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A Linear–Time Algorithm for Computing the Complete Forcing Number and the Clar Number of Catacondensed Hexagonal Systems

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Abstract

Let G be a graph with edge set $E(G)$ that admits a perfect matching M. A *forcing set* of M is a subset of M contained in no other perfect matching of G. A *complete forcing set* of G, recently introduced by Xu *et al.* [Complete forcing numbers of catacondensed hexagonal systems, *J. Comb. Optim.*, doi: 10.1007/s10878-013-9624-x], is a subset of $E(G)$ to which the restriction of any perfect matching M is a forcing set of M. The minimum possible cardinality of a complete forcing set of G is the *complete forcing number* of G. In this article, we prove theorems for general graphs about explicit relations between the complete forcing numbers under the operation of identifying edges. Regarding its applications to a catacondensed hexagonal system, we prove an unexpectedly linear relationship between the complete forcing number and the Clar number, an important concept on Clar's aromatic sextet theory in chemistry, propose a linear-time algorithm for computing the complete forcing number and the Clar number and, finally, give an exponential sharp lower bound on the number of minimum complete forcing sets.

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1 Introduction

A *perfect matching* of a graph is a set of disjoint edges that covers all vertices of the graph. Perfect matchings arose in the dimer problem of statistical physics, Kekulé structures of organic chemistry and in the personnel assignment problem of operations research [14]. The number of Kekulé structures (i.e., perfect matchings) of a benzenoid hydrocarbon can measure its stability [4]. The idea of "forcing" has long been used in many research fields in graph theory and combinatorics [7, 15], and its application to a perfect matching M of a graph first appeared in Ref. [8] by Harary, Klein, Živković, that is, a subset S of M forces exactly one perfect matching of G, namely, M. In other words, then S occurs simultaneously in no other perfect matching. Such an S is called a *forcing set* of M. The minimum possible cardinality of S is called the *forcing number* of M. The forcing number can trace its origin back to the papers [11, 17] in the study of molecular resonance structures by Randić and Klein in the chemical literature, where the forcing number was introduced under the name of "innate degree of freedom" of a Kekulé structure. Adams *et al.* proved [1] the problem of finding the forcing number of a perfect matching in a bipartite graph with maximum degree 3 is NP-complete. For more results on the forcing number, we refer the reader to Refs. [2, 12, 13, 16, 18, 27].

Forcing sets and forcing numbers 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. Vukičević *et al.* [20, 21] introduced the concept of *global* (or *total*) *forcing set* from the "global" point of view, i.e., concerning all perfect matchings instead of a particular perfect matching, which is defined as a subset S of $E(G)$ on which there are no two distinct perfect matchings coinciding, i.e., the restriction of the characteristic function of perfect matchings to S is an injection. On the other hand, Klein and Randić [11] proposed *the degree of freedom* of a graph from the "global" point of view, defined as the sum of forcing numbers over all perfect matchings of a graph. Again, combining the "forcing" and "global" ideas, Xu *et al.* [22] first proposed studying a structure concerning all perfect matchings instead of a particular perfect matching, namely a subset S of $E(G)$ to which the restriction of every perfect matching is a forcing set of the perfect matching. Such an S is called a *complete forcing set* of G. The minimum possible cardinality of a complete forcing set is called the *complete forcing number* of G. To a certain extent, the complete forcing number of a graph gives some sort of identification of the minimal amount of "information" required to specify forcing sets of perfect matchings of the graph. Also, they established some initial results about complete forcing sets and the complete forcing number of a graph, including a necessary and sufficient condition for a set to be a complete forcing set of a graph, and proving that a complete forcing set of a graph is also a global forcing set and the converse is not true by a counterexample.

