MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **60** (2008) 193-216

ISSN 0340 - 6253

On elementary benzenoid graphs: new characterization and structure of their resonance graphs

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(Received November 20, 2007)

Abstract

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 one. A benzenoid graph G is elementary if every edge belongs to a 1-factor of G. The vertex set of the resonance graph of a benzenoid graph G consists of 1-factors of G, two 1-factors being adjacent whenever their symmetric difference forms the edge set of a hexagon of G. The resonance graphs of benzenoid graphs are partial

*Supported by the Ministry of Science of Slovenia under the grant 0101-P-297.

cubes (as well as median graphs). The τ-graph G^τ of a partial cube G has the equivalence classes of the Djoković-Winkler relation Θ as vertices, two classes E and F being adjacent if some edges $e \in E$ and $f \in F$ induce a convex P_3. We show a new characterization of elementary benzenoid graphs based on 4-tiling. We also present a decomposition theorem for the resonance graph of a benzenoid graph without a coronene. Moreover, we show that the τ-graph of the resonance graph of a benzenoid graph without a coronene is closely related to 4-tiling.

1 Introduction

Benzenoid graphs (molecular graphs of benzenoid hydrocarbons) are one of the most examined classes of graphs within the chemical graph theory. The interested reader is invited to consult the books [2, 6] dedicated to these graphs and a sample of papers on different aspects of these graphs [3, 7, 10, 11, 15].

The concept of a resonance graph has been introduced in chemistry by Gründler [8, 9] and later reinvented by El-Basil [4, 5] as well as by Randić with co-workers [24, 25]. Independently, Zhang et al. introduced this concept to mathematics, more precisely to graph theory, under the name Z-transformation graphs [29]. Resonance graphs of benzenoid graphs have been studied in [29], where it is established that such graphs (with the understanding that they contain at least one vertex) are connected, bipartite, and either isomorphic to a path or have girth 4. An extensive survey on resonance graphs of plane bipartite graphs was presented by Zhang [28]. Restricting to the catacondensed benzenoid graphs even more is known about the structure of their resonance graphs. Particularly, every such graph possesses a Hamilton path [1, 16] and belongs to the class of median graphs [18]. The latter result makes up the basis for an algorithm that assigns a binary code to every 1-factor of a catacondensed benzenoid graph [17, 23]. Recently Lam et al. [19] generalized these results by showing that the resonance graph of a plane weakly-elementary bipartite graph is a median graph. Since benzenoid graphs are all weakly-elementary, the resonance graph of an arbitrary benzenoid graph is median as well.

The relation Θ on the edge set of a graph plays a very important role in many graph theoretical concepts and results. It is intrinsically connected with partial cubes and enables several characterizations and recognition algorithms for this class of graphs. Moreover, since a benzenoid graph is a partial cube, the relation Θ induces several interesting applications in chemical graph theory (cf. [13, 14]).

The transitivity of the relation Θ in partial cubes admits the concept of τ graph. This concept also found a very appealing application in mathematical chemistry. In [27] one of the authors proposed a characterization of the resonance graphs of catacondensed benzenoid graphs as those median graphs for which G^τ is a tree T with largest degree at most 3 such that the vertices of T of degree 3 correspond to the peripheral Θ-classes of G.

In the next section we formally introduce the concepts and notations of this paper. In Section 3 we give a new characterization of elementary benzenoid graphs with the concept of 4-tilings. A decomposition theorem of the resonance graphs of elementary benzenoid graphs without a coronene as a subgraph is presented in Section 4. In the final section we explore some properties of elementary benzenoid graphs connected to the τ-graphs of their resonance graphs and 4-tilings.

2 Preliminaries

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. A *coronoid* is a connected subgraph of a benzenoid graph such that every edge belongs to at least one hexagon and it contains at least one non-hexagonal interior face. A benzenoid graph G is *catacondensed* if any triple of hexagons of G has empty intersection. In our case, benzenoid graphs are drawn in such way (where important) that we have vertical edges and the peaks are colored black.

A graph G is called *bipartite* if it is connected and its vertex set can be divided in two disjont 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.

A *matching* of a graph G is a set of pairwise independent edges. A matching is a 1-*factor*, 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 planar 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.

It is well known that benzenoid graphs and catacondensed benzenoid graphs are weakly elementary and elementary, respectively.

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

Let G be a benzenoid graph. Then the vertex set of the *resonance graph* $R(G)$ of G consists of the 1-factors of G, two 1-factors being adjacent whenever their symmetric difference forms the edge set of a hexagon of G. In Figure 1 the resonance graph of pyrene is shown, with the vertices being its 1-factors (double edges). The numbers next to the edges refer to the Θ-class to which the edge belongs.

The *hypercube* of order n and denoted Q_n is the graph $G = (V, E)$ where the vertex set $V(G)$ is the set of all binary strings $b_{n-1}, \ldots b_1, b_0$. Two vertices $x, y \in V(G)$ are adjacent in Q_n if and only if $H(x, y) = 1$.

Isometric subgraphs of hypercubes are called *partial cubes.*

For a triple of vertices u, v and w of given graph G, a vertex x of G is a *median* of u, v and w if x lies simultaneously on shortest paths joining u and v, v and w, and w and u, respectively. If G is connected and every triple of vertices admits a unique median, then G is a *median graph.* It is well known that median graphs are partial cubes.

Let G be a connected graph and $e = xy$, $f = uv$ be two edges of G. We say e is in the Djoković-Winkler relation Θ to f if $d(x, u) + d(y, v) \neq d(x, v) + d(y, u)$. Θ is reflexive and symmetric, but need not be transitive. Note that in partial cubes Θ is transitive and therefore an equivalence relation.

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*) if every edge of C belonging to M goes from white (black) end-vertex to black (white) end-vertex by the clockwise orientation of C.

