

# The Distinguishing Number and the Distinguishing Index of Graphs from Primary Subgraphs

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## ABSTRACT

The distinguishing number (index)  $D(G)$  ( $D'(G)$ ) of a graph  $G$  is the least integer  $d$  such that  $G$  has a vertex labeling (edge labeling) with  $d$  labels that is preserved only by the trivial automorphism. Let  $G$  be a connected graph constructed from pairwise disjoint connected graphs  $G_1, \dots, G_k$  by selecting a vertex of  $G_1$ , a vertex of  $G_2$ , and identifying these two vertices. Then continue in this manner inductively. We say that  $G$  is obtained by point-attaching from  $G_1, \dots, G_k$  and that  $G_i$ 's are the primary subgraphs of  $G$ . In this paper, we consider some particular cases of these graphs that are of importance in chemistry and study their distinguishing number and distinguishing index.

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## 1. INTRODUCTION

We first introduce some notations and terminology which is needed for the paper. A molecular graph is a simple graph such that its vertices correspond to the atoms and the edges to the bonds of a molecule. Let  $G = (V, E)$  be a graph. We use the standard graph notation [7]. In particular,  $Aut(G)$  denotes the automorphism group of  $G$ . The set of the vertices adjacent in  $G$  to a vertex of a vertex subset  $W \subseteq V$  is the open neighborhood  $N_G(W)$  of  $W$ . The closed neighborhood  $G[W]$  also includes all vertices of  $W$  itself. In case of a singleton set  $W = \{v\}$  we write  $N_G(v)$  and  $N_G[v]$  instead of  $N_G(\{v\})$  and  $N_G[\{v\}]$ , respectively. We omit the subscript when the graph  $G$  is clear from the context. The complement of  $N[v]$  in  $V(G)$  is denoted by  $\overline{N[v]}$ .

In theoretical chemistry, molecular structure descriptors, also called topological indices, are used to understand the properties of chemical compounds. The Wiener index is

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one of the oldest descriptors concerned with the molecular graph [11]. By now there are many different types of such indices for a general graph  $G=(V,E)$ , see for example [3]. Here, apart from the topological index, we are interested in computing the distinguishing number and the distinguishing index. A labeling of  $G$ ,  $\varphi: V \rightarrow \{1,2,\dots,r\}$ , is  $r$ -distinguishing, if no non-trivial automorphism of  $G$  preserves all of the vertex labels. Formally,  $\varphi$  is  $r$ -distinguishing if for every non-trivial  $\sigma \in \text{Aut}(G)$ , there exists  $x$  in  $V$  such that  $\varphi(x) \neq \varphi(\sigma(x))$ . The distinguishing number of a graph  $G$  is the minimum number  $r$  such that  $G$  has a labeling that is  $r$ -distinguishing. This number has defined by Albertson and Collins [1]. Similar to this definition, Kalinowski and Pilśniak [8] have defined the distinguishing index  $D'(G)$  of  $G$  which is the least integer  $d$  such that  $G$  has an edge colouring with  $d$  colours that is preserved only by a trivial automorphism.

In this paper, we consider the distinguishing number and the distinguishing index on graphs that contain cut-vertices. Such graphs can be decomposed into subgraphs that we call primary subgraphs. Blocks of graphs are particular examples of primary subgraphs, but a primary subgraph may consist of several blocks. For convenience, the definition of these kind of graphs will be given in the next section. In Section 2, the distinguishing number and the distinguishing index of some graphs are computed from their primary subgraphs. In Section 3, we apply the results of Section 2, in order to obtain the distinguishing number and the distinguishing index of families of graphs that are of importance in chemistry.

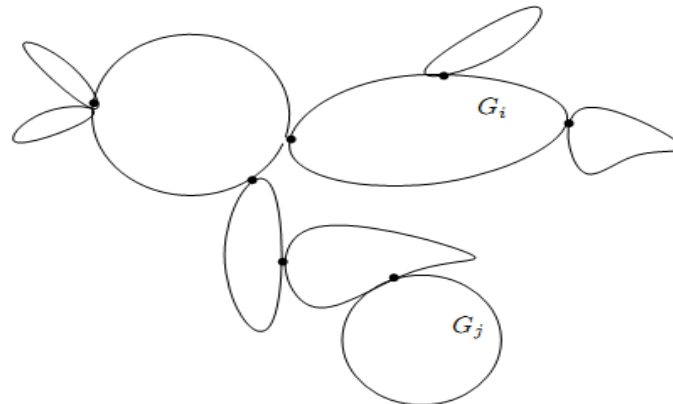
## 2. THE DISTINGUISHING NUMBER (INDEX) OF SOME GRAPHS FROM PRIMARY SUBGRAPHS

Let  $G$  be a connected graph constructed from pairwise disjoint connected graphs  $G_1, \dots, G_k$  as follows: Select a vertex of  $G_1$ , a vertex of  $G_2$ , and identify these two vertices and continue in this manner inductively. Note that the graph  $G$  constructed in this way has a tree-like structure and the  $G_i$ 's being its building stones, see Figure 1. Usually, we say that  $G$  is obtained by point-attaching from  $G_1, \dots, G_k$  and that  $G_i$ 's are the primary subgraphs of  $G$ . A particular case of this construction is the decomposition of a connected graph into blocks [3]. In this section, we consider some particular cases of these graphs and study their distinguishing number and index.

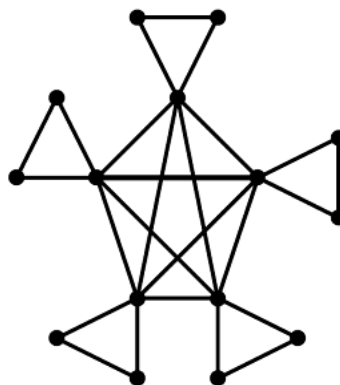
As an example of point-attaching graph, consider the graph  $K_m$  and  $m$  copies of  $K_n$ . By definition, the graph  $Q(m,n)$  is obtained by identifying each vertex of  $K_m$  with a vertex of a unique  $K_n$ . The graph  $Q(5,3)$  is shown in Figure 2.