Let G be a hexagonal system, $\mathcal{H}$ a set of disjoint hexagons in G. $\mathcal{H}$ is called a *resonant set* (or *sextet pattern*) if the subgraph of G obtained from G by deleting vertices in $\mathcal{H}$ together with their incident edges has a perfect matching or is empty. A *Clar formula* is a resonant set of maximum possible size. The *Clar number*, denoted by $Cl(G)$, of G is the cardinality of a Clar formula of G. The concept of resonant pattern originates from Clar's aromatic theory [3]. Within benzenoid hydrocarbon isomers, one with larger Clar number is chemically and thermodynamically more stable. Klažar *et al.* [10] proposed a simple paper-and-pencil method for determining the Clar number of a catacondensed hexagonal system. An integer linear programming was proposed by Hansen and Zheng [9] to compute the Clar number of hexagonal systems. For other researches on the Clar number, see Refs. [19, 23, 25, 26].

Concerning the difficulty of the computation of complete forcing numbers, we hope to express the complete forcing number of a graph in terms of complete forcing numbers of its subgraphs. Motivated by this idea, in this article we discuss the decomposition of a graph into smaller subgraphs, which has been an area of considerable interest in graph theory, and give relations between the complete forcing number of a graph and the complete forcing numbers of the subgraphs obtained by splitting an edge whose endpoints constitute a cutset. As their applications, we prove an unexpectedly linear relationship between the complete forcing number and the Clar number of a catacondensed hexagonal system G and propose a linear-time algorithm for computing the complete forcing number and the Clar number of G. Finally we give an exponential sharp lower bound on the number of minimum complete forcing sets of G.

The present paper is organized as follows. In the next section, we formally define complete forcing sets, the complete forcing number of a graph, catacondensed hexagonal systems, along with other graph-theoretic terms relevant to our subject. In Section 3, we give a necessary and sufficient condition for complete forcing sets and theorems about relations between complete forcing numbers under graph edge-identification. In Section

4, we provide and prove our main results on catacondensed hexagonal systems G: a linear relationship between the complete forcing number and the Clar number of G, a linear algorithm for computing the complete forcing number and the Clar number of G, and an exponential sharp lower bound on the number of minimum complete forcing sets of G. We conclude this article in Section 5.

2 Preliminaries

Each graph G with edge set $E(G)$ and vertex set $V(G)$ in this paper is simple and has perfect matchings. For all terms and notation used but not defined here we refer the reader to the textbook [5].

A *hexagonal system* (or *benzenoid system*, *polyhex graph*) is a connected graph without cut vertices embedded into the regular hexagonal lattice in the plane, and in which all internal faces are regular hexagons. Note that hexagonal systems are bipartite. A hexagonal system is *catacondensed* if there are no three hexagons sharing one common vertex, i.e., all vertices lie on the boundary of the non-hexagonal external face. A *hexagonal chain* is a catacondensed hexagonal system in which no hexagon is adjacent to three hexagons.

Let G be a catacondensed hexagonal system. An edge e in G is called *shared* if e is contained in two hexagons. A hexagon r of G has zero, one, two or three neighbouring hexagons. If r has zero or one neighbouring hexagon, it is said to be *terminal*, and if it has three neighbouring hexagons, to be *branched*. A hexagon which is adjacent to exactly two other hexagons is a *kink* if it has two adjacent vertices of degree 2, and is *linear* otherwise. A hexagonal chain with no kinks is said to be *linear*. A *segment* is a maximal linear hexagonal chain in G, including the kinks and/or terminal hexagons and/or branched hexagons at its end. If a segment L contains a terminal hexagon, L is called *terminal*.

Let S_1, S_2 be two subsets of a set. The *symmetric difference*, denoted by $S_1 \oplus S_2$, of S_1 and S_2 is the set of elements belonging to exactly one of S_1 and S_2.

Let G be a connected graph with a perfect matching. A subgraph H of G is *nice* if $G - V(H)$ contains a perfect matching. It is obvious that an even cycle C of G is *nice* if and only if C is exactly the symmetric difference of some two perfect matchings M_1 and M_2 of G, i.e., $C = M_1 \oplus M_2$; Let C be an even cycle. A set of alternative edges on C is called a *type-set* of C. Alternatively, each type-edge of an even cycle C is a perfect matching of C.

