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Complete forcing numbers of catacondensed phenylene systems

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Abstract. Combining "forcing" and "global" idea, Xu et al. proposed the concepts: complete forcing set and complete forcing number of perfect matchings of graph. In this paper, we give explicit formulae for the complete forcing numbers of phenylene chains and catacondensed phenylene systems, respectively. Moreover, we present an algorithm to find the minimum complete forcing sets of these graphs.

1. Introduction

The root of the concept of "forcing set" can be traced back to the study of resonance structures in mathematical chemistry where it was introduced under the name of the innate degree of freedom[10, 15], and "forcing" has been applied in many research fields, such as graph theory and combinatorial mathematics [4, 6, 13]. Harary et al. first applied the idea of "forcing" to perfect matching [8]. Subsequently, global forcing set, global forcing number, complete forcing set and complete forcing number of perfect matchings of graph has been proposed and studied by scholars.

Forcing edge and forcing number were first proposed by Harary et al. in 1991, they studied the forcing number and perfect matching vector of perfect matching of polyhex (also known as the hexagonal system) [8]. The roots of these concepts can be traced back to 1985-1987, Randić and Klein's research, where the forcing number was introduced under the name of "innate degree of freedom" of a Kekulé structure (namely, a perfect matching of graph in mathematics), which plays an important role in the resonance theory of chemistry [10, 15]. In the past two decades, more and more scholars have studied forcing set (including forcing edges, forcing faces, etc.) and forcing numbers of graphs. The scope of graphs considered has been expanded from hexagonal system to all kinds of bipartite graphs and non-bipartite graphs. In 1998, Pachter and Kim studied a class of bipartite graphs with cyclic packing property and proved that the forcing number of any perfect matching M in such graphs, it can be obtained by calculating the maximum numbers of disjoint M-alternating cycles [14]. In 2002, Riddle used the trailing vertex method gave the lower bound of the forcing number of bipartite graphs [16]. Zhang et al. extensively studied the plane elementary bipartite

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graph and generalized many important results in hexagonal system to plane elementary bipartite graph. In particular, they extended the concept of forced edge of hexagonal system to connected plane bipartite graph. Furthermore, the concept of Z-transformation graph was extended to planar bipartite graphs, which plays an important role in studying the forcing edges and forcing faces of planar bipartite graphs including hexagonal systems [24]. For the study of forcing numbers of perfect matchings of non-bipartite graphs, Zhang et al. studied the forcing numbers of perfect matchings of non-bipartite fullerene graphs in 2010 [25]. On the basis of previous studies [25], in 2021, Shi et al. found a special fullerene graph F_{24} with a minimum forcing number of 2. By means of construction, they described all fullerenes graphs with forcing number 3 [17].

Forcing set and forcing number of perfect matching of graph are defined from "local", that is, by a particular perfect matching of graph. In 2004, Vukičecić and Sedlar introduced the concept of "global" from the perspective of all perfect matchings of graph, proposed the concepts of total forcing set and total forcing number of perfect matching of graph [18]. In 2007, Vukičecić and Došlić introduced equivalent definitions of total forcing set and total forcing number: global forcing set and global forcing number of perfect matchings of graph. Methods to calculate the global forcing numbers of perfect matchings of two kinds of composite graph, grid graph and complete graph were given [19]. On the research of Došlić [19], in 2012, Cai and Zhang improved some results of Došlić, and obtained the global forcing number of catafused coronoid containing n hexagons is n or $n-1$. In addition, by some properties of nice cycle and nice subgraph, they cleverly solved some open problems proposed by Došlić [1]. In 2014, Liu and Xu et al. studied the global forcing numbers of perfect matchings of handgun-shaped benzenoid systems and their calculation formulae [11]. Furthermore, in 2018, Vukičecić and Zhao et al. extended the concept of global forcing number and global forcing set to maximal matchings of graph, and obtained some results similar to perfect matchings. The upper and lower bounds of global forcing numbers for maximal matchings of graph were given. The global forcing numbers of maximal matchings of trees and complete graphs were given respectively [20].

