

The matching interdiction problem in dendrimers

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ABSTRACT The purpose of the matching interdiction problem in the weighted graph G is to find a subset of vertices $R^* \subseteq V$ such that the weight of the maximum matching in the graph $G[V \setminus R^*]$ is minimized. According to the maximum matching in G , an approximate solution, denoted by R , for this problem is presented. Suppose that $\nu(G)$ is the weight of the maximum matching in G . In this paper, we consider dendrimers as graphs such that the weights of edges are the bond lengths. We obtain the maximum matching in some types of dendrimers. Then, we compute the value of $(\nu(G) - \nu(G[V \setminus R^*])) / (\nu(G) - \nu(G[V \setminus R]))$ for them. It is shown that this ratio in these classes of dendrimers is equal to the maximum value.

KEYWORDS Matching · interdiction · dendrimer.

1. INTRODUCTION

This paper is based on two concepts in mathematics and chemistry: interdiction and dendrimer. First, we explain these concepts.

In the network interdiction problems, there are two inconsistent forces, the follower and interdictor. The follower tries to optimize the objective function by considering some constraints in the problem. The interdictor attempts to prevent the action of the follower. The interdictor does this act by deleting arcs or vertices of the network. Also, the interdictor requires a budget to destroy the arcs or vertices of the network that it is called the interdiction budget. The network interdiction problem has been introduced in the 1960s [1,2]. The interdiction problem is expressed on some problems such as the maximum flow network, the connectivity, the matching, the independent sets and so on [3-6]. In the

maximum flow network interdiction problem, the follower maximizes the flow in the network. While, the interdictor tries to minimize the maximum flow by deleting arcs of network so that the cost of deleting arcs is not more than the interdiction budget. In 1993, Wood [3] presented an integer linear programming model for the maximum flow network interdiction problem such that this model has been used in many papers [7,8]. He used the concept of interdiction to decrease the disruptions in the electric power grids [9]. These disruptions are created by terrorist attacks. In 2010, Zenklusen [5] introduced the matching interdiction problem. The purpose of this problem is to remove a set of vertices such that the weight of the maximum matching in the new graph is minimized. Zenklusen [5] presented an approximate solution for this problem. Also, he showed that this problem is NP-complete on graphs with unit weights and interdiction costs. The matching interdiction problem can be considered on the edges of graph. It has been shown which this problem is NP-complete on simple bipartite graphs with unit weights and interdiction costs. The definition of interdiction in the independent sets is similar to definition of the matching interdiction problem [6]. Also, Shen et al. [4] presented an interdiction problem in graphs. The purpose was to remove a subset of vertices in the graph such that the disconnectivity of graph is maximized. They introduced three metrics for measuring the connectivity of graph.

Dendrimers are nanostructures that are used in the biomedicine fields. Dendrimers have a central core and are constructed by repetitive processes. The branches similar to tree are added to them in each step [10,11]. In other words, dendrimers have three Structural components: core, branches and end groups [12]. Research on dendrimers began in the 1970s. Dendrimers are produced by two methods: convergent and divergent. In the convergent approach, dendrimers are made from the end groups. In divergent approach, dendrimers grow from the core of molecule [13]. Dendrimers have the applications and properties that we express some of them [13]:

1. Dendrimer can be a therapeutic agent for example in cancer.
2. Dendrimer is an agent in the delivery of drug.
3. Physical imprisonment of molecules and atoms can be done within dendrimers.
4. Dendrimers can be used in gene therapy.
5. The ibuprofen can be encapsulated by some dendrimers.

According to structure of dendrimers, they are considered as graphs. Therefore, some mathematical problems are expressed on dendrimers. For example, the atom-bond connectivity and geometric arithmetic indices of some dendrimers have been calculated in [14]. Also, the PI index in some structures has been obtained [15]. In this paper, we consider some types of dendrimers such as Pan and Ford's amphiphilic dendrimer, Alkylsilane dendrimer, Styrylbenzene dendrimer and aromatic-based, all-hydrocarbon dendrimer. Pan and Ford introduced a structure that has the hydrophobic and hydrophilic terminal chains and is used as catalysts in aqueous media [16,17]. This dendrimer is depicted in Figure 1. Roovers et al. [18] synthesized a series of carbosilane dendrimers

using Pt-mediated silane alkenylation and vinylation, see Figure 2. Iranmanesh et al. [19] computed the Szeged index of Styrylbenzene dendrimer, depicted in Figure 3. In Figure 4, an aromatic-based, all-hydrocarbon dendrimer is depicted. This dendrimer is prepared in gram quantities and its thermal stability in air is at least 350°C [20]. In this paper, first we obtain the weight of the maximum matching in these dendrimers such that weights of edges are the bond lengths. Then, the approximate and optimal solutions of the matching interdiction problem are obtained for them. Also, we compute a special ratio which is defined in [5] for this problem.