The following theorems give the distinguishing number and the distinguishing index of  $Q(m,n)$ . A key point for proving these theorems is that under every automorphism  $f$  of  $Q(m,n)$ , the set of the vertices of  $K_m$  are mapped to itself and the copies of  $K_n$  to themselves, only with respect to the degrees of the vertices. In fact, if  $f$  maps the vertex  $v_i$  of  $K_m$  to the

vertex  $v_j$  of  $K_m$ , then the restriction of  $f$  to the copy of  $K_n$  corresponding to the vertex  $v_i$  is an automorphism of the copy of  $K_n$  corresponding to the vertex  $v_j$ .



**Figure 1.** The graph  $G$  obtained by point-attaching from  $G_1, \dots, G_k$ .



**Figure 2.** The graph  $Q(5,3)$ .

**Theorem 2.1.** *The distinguishing number of  $Q(m,n)$  is*

$$D(Q(m,n)) = \min\{r : r \binom{r}{n-1} \geq m\}.$$

**Proof.** We denote the vertices of  $K_m$  by  $v_1, \dots, v_m$  and the vertices of corresponding  $K_n$  to the vertex  $v_i$  by  $w_1^{(i)}, \dots, w_{n-1}^{(i)}$  where  $i = 1, \dots, m$ . In an  $r$ -distinguishing labeling, each of the vertices  $w_1^{(i)}, \dots, w_{n-1}^{(i)}$  must have a different label. Also, each of  $n$ -ary consisting of a vertex of  $K_m$  and  $n-1$  vertices of its corresponding  $K_n$  must have a different ordered  $n$ -ary of labels. There are  $r \binom{r}{n-1}$  possible ordered  $n$ -ary of labels using  $r$  labels, hence

$$D(Q(m,n)) = \min\{r : r \binom{r}{n-1} \geq m\},$$

proving the result. ■

**Theorem 2.2.** *The distinguishing index of  $Q(m,n)$  is 2.*

**Proof.** We prove the theorem in the following three cases:

**Case 1.** If  $m \geq 6$  and  $n \geq 6$ , then since  $D'(K_n) = D'(K_m) = 2$ , we label the edges of  $K_m$  and copies of  $K_n$  in a distinguishing way with two labels. This labeling is distinguishing because if  $f$  is an automorphism of  $Q(m,n)$  preserving the labeling, then with respect to the distinguishing labeling of  $K_m$  we conclude that the vertices of  $K_m$  is fixed under  $f$  such that it moves the vertices of  $K_m$ . By a similar argument, we can conclude that  $f$  is the identity automorphism on vertices of  $K_n$ , and so on  $Q(m,n)$ .

**Case 2.** If  $m \geq 6$  and  $n < 6$ , then we label the edges of  $K_m$  in a distinguishing way with two labels. Since  $n < 6$ , we can label the edges of every copy of  $K_n$  with two labels such that the sets consisting the incident edges to  $w_j^{(i)}$ ,  $j = 1, \dots, n-1$  have different number of label 2 for all  $i = 1, \dots, m$ . Hence the vertices  $w_j^{(i)}$ ,  $j = 1, \dots, n-1$  are fixed under each automorphism of  $G$  preserving the labeling. Now since the vertices of  $K_m$  have been labeled distinguishingly, we conclude that these vertices are fixed under each automorphism of  $G$  preserving the labeling. Hence, we have a distinguishing labeling for  $Q(m,n)$  as prior case.

**Case 3.** If  $m < 6$ , then we can label the edges of  $K_m$  with two labels such that there exist two vertices of  $K_m$  have the same number of label 2 and 1 in label of their incident edges. Let these two vertices be  $v_1$  and  $v_2$ . We label the edges of  $K_n$  corresponding to  $v_t$ ,  $t = 1, 2$  with two labels such that

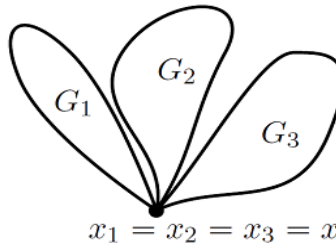
1. The sets consisting the incident edges to  $w_j^{(t)}$ ,  $j = 1, \dots, n-1$  have different number of label 2, where  $t = 1, 2$ .
2. The number of label 2 that have been used for the labeling of edges of  $K_n$  corresponding to  $v_1$  and  $v_2$  are distinct.

So this labeling is distinguishing. Using these three cases we have the result. ■

Now, we present several constructions of graphs and study their distinguishing number and distinguishing index. These constructions will in turn be used in the next section where chemical applications will be given. Most of the following constructions have been stated in [3].

**2.1. BOUQUET OF GRAPHS**

Let  $G_1, G_2, \dots, G_k$  be a finite sequence of pairwise disjoint connected graphs and let  $x_i \in V(G_i)$ . By definition, the bouquet  $G$  of the graphs  $\{G_i\}_{i=1}^k$  with respect to the vertices  $\{x_i\}_{i=1}^k$  is obtained by identifying the vertices  $x_1, x_2, \dots, x_k$  (see Figure 3 for  $k = 3$ ).



**Figure 3.** A bouquet of three graphs.

**Theorem 2.3.** *Let  $G$  be the bouquet of the graphs  $\{G_i\}_{i=1}^k$  with respect to the vertices  $\{x_i\}_{i=1}^k$  then*

- (i)  $D(G) \leq \sum_{i=1}^k D(G_i)$ ,
- (ii)  $D'(G) \leq \sum_{i=1}^k D'(G_i)$ .

**Proof.** (i) We label the vertices of graph  $G_1$  with labels  $\{1, \dots, D(G_1)\}$  in a distinguishing way. Next we label the vertices of graph  $G_j$  ( $2 \leq j \leq k$ ) except the vertex  $x$  with labels  $\{(\sum_{i=1}^{j-1} D(G_i)) + 1, \dots, (\sum_{i=1}^{j-1} D(G_i)) + D(G_j)\}$  in a distinguishing way. This labeling is distinguishing, because if  $f$  is an automorphism of  $G$  preserving the labeling then by the method of labeling we have  $f(V(G_i)) = V(G_i)$  where  $i = 1, \dots, k$ . Since every  $G_i$  is labeled distinguishingly,  $f|_{V(G_i)}$  is the identity, and so  $f$  is the identity automorphism on  $G$ . We used  $\sum_{i=1}^k D(G_i)$  labels, and hence the result follows.