Combining "forcing" and "global forcing" ideals, in 2015, Xu et al. proposed the new concepts complete forcing set and complete forcing number of perfect matchings of graph. Using properties of nice cycle, they gave sufficient and necessary condition of an edge subset to be a complete forcing set. They researched complete forcing numbers and complete forcing sets of perfect matchings of hexagonal chain and catacondensed hexagonal system respectively. The exact formulae for calculating the complete forcing numbers of those two kinds graphs are given, and the method for finding the minimum complete forcing set was also given [21].

Based on the above research [21], using similar methods, Xu et al. presented an expression to calculate complete forcing numbers and a method to find the minimum complete forcing set of perfect matchings of primitive coronoids [22]. Motivated by the study of Xu [21], Chan et al. proved the linear relationship between the complete forcing number and Clar number of catacondensed hexagonal system. They also gave a linear time algorithm for calculating the complete forcing number of perfecting matchings and clar number of catacondensed hexagonal system [3].

Recently, Liu and Bian et al.(2021) studied complete forcing number of perfect matchings of spiro hexagonal system, gave its calculating formula, and obtained some inequality relations of global forcing number of spiro hexagonal system [12]. Subsequently, in 2021, Xue and Bian et al. researched minimum complete forcing set and complete forcing number of perfect matchings of random multiple chains, and provided a method to find the minimum complete forcing set [23]. In 2021, He and Zhang used elementary edge-cut cover and graph decomposition obtained the upper bound and lower bound of complete forcing numbers of perfect matchings of general hexagonal systems respectively. And used those methods, they got some formulas for complete forcing numbers of hexagonal systems [9]. Chang et al. (in 2021) discussed the complete forcing number of perfect matchings of rectangular polynominoes (grid), and gave the calculation formula of complete forcing number that related to its length [2].

This paper is organized as follows. In the next section, we will give preliminary knowledge and conclusion concerning complete forcing set and complete forcing number of perfect matchings of graph. In section 3, we will give explicit formulas of the complete forcing numbers of phenylene chains. In section 4, we will give an explicit formula for the complete forcing numbers of catacondesed phenylene systems.

2. Preliminaries

A *hexagonal system* is a connected graph without cut vertices embedded into the regular hexagonal lattice in plane, and in which all inner faces are regular hexagons. A hexagonal system is *catacondensed* if there no three hexagons sharing one common vertex.

Let H be a catacondensed hexagonal system. A hexagon r of H has one neighbouring hexagon, then it is said to be *terminal*, and if it has three neighbouring hexagons, to be *branched*. A hexagon r being adjacent to exactly two other hexagons is *kink* if r possess two adjacent vertices of degree 2, and is linear otherwise. A catacondensed hexagonal system with no branched hexagon is said to be a *hexagonal chain*. A hexagonal chain with no kinks is said to be a *linear chain*. The number of hexagons in hexagonal chain is called its *length*. An edge is *shared* if it contained in two hexagons.

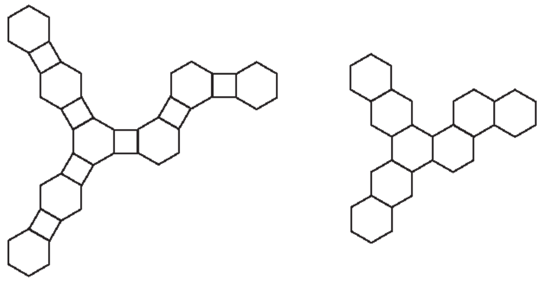

Fig. 1: A phenylene system and its squeeze.

Let G be a catacondensed hexagonal system with at least two hexagons. If we add quadrilaterals (face where boundary is a 4-cycle) between all pair of adjacent hexagons of G obtained graph $G^{'}$ is called *phenlene syetem*. We say that G is the *hexagonal squeeze* of $G^{'}$. A phenylene system containing n hexagons is called an $[n]$-phenylene system. Clearly, there is one to one correspondence between a phenylene system and its hexagonal squeeze, both possesses the same number of hexagons, see Fig.1. A phenylene system with n hexagons possess $n-1$ squares.

