MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **63** (2010) 393-400

ISSN 0340 - 6253

An optimal perfect matching with respect to the Clar problem in 2-connected plane bipartite graphs

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(Received June 4, 2008)

Abstract

We provide an optimality criteria for a perfect matching with respect to the Clar problem in 2-connected plane bipartite graphs.

1 Introduction

The class of graphs considered here are the 2-connected plane bipartite graphs with perfect matchings. We use $G \equiv G(V, E, F)$ to denote an arbitrary graph in this class, where V is the set of vertices, E is the set of edges and F is the set of inner faces. It will be assumed that the vertices of G are bi-colored, black and white say, such that the end vertices of each edge have different colors. A special type of 2-connected plane bipartite graphs are the so-called hexagonal systems. A *hexagonal system* is a 2-connected plane graph in which every inner face is a regular hexagon of side length one. Hexagonal systems with perfect matchings, i.e., Kekuléan benzenoid systems, are interesting graphs in chemical graph theory [1, 2] since they represent the chemical compounds known as benzenoid hydrocarbons. Throughout this paper, the examples provided are drawn from these graphs.

An interesting optimization problem in 2-connected plane bipartite graphs with perfect matchings is the so-called Clar problem, a definition [3] of which follows. Let P be a set of inner faces of G. We call P a *resonant set* of G (or a *generalized Clar formula* of G) if the faces in P are pair-wise disjoint and there exists a perfect matching of G that contains a perfect matching of each face in P. Let us recall here that every perfect matching of G contains a perfect matching of an inner face of G [4, 5]. The maximum of the cardinalities of all the resonant sets is called the *Clar number* [6]. It was Clar [7] who noticed the significance of this number in the chemistry of benzenoid hydrocarbons. A *maximum cardinality* resonant set (or a *Clar formula*) is a resonant set whose cardinality is the Clar number. By solving the *Clar problem*, we mean obtaining a maximum cardinality resonant set.

The Clar problem can be solved in polynomial time using linear programming algorithms [8, 9, 10, 5]. However, no polynomial-time combinatorial algorithm is available for the Clar problem. The purpose of this paper is to contribute to the development of such an algorithm within the framework described in [11]. Here, it should be noted that polynomial-time combinatorial algorithms for the Clar problem in two special classes of hexagonal systems with perfect matchings do exist [5, 12, 13]. In the remainder of this section, the framework suggested in [11] to solve the Clar problem is reviewed and the contribution of this paper is further specified, but more definitions are needed.

Let M a perfect matching of G and P be a set of inner faces of G. We call P an *M-resonant set* of G if the faces in P are pair-wise disjoint and the perfect matching M contains a perfect matching of each face in P. It is noted that a set of inner faces of G is resonant if and only if it is M-resonant for some perfect matching M [11]. A *maximum cardinality* M-resonant set is an M-resonant set whose cardinality is the maximum of the cardinalities of all the M-resonant sets. It is noted that a maximum cardinality M-resonant set for some perfect matching M is not necessarily a maximum cardinality resonant set [11]. A perfect matching M is *optimal* with respect to the Clar problem if the maximum of the cardinalities of all the M-resonant sets is the Clar number.

The Clar problem can be solved in two stages [11]. We obtain a perfect matching M that is optimal with respect to the Clar problem and then obtain a maximum cardinality M-resonant set. It was shown [11] that a maximum cardinality M-resonant set can be obtained in polynomial time by a combinatorial algorithm. This paper provides optimality criteria for a perfect matching with respect to the

Clar problem. In order to present this optimality criteria, we need to introduce an optimization problem on 2-connected plane bipartite graphs with perfect matching that is closely related to the Clar problem. It is the minimum weight cut cover problem. This will be the subject of section 2 and the optimality criteria will be given in section 3. For graph theory terminology, the reader is referred to [14].

