properties. Therefore, computation of the number of k -matchings of various molecular structures has importance. Two methods, one for computing the number of the Hosoya index of catacondensed benzenoid systems and the other for the number of k -matchings in benzenoid chains (unbranched catacondensed benzenoid systems), have been presented so far. In this paper, a method based on some transfer matrices to compute the number of k -matchings of arbitrary (both unbranched and branched) catacondensed benzenoid systems is presented. Moreover, some algorithms are designed to keep the applicability of the method the same as k increases.

1 Introduction

Let $G = (V, E)$ be a graph. Edges without any common vertex are called independent edges. A set containing independent edges of G is called a matching. If a matching contains k independent edges, then it is called a

k -matching. The number of all possible k -matchings in G is called the k -matching number and let us denote by $p(G, k)$. When $0 \leq k \leq 6$, works on the number of k -matchings for certain graphs can be found in [1, 6, 7, 20, 21]. [11] The Hosoya index (Z index) of G was defined by Haruo Hosoya in 1971 as follows:

$$Z(G) = \sum_{k \geq 0} p(G, k).$$

The Hosoya index correlated with various thermodynamic properties of some molecules is the subject of lots several studies in mathematical chemistry, more details can be found in [8, 22].

Molecular graphs of benzenoid hydrocarbons are called benzenoid systems. Formally, a benzenoid system is a finite 2-connected graph whose each bounded region is a regular hexagon. An edge that is adjacent to only a hexagon is called an external edge. The perimeter of a benzenoid system is the cycle that contains all external edges of the benzenoid system. All vertices that belong to the perimeter are called external vertices, otherwise internal [9]. A benzenoid system that has no internal vertex is called a catacondensed benzenoid system, otherwise a pericondensed benzenoid system. A catacondensed benzenoid system in which each hexagon is adjacent to at most two hexagons is called a benzenoid chain, for details we refer to [9].

Many studies have been made on the k -matchings and the Hosoya indices of various benzenoid systems and polygonal systems, some of them can be seen in [2–5, 10, 13, 14, 23, 24].

The operator technique and the transfer matrix technique have great importance for solving several enumeration problems such as matchings. Some of the studies in which these techniques are used can be viewed in [12, 18, 19]. Hosoya and Ohkami achieved the recurrence equations of matching polynomials of some benzenoid chains by using the operator technique in [12]. Randić et al. gave an algorithm by which matching polynomials of arbitrary benzenoid chains can be obtained by using the transfer matrix technique in [19].

In [5], R. Cruz et al. gave a method based on a suitable multiplication of some transfer matrices with dimension 4×4 and a vector to compute

the Hosoya index of arbitrary catacondensed benzenoid systems. In [15], a method for enumerating independent sets in benzenoid chains was presented, based on an appropriate multiplication of three transfer matrices and a vector. Moreover, methods based on the transfer matrix technique were raised for computations of the Merrifield–Simmons indices of both benzenoid chains and double benzenoid chains in [16]. Analogously, the Hosoya and Merrifield–Simmons indices of two special pericondensed benzenoid systems were calculated by utilizing methods each based on various transfer matrices in [17]. In [14], for each $k \geq 0$, a method based on three transfer matrices was given to compute $p(G, k)$ in arbitrary benzenoid chains (unbranched catacondensed benzenoid systems). In this paper, in addition to the presented method in [14], we also focus on the hexagons that are adjacent to three hexagons in catacondensed benzenoid systems. Thus, for every $k \geq 0$, we present a method for computing $p(G, k)$ in arbitrary (both unbranched and branched) catacondensed benzenoid systems by adding five new transfer matrices to the previously given method in [14].

2 Computing $p(G, k)$ in catacondensed benzenoid systems

There are two useful recurrence relations to obtain the number of k -matchings in G as follows:

$$p(M \cup H, k) = p(M, k)p(H, 0) + p(M, k-1)p(H, 1) + \cdots + p(M, 0)p(H, k), \quad (1)$$

where $G = M \cup H$ and M, H are connected components of G . Furthermore,

$$p(G, k) = p(G - ij, k) + p(G - i - j, k - 1) \quad (2)$$

for an edge ij , more details can be found in [12].

