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Research article

Computation method of the Hosoya index of primitive coronoid systems

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Abstract: Coronoid systems are natural graph representations of coronoid hydrocarbons associated with benzenoid systems, but they differ in that they contain a hole. The Hosoya index of a graph G is defined as the total number of independent edge sets, that are called k-matchings in G.
The Hosoya index is a significant molecular descriptor that has an important position in QSAR and QSPR studies. Therefore, the computation of the Hosoya index of various molecular graphs is needed for making progress on investigations. In this paper, a method based on the transfer matrix technique and the Hosoya vector for computing the Hosoya index of arbitrary primitive coronoid systems is presented. Moreover, the presented method is customized for hollow hexagons by using six parameters. As a result, the Hosoya indices of both each arbitrary primitive coronoid system and also each hollow hexagon can be computed by means of a summation of four selected multiplications consisting of presented transfer matrices and two vectors.

Keywords: Hosoya index; coronoid systems; primitive coronoid systems; hollow hexagons

1. Introduction

Benzenoid hydrocarbons are defined as unsaturated, condensed and fully conjugated hydrocarbons formed by just hexagons [1]. Hexagonal systems, in other words benzenoid systems, are molecular graphs of benzenoid hydrocarbons. They are defined as finite 2-connected graphs in which all closed regions are mutually congruent regular hexagons.

Benzenoid systems have vertices that can belong to one, two or three hexagons. Vertices belonging to three hexagons are called internal vertices, otherwise are called external vertices. A benzenoid system in which all vertices are external vertices is called a catacondensed benzenoid system, otherwise it is called a pericondensed benzenoid system. An unbranched catacondensed benzenoid system is called a benzenoid chain.

The plane can be fully covered by a hexagonal lattice consisting of an infinite number of mutually congruent regular hexagons. A hexagonal lattice can be seen in the background in the first graph of Figure 1, and honey combs are a clear example of this. Let C be a cycle on the hexagonal lattice. Then, all vertices and edges lying on C and in the interior of C constitute a benzenoid system. Coronoid systems are molecular graphs of coronoid hydrocarbons, also called benzenoid-like systems. The definition made for benzenoid systems can be easily adapted to coronoid systems. Let us assume that C^1 and C^2 are two cycles on the hexagonal lattice, where C^2 is fully embraced by C^1. The vertices and edges lying on C^2 and in the interior of C^2 are called the corona hole. The number of vertices and edges of C^2 must be at least 10, so each coronoid system must have at least eight hexagons. A coronoid system is formed by the vertices and edges lying on C^1 and C^2 as well as in the interior of C^1, but outside of C^2 as shown in Figure 1. The cycles C^2 and C^1 are the inner perimeter and the outer perimeter of the coronoid system, respectively. Moreover, the dualist graph of the coronoid system presented in the first and second graphs of Figure 1 can be seen in the third graph of Figure 1.

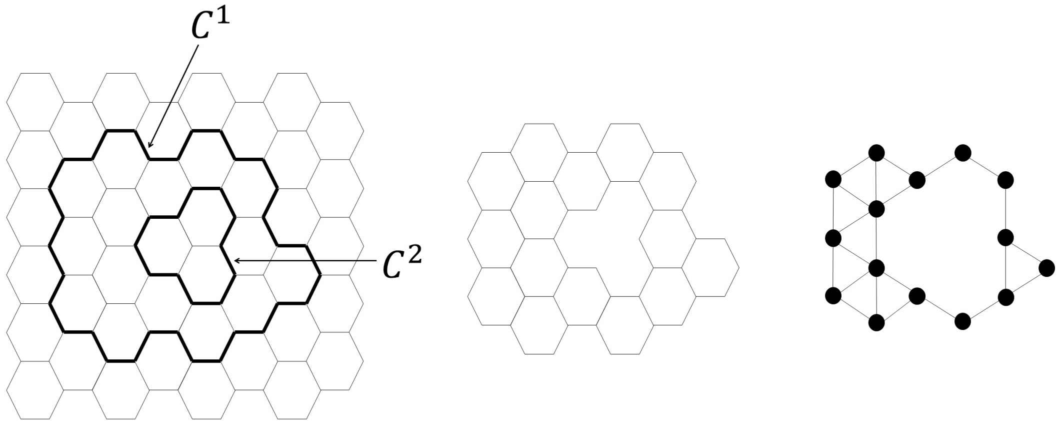

Figure 1. Hexagonal lattice, coronoid system and dualist graph of the coronoid system.