(ii) A similar argument yields that  $D'(G) \leq \sum_{i=1}^k D'(G_i)$ . ■

The bounds of Theorem 2.3 are sharp. If the graphs  $\{G_i\}_{i=1}^k$  are the star graphs  $\{K_{1, n_i}\}_{i=1}^k$  ( $n_i \geq 3$ ) and  $\{x_i\}_{i=1}^k$  are the central points of  $\{K_{1, n_i}\}_{i=1}^k$ , respectively, then the bouquet of  $\{K_{1, n_i}\}_{i=1}^k$  with respect to their central points is the star graph  $K_{1, n_1 + \dots + n_k}$ . Since the distinguishing number and index of the star graph  $K_{1, n}$  is  $n$ , both bounds of above theorem are sharp.

### 2.1.1. DUTCH-WINDMILL GRAPHS

Here we consider another kind of point-attaching graphs and study their distinguishing number and distinguishing index. The dutch windmill graph  $D_n^k$  is the graph obtained by taking  $n$  ( $n \geq 2$ ) copies of the cycle graph  $C_k$  ( $k \geq 3$ ) with a vertex in common (see Figure 4). For  $k = 3$ , the graph  $D_n^3$  is called the friendship graph and is denoted by  $F_n$ . The distinguishing number and the distinguishing index of the friendship graph have been studied in [2]. The following theorem gives the distinguishing number and the distinguishing index of  $F_n$ .

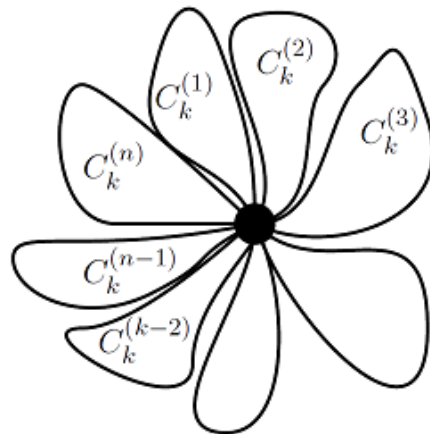
**Theorem 2.4.** [2]

- (i) The distinguishing number of the friendship graph  $F_n$  ( $n \geq 2$ ) is

$$D(F_n) = \lceil \frac{1 + \sqrt{8n + 1}}{2} \rceil.$$

- (ii) Let  $a_n = 1 + 27n + 3\sqrt{81n^2 + 6n}$ . For every  $n \geq 2$ ,

$$D'(F_n) = \lceil \frac{1}{3}(a_n)^{\frac{1}{3}} + \frac{1}{3(a_n)^{\frac{1}{3}}} + \frac{1}{3} \rceil.$$



**Figure 4.** Dutch windmill graph  $D_n^k$ .

To obtain the distinguishing number and the distinguishing index of the dutch windmill graph  $D_n^k$ , we first prove the following theorem:

**Theorem 2.5.** *The order of the automorphism group of  $D_n^k$  is  $|Aut(D_n^k)| = n!2^n$ .*

**Proof.** To obtain the automorphism group of  $D_n^k$ , let to denote the central vertex by  $w$  and the vertices of  $i$ -th cycle  $C_k$  (which we call it a blade) of  $D_n^k$  by  $V_i$  ( $1 \leq i \leq n$ ). The vertex  $w$  should be mapped to itself under automorphisms of  $D_n^k$ . In fact every element of the automorphism group of  $D_n^k$  is of the form

$$h_\sigma(v) = \begin{cases} f_1(v) & \text{if } v \in V_1 \\ \vdots \\ f_n(v) & \text{if } v \in V_n \end{cases}$$

where  $\sigma \in S_n$ . If we denote the vertices of  $i$ -th blade except the central vertex, by  $v_1^{(i)}, \dots, v_{k-1}^{(i)}$ , then every function  $f_i : V_i \rightarrow \sigma(V_i)$  has one of the following two forms:

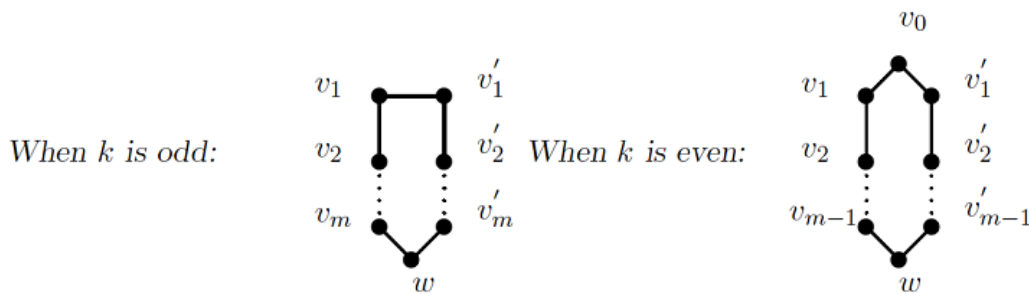
$$\begin{cases} v_1^{(i)} \mapsto v_1^{\sigma(i)} \\ v_2^{(i)} \mapsto v_2^{\sigma(i)} \\ \vdots \\ v_{k-1}^{(i)} \mapsto v_{k-1}^{\sigma(i)} \end{cases} \quad \begin{cases} v_1^{(i)} \mapsto v_{k-1}^{\sigma(i)} \\ v_2^{(i)} \mapsto v_{k-2}^{\sigma(i)} \\ \vdots \\ v_{k-1}^{(i)} \mapsto v_1^{\sigma(i)} \end{cases}$$

Therefore,  $|Aut(D_n^k)| = n!2^n$ . ■

**Theorem 2.6.** Let  $D_n^k$  be Dutch windmill graph such that  $n \geq 2$  and  $k \geq 3$ . Then we have

$$D(D_n^k) = \min\{r : \frac{r^{k-1} - r^{\lceil \frac{k-1}{2} \rceil}}{2} \geq n\}.$$

**Proof.** If  $k$  is odd, then there is a natural number  $m$  such that  $k = 2m + 1$ . We can consider a blade of  $D_n^k$  as in Figure 5.