Let us call the boundary of the infinite face of G the *outer boundary* or the *outer cycle.*

Let G be a plane bipartite graph. Let $\mathcal{M}(G)$ denote the set of all 1-factors of G. It was shown in [31] that G has a unique 1-factor $M_{\hat{0}}$ such that G has no proper $M_{\hat{0}}$-alternating cycles. We call $M_{\hat{0}}$ the *minimal 1-factor* of G, since $M_{\hat{0}}$ is the minimal element of the poset induced by $\mathcal{M}(G)$

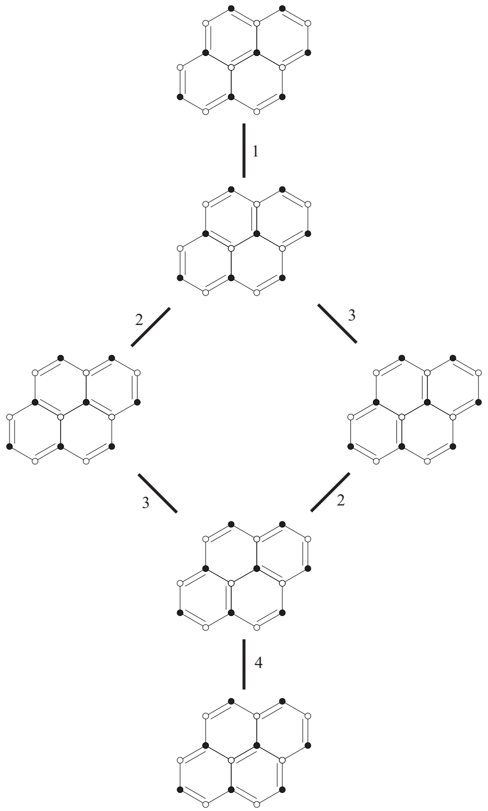

Figure 1: The resonance graph of pyrene.

[19, 20]. 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 1. *[26] 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 [22]. In [32] Zhang and Zhang evolved this concept and presented the so-called reducible face decomposition. This decomposition can serve as a construction method for 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 $G_{r-1} = x + P_1 + P_2 + \ldots + P_{r-1}$ 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 $G_r = x + P_1 + P_2 + \ldots + P_r$ is called an *(bipartite) ear decomposition* of G_r. It was shown in [21] that a bipartite graph is elementary if and only if it has an (bipartite) ear decomposition.

An ear decomposition $(G_1, G_2, \ldots, G_r(= G))$ (equivalently, $G = x + P_1 + P_2 + \ldots + P_r$) 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 $2 \leq i \leq r$.

It was proved in [32] 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 result 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 nonempty intersection. Let G be a plane 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 edges of P. 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 [32].

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

Theorem 1. *[26] Let G be an elementary benzenoid graph. Then h is a reducible hexagon of G if and only if the following holds*

(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 Characterization of elementary benzenoid graphs

In this section we will characterize elementary benzenoid graphs with the concept of a 4-tiling.

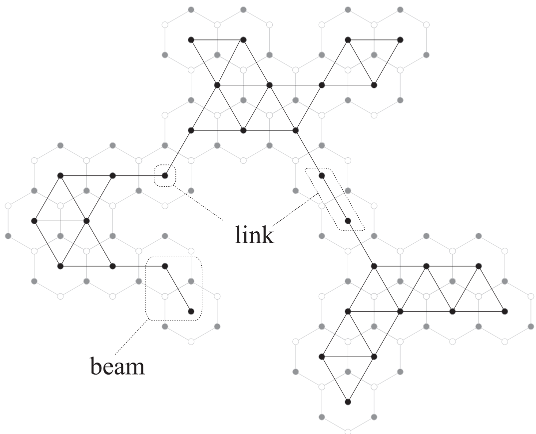

Figure 2: A benzenoid graph with its inner dual.

The vertices of the *inner dual* of G are the finite faces of G, two vertices being adjacent if and only if the corresponding faces share an edge in G. The inner dual of a benzenoid graph, denoted $I(G)$, is a subgraph of the regular triangular grid (see Fig. 2). Clearly, the inner dual of a catacondensed benzenoid graph is a tree with maximum vertex degree three.

A subgraph H of G is a *block* of G if H is a maximal subgraph without cut vertices or edges whose removal increases the number of components of G.

Let G be a benzenoid graph. The subgraph of G that corresponds to the block of the inner dual of G is called a *pericondensed component* of G. By removing the pericondensed components from G we obtain a graph that we call a *catacondensed forest* of G, while its connected component is called a *catacondensed tree*.

A catacondensed tree is called a *link* if it joins the vertices of two pericondensed components and a *beam* otherwise. These definitions are illustrated in Fig. 2.

Proposition 2. *A benzenoid graph G is elementary if and only if every pericondensed component of G is elementary.*

Proof. If G has no pericondensed components, then G is catacondensed and the proposition clearly holds. Suppose then that G is pericondensed.

Suppose there is an elementary benzenoid graph that possesses a pericondensed component which is not elementary. Let G be such a graph with the smallest number of hexagons. Let H denote its non-elementary pericondensed component and let h be a reducible hexagon of G. Then h has to be in H, otherwise $G-h$ is elementary with a non-elementary pericondensed component contradicting the minimality of G. By the same argument $H-h$ has to be elementary. It follows that H is also elementary and h is its reducible face. Since we obtained a contradiction this part of the proof is completed.