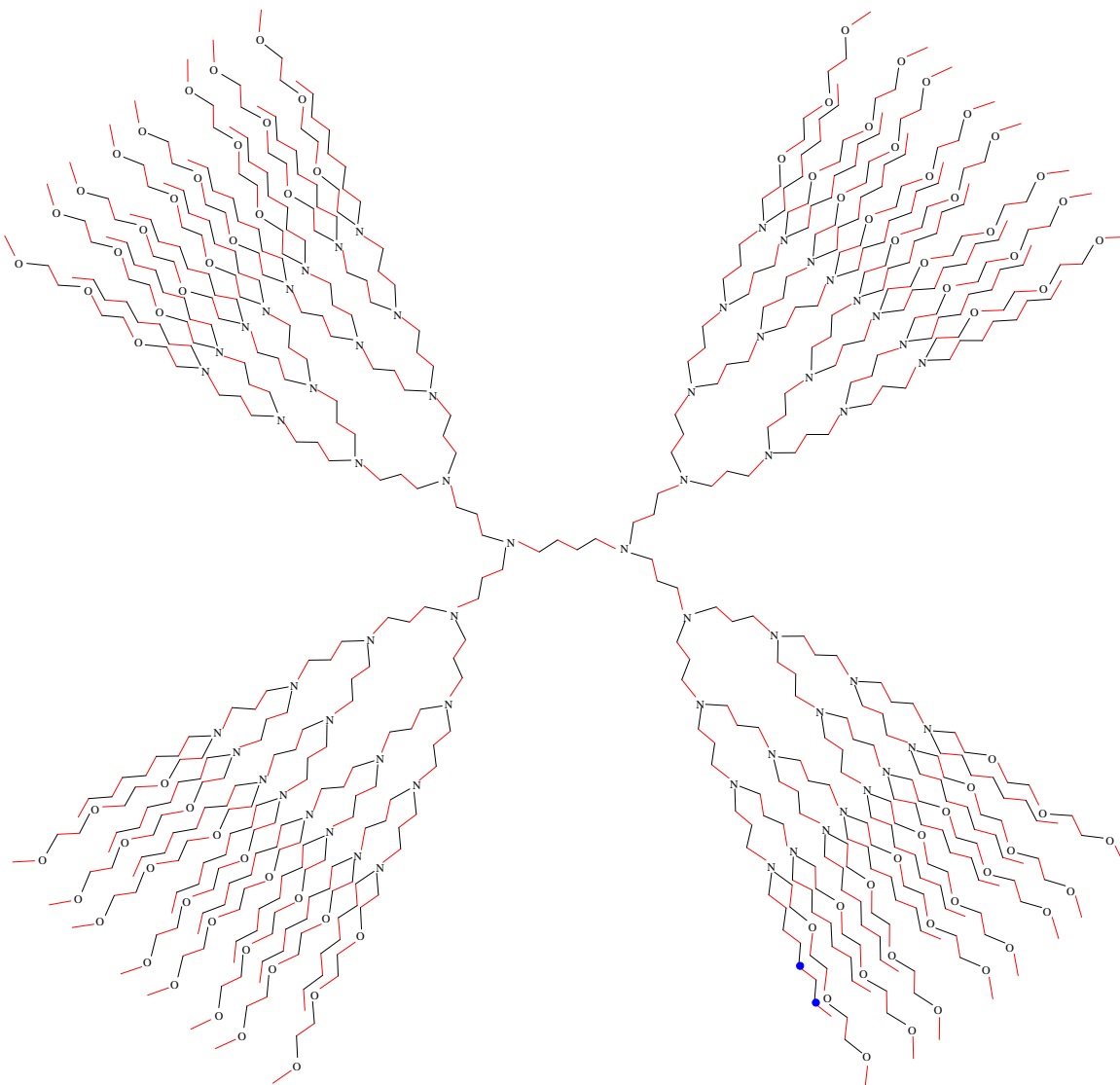


Figure 1. Pan and Ford's Amphiphilic Dendrimer.

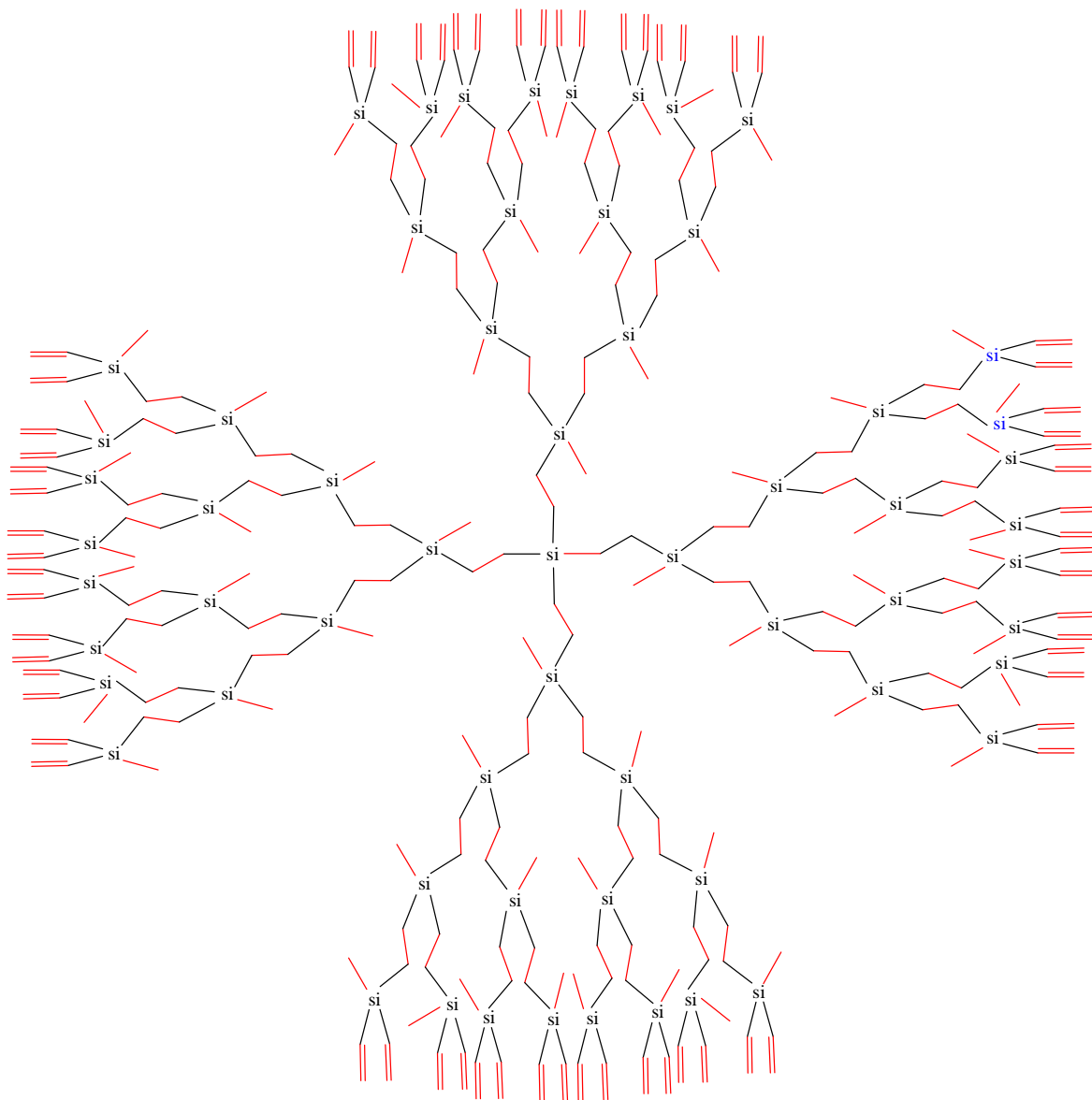


Figure 2. An Alkyldisilane Dendrimer.