**Figure 5.** The considered polygon (or a cycle of size  $k$ ) in the proof of Theorem 2.6.

Let  $(x_1^{(i)}, x_{1'}^{(i)}, \dots, x_m^{(i)}, x_{m'}^{(i)})$  be the label of vertices  $(v_1, v_{1'}, \dots, v_m, v_{m'})$  of the  $i$ -th blade where  $1 \leq i \leq n$ . Suppose

$$L = \{(x_1^{(i)}, x_{1'}^{(i)}, \dots, x_m^{(i)}, x_{m'}^{(i)}) \mid 1 \leq i \leq n, x_j^{(i)}, x_{j'}^{(i)} \in \mathbb{N}, 1 \leq j \leq m\}$$

is a labeling of the vertices of  $D_n^k$  except its central vertex. In an  $r$ -distinguishing labeling we must have: There exists  $j \in \{1, \dots, m\}$  such that  $x_j^{(i)} \neq x_{j'}^{(i)}$  for all  $i \in \{1, \dots, n\}$ . For  $i_1 \neq i_2$  we must have  $(x_1^{(i_1)}, x_{1'}^{(i_1)}, \dots, x_m^{(i_1)}, x_{m'}^{(i_1)}) \neq (x_1^{(i_2)}, x_{1'}^{(i_2)}, \dots, x_m^{(i_2)}, x_{m'}^{(i_2)})$  and

$$(x_1^{(i_1)}, x_{1'}^{(i_1)}, \dots, x_m^{(i_1)}, x_{m'}^{(i_1)}) \neq (x_{1'}^{(i_2)}, x_1^{(i_2)}, \dots, x_{m'}^{(i_2)}, x_m^{(i_2)}).$$

There are  $(r^{2m} - r^m)/2$  possible  $(2m)$ -arrays of labels using  $r$  labels satisfying (i) and (ii), hence  $D(D_n^k) = \min\{r : \frac{r^{2m} - r^m}{2} \geq n\}$ .

If  $k$  is even, then there is a natural number  $m$  such that  $k = 2m$ . We can consider a blade of  $D_n^k$  as in Figure 5. Let  $(x_0^{(i)}, x_1^{(i)}, x_{1'}^{(i)}, \dots, x_{m-1}^{(i)}, x_{m-1}^{(i)})$  be the label of vertices  $(v_0, v_1, v_{1'}, \dots, v_{m-1}, v_{m-1}')$  of  $i$ -th blade where  $1 \leq i \leq n$ . Suppose that  $L = \{(x_0^{(i)}, x_1^{(i)}, x_{1'}^{(i)}, \dots, x_{m-1}^{(i)}, x_{m-1}^{(i)}) \mid 1 \leq i \leq n, x_0^{(i)}, x_j^{(i)}, x_{j'}^{(i)} \in \mathbb{N}, 1 \leq j \leq m-1\}$  is a labeling of the vertices of  $D_n^k$  except its central vertex. In an  $r$ -distinguishing labeling there exists  $j \in \{1, \dots, m-1\}$  such that  $x_j^{(i)} \neq x_{j'}^{(i)}$  for all  $i \in \{1, \dots, n\}$ . For  $i_1 \neq i_2$  we must have

$$(x_0^{(i_1)}, x_1^{(i_1)}, x_{1'}^{(i_1)}, \dots, x_{m-1}^{(i_1)}, x_{m-1}^{(i_1)}) \neq (x_0^{(i_2)}, x_1^{(i_2)}, x_{1'}^{(i_2)}, \dots, x_{m-1}^{(i_2)}, x_{m-1}^{(i_2)}),$$

$$(x_0^{(i_1)}, x_1^{(i_1)}, x_{1'}^{(i_1)}, \dots, x_{m-1}^{(i_1)}, x_{m-1}^{(i_1)}) \neq (x_0^{(i_2)}, x_{1'}^{(i_2)}, x_1^{(i_2)}, \dots, x_{m-1}^{(i_2)}, x_{m-1}^{(i_2)}).$$

There are  $(r^{2m-1} - r^m)/2$  possible  $(2m-1)$ -arrays of labels using  $r$  labels satisfying (i) and (ii) ( $r$  choices for  $x_0$  and  $(r^{2(m-1)} - r^{m-1})/2$  choices for  $x_1^{(i_1)}, x_{1'}^{(i_1)}, \dots, x_{m-1}^{(i_1)}, x_{m-1}^{(i_1)}$ ), hence  $D(D_n^k) = \min\{r : \frac{r^{2m-1} - r^m}{2} \geq n\}$ . ■

**Corollary 2.7.** Let  $D_n^k$  be the dutch windmill graph such that  $n \geq 2$  and  $k \geq 3$ . If

$$k = 2m + 1, \text{ then } D(D_n^k) = \lceil \sqrt[m]{\frac{1 + \sqrt{8n + 1}}{2}} \rceil.$$

**Proof.** It is easy to see that  $\min\{r : \frac{r^{2m} - r^m}{2} \geq n\} = \lceil \sqrt[m]{\frac{1 + \sqrt{8n + 1}}{2}} \rceil$ . So the result follows from Theorem 2.6. ■

The following theorem implies that to study the distinguishing index of  $D_n^k$ , it suffices to study its distinguishing number and vice versa.

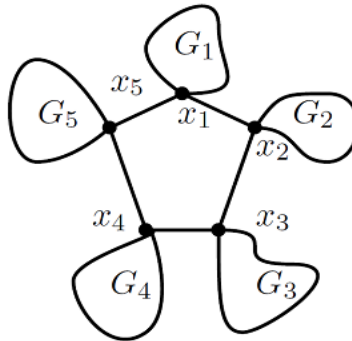


**Theorem 2.8.** Let  $D_n^k$  be the dutch windmill graph such that  $n \geq 2$  and  $k \geq 3$ . Then  $D'(D_n^k) = D(D_n^{k+1})$ .

