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Anti–Forcing Number of Some Specific Graphs

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ABSTRACT

Let G be a simple connected graph. A perfect matching (or Kekulé structure in chemical language) of G is a set of disjoint edges which covers all vertices of G. The anti–forcing number of G is the smallest number of edges such that the remaining graph obtained by deleting these edges has a unique perfect matching and is denoted by $af(G)$. In this paper we consider some specific graphs that are of importance in chemistry and study their anti–forcing numbers.

1. INTRODUCTION

All graphs considered in this paper are undirected and simple. Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. A perfect matching or 1–factor (or Kekulé structure in chemical literature) of G is a set of disjoint edges which covers all vertices of G. Perfect matching has many practical applications, such as in dimer problem of statistical physics, Kekulé structures in organic chemistry and personnel assignment of operations research, etc. For more details on perfect matching, we refer the reader to see [8].

In 2007, Vukičević and Trinajstić [9,10] introduced the anti–forcing number of a graph G with perfect matching M. A set $S \subseteq M$ is called a forcing set of M if S cannot be contained in another perfect matching of G other than M. The forcing number (or innate degree of freedom) of M is defined as the minimum size of all forcing sets of M, denoted by $f(G,M)$ [5, 6]. The minimum forcing number of G is the minimum value of the

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forcing numbers of all perfect matchings of G, denoted by $f(G)$. Zhang et al. [11] proved that the minimum forcing number of fullerenes has a lower bound three and there are infinitely many fullerenes achieving this bound. For $S \subseteq E(G)$, let $G-S$ denote the graph obtained by removing S from G. Then S is called an anti–forcing set if $G-S$ has a unique perfect matching. The cardinality of a smallest anti–forcing set is called the anti–forcing number of G, denoted by $af(G)$. An edge e of G is called an anti–forcing edge if $G-e$ has a unique perfect matching. Note that $af(G)=|E(G)|$ if and only if G does not have any perfect matching. A graph G is called odd or even graph, if the number of vertices of G is odd or even, respectively.

Recently, Lei et al. [7] defined the anti–forcing number of a perfect matching M of a graph G as the minimal number of edges not in M whose removal to make M as a single perfect matching of the resulting graph, denoted by $af(G,M)$. By this definition, the anti–forcing number of a graph G is the smallest anti–forcing number over all perfect matchings of G.

In the next section, after computing the anti–forcing number of some specific graphs, the anti–forcing number of the link and the chain of graphs are discussed. Also we study the anti–forcing number of chain triangular cactus and chain square cactus as a special kind of the chain of graphs that are of importance in chemistry. In Section 3, we consider two graph operations, the join and the corona of two graphs and obtain some relations between the anti–forcing number of two graphs G_1 and G_2 and the anti–forcing number of the join and the corona of them under some suitable assumptions. Finally, in Section 4, we compute the anti–forcing number of some dendrimers.

2. ANTI–FORCING NUMBER OF SPECIFIC GRAPHS

In this section, we shall compute the anti–forcing number of some specific graphs. First we consider some certain graphs such as paths, cycles, wheels, friendship and Dutch–windmill graphs. The following example gives the anti–forcing number of path, cycle and wheel graphs.

Example 2.1 Let P_n, C_n and W_n be a path, cycle and wheel of order n, respectively. We have

$$af(P_n)=\begin{cases} n-1 & 2\nmid n \\ 0 & 2|n \end{cases},\quad af(C_n)=\begin{cases} n & 2\nmid n \\ 1 & 2|n \end{cases} \text{ and } af(W_n)=\begin{cases} 2(n-1) & 2\nmid n \\ 2 & 2|n \end{cases}.$$

As another specific graph, we consider friendship graph F_n which is a graph that can be constructed by coalescence n copies of the cycle graph C_3 with a common vertex. It is obvious that this graph does not have any perfect matching and so

$af(F_n)=|E(F_n)|=3n$. For the stars graphs $K_{1,n}$ there is no perfect matching, thus $af(S_n)=n$, for $n\geq 2$ and $af(K_{1,1})=0$. Also for the n–book graph B_n which can be constructed by joining n copies of the cycle graph C_4 with a common edge $\{u,v\}$, $af(B_n)=1$.