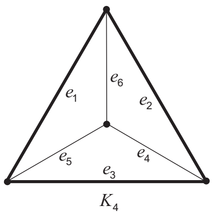

Fig. 1: A minimum complete forcing set $\{e_1, e_2, e_3\}$ in K_4 is indicated by bold lines. Hence $cf(K_4) = 3$.

The following is a basic property of catacondensed hexagonal systems.

Lemma 2.1. *[4, 6] Let G be a catacondensed hexagonal system. Then G has a perfect matching and each hexagon in G is nice.*

Let G be a catacondensed hexagonal system with a hexagon r. (Hexagon r is necessarily nice by Lemma 2.1.) If r is a kink or branched hexagon, then all shared edges of r belong to one common type-set of r, while two shared edges of a linear hexagon r belong to two distinct type-sets of r.

Let G be a connected graph with edge set $E(G)$ and a perfect matching M. A *forcing set* of M is a subset of M contained in no other perfect matching of G. It follows that the empty set is a forcing set of M if and only if M is the unique perfect matching of G. A *complete forcing set* of G is a subset S of $E(G)$ of which, for any perfect matching M, the restriction to M is a forcing set of M. Obviously, any set containing a complete forcing set of G, particularly $E(G)$, is also a complete forcing set of G. A complete forcing set of the smallest cardinality is called a *minimum complete forcing set*, and its cardinality is the *complete forcing number* of G, denoted by $cf(G)$.

As an illustrative example we consider K_4 shown in Fig. 1 (see Refs. [20, 22], Fig. 1). It contains three different perfect matchings: $M_1 = \{e_1, e_4\}$, $M_2 = \{e_2, e_5\}$, $M_3 = \{e_3, e_6\}$. It is easy to see that the restriction of every perfect matching M to $S = \{e_1, e_2, e_3\}$ is a forcing set of M. Hence S is a complete forcing set of K_4. Since the intersection of S and every perfect matching is nonempty and $\{M_1, M_2, M_3\}$ is a partition of the edge set of K_4, S of cardinality 3 is a minimum complete forcing set. Hence, $cf(K_4) = 3$.

3 Complete forcing numbers under graph edge–identification

First, we recall a necessary and sufficient condition for a complete forcing set of a graph shown in [22].

Theorem 3.1. *[22] Let G be a connected graph with edge set $E(G)$ and a perfect matching. Then $S \subseteq E(G)$ is a complete forcing set of G if and only if for any nice cycle C in G, the intersection of S and each type-set of C is non-empty.*

Now we show another necessary and sufficient condition for a complete forcing set of a connected graph with a perfect matching.

Theorem 3.2. *Let G be a connected graph with edge set $E(G)$ and a perfect matching. Then $S \subseteq E(G)$ is a complete forcing set of G if and only if for each nice subgraph H with a perfect matching of G, the restriction of S to H is a complete forcing set of H.*

Proof. Sufficiency ("$\Longleftarrow$"). Since G itself is a nice subgraph of G (i.e., let $H = G$), S is a complete forcing set of G.

Necessity ("$\Longrightarrow$"). Let S be a complete forcing set of G, H a nice subgraph with a perfect matching of G, and S' the restriction of S to H. We need to prove that S' is a complete forcing set of H. Suppose to the contrary that S' is not a complete forcing set of H. That is, by Lemma 3.1 S' does not intersect a type-set of a nice cycle C of H. Since C is also a nice cycle of G, S does not intersect a type-set of a nice cycle C of G, a contradiction. □

We now give some results about the complete forcing numbers under graph edge-identification.