**Proof.** Since the effect of every automorphism of  $D_n^{k+1}$  on its non-central vertices is exactly the same as the effect of an automorphism of  $D_n^k$  on its edges and vice versa, so if we consider the label of non-central vertices of  $D_n^{k+1}$  as the label of edges of  $D_n^k$  and vice versa, then we have  $D'(D_n^k) = D(D_n^{k+1})$ . ■

**2.2. CIRCUIT OF GRAPHS**

Let  $G_1, G_2, \dots, G_k$  be a finite sequence of pairwise disjoint connected graphs and let  $x_i \in V(G_i)$ . By definition, the circuit  $G$  of the graphs  $\{G_i\}_{i=1}^k$  with respect to the vertices  $\{x_i\}_{i=1}^k$  is obtained by identifying the vertex  $x_i$  of the graph  $G_i$  with the  $i$ -th vertex of the cycle graph  $C_k$  ([3]). See Figure 6 for  $k = 5$ .



**Figure 6.** A circuit of five graphs.

**Theorem 2.9.** Let  $G$  be circuit graph of the graphs  $\{G_i\}_{i=1}^k$  with respect to the vertices  $\{x_i\}_{i=1}^k$ . Then

- i)  $D(G) \leq \max\{\max\{D(G_i)\}_{i=1}^k, D(C_k)\}$
- ii)  $D'(G) \leq \max\{\max\{D'(G_i)\}_{i=1}^k, D'(C_k)\}$ .

**Proof.** It is known that  $D(C_k) = D'(C_k) = 3$  for  $k = 3, 4, 5$ , and  $D(C_k) = D'(C_k) = 2$  for  $k \geq 6$ .

(i) We label the vertices of  $C_k$  with the labels  $\{1, \dots, D(C_k)\}$  and vertices of every  $G_i$  ( $1 \leq i \leq k$ ) with the labels  $\{1, \dots, D(G_i)\}$  in a distinguishing way, respectively. This labeling is distinguishing for  $G$ , because if  $f$  is an automorphism of  $G$  preserving the labeling, then we have two following cases:

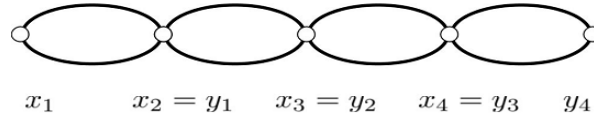
1. If the restriction of  $f$  to the set  $V(C_k)$  is  $V(C_k)$ , then for all  $i$  we have  $f|_{V(G_i)} = V(G_i)$ . Since we labeled  $C_k$  distinguishingly,  $f|_{V(C_k)}$  is the identity automorphism. In this case  $f$  is the identity automorphism on  $G$ , because each of  $G_i$  is labeled in a distinguishing way. We used  $\max\{\max\{D(G_i)\}_{i=1}^k, D(C_k)\}$  labels, and so the result follows.
2. Suppose that there exists the vertex  $x$  of  $C_k$  such that for some  $i$ ,  $f(x) = y$  where  $y \in V(G_i) \setminus V(C_k)$  and  $x \notin V(G_i)$ , then  $f(V(C_k)) \subseteq V(G_i)$ , i.e.,  $G_i$  contains a copy of  $C_k$ . The label of vertex  $y$  can be  $l \in \{1, \dots, D(G_i)\}$  and label  $x$  can be  $l' \in \{1, 2, 3\}$ . By assigning two different labels to  $x$  and  $y$  we get a distinguishing labeling.

(ii) A similar argument yields that  $D'(G) \leq \max\{\max\{D'(G_i)\}_{i=1}^k, D'(C_k)\}$ . In fact, we label the edges of  $C_k$  with the labels  $\{1, \dots, D'(C_k)\}$  and edges of every  $G_i$  ( $1 \leq i \leq k$ ) with the labels  $\{1, \dots, D'(G_i)\}$  in a distinguishing way, respectively. This labeling is distinguishing for  $G$ , because if  $f$  is an automorphism of  $G$  preserving the labeling, then we have two following cases:

1. If the restriction of  $f$  to the set  $V(C_k)$  is  $V(C_k)$ , then for all  $i$  we have  $f|_{V(G_i)} = V(G_i)$ . Since we labeled  $C_k$  distinguishingly,  $f|_{V(C_k)}$  is the identity automorphism. In this case  $f$  is the identity automorphism on  $G$ , because each of  $G_i$  is labeled in a distinguishing way. We used  $\max\{\max\{D'(G_i)\}_{i=1}^k, D'(C_k)\}$  labels, and so the result follows.
2. Suppose that there exists the vertex  $x$  of  $C_k$  such that for some  $i$ ,  $f(x) = y$  where  $y \in V(G_i) \setminus V(C_k)$  and  $x \notin V(G_i)$ , then  $f(V(C_k)) \subseteq V(G_i)$ , i.e.,  $G_i$  contains a copy of  $C_k$ . The label of the incident edges with vertex  $y$  can be  $l \in \{1, \dots, D'(G_i)\}$  and label of the incident edges with  $x$  can be  $l' \in \{1, 2, 3\}$ . By assigning two different sequences of labels to the incident edges with  $x$  and  $y$  we get a distinguishing labeling ■

**2.3. CHAIN OF GRAPHS**

Let  $G_1, G_2, \dots, G_k$  be a finite sequence of pairwise disjoint connected graphs and let  $x_i, y_i \in V(G_i)$ . By definition (see [9, 10]) the chain  $G$  of the graphs  $\{G_i\}_{i=1}^k$  with respect to the vertices  $\{x_i, y_i\}_{i=1}^k$  is obtained by identifying the vertex  $y_i$  with the vertex  $x_{i+1}$  for  $i \in [k - 1]$  (also see [3]). See Figure 7 for  $k = 4$ .