A coronoid system having no internal vertices is called a *catacondensed coronoid system*, otherwise it is called a *pericondensed coronoid system* [1].

In general, 12 hexagon fusion types are allowed in a coronoid system [2]. In this paper, two types will be needed, A_2 and L_2 shown in Figure 2.

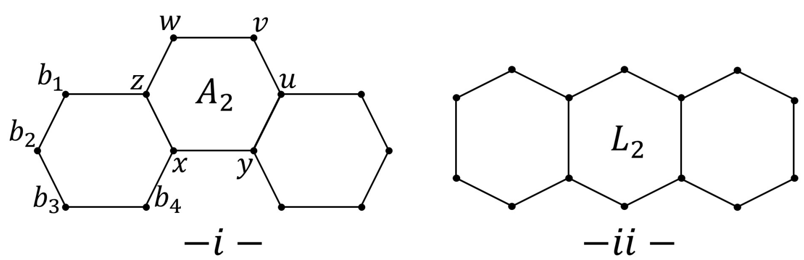

Figure 2. A_2 and L_2 types.

A catacondensed coronoid system consisting of annelated hexagons with A_2 and L_2 fusion types, that is, angular and linear annelated hexagons, is called a *primitive coronoid system* [1]. Each hexagon having A_2 fusion type is called a corner. There exist two corner types that are called intruding and protruding. While a corner having three edges on the inner perimeter is called intruding, a corner having three edges on the outer perimeter is called protruding.

A primitive coronoid system with exatly six corners is called *hollow hexagon* and all corners of it are protruding. A segment of a primitive coronoid system is defined as a linear benzenoid chain between two corners inclusive. The number of hexagons in a segment is defined as the length of the segment. In a hollow hexagon there are six segments with length $a+1, b+1, c+1, d+1, e+1$ and $f+1$. Note that a, b, c, d, e and f are the numbers. An example of a hollow hexagon can be seen in Figure 3, where $a = 1, b = 4, c = 3, d = 2, e = 3, f = 4$. We denote by $HH(a, b, c, d, e, f)$ the hollow hexagon with parameters a, b, c, d, e, f.

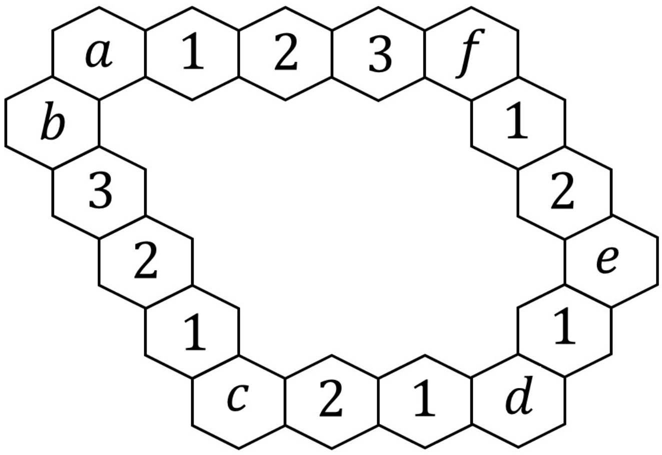

Figure 3. A hollow hexagon and its parameters.

More detailed and informative notions about benzenoid and coronoid systems can be found in [1–4].

The Hosoya index is one of the most significant tools in theoretical chemistry for predicting some thermodynamic properties of molecules and is defined as

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

where $p(G, k)$ is the total number of possible ways in which k mutually independent edges can be selected in G, see [5]. We refer [6, 7] for chemical importance and further investigations.

Benzenoid and coronoid systems have been studied extensively, from simple to complex, by both mathematicians and chemists due to their importance. In mathematical chemistry, there are important studies on the effort to compute various properties of these systems, some of them listed in [8–21].

Different techniques have been utilized to study various topological indices. Some spectral techniques have been used in the study of various topological indices, see [22, 23]. Besides, the transfer matrix technique has made it easy to solve many combinatoric and enumeration problems in mathematical chemistry so far. Two important studies in which this technique has been used can be seen in [19, 20].

In this paper, we propose a method based on a summation of four appropriate multiplications of some transfer matrices by some vectors to compute the Hosoya index of arbitrary primitive coronoid systems by using two important recurrence relations and the Hosoya vector defined in [12]. After that, we customize the method for hollow hexagons by using the parameters a, b, c, d, e and f.