Let G be a benzenoid graph such that every pericondensed component of G is elementary. Since G is not a coronoid system, it is not difficult to see, that G possesses at least one pericondensed component with at most one link. Let P denote this pericondensed component and let L denote its link. The beams are clearly elementary, therefore we can use Theorem 1 and proceed as follows:

1. Find a reducible sequence of hexagons for each beam of P, such that the last hexagon of the reducible sequence is adjacent to a hexagon of P and remove the hexagons of that sequence from the graph.
2. Find a reducible sequence of hexagons for P such that the last hexagon of the reducible sequence is adjacent to a hexagon of L and remove the hexagons of that sequence from the graph. If P intersects with an adjacent pericondensed component, then find a reducible sequence of hexagons for P such that the last hexagon of the reducible sequence is the common hexagon and remove the hexagons of that sequence (with the exception of the common hexagon) from the graph.

We then repeat the steps above till the last hexagon. Since this procedure defines a reducible sequence of hexagons of G (and the corresponding ear decomposition), G is elementary and the assertion follows. $\square$

The edge e of $I(G)$ is *peripheral*, if it belongs to the infinite face of $I(G)$ and *internal*, otherwise. If h is a hexagon of a benzenoid graph, then h will also denote the corresponding vertex of $I(G)$.

Let $I(G)$ be the inner dual of a benzenoid graph G and let S denote a subset of internal edges of $E(I)$. Then S is a *4-tiling* of G if $I(G) \setminus S$ is the graph where every finite face is a 4-cycle. If S is a *4-tiling* of G then we set $I_4(G) := I(G) \setminus S$ (cf. Figure 3).

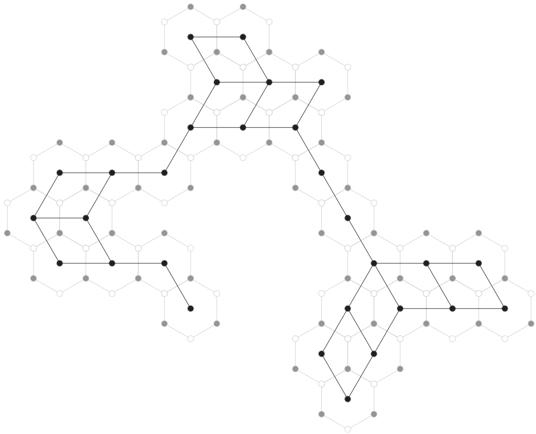

Figure 3: A benzenoid graph with its 4-tiling.

Let G be a benzenoid graph with a 4-tiling. The walk in a clockwise direction along the vertices of $I_4(G)$ induces three types of turns. The turns and the corresponding hexagons are denoted $\frac{\pi}{3}$, $\frac{2\pi}{3}$, and $-\frac{\pi}{3}$ in a natural way. All turns are depicted in Figure 4.

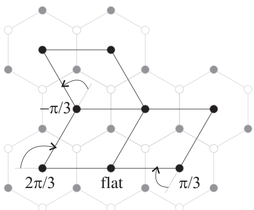

Figure 4: Turns.

Let G be a benzenoid graph with a 4-tiling and let C be the outer cycle of G. Let h be a hexagon that corresponds to a vertex of C. Then the hexagon h is called *removable* if

- h is a $\frac{\pi}{3}$ turn and the corresponding vertex in $I(G) \setminus S$ is of degree two, or
- h is a $-\frac{\pi}{3}$ turn and the corresponding vertex in $I(G) \setminus S$ is of degree three.

Note that a $\frac{\pi}{3}$ turn and a $-\frac{\pi}{3}$ turn in Fig. 4 are both removable.

Lemma 1. *A benzenoid graph G with a pericondensed component that possesses a 4-tiling has at least one removable hexagon.*

Proof. Let P be a pericondensed component of G and let T denote the set of all turns of P. We first state the following Facts which can be easily proved with figures:

1. The boundary of P cannot have two consecutive $\frac{2\pi}{3}$ turns (cf. Fig. 5).

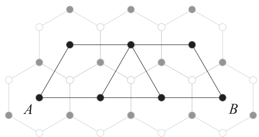

Figure 5: Two consecutive $\frac{2\pi}{3}$ turns A and B.

2. One of two consecutive $\frac{\pi}{3}$ turns is always removable (cf. Fig. 6).

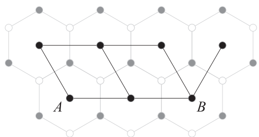

Figure 6: Two consecutive $\frac{\pi}{3}$ turns A and B.

3. A $\frac{\pi}{3}$ turn adjacent to a $\frac{2\pi}{3}$ turn is always removable (cf. Fig. 7).

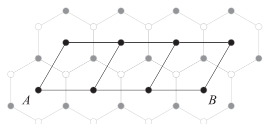

Figure 7: A $\frac{\pi}{3}$ turn B adjacent to a $\frac{2\pi}{3}$ turn A.

4. A $-\frac{\pi}{3}$ turn adjacent to two $\frac{2\pi}{3}$ turns is always removable (cf. Fig. 8).

5. If a $-\frac{\pi}{3}$ turn is adjacent to two $\frac{\pi}{3}$ turns then at least one of them is removable (cf. Fig. 9).

6. If a $-\frac{\pi}{3}$ turn is adjacent to a $\frac{\pi}{3}$ turn and to a $\frac{2\pi}{3}$ turn, then one of the former two is removable (cf. Fig. 10).

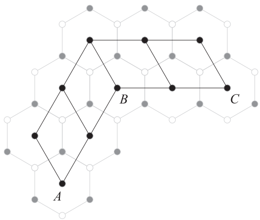

Figure 8: A $-\frac{\pi}{3}$ turn B adjacent to two $\frac{2\pi}{3}$ turns A and C.

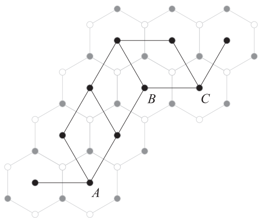

Figure 9: A $-\frac{\pi}{3}$ turn B adjacent to two $\frac{\pi}{3}$ turns A and C.

