Kekulé Patterns and Clar Patterns in Bipartite Plane Graphs

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Received May 11, 1995[⊗]

Let G be a finite bipartite plane graph. In a chemical context, a set of pairwise disjoint edges that cover all vertices of G (i.e., a perfect matching of G) is called a *Kekulé pattern* of G, and a set of pairwise disjoint cells of G such that the deletion of all vertices incident to these cells results in a graph that has a Kekulé pattern, or is empty, is called a *Clar pattern* of G. Let $k(G)$ and $c(G)$ denote the number of Kekulé patterns and of Clar patterns of G, respectively. It is shown that $k(G)$ is not smaller than $c(G)$ and that equality holds if G is an outerplane graph. This result generalizes a well-known proposition of the theory of benzenoid hydrocarbons; the proof uses a new idea.

1. INTRODUCTION

1.1. Chemical Background. During the last two decades, applications of graph theory to benzenoids (polycyclic aromatic hydrocarbons; see Figure 1) have raised great interest in general resonance theory. With this respect, W. C. Herndon's work[1,2] and the conjugated circuit model of M. Randić[3,4] are particularly important. The sextet polynomial found by H. Hosoya and T. Yamaguchi[5] allows a systematic enumeration of Kekulé patterns in catacondensed benzenoids (Figure 1); it reflects essential parts of E. Clar's sextet theory.[6] Applications of the sextet polynomial concept in various directions can be found, e.g., in refs 7–10; generalizing the sextet polynomial, I. Gutman[11,12] and P. John[13] defines the so-called "cell polynomial" for polycyclic unsaturated (in particular, for catacondensed) hydrocarbons.

In Clar's sextet theory, Clar patterns play a central role. In particular, the following proposition has been proved.[11,14,15]

(*) For any benzenoid B, the number of Kekulé patterns of its molecular graph is not smaller than the number of Clar patterns. If B is catacondensed, then these two numbers coincide.

In this paper, it is shown that this proposition (*) generalizes to arbitrary bipartite plane graphs; the proof, however, needs a new idea. Therefore, the authors have found it worth presenting the general theorem and its proof.

1.2. Terminology and Notation. All graphs considered in this paper are finite planar graphs that are allowed to have multiple edges. A *plane graph* is an (intersection-free) embedding of a planar graph in the Euclidean plane. A finite face **f** of the plane graph G is called a *cell* if the boundary of **f** is a circuit. The (edge set of the) boundary circuit of a cell **z** is denoted by z. The boundary b of the infinite face is briefly referred to as the *boundary of G*. An edge is a *boundary edge* if it belongs to b; otherwise, it is an *internal* edge.

An *outerplane graph* is a connected plane graph all of whose vertices lie on its boundary; an *outerplane map* is an outerplane graph whose boundary is a circuit (Figure 1, part 1.1).

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[⊗] Abstract published in *Advance ACS Abstracts*, October 15, 1995.

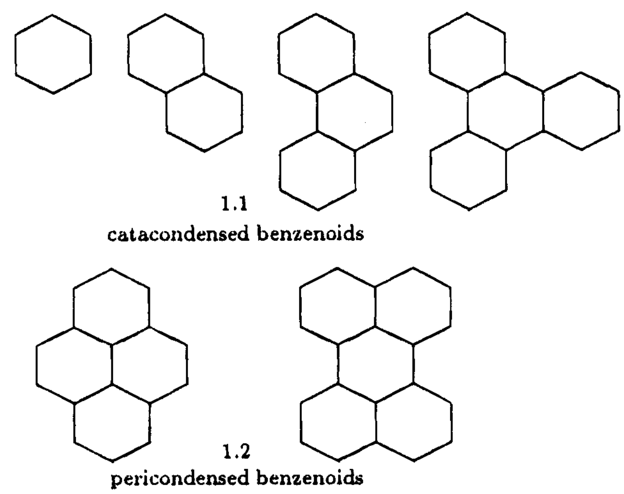

Figure 1. Examples of benzenoids.

A set of pairwise disjoint edges of a graph G that cover all vertices of G (i.e., a perfect matching, or 1-factor, of G) is called a *Kekulé pattern* or, briefly, a *k-pattern* of G.