2. The Hosoya index of primitive coronoid systems

The most commonly used recurrence relations for computing the Hosoya index of G can be found in [7] and they are as follows:

$$Z(G) = \prod_{i=1}^{k} Z(G_i), \tag{2.1}$$

where $G_1, G_2, \ldots, G_k$ are the connected components of G;

$$Z(G) = Z(G - cd) + Z(G - c - d), \tag{2.2}$$

where cd is an edge of G.

Let us recall the definition of the Hosoya vector of G at an edge that has been introduced in [12].

Definition 2.1. *[12] Let G be a graph with an edge $e = cd$. The Hosoya vector of G at $e = cd$ is*

$$Z_{cd}(G) = [Z(G), Z(G - c), Z(G - d), Z(G - c - d)]^T .$$

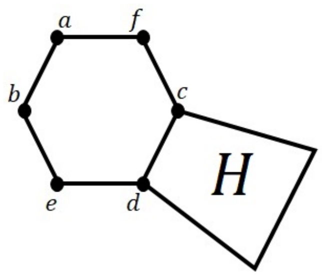

Figure 4. Graph G used in Lemma 2.1.

Proposition 2.1. *[12] Let G be the graph given in Figure 4, where H is an arbitrary subgraph. Then*

$$Z_{ab}(G) = Q \cdot Z_{cd}(H), \ \text{where } Q = \begin{bmatrix} 5 & 3 & 3 & 2 \\ 2 & 2 & 1 & 1 \\ 2 & 1 & 2 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

Proposition 2.2. *[12] Let G be the graph given in Figure 4, where H is an arbitrary subgraph. Then*

$$Z_{be}(G) = \left[E_i \cdot Z_{af}(K_2)\right]_i Z_{dc}(H), \ \text{where } K_2 \text{ denotes the edge } af,$$

$$i = 1,2,3,4 \text{ and } E_1 = \begin{bmatrix} 2 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \ E_2 = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \ E_3 = \begin{bmatrix} 0 & 0 & 2 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \ E_4 = \begin{bmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

The next lemma is a natural result of Proposition 2.1 and Proposition 2.2. The following matrices play an important role in the next lemma:

$$Q = \begin{bmatrix} 5 & 3 & 3 & 2 \\ 2 & 2 & 1 & 1 \\ 2 & 1 & 2 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}, \ P = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \ S_0 = \begin{bmatrix} 5 & 3 & 3 & 2 \\ 2 & 2 & 1 & 1 \\ 3 & 0 & 2 & 0 \\ 2 & 0 & 1 & 0 \end{bmatrix}. \tag{2.3}$$

Lemma 2.1. *Let G be the graph given in Figure 4, where H is an arbitrary subgraph. Then*

1. $Z_{ab}(G) = Q \cdot Z_{cd}(H)$.
2. $Z_{fa}(G) = P \cdot S_0 \cdot Z_{cd}(H)$.
3. $Z_{be}(G) = S_0 \cdot P \cdot Z_{cd}(H)$.

Recall that if the subgraph H in Figure 4 is the edge cd, then

$$Z_{cd}(H) = Z_{cd}(K_2) = X_0 = (2, 1, 1, 1)^T,$$

where K_2 denotes the graph consisting of only one edge.

Now we introduce an algorithm for computing the Hosoya index of an arbitrary primitive coronoid system.