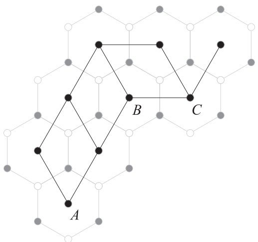

Figure 10: A $-\frac{\pi}{3}$ turn B adjacent to a $\frac{\pi}{3}$ turn C and to a $\frac{2\pi}{3}$ turn A.

In order to conclude the proof, observe three consecutive turns in the boundary of P. Note first that from Fact 1 it follows that all triplets with two consecutive $\frac{2\pi}{3}$ turns can be neglected. Moreover, from Facts 2 - 5 follows that any other triplet with at most one $-\frac{\pi}{3}$ turn induces a removable hexagon. It remains to explore the cases with two or three $-\frac{\pi}{3}$ turns. Note that sum of the values of a triplet of this kind is at most zero. Since the sum of values of turns in T must equal 2π, it is straightforward to conclude that P contains at least one triplet with at most one $-\frac{\pi}{3}$ turn. That concludes the proof. $\square$

Theorem 2. *A benzenoid graph G is elementary if and only if G admits a 4-tiling.*

Proof. Let G be an elementary benzenoid graph. The proof that G admits a 4-tiling is by induction on the number of hexagons r. If $r \leq 4$, the claim clearly holds. Let then G denote an elementary benzenoid graph with $r > 4$ hexagons. From the reducible face decomposition follows that $G = G_r = G_{r-1} + P_r$, where P_r is of length 1, 3 or 5. Let I and I_{r-1} denote the inner dual of G and G_{r-1}, respectively. By the inductive hypothesis, G_{r-1} admits a 4-tiling. Let us denote it S_{r-1}.

a) $|P_r| = 5$. The new hexagon h has exactly one neighbor denoted h' in G. Therefore I is obtained from I_{r-1} by adding the edge hh'. Since I and I_{r-1} has the same set of finite faces, S_{r-1} is also a 4-tiling of G.

b) $|P_r| = 3$. The new hexagon h has exactly three neighbors h_1, h_2 and h_3 in G. Since h_1, h_2 and h_3 are peripheral in G_{r-1}, the edges h_1h_2 and h_2h_3 are in $I_{r-1} - S_r$. I is obtained from I_{r-1} by adding the edges hh_1, hh_2 and hh_3. It is straightforward to see that $S_{r-1} \cup \{hh_2\}$ is a 4-tiling of G.

c) $|P_r| = 5$. The new hexagon h has exactly five neighbors h_1, h_2, h_3, h_4 and h_5 in G. Analogously as above we can see that $S_{r-1} \cup \{hh_2, hh_4\}$ is a 4-tiling of G.

Since a 4-tiling can be obtained in all three cases, this part of the proof is done.

Let G be a benzenoid graph that admits a 4-tiling S and let I be the inner dual of G. By Proposition 2, we can without loss of generality suppose that G has exactly one pericondensed component and no beams. It is straightforward to check that the graph that admits a 4-tiling with exactly one 4-cycle is elementary.

Suppose now that an elementary benzenoid graph that admits a 4-tiling which is not elementary exists. Let G be such a graph with the smallest number of hexagons. From Lemma 1 it follows that G has at least one removable hexagon. Denote it h. Suppose that h is a $\frac{\pi}{3}$ turn and let e be the edge of S with one end in the vertex that corresponds to h. It is straightforward to see that $S \setminus e$ is a 4-tiling of $G - h$. By the assumption, $G - h$ is elementary. However, h induces an ear of G, implying that G is elementary and we obtained a contradiction. Since the proof that the case with h is a $-\frac{\pi}{3}$ turn leads to a contradiction is analogous, the assertion follows. $\square$

4 Decomposition

Let $\mathcal{F}$ be the set of all finite faces of a graph 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. Particularly, $M_{\hat{0}}$ is constantly zero, i.e. every value on the inner faces is 0.

Lemma 2. *[19] 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 $\mathcal{F}$.*

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 in [19] that the resonance graph of a plane elementary bipartite graph is a median graph. Moreover, if G is a benzenoid graph with p hexagons and without a coronene (see Fig. 11), then ϕ is an isometric embbeding of $R(G)$ into Q_p.

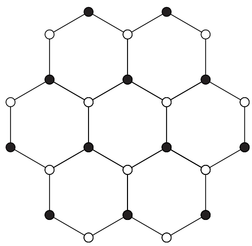

Figure 11: The coronene.

Lemma 3. *Let e be an edge on the boundary of an elementary benzenoid graph G and let h be the hexagon of G containing e. Let $e \in M'$ and let $\phi_{M'}(h) = i$, $i = 0, 1$. If M is an arbitrary 1-factor of $R(G)$, then $\phi_M(h) = i$ if and only if M contains e.*

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

Suppose that a 1-factor M containing e such that $\phi_M(h) = 1$ 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 $\phi_{M_i}(h) = 0$ and $\phi_{M_{i+1}}(h) = 1$. Thus, for every $j = 1, \ldots, i-1, i+1, \ldots, k$, $M_j \oplus M_{j+1} \neq h$. Since e does not belong to any other hexagon but h, M_i and M_{i+1} must contain e. But then $M_i \oplus M_{i+1} \neq h$ and we obtain a contradiction.

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

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

Let C denote the outer boundary cycle of 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.

From Lemma 3 and Proposition 1 we obtain the following

Corollary 1. *Let h be a peripheral hexagon and M a 1-factor of an elementary graph G. Then $\phi_M(h) = 1$ ($\phi_M(h) = 0$) if and only if a proper (improper) edge on the common boundary of h and G belongs to M.*

Let H be a fixed subgraph of a graph G, $H \subseteq G$. The *peripheral expansion* $\mathrm{pe}(G; H)$ of G with respect to H is the graph obtained from the disjoint union of G and an isomorphic copy of H, in which every vertex of the copy of H is joined by an edge with the corresponding vertex of $H \subseteq G$.