Theorem 3.3. *Let G be a connected graph with two nice subgraphs G_1 and G_2 such that $G = G_1 \cup G_2$ and the intersection of G_1 and G_2 is an edge $e = v_1v_2$ (see Fig. 2). Then*

$$cf(G_1) + cf(G_2) - 1 \leqslant cf(G) \leqslant cf(G_1) + cf(G_2), \tag{1}$$

and

(1). $cf(G) = cf(G_1) + cf(G_2)$ if and only if either e is not contained in any minimum complete forcing set in G_1 or e is not contained in any minimum complete forcing set in

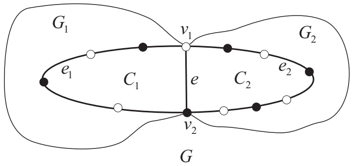

Fig. 2: Illustration for the proof of Claim in Theorem 3.3. Vertices on the nice cycle C in G can be represented by white and black points.

G_2,

(2). $cf(G) = cf(G_1)+cf(G_2)-1$ *if and only if both* G_1 *and* G_2 *contain minimum complete forcing sets which contain* e.

Proof. We first prove the inequality (1).

Upper bound. For $i = 1, 2$, let S_i be a complete forcing set of G_i. Then

Claim. The union $S = S_1 \cup S_2$ of S_1 and S_2 is a complete forcing set of G.

By Theorem 3.1, it is sufficient to prove that there is a nonempty intersection of S and any type-set of any nice cycle C of G.

If C is completely contained in G_1 or G_2, say G_1, then it is easily proven that C is also a nice cycle of G_1 by the structure of G. Since S_1 is a complete forcing set of G_1, the intersection of S_1 and any type-set of C is non-empty by Theorem 3.1. Thus the intersection of S ($\supseteq S_1$) and any type-set of C is non-empty. Otherwise, we assume that C is not contained entirely in G_1 or G_2. C must pass through the vertices v_1 and v_2 but not the edge e by the structure of G. The addition of e to C creates two cycles containing e, one entirely in G_1, say C_1, and the other, say C_2, entirely in G_2 (see Fig. 2). Then for $i = 1, 2$, C_i is nice in G_i by the nicety of C. So by the definition of S_i, $1 \leqslant i \leqslant 2$, the intersection of S_i and the type-set of C_i not containing e is non-empty; we denote by e_i one edge in the intersection. It is easily proven that e_1 and e_2 in S belong to two different type-sets of C by using e serving as a link.

For $i = 1, 2$, if S_i is minimal, then by the claim, we have $cf(G) \leqslant |S| \leqslant |S_1| + |S_2| = cf(G_1) + cf(G_2)$. So we have proved the upper bound on $cf(G)$.

Lower bound. Let S be a minimum complete forcing set of G. Let $S_i = S \cap G_i$ for $i = 1, 2$. By Theorem 3.2, S_i is a complete forcing set of G_i. Combined with $S_1 \cap S_2 \subseteq \{e\}$ and $S = S_1 \cup S_2$, we have $cf(G_1) + cf(G_2) - 1 \leqslant |S_1| + |S_2| - 1 \leqslant |S| = cf(G)$.

In what follows we prove the statements (1) and (2). By the inequality (1), we know two statements (1) and (2) are equivalent. So it is sufficient to prove one of these statements. Here we prove Statement (1).

Necessity ("$\Longrightarrow$"). Assume to the contrary that, for $i = 1, 2$, G_i has a minimum complete forcing set containing e, denoted by S_i. Then $S_1 \cap S_2 = \{e\}$ and $S = S_1 \cup S_2$ is a complete forcing set of G by the claim in Theorem 3.3. Hence $cf(G) \leqslant |S| = |S_1| + |S_2| - 1 = cf(G_1) + cf(G_2) - 1$, which contradicts the assumption.

Sufficiency ("$\Longleftarrow$"). Assume to the contrary that $cf(G) = cf(G_1) + cf(G_2) - 1$ by Theorem 3.3. We distinguish two cases.

Case 1. There exists a minimum complete forcing set S containing e in G.