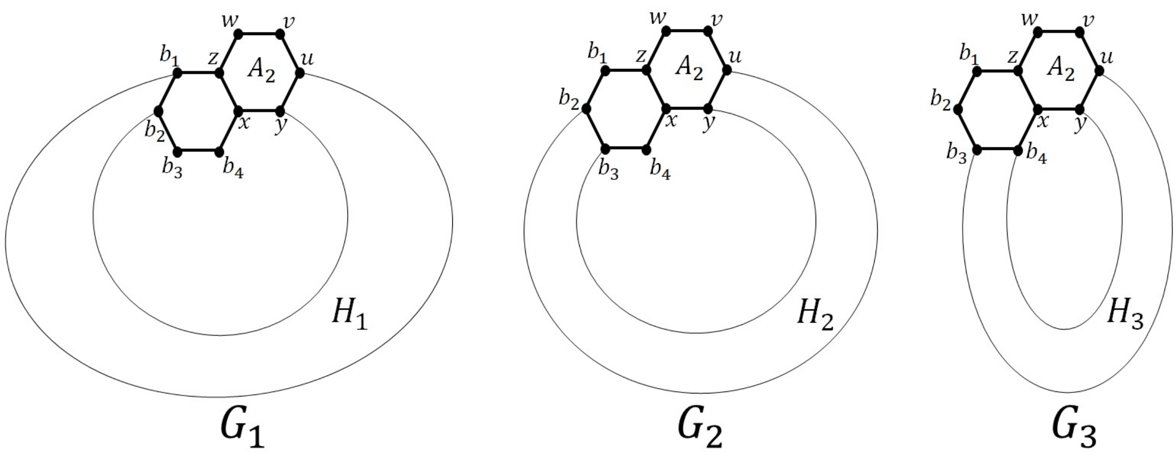

Figure 5. Three possible configurations of primitive coronoid systems.

It is known that any primitive coronoid system contains at least six hexagons with fusion type A_2. Thus, choosing an angular hexagon in a primitive coronoid system results in three possible configurations G_1, G_2 and G_3, as depicted in Figure 5. For $i \in \{1, 2, 3\}$, let H_i denotes the benzenoid chain starting at the edge uy and ending at the edge $b_i b_{i+1}$.

Note that for each $i \in \{1, 2, 3\}$, using the results in [12], one can compute the Hosoya vector of H_i at the edge uy as follows

$$Z_{uy}(H_i) = M \cdot Z_{b_i b_{i+1}}(K_2) = M \cdot X_0,$$

where M is a product of matrices of type Q, P, S_0.

We now present our main result.

Theorem 2.1. *Let G_i be a primitive coronoid system with $i \in \{1, 2, 3\}$, depicted in Figure 5. Let H_i denotes the benzenoid chain starting at the edge uy and ending at the edge b_ib_{i+1}. If H_i has the Hosoya vector*

$$Z_{uy}(H_i) = M \cdot X_0,$$

then

$$Z(G_i) = \sum_{k=1}^{4} e_k^T \cdot M \cdot Z_{b_ib_{i+1}}(F_k),$$

where M is a product of matrices of type Q, P, S_0, the graphs F_1, F_2, F_3, F_4 are depicted in Figure 6 and e_1, e_2, e_3, e_4 are the canonical vectors in $\mathbb{R}^4$.

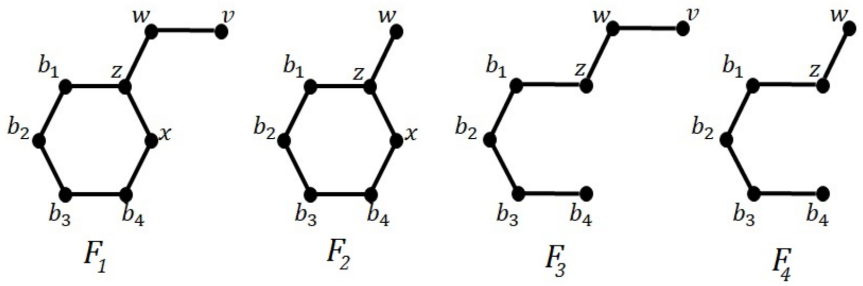

Figure 6. Graphs $F_1 = F$, $F_2 = F - v$, $F_3 = F - x$ and $F_4 = F - v - x$ used in Theorem 2.1

Proof. Let G_i be the graph given in Figure 5 for $i \in \{1, 2, 3\}$. Using recurrence relation (2.2) we obtain

$$Z(G_i) = Z(G_i - xy - uv) + Z(G_i - xy - u - v) + Z(G_i - x - y - uv) + Z(G_i - x - y - u - v). \quad (2.4)$$