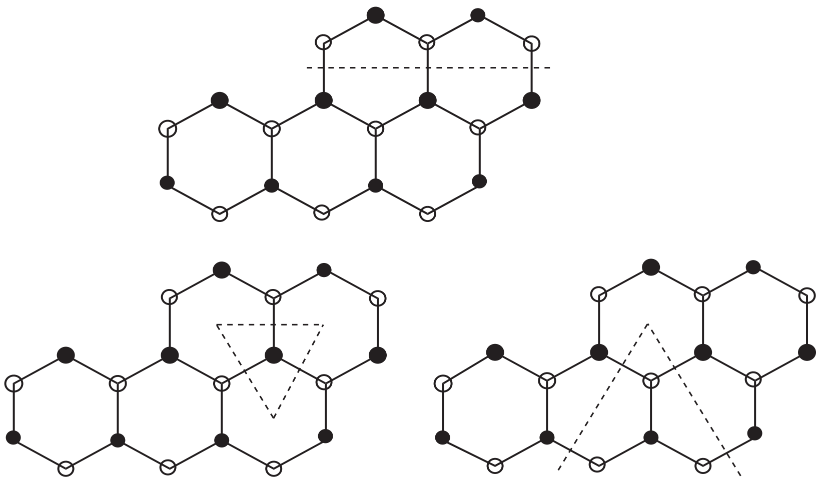


Figure 1: Closed cut lines.

2 The minimum weight cut cover problem

Let G^* be a plane dual of G. Let C be a cycle of G^* and E_C be the set of edges of G intersected by C. It can be easily seen that $G - E_C$ has exactly two components. The cycle C is called a *closed cut line* of G if all the edges of E_C are incident with black vertices of one of the components of $G - E_C$ and white vertices of the other one [6, 15]. Fig. 1 shows examples of closed cut lines of benzo[a]pyrene.

A closed cut line of G *intersects* a face of G if the vertex of G^* corresponding to the face is one of the vertices of the closed cut line. A *cut cover* [6] of G is a set of closed cut lines of G such that each inner face of G is intersected by a closed cut line in the set; it is *perfect* if each inner face is intersected by exactly one closed cut line. Fig. 2 shows both a perfect cut cover and a cut cover that is not perfect.

For every closed cut line C of G, the number of matched edges of G intersected by C is independent of the perfect matching [6, 5, 9] and is called the *weight* of

C. The *weight* of a cut cover is the sum of the weights of its closed cut lines. A *minimum weight* cut cover is a cut cover whose weight is the minimum of the weights of all the cut covers.

Hansen and Zheng [6] showed that for a hexagonal system with perfect matchings, the maximum cardinality of a resonant set is at most the minimum weight of a cut cover and conjectured that equality holds. Abeledo and Atkinson [5, 9] proved the conjecture for 2-connected plane bipartite graphs with perfect matchings; that is,

Theorem 2.1 ([5, 9]). *Let G be a 2-connected plane bipartite graph with perfect matchings. The maximum of the cardinalities of all the resonant sets of G is equal to the minimum of the weights of all the cut covers of G.*

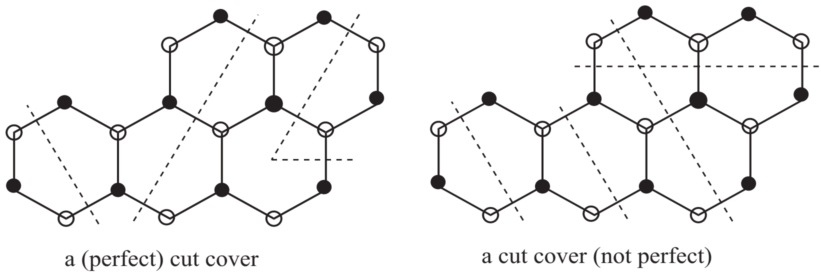


Figure 2: Cut covers.

3 The optimality criteria

Remark 3.1 ([5]). If a closed cut line of G, C say, intersects a face of G, then E_C contains exactly two edges of the boundary of that face. Moreover, if the boundary of that face is M-alternating, where M is a perfect matching of G, then exactly one of these two edges is matched.

Remark 3.2. Given a perfect matching of G and a cut cover $\mathcal{C}$ of G, the *contribution* of a matched edge e to the weight of $\mathcal{C}$ is the number of closed cut lines in $\mathcal{C}$ that intersect e. The sum of the contributions of all the matched edges is the weight of the cut cover $\mathcal{C}$.

Lemma 3.3. *Let G be a 2-connected plane bipartite graph with perfect matchings. Let $\mathcal{C}$ be a minimum weight cut cover of G. Let M be a perfect matching of G*

that is optimal with respect to the Clar problem. For every maximum cardinality M-resonant set P of G, every matched edge not in the boundary of a face in P is not intersected by a closed cut line in $\mathcal{C}$.