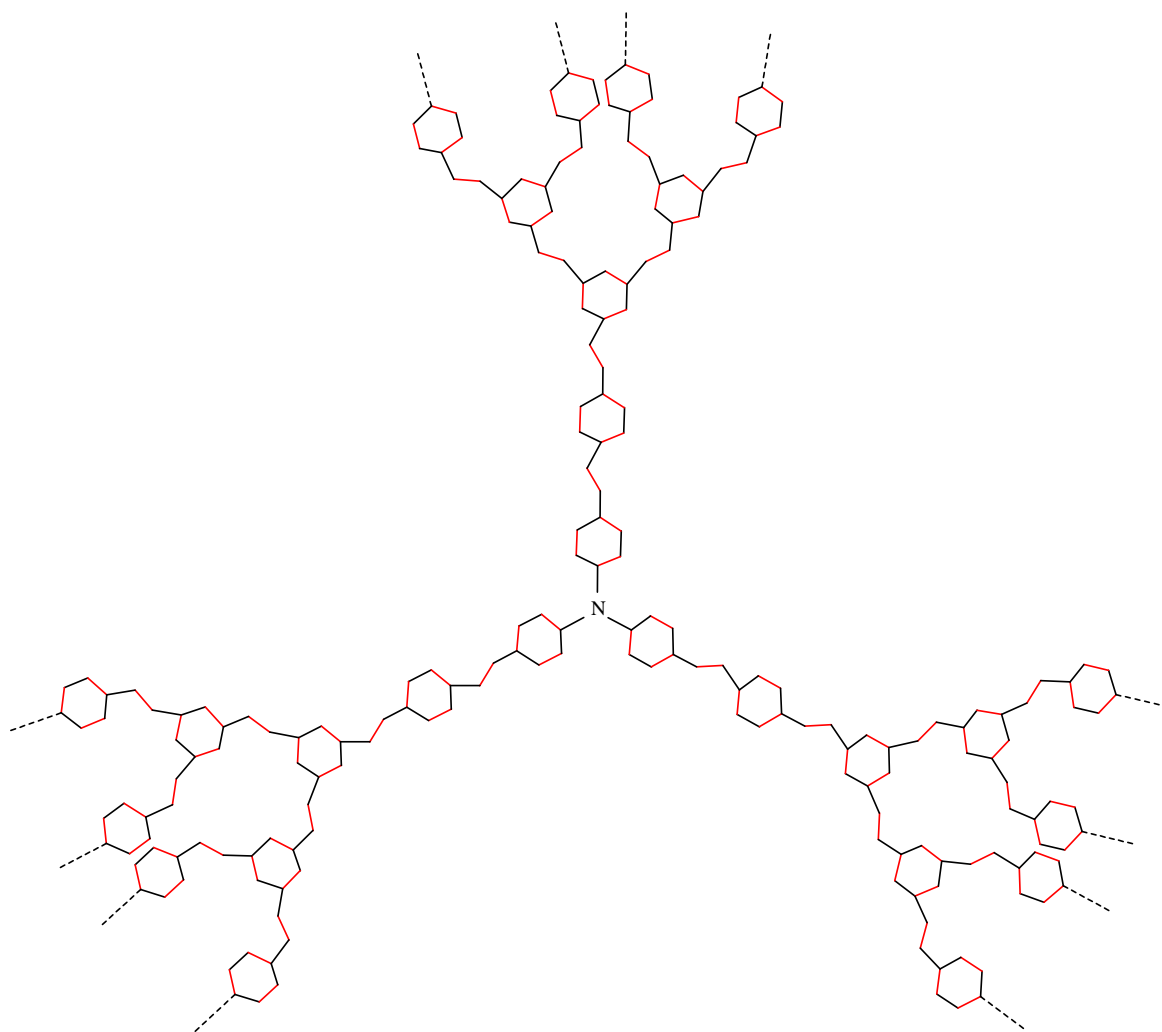


Figure 3. A Styrylbenzene Dendrimer.

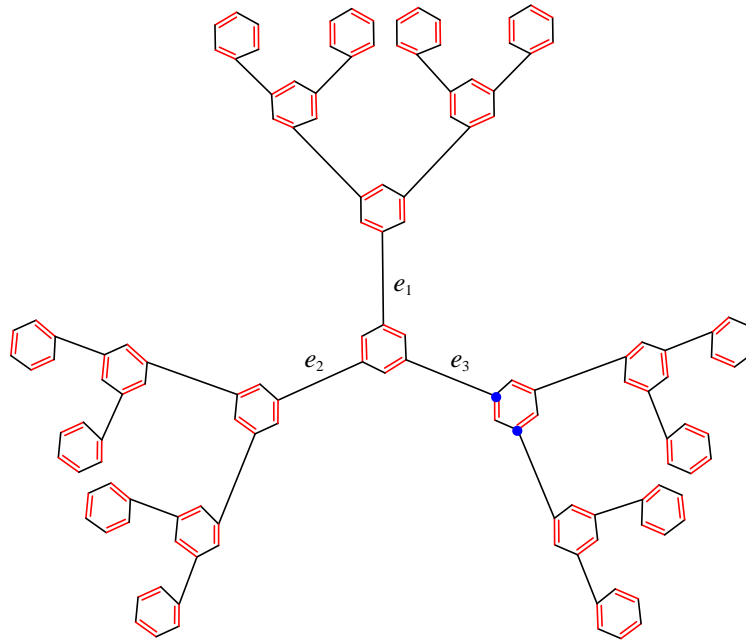


Figure 4. An Aromatic-Based, All-Hydrocarbon Dendrimer.