Let $Wd(k,n)$ be an undirected graph, constructed for $k\geq 2$ and $n\geq 2$ by joining n copies of the complete graph K_k at a shared vertex. We have $|V(G)|=(k-1)n+1$, $|E(G)|=1/2kn(k-1)$ (see [4]). We have the following theorem for the anti–forcing number of $Wd(k,n)$.

Theorem 2.2 $af(Wd(k,n))=\frac{1}{2}kn(k-1)$.

Proof. Suppose that n is even. Obviously, for every k, $Wd(k,n)$ is an odd graph and so the graph does not have any perfect matching. It implies that for every k, $af(Wd(k,n))=1/2kn(k-1)$. Now assume that n is odd, then for odd k, the order of $Wd(k,n)$ is odd too and hence the graph does not have any perfect matching. For even k, using Tutte's Theorem we have the same result. So we can conclude that $af(Wd(k,n))=1/2kn(k-1)$. ■

Here, we consider some graphs with specific construction that are of importance in chemistry and study their anti–forcing number. First we define the link of graphs.

Definition 2.3 [3] Let G_1, G_2, ..., G_k be a finite sequence of pairwise disjoint connected graphs and let $x_i, y_i \in V(G_i)$. 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 an edge the vertex y_i of G_i with the vertex x_{i+1} of G_{i+1} for all $i=1,2,...,k-1$ (see Figure 1 for $k=4$).

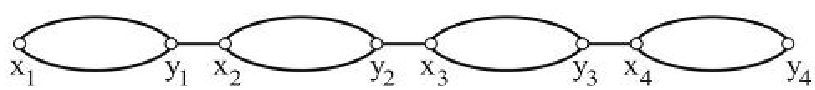

Figure 1: A link of four graphs.

Theorem 2.4 Let $L(G_1,G_2,...,G_k)$ be the link of k graphs $G_1,G_2,...,G_k$. If every G_i $(1\leq i\leq k)$ has perfect matching, then

$$af(L(G_1,G_2,...,G_k)) = \sum_{i=1}^{k} af(G_i).$$

Proof. It sufficies to prove the theorem for $k=2$. Let G_1 and G_2 be two graphs with perfect matching. Let $x_1 \in V(G_1)$, $x_2 \in V(G_2)$ and $L(G_1,G_2)$ be the link of these two graphs obtained by joining an edge the vertex x_1 with the vertex x_2. Suppose that S_1 and S_2 have the smallest cardinality over all anti–forcing sets of graphs G_1 and G_2, respectively. So $af(G_1) = |S_1|$ and $af(G_2) = |S_2|$. It is obvious that the edge x_1x_2 does not belong to any perfect matching of $L(G_1,G_2)$. So if S has the smallest cardinality over all anti–forcing sets of graph $L(G_1,G_2)$, then $S = S_1 \cup S_2$ and so,

$$af(L(G_1,G_2)) = |S| = |S_1| + |S_2| = af(G_1) + af(G_2),$$

which completes our argument. ■

Note that if there exist $1 \le i \le k$ such that G_i does not have any perfect matching, then Theorem 2.4 is not true. For example, $af(L(P_3,C_4,C_4)) = 12$, but $af(P_3) + 2af(C_4) = 4$. Now, we consider the chain of graphs and study the anti–forcing number of them for different cases.

Definition 2.5 [3] Let $G_1,G_2,...,G_k$ be a finite sequence of pairwise disjoint connected graphs and let $x_i, y_i \in V(G_i)$. 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 $1 \le i \le k-1$, see Figure 2 for $k=4$.

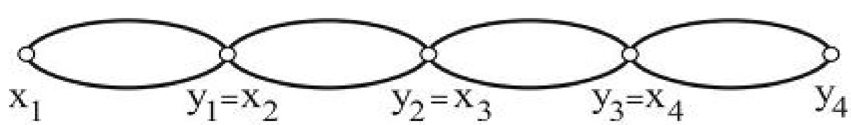

Figure 2: A chain of four graphs.

