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Complete Forcing Numbers of Polyphenyl Systems

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ABSTRACT The idea of "forcing" has long been used in many research fields, such as colorings, orientations, geodetics and dominating sets in graph theory, as well as Latin squares, block designs and Steiner systems in combinatorics [D. Donovan, E. S. Mahmoodian, C. Ramsay, A. P. Street, Defining sets in combinatorics: A survey, in: C. D. Wensley (Ed.), Surveys in Combinatorics, Cambridge Univ. Press, 2003, pp. 115–174]. Recently, the forcing on perfect matchings has been attracting more researchers' attention. A forcing set of a perfect matching M of a graph G is a subset of M contained in no other perfect matchings of G. A global forcing set of G, introduced by Vukičević et al., is a subset of E(G) on which there are distinct restrictions of any two different perfect matchings of G. Combining the above "forcing" and "global" ideas. Xu et al. in [Complete forcing numbers of catacondensed benzenoid, *J. Combin. Optim.* **29** (2015) 803–814.] introduced a complete forcing set of G defined 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. In this paper, we give the explicit expressions for the complete forcing number of several classes of polyphenyl systems.

KEYWORDS Complete forcing number • polyphenyl system • global forcing number.

1. INTRODUCTION

The molecular graphs (or more precisely, the graphs representing the carbon-atoms) of polyphenyls are called the polyphenyl systems. This kind of macrocyclic aromatic hydrocarbons called polyphenyls and their derivatives attracted the attention of chemists for many years [3, 4, 5]. The derivatives of polyphenyls are very important organic chemicals, which can be used in organic synthesis, drug synthesis, heat exchanger, etc. Biphenyl compounds also have extensive industrial applications. For example, 4,4–bis (chloromethyl) biphenyl can be used for the synthesis of brightening agents. Especially, polychlorinated biphenyls (PCBs) can be applied in print and dyeing extensively [6, 7]. On the other side, PCBs are dangerous organic pollutants, which lead to global pollution. Many years ago, a series of physical properties were discussed [8–13].

A perfect matching M (or Kekulé structure, 1-factor) of a graph G is a set of independent edges such that every vertex of G is incident with exactly one edge in M.

Let G be a graph with edge set $E(G)$ that admits a perfect matching M. A forcing set of M is a subset S of M contained in no other perfect matchings of G. The minimum possible cardinality of forcing set S is called the forcing number of M.

The notions of a forcing edge and the forcing number of a perfect matching first appeared in 1991 in a paper of Harary, Klein and Živković [14]. The root of these concepts can be traced to the works [15, 16] by Randić and Klein in 1985−1987, where the forcing number was introduced under the name of "innate degree of freedom" of a Kekulé structure, which plays an important role in the resonance theory in chemistry.

Over the past two decades, more and more mathematicians were attracted to the study on forcing sets (including forcing edges and forcing faces, etc) and the forcing numbers of perfect matchings of a graph. The scope of graphs in consideration has been extended from polyhexes to various bipartite graphs and non-bipartite graphs.

Some varied topics such as global (or total) forcing matchings and anti-forcing matching also emerged.

Klein and Randić [15] 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, and showed by evidence that the degree of freedom of a chemical graph actually measures graphical characteristics distinct from those measured by a couple of common resonance energy estimators. Because of extensive industrial and medical applications, one class of chemical graph-macrocyclic aromatic hydrocarbons called polyphenyls and their derivatives attracted the attention of chemists for many years [3, 4, 5]. A series of linear and branched polyphenyls and their derivatives were synthesized and some physical properties were discussed [8−13].