Let Z be a subset of the cell set of a finite bipartite plane graph G and denote by $G - Z$ the plane graph obtained by removing from G all vertices incident to the cells in Z and all edges incident to these vertices. If the cells in Z are pairwise disjoint and $G - Z$ has a k-pattern or is empty, then Z is called a *Clar pattern* or, briefly, a *c-pattern* of G (Figure 2). Note that Z is allowed to be empty.

Let $\mathcal{K}(G)$ and $\mathcal{C}(G)$ denote the set of k-patterns and the set of c-patterns of G, respectively. Let $k(G) = |\mathcal{K}(G)|$, $c(G) = |\mathcal{C}(G)|$.

2. THEOREM

For any finite bipartite plane graph G, $k(G) \geq c(G)$ where equality holds if G is outerplane.

3. PROOF

3.1. Preliminaries. Let $\mathcal{B}$ denote the set of all finite connected bipartite plane graphs that have a k-pattern. It suffices to prove the theorem for plane graphs $B \in \mathcal{B}$.

Let $B \in \mathcal{B}$. The vertex set of B has a unique partition into two classes, say X and Y, such that each edge of B connects a vertex in X with a vertex in Y. Orient all edges

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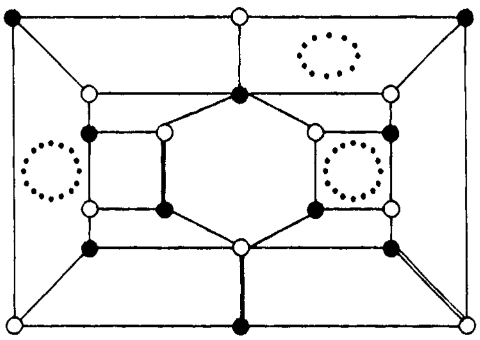

Figure 2. The cells marked by a dotted circle form a c-pattern.

from X to Y and let ω be the orientation of B so obtained. With respect to ω, each edge has a left bank and a right bank: mark the left bank "+" and the right bank, "−". Note that any two banks that lie in the same face and are consecutive on its boundary are marked differently (Figure 3). Interchanging X and Y is equivalent to interchanging + and −, thus there are precisely two such markings which we will call *the nice markings* of B. The pair of the nice markings of B is denoted by $\mu(B)$.

Let $B \in \mathscr{B}$ and $m \in \mu(B)$; let B' be a connected subgraph of B and $m|_{B'}$ the restriction of m to B'.

Observation 1. $m|_{B'} \in \mu(B')$. (Immediate.)

Corollary 1. *Let c be a circuit of B and let $m \in \mu(B)$. Then the banks of the edges of c that lie in the interior of c are marked alternatingly + and −.*

We shall now prove three lemmas from which the theorem immediately follows.

3.2. Positive cells. Let $B \in \mathscr{B}$, $m \in \mu(B)$; let $\mathbf{z}$ be a cell of B let z^+ denote the set of those edges of z whose banks in the interior of z (i.e., in $\mathbf{z}$) are marked +. Let $K \in \mathscr{K}(B)$.

Cell $\mathbf{z}$ is called *(m, K)-positive* if $z^+ \subseteq K$. Let $Z^+ (B; m, K)$ denote the set of (m, K)-positive cells of B (Figure 3). Clearly, the cells in $Z^+ (B; m, K)$ are pairwise disjoint.

Lemma 1. *Let $B \in \mathscr{B}$, $m \in \mu(B)$, and $K \in \mathscr{K}(B)$. Then $Z+ (B; m, K) \in \mathscr{C}(B)$.*

Proposition 1. *Let $B \in \mathscr{B}$, $m \in \mu(B)$. Then there is a k-pattern $K_0 \in \mathscr{K}(B)$ such that $Z^+ (B; m, K_0) = \varnothing$.*

Proof. Assume that the assertion is not true. Then, for every $K \in \mathscr{K}(B)$, there is an (m, K)-positive cell; for each K, select such a cell and denote it by $\mathbf{z}(K)$. Let $F(K)$ be the k-pattern obtained from K by interchanging in $z(K)$ the edges belonging to K with the edges not belonging to K.

Select an arbitrary k-pattern $K_1^* \in \mathscr{K}(B)$; iterating the application of F, we obtain an infinite sequence $s^* = (K_1^*, K_2^*, ...)$ where $K_{n+1}^* = F(K_n^*)$. The number of k-patterns being finite, s^* must become periodic, i.e., there are integers p and q such that $K_1^*, K_2^*, ..., K_{q+p-1}^*$ are pairwise distinct and $K_{q+p}^* = K_q^*$.