Theorem 2.6 Let $C(G_1,G_2,...,G_k)$ be the chain of k graphs $G_1,G_2,...,G_k$.

i. If $G_1,G_2,...,G_k$ are odd graphs, then $af(C(G_1,G_2,...,G_k)) = \sum_{i=1}^{k} |E(G_i)|$.

ii. If $G_1,G_2,...,G_k$ are even graphs, then for every even k we have

$$af(C(G_1,G_2,...,G_k)) = \sum_{i=1}^{k} |E(G_i)|.$$

Proof.

i. It can easily verified that $|V(C(G_1,G_2,...,G_k))|=\sum_{i=1}^{k}|V(G_i)|-(k-1)$. Thus in this case, for every k, $C(G_1,G_2,...,G_k)$ is an odd graph and so
$$af(C(G_1,G_2,...,G_k))=|E(C(G_1,G_2,...,G_k))|.$$
Since $|E(C(G_1,G_2,...,G_k))| = \sum_{i=1}^{k}|E(G_i)|$, we have the result.

ii. It is easy to see that in this case the chain graph $C(G_1,G_2,...,G_k)$ is an odd graph and so we have the result.

Hence the result. ■

Remark 2.7 Theorem 2.6(ii), is not true for odd k. For example, $af(C(P_2,P_4,P_2))=0$ and $af(C(P_2,P_4,C_4))=1$.

As special cases of chain graphs, we can consider cactus chains. A cactus graph is a connected graph in which no edge lies in more than one cycle. Consequently, each block of a cactus graph is either an edge or a cycle. If all blocks of a cactus G are cycles of the same size k, the cactus is k–uniform. A triangular cactus is a graph whose blocks are triangles, i.e., a 3–uniform cactus. A vertex shared by two or more triangles is called a cut–vertex. If each triangle of a triangular cactus G has at most two cut–vertices, and each cut–vertex is shared by exactly two triangles, we say that G is a chain triangular cactus. The number of triangles in G is called the length of the chain. An example of a chain triangular cactus is shown in Figure 3.

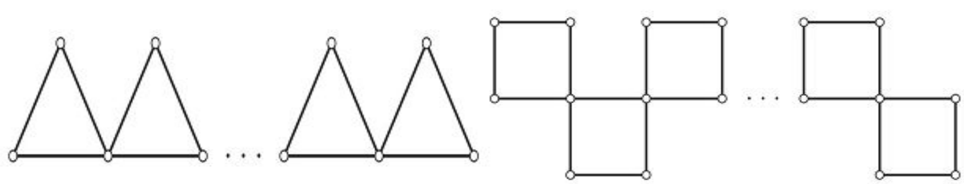

Figure 3:A chain triangular cactus T_n and square cactus O_n, respectively.

Obviously, all chain triangular cactus of the same length are isomorphic. Hence, we denote the chain triangular cactus of length n by T_n. clearly, a chain triangular cactus of length n has $2n+1$ vertices and $3n$ edges [1]. Since T_n does not have any perfect matching, we have $af(T_n)=3n$.

By replacing triangles in chain triangular chain T_n by cycles of length 4, we obtain cactus whose every block is C_4 as shown in Figure 3. We call such cactus, square cactus and denote a chain square cactus of length n by O_n [1].

Theorem 2.8 Let O_n be a chain square cactus. We have

I. If n is even, then $af(O_n) = 4n$.

II. If n is odd, then $af(O_n) = \frac{n+1}{2}$.

Proof.

I. By Tutte's Theorem, there is no perfect matching for O_n in this case and so $af(O_n) = 4n$.

II. For this case the anti–forcing number of O_n is equal with the anti-forcing number of $L(\underbrace{C_4,...,C_4}_{(\frac{n+1}{2})-times})$. Since $af(C_4) = 1$, so we have the result by Theorem 2.4.

This proves the theorem. ■

3. ANTI–FORCING NUMBER OF SOME OPERATIONS OF GRAPHS

In this section, we shall study the anti–forcing number of some operations of two graphs. First we consider the join of two graphs. The join $G_1 + G_2$ of graphs G_1 and G_2 with disjoint point sets $V(G_1)$ and $V(G_2)$ and edge sets $E(G_1)$ and $E(G_2)$ is the graph union $G_1 \cup G_2$ together with all the edges joining $V(G_1)$ and $V(G_2)$. The following theorem gives a lower bound for the anti–forcing of join of two graphs.

