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1-FACTORS AND CHARACTERIZATION OF REDUCIBLE FACES OF PLANE ELEMENTARY BIPARTITE GRAPHS

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Abstract

As a general case of molecular graphs of benzenoid hydrocarbons, we study plane bipartite graphs with Kekulé structures (1-factors). A bipartite graph G is called elementary if G is connected and every edge belongs to a 1-factor of G. Some properties of the minimal and the maximal 1-factor of a plane elementary graph are given.

A peripheral face f of a plane elementary graph is reducible, if the removal of the internal vertices and edges of the path that is the intersection of f and the outer cycle of G results in an elementary graph. We characterize the reducible faces of a plane elementary bipartite graph. This result generalizes the characterization of reducible faces of an elementary benzenoid graph.

Keywords: plane elementary bipartite graph, reducible face, perfect matching, 1-factor, benzenoid graph.

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1. Introduction

Benzenoid graphs (molecular graphs of benzenoid hydrocarbons) are one of the most studied classes of graphs within the chemical graph theory since they represent the chemical compounds known as benzenoid hydrocarbons. For basic characteristics of these structures interested reader is invited to consult the books [1, 3] and a sample of papers [2, 4, 5, 6] with various results on these graphs.

A necessary condition for a benzenoid hydrocarbon to be (chemically) stable is that it possesses Kekulé structures, which describe the distribution of so called

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π-electrons. A Kekulé structure of a conjugated molecule can be represented by a 1-factor (or a perfect matching) of the underlying molecular graph. Particularly, the skeleton of carbon atoms in a benzenoid hydrocarbon is a benzenoid graph. One of the central problems in this area is to find the number of 1-factors/Kekulé structures of a benzenoid graph in order to relate this number to forecast some physico-chemical properties of the underlying compound [3].

On the other hand, some problems involving Kekulé structures of benzenoid hydrocarbons can be extended to 1-factors of some more general classes of graphs, such as hexagonal, bipartite, and plane bipartite graphs. In this paper we will consider plane elementary graphs which embrace elementary benzenoid graphs.

In the next section we formally introduce the concepts and notations of this paper. In Section 3 we show some properties of the so-called minimal and maximal 1-factor of a plane elementary graph. Finally in Section 4 we extend some results previously obtained for elementary benzenoid graphs to plane elementary graphs.

2. Preliminaries

A *matching* of a graph G is a set of pairwise independent edges. A matching is a 1*-factor* or a *perfect matching*, if it covers all the vertices of G. If M is a 1-factor of G and H a subgraph of G then M_H denotes the restriction of M to H.

A bipartite graph G is called *elementary* if G is connected and every edge belongs to a 1-factor of G. *Elementary components* of G are components of the graph obtained from G by removing those edges of G that are not contained in any 1-factor. G is called *weakly elementary* if every inner face of every elementary component of G is still a face of the original G. Note that all elementary graphs are also weakly elementary.

A *benzenoid graph* is a finite connected graph with no cut vertices in which every interior region is bounded by a regular hexagon of a side length 1. It is well known that benzenoid graphs are weakly elementary.

Let G be plane bipartite graph. Let us call the boundary of the infinite face of G the *outer boundary* or the *outer cycle*. A cycle (face) of a graph G is said to be *resonant*, if the edges of the cycle (face) appear successively in and off some 1-factor of G.

Theorem 1 [11, 17]**.** *Assume that a* 2*-connected plane bipartite graph G is weakly elementary. Then the following statements are equivalent:*

1. *G is elementary,*
2. *each interior face of G is resonant,*
3. *the outer cycle of G is resonant.*

Let G be a plane bipartite graph. We always color properly all vertices of G with two colors, black and white, so that two end vertices of each edge are of different colors.

The symmetric difference of finite sets A and B is defined as $A \oplus B := (A \cup B) \setminus (A \cap B)$.