A *perfect matching* (or 1-factor) of G is a set of independent edges of G covering all vertices of G. An edge of G is *termed allowed* if it lies in some perfect matching of G and forbidden otherwise. A graph G is said to be *elementary* if all its allowed edges form a connected subgraph of G.

The boundary of a finite face of G is called a *ring* if it is a cycle of G. A cycle C of G is called *M-alternating* if the edges of C appear alternately in M and $E(G)\backslash M$. A face f of G is said to be *resonant* if G has a perfect matching M such that the boundary of f is an M alternating cycle. The *symmetric difference* of two finite set M_1 and M_2 is defined by $M_1 \oplus M_2 = (M_1 \cup M_2)\backslash(M_1 \cap M_2)$.

A subgraph H of G is said to be *nice* if $G - V(H)$ has a perfect matching. Let G be a bipartite graph with a perfect matching M and a cycle C. If the edges of C appear alternating in M and $E(G)\backslash M$, then we say that C is an M-alternating cycle. It is obvious that a cycle of G is nice if and only if there is a perfect matching M of G such that C is an M-alternating cycle. If M_1 and M_2 are two different perfect matchings, then the symmetric difference $M_1 \oplus M_2$ consists of mutually disjoint (M_1, M_2)-alternating cycles. Let G be a plane bipartite graph and C the boundary of a face f of G. If G has a perfect matching M such that C is an M-alternating cycle, then C and f will be called an *M-resonant cycle* and *face*, respectively. That is, a face is resonant if and only if the boundary of it is a nice cycle.

Let G be a graph with edge set $E(G)$ that admit a perfect matching M. A *forcing set* of M is a subset of M contained in no other perfect matchings of G. The minimum cardinality of forcing sets of M is called *forcing number* (or innate degree of freedom) of M. The sum of forcing numbers over all perfect matchings of G is called the degree of freedom of G, denoted by $df(G)$. Forcing set and forcing number of perfect matchings of a graph G with edge set $E(G)$ are defined by the "local" approach, i.e., defined with respect to a particular perfect matching of G. The concept of *global forcing set* of G from the "global" point of view, i.e., concerning all perfect matching instead of a particular perfect matching, which is defined as a subset S of $E(G)$ on which there no two distinct perfect matching coinciding. The minimum cardinality of global forcing sets of G is called *the global forcing number* of G, denoted by $gf(G)$. Combing the above "forcing" and "global" ideals, Xu et al. introduced and defined a *complete forcing set* of G as a subset of $E(G)$ on which the restriction of any perfect matching M of G is a forcing set of M. The minimum cardinality of complete forcing sets is *the complete forcing number* of G, denoted by $cf(G)$.

As an illustrative example, we consider K_4 shown in Fig.2. K_4 contains three different perfect matching: $M_1 = \{e_1, e_4\}$, $M_2 = \{e_2, e_5\}$, $M_3 = \{e_3, e_6\}$. It is easy to say that the restriction of every perfect matching M on $S = \{e_1, e_2, e_3\}$ is a forcing set of M. Since every complete forcing set contains at least one edge of every perfect matching of K_4, S is a complete forcing set with the minimum cardinality. Hence, $cf(G) = 3$. It can be see that only one edge is taken from each of the three set M_1, M_2, M_3 to form a set, which are all complete forcing set with minimum cardinality. The intersection of every perfect matching of K_4 with set $S_1 = \{e_1.e_2\}$ are not equal. It is easy to verify that S_1 is one of the minimum set with this property. Then S_1 ia a global forcing set with the minimum cardinality, $gf(G) = 2$. It can be seen that from any two sets of three sets M_1, M_2, M_3, only one edge is taken respectively to from a set with cardinality 2, which are all global forcing sets with minimum cardinality.

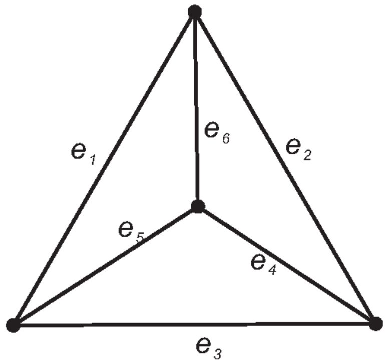

Fig. 2: The complete graph K_4.