Let G be an elementary benzenoid graph and h a reducible hexagon of G. Then the periphery of h contains one, three, or five edges. We say that h is of type T1, T3 and T5, respectively. Furthermore, reducible hexagons of type T5, T3 and T1 have one, three and five adjacent hexagons, respectively. These hexagons will be denoted consecutively with $h_1, h_2, \ldots, h_5$ in the clockwise direction with respect to the boundary of $G - h$.

Let G be an elementary benzenoid graph and h its reducible hexagon. Let P denote the path induced by the intersection of h and $G - h$. We say that h is a *proper (improper)* reducible hexagon of G if P starts with a white (black) vertex with regard to the clockwise orientation of the boundary of $G - h$.

We are ready now to state the decomposition theorem for elementary benzenoid graphs which do not posses a coronene as a subgraph.

Theorem 3. *Let G be an elementary benzenoid graph without a coronene as a subgraph and h a reducible hexagon of G. Then $R(G) = \mathrm{pe}(R(G-h); X)$. If h is improper (proper) then a 1-factor M is a vertex of X if and only if $\phi_M(h_i) = 1$ ($\phi_M(h_i) = 0$) for each hexagon h_i adjacent to h.*

Proof. Let $M'_{\hat{0}}$ and $M_{\hat{0}}$ denote the minimal 1-factor of $R(G-h)$ and $R(G)$, respectively. We will prove the theorem for a reducible hexagon of type T5, T3, and T1.

(i) If h is of type T5, then h possesses only one adjacent hexagon (denoted h_1). Denote the vertices of h with $v_0, v_1, \ldots v_5$ in a clockwise direction, such that the common edge of h and h_1 has the end-vertices v_0 and v_1 (see Fig. 12). Suppose first that h is proper.

Thus, the edge v_0v_1 does not belong to $M'_{\hat{0}}$. We first prove that $R(G) = \mathrm{pe}(G-h; X)$. Clearly, $M'_{\hat{0}} \cup \{v_2v_3, v_4v_5\}$ is a 1-factor of G. Furthermore, since $M'_{\hat{0}}$ is the minimal 1-factor

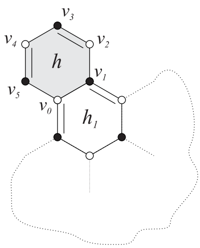

Figure 12: Reducible hexagon of type T5

of $G-h$ and the newly introduced edges do not form a proper cycle in G, it follows that $M'_{\hat{0}} := M'_{\hat{0}} \cup \{v_2v_3, v_4v_5\}$ is the minimal 1-factor of G.

Since G is a benzenoid graph without a coronene as a subgraph, ϕ is an isometric embedding of $R(G)$ into a hypercube. Let A denote the set of binary strings. We then state: $A^i := \{si; s \in A\}$, $i = 0, 1$. In other words, the binary strings of A^0 are obtained by adding 0 to every string of V.

Let the string s correspond to a factor of $R(G-h)$ and let the string si, $i = 0, 1$ correspond to a factor of $R(G)$. Figure 12 shows that s corresponds to a 1-factor of $V(R(G-h))$ if and only if $s0$ corresponds to a 1-factor of $V(R(G))$. In other words, $V^0(R(G-h)) \subseteq V(R(G))$. Let X be the set of all vertices of $V(R(G-h))$, such that the last bit of the corresponding binary string representing the hexagon h_1, equals 1. We will show that $V(R(G)) = V^0(R(G-h)) \cup X^1$. In particular, we need to determine when a string s of $V(R(G-h))$ admits that the string $s1$ is a vertex of G. Let M and M' denote 1-factors of G that correspond to $s0$ and $s1$, respectively. If $s0$ is adjacent to $s1$, then $M \oplus M' = h$. This implies that v_0v_1 must belong to M. Furthermore, from Proposition 3 and Corollary 1 it follows that $\phi_M(h_1) = 1$. It is left to confirm that $\phi_M(h_1) = 1$ if $\phi_M(h) = 1$. Note first that by Corollary 1 the edge v_1v_2 belongs to every 1-factor M with $\phi_M(h) = 1$. But then the adjacent edge of h_1 is not in M which implies that $\phi_M(h_1) = 1$. It follows that $R(G) = \mathrm{pe}(R(G-h); X)$ and this case is settled.

If h is proper, observe instead of the minimal 1-factors the maximal 1-factors of G and $G-h$. The proof then goes analogously as above.

(ii) If h is of type $T3$, then h possesses exactly three adjacent hexagons denoted h_1, h_2, and h_3.

Suppose first that h is proper. Denote its vertices consecutively $v_0, v_1, \ldots v_5$ with regard to the clockwise direction of the boundary of $G-h$ such that the first vertex of the intersection of h and $G-h$ is denoted v_0 (see Fig. 13). Note that the edge v_2v_1 belongs to $M'_{\hat{0}}$ when h is proper.

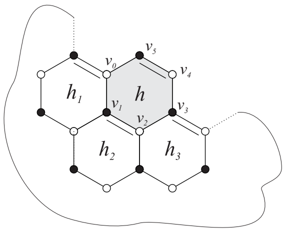

Figure 13: Reducible hexagon of type T3.

Let the string s correspond to a factor of $R(G-h)$ and let the string si, $i = 0, 1$ correspond to a factor of $R(G)$. Clearly, s corresponds to a 1-factor of $V(R(G-h))$ if and only if $s0$ corresponds to a 1-factor of $V(R(G))$. Note that the peripheral edges of h_1 and h_3, adjacent to v_0 and v_3, respectively, belong to both of $M_{\hat{0}}$ and $M'_{\hat{0}}$.