Let G be a plane bipartite graph. Then the vertex set of the *resonance graph* $R(G)$ (also called the *Z-transformation* graph, see e.g. [14]) of G consists of the 1-factors of G, two 1-factors being adjacent whenever their symmetric difference forms the edge set of an interior face of G. The construction of the resonance graph of a simple benzenoid graph is presented in Figure 1.

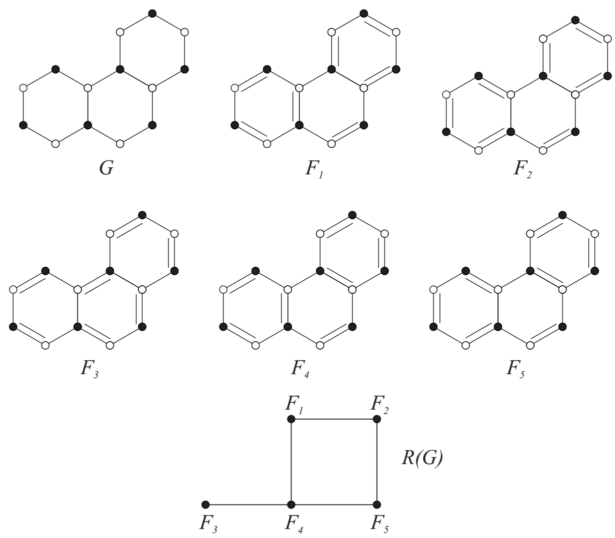

Figure 1. Benzenoid graph G, 1-factors F_1, F_2, F_3, F_4, F_5 of G, and its resonance graph $R(G)$.

Let C denote a cycle of a bipartite graph G. We say an edge of C is *proper* (*improper*) if it goes from white (black) to black (white) end-vertex by the clockwise orientation of C.

Let M be a 1-factor of G. A cycle C is *M-alternating* if edges of C appear alternately in and off the M. An M-alternating cycle C of G is said to be *proper* (*improper*) [16] if every edge of C belonging to M is proper (improper). A 1-factor M is said to be *peripheral* if the outer cycle of G is M-alternating.

Let G be a plane bipartite graph. The set of all 1-factors of G is denoted as $\mathcal{M}(G)$, or simply $\mathcal{M}$ when the considered graph G is obvious.

The *resonance digraph* $\vec{R}(G)$ is defined [15, 14] as a digraph on $\mathcal{M}(G)$ such that there exists an arc from M_1 to M_2 provided that $M_1 \oplus M_2$ is a proper (improper) M_1 (M_2)-alternating cycle that is an inner facial boundary of G.

Ignoring directions of arcs of $\vec{R}(G)$ we get the usual resonance graph [7, 10]. For a plane bipartite graph G, $\vec{R}(G)$ is the Hasse diagram of $\mathcal{M}(G)$ [8].

It was shown that G has a unique 1-factor $M_{\hat{0}}$ such that G has no proper $M_{\hat{0}}$-alternating cycles [16]. We call $M_{\hat{0}}$ the *minimal 1-factor* of G, since $M_{\hat{0}}$ is the minimal element of the poset induced by $\mathcal{M}(G)$ [15, 8]. In addition, G has a unique 1-factor $M_{\hat{1}}$ such that G has no improper $M_{\hat{1}}$-alternating cycles. $M_{\hat{1}}$ is called the *maximal* 1*-factor* of G.

Proposition 2 [12]**.** *Let G be an elementary benzenoid graph. Then the outer cycle of G is improper $M_{\hat{0}}$-alternating as well as proper $M_{\hat{1}}$-alternating.*

An important property of elementary bipartite graphs is the bipartite ear decomposition [9]. Zhang and Zhang evolved this concept and presented the so-called reducible face decomposition [17].

It was proved [17] that a plane bipartite graph G is elementary if and only if G has a reducible face decomposition starting with the boundary of any interior face of G. This gives the construction method for plane elementary bipartite graphs: starting with some face, then adding one new face at each step gives any plane elementary bipartite graph. A face f of a plane bipartite graph G is *peripheral* if the peripheries of G and f have a path of positive length in common. Let G be a plane elementary bipartite graph. Let f be a peripheral face of G and P a common path of the peripheries of f and G. Let $G - f$ denote the resultant subgraph of G by removing the internal vertices and the corresponding incident edges of P. Note that P can be a path on two vertices therefore no internal vertices exist, yet in this case we can remove only the edge between these two vertices. If $G - f$ is elementary than we call f a *reducible face* of G.