Theorem 3.1 Let G_1 and G_2 be two simple graphs. Then we have

$$af(G_1 + G_2) \geq af(G_1) + af(G_2).$$

Proof. Suppose that S_1, S_2 and S have the smallest cardinality over all anti–forcing sets of graphs G_1, G_2 and $G_1 + G_2$, respectively. So $af(G_1) = |S_1|$, $af(G_2) = |S_2|$ and $af(G_1 + G_2) = |S|$. By definition of $G_1 + G_2$, $|V(G_1 + G_2)| = |V(G_1)| + |V(G_2)|$ and $|E(G_1 + G_2)| > |E(G_1)| + |E(G_2)|$. Thus for the choosing the perfect matchings of $G_1 + G_2$, we have more possibilities than the number of perfect matching of G_1 plus the number of perfect matchings of G_2. It means that $|S| \geq |S_1| + |S_2|$ and so we have the result. ■

Remark 3.2 The lower bound in Theorem 3.1 is sharp. For example $af(C_3+C_3)=6=af(C_3)+af(C_3)$. Also, if G_1 is an odd graph and G_2 is an even graph, then

$$af(G_1+G_2)>af(G_1)+af(G_2).$$

Because for odd graph G_1, we have $af(G_1)=|E(G_1)|$ and for even graph G_2, $af(G2)\leq|E(G2)|$. Also G_1+G_2 is an odd graph. So

$$af(G1+G2)=|E(G1+G2)|>|E(G1)|+|E(G2)|\geq af(G1)+af(G2).$$

Here, we consider the corona of two graphs and then we study the anti–forcing number of them. We recall that the corona of two graphs G_1 and G_2, written as $G_1\circ G_2$, is the graph obtained by taking one copy of G_1 and $|V(G_1)|$ copies of G_2, and then joining the *i*-th vertex of G_1 to every vertex in the *i*-th copy of G_2.

Theorem 3.3 Let G_1 and G_2 be two simple graphs. If both of G_1 and G_2 have perfect matching, then

$$af(G_1\circ G_2)=af(G_1)+|V(G_1)|\,af(G_2).$$

Proof. Suppose that S_1 and S_2 have the smallest cardinality over all anti–forcing sets of graphs G_1 and G_2, respectively. So $af(G_1)=|S_1|$ and $af(G_2)=|S_2|$. Let $V(G_1)=\{x_1,x_2,...,x_n\}$ and $V(G_2)=\{y_1,y_2,...,y_m\}$. For every $1\leq i\leq n$ and every $1\leq j\leq m$, the edge x_iy_j cannot be in the perfect matchings of $G_1\circ G_2$. Let S has the smallest cardinality over all anti–forcing sets of graph $G_1\circ G_2$. Then

$$S=S_1\cup\underbrace{S_2\cup...\cup S_2}_{|V(G_1)|-times}$$

and we have

$$af(G_1\circ G_2)=|S|=|S_1|+|V(G_1)||S_2|=af(G_1)+|V(G_1)|\,af(G_2).$$

This completes the proof. ■

Clearly, If G_1 has a unique perfect matching, then $af(G_1\circ G_2)=|V(G_1)|\,af(G_2)$ and if G_2 has a unique perfect matching, then $af(G_1\circ G_2)=af(G_1)$. For example $af(C_4\circ P_2)=1$ and $af(P_2\circ C_4)=2$.

Now this question comes to mind: what happens to the anti–forcing number of graph $G_1 o G_2$, when at least one of the G_1 or G_2 does not have any perfect matching? It can easily verified that if only G_1 does not have any perfect matching, then the graph $G_1 o G_2$ does not have any perfect matching too and so $af(G_1 o G_2)=|E(G_1 o G_2)|$. But if G_2 does not have perfect matching, then the anti–forcing number of $G_1 o G_2$ just depends on G_2, because assume that $u\in V(G_1)$ and $(G_2)_u$ be a copy of G_2 such that the vertex u is adjacent to every vertex of $(G_2)_u$. Since G_2 does not have any perfect matching, then it has at least one unsaturated vertex. Without loss of generality we can suppose that $v \in V((G_2)_u)$ is the unsaturated vertex of $(G_2)_u$. Then $uv \in M$ where M is a maximum matching of graph $G_1 o G_2$. Thus every vertex of G_1 in M is saturated by the edges that connect G_1 with G_2. In the following propositions, we consider the anti–forcing number of $G_1 o G_2$, when G_2 is a path, cycle or wheel of odd order n, respectively.