It is easy to see that

1. $Z(G_i - xy - uv)$ is the first component of the Hosoya vector of the graph $G_i - xy - uv$ at edge uy. Then
$$Z(G_i - xy - uv) = e_1^T Z_{uy}(G_i - xy - uv) = e_1^T \cdot M \cdot Z_{b_ib_{i+1}}(F_1).$$
2. $Z(G_i - xy - u - v)$ is the second component of the Hosoya vector of the graph $G_i - xy - v$ at edge uy. Then
$$Z(G_i - xy - u - v) = e_2^T Z_{uy}(G_i - xy - v) = e_2^T \cdot M \cdot Z_{b_ib_{i+1}}(F_1 - v).$$
3. $Z(G_i - x - y - uv)$ is the third component of the Hosoya vector of the graph $G_i - x - uv$ at edge uy. Then
$$Z(G_i - x - y - uv) = e_3^T Z_{uy}(G_i - x - uv) = M \cdot Z_{b_ib_{i+1}}(F_1 - x).$$
4. $Z(G_i - x - y - u - v)$ is the fourth component of the Hosoya vector of the graph $G_i - x - v$ at edge uy. Then
$$Z(G_i - x - y - u - v) = e_4^T Z_{uy}(G_i - v - x) = e_4^T \cdot M \cdot Z_{b_ib_{i+1}}(F_1 - v - x).$$

Replacing in (2.4) we are done. □

In Table 1 we present the Hosoya vectors $Z_{b_ib_{i+1}}(F_k)$ for $i \in \{1,2,3\}$ and $k \in \{1,2,3,4\}$. These values are calculated using Lemma 2.1

Table 1. Hosoya vectors $Z_{b_ib_{i+1}}(F_k)$ for $i \in \{1,2,3\}$ and $k \in \{1,2,3,4\}$.

i	$Z_{b_ib_{i+1}}(F_1)$	$Z_{b_ib_{i+1}}(F_2)$	$Z_{b_ib_{i+1}}(F_3)$	$Z_{b_ib_{i+1}}(F_4)$
1	$[44,21,19,13]^T$	$[26,13,11,8]^T$	$[21,9,10,6]^T$	$[13,6,6,4]^T$
2	$[44,19,20,12]^T$	$[26,11,12,7]^T$	$[21,10,8,5]^T$	$[13,6,5,3]^T$
3	$[44,20,19,12]^T$	$[26,12,11,7]^T$	$[21,10,13,8]^T$	$[13,5,8,5]^T$

Example 2.1. *Now we give an illustration of the use of Theorem 2.1. Let G be the primitive coronoid system shown in Figure 7. Note that G corresponds to configuration G_3 shown in Figure 5. The Hosoya vector of H_3 at uy is*

$$Z_{uy}(H_3) = M \cdot X_0,$$

where

$$M = Q \cdot Q \cdot P \cdot S_0 \cdot S_0 \cdot P \cdot S_0 \cdot P \cdot Q \cdot S_0 \cdot P \cdot Q \cdot S_0 \cdot P \cdot Q \cdot P \cdot S_0 \cdot Q \cdot S_0 \cdot P \cdot Q \cdot S_0 \cdot P \cdot S_0 \cdot P \cdot Q \cdot P \cdot S_0.$$

By Theorem 2.1, using Table 1, we obtain

$$\begin{aligned} Z(G) &= \sum_{k=1}^{4} e_k^T \cdot M \cdot Z_{b_3b_4}(F_k) \\ &= [1,0,0,0] \cdot M \cdot [44,20,19,12]^T + [0,1,0,0] \cdot M \cdot [26,12,11,7]^T \\ &\quad + [0,0,1,0] \cdot M \cdot [21,10,13,8]^T + [0,0,0,1] \cdot M \cdot [13,5,8,5]^T \\ &= 2\,217\,936\,358\,652\,483\,532. \end{aligned}$$