If G is a plane elementary bipartite graph with at least two finite faces, then G has at least two reducible faces [17].

The reducible hexagons of an elementary benzenoid graph can be characterized as follows.

Theorem 3 [12]**.** *Let G be an elementary benzenoid graph. Then h is a reducible hexagon of G if and only if the following hold*

(i) *the common periphery of h and G is a path of odd length and*

(ii) *G admits a peripheral* 1*-factor M such that the edges of h form an M-alternating cycle.*

3. Minimal and Maximal 1-factor

Let G be a plane bipartite graph. Let $\mathcal{F}$ be the set of all finite faces of G. For each $M \in \mathcal{M}$, a function ϕ_M is defined on $\mathcal{F}$ as follows: for any $f \in \mathcal{F}$, $\phi_M(f)$ is the number of cycles in $M \oplus M_{\hat{0}}$ with f in their interiors. Note that f is regarded as the set of edges bounding the face.

Lemma 4 [15]**.** *For M, $M' \in \mathcal{M}$, M and M' are adjacent in $R(G)$ if and only if $|\phi_M(f) - \phi_{M'}(f)| = 1$ for $f = f_0$, where f_0 is an inner face bounded by the cycle $M \oplus M'$ and 0 for the other faces in $\mathcal{F}$.*

In other words, M and M' are adjacent in $R(G)$ if and only if $M \oplus M'$ forms an inner face f_0 of G and f_0 is both M and M'-alternating.

Since 1-factors compile pairwise independent edges, all the cycles induced by $M \oplus M_{\hat{0}}$ have to be disjoint. It follows that for every peripheral face f, $\phi_M(f)$ is either 1 or 0.

It was shown [15] that the resonance graph of a plane elementary graph is a median graph.

The following lemma generalizes the result on elementary benzenoid graphs [13]. The proof goes analogously, however, for the sake of completeness, we repeat the arguments.

Lemma 5. *Let e be an edge on the boundary of a plane elementary graph G and let f be the face of G containing e. Let $e \in M'$ and let $\phi_{M'}(f) = i$, $i = 0, 1$. If M is an arbitrary 1-factor of $R(G)$, then $\phi_M(f) = i$ if and only if M contains e.*

Proof. Let $\phi_{M'}(f) = 0$.

Suppose that a 1-factor M containing e such that $\phi_M(f) = 1$ exists. Let then $M' = M_1, M_2, \ldots, M_k = M$ denote a shortest path between M and M' in $R(G)$. Since $R(G)$ is a partial cube (and a median graph), there exists exactly one pair M_i, M_{i+1} such that $\phi_{M_i}(f) = 0$ and $\phi_{M_{i+1}}(f) = 1$. Thus, for every $j = 1, \ldots, i-1, i+1, \ldots, k$, $M_j \oplus M_{j+1} \neq f$. Since e does not belong to any other face but f, M_i and M_{i+1} must contain e. But then $M_i \oplus M_{i+1} \neq f$ and we obtain a contradiction.

Suppose that such a 1-factor M not containing e with $\phi_M(f) = 0$ exists. Let then $M' = M_1, M_2, \ldots, M_r = M$ denote a shortest path between M and M' in $R(G)$. $R(G)$ is a partial cube, thus for every $i = 1, \ldots, r-1$, $M_i \oplus M_{i+1} \neq f$. Since e does not belong to any other face but f, M_r must contain e and again we obtain a contradiction.

If $\phi_{M'}(f) = 1$, the proof goes analogously. ■

The following lemmas are illustrated by the example shown in Figure 2.