Let $S_i = S \cap G_i$ for $i = 1, 2$. Then S_i is a complete forcing set of G_i by Theorem 3.2 and $S_1 \cap S_2 = \{e\}$. Then

$$cf(G_1) + cf(G_2) - 1 \leqslant |S_1| + |S_2| - 1 = |S| = cf(G_1) + cf(G_2) - 1. \tag{2}$$

Hence the equality holds in Eq. (2) and further S_i is a minimum complete forcing set of G_i containing e for $i = 1, 2$, which contradicts the assumption.

Case 2. e is not contained in any minimum complete forcing set in G.

Let S be a minimum complete forcing set of G and denote $S_i = S \cap G_i$ for $i = 1, 2$. Then $S_1 \cap S_2 = \emptyset$ and S_i is a complete forcing set of G_i by Theorem 3.2. we have $cf(G_1) + cf(G_2) \leqslant |S_1| + |S_2| = |S| = cf(G) = cf(G_1) + cf(G_2) - 1$, a contradiction. □

4 A linear relationship between the complete forcing number and the Clar number and a linear-time algorithm for their computation

For catacondensed hexagonal systems, there exists a particular necessary and sufficient condition for complete forcing sets as follows.

Theorem 4.1. *[22] Let G be a catacondensed hexagonal system with edge set $E(G)$. Then $S \subseteq E(G)$ is a complete forcing set of G if and only if S and two type-sets of each hexagon in G have a nonempty intersection, respectively.*

Theorem 4.2. *[22] Let L be a linear hexagonal chain with n hexagons. Then $cf(L) = n + 1$.*

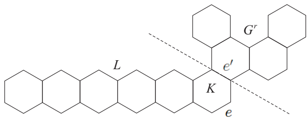

Fig. 3: Illustration for the proof of Lemma 4.4.

Lemma 4.3. *Let L be a linear hexagonal chain with n hexagons ($n \geqslant 1$). Then every minimum complete forcing set of L consists of the $n-1$ shared edges and two additional edges, lying respectively in the type-set of its terminal hexagon(s) containing no shared edges. Thus L has precisely nine minimum complete forcing sets.*

Proof. Assume to the contrary that there exists a minimum complete forcing set S of L which does not contain a shared edge e. Then e divides L into two linear hexagonal chains L_1 and L_2. Note that the total number of hexagons in L_1 and L_2 is n. By Theorem 3.2, the restriction of S to L_1 (resp., to L_2) is a complete forcing set in L_1 (resp., to L_2), denoted by S_1 (resp., S_2). Then S_1 (resp. S_2) does not contain e and hence $|S| = |S_1| + |S_2|$. Again combined with Theorem 4.2, we have $n+1 = cf(L) = |S| = |S_1| + |S_2| \geqslant cf(L_1) + cf(L_2) = n+2$, a contradiction.

As there are totally $n-1$ shared edges in L, combined with Theorem 4.2, S has two edges other than shared edges. It directly follows from Theorem 4.1 that these two edges belong respectively to the type-set of its terminal hexagon(s) containing no shared edges. Since each type-set of a terminal hexagon containing no shared edges has three edges, L has precisely $3 \times 3 = 9$ minimum complete forcing sets. □

Lemma 4.4. *Let L be a terminal segment containing a kink K as one of its ends in a catacondensed hexagonal system G. We denote by e, e' the two edges in the type-set of K containing shared edges (see Fig. 3) such that e is not shared. Then no minimum complete forcing set in G contains e.*

Proof. We denote by G^r the subgraph of G separated along e' inclusive other than L. Let S be a minimum complete forcing set of G.