**Figure 7.** A chain of graphs.

**Theorem 2.10.** Let  $G$  be the chain of the graphs  $\{G_i\}_{i=1}^k$  with respect to the vertices  $\{x_i, y_i\}_{i=1}^k$ . Then

- i)  $D(G) \leq \max\{\max\{D(G_i)\}_{i=1}^k, \max\{\deg_G x_i\}_{i=2}^k\}$ ,
- ii)  $D'(G) \leq \max\{\max\{D'(G_i)\}_{i=1}^k, \max\{\deg_G x_i\}_{i=2}^k\}$ .

**Proof.** A shortest path between  $x_1$  and  $y_k$  is made by connecting shortest paths between  $x_i$  and  $y_i$  for  $i = 1, \dots, k$ . If  $f$  is an automorphism of  $G$ , then we have the two following cases:

- 1. There exists  $i$  ( $1 \leq i \leq k$ ) such that  $f(x_i) \neq x_i$ . Thus a shortest path between  $x_1$  and  $y_k$  is not fixed under  $f$ , and so  $f(x_1) = y_k$  or  $f(y_k) = x_1$ .
- 2. For all  $i$ ,  $f(x_i) = x_i$ , and so  $f(N_G(x_i)) = N_G(x_i)$ .

(i) Now we want to present a distinguishing vertex labeling for  $G$ . For this purpose we label the vertex  $x_1$  with label 1 and the vertex  $y_k$  with label 2, next we label all vertices adjacent to  $x_i$ , with  $\deg_G x_i$  different labels where  $i = 2, \dots, k$ . The remaining vertices of every  $G_i$  are labeled with labels  $\{1, \dots, D(G_i)\}$  in a distinguishing way, respectively. This labeling is distinguishing, because if  $f$  is an automorphism of  $G$  preserving the labeling then the two following cases may occur:

- (a) There exists  $i$  ( $1 \leq i \leq k$ ) such that  $f(x_i) \neq x_i$ . Thus by (a) we have  $f(x_1) = y_k$  or  $f(y_k) = x_1$ . Since we label the vertices  $x_1$  and  $y_k$  with two different labels, so this case can not occur.

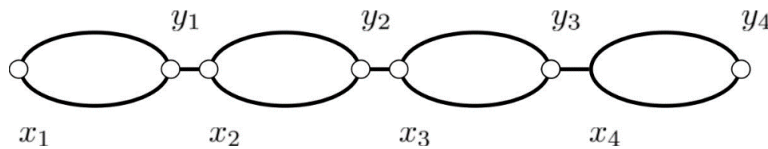
(b) For all  $i$ ,  $f(x_i) = x_i$ , and so by (b) we have  $f(N_G(x_i)) = N_G(x_i)$ . Since adjacent vertices to every  $x_i$  are labeled differently, so  $f|_{N_G(x_i)}$  is the identity automorphism. On the other hand since  $f(N_G[x_i]) = N_G[x_i]$ , hence  $f|_{V(G_i)} = V(G_i)$ , and thus  $f|_{V(G_i)}$  is the identity automorphism, because we labeled the vertices in  $\overline{N_{G_i}(x_i)}$  distinguishingly. Therefore  $f$  is the identity automorphism on  $G$ . Since

we used  $\max\{\max\{D(G_i)\}_{i=1}^k, \max\{\deg_G x_i\}_{i=2}^k\}$  labels, the Part (i) follows.

(ii) First we label all edges incident to  $x_1$  with label 1, and all edges incident to  $y_k$  with label 2. Next we label all edges incident to  $x_i$ , with  $\deg_G x_i$  different labels where  $i = 2, \dots, k$ . The remaining edges of every  $G_i$  are labeled with labels  $\{1, \dots, D'(G_i)\}$  in a distinguishing way, respectively. As Case (i) we can prove this labeling is distinguishing, and that  $D'(G) \leq \max\{\max\{D'(G_i)\}_{i=1}^k, \max\{\deg_G x_i\}_{i=2}^k\}$ . ■

**2.4. LINK OF GRAPHS**

Let  $G_1, G_2, \dots, G_k$  be a finite sequence of pairwise disjoint connected graphs and let  $x_i, y_i \in V(G_i)$ . By definition (see [5]), the link  $G$  of the graphs  $\{G_i\}_{i=1}^k$  with respect to the vertices  $\{x_i, y_i\}_{i=1}^k$  is obtained by joining by an edge the vertex  $y_i$  of  $G_i$  with the vertex  $x_{i+1}$  of  $G_{i+1}$  for all  $i = 1, 2, \dots, k - 1$  (see Figure 8 for  $k = 4$ ).



**Figure 8.** A link of graphs.

**Theorem 2.11.** *Let  $G$  be the link of the graphs  $\{G_i\}_{i=1}^k$  with respect to the vertices  $\{x_i, y_i\}_{i=1}^k$ . Then*

- (i)  $D(G) \leq \max\{D(G_i)\}_{i=1}^k$ ,
- (ii)  $D'(G) \leq \max\{D'(G_i)\}_{i=1}^k$ .

**Proof.** A shortest path between  $x_1$  and  $y_k$  is made by connecting shortest paths between  $x_i$  and  $y_i$  for  $i = 1, \dots, k$ , altogether the edges  $y_i x_{i+1}$  where  $i = 1, \dots, k-1$ . If  $f$  is an automorphism of  $G$ , then we have the two following cases:

1. There exists  $i$  ( $1 \leq i \leq k$ ) such that  $f(x_i) \neq x_i$ . Thus a shortest path between  $x_1$  and  $y_k$  is not fixed under  $f$ , and so  $f(x_1) = y_k$  or  $f(y_k) = x_1$ .

2. For all  $i$ ,  $f(x_i) = x_i$ , and so  $f(y_i) = y_i$ , and hence  $f(V(G_i)) = V(G_i)$ .

(i) Now we want to present a distinguishing vertex labeling for  $G$ . For this purpose we label the vertex  $x_1$  with label 1 and the vertex  $y_k$  with label 2. The vertices of every  $G_i$  are labeled with labels  $\{1, \dots, D(G_i)\}$  in a distinguishing way, respectively. This labeling is distinguishing, because if  $f$  is an automorphism of  $G$  preserving the labeling then the two following cases may occur:

(a) There exists  $i$  ( $1 \leq i \leq k$ ) such that  $f(x_i) \neq x_i$ . Thus by (a) we have  $f(x_1) = y_k$  or  $f(y_k) = x_1$ . Since we labeled the vertices  $x_1$  and  $y_k$  with two different labels, so this case can not occur.