2. BASIC FACTS

Let $G = (V_G, E_G)$ be an undirected connected graph such that V_G and E_G are the sets of vertices and edges, respectively. An edge in G is denoted by (i, j) , where $i, j \in V_G$. Each edge $(i, j) \in E_G$ has a weight $w(i, j) > 0$. Two edges with a common vertex in G are called adjacent. The matching M in G is a set of nonadjacent edges in G . The weight of the matching M is defined as follows:

$$w(M) = \sum_{e \in M} w(e).$$

The matching M_G is called the maximum matching in G if $w(M_G) \geq w(M)$, for every matching M in G . Let $M_G = \{e_1, \dots, e_k\}$ such that $w(e_1) \geq \dots \geq w(e_k)$. The weight of the maximum matching M_G is denoted by $\nu(G)$. Let

$$\nu(G[V_G \setminus R_G^*]) = \text{Min}\{\nu(G[V_G \setminus R]) \mid R \subseteq V_G, |R| = 2\}.$$

R_G^* is called the optimal interdiction set of G . If $e_1 = (i_1, j_1)$, the set $R_G = \{i_1, j_1\}$ is called the approximate interdiction set of G . Notice that $M_G \setminus e_1$ is a maximum matching in $G[V_G \setminus R_G]$. Therefore,

$$\nu(G) - \nu(G[V_G \setminus R_G]) = w(e_1). \quad (1)$$

Now, e_G is defined as follows:

$$e_G = \frac{v(G) - v(G[V_G \setminus R_G^*])}{v(G) - v(G[V_G \setminus R_G])}$$

It has been shown that $e_G \leq 2$ [5].

We consider dendrimers as graphs as follows:

1. The atoms in dendrimer are the vertices of graph that are called by their first letter. The vertices without name are Carbon.
2. The covalent bonds between atoms in dendrimer are the edges of graph.
3. The weight of each edge is equal to the bond length between two atoms. Some bond lengths that are used in this paper are presented in Table 1 [21].

Table 1. The Bond Lengths.

Bond	Bond length (pm)
C–N	$w_1 = 147$
C–C (in hydrocarbons)	$w_2 = 154$
C–O	$w_3 = 143$
Si–C	$w_4 = 186$
C=C	$w_5 = 134$
C–C (in benzene)	$w_6 = 139$

3. MAIN RESULTS

In this section, we obtain e_G for the dendrimers in Figures 1 – 4. Notice that the elements of set R_G^* are denoted by the blue points or atoms and the elements of set M_G are denoted by red edges in these dendrimers.

3.1. PAN AND FORD'S AMPHIPHILIC DENDRIMER

Consider the sequence of graphs $\{G_n\}_{n=1}^5$ which is depicted in Figure 5. The weight of the maximum matching in G_n , where $1 \leq n \leq 5$, is equal to:

$$v(G_n) = \begin{cases} (2^n - 1)(w_1 + w_2) & n = 1, 2, 3, 4, \\ v(G_4) + 8(3w_3 + 6w_2) & n = 5. \end{cases}$$

In other words,

$$v(G_n) = \begin{cases} (2^n - 1)(w_1 + w_2) & n = 1, 2, 3, 4, \\ 15w_1 + 63w_2 + 24w_3 & n = 5. \end{cases}$$

We consider two blue vertices of the graph G_5 in Figure 5 as u and v . The following relation holds for the graph G_5 :

$$v(G_5[V_{G_5} \setminus \{u, v\}]) = v(G_5) - 2w_2. \quad (2)$$

Claim 1. $R_{G_5}^* = \{u, v\}$.

Proof of Claim 1. Let $V' \subseteq V_{G_5}$ such that $|V'| = 2$ and $M = \{(i, j) \in M_{G_5} \mid i \in V' \text{ or } j \in V'\}$. Hence, $|M| \leq 2$. According to the structure of graph G_5 , it is obvious that $M_{G_5} \setminus M$ is a matching in $G_5 \setminus V'$. We denote this matching as M'_{G_5} . Therefore,

$$w(M'_{G_5}) = v(G_5) - \sum_{(i,j) \in M} w(i, j).$$

The weights of edges in G_5 are w_1 , w_2 and w_3 . Since $w_3 < w_1 < w_2$, we have $2w_2 \geq \sum_{(i,j) \in M} w(i, j)$. Therefore, the following relations hold:

$$\begin{aligned} v(G_5) - 2w_2 &\leq v(G_5) - \sum_{(i,j) \in M} w(i, j) \\ &= w(M'_{G_5}) \\ &\leq v(G_5 \setminus V'). \end{aligned} \quad (3)$$

Using Eqs. (2) and (3), we have the following relation:

$$v(G_5[V_{G_5} \setminus \{u, v\}]) \leq v(G_5 \setminus V').$$

Since V' is an arbitrary subset of vertices, then $R_{G_5}^* = \{u, v\}$. The Claim follows. \blacksquare

Suppose that the Pan and Ford's amphiphilic dendrimer in Figure 1 is denoted by D_1 . The graph G_5 is a subgraph of D_1 . By the maximum matching in G_5 , the weight of the maximum matching in D_1 is obtained as follows:

$$\begin{aligned} v(D_1) &= 4v(G_5) + 2w_1 + w_2 \\ &= 62w_1 + 253w_2 + 96w_3. \end{aligned}$$

Also, $R_{D_1}^* = R_{G_5}^* = \{u, v\}$ and the following relation holds:

$$v(D_1[V_{D_1} \setminus R_{D_1}^*]) = v(D_1) - 2w_2.$$

According to Eq. (1), we have:

$$v(D_1[V_{D_1} \setminus R_{D_1}]) = v(D_1) - w_2.$$

Therefore, e_{D_1} is obtained as follows:

$$\begin{aligned}
e_{D_1} &= \frac{v(D_1) - (D_1[V_{D_1} \setminus R_{D_1}^*])}{v(D_1) - (D_1[V_{D_1} \setminus R_{D_1}])} \\
&= \frac{v(D_1) - v(D_1) + 2w_2}{v(D_1) - v(D_1) + w_2} \\
&= 2.
\end{aligned}$$