If $e' \in S$, then $e \notin S$ by the choice of S and Theorem 4.1. Otherwise, we assume that $e' \notin S$. Let S_1, S_2 be the restrictions of S to L, G^r, respectively. Then $|S| = |S_1| + |S_2|$ and S_1, S_2 are complete forcing sets of L, G^r, respectively, by Theorem 3.2. So we have

$$cf(G) = |S| = |S_1| + |S_2| \geqslant cf(L) + cf(G^r).$$

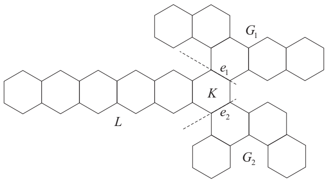

Fig. 4: Illustration for the proof of Theorem 4.5.

Again combined with Theorem 3.3, equality holds in the inequality above. So S_1 is a minimum complete forcing set of L. Note that there are at least two hexagons in L. By Lemma 4.3, $e \notin S_1$, so, $e \notin S$. □

Theorem 4.5. *Let G be a catacondensed hexagonal system with a terminal segment L containing a kink or branched hexagon K. G is decomposed into L and residuals G_1, G_2 along two shared edges, denoted by e_1, e_2, of K (see Fig. 4) (called a* terminal decomposition. *Note that if K is a kink, then one of G_1, G_2, say G_2, is empty). Then $cf(G) = cf(L) + cf(G_1)$ in the case of the kink K and $cf(G) = cf(L) + cf(G_1) + cf(G_2)$ in the case of the branched hexagon K.*

Proof. If K is a kink, i.e., G_2 is empty, then no minimum complete forcing set of L contains e_1 by Lemma 4.3. Hence by Theorem 3.3 (1), $cf(G) = cf(L) + cf(G_1)$. If K is branched, we make two inverse operations of edge-identifications of G into L, G_1, and G_2. First, along the edge e_1, we decompose G into G_1 and the residual G^r consisting of L and G_2 (including e_1). By Lemma 4.4, no minimum complete forcing set of G^r contains e_1. By Theorem 3.3 (1), $cf(G) = cf(G_1) + cf(G^r)$. Similarly, we decompose G^r into L and G_2 along e_2, by Lemma 4.3, no minimum complete forcing set of L contains e_2 (note that L contains at least two hexagons). By Theorem 3.3 (1), $cf(G^r) = cf(L) + cf(G_2)$. Combining the two equalities above, we get $cf(G) = cf(L) + cf(G_1) + cf(G_2)$. This completes the proof. □

Proposition 4.6. *Let G be a catacondensed hexagonal system. Then G can be decomposed into a series of linear hexagonal chains by successively terminal decompositions for current components other than linear hexagonal chains.*

Proof. We can make one further terminal decomposition whenever there exist kinks or branched hexagons in current graphs. Thus we ultimately arrive at a series of linear hexagonal chains. □

Since there are various linear hexagonal chains arising in current terminal decomposition procedure, eventually there are various series of linear hexagonal chains as in Proposition 4.6 for a given catacondensed hexagonal system. But we have the following result.

Corollary 4.7. *Let G be a catacondensed hexagonal system with n hexagons. Then the number of linear hexagonal chains into which G can be decomposed as in Proposition 4.6 is constant and is equal to $cf(G) - n$.*

Proof. We take one series of linear hexagonal chains, say, $H_1, H_2, \cdots, H_t$ for some integer t, as in Proposition 4.6. By Theorem 4.5, we have

$$cf(G) = \sum_{i=1}^{t} cf(H_i).$$

By Theorem 4.2, we know each $cf(H_i)$ is equal to the number of hexagons, denoted by h_i, in H_i plus one. Note that $n = \sum_{i=1}^{t} h_i$. Hence we have $cf(G) = \sum_{i=1}^{t}(h_i + 1) = \sum_{i=1}^{t}(h_i) + t = n + t$, i.e., $t = cf(G) - n$. So t is constant for a given catacondensed hexagonal system. □

Let G be a catacondensed hexagonal system. We denote by $t(G)$ the number of linear hexagonal chains into which G can be decomposed as in Proposition 4.6.

Combining Theorems 4.2 and 4.5, we easily obtain the following result.