Lemma 6. *Let G be a plane elementary graph. Then the minimal* (*maximal*) *1-factor of G does not admit a proper* (*improper*) *edge of the outer cycle of G.*

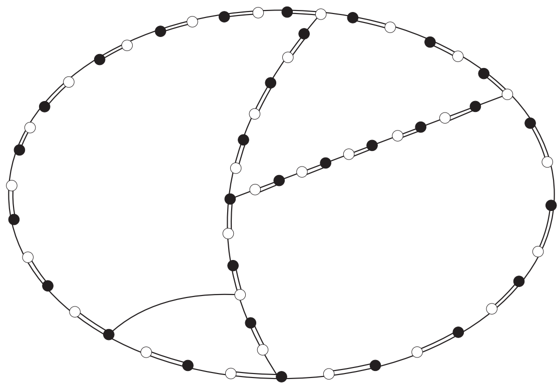

Figure 2. A plane elementary graph with its minimal 1-factor.

Proof. Let C denote the outer cycle of G. Suppose that the minimal 1-factor $M_{\hat{0}}$ contains a proper edge e of C. Let e belong to the face f of G. Obviously, $\phi_{M_{\hat{0}}}(f) = 0$ and $\phi_{M_{\hat{1}}}(f) = 1$. Let $M_{\hat{0}} = M_1, M_2, \ldots, M_k = M_{\hat{1}}$ denote a shortest path between $M_{\hat{0}}$ and $M_{\hat{1}}$ in $R(G)$. Since $R(G)$ is a partial cube (and a median graph), there exists exactly one pair M_i, M_{i+1} such that $\phi_{M_i}(f) = 0$ and $\phi_{M_{i+1}}(f) = 1$. Note that by Lemma 5 the 1-factor M_{i+1} does not contain e. Moreover, M_i does contain e. But then f cannot be improper (proper) M_i (M_{i+1})-alternating and we obtain a contradiction.

The proof for the maximal 1-factor of G is analogous. ■

Lemma 7. *Let G be a plane elementary bipartite graph. Then the minimal* (*maximal*) 1*-factor of G contains every improper* (*proper*) *edge of the outer cycle of G.*

Proof. Let C denote the outer cycle of G. Suppose that the minimal 1-factor $M_{\hat{0}}$ does not contain an improper edge e of C. Let e belong to the face f of G. Obviously, $\phi_{M_{\hat{0}}}(f) = 0$ and $\phi_{M_{\hat{1}}}(f) = 1$. From Lemma 5 it follows that $M_{\hat{1}}$ does contain e. But e is improper and by Lemma 6 we obtain a contradiction.

The proof for the maximal 1-factor of G is analogous. ■

From Lemma 6 and Lemma 7 we obtain the following

Proposition 8. *Let G be a plane elementary bipartite graph. Then the outer cycle of G is improper $M_{\hat{0}}$-alternating as well as proper $M_{\hat{1}}$-alternating.*

Corollary 9. *Let f be a peripheral face and M a* 1*-factor of a plane elementary bipartite graph G. Then $\phi_M(f) = 1$ ($\phi_M(f) = 0$) if and only if a proper* (*improper*) *edge on the common boundary of f and the outer cycle of G belongs to M.*

4. Characterization of Reducible Faces

Theorem 10. *Let G be a plane elementary graph. Then f is a reducible face of G if and only if the following hold*

(i) *the common periphery of f and G is a path P of odd length and*

(ii) *G admits a peripheral 1-factor M such that the edges of f form an M-alternating cycle.*

Proof. Note that (i) is a necessary condition which follows from the definition of reducible faces.

Suppose that f is a reducible face of a plane elementary graph G. Since G is elementary and f is its reducible face then $G' = G - f$ is also elementary. By Theorem 1 a peripheral 1-factor M' of G' exists. Let C' denote the outer cycle of G'.