(b) For all  $i$ ,  $f(x_i) = x_i$ , and so by (b) we have  $f(y_i) = y_i$  and  $f(V(G_i)) = V(G_i)$ . Hence  $f|_{V(G_i)}$  is the identity automorphism, because we labeled the vertices of each  $G_i$  distinguishingly. Therefore  $f$  is the identity automorphism on  $G$ . Since we used  $\max\{D(G_i)\}_{i=1}^k$  labels, the Part (i) follows.

(ii) We first label all edges incident to  $x_1$  with label 1, and all edges incident to  $y_k$  with label 2. The edges of every  $G_i$  are labeled with labels  $\{1, \dots, D'(G_i)\}$  in a distinguishing way, respectively. As Case (i) we can prove this labeling is distinguishing, and that  $D'(G) \leq \max\{D'(G_i)\}_{i=1}^k$ . ■

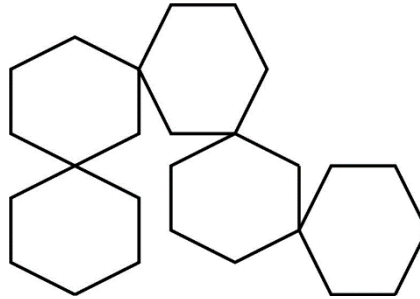
### 3. DISTINGUISHING LABELING OF GRAPHS THAT ARE OF IMPORTANCE IN CHEMISTRY

In this section, we apply the previous results in order to obtain the distinguishing number and the distinguishing index of families of graphs that are of importance in chemistry.

#### 3.1. SPIRO-CHAINS

Spiro-chains are defined in [4] page 114. Making use of the concept of chain of graphs, a spiro-chain can be defined as a chain of cycles. We denote by  $S_{q,h,k}$  the chain of  $k$  cycles

$C_q$  in which the distance between two consecutive contact vertices is  $h$  (see  $S_{6,2,5}$  in Figure 9, [3]).



**Figure 9.** Spiro-chain  $S_{6,2,5}$ .

**Theorem 3.1.** *The distinguishing number of spiro-chains is 2, except  $D(S_{3,1,2}) = 3$ .*

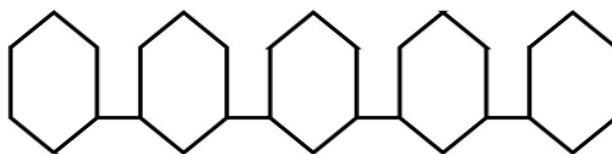
**Proof.** Since spiro-chains are as a chain of cycles, we follow the notation of attached vertices as denoted in the chain of graphs in Figure 7. We assign the vertex  $x_1$ , label 1, and the vertices  $y_1, \dots, y_k$ , label 2. Next we assign non-labeled vertices on path of length  $h$  between  $x_i$  and  $y_i$ , label 1 and assign the non-labeled vertices on path of length  $k - h$  between  $x_i$  and  $y_i$ , the label 2, where  $1 \leq i \leq k$ . This labeling is distinguishing, because with respect to the label of  $x_1$  and  $y_k$ , every  $C_k$  is mapped to itself. Now regarding to the label of vertices of each  $C_k$ , we can conclude that the identity automorphism is the only automorphism of  $G$  preserving the labeling. So  $D(G) = 2$ . It can be seen that  $S_{3,1,2}$  is friendship graph  $F_2$ , so  $D(S_{3,1,2}) = 3$  by Theorem 2.4. ■

**Theorem 3.2.** *The distinguishing index of spiro-chains is 2.*

**Proof.** We label the two edges incident to  $x_1$  with label 1, and the two edges incident to  $y_k$  with label 2. Next we assign non-labeled edges on path of length  $h$  between  $x_i$  and  $y_i$ , label 1 and assign the non-labeled edges on path of length  $k - h$  between  $x_i$  and  $y_i$ , label 2 where  $1 \leq i \leq k$ . Similar to the proof of Theorem 3.1, this labeling is distinguishing. So  $D'(G) = 2$ . ■

### 3.2. POLYPHENYLENES

Similar to the definition of the spiro-chain  $S_{q,h,k}$ , we can define the graph  $L_{q,h,k}$  as the link of  $k$  cycles  $C_q$  in which the distance between the two contact vertices in the same cycle is  $h$ . (See Figure 10 for  $L_{6,2,5}$ ).



**Figure 10.** Polyphenylenes  $L_{6,2,5}$ .

The following theorem shows that polyphenylenes can be distinguished by two labels.

#### Theorem 3.3.

- (i) The distinguishing number of polyphenylenes is 2.
- (ii) The distinguishing index of polyphenylenes is 2.

#### Proof.

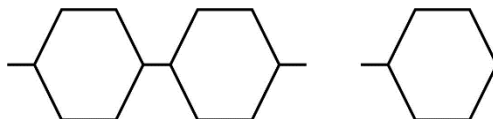
- (i) The proof is exactly similar to the proof of Theorem 3.1.
- (ii) Since polyphenylenes are as a link of cycles, we follow the notation of attached vertices as denoted in the link of graphs in Figure 7. We label the edge  $x_1y_1$  with label 1, and the edges  $x_2y_2, \dots, x_ky_k$  with label 2. Next we assign the non-labeled edges of every  $C_k$  on path of length  $h$  between  $x_i$  and  $y_i$ , label 1 where  $1 \leq i \leq k$ , and we label the rest of edges of  $C_k$  with label 2. It can be seen that this labeling is distinguishing. This proves that  $D'(G) = 2$ .