Theorem 4.8. *Let G be a catacondensed hexagonal system with n hexagons. Then $cf(G) = n + t(G)$.*

In study of the Clar number of a catacondensed hexagonal system, Klavžar *et al.* [10] also considered a kind of decomposition associated with a catacondensed hexagonal system, which is essentially the terminal decomposition we used, and gave a remarkably simple recursive method (i.e., *Rules* 1 and 2 in the original paper) for determining the Clar number of a catacondensed hexagonal system, from which the following result is easily obtained.

Lemma 4.9. *[10] Let G be a catacondensed hexagonal system. Then $Cl(G) = t(G)$.*

Hence, combining Theorem 4.8 and Lemma 4.9, we give a close relationship between the complete forcing number and the Clar number of a catacondensed hexagonal system as follows.

Theorem 4.10. *Let G be a catacondensed hexagonal system with n hexagons, $cf(G)$, $Cl(G)$ the complete forcing number and the Clar number of G, respectively. Then*

$$cf(G) = Cl(G) + n.$$

By Theorem 4.8 and Lemma 4.9, we can give a linear-time algorithm for the complete forcing number and the Clar number of a catacondensed hexagonal system as follows.

Algorithm A (*Computing the complete forcing number and the Clar number of a catacondensed hexagonal system*)

Input: a catacondensed hexagonal system G with n hexagons.

Output: the complete forcing number cf and the Clar number Cl of G.

Initialize a set TH as the set of terminal hexagons in G; $cf \leftarrow n$; $Cl \leftarrow 0$.

while $TH \neq \emptyset$ **do**

choose a terminal segment L with hexagons h, h' as their ends;

add non-branched hexagons outside L adjacent to h or h' into TH;

delete h, h' from TH;

$G \leftarrow$ the subgraph of G entirely consisting of hexagons not in L;

$cf \leftarrow cf + 1, Cl \leftarrow Cl + 1$,

end while

Return cf, Cl.

Theorem 4.11. *Algorithm A runs in $O(n)$ time.*

Proof. Take any terminal hexagon K_1 from the set of terminal hexagons in $G_1 = G$. We explore the terminal segment L_1 containing K_1 with l_1 hexagons, which is implemented in $O(l_1)$ time. We delete all hexagons in L_1 from G_1 (but not shared edges with the other parts) and denote the resulting graph with $n - l_1$ hexagons by G_2 and update the set of terminal hexagons in G_2 in $O(1)$ time. We continue until we are left with the empty graph and get a series of linear hexagonal chains $L_1, L_2, \cdots, L_t$ with $l_1, l_2, \cdots, l_t$ hexagons, respectively. Note that $n = l_1 + l_2 + \cdots + l_t$. Hence the total time we need is $O(l_1 + l_2 + \cdots + l_t + t) = O(n)$. □

An example: A catacondensed hexagonal system G with 16 hexagons in Fig. 5 can be decomposed into eight linear hexagonal chains. So $t(G) = 8$. By Theorem 4.8 and Lemma

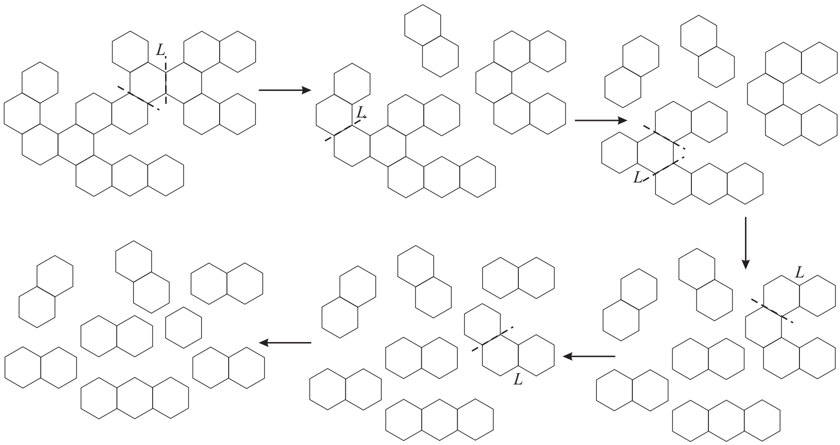

Fig. 5: A catacondensed hexagonal system G with 16 hexagons. G can be decomposed into eight linear hexagonal chains by terminal decompositions. By Theorem 4.8 and Lemma 4.9, $cf(G) = 16 + 8 = 24, Cl(G) = 8$.