Let M and $\hat{M}$ denote the 1-factors of G that correspond to $s0$ and $s1$, respectively. $s0$ is adjacent to $s1$, thus $M \oplus \hat{M} = h$. This implies that v_0v_1 and v_2v_3 must belong to M. Thus, from Corollary 1 it follows that $\phi_M(h_1) = \phi_M(h_3) = 1$. Furthermore, h_2 is peripheral implying by Corollary 1 that $\phi_{M_{G-h}}(h_2) = \phi_M(h_2) = 1$.

It is left to confirm that for every 1-factor M with $\phi_M(h) = 1$ follows that $\phi_M(h_1) = \phi_M(h_2) = \phi_M(h_3) = 1$. Note first that by Corollary 3 the edge v_0v_5 and the edge v_3v_4 have to belong to all 1-factors M with $\phi_M(h) = 1$. But then the peripheral edge of h_1 with end vertex v_0 and the peripheral edge of h_3 with end vertex v_3 do not belong to any 1-factor M with $\phi_M(h) = 1$ and we have $\phi_M(h_1) = \phi_M(h_3) = 1$.

Suppose now that a 1-factor M with $\phi_M(h) = 1$ and $\phi_M(h_2) = 0$ exists. Let $\hat{M}$ denote a 1-factor of G with $\phi_{\hat{M}}(h) = 1$ which is adjacent to a 1-factor $\tilde{M}$ with $\phi_{\tilde{M}}(h) = 0$. We have already shown that $\phi_{\hat{M}}(h_2) = 1$. Moreover, the edge v_1v_2 belongs to $\hat{M}$. Let then $\hat{M} = M_1, M_2, \ldots, M_k = M$ denote a shortest path between $\hat{M}$ and M in $R(G)$. Since $R(G)$ is a partial cube, exactly one pair M_i, M_{i+1} such that $\phi_{M_i}(h_2) = 1$ and $\phi_{M_{i+1}}(h_2) = 0$. Thus, for every $j = 1, \ldots, i-1$, $M_j \oplus M_{j+1} \neq h_2$. Moreover, since $\phi_M(h) = \phi_{\hat{M}}(h) = 1$, for every $j = 1, \ldots, i-1$, $M_j \oplus M_{j+1} \neq h$. Note that v_1v_2 does not belong to any other hexagon but h and h_2, therefore M_i must contain v_1v_2. But then M_i must form a proper M_i-cycle in h_2 and we obtain a contradiction.

We proved that $R(G) = \mathrm{pe}(R(G-h); X)$, where for every 1-factor M of X we have $\phi_M(h_1) = \phi_M(h_2) = \phi_M(h_3) = 1$, thus, this part of the proof is complete.

If h is improper, observe instead of the minimal 1-factors the maximal 1-factors of G and $G - h$. The proof then goes analogously as above.

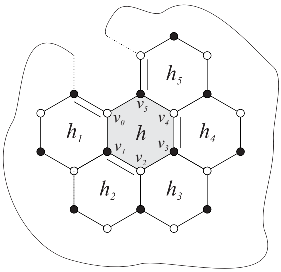

Figure 14: Reducible hexagon of type T1.

(iii) Suppose first that h is proper. If h is of type T1, then h possesses exactly five adjacent hexagons denoted h_1, h_2, h_3, h_4, and h_5 (see Fig. 14).

Denote the vertices of h with $v_0, v_1, \ldots v_5$ with respect to the clockwise direction of the boundary of $G - h$ such that the first vertex of the intersection of h and $G - h$ is denoted v_0 (see Fig. 14). Note that the edge v_1v_2 belongs to $M'_{\hat{0}}$ when h is proper.

Let the string s correspond to a factor of $R(G-h)$ and let the string si, $i = 0, 1$ correspond to a factor of $R(G)$. Clearly, s corresponds to a 1-factor of $V(R(G-h))$ if and only if $s0$ corresponds to a 1-factor of $V(R(G))$.

Let M and $\hat{M}$ denote the 1-factors of G that correspond to $s0$ and $s1$, respectively. $s0$ is adjacent to $s1$, thus $M \oplus M' = h$. Using analogous arguments as in case (ii) we obtain that $\phi_M(h_1) = \phi_M(h_2) = \phi_M(h_3) = \phi_M(h_4) = \phi_M(h_5) = 1$. Analogously we also confirm that for every 1-factor M' with $\phi_{M'}(h) = 1$ follows that $\phi_{M'}(h_1) = \phi_{M'}(h_2) = \phi_{M'}(h_3) = \phi_{M'}(h_4) = \phi_{M'}(h_5) = 1$. This proves that $R(G) = \mathrm{pe}(R(G-h); X)$, where for every 1-factor M of X we have $\phi_M(h_1) = \phi_M(h_2) = \phi_M(h_3) = \phi_M(h_4) = \phi_M(h_5) = 1$.

If h is improper, then again observe the maximal 1-factors of G and $G - h$.

Since we elaborated all three cases, the proof is complete. □

5 τ graph

The transitivity of the relation Θ in partial cubes allows the concept of τ graph.

Let e and f be two edges of a graph G. Then e and f are in relation τ if $e = f$ or if they form a convex path on three vertices. For a partial cube G its τ-graph G^τ is defined as follows. $V(G^\tau)$ consists of the Θ-equivalence classes of G, where Θ-classes E and F are adjacent whenever $E \neq F$ and there exist edges $e \in E$ and $f \in F$ with $e \,\tau\, f$.