3.2. ALKYL SILANE DENDRIMER

Consider the sequence of graphs $\{S_n\}_{n=1}^5$, depicted in Figure 6. The weight of the maximum matching in S_n , where $1 \leq n \leq 5$, is equal to:

$$v(S_n) = \begin{cases} 2w_4 & n = 1, \\ 2^n w_4 + (2^{n-1} - 2)w_2 & n = 2, 3, 4, \\ 16w_4 + 14w_2 + 16w_5 & n = 5. \end{cases}$$

We consider two blue atoms in the graph S_5 in Figure 6 as u and v . Similar to Claim 1, we can prove that the optimal interdiction set in the graph S_5 is $R_{S_5}^* = \{u, v\}$. Therefore, we have the following relation:

$$v(S_5[V_{S_5} \setminus R_{S_5}^*]) = v(S_5) - 2w_4.$$

Suppose that the Alkylsilane dendrimer in Figure 2 is denoted by D_2 . The graph S_5 is a subgraph of D_2 . Using the maximum matching in S_5 , the weight of the maximum matching in D_2 is equal to $4v(S_5) - 3w_4 + 3w_2$ or $4v(S_5) - 4w_4 + 4w_2$. Since $w_4 > w_2$, we have:

$$\begin{aligned}
v(D_2) &= 4v(S_5) - 3w_4 + 3w_2 \\
&= 61w_4 + 59w_2 + 64w_5.
\end{aligned}$$

Also, the optimal interdiction set in the graph D_2 is $R_{D_2}^* = R_{S_5}^*$ and it is obvious that

$$v(D_2[V_{D_2} \setminus R_{D_2}^*]) = v(D_2) - 2w_4.$$

On the other hand, by Eq. (1) we have:

$$v(D_2[V_{D_2} \setminus R_{D_2}]) = v(D_2) - w_4.$$

Therefore, e_{D_2} is obtained as follows:

$$\begin{aligned}
e_{D_2} &= \frac{v(D_2) - (D_2[V_{D_2} \setminus R_{D_2}^*])}{v(D_2) - (D_2[V_{D_2} \setminus R_{D_2}])} \\
&= \frac{v(D_2) - v(D_2) + 2w_4}{v(D_2) - v(D_2) + w_4} \\
&= 2.
\end{aligned}$$

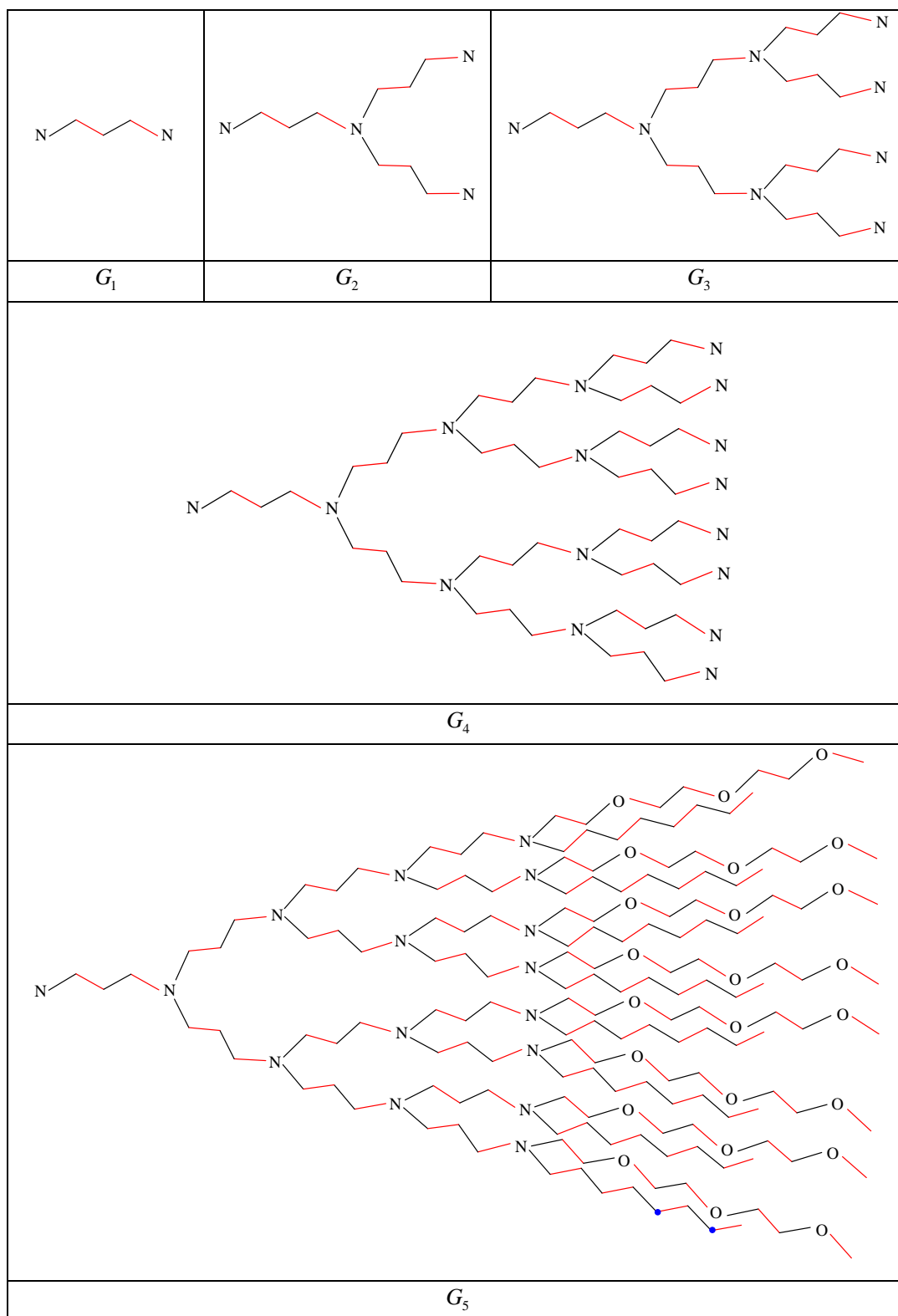


Figure 5. The Sequence of Graphs $\{G_n\}_{n=1}^5$.