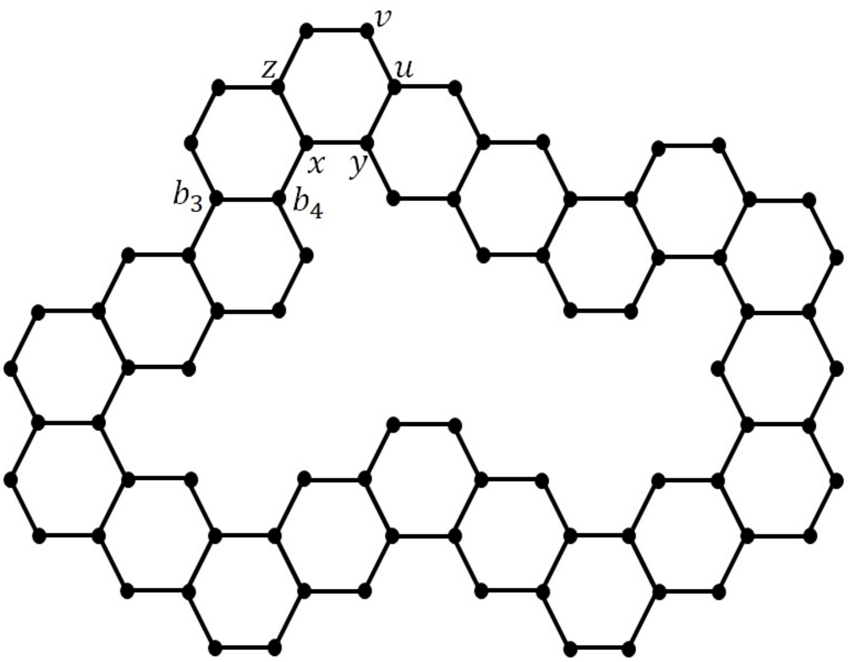

Figure 7. Primitive coronoid system G.

Next we find the Hosoya index of a hollow hexagon $HH(a, b, c, d, e, f)$. We may assume that $a > 1$ since the size of the corona hole must be at least 10. The general form of hollow hexagons is depicted in Figure 8.

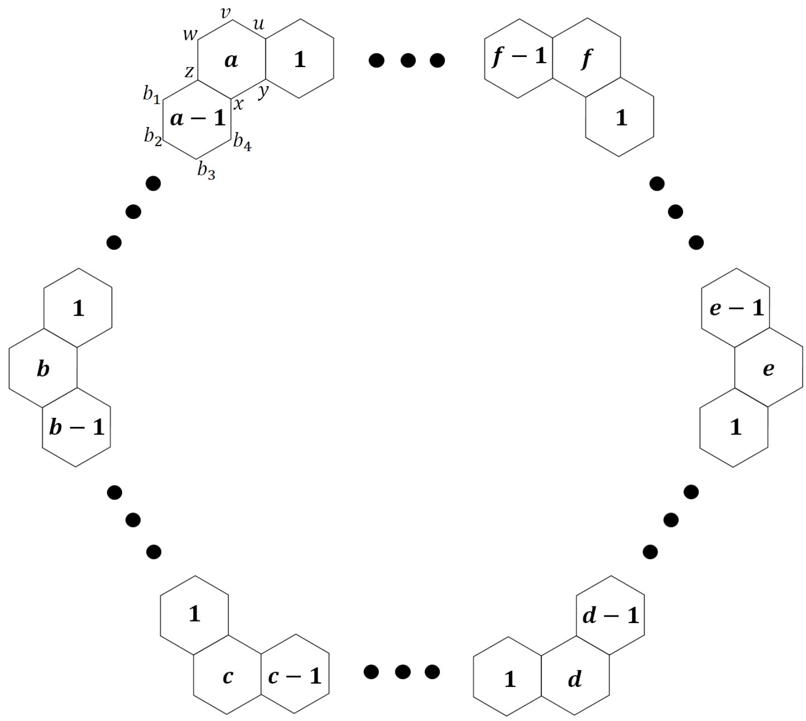

Figure 8. General form of a hollow hexagon.

Theorem 2.2. *Let $HH = HH(a, b, c, d, e, f)$ be a hollow hexagon. Then*

$$Z(HH) = \sum_{k=1}^{4} e_k^T \cdot M \cdot Z_{b_2 b_3}(F_k),$$

where

$$M = Q^{f-1} \cdot S_0 \cdot P \cdot Q^{e-1} \cdot S_0 \cdot P \cdot Q^{d-1} \cdot S_0 \cdot P \cdot Q^{c-1} \cdot S_0 \cdot P \cdot Q^{b-1} \cdot S_0 \cdot P \cdot Q^{a-2}.$$

Proof. Let $HH = HH(a, b, c, d, e, f)$ be a hollow hexagon as shown in Figure 8 and H_2 denotes the hexagonal chain starting at the edge uy and ending at the edge $b_2 b_3$. Since each hollow hexagon has just protruding corners, using Lemma 2.1, the Hosoya vector of H_2 at edge uy is

$$Z_{uy}(H_2) = M \cdot X_0,$$

where

$$M = Q^{f-1} \cdot S_0 \cdot P \cdot Q^{e-1} \cdot S_0 \cdot P \cdot Q^{d-1} \cdot S_0 \cdot P \cdot Q^{c-1} \cdot S_0 \cdot P \cdot Q^{b-1} \cdot S_0 \cdot P \cdot Q^{a-2}.$$