Corollary 2.1. *[24] Let G be a plane elementary bipartite graph with a perfect matching M and C be an M-alternating cycle. Then there exists an M-resonant face in the interior of C.*

Theorem 2.2. *[21] Let G be a graph with edge set E(G) and M be a perfect matching of G. Then $S \subseteq E(G)$ is a complete forcing set of G if and only if for any nice cycle C of G, the intersection of S and each-type-edges of C is nonempty.*

3. Complete forcing number of phenylene chain

Lemma 3.1. *Let G be a catacondensed phenylene system with a cycle C, and M be a perfect matching of G. Suppose that $M(C)$ are one type-edges of C. Then there exists a hexagon h or a square s contained in C such that $M(C) \cap E(h)$ are one type-edges of h, or $M(C) \cap E(s)$ are one type-edges of s.*

Proof. We know that every edge of $E(G)$ is allowed, and catacondensed phenylene system G is a bipartite graph, then G is a plane elementary bipartite graph. G has perfect matching. For any cycle C of G is an even cycle, there exists a perfect matching M such that C is an M-alternating cycle. Let $M(C)$ be one type-edges of C. From Corollary 2.1, there exists an M-resonant face hexagon h or square s contained in C, such that $M(C) \cap E(h)$ are one type-edges of h, or $M(C) \cap E(s)$ are one type-edges of s.

Theorem 3.2. *Let G be a catacondensed phenylene system with edge set E(G). Then $S \subseteq E(G)$ is a complete forcing set of G if and only if S has a nonempty intersection with either of two type-edges of each hexagon h and square s in G.*

Proof. We known that every hexagon and square in catacondensed phenylene system G is nice. From Theorem 2.2, the necessity is obvious. Next, we prove the sufficiency.

Suppose that M is a perfect matching of G and $S \subseteq E(G)$ has a nonempty intersection with either of two type edges of each hexagon h and square s in G. From Theorem 2.2, we show that for any nice cycle C of G, S has a nonempty intersection with either of two type-edges of C, say $M(C)$, $S \cap M(C) \neq \emptyset$. From Lemma 3.1, C contain a face f (hexagon or square) is one of two type-edges of the boundary of f. According to the definition of set S, S has a nonempty intersection with either two type-edges of each hexagon and square of G. From Theorem 2.2, the sufficiency has proved. □

Let G be a catacondensed phenylene system with hexagon h, the shared edges in a kink hexagon h or a branched hexagon h belong to one common type-edge of h, while the two shared edges in a linear hexagon h belong to distinct type-edges of h.

Suppose that S is a complete forcing set of a catacondensed phenylene system with a hexagon h and an edge $e \in E(h)$. If e is not in S, then we say h contribute 0 to $|S|$ in term of e, if e is in S and shared by h and the other hexagon h', then we say h contribute $\frac{1}{2}$ to S in term of e. If e is in S and not shared, then we say h contribute 1 to $|S|$ in terms of e. The contribution of a whole hexagon h to S is defined as the sum of contribution in term of e over all edges e of $E(h)$.

Theorem 3.3. *Let H be a phenylene chain with n hexagons, then $cf(H) = 3n - 1$.*

Proof. We first prove $cf(H) \geqslant 3n - 1$, and then construct a complete forcing set S with cardinality $3n - 1$.

Let n^* be the number of kink hexagons of H. According to the two shared edges of a kink hexagon belong to one common type-edges, the two shared edges in a linear hexagon belong to distinct type-edges. From Theorem 3.2, we known that every terminal hexagon in H contribute at least $1 + \frac{1}{2} = \frac{3}{2}$ to $|S|$, every linear hexagon contribute at least $\frac{1}{2} + \frac{1}{2} = 1$ to $|S|$, and every kink hexagon contribute at least $1 + \frac{1}{2} = \frac{3}{2}$ to $|S|$. So all non-kink hexagons in H have total contribute at least $\frac{3}{2} \times 2 + (n - n^* - 2) \times 1 = n - n^* + 1$, all kink hexagons have total contribute at least $\frac{3}{2}n^*$.