Proof. Let P be a maximum cardinality M-resonant set of G. Assume that a matched edge not in the boundary of a face in P is intersected by a closed cut line in $\mathcal{C}$. It follows from Remarks 3.1 and 3.2 that the weight of $\mathcal{C}$ exceeds the cardinality of P. Since M is optimal with respect to the Clar problem, P is a maximum cardinality resonant set of G. Hence, the weight of a minimum weight cut cover of G exceeds the cardinality of a maximum cardinality resonant set of G, a contradiction to Theorem 2.1. $\square$

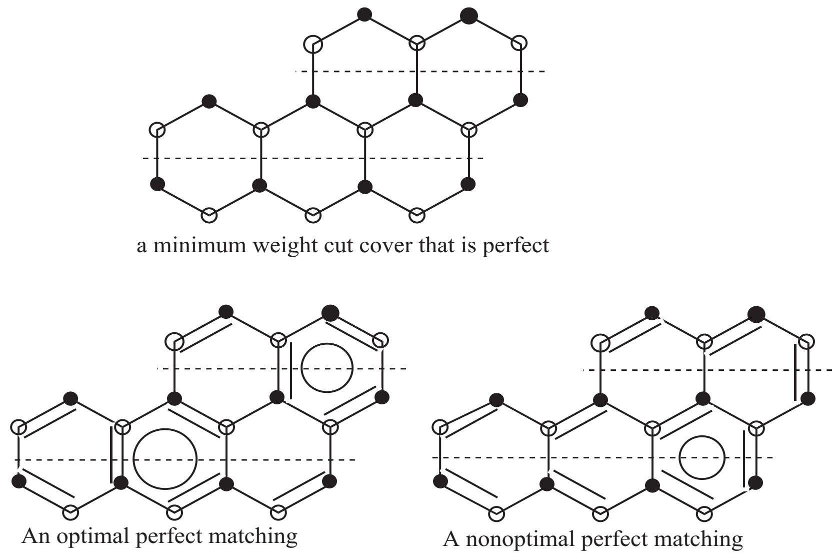


Figure 3: An application of Theorem 3.4.

Theorem 3.4. *Let G be a 2-connected plane bipartite graph with perfect matchings. Let $\mathcal{C}$ be a minimum weight cut cover of G that is perfect. Let M be a perfect matching of G. The following statements are equivalent.*

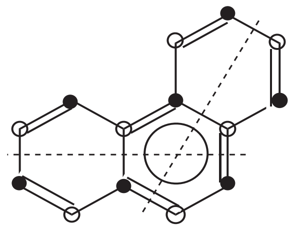
i. The perfect matching M is optimal with respect to the Clar problem.

ii. For every maximum cardinality M-resonant set P of G, every matched edge not in the boundary of a face in P is not intersected by a closed cut line in $\mathcal{C}$.

iii. *There exists a maximum cardinality M-resonant set P of G such that every matched edge not in the boundary of a face in P is not intersected by a closed cut line in $\mathcal{C}$.*

Proof. (i) implies (ii): This follows from Lemma 3.3. (ii) implies (iii): This is obvious. (iii) implies (i): Let P be a maximum M-resonant set of G such that every matched edge not in the boundary of a face in P is not intersected by a closed cut line in $\mathcal{C}$. Since $\mathcal{C}$ is a perfect cut cover, it follows from Remarks 3.1 and 3.2 that the weight of $\mathcal{C}$ is equal to the cardinality of P. By Theorem 2.1, this implies that P is a maximum cardinality resonant set. Hence, the perfect matching M is optimal with respect to the Clar problem. □

Here it is further clarified how to use Theorem 3.4 to determine whether a given perfect matching is optimal with respect to the Clar problem. It should be emphasized that a minimum weight cut cover that is perfect, $\mathcal{C}$ say, should be available to apply Theorem 3.4. Given a perfect matching M, a maximum cardinality M-resonant set, P say, is constructed. If every matched edge not in the boundary of a face in P is not intersected by a closed cut line in $\mathcal{C}$ then the perfect matching is optimal with respect to the Clar problem, otherwise it is not. Figure 3 illustrates an application of Theorem 3.4.



Phenanthrene: Clar number=2

Figure 4: When Theorem 3.4 fails.

Remark 3.5. Theorem 3.4 fails if the condition that the minimum weight cut cover should be perfect is relaxed. Figure 4 shows a minimum weight cut cover that is *not* perfect, $\mathcal{C}$ say, a perfect matching, M say, and a maximum cardinality M-resonant set, P say. It is clear that every matched edges not in the boundary of a hexagon in P is not intersected by a closed cut line in $\mathcal{C}$, yet the perfect matching M is not optimal with respect to the Clar problem.

Acknowledgment

A revised version of this paper was prepared during the author's visit to the mathematics section of The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy.

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