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Regular coronoids and 4-tilings

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ABSTRACT

A benzenoid is a finite connected plane graph with no cut vertices in which every interior region is bounded by a regular hexagon of side length one. A coronoid G is a connected subgraph of a benzenoid such that every edge lies in a hexagon of G and G contains at least one non-hexagon interior face, which should have a size of at least two hexagons. A polyhex is either a benzenoid or a coronoid. A coronoid is said to be regular if it can be generated from a single hexagon by a series of specific additions of hexagons. The vertices of the inner dual $I(G)$ of a polyhex G are the centers of all hexagons of G, two vertices being adjacent if and only if the corresponding hexagons share an edge in G. The graph $I_S(G)$ is obtained from $I(G)$ by removing a set of internal edges S. A polyhex G admits a 4-tiling, if every triple of pairwise adjacent hexagons of G belongs to a 4-cycle face of $I_S(G)$. We show that a coronoid G admits a 4-tiling if and only if G is regular. This fact enables us to prove that a coronoid G is regular if and only if G can be generated from a single hexagon by a series of normal additions plus corona condensations of mode A_2. This result confirms Conjecture 6 stated in [9].

1. Introduction and preliminaries

A *benzenoid system* or a *hexagonal system* or simply a *benzenoid* is a finite connected plane graph with no cut vertices in which every interior region is bounded by a regular hexagon of a side length one. A benzenoid graph G is *catacondensed* if any triple of hexagons of G has empty intersection, otherwise it is *pericondensed*.

A coronoid G is a connected subgraph of a hexagonal system such that every edge lies in a hexagon of G and G contains at least one non-hexagon interior face (called *corona hole*), which should have a size of at least two hexagons. A coronoid is said to be *single* if it contains exactly one hole. A *polyhex* is either a benzenoid or a coronoid.

In general, coronoids can be regarded as benzenoids with holes. Since benzenoids and coronoids have counterparts in what are called benzenoid and coronoid hydrocarbons, the studies of such systems are of significant chemical relevance [1,2].

The paper is organized as follows. In the sequel of this section we give basic definitions and concepts needed in this paper. In Section 2, the main result of this paper is presented: we show that a coronoid G admits a 4-tiling if and only if G is regular. We use this result in the last section of the paper presenting the theorem which shows that a single coronoid is regular if and only if it can be generated from a single hexagon by a series of normal additions plus only one corona condensation of mode A_2. As a corollary to this result, we show that a coronoid G is regular if and only if G can be generated from a single hexagon by a series of normal additions plus corona condensations of mode A_2. This corollary confirms Conjecture 6 stated in [9].

A *matching* of a graph G is a set of pairwise independent edges. If a matching covers all the vertices of G, then it is called *perfect*. In the chemical graph theory, perfect matchings are called *Kekulé structures*. For benzenoids or coronoids, *Kekulean*

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systems are those which possess a Kekulé structure. A Kekulean system is called *normal* if every edge is contained in a Kekulé structure; essentially disconnected otherwise. A normal benzenoid is also called *elementary*.

Let M be a perfect matching of graph G. A cycle C is of G is M-*alternating* if edges of C appear alternately in and off the M.

A graph G is called *bipartite* if its vertex set can be divided in two disjoint sets V_1 and V_2 such that $V_1 \cup V_2 = V(G)$ and no two vertices from the same set are joined by an edge. If $u \in V_1$ and $v \in V_2$, then we say that u and v are of different *colors*. Every benzenoid graph G is clearly bipartite. A bipartite graph G is called *elementary* if G is connected and every edge belongs to a perfect matching of G.

The *periphery* of a polyhex consists of the boundaries of all non-hexagon faces of G, i.e., the boundary of the infinite face of G and the boundaries of corona holes of G. The boundary of the infinite face of G is called the *boundary of* G.

Let f denote a face of a plane elementary bipartite graph G such that the peripheries of G and f have a nonempty intersection. Let then $G-f$ denote the resultant subgraph of G by removing the edges and internal vertices of paths that the peripheries of G and f have in common.

A hexagon h of a polyhex G is called a *pendant hexagon* if a common path of the peripheries of h and G is a path of length five.

A hexagon h of a polyhex G is *peripheral* if the peripheries of G and h have a nonempty intersection and *internal* otherwise.