For convenience, we specify that for a kink hexagon or terminal hexagon h, we take one type-edges of h is the shared edge between h and the adjacent square to the right side of h. From Theorem 3.2, every square contribute at least $1 + \frac{1}{2} = \frac{3}{2}$, and on this basis, the square between two adjacent linear hexagons, or square between adjacent linear and terminal hexagons, or from left to right square between adjacent kink hexagon and non-kink hexagon (that is, it has order) contributes more than $\frac{1}{2}$ to $|S|$. So, all squares contribute at least $\frac{3}{2}(n - 1) + \frac{1}{2}(n - n^* - 1)$.

From above, we have

$$
\begin{aligned}
cf(H) &\geqslant n - n^* + 1 + \frac{3}{2}n^* + \frac{3}{2}(n-1) + \frac{1}{2}(n - n^* - 1) \\
&= 3n - 1.
\end{aligned}
$$

In what follow, we construct a complete forcing set S with cardinality of $|S| = 3n - 1$. For any linear or terminal hexagon, in the case of type-edges with shared edge in it, we selected shared edge into S, for the other type-edges of terminal hexagons any one edge can be selected into S. For every kink hexagon, we selected the shared edge of kink hexagon and the adjacent square to the right side of this kink hexagon, for any other type-edges of kink hexagon, we selected either one edge into S. For square, based on the above selection of edges, we selected any one edge for the other type-edges into S. See example. It is easy to prove that such an S is a complete forcing set of H with $|S| = 3n - 1$.

Note 3.1. *We can also give the proof of Theorem 3.3 by induction on n.*

In fact, for $n = 1, 2, 3$, the conclusion is clearly true. Assume that this is true when $n = k$, that is $cf(H) = 3k - 1$. Let's verify when $n = k + 1$. The phenylene chain H_{k+1} with $k + 1$ hexagons is equivalent to adding a square and a hexagon to phenylene chain H_k, see Fig.3. From Theorem 3.2, the minimum complete forcing set of H_{k+1} has three more edges based on the minimum complete forcing set of H_k. That is $cf(H_{k+1}) = cf(H_k) + 3 = 3k - 1 + 3 = 3(k + 1) - 1$. Conclusion of Theorem 3.3 is proved.

From Theorem3.2, Theorem3.3 and Note3.1, we can give a linear-time algorithm to computer the complete forcing number of a phenylene chain as follows.

Algorithm A (Computing the complete forcing number of a phenylene chain)
Input: a phenylene chain H with n hexagons.
Output: the complete forcing number $ch(H)$ of H.
Initialize a set T as the set of terminal hexagons in H with $|T| = 2$ or 1; $cf(H) = 0$.
While $T \neq \emptyset$ **do**
If $|T| = 2$
  choose a terminal hexagon h and the square s adjacent to h;
  delete h from T, add hexagon h' that adjacent to square s except h into T,
  $H \leftarrow$ the subgraph of H that not contains h and s;
  $cf(H) \leftarrow cf(H) + 3$;
else $|T| = 1$
  $cf(H) \leftarrow cf(H) + 2$;
  end if
end while

Theorem 3.4. *Algorithm A runs in $O(n)$ time.*

Proof. Take any terminal hexagon h from the set of terminal hexagons in $H_1 = H$. We explore the terminal hexagon h and the square s that adjacent to h, which is implemented in $O(2)$ time. We delete h and s from G_1 (but not shared edges with the other part) and denote the resulting graph with $n-1$ hexagon by G_2 and update the set of terminal hexagons in G_2 in $O(1)$ time. We continue until there are left with the empty graph. Hence the total time we need is $O(2(n-1) + n) = O(n)$.

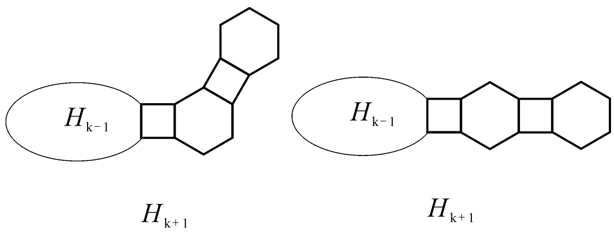

Fig. 3: Two ways of constructing H_{k+1} from H_k.