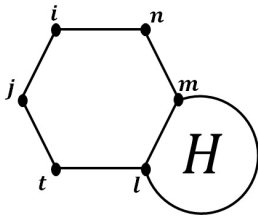


Figure 1. Graph in Theorems 1 and 3

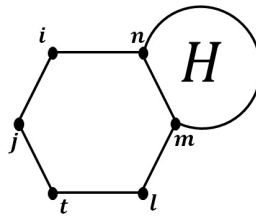


Figure 2. Graph used in Theorem 2

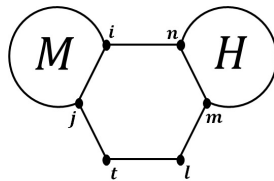


Figure 3. Graph used in Theorem 4

Let us recall the k -matching vector of G defined at a given edge in [14].

Definition 1. Let G be a graph and ij be an edge of G . The k -matching vector of G at the edge ij is defined as

$$p_{ij}(G, k) = \begin{pmatrix} p(G, k) \\ p(G, k - 1) \\ \vdots \\ p(G, 0) \\ p(G - i, k) \\ p(G - i, k - 1) \\ \vdots \\ p(G - i, 0) \\ p(G - j, k) \\ p(G - j, k - 1) \\ \vdots \\ p(G - j, 0) \\ p(G - i - j, k) \\ p(G - i - j, k - 1) \\ \vdots \\ p(G - i - j, 0) \end{pmatrix}.$$

In [14], for every $k \geq 0$, the number of k -matchings in benzenoid chains is computed by using three theorems. First of all, Let us recall them.

Theorem 1. [14] *Let G be a graph derived by fusing a hexagon and a graph H at the edge ml (See Fig. 1). Then*

$$p_{ij}(G, k) = Q_1 \cdot p_{ml}(H, k)$$

where Q_1 is a transfer matrix with dimension $(4k+4) \times (4k+4)$ as follows:

$$\begin{pmatrix} 1 & 3 & 1 & 0 & \cdots & 0 & 0 & 1 & 2 & 0 & \cdots & 0 & 0 & 1 & 2 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & 0 & \cdots & 0 \\ 0 & 1 & 3 & 1 & \cdots & 0 & 0 & 0 & 1 & 2 & \cdots & 0 & 0 & 0 & 1 & 2 & \cdots & 0 & 0 & 0 & 0 & 1 & 1 & \cdots & 0 \\ \vdots & \\ 0 & \cdots & 0 & 1 & 3 & 1 & 0 & \cdots & 0 & 0 & 1 & 2 & 0 & \cdots & 0 & 1 & 2 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\ 0 & \cdots & 0 & 0 & 1 & 3 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & 0 & \cdots & 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 \\ \hline 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \\ 0 & \cdots & 0 & 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\ 0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \hline 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 1 & \cdots & 0 & 0 & 0 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \\ 0 & \cdots & 0 & 1 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & \cdots & 0 & 1 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\ 0 & \cdots & 0 & 0 & 1 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \hline 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \\ 0 & \cdots & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & \cdots & 0 & 1 & 0 & 0 & 0 & 0 & \cdots & 0 & 1 \\ 0 & \cdots & 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}.$$

Theorem 2. [14] *Let G be a graph derived by fusing a hexagon and a graph H at the edge nm (See Fig. 2). Then*

$$p_{ij}(G, k) = Q_2 \cdot p_{nm}(H, k)$$

where Q_2 is a transfer matrix with dimension $(4k+4) \times (4k+4)$ as follows:

$$\begin{aligned}
p(G, k) &= p(G - ni - ml - jt, k) + p(G - ni - ml - j - t, k - 1) \\
&+ p(G - ni - m - l - jt, k - 1) + p(G - ni - m - l - j - t, k - 2) \\
&+ p(G - n - i - ml - jt, k - 1) + p(G - n - i - ml - j - t, k - 2) \\
&+ p(G - n - i - m - l - jt, k - 2) + p(G - n - i - m - l - j - t, k - 3) \\
&= p(P_2 \cup M \cup H, k) + p(M - j \cup H, k - 1) + p(M \cup H - m, k - 1) \\
&+ p(M - j \cup H - m, k - 2) + p(P_2 \cup M - i \cup H - n, k - 1) \\
&+ p(M - i - j \cup H - n, k - 2) + p(M - i \cup H - n - m, k - 2) \\
&+ p(M - i - j \cup H - n - m, k - 3) = (p(M, k) + p(M, k - 1) \\
&+ p(M - j, k - 1))p(H, 0) + (p(M, k - 1) + p(M, k - 2) \\
&+ p(M - j, k - 2))p(H, 1) + \cdots + (p(M, 1) + p(M, 0) + p(M - j, 0))p(H, k - 1) \\
&+ p(M, 0)p(H, k) + (p(M, k - 1) + p(M - j, k - 2))p(H - m, 0) \\
&+ (p(M, k - 2) + p(M - j, k - 3))p(H - m, 1) + \cdots \\
&+ (p(M, 1) + p(M - j, 0))p(H - m, k - 2) + p(M, 0)p(H - m, k - 1) \\
&+ (p(M - i, k - 1) + p(M - i, k - 2) + p(M - i - j, k - 2))p(H - n, 0) \\
&+ (p(M - i, k - 2) + p(M - i, k - 3) + p(M - i - j, k - 3))p(H - n, 1) + \cdots \\
&+ (p(M - i, 1) + p(M - i, 0) + p(M - i - j, 0))p(H - n, k - 2) \\
&+ p(M - i, 0)p(H - n, k - 1) + (p(M - i, k - 2) \\
&+ p(M - i - j, k - 3))p(H - m - n, 0) + (p(M - i, k - 3) \\
&+ p(M - i - j, k - 4))p(H - m - n, 1) + \cdots + (p(M - i, 1) \\
&+ p(M - i - j, 0))p(H - m - n, k - 3) + p(M - i, 0)p(H - m - n, k - 2).
\end{aligned}$$

Then we get $p(G, k) = [A_1 \cdot p_{ji}(M, k)]^T \cdot p_{mn}(H, k)$, where A_1 is as defined above, by arranging the equation above and by using the definitions of $p_{ji}(M, k)$ and $p_{mn}(H, k)$. Secondly we calculate $p(G - t, k)$ as the following:

$$\begin{aligned}
p(G - t, k) &= p(G - t - ni - ml, k) + p(G - t - ni - m - l, k - 1) \\
&+ p(G - t - n - i - ml, k - 1) + p(G - t - n - i - m - l, k - 2) \\
&= p(M \cup H, k) + p(M \cup H - m, k - 1) + p(M - i \cup H - n, k - 1) \\
&+ p(M - i \cup H - n - m, k - 2) = p(M, k)p(H, 0) + p(M, k - 1)p(H, 1) \\
&+ \cdots + p(M, 1)p(H, k - 1) + p(M, 0)p(H, k) + p(M, k - 1)p(H - m, 0) \\
&+ p(M, k - 2)p(H - m, 1) + \cdots + p(M, 1)p(H - m, k - 2) \\
&+ p(M, 0)p(H - m, k - 1) + p(M - i, k - 1)p(H - n, 0) \\
&+ p(M - i, k - 2)p(H - n, 1) + \cdots + p(M - i, 1)p(H - n, k - 2)
\end{aligned}$$

$$\begin{aligned}
& + p(M-i, 0)p(H-n, k-1) + p(M-i, k-2)p(H-m-n, 0) \\
& + p(M-i, k-3)p(H-m-n, 1) + \cdots + p(M-i, 1)p(H-m-n, k-3) \\
& + p(M-i, 0)p(H-m-n, k-2).
\end{aligned}$$