Gutman [17] showed that the values which the Wiener indices of isometric polyphenyls may assume are all congruent modulo 36. Bian and Zhang [18, 19] determined the polyphenyl chain with minimum and maximum Wiener (or edge-Wiener) indices among all the polyphenyl chains with n hexagons. Li and Bian [20] gave the extremal polyphenyl chains concerning k-matchings and k-independent sets. In 2013, Ma and Bian [21] also gave the extremal polyphenyl spiders concerning k-matchings and k-independent sets. A complete forcing set of G, introduced by Xu et al. [2] recently, is a subset of $E(G)$ on which the restriction of any perfect matching is a forcing set of the perfect matching. The minimum possible cardinality of complete forcing sets of G is the complete forcing number of G, denote it by $cf(G)$. Xu et al. gave an expression for the complete forcing number of a hexagonal chain and a recurrence relation for complete forcing number of cata-condensed hexagonal system. In 2014, Xu et al. [22] by the constructive proof, gave an explicit analytical expression for the complete forcing number of a primitive coronoid, a circular single chain consisting of congruent regular hexagons.

Based on these works, in this paper, we give the explicit expressions for the complete forcing number of several classes of polyphenyl systems.

2. Preliminaries

All graphs in this paper are simple connected and have perfect matchings. For all terms and notations used but not defined here, we refer the reader to the textbooks [23, 24].

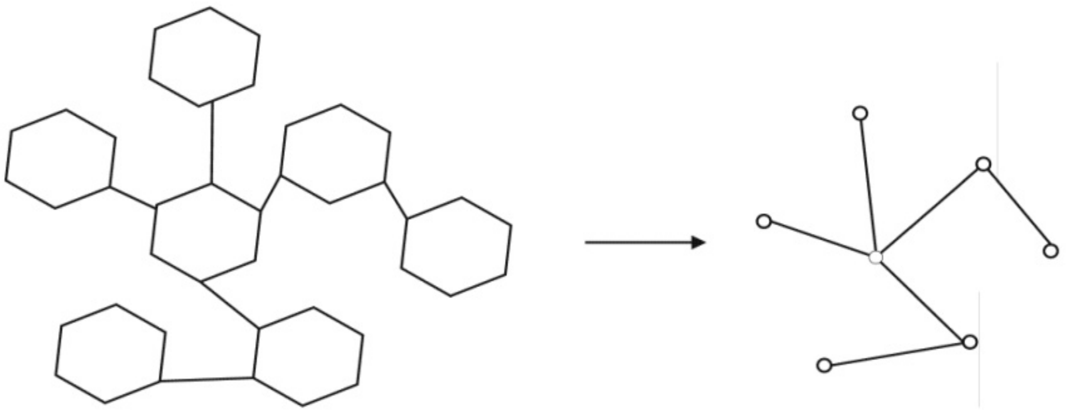

Figure 1. A tree-like polyphenyl system and corresponding tree.

A polyphenyl system *H* is said to be tree-like (see Figure 1), if each vertex of *H* lies in a hexagon and the graph obtained by contracting every hexagon into a vertex in original molecular graph is a tree.

A hexagon *r* of a tree-like polyphenyl system may have one, two, three, four, five or six neighboring hexagons. If *r* has one neighboring hexagon, then it is said to be terminal, and internal otherwise. Also it is branched if it has three or more neighboring hexagons.

Definition 1. If every hexagon in a polyphenyl system has exactly two neighboring hexagons, then it is called primitive coronoid polyphenyl system. The set of primitive coronoid polyphenyl systems with *n* hexagons is denoted by CH_n (see Figure 2).

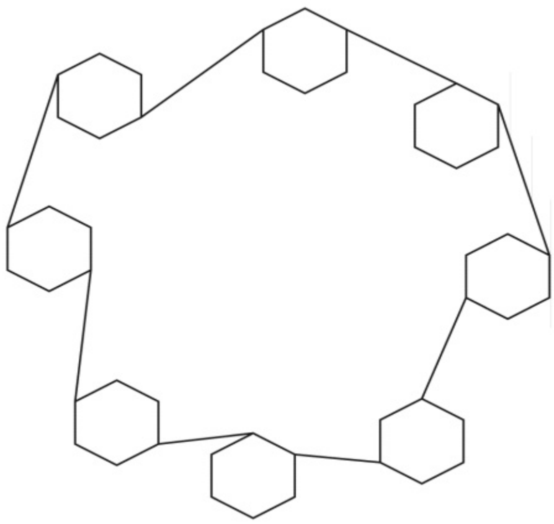

Figure 2. A primitive coronoid polyphenyl system with 8 hexagons.