■

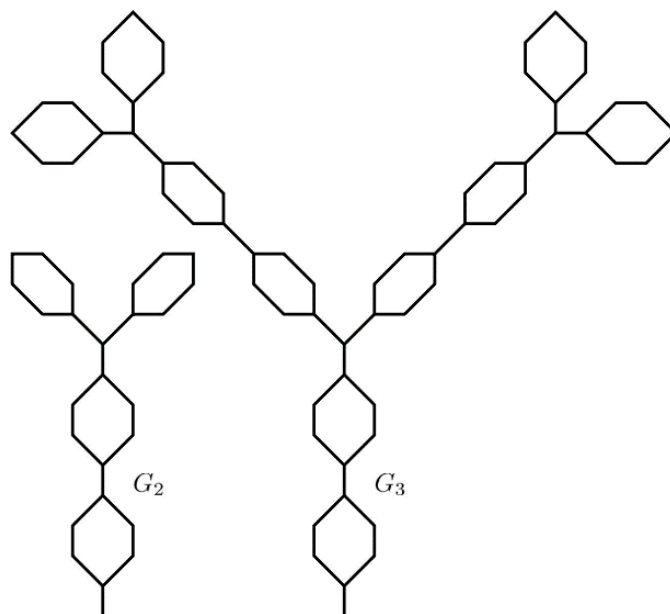
### 3.3. NANOSTAR DENDRIMERS

Dendrimers are large and complex molecules with well tailored chemical structures. These are key molecules in nanotechnology and can be put to good use. We intend to derive the distinguishing number and the distinguishing index of the nanostar dendrimer  $ND_k$  defined in [6]. In order to define  $ND_k$ , we follow [3]. First we define recursively an auxiliary family of rooted dendrimers  $G_k$  ( $k \geq 1$ ). We need a fixed graph  $F$  defined in Figure 11; we

consider one of its endpoint to be the root of  $F$ . The graph  $G_1$  is defined in Figure 11, the leaf being its root. Now we define  $G_k$  ( $k \geq 2$ ) as the bouquet of the following three graphs:  $G_{k-1}, G_{k-1}$ , and  $F$  with respect to their roots; the root of  $G_k$  is taken to be its unique leaf (see  $G_2$  and  $G_3$  in Figure 12). Finally, we define  $ND_k$  ( $k \geq 1$ ) as the bouquet of three copies of  $G_k$  with respect to their roots. See a nanostar dendrimer  $ND_n$  depicted in Figure 13.



**Figure 11.** The graphs  $F$  and  $G_1$ , respectively.



**Figure 12.** The graphs  $G_2$  and  $G_3$ , respectively.

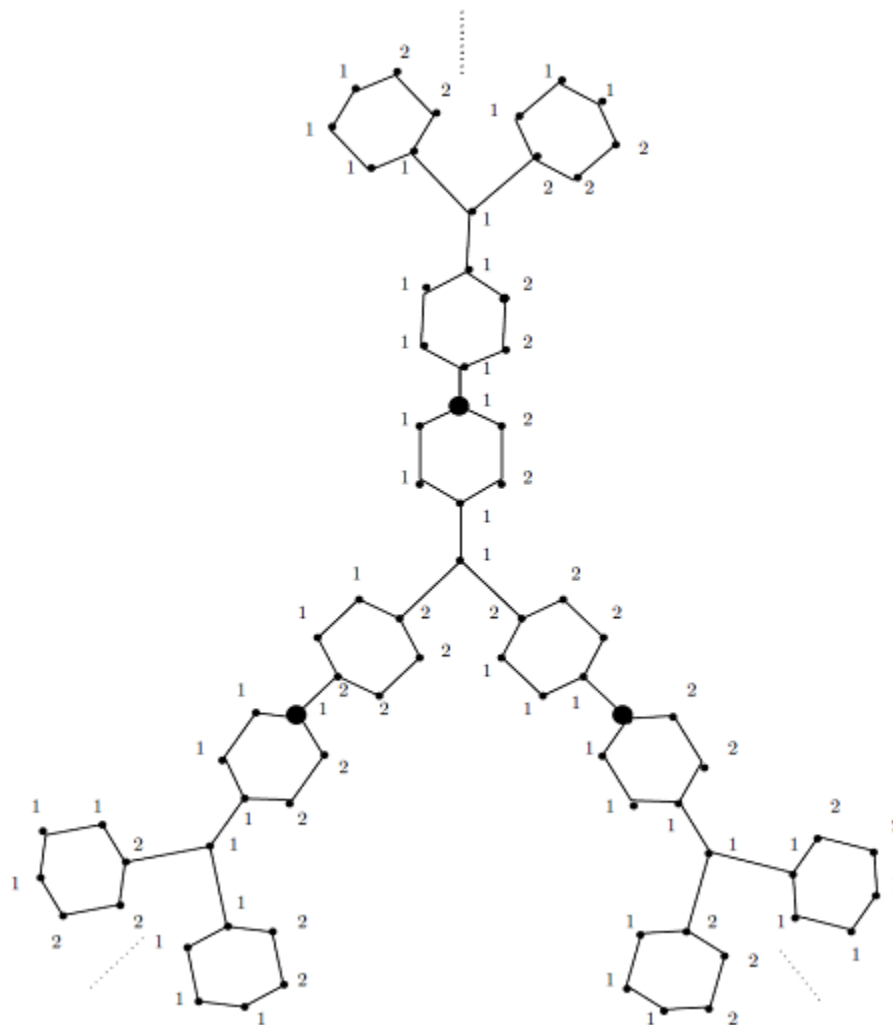
Here we compute the distinguishing number and the distinguishing index of this infinite class of dendrimers.

**Theorem 3.4.** *The distinguishing number and index of nanostar dendrimer graph is 2.*

**Proof.** Since the nanostar dendrimer graph is symmetric, i.e., the graph has a non-identity automorphism, so  $D(ND_n) > 1$ . In Figure 13, we presented a 2-labeling of vertices of  $ND_n$



Considering the automorphisms of  $ND_n$ , it can directly follow that the labeling is distinguishing. A similar argument also yields  $D'(ND_n) = 2$ . ■



**Figure 13.** The 2 -distinguishing labeling of vertices of  $ND_n$ .

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