Then we get $p(G-t, k) = [A_2 \cdot p_{ji}(M, k)]^T \cdot p_{mn}(H, k)$, where A_2 is as defined above by arranging the equation above and by using the definitions of $p_{ji}(M, k)$ and $p_{mn}(H, k)$. Thirdly we calculate $p(G-l, k)$ as below:

$$\begin{aligned}
p(G-l, k) & = p(G-l-ni-jt, k) + p(G-l-ni-j-t, k-1) \\
& + p(G-l-n-i-jt, k-1) + p(G-l-n-i-j-t, k-2) \\
& = p(M \cup H, k) + p(M-j \cup H, k-1) + p(M-i \cup H-n, k-1) \\
& + p(M-i-j \cup H-n, k-2) = (p(M, k) + p(M-j, k-1))p(H, 0) \\
& + (p(M, k-1) + p(M-j, k-2))p(H, 1) + \cdots \\
& + (p(M, 1) + p(M-j, 0))p(H, k-1) + p(M, 0)p(H, k) + (p(M-i, k-1) \\
& + p(M-i-j, k-2))p(H-n, 0) \\
& + (p(M-i, k-2) + p(M-i-j, k-3))p(H-n, 1) + \cdots \\
& + (p(M-i, 1) + p(M-i-j, 0))p(H-n, k-2) \\
& + p(M-i, 0)p(H-n, k-1).
\end{aligned}$$

Then we get $p(G-l, k) = [A_3 \cdot p_{ji}(M, k)]^T \cdot p_{mn}(H, k)$ where A_3 is as defined above by arranging the equation above and by using the definitions of $p_{ji}(M, k)$ and $p_{mn}(H, k)$. Finally, we calculate $p(G-t-l, k)$ as follows:

$$\begin{aligned}
p(G-t-l, k) & = p(G-t-l-ni, k) + p(G-t-l-n-i, k-1) \\
& = p(M \cup H, k) + p(M-i \cup H-n, k-1) \\
& = p(M, k)p(H, 0) + p(M, k-1)p(H, 1) + \cdots + p(M, 1)p(H, k-1) \\
& + p(M, 0)p(H, k) + p(M-i, k-1)p(H-n, 0) \\
& + p(M-i, k-2)p(H-n, 1) + \cdots + p(M-i, 1)p(H-n, k-2) \\
& + p(M-i, 0)p(H-n, k-1).
\end{aligned}$$

Then we get $p(G-t-l, k) = [A_4 \cdot p_{ji}(M, k)]^T \cdot p_{mn}(H, k)$ where A_4 is as defined above by arranging the equation above and by using the definitions of $p_{ji}(M, k)$ and $p_{mn}(H, k)$. ■

In Theorem 4, observe that each $[(A_b \cdot p_{ji}(M, k))_b]^T$ is a $1 \times (4k + 4)$ dimensional vector. Then we construct a new matrix, the vectors $[A_1 \cdot p_{ji}(M, k)]^T$, $[A_2 \cdot p_{ji}(M, k)]^T$, $[A_3 \cdot p_{ji}(M, k)]^T$ and $[A_4 \cdot p_{ji}(M, k)]^T$ are written in the first row, $(k+2)$ -th row, $(2k+3)$ -th row and $(3k+4)$ -th

row of the matrix, respectively. After that, the echelon forms of sixteen submatrices in the matrix are obtained similar to the forms of the matrices Q_1, Q_2, Q_3 given in Theorems 1, 2 and 3. Let us call the newly formed matrix by S . As a result, we achieve the next corollary:

Corollary. *Let G be a graph derived by fusing the graphs M, H with a hexagon at the edges ji and mn , respectively see Fig. 3. Then*

$$p_{tl}(G, k) = S \cdot p_{mn}(H, k)$$

where S is a transfer matrix with dimension $(4k+4) \times (4k+4)$ as explained above.

Proof. Proof is obtained by utilizing Theorem 4 and the structure of the matrix S . ■

3 Algorithms

It is clear that it is easy to form the matrices Q_1, Q_2, Q_3 and the vector $p_{st}(P_2, k)$, where st is an edge of P_2 , for $k = 0, 1, 2$. In [14], two algorithms have been presented in MATLAB that run according to entered value $k \geq 3$, one is used for obtaining the transfer matrices Q_1, Q_2, Q_3 and the other for obtaining $p_{ij}(P_2, k)$. In this section, we designed five algorithms in MATLAB to obtain five transfer matrix forms W, S, A_1, A_2, A_3 and A_4 directly for $k \geq 3$. Thanks to the algorithms, the method can be applied to any catacondensed benzenoid system efficiently, regardless of the size of k .