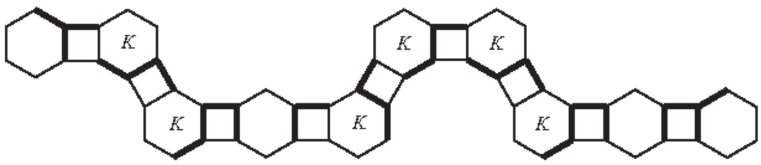

Fig. 4: A phenylene chain with 10 hexagons, with their kinks indicated by placing letter 'K' at centers of them. The complete forcing set indicated by *bold edges* has minimum cardinality 29.

4. Complete forcing number of catacondensed phenylene system

In this subsection we study complete forcing numbers of catacondensed phenylene systems.

A branched hexagon h in a catacondensed phenylene system G is called *terminal* if two of its three branches contain no branched hexagons of G, which are denoted by $C^1_G(h)$ and $C^2_G(h)$. According to the terminal branched hexagon h, we decompose G into two smaller constituents by deleting the two unshared edges e_1, e_2 of the square which between hexagon h and hexagon in $C^1_G(h)$ or $C^2_G(h)$, one is a phenylene chain, denoted by $G^c(h)$, the other is its residual, denoted by $G^r(h)$.

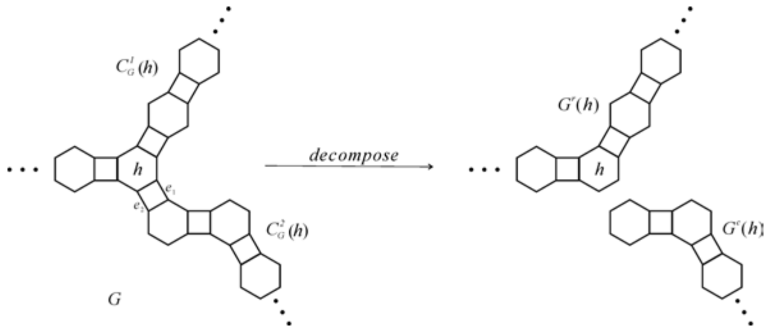

Fig. 5: Illustration for decomposition of a catacondensed phenylene system G.

Theorem 4.1. *Let G be a catacondensed phenylene system, h a terminal branched hexagon of G. Then* $cf(G) = cf(G^c(h)) + cf(G^r(h)) + 1$.

Proof. Let S be a minimum complete forcing set of G. It is evident that restrictions of S on $G^c(h)$ and $G^r(h)$ are minimum complete forcing set of $G^c(h)$ and $G^r(h)$ respectively. In turn, let S_1 be a minimum complete forcing set of $G^c(h)$, S_2 is a minimum complete forcing set of $G^r(h)$. Then $S_1 \cup S_2 \cup \{e_1\}(\text{or}\{e_2\})$ is a minimum complete forcing set of G. So $cf(G) = cf(G^c(h)) + cf(G^r(h)) + 1$. □

Corollary 4.2. *Let G be a catacondensed phenylene system with n hexagons, then* $cf(G) = 3n - 1$.

Proof. Let l be the number of branched hexagons of a catacondensed phenylene system G. According to the decomposition of above, we will have $l + 1$ phenylene chains, and l squares in G are reduced. We assume that lengths of those $l + 1$ phenylene chains are $k_1, k_2, \ldots, k_{l+1}$, then $k_1 + k_2 + \cdots + k_{l+1} = n$. From Theorem 4.1 and From Theorem 3.3, we have

$$\begin{aligned} cf(G) &= 3k_1 - 1 + 3k_2 - 1 + \cdots + 3k_{l+1} - 1 + l \\ &= 3(k_1 + k_2 + \cdots + kl + 1) - (l + 1) + l \\ &= 3n - 1. \end{aligned}$$

From Theorem4.1 and Corollary4.2, we can give a linear-time algorithm to complete forcing number of a catacondensed phenylene system as follows.