Definition 2. A tree-like polyphenyl system without branched hexagons is called a polyphenyl chain. A polyphenyl chain with *n* hexagons is denoted by H_n (see Figure 3).

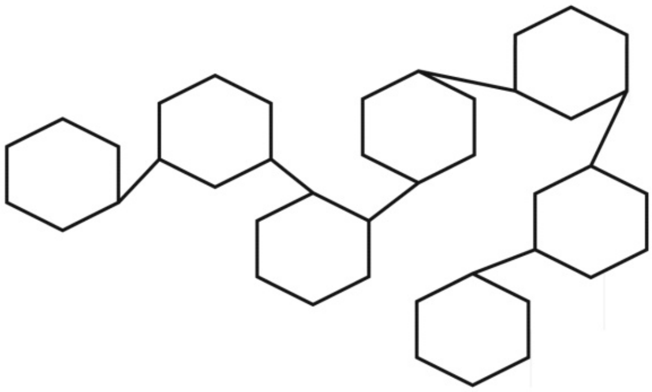

Figure 3. A polyphenyl chain with 7 hexagons.

For a hexagon *C*, two vertices *u* and *v* of *C* are said to be in ortho–position if they are adjacent in *C*. If two vertices are at distance 2, they are in meta–position. Finally, if *u* and *v* are at distance 3, we say that they are in para–position. Examples of pairs of vertices in ortho–, meta–, and para–position are shown in Figure 4.

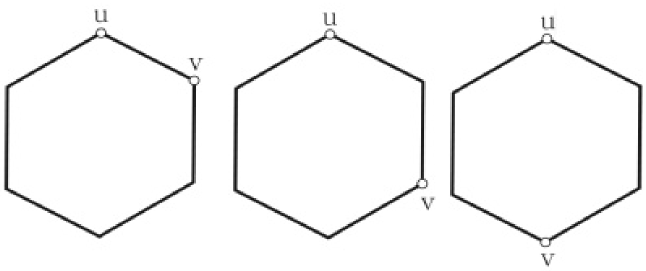

Figure 4. Orhto–, meta–, and para–positions of vertices u and v in C.

An internal hexagon *C* in a polyphenyl chain is called ortho–hexagon, meta–hexagon, or para–hexagon, if the two vertices of *C* incident with two edges which connect other two hexagons are in ortho–, meta–, or para–position, respectively.

Following Lovász and Plummer [24], an edge of *G* is said to be allowed if it is contained in some perfect matching of *G* and forbidden otherwise.

Theorem 1. *Let H be a tree-like polyphenyl system with n hexagons. Then we have cf*(*H*) = 2*n*.

Proof. Suppose that *H* is a tree-like polyphenyl system with *n* hexagons.

First we claim that every edge incident with the terminal hexagons is forbidden edge. In fact, if an edge incident with a terminal hexagon *C* is allowed edge, then it lies in some perfect matching *M* of *H*, hence, the number of the rest of vertices in *C* besides the vertex incident with the allowed edge is odd, which contradicts that *H* has the perfect matching.

We can delete all edges incident with terminal hexagons, and obtain the resulting graph, which consists of a small tree-like polyphenyl system and some independent hexagons.

Now we consider the small tree-like polyphneyl system, we also can show that every edge incident with the terminal hexagons of the small polyphenyl system is forbidden edge, then we delete all edges incident with terminal hexagons of the small tree-like polyphenyl system again. By iterating the same proceed, until the resulting graph is an independent hexagon. We can conclude that all edges between the two hexagons are forbidden edges, and the edges lie in every hexagon are allowed edges of H. Moreover, there are two perfect matchings in each hexagon, the union of perfect matching of each hexagon will be a perfect matching of H, and the number of perfect matching of H is $2n$.