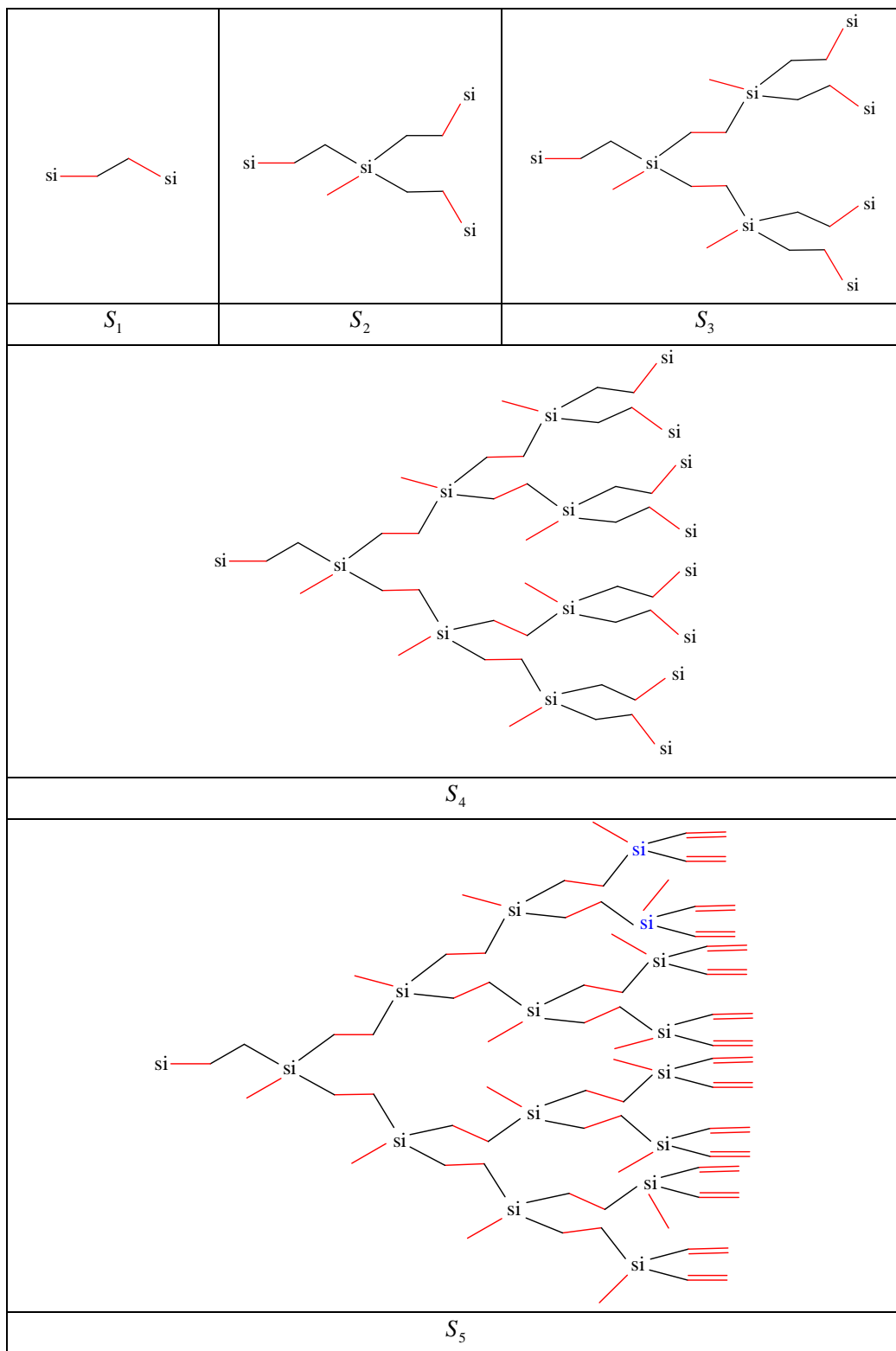


Figure 6. The Sequence of Graphs $\{S_n\}_{n=1}^5$.

3.3. STYRYLBENZENE DENDRIMER

Consider the sequence of graphs $\{H_n\}_{n=1}^{\infty}$, depicted in Figure 7. The number of hexagons in H_n , for every $n \geq 1$, is equal to $2^n - 1$. The weight of every edge in H_n , where $n \geq 1$, is equal to w_2 . Hence, the weight of the maximum matching in H_n is equal to:

$$v(H_n) = 4(2^n - 1)w_2, \quad \forall n \geq 1.$$

We consider two blue vertices in the sequence of graphs $\{H_n\}_{n=1}^{\infty}$ in Figure 7 as u and v . Similar to Claim 1, we can show that $R_{H_n}^* = \{u, v\}$, for every $n \geq 1$. Therefore, we have:

$$v(H_n[V_{H_n} \setminus R_{H_n}^*]) = v(H_n) - 2w_2, \quad \forall n \geq 1.$$

Now, consider the graph H in Figure 8. When n is large, H_n is the subgraph of H . Therefore, the weight of the maximum matching in the graph H is as follows:

$$\begin{aligned} v(H) &= v(H_n) + 7w_2 \\ &= (2^{n+2} + 3)w_2. \end{aligned} \quad (4)$$

We consider two blue vertices of the graph H in Figure 8 as u' and v' . The graph $H[V_H \setminus \{u', v'\}]$ is disconnected with two components. Since H_n is a component of this graph, then:

$$v(H[V_H \setminus \{u', v'\}]) = v(H_n) + 5w_2. \quad (5)$$

Similar to Claim 1, we can conclude that $R_H^* = \{u', v'\}$. Now, consider the Styrylbenzene dendrimer in Figure 3 that is denoted by D_3 . Since H is a subgraph of D_3 , it follows:

$$\begin{aligned} v(D_3) &= 3v(H) \\ &= 3(2^{n+2} + 3)w_2. \end{aligned} \quad (6)$$