By Theorem 2.1 we are done. □

Example 2.2. *Now we find the Hosoya index of all the hollow hexagons with* 12 *hexagons by using Theorem 2.2. These hollow hexagons are depicted in Figure 9.*

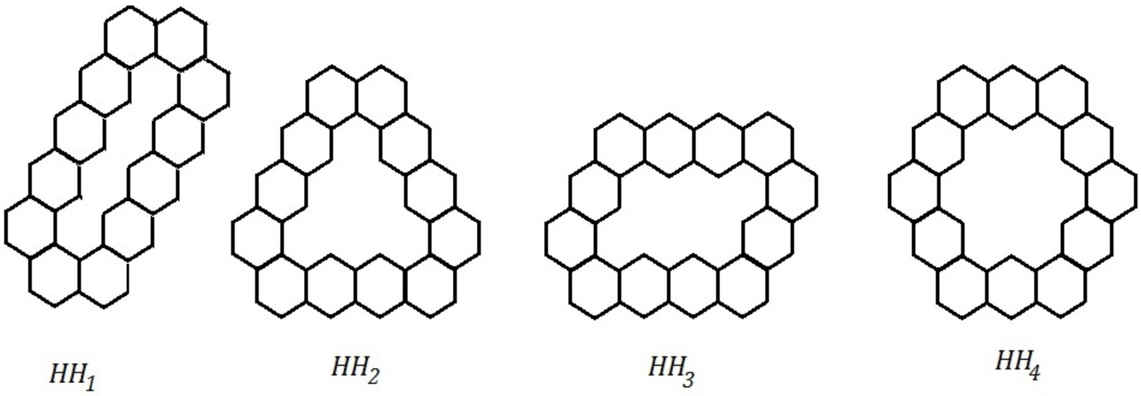

Figure 9. Hollows hexagons with 12 hexagons.

Let

$$\begin{aligned}
M_1 &= S_0 \cdot P \cdot S_0 \cdot P \cdot Q^3 \cdot S_0 \cdot P \cdot S_0 \cdot P \cdot S_0 \cdot P \cdot Q^2,\\
M_2 &= S_0 \cdot P \cdot Q^2 \cdot S_0 \cdot P \cdot S_0 \cdot P \cdot Q^2 \cdot S_0 \cdot P \cdot S_0 \cdot P \cdot Q,\\
M_3 &= Q^2 \cdot S_0 \cdot P \cdot S_0 \cdot P \cdot Q \cdot S_0 \cdot P \cdot Q^2 \cdot S_0 \cdot P \cdot S_0 \cdot P,\\
M_4 &= Q \cdot S_0 \cdot P \cdot Q \cdot S_0 \cdot P \cdot Q \cdot S_0 \cdot P \cdot Q \cdot S_0 \cdot P \cdot Q \cdot S_0 \cdot P.
\end{aligned}$$

The Hosoya index of these hollow hexagons are

$$\begin{aligned}
Z(HH_1) &= Z(HH(4,1,1,4,1,1)) = \sum_{k=1}^{4} e_k^T \cdot M_1 \cdot Z_{b_2b_3}(F_k) = 98034534619.\\
Z(HH_2) &= Z(HH(3,1,3,1,3,1)) = \sum_{k=1}^{4} e_k^T \cdot M_2 \cdot Z_{b_2b_3}(F_k) = 98366058276.\\
Z(HH_3) &= Z(HH(2,1,3,2,1,3)) = \sum_{k=1}^{4} e_k^T \cdot M_3 \cdot Z_{b_2b_3}(F_k) = 98902242744.\\
Z(HH_4) &= Z(HH(2,2,2,2,2,2)) = \sum_{k=1}^{4} e_k^T \cdot M_4 \cdot Z_{b_2b_3}(F_k) = 99914817684.
\end{aligned}$$

3. Conclusion

In this research, we have presented a method based on the transfer matrix technique and the Hosoya vector by using two significant recurrence relations. The supremacy of the method is that the Hosoya index of an arbitrary primitive coronoid benzenoid system and also an arbitrary hollow hexagon can be computed by a sum of four products of 4×4 dimensional transfer matrices with some vectors. In the implementation of the method according to a primitive coronoid system and a hollow hexagon, each of the four multiplication selections of the transfer matrices and vectors must be chosen according to the primitive coronoid system and the hollow hexagon then the method is applied simply. Besides, the method can be generalized for arbitrary catacondensed coronoid systems in further investigations.

Conflict of interest

The authors declare there is no conflict of interest.

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