Let $K_1 = K_q^*$ and, as before, form the sequence $s = (K_1, K_2, ...)$ where $K_{n+1} = F(K_n)$. Clearly, s is strictly periodic with primitive period p. Thus, $z(K_{n+p}) = \mathbf{z}(K_n)$ for any integer n. Let $r \in \{1, 2, ..., p\}$ and let $\mathbf{f}$ be a face having an edge, say e, in common with $\mathbf{z}(K_r)$. If e does (does not) belong to K_r then e does not (does) belong to $K_{r+1} = F(K_r)$, but it does (does not) belong to $K_{r+p} = K_r$. This implies that $\mathbf{f}$ coincides with one of the cells $\mathbf{z}(K_{r+1})$, $\mathbf{z}(K_{r+2})$, ..., $\mathbf{z}(K_{r+p-1})$ and, therefore, is a member of the set $S = \{\mathbf{z}(k_1), \mathbf{z}(K_2), ..., \mathbf{z}(K_p)\}$. Thus every face that has an edge in common with one of the cells in $\mathbf{S}$ is itself a member of $\mathbf{S}$. We conclude that all faces of B, including the infinite face, are elements of $\mathbf{S}$, a contradiction.

Remark: For $B \in \mathscr{B}$ and $m \in \mu(B)$, we define the *m-transformation graph* $T = T_m(B)$ as a directed graph as follows: the set of vertices of T is the set of $\mathscr{K}(B)$; there is an arc from K_i to K_j if B has an (m, K_i)-positive cell $\mathbf{z}$ such that $K_j = (K_i - z^+) \cup (z - z^+)$.

By the proof of proposition 1, T has no directed circuits, i.e., it is acyclic. This proposition is related to a result of Gutman et al.,[14] see also Zhang et al.[16,17]

Lemma 2. *Let $B \in \mathscr{B}$, $m \in \mu(B)$, and $C \in \mathscr{C}(B)$. Then there is a $K \in \mathscr{K}(B)$ such that $C = Z^+ (B; m, K)$.*

Proof. Let $C = \{\mathbf{z}_1, \mathbf{z}_2, ..., \mathbf{z}_k\}$. Let $G' = B - C$ have components $B_1, B_2, ..., B_h$ and let $m_i = m|_{B_i}$, $i = 1, 2, ..., h$. By proposition 1, there is a k-pattern $K_i \in \mathscr{K}(B_i)$ such that $Z^+ (B_i, m_i, K_i) = \varnothing$ ($i = 1, 2, ..., h$). Let $K' = \cup_{i=1}^{h} K_i$ and $K'' = \cup_{j=1}^{k} z_j^+$. Then $K = K' \cup K''$ is a k-pattern of B satisfying $Z^+(B; m, K) = C$.

3.3. Outerplane Graphs. Let $v(B), f(B), e(B); i(B), b(B)$, and $z(B)$ be the number of vertices, faces, edges; internal edges, boundary edges, and cells of $B \in \mathscr{B}$, respectively. Clearly, $e(B) = b(B) + i(B)$; by Euler's formula, $v(B) + f(B) = e(B) + 2$, thus $f(B) - 1 = b(B) - v(B) + i(B) + 1$.

Observation 2. *For any outerplane map M, $z(M) = f(M) - 1$, $v(M) = b(M)$.* (Immediate.)

Corollary 2. $z(M) = i(M) + 1$.