Algorithm B (Computing the complete forcing number of a cata-condensed phenylene system)
Input: a cata-condensed phenylene system G with n hexagons.
Output: the complete forcing number $cf(G)$ of G.
Initialize a set T as the set of branched hexagons in G; $cf(G) = 0$.
While $T \neq \emptyset$ **do**
choose a terminal branched hexagon $h \in T$;
decompose G into subgraphs $C^r_G(h)$ and $C^c_G(h)$ to get a phenylene chain, which is denoted as H, (see Fig.6);
$T \leftarrow T - h$;
$G \leftarrow G \backslash H$;
$cf(G) \leftarrow cf(G) + cf(H) + 1$;

end while

In order to better explain Theorem 4.1 and Corollary 4.2, we will give the following example. The above notations will continue to be used.

Example 4.3. *Let G be a catacondensed phenylene system with* 13 *hexagons, and the decompositions of G are shown in Fig.6.*

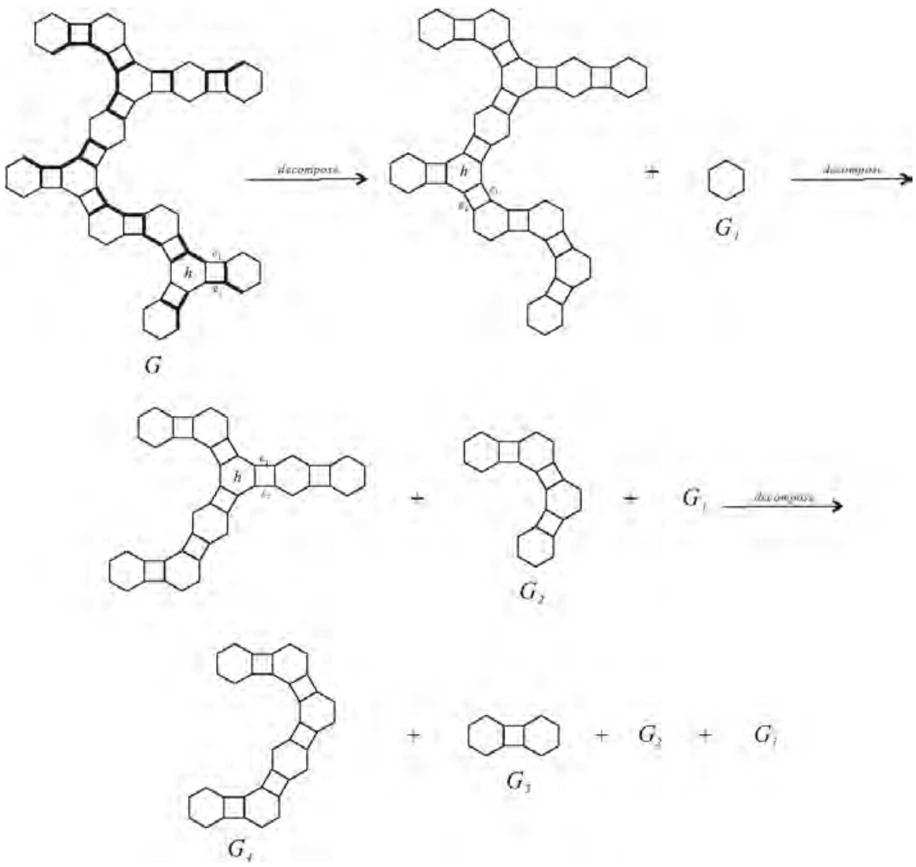

Fig. 6: An application of Theorem 4.1 to a catacondensed phenylene system. G can be decomposed into G_1, G_2, G_3, G_4. A minimum complete forcing set of G is indicated by bold edges.

Obviously, $l = 3$ for G. After the decomposition of G, $k_1 = 1, k_2 = 4, k_3 = 2, k_4 = 6$. Then

$$\begin{aligned} cf(G) &= cf(G_1) + cf(G_2) + cf(G_3) + cf(G_4) + l \\ &= 3k_1 - 1 + 3k_2 - 1 + 3k_3 - 1 + 3k_4 - 1 + 3 \\ &= 38. \end{aligned}$$

On the other hand, $cf(G) = 3n - 1 = 3 \times 13 - 1 = 38$.

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