By Eq. (1), we have the following relation:

$$v(D_3[V_{D_3} \setminus R_{D_3}]) = v(D_3) - w_2.$$

The optimal interdiction set in D_3 is the similar to the optimal interdiction set in the graph H . According to Eqs. (4), (5) and (6), we have:

$$\begin{aligned} v(D_3[V_{D_3} \setminus R_{D_3}^*]) &= 2v(H) + v(H[V_H \setminus R_H^*]) \\ &= v(D_3) - 2w_2. \end{aligned}$$

Hence, e_{D_3} is obtained as follows:

$$\begin{aligned} e_{D_3} &= \frac{v(D_3) - (D_3[V_{D_3} \setminus R_{D_3}^*])}{v(D_3) - (D_3[V_{D_3} \setminus R_{D_3}])} \\ &= \frac{v(D_3) - v(D_3) + 2w_2}{v(D_3) - v(D_3) + w_2} \\ &= 2. \end{aligned}$$

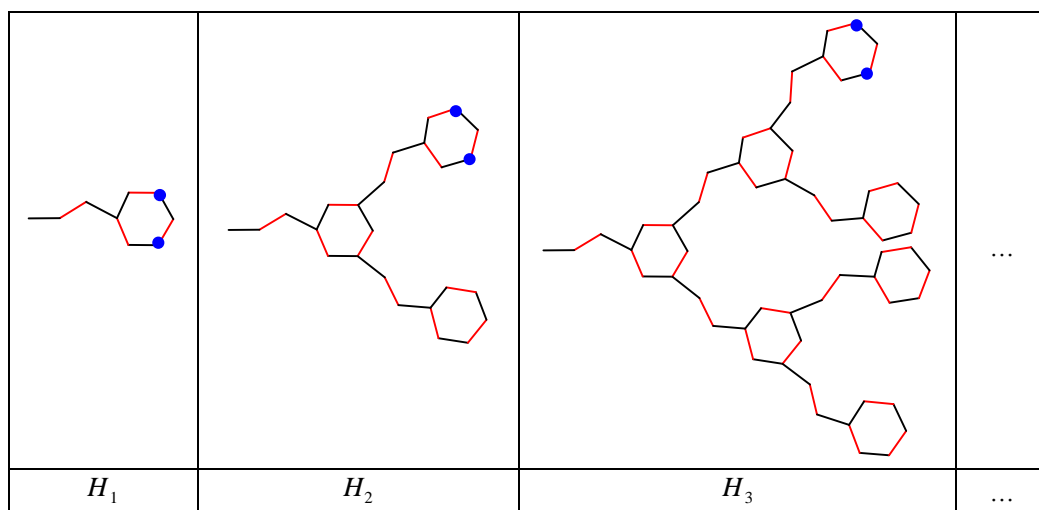


Figure 7. The Sequence of Graphs $\{H_n\}_{n=1}^\infty$.

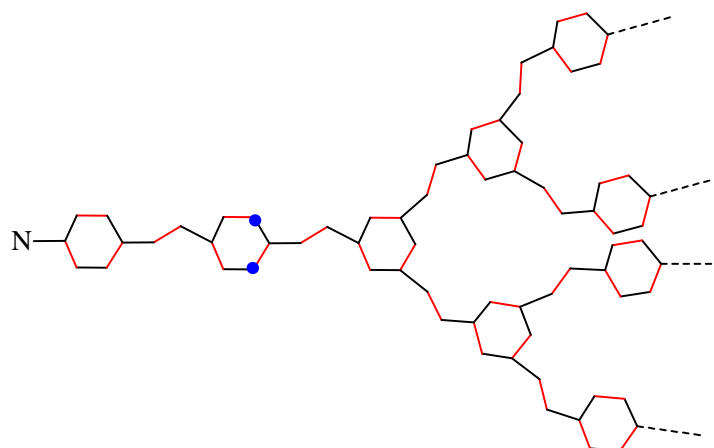


Figure 8. The Graph H .

3.4. AROMATIC-BASED, ALL-HYDROCARBON DENDRIMER

Consider the sequence of graphs $\{A_n\}_{n=1}^3$ which is depicted in Figure 9. The weight of the maximum matching in A_n , for every $1 \leq n \leq 3$, is equal to:

$$\begin{aligned} v(A_n) &= w_2 + (3(2^n - 2) + 2)w_6 \\ &= w_2 + (3 \times 2^n - 4)w_6. \end{aligned}$$

Consider the sequence of graphs $\{B_n\}_{n=1}^3$, depicted in Figure 10. The weight of the maximum matching in B_n , for every $1 \leq n \leq 3$, is equal to:

$$v(B_n) = 3(2^n - 1)w_6.$$

Suppose that the dendrimer in Figure 4 is denoted by D_4 . A_3 and B_3 are the subgraphs of D_4 . There are four cases for the maximum matching in D_4 as follows:

1. M_1 is the maximum matching of D_4 inclusive an edge of the set $\{e_1, e_2, e_3\}$. In this case, the weight of M_1 is equal to:

$$\begin{aligned} w(M_1) &= v(A_3) + 2v(B_3) + 2w_6 \\ &= w_2 + 64w_6. \end{aligned}$$

2. M_2 is the maximum matching of D_4 inclusive two edges of the set $\{e_1, e_2, e_3\}$. In this case, the weight of M_2 is equal to:

$$\begin{aligned} w(M_2) &= 2v(A_3) + v(B_3) + w_6 \\ &= 2w_2 + 62w_6. \end{aligned}$$