For the transfer symmetry matrix W , the steps must be added consecutively before step $L(1, :) = L1$ as follows:

$$L1 = \text{zeros}(1, 4 * k + 4); L1(1) = 1; L2 = \text{zeros}(1, 4 * k + 4); L2(2 * k + 3) = 1; L3 = \text{zeros}(1, 4 * k + 4); L3(k + 2) = 1; L4 = \text{zeros}(1, 4 * k + 4); L4(3 * k + 4) = 1;$$

For the transfer matrix S , the vectors $[(A_b \cdot p_{ji}(M, k))_b]^T$ that are mentioned after the proof of Theorem 4 must be assigned to Lb where $b = 1, 2, 3, 4$, respectively. Then let us present the algorithms to get A_b , where $b = 1, 2, 3, 4$.

Algorithm 1: Algorithm to set the transfer matrix forms W and S for corresponding k .

Input: Enter the value of $k \geq 3$.

Result: Required echelon matrix form according to the rows $1, k+2, 2k+3$ and $3k+4$.

$L = \text{zeros}(4 * k + 4, 4 * k + 4)$;

"If the desired matrix is W , then the steps given after this algorithm will be added to this part, otherwise there are not any required steps to add to this part."

$L(1, :) = L1$;

$L(k+2, :) = L2$;

$L(2 * k + 3, :) = L3$;

$L(3 * k + 4, :) = L4$;

for from $i = 1$ to $k + 1$ **do**

for from $j = i$ to k **do**

$L(i+1, j+1) = L(i, j)$;

$L(i+1, j+k+2) = L(i, j+k+1)$;

$L(i+1, j+2 * k + 3) = L(i, j+2 * k + 2)$;

$L(i+1, j+3 * k + 4) = L(i, j+3 * k + 3)$;

end

end

for from $i = k + 2$ to $2 * k + 1$ **do**

for from $j = 1$ to k **do**

$L(i+1, j+1) = L(i, j)$;

$L(i+1, j+k+2) = L(i, j+k+1)$;

$L(i+1, j+2 * k + 3) = L(i, j+2 * k + 2)$;

$L(i+1, j+3 * k + 4) = L(i, j+3 * k + 3)$;

end

end

for from $i = 2 * k + 3$ to $3 * k + 2$ **do**

for from $j = 1$ to k **do**

$L(i+1, j+1) = L(i, j)$;

$L(i+1, j+k+2) = L(i, j+k+1)$;

$L(i+1, j+2 * k + 3) = L(i, j+2 * k + 2)$;

$L(i+1, j+3 * k + 4) = L(i, j+3 * k + 3)$;

end

end

for from $i = 3 * k + 4$ to $4 * k + 3$ **do**

for from $j = 1$ to k **do**

$L(i+1, j+1) = L(i, j)$;

$L(i+1, j+k+2) = L(i, j+k+1)$;

$L(i+1, j+2 * k + 3) = L(i, j+2 * k + 2)$;

$L(i+1, j+3 * k + 4) = L(i, j+3 * k + 3)$;

end

end

Example 1. Let G be a catacondensed benzenoid system as shown in Fig.

4.

Algorithm 2: Algorithm to set the transfer matrix A_1 for corresponding k .

Input: Enter the value of $k \geq 3$.

Result: The transfer matrix A_1 for corresponding k .

$A1 = \text{zeros}(4 * k + 4, 4 * k + 4)$;

$t1 = 0$;

for from $i = 2$ to $k + 1$ **do**

$A1(1, k + 1) = 1$;

$A1(i, k + 3 - i) = 1$;

$A1(i, k + 2 - i) = 1$;

$A1(i, 2 * k + 2 - t1) = 1$;

$t1 = t1 + 1$;

end

$t2 = 1$;

for from $i = k + 4$ to $2 * k + 2$ **do**

$A1(k + 3, k + 1) = 1$;

$A1(i, k + 1 - t2) = 1$;

$A1(i, 2 * k + 3 - t2) = 1$;