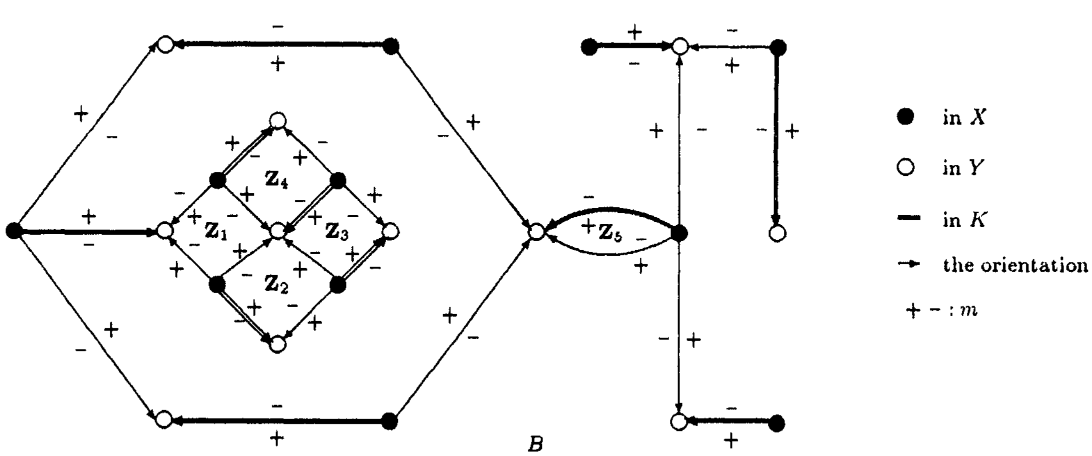

Figure 3. A plane bipartite graph $B \in \mathscr{B}$ with a k-pattern K, an orientation ω, and a nice marking m. The cell set is $\{\mathbf{z}_1, \mathbf{z}_2, \mathbf{z}_3, \mathbf{z}_4, \mathbf{z}_5\}$. Cells $\mathbf{z}_3$, $\mathbf{z}_5$ are, and cells $\mathbf{z}_1$, $\mathbf{z}_2$, $\mathbf{z}_4$ are not, (m, K)-positive, thus $Z^+(B; m, K) = \{\mathbf{z}_3, \mathbf{z}_5\}$. Here $k(B) = c(B) = 8$.

Lemma 3. *Let $B \in \mathscr{B}$ be a bipartite outerplane graph and $m \in \mu(B)$. Let $K_1, K_2 \in \mathscr{K}(B)$ satisfy $Z^+(B; m, K_1) = Z^+(B; m, K_2)$. Then $K_1 = K_2$.*

Proof. Assume $K_1 \neq K_2$. Let $G' = B - Z^+(B; m, K_1)$; clearly, $K_1' = K_1|_{G'}$ and $K_2' = K_2|_{G'}$ are distinct k-patterns of G'. The edges of G' that are in K_1' or K_2' but not in both form disjoint (K_1', K_2')-alternating circuits; let c be one of them. The subgraph M of G' consisting of c and the edges in the interior of c (which, clearly, do not belong to K_1' or K_2') is a bipartite outerplane map with nice marking $m|_M$. Note that $c = K_1'' \cup K_2''$ where $K_1'' = K_1'|_M = K_1|_M$ and $K_2'' = K_2'|_M = K_2|_M$ are disjoint k-patterns of M. By corollary 1, the banks of the edges of c that lie in the interior of c are marked + and − alternatingly: without loss of generality assume that those of these banks marked + belong to edges of K_1''. Let $\mathbf{z}_1, \mathbf{z}_2, ..., \mathbf{z}_k$ be the cells of M; note that each cell $\mathbf{z}_j$ is also a cell of G', therefore, $\mathbf{z}_j \notin Z^+(B; m, K_1)$ implying $|K_1'' \cap z_j| = |K_1 \cap z_j| \leq |z_j|/2 - 1, j = 1, 2, ..., k$. We obtain

$$
\begin{aligned}
v(M)/2 = |K_1''| &= \sum_{j=1}^{k} |K_1'' \cap z_j| \leq \sum_{j=1}^{k} (|z_j|/2 - 1) \\
&= 1/2 \sum_{j=1}^{k} |z_j| - k = b(M)/2 + i(M) - k \\
&= v(M)/2 + i(M) - k
\end{aligned}
$$

thus $i(M) \geq k = z(M)$, contradicting corollary 2.

3.4. The Final Step. Let $B \in \mathscr{B}$ and $m \in \mu(B)$; set $\tilde{\mathscr{C}} = \{Z^+(B; m, K) | K \in \mathscr{K}(B)\}$.

By lemmas 1 and 2, $\tilde{\mathscr{C}} = \mathscr{C}(B)$, thus $k(B) \geq c(B)$.

If B is outerplane, then, by lemma 3, the elements $Z^+(B; m, K)$ of $\tilde{\mathscr{C}}$ are pairwise distinct, thus there is a (1,1)-correspondence between $\mathscr{K}(B)$ and $\mathscr{C}(B)$ implying $k(B) = c(B)$.

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CI950047H