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CHARACTERIZATION OF RESONANCE GRAPHS OF CATACONDENSED HEXAGONAL GRAPHS

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Abstract. A characterization of the resonance graphs of catacondensed hexagonal graphs is presented. The characterization is the basis for an algorithm that recognizes the resonance graph of a catacondensed hexagonal graph. Moreover, a modified algorithm can be applied to recognize Fibonacci cubes, a new topology for the interconnection of multicomputers.

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1. INTRODUCTION

The concept of the resonance graphs was first raised by Gründler [3, 4] and was then re-invented by El Basil [1, 2] and, independently, by Randić [16, 17]. Loosely speaking, the concept models the interaction of two Kekulé structures (of benzenoid hydrocarbons) that differ in the position of three double bonds [12]. In addition to this, Zhang, Guo and Chen [19] introduced resonance graphs under the name Z-transformation graphs and established their basic mathematical properties. It was found that the resonance graphs of catacondensed benzenoid graphs as well as the resonance graphs of more general hexagonal graphs possess a lot of structure, see [13] and the references therein. Note that the concept of the resonance graphs is not restricted to catacondensed benzenoids, but to benzenoids that possess 1-factor. Hovewer, catacondensed hexagonal graphs always possess 1-factors. Moreover, Gutman [5] showed that a catacondensed hexagonal graph with h hexagons has at least $h+1$ 1-factors.

By a *hexagonal graph* we mean a simple 2-connected plane graph in which all inner faces are hexagons (and all hexagons are faces), such that two hexagons are either disjoint or have exactly one common edge, and no three hexagons share a common edge. A hexagonal graph G is *catacondensed* if any triple of hexagons of G has empty intersection. See also [6, 7].

Let G be a hexagonal 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. For instance, the construction of the resonance graph of the benzo[c]phenanthrene is presented in Fig. 1. We also set $R(K_2) = R(K_1) = K_1$, where K_n denotes the complete graph on n vertices.

The Fibonacci cubes represent a new communication network that possess many suitable properties that are important in network design and application. Its major advantage is that it uses fewer links than the comparable hypercube, while its size does not increase as fast as the hypercube. Moreover, the Fibonacci cubes can efficiently emulate many hypercube algorithms [8]. The Fibonacci cubes possess a valuable recursive structure tightly associated with the Fibonacci numbers. In addition, the Fibonacci cubes are precisely the resonance graphs of fibonaccenes, i.e. a subclass of catacondensed hexagonal graphs [14].

The paper is structured as follows. Section 2 contains basic definitions concerning the resonance graph of catacondensed hexagonal graphs. The characterization for the resonance graphs of catacondensed hexagonal graphs needed for the recognition algorithm is described is Section 3. In Section 4 an algorithm for recognizing the resonance graphs of catacondensed hexagonal graphs with time bound $O(mn)$ is presented. Moreover, the

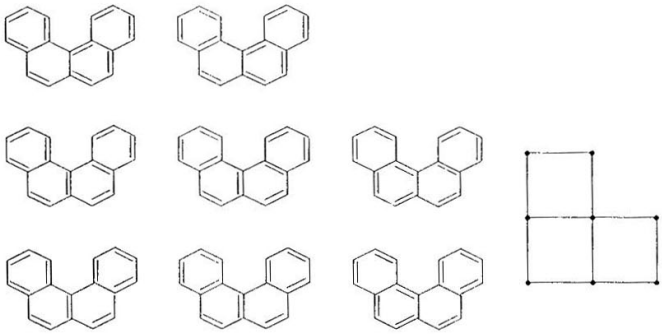

Figure 1: Kekulé structures and the resonance graph of benzo[c]phenanthrene.

algorithm can be modified in order to recognize the Fibonacci cubes with the same time bound.