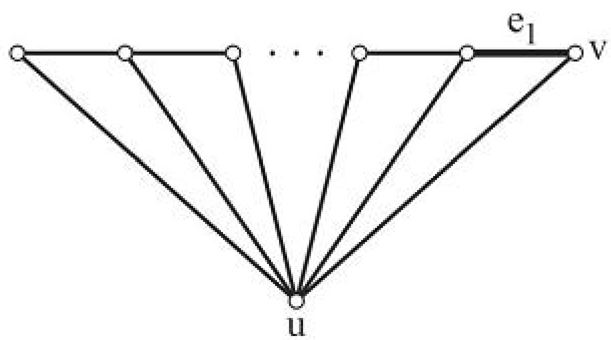

Figure 4: The $K_1 \circ P_n$ in the proof of Proposition 3.4.

Proposition 3.4 Let G be a simple graph and P_n a path of odd order n. We have

$$af(G \circ P_n) = |V(G)|.$$

Proof. Let $u \in V(G)$ and $(P_n)_u$ be a copy of P_n with the vertex set $\{v_1,...,v_n\}$ such that the vertex u is adjacent to all vertices of $(P_n)_u$. It can easily verified that if v is one of the vertices in the set $\{v_1, v_3,...,v_n\}$, then the edge uv belongs to a perfect matching of graph $G \circ P_n$. Since $P_n - v$ has unique perfect matching and there exist (n+1)/2 ways to choose vertex $v \in V(P_n)$, so we can conclude that the number of perfect matchings of $K_1 \circ P_n$ is equal to (n+1)/2. Also n is odd and so the perfect matching of $G \circ P_n$ does not related to the perfect matching of G. Thus the number of perfect matchings of $G \circ P_n$ is equal to $[(n+1)/2]^{|V(G)|}$. Let $S = \{e_1\}$ (see Figure 4). Then S has the smallest cardinality over all anti–forcing sets of graph $K_1 \circ P_n$. So for each odd n, we have $af(K_1 \circ P_n) = 1$. Obviously, the number of graphs $K_1 \circ P_n$ is equal to $|V(G)|$ and this implies the result. ■

Proposition 3.5 Let G be a simple graph and C_n be a cycle of odd order n. We have

$$af(G \circ C_n) = 2|V(G)|.$$

Proof. Let $u \in V(G)$ and $(C_n)_u$ be a copy of C_n such that the vertex u is adjacent to every vertex of $(C_n)_u$. Suppose that $v \in V((C_n)_u)$ and uv belongs to one of the perfect matchings of graph $G \circ C_n$. Since $C_n - v = P_{n-1}$, so $C_n - v$ has an unique perfect matching. Also to choose vertex $v \in V(C_n)$ we have n possibilities. Note that since n is odd, thus the perfect matching of $G \circ C_n$ does not related to the perfect matching of G and we can conclude that the number of perfect matchings of $G \circ C_n$ is equal to $n^{|V(G)|}$. Let $S = \{e_1, e_2\}$ be as shown in Figure 5. Clearly, S has the smallest cardinality over all anti–forcing sets of graph $K_1 \circ C_n$. So for every odd n, we have $af(K_1 \circ C_n) = 2$. Also the number of graphs $K_1 \circ C_n$ is equal to $|V(G)|$. So we have the result. ∎

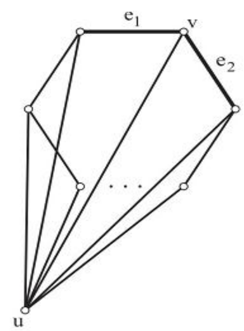

Figure 5: The graph with $S = \{e_1, e_2\}$ in the proof of Proposition 3.5.