Suppose P is a path from a black to a white vertex in the clockwise direction of the outer cycle C of G. Note that C' is either proper or improper M'-alternating. If C' is improper M'-alternating, we set $M' := M' \oplus C'$ (M' now contains all proper edges of C'). Let M_P denote the set of all proper edges of P. Since both end-vertices of P are in M', clearly $M = M' \cup M_P$ is a peripheral 1-factor of G, see Figure 3a. It follows that $M \oplus C$ is also a peripheral 1-factor of G, moreover edges of f form a $M \oplus C$-alternating cycle, see Figure 3b.

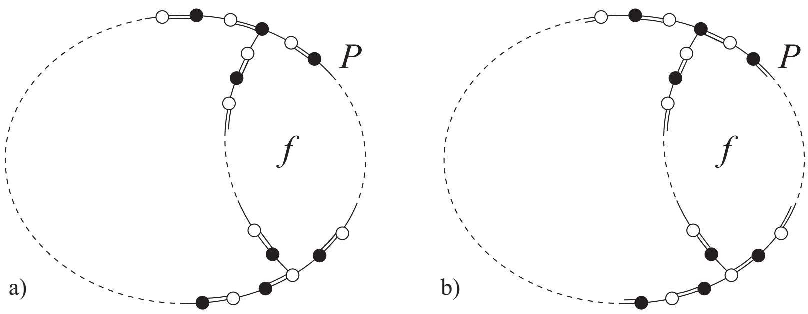

Figure 3. P is a path from a black to a white vertex.

If P is a path from a white to a black vertex in the clockwise direction of C', consider the peripheral 1-factor M' of G' such that it contains all improper edges of C'. Let now the set M_P be the set of all improper edges of P, see Figure 4a. Again, $M = M' \cup M_P$ is a peripheral 1-factor of G and the edges of f form a $M \oplus C$-alternating cycles, see Figure 4b. This concludes the if part of the proof.

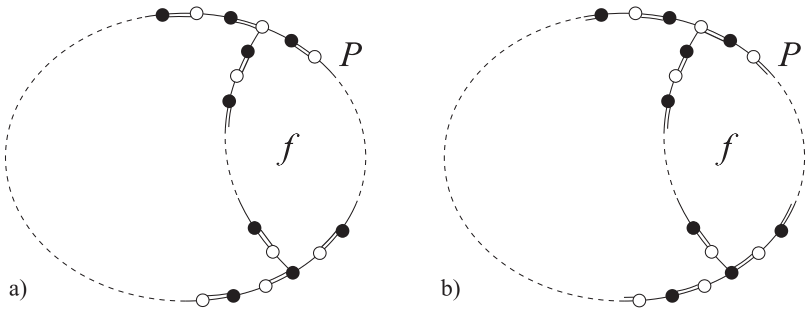

Figure 4. P is a path from a white to a black vertex.

For the converse let G admit a peripheral 1-factor M such that the edges of f form a M-alternating cycle. If C is a proper M-alternating cycle (Figure 4b) then the path P goes from a white to a black vertex in the clockwise direction of C. Consider now $M' = M \oplus C$ restricted to $G' = G - f$. Clearly, M' is a peripheral 1-factor of G' and from Theorem 1 it follows that G' is a plane elementary graph. We have proven that f is a reducible face of G.

On the other hand, if C is an improper M-alternating cycle (Figure 3b), then the path P goes from a black to a white vertex in the clockwise direction of C. Again, considering $M' = M \oplus C$ restricted to $G' = G - f$ we see that M' is a peripheral 1-factor of G'. Form Theorem 1 it follows that G' is elementary and f a reducible face of G. ∎

Corollary 11. *Let G be a plane elementary graph and let $M_{\hat{0}}$, $M_{\hat{1}}$, and C be the minimal 1-factor, the maximal 1-factor and the outer cycle of G, respectively. Then at least one of 1-factors: $M_{\hat{0}}$, $M_{\hat{1}}$, $M_{\hat{0}} \oplus C$, and $M_{\hat{1}} \oplus C$ admits a reducible face of G.*

Proof. For a peripheral 1-factor in the proof of Theorem 10 one can take $M_{\hat{0}}$ or $M_{\hat{1}}$. ∎

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