Let h be a peripheral hexagon of an elementary benzenoid graph G. If $G-h$ is elementary, then we call h a *reducible hexagon* of G. It is well known that an elementary benzenoid graph admits at least two reducible hexagons [7,10]. The sequence of hexagons $h_1, h_2, h_3, \ldots, h_r$ is called *reducible* if h_i is a reducible hexagon of G_i such that $G_r = G, G_{i-1} = G_i - h_i, i = r, r-1, \ldots, 2$ and $h_1 = G_1$.

The sequence of reducible hexagons of elementary benzenoid graphs has another explanation with respect to a broader class of elementary bipartite graphs. Let x be an edge. Join its end vertices by a path P_1 of odd length (first ear). Then proceed inductively to build a sequence of bipartite graphs as follows: if $G_{r-1} = x+P_1+P_2+\cdots+P_{r-1}$ has already been constructed, add the rth *ear* P_r (of odd length) by joining any two vertices of different colors in G_{r-1} such that P_r has no internal vertices in common with G_{r-1}. The decomposition $G_r = x + P_1 + P_2 + \cdots + P_r$ is called an *(bipartite) ear decomposition* of G_r.

A bipartite graph is elementary if and only if it has an (bipartite) ear decomposition [3,4].

Zhang and Zhang [10] narrowed the concept of an ear decomposition for plane elementary bipartite graphs as follows. An ear decomposition $(G_1, G_2, \ldots, G_r(= G))$ (equivalently, $G = x + P_1 + P_2 + \cdots + P_r$) of a plane elementary bipartite graph G is called a *reducible face decomposition* (RFD) if G_1 is the boundary of an interior face of G and the ith ear P_i lies in the exterior of G_{i-1} such that P_i and a part of the periphery of G_{i-1} surround an interior face of G for all $2 \le i \le r$.

For a reducible face decomposition $G = x + P_1 + \cdots + P_r$, every P_i and a path with odd length on the boundary of G_{i-1} surround an interior face s_i. Hence a RFD of G is also associated with a sequence $s_1, \ldots, s_r$ of all the interior faces of G such that $G_{i-1} = G_i - s_i$. We say that s_i is a *reducible face* of G_i.

Theorem 1 ([10]). *Let G be a plane bipartite graph other than K_2. Then G is elementary if and only if G has a reducible face decomposition starting with the boundary of any interior face of G.*

Theorem 2 ([10]). *Let G be a plane elementary bipartite graph with at least three finite faces. Then G has at least two reducible faces.*

If G is an elementary benzenoid graph, then an ear P_i of a reducible face decomposition $(G_1, G_2, \ldots, G_r(= G))$ together with a part on the perimeter of the infinite face forms a new hexagon, say h_i, of G_i. Note that P_i is of length five, three or one. In other words, h_i admits one, three, or five adjacent hexagons in G_i; therefore we say that we obtain G_i from G_{i-1} such that the added hexagon acquires the mode L_1, L_3 or L_5, respectively (see Fig. 1). If an added hexagon acquires one of these modes, then we also speak about a *normal addition*.

Theorems 1 and 2 together with the above discussion yield the following result.

Theorem 3. *Any normal benzenoid with $r+1$ hexagons can be generated from a normal benzenoid with r hexagons by a normal addition of one hexagon.*

In order to construct normal coronoids, the situation is little more involved. Beside normal additions, four modes of *corona condensation* are needed: L_2, L_4, A_2 and A_3 (see Fig. 1). Normal coronoids are divided into two types: regular and half essentially disconnected. A coronoid is said to be *regular* if it can be generated from a single hexagon by a series of normal additions plus corona condensations of modes L_2 or A_2 and *non-regular* otherwise. Note that every regular coronoid is also normal. Normal coronoids that are not regular are called *half essentially disconnected*. A necessary and sufficient condition for a coronoid to be regular is given in [5].

Let G be a polyhex. We will say that G is *regular* if G is a regular coronoid or G is an elementary benzenoid graph.

Let G be a plane elementary bipartite graph. Two faces of G are said to be *disjoint* if their boundaries do not intersect; adjacent otherwise. Let F be a non-empty set of specified faces of G. The faces in F are called *forbidden* if faces in F are pairwise disjoint. The other faces of G are called *allowed faces*.

Zhang proposed an analog to the RFD for a 2-connected plane bipartite graph with forbidden faces G where the sequence of graphs which results in G is build by adding allowed faces of G. The addition of an allowed face in this process is called the *regular addition* (see [9] for the details). If a plane elementary bipartite graph G with forbidden faces can be generated from