3. M_3 is the maximum matching of D_4 inclusive the edges e_1 , e_2 and e_3 . In this case, the weight of M_3 is equal to:

$$\begin{aligned} w(M_3) &= 3v(A_3) \\ &= 3w_2 + 60w_6. \end{aligned}$$

4. M_4 is the maximum matching of D_4 such that it is not inclusive the edges e_1 , e_2 and e_3 . In this case, the weight of M_4 is equal to:

$$\begin{aligned} w(M_4) &= 3v(B_3) + 3w_6 \\ &= 66w_6. \end{aligned}$$

By the above four cases, we have:

$$w(M_4) > w(M_1) > w(M_2) > w(M_3).$$

Therefore, M_4 is the maximum matching in the graph D_4 and $v(D_4) = 66w_6$. Consider the subgraph D of D_4 where has been depicted in Figure 11. There exist three cases for the maximum matching in D :

1. The maximum matching of D is inclusive an edge of set $\{e_1, e_2\}$. The weight of this matching is equal to:

$$v(A_3) + v(B_3) + 2w_6 = w_2 + 43w_6.$$

2. The maximum matching of D is inclusive edges e_1 and e_2 . The weight of this matching is equal to:

$$2v(A_3) + w_6 = 2w_2 + 41w_6.$$

3. The maximum matching of D is not inclusive edges e_1 and e_2 . The weight of this matching is equal to:

$$2v(B_3) + 3w_6 = 45w_6.$$

By the above three cases, the weight of the maximum matching in D is equal to $v(D) = 45w_6$. We consider two blue vertices in the graph D_4 in Figure 4 as u and v .

Similar to Claim 1, we can show that $R_{D_4}^* = \{u, v\}$. Therefore,

$$v(D_4[V_{D_4} \setminus R_{D_4}^*]) = v(D_4) - 2w_6.$$

Also, using Eq. (1) we have:

$$v(D_4[V_{D_4} \setminus R_{D_4}]) = v(D_4) - w_6.$$

Therefore, e_{D_4} is obtained as follows:

$$\begin{aligned} e_{D_4} &= \frac{v(D_4) - (D_4[V_{D_4} \setminus R_{D_4}^*])}{v(D_4) - (D_4[V_{D_4} \setminus R_{D_4}])} \\ &= \frac{v(D_4) - v(D_4) + 2w_6}{v(D_4) - v(D_4) + w_6} \\ &= 2. \end{aligned}$$

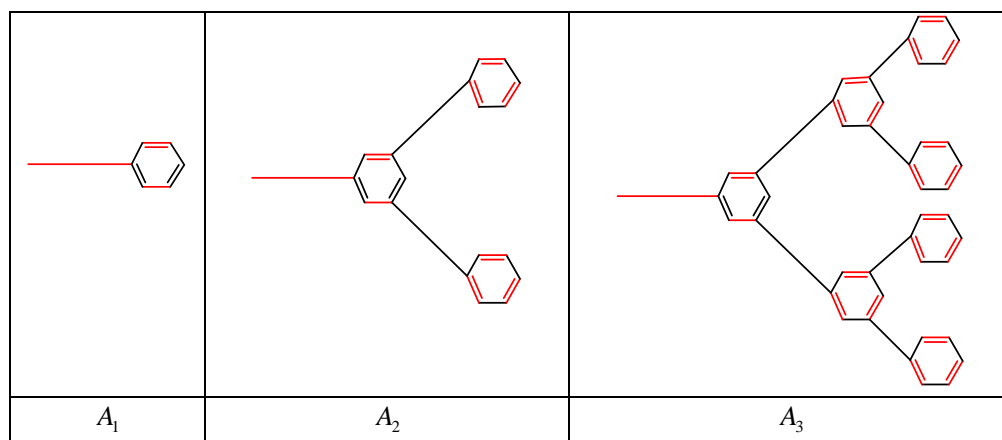


Figure 9. The Sequence of Graphs $\{A_n\}_{n=1}^3$.

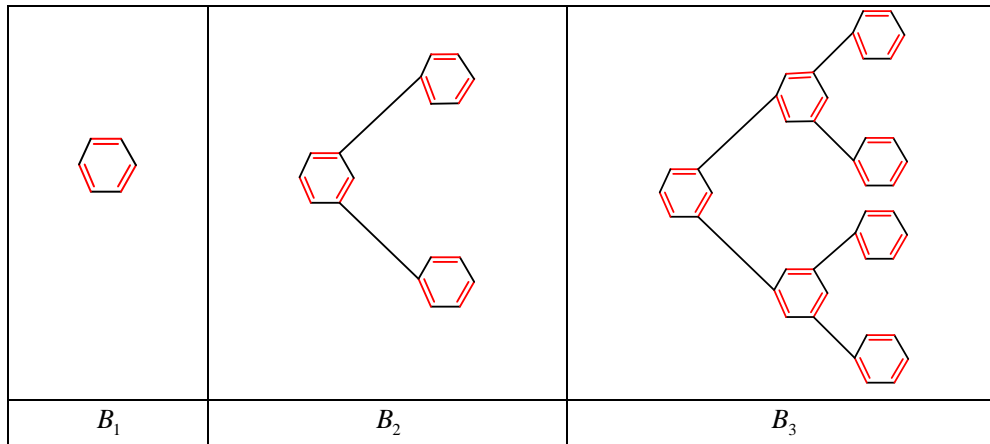


Figure 10. The Sequence of Graphs $\{B_n\}_{n=1}^3$.

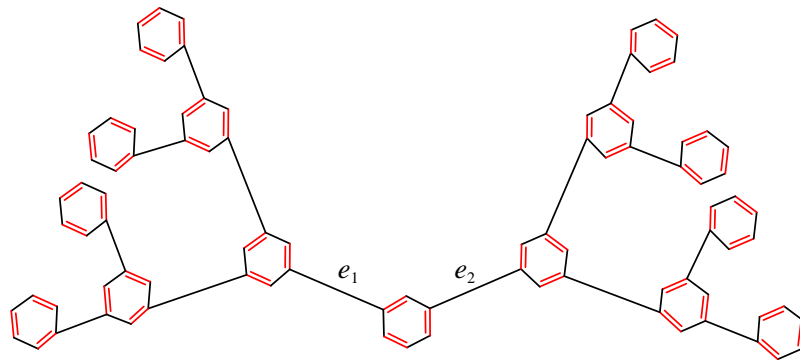


Figure 11. The Graph D .

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