$t2 = t2 + 1$;

end

$t3 = 0$;

for from $i = 2 * k + 5$ to $3 * k + 3$ **do**

$A1(2 * k + 4, 3 * k + 3) = 1$;

$A1(i, 3 * k + 3 - t3) = 1$;

$A1(i, 3 * k + 2 - t3) = 1$;

$A1(i, 4 * k + 4 - t3) = 1$;

$t3 = t3 + 1$;

end

$t4 = 0$;

for from $i = 3 * k + 7$ to $4 * k + 4$ **do**

$A1(3 * k + 6, 3 * k + 3) = 1$;

$A1(i, 3 * k + 2 - t4) = 1$;

$A1(i, 4 * k + 4 - t4) = 1$;

$t4 = t4 + 1$;

end

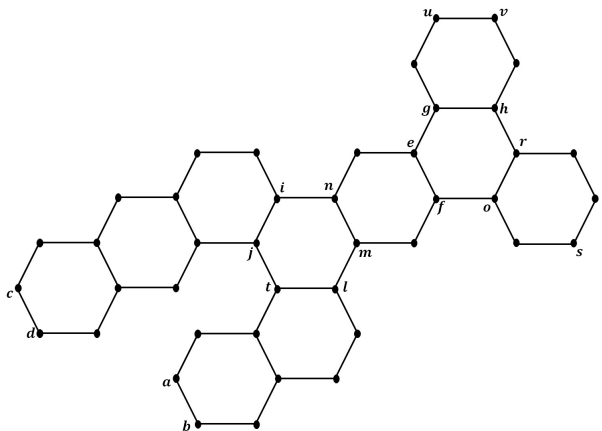


Figure 4. A catacondensed benzenoid system

Algorithm 3: Algorithm to set the transfer matrix A_2 for corresponding k .

Input: Enter the value of $k \geq 3$.
Result: The transfer matrix A_2 for corresponding k .
 $A_2 = \text{zeros}(4 * k + 4, 4 * k + 4)$;
for *from* $i = 1$ *to* $k + 1$ **do**
 | $A_2(i, k + 3 - i - 1) = 1$;
end
 $t_2 = 0$;
for *from* $i = k + 3$ *to* $2 * k + 2$ **do**
 | $A_2(i, k + 1 - t_2) = 1$;
 | $t_2 = t_2 + 1$;
end
 $t_3 = 0$;
for *from* $i = 2 * k + 4$ *to* $3 * k + 3$ **do**
 | $A_2(i, 3 * k + 3 - t_3) = 1$;
 | $t_3 = t_3 + 1$;
end
 $t_4 = 0$;
for *from* $i = 3 * k + 6$ *to* $4 * k + 4$ **do**
 | $A_2(i, 3 * k + 3 - t_4) = 1$;
 | $t_4 = t_4 + 1$;
end

Algorithm 4: Algorithm to set the transfer matrix A_3 for corresponding k .

Input: Enter the value of $k \geq 3$.
Result: The transfer matrix A_3 for corresponding k .
 $A_3 = \text{zeros}(4 * k + 4, 4 * k + 4)$;
 $t_1 = 0$;
for *from* $i = 2$ *to* $k + 1$ **do**
 | $A_3(1, k + 1) = 1$;
 | $A_3(i, k + 2 - i) = 1$;
 | $A_3(i, 2 * k + 2 - t_1) = 1$;
 | $t_1 = t_1 + 1$;
end
 $t_2 = 0$;
for *from* $i = 2 * k + 5$ *to* $3 * k + 3$ **do**
 | $A_3(2 * k + 4, 3 * k + 3) = 1$;
 | $A_3(i, 3 * k + 2 - t_2) = 1$;
 | $A_3(i, 4 * k + 4 - t_2) = 1$;
 | $t_2 = t_2 + 1$;
end

Algorithm 5: Algorithm to set the transfer matrix A_4 for corresponding k .