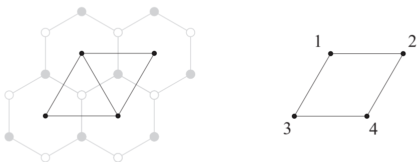

Figure 15: The inner dual of pyrene (left) and the τ-graph (right) of the pyrene's resonance graph.

In [27] it was shown that if G is the resonance graph of a catacondensed hexagonal graph H, then G^τ is isomorphic to the inner dual of H. This result leads to the characterization of the resonance graphs of catacondensed benzenoid graphs as those median graphs G for which G^τ is a tree T with largest degree at most 3 such that the vertices of T of degree 3 correspond to the peripheral Θ-classes of G.

In Figure 15 we can see that the inner dual of pyrene differs from the τ-graph of the resonance graph of the pyrene. The Θ-classes of the τ graph are labeled as in Figure 1. We can see in Fig. 15 that the inner dual of a pericondensed benzenoid graph G does not coincide with $R(G)^{\tau}$. However, the τ graph of the resonance graph of the graph from the figure is isomorphic to $I_4(G)$. We will show in the sequel, that the same can be proved for every benzenoid graph which does not posses a coronene.

We proved in Theorem 3 that $R(G) = \mathrm{pe}(R(G-h); X)$. Note that the ends of the newly introduced edges induce a Θ-class E in $\mathrm{pe}(G; H)$. Moreover, a subgraph of $\mathrm{pe}(G; H)$ induced by the edges of E is isomorphic to $H \Box K_2$. This fact implies the following lemma.

Lemma 4. *Let E be the Θ-class induced by the peripheral expansion $pe(G; H)$ and let E' be a Θ-class induced by an edge of H. Then E and E' are disjoint in $R(G)^{\tau}$.*

In order to prove the next theorem we will need the following lemma.

Lemma 5. *Let G be an elementary benzenoid graph and let h be a hexagon of G such that its set of peripheral edges, denoted $E_p(h)$, induces a cut in G. Let G_1 and G_2 denote the connected components of G induced by $E_p(h)$ and let h_1 and h_2 denote the hexagons of G_1 and G_2, respectively, both adjacent to h. If G admits a 1-factor M with $\phi_M(h_1) = \phi_M(h_2) = 0$ and $\phi_M(h) = 1$ then a 1-factor M_1 in G, such that $\phi_{M_1}(h_1) = \phi_{M_1}(h) = 1$ and $\phi_{M_1}(h_2) = 0$ always exist.*

Proof. Let G admit a 1-factor M with $\phi_M(h_1) = \phi_M(h_2) = 0$ and $\phi_M(h) = 1$. Since G contains the maximal 1-factor, G must admit a 1-factor M' with $\phi_{M'}(h_2) = \phi_{M'}(h) = \phi_{M'}(h_1) = 1$. Since the resonance graph of G is connected, the claim of the lemma must hold for at least one of the connected components induced by $E_p(h)$. Let then M_2 denote a 1-factor in G, such that $\phi_{M_2}(h_2) = \phi_{M_2}(h) = 1$ and $\phi_{M_2}(h_1) = 0$. Since $\phi_M(h) = \phi_{M'}(h) = \phi_{M_2}(h) = 1$, from Corollary 3 it follows that M_2, M' and M contain the very same edges of $E_p(h)$. Now we set $M_1 := (M' \setminus E(G_1)) \cup (M \cap E_p(h)) \cup (M_2 \setminus E(G_2))$. Since $E_p(h)$ induces a cut of G, it follows that M_1 is a 1-factor of G with $\phi_{M_1}(h_1) = \phi_{M_1}(h) = 1$ and $\phi_{M_1}(h_2) = 0$ and the assertion follows. $\square$

In the next theorem we will use the notation $N_G(v)$ for the neighborhood for a vertex v of a graph G.

Let G be an elementary benzenoid graph without a coronene as a subgraph and h a reducible hexagon of G. Let us again denote the hexagons adjacent to h consecutively with $h_1, h_2, \ldots, h_5$ in the clockwise direction with respect to the boundary of $G - h$. Since ϕ is an isometric embedding of $R(G)$ into a hyper cube, every hexagon of G correspond to exactly one Θ-class of $R(G)$. Let then Θ-classes $E_h, E_1, E_2, \ldots, E_5$ correspond to the hexagons $h, h_1, h_2, \ldots, h_5$, respectively.

Theorem 4. *Let G be an elementary benzenoid graph without a coronene as a subgraph and h a reducible hexagon of G. Then*

(i) $N(E_h)_{R(G)^\tau} = \{E_1\}$, if h is of type T5,

(ii) $N(E_h)_{R(G)^\tau} = \{E_1, E_3\}$, if h is of type T3,

(iii) $N(E_h)_{R(G)^\tau} = \{E_1, E_3, E_5\}$, if h is of type T1.

Proof. *(i)* If h is of type T5, then h possesses only one adjacent hexagon denoted h_1. From Theorem 3 it follows that $R(G) = \mathrm{pe}(R(G-h); X)$. Moreover, the newly introduced edges connecting X and its copy in $R(G)$ belong to the same Θ-class which corresponds to the new hexagon h. Let X' be the copy of X in $\mathrm{pe}(R(G); X)$. Note that X and X' both contain all Θ-classes of $R(G)$ except E_h and E_1. Furthermore, if E is one of these Θ-classes, then from Lemma 4 it follows that E is not adjacent to E_h.

Finally, since $R(G)$ is connected, in X exists a vertex v adjacent to the vertex v'' in $R(G) \setminus (X \cup X')$. Let v' denote the copy of v in X'. Clearly, vv' and vv'' do not lie on a common 4-cycle. Therefore, E_h and E_1 are adjacent in $R(G)^\tau$ and this part of the proof is complete.