Proposition 3.6 Let G be a simple graph and W_n a wheel of odd order n. We have

$$af(G \circ W_n) = 4|V(G)|.$$

Proof. Let $u \in V(G)$ and $(W_n)_u$ be a copy of W_n such that u is adjacent to every vertex of $(W_n)_u$. Suppose that $v \in V((W_n)_u)$ and uv belongs to one of the perfect matchings of graph $G \circ W_n$. If $v \in C_{n-1}$, then to choose other edges of perfect matching of $K_1 \circ W_n$, we have (n−1)/2 possibilities and if $v \in K_1$, then there exist two possibilities to choose other edges of perfect matching of $K_1 \circ W_n$. Since n is odd, so the perfect matching of $G \circ W_n$ does not related to the perfect matching of G. Also C_{n-1} have $n-1$ vertices. Thus to choose perfect matching of $G \circ W_n$, we have $[1/2(n-1)^2 + 2]^{|V(G)|}$ possibilities. Let $S = \{e_1, e_2, e_3, e_4\}$ as shown in Figure 6. Observe that S has the smallest cardinality over all anti–forcing sets of graph $K_1 \circ W_n$. Then for every odd n, $af(K_1 \circ W_n) = |S| = 4$ and we can conclude that $af(G \circ W_n) = 4|V(G)|$.

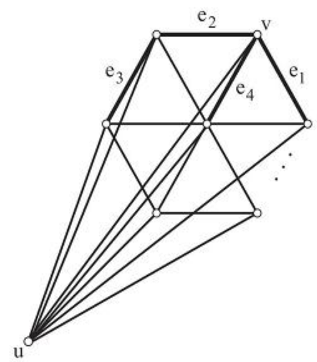

Figure 6: The graph with $S = \{e_1, e_2, e_3, e_4\}$ in the proof of Proposition 3.6.

4. ANTI–FORCING NUMBER OF SOME DENDRIMERS

Dendrimers are hyper–branched macromolecules, with a rigorously tailored architecture. They can be synthesized, in a controlled manner, either by a divergent or a convergent procedure. Dendrimers have gained a wide range of applications in supra–molecular chemistry, particularly in host guest reactions and self–assembly processes. Their applications in chemistry, biology and nano–science are unlimited [2].

In this section, we shall find the anti–forcing number of certain polyphenylene dendrimers. First we obtain the anti–forcing number of the first kind of dendrimer of generation 1–3 that has grown n stages.We denote this graph by $D_3[n]$. Figure 7 shows the first kind of dendrimer of generation 1–3 has grown 3 stages $D_3[n]$. Also we shall study the anti–forcing number of the first kind of dendrimer which has grown n steps denoted $D_1[n]$. Figure 7 shows $D_1[4]$. Note that there are three edges between each two cycle C_6 in this dendrimer.

Theorem 4.1

(i) Let $D_3[n]$ be a kind of dendrimer of generation 1–3 that has grown n stages. Then $af(D_3[n]) = 3 \times 2^{n+4} - 24.$

(ii) Let $D_1[n]$ be a kind of dendrimer that has grown n stages. Then $af(D_1[n]) = 9 \times 2^{n+1} - 11.$

Proof.

(i) It follows from Tutte's Theorem.

(ii) It can be observe that from Figure 7 that $D_1[n]$ is an odd graph. So $af(D_1[n]) = |E(D_1[n])| = 25 + \sum_{i=1}^{n-1} (18 \times 2^i).$