By definition of complete forcing number, we take any two adjacent edges in every hexagon, the set of these edges will be a complete forcing set of H. Then we have $cf(H) = 2n$. ■

Since the polyphenyl chain can be viewed as a special tree-like polyphenyl system, as a corollary of Theorem 1, we easily have the following result.

Corollary 2. *Let H_n be any polyphenyl chain with n hexagons. Then we have $cf(H_n) = 2n$.*

For a primitive coronoid polyphenyl system *CH*, the meta–hexagon in *CH* will affect the number of perfect matchings of *CH*, according to whether *CH* has meta–hexagons or not, we distinguish the following two cases.

Theorem 3. *Let CH_n be a primitive coronoid polyphenyl system with n hexagons such that CH_n has no meta–hexagons. Then we have $cf(CH_n) = 2n + 1$.*

Proof. By the assumption, any hexagon C of CH_n is either ortho–hexagon or para–hexagon, so the two vertices of C incident with two edges which connect other two hexagons are in ortho–position or para–position.

First, we claim that G has a perfect matching M consisting of edges connecting two hexagons with the remainder two independent edges of every hexagon by deleting the two ortho– (or para–) position vertices of C. Moreover, every hexagon has two perfect matchings, the union of a perfect matching of every hexagon will be a perfect matching of CH_n. So the number of perfect matchings of CH_n is $2n + 1$.

We can obtain a complete forcing set of CH_n by taking any one edge connecting two hexagons and two adjacent edges of every hexagon in CH_n. Hence, the complete forcing number of CH_n is $2n + 1$. ■

Theorem 4. *Let CH_n be any primitive coronoid polyphenyl system with n hexagons such that CH_n has at least one meta–hexagon. Then we have $cf(CH_n) = 2n$.*

Proof. According to assumption, CH_n has at least one meta–hexagon C. We claim that none of the two edges incident with the two meta-position vertices of C is allowed edge. In fact, if one of the two edges is allowed edge, then it must be matched by some perfect matching M of CH_n, in this case, the remainder vertices of C besides the vertex incident with the allowed edge cannot be completely matched by M, which contradicts that M is a perfect matching of CH_n.

So, the vertices of every hexagon in CH_n must be matched by themselves in M, namely, any edge connecting two hexagons must be forbidden edge of CH_n. The resulting graph is the set of independent hexagons by deleting all the forbidden edges of CH_n. It is clear that the number of perfect matchings of CH_n is $2n$, and we can obtain the complete forcing set of CH_n by taking two adjacent edges of every hexagon of CH_n. Hence, the complete forcing number of CH_n is $2n$. ■

4. CONCLUDING REMARKS

In this section, we discuss the global forcing number of the polyphenyl system. For a simple connected graph G with a perfect matching, let $M(G)$ denote the set of all perfect matchings in G, and $f : M(G) \rightarrow \{0, 1\}^{|E(G)|}$ a characteristic function of perfect matchings of G. Any set $S \subseteq E(G)$ such that $f|S$ is an injection is called a global forcing set in G, and the cardinality of smallest such S is called the global forcing number of G. Tomislav Došlić et al. showed that the global forcing number of graph G has lower bound $\lceil \log_2|M(G)| \rceil$ and upper bound $|E(G)| - |V(G)| + 1$. We can easily show that the lower and upper bounds of the global forcing number for a tree-like polyphenyl system with n hexagons (in particular a polyphenyl chain with n hexagons) and a primitive coronoid polyphenyl system with n hexagons which has no meta- hexagons are all tight. And the global forcing number of a tree-like polyphenyl system with n hexagons (in particular a polyphenyl chain with n hexagons) is n, the global forcing number of a primitive coronoid polyphenyl system with n hexagons which has no meta–hexagons is $n+1$. For a primitive coronoid polyphenyl system with n hexagons which has at least one meta–hexagon, only the lower bound of the global forcing number for this primitive coronoid polyphenyl system is tight, and the global forcing number of it is n. These results are similar to that of the complete forcing number of the polyphenyl system.

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