4.9,

$$cf(G) = 16 + 8 = 24, Cl(G) = 8.$$

In what follows, we give an exponential sharp lower bound on the number of minimum complete forcing sets of a catacondensed hexagonal system G with n hexagons in terms of $cf(G)$ and n.

Theorem 4.12. *Let G be a catacondensed hexagonal system with n hexagons. Then the number of minimum complete forcing sets is at least $9^{cf(G)-n}$. Equality holds if G is a linear hexagonal chain.*

Proof. Let $\{H_1, H_2, \cdots, H_{cf(G)-n}\}$ be any series of linear hexagonal chains as in Proposition 4.6 associated with G. We denote by S_i a minimum complete forcing set of H_i for $1 \leqslant i \leqslant cf(G) - n$. Let $S = \cup_{i=1}^{cf(G)-n} S_i$. By Theorem 4.1, we know that S is a complete forcing set of G. $|S| \leqslant \sum_{i=1}^{cf(G)-n} |S_i| = \sum_{i=1}^{cf(G)-n} cf(H_i) = cf(G)$. Hence the equality holds in the inequality above. So S is a minimum complete forcing set of G. By Lemma 4.3, S is a disjoint union of $S_1, S_2, \cdots, S_{cf(G)-n}$ and each S_i has nine choices. So S has at least $9^{cf(G)-n}$ distinct choices. This completes the proof. □

5 Concluding remarks

In this paper we discussed the calculation of the complete forcing numbers of graphs, the close relationship between the complete forcing number and the Clar number, and a remarkably simple method for their calculations. First we gave a necessary and sufficient condition for complete forcing sets, then a result on the complete forcing numbers under graph edge-identifications (i.e., Theorem 3.3) and introduced a decomposition for a catacondensed hexagonal system G. Regarding their applications, we first decompose G into a set of linear hexagonal chains by arbitrarily choosing terminal segments (i.e., terminal decompositions) and prove the number of these obtained linear hexagonal chains for any such terminal decomposition are constant for any given catacondensed hexagonal system G and further gave an unexpectedly linear relationship between the complete forcing number and the Clar number of G and ultimately gave a linear-time algorithm for computing the complete forcing number and the Clar number of G. Finally we offered an exponential sharp lower bound on the number of minimum complete forcing sets of G with n hexagons in terms of n and the complete forcing number of G.

In deed, about the calculation of the complete forcing numbers of catacondensed hexagonal systems, Xu *et al.* [22] decomposed G into a series of hexagonal chains by choosing a special branched hexagon K in the current graph and separating the component containing K into two parts along a special shared edge of K at each step, then expressed the complete forcing number of G as the sum of all complete forcing numbers of these hexagonal chains. The complete forcing number of each hexagonal chain can be obtained by considering the construction of each hexagonal chain. There are two main differences between two methods for the calculation of the complete forcing numbers of catacondensed hexagonal systems. In order to carry out decompositions, we chose randomly terminal segments in the current paper, while, in [22], branched hexagons and decompositions were chosen in the special manner. On the other hand, there was a simple formula (i.e., Theorem 4.2) for calculating the complete forcing number of a linear hexagonal chain in terms of the number of hexagons, but no such a simple formula for the complete forcing number of a hexagonal chain. Combining the two advantages, we gave a linear-time algorithm for computing complete forcing numbers of catacondensed hexagonal systems.

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