This completes our argument. ■

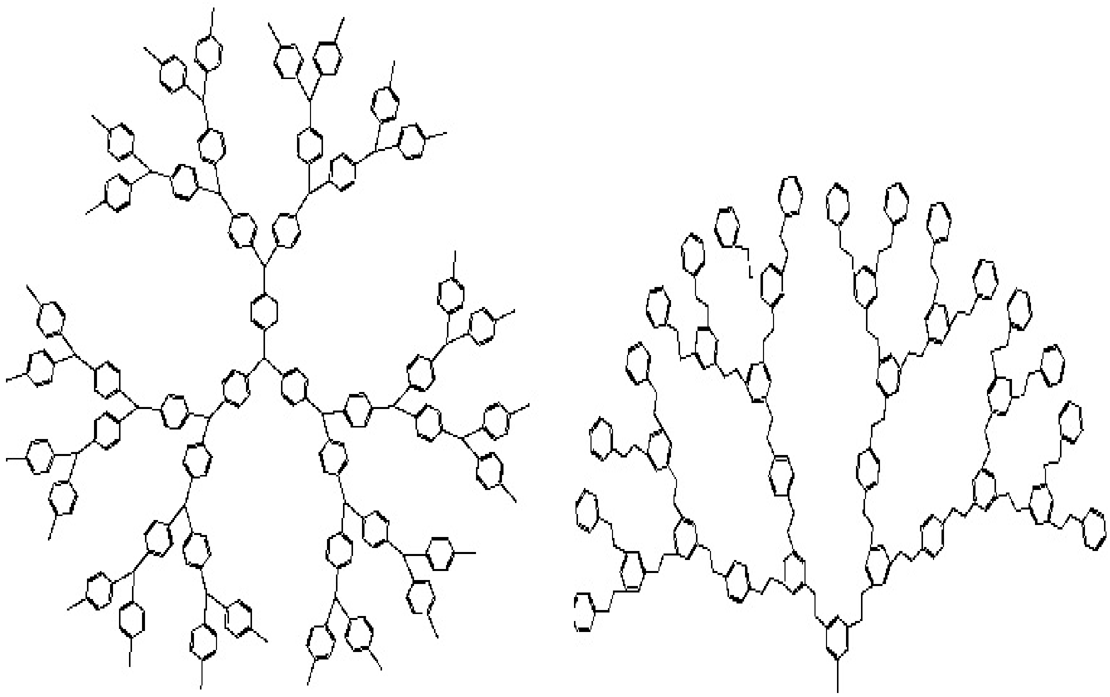

Figure 7: The dendrimers $D_3[3]$ and $D_1[4]$, respectively.

Finally we consider another type of polyphenylene dendrimer by construction of dendrimer generations G_n that has grown n stages. We simply denote this graph by $PD_2[n]$. Figure 8 shows the generations G_3 that has grown 3 stages.

Theorem 4.2 Let $PD_2[n]$ be a type of polyphenylene dendrimer by construction of dendrimer generations G_n that has grown n stages. Then we have

$$af(PD_2[n]) = 2 + \sum_{i=1}^{n}(5\times 2^{i+1}).$$

Proof. As you see in Figure 8,

$$PD_2[n] = L(\underbrace{C_6, C_6, \ldots, C_6}_{(2+\sum_{i=1}^{n}5\times 2^{i+1})-times}).$$

Now the result follows from Theorems 2.1 and 2.4. ■

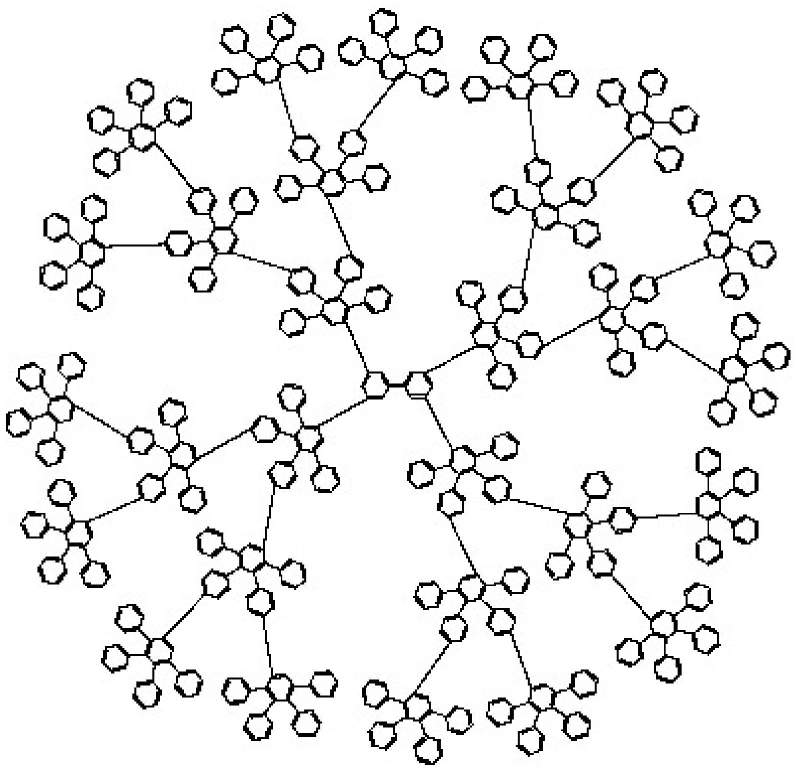

Figure 8: Polyphenylene dendrimer of generations G_3 that has grown 3 stages.

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