(ii) If h is of type T3, then h possesses exactly three adjacent hexagons denoted h_1, h_2, and h_3. Suppose first that h is proper.

We proved in Theorem 3 that $R(G) = \mathrm{pe}(R(G-h); X)$, where for every 1-factor M of X we have $\phi_M(h_1) = \phi_M(h_2) = \phi_M(h_3) = 1$. The newly introduced edges connecting X and its copy in $R(G)$ belong to the same Θ-class which corresponds to the new hexagon h. Let X' be the copy of X in $\mathrm{pe}(R(G); X)$. Note that X and X' both contain all Θ-classes of $R(G)$ except E_h, E_1, E_2, and E_3. If E is a Θ-class from X, then from Lemma 4 it follows that E is not adjacent to E_h in $R(G)^\tau$. Denote the vertices of h with $v_0, v_1, \ldots v_5$ as defined in the proof of Theorem 3 (see Fig. 13). In order to prove that E_2 cannot be adjacent to E, note that every 1-factor

M in X contains the edges v_0v_1 and v_2v_3. This yields that the edge v_1v_2 cannot belong to any 1-factor $M' \in G \setminus X'$ adjacent to M with $\phi_{M'}(h_1) = 1$ or $\phi_{M'}(h_3) = 1$. Since v_1v_2 is a boundary edge of $G - h$, from Corrolary 1 it follows that $\phi_{M'_{G-h}}(h_2) = \phi_{M'}(h_2) = 1$.

We conclude the proof by showing that that both of E_1 and E_3 are adjacent to E_h in $R(G)^\tau$. In other words, we claim that a 1-factor M_1 with $\phi_{M_1}(h_1) = 0$ and $\phi_{M_1}(h_2) = \phi_{M_1}(h_3) = 1$ as well as a 1-factor M_2 with $\phi_{M_1}(h_3) = 0$ and $\phi_{M_2}(h_2) = \phi_{M_2}(h_1) = 1$ exist. But since the peripheral edges of h_2 induce a cut of $G - h$, by Lemma 5 $G - h$ (as well as G) admits the 1-factors of interest and this part of the proof is complete.

If h is improper, then $R(G) = \mathrm{pe}(R(G - h); X)$, where for every 1-factor M of X we have $\phi_M(h_1) = \phi_M(h_2) = \phi_M(h_3) = 0$. The proof goes analogously.

(iii) If h is of type T1, then h possesses exactly five adjacent hexagons denoted h_1, h_2, h_3, h_4, and h_5. Suppose first that h is proper. We proved in Theorem 3 that $R(G) = \mathrm{pe}(R(G - h); X)$, where for every 1-factor M of X we have $\phi_M(h_1) = \phi_M(h_2) = \phi_M(h_3) = \phi_M(h_4) = \phi_M(h_5) = 1$. The newly introduced edges connecting X and its copy in $R(G)$ belong to the same Θ-class which corresponds to the new hexagon h. Let X' be the copy of X in $\mathrm{pe}(R(G); X)$. Note that X and X' both contain all Θ-classes of $R(G)$ except E_1, E_2, E_3, E_4, and E_5.

If E is a Θ-class from X, then from Lemma 4 it follows that E is not adjacent to E_h in $R(G)^\tau$. In order to prove that E_2 cannot be adjacent to E, note that every 1-factor M in X contains the edges v_0v_1, v_2v_3, and v_4v_5. This yields that the edge v_1v_2 cannot belong to any 1-factor $M' \in G \setminus X'$ adjacent to M with $\phi_{M'}(h_1) = 1$ or $\phi_{M'}(h_3) = 1$. Since v_1v_2 is a boundary edge of $G - h$, from Corollary 1 follows that $\phi_{M'_{G-h}}(h_2) = \phi_{M'}(h_2) = 1$. A similar argument shows that E_4 cannot be adjacent to E.

In order to conclude the proof by showing that all of E_1, E_3, and E_5 are adjacent to E_h in $R(G)^\tau$, we invoke that the peripheral edges of h_2 and h_4 both induce a cut of $G - h$. Then Lemma 5 again yields that $G - h$ (as well as G) admits the 1-factors adjacent to E_1, E_3, and E_5.

If h is improper, the proof goes analogously.

Since we settled all three cases, the proof is complete. $\square$

Corollary 2. *Let G be an elementary benzenoid graph without a coronene as a subgraph. Then G admits a 4-tiling S such that $R(G)^\tau$ embedded in $I(G)$ in a natural way equals $I(G) \setminus S$.*

Proposition 3. *Let G be an elementary benzenoid graph without a coronene as a subgraph. Then G has a unique 4-tiling.*

Proof. Note first that a 4-tiling induced by $R(G)^{\tau}$ is unique. It is trivial to check the claim for catacondensed benzenoid graph graphs. Suppose that an elementary benzenoid graph without a coronene as a subgraph that admits at least two different 4-tilings exists. Let G denote such a graph with the smallest number of hexagons. Let S_1 denote the 4-tiling induced by $R(G)^{\tau}$. By assumption G has at least one another 4-tiling. Let us denote it S_2. From Lemma 1 and the proof of Theorem 2 follows that G possesses a removable hexagon h with regard to S_2. Note that h is also a reducible hexagon of G. Suppose that h is a $\frac{\pi}{3}$ turn with regard to S_2 and let e be the edge of S_2 with one end in the vertex that corresponds to h. It is straightforward to see that $S_2 \setminus e$ is a 4-tiling of $G - h$. By the assumption, $G - h$ is elementary graph that admits exactly one 4-tiling. In other words, $S_2 \setminus e$ equals the 4-tiling induced by $R(G-h)^{\tau}$. By Theorem 4, since h is a reducible hexagon of G, S_2 is also induced by $R(G)^{\tau}$. But then S_2 equals S_1 and the proof is complete.

□

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