Input: Enter the value of $k \geq 3$.
Result: The transfer matrix A_4 for corresponding k .
 $A_4 = \text{zeros}(4 * k + 4, 4 * k + 4)$;
for *from* $i = 1$ *to* $k + 1$ **do**
 | $A_4(i, k + 3 - i - 1) = 1$;
end
 $t_3 = 0$;
for *from* $i = 2 * k + 4$ *to* $3 * k + 3$ **do**
 | $A_4(i, 3 * k + 3 - t_3) = 1$;
 | $t_3 = t_3 + 1$;
end

Then let us calculate the number of 22-matchings $p(G, 22)$ in G by utilizing the vector $p_{ab}(G, 22)$, Theorems 1, 2, 3, 4, Lemma 1 and Cor. 2:

$$\begin{aligned}
 p_{ab}(G, 22) &= Q_1 \cdot Q_2 \cdot p_{tl}(H^I, 22) \\
 &= Q_1 \cdot Q_2 \cdot S_1 \cdot p_{mn}(H^{II}, 22) \\
 &= Q_1 \cdot Q_2 \cdot S_1 \cdot W \cdot p_{nm}(H^{III}, 22) \\
 &= Q_1 \cdot Q_2 \cdot S_1 \cdot W \cdot Q_1 \cdot p_{ef}(H^{III}, 22) \\
 &= Q_1 \cdot Q_2 \cdot S_1 \cdot W \cdot Q_1 \cdot S_2 \cdot p_{or}(H^{IV}, 22) \\
 &= Q_1 \cdot Q_2 \cdot S_1 \cdot W \cdot Q_1 \cdot S_2 \cdot Q_1 \cdot p_{st}(P_2, 22)
 \end{aligned}$$

where $H^I, H^{II}, H^{III}, H^{IV}$ are corresponding subgraphs and S_1, S_2 are the transfer matrices that are used for reducing hexagons with three adjacent hexagons in the system. After getting the equation above, we use the algorithms (in MATLAB) to get Q_1, Q_2, S_1, W, S_2 and $p_{st}(P_2, 22)$ and we have the result as follows:

$p_{ab}(G, 22)$	= [0	132	9662	227594	2601131	17152998
72097837	206026293	418537074	624169412	699551840	599344823	397202204
205121448	82799431	26093309	6380478	1195807	168219	17161
1197	51	1	0	0	438	21082
369381	3287480	17385527	59871421	142415419	243596100	308231313
294388422	215204058	121478142	53174123	18042957	4720320	941067
140091	15052	1101	49	1	0	0
380	19152	345269	3130628	16782604	58393615	139985347
240819370	305973103	293061790	214637443	121302606	53135185	18036943
4719707	941030	140090	15052	1101	49	1
0	0	48	3582	83621	937422	6012090
24374973	66620034	128290722	179643581	187135760	147390044	88720330
41055807	14620910	3990013	825501	126970	14043	1054
48	1] ^T .					

As a consequence, the numbers of k -matchings are obtained as $p(G, 22) = 0$, $p(G, 21) = 132$, $p(G, 20) = 9662$, $p(G, 19) = 227594$, $p(G, 18) = 2601131$, $p(G, 17) = 17152998$, $p(G, 16) = 72097837$, $p(G, 15) = 206026293$, $p(G, 14) = 418537074$, $p(G, 13) = 624169412$, $p(G, 12) = 699551840$, $p(G, 11) = 599344823$, $p(G, 10) = 397202204$, $p(G, 9) = 205121448$, $p(G, 8) = 82799431$, $p(G, 7) = 26093309$, $p(G, 6) = 6380478$, $p(G, 5) = 1195807$, $p(G, 4) = 168219$, $p(G, 3) = 17161$, $p(G, 2) = 1197$, $p(G, 1) = 51$ and $p(G, 0) = 1$.

Furthermore, since $p(G, 22) = 0$ the Hosoya index of G is equal to 3358698102 by the definition of the Hosoya index. In the example, for every $0 \leq k \leq 22$ each number of k -matchings number in G has been

obtained by Lemma 1, Theorems 1, 2, 3, 4 and Cor. 2. In addition to the number of k -matchings in arbitrary catacondensed benzenoid system, it is clear that the Hosoya index of arbitrary catacondensed benzenoid system and the Hosoya indices of some subgraphs of it are achieved by using the method.

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