2. PRELIMINARIES

A hexagon of a catacondensed hexagonal graph can share an edge with at most three other hexagons. According to this, we will say that a *hexagon is of degree tree, two, or one*, respectively. A hexagon of degree one is also called *pendant*. The edge of a pendant hexagon that is shared with another hexagon will be called a *join edge*. In Fig. 2 we see a catacondensed hexagonal graph G. Its hexagons A_1, A_2, and A_3 are of degree one, two, and tree, respectively.

If A is a hexagon of a catacondensed hexagonal graph of degree two, then A possesses two vertices of degree two. A is called *angularly connected*, if these two vertices are adjacent and A is called *linearly connected* otherwise. In Fig. 2 we see hexagons A_+ and A_2 of degree two, the former is angularly connected and the latter is linearly connected.

A *hexagonal chain* is an unbranched catacondensed hexagonal graph, i.e., no hexagon is of degree three.

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. For a graph G, let $\mathcal{F}(G)$ be the set of its 1-factors.

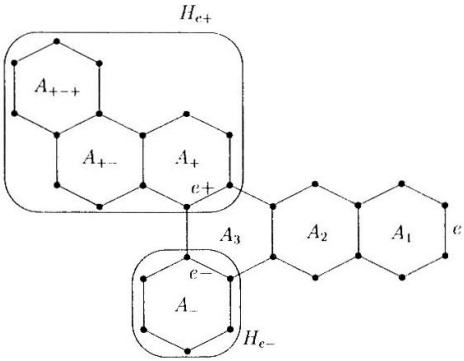

Figure 2: Catacondensed hexagonal graph H.

In addition, if $e_1, e_2, \ldots, e_n$ and e are fixed edges of G, let $\mathcal{F}(G; e_1, e_2, \ldots, e_n, \overline{e})$ denotes the set of those 1-factors of G that contain $e_1, e_2, \ldots, e_n$ and do not contain e.

Let $G = (V(G), E(G))$ be a graph. A *walk* is a sequence of vertices $v_1, v_2, \ldots, v_n$ and edges $v_i v_{i+1}$, $1 \leq i \leq n-1$. A *path* on n vertices is a walk on n different vertices and denoted P_n. For $u, v \in V(G)$, $d_G(u, v)$ or $d(u, v)$ denotes the length of a shortest path in G from u to v.

The *Cartesian product* $G \Box H$ of graphs G and H is the graph with the vertex set $V(G) \times V(H)$ and $(a, x)(b, y) \in E(G \Box H)$ whenever $ab \in E(G)$ and $x = y$, or $a = b$ and $xy \in E(H)$.

It is well known that the Cartesian product is associative, cf. [10, Proposition 1.36]. Hence the Cartesian product of graphs $G_1, G_2, \ldots, G_k$ can be written as $G_1 \Box G_2 \Box \cdots \Box G_k$. The vertex set of such a product is then the set of all k-tuples $(u_1, u_2, \ldots, u_k)$, where $u_i \in G_i$, while $(u_1, u_2, \ldots, u_k)$ is adjacent to $(v_1, v_2, \ldots, v_k)$ whenever there is an index j such that $u_j v_j$ is an edge of G_j and $u_i = v_i$ for all $i \neq j$. The *n-cube* Q_n (or the *n-dimensional hypercube*) is the graph whose vertices are all binary words of length n, two words being adjacent whenever they differ in precisely one place. In other words, Q_n is just the Cartesian product of n copies of K_2.

If H is a subgraph of G, such that $d_H(u, v) = d_G(u, v)$ for all $u, v \in H$, then H is an isometric subgraph. Isometric subgraphs of hypercubes are called *partial cubes*.

Let G be a connected graph and $e = xy$, $f = uv$ be two edges of G. We say e is in 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. We denote its transitive closure by Θ^*. Winkler [18] proved that G is a partial cube if and only if G is bipartite and $\Theta^* = \Theta$.

For a triple of vertices u, v and w of a 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. If G is connected and every triple of vertices admits a unique median, then G is a *median graph*.

For an edge ab of G we write

$$\begin{aligned}
W_{ab} &= \{w \in V \mid d(a,w) < d(b,w)\},\\
W_{ba} &= \{w \in V \mid d(b,w) < d(a,w)\},\\
F_{ab} &= \{xy \mid xy \text{ edge of } G \text{ with } x \text{ in } W_{ab} \text{ and } y \text{ in } W_{ba}\},\\
U_{ab} &= \{w \in W_{ab} \mid w \text{ is the end vertex of an edge in } F_{ab}\},\\
U_{ba} &= \{w \in W_{ba} \mid w \text{ is the end vertex of an edge in } F_{ab}\}\ .
\end{aligned}$$

For $X \subseteq V(G)$ let $G[X]$ denotes the subgraph of G induced by the set X.

Let ab be an edge of a median graph G for which $U_{ab} = W_{ab}$. Then $G[W_{ab}]$ is called *a peripheral subgraph* of G.

A Θ-class E of a median graph G is called *peripheral* if at least one of $G[W_{ab}]$ and $G[W_{ba}]$ is peripheral for $ab \in E$. E is *internal* if it is not peripheral.

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 $H \subseteq G$. Note that the ends of the newly introduced edges induce a subgraph of $\mathrm{pe}(G;H)$ isomorphic to $H \Box K_2$.

A *peripheral contraction* is just the inverse operation of the expansion, i.e., G is a peripheral contraction of $\mathrm{pe}(G;H)$.

Let e be an edge of a hexagonal graph G. Then the *cut* C_e corresponding to e is the set of edges so that with every edge e' of C_e also the opposite edge with respect to a hexagon containing e' belongs to C_e. As hexagonal graphs admits isometric embeddings into hypercubes [11], C_e can also be described as the equivalence class of the relation Θ containing e.

3. CHARACTERIZATION

In this section we present our main theorem. We first recall some notations concerning catacondensed hexagonal graph introduced in [13].

Let H be a catacondensed hexagonal graph and e an edge of H with ends of degree two. Let $e = e_0, e_1, \ldots, e_n$ be the edges of the cut C_e, and let $A_1 = A, A_2, \ldots, A_n$ be the corresponding hexagons. Let $e+$ and $e-$ be the edges of A_n incident to e_n, where

$e+$ is the right edge looking from $e = e_0$ to e_n while $e-$ is the left edge, and let A_+ and A_- be the corresponding hexagons. Remove now from H the hexagons $A_1, \ldots, A_n$, except $e+$ and $e-$. Then the remaining graph consists of two connected components H_{e+} and H_{e-}, where $e+ \in H_{e+}$ and $e- \in H_{e-}$. Note that any of H_{e+} and H_{e-} is either a catacondensed hexagonal graph or a K_2. These notations are illustrated in Fig. 2. If H_{e+} is a catacondensed hexagonal graph, we repeat the described construction on H_{e+}, where the construction begins with $e+$. In this way we obtain two connected subgraph of H denoted H_{e++} and H_{e+-}. Similarly, if H_{e-} is a catacondensed hexagonal graph, then we repeat the construction on H_{e-}, starting with $e-$, to obtain connected subgraphs H_{e-+} and H_{e--}. In the case that $H_{e+} = K_2$ we set $H_{e++} = K_1$ and $H_{e+-} = K_1$, and if $H_{e-} = K_2$ we set $H_{e-+} = K_1$ and $H_{e--} = K_1$.

Klavžar, Žigert and Brinkmann [15] proved that the resonance graph $R(H)$ of a catacondensed benzenoid graph H can be isometrically embedded into the h-dimensional hypercube Q_h, where h is the number of hexagons of H. With other words, they proved that the resonance graph $R(H)$ of a catacondensed benzenoid graph H is a partial cube where the number of Θ-classes corresponds to the number of hexagons of H. In fact, they showed an even stronger statement, namely that $R(H)$ is a median graph.

Klavžar, Vesel and Žigert [13] closely examined the structure of the resonance graphs of hexagonal graphs and proved the following decomposition theorem.

Theorem 1 *Let H be a catacondensed hexagonal graph and e an edge with ends of degree two with $|C_e| = n+1$, where $n \geq 1$. Let $Y = R(H)[\mathcal{F}(H;e)]$, $X = R(H)[\mathcal{F}(G;e,e+,e-)]$, and X_1 the copy of X in Y_0 (the first Y-layer of $Y \Box P_n$). Then*

$$R(H) = \mathrm{pe}(Y \Box P_n;\, X_1)\,.$$

Moreover,

(i) $Y = R(H_{e+}) \Box R(H_{e-})$ *and*
(ii) $X_1 = X = R(H_{e++}) \Box R(H_{e+-}) \Box R(H_{e-+}) \Box R(H_{e--})$.

Let H be a catacondensed hexagonal graph and e the edge with ends of degree two with $|C_e| = n+1$, where $n \geq 1$. The decomposition theorem is proved using the fact that for $i = 1, 2, \ldots, n-1$, a 1-factor $f_i \in \mathcal{F}(H; e_i)$ is adjacent (in $R(H)$) to exactly one 1-factor $f_{i-1} \in \mathcal{F}(H; e_{i-1})$ and to exactly one 1-factor $f_{i+1} \in \mathcal{F}(H; e_{i+1})$. Moreover, the symmetric difference of f_{i-1} and f_i is the edge set of A_i, while the symmetric difference of f_i and f_{i+1} is the edge set of A_{i+1}. Similarly, the edges of A_{n-1} form the symmetric difference of f_{n-2} and f_{n-1} as well as the edges of A_1 form the symmetric difference of f_0 and f_1. A 1-factor $f_n \in \mathcal{F}(H; e_n)$ is adjacent to exactly one 1-factor f from $\mathcal{F}(H; e_{n-1})$ and the symmetric difference of f_n and f is the edge set of A_n, cf. Fig. 7 in [13].

With other words, for $i = 1, 2, \ldots, n$ every hexagon A_i corresponds to the unique Θ-class in $R(H)$ consisted of the edges joining $\mathcal{F}(H; e_{i-1})$ and $\mathcal{F}(H; e_i)$.

Consider now the structure of $R(H)[\mathcal{F}(H; e_{n-1})]$ versus $R(H)[\mathcal{F}(H; e_{n-1}, e+, e-)]$. We know from the decomposition theorem and from the discussion above that $R(H)[\mathcal{F}(H; e_{n-1})]$ contains a copy of $R(H)[\mathcal{F}(H; e_n)]$ with the vertex set $\mathcal{F}(H; e_{n-1}, e+, e-)$. Note also that $R(H)[\mathcal{F}(H; e_{n-1})] = R(H_{e+})\Box R(H_{e-})$ and
$R(H)[\mathcal{F}(H; e_{n-1}, e+, e-)] = R(H_{e++})\Box R(H_{e+-})\Box R(H_{e-+})\Box R(H_{e--})$.

We distinguish three cases now.

(a) $H_{e+} = H_{e-} = K_2$. Then $\mathcal{F}(H; e_{n-1}, e+, e-) = \mathcal{F}(H; e_{n-1}) = \mathcal{F}(H; e_n) = K_1$.

(b) Exactly one of H_{e+} and H_{e-} equals K_2. Suppose $H_{e+} \neq K_2$. Then from Theorem 1 follows $\mathcal{F}(H; e_{n-1}, e+, e-) = \mathcal{F}(H; e_{n-1}, e+)$. Note that $\mathcal{F}(H; e_{n-1}) = \mathcal{F}(H; e_{n-1}, e+) + \mathcal{F}(H; e_{n-1}, \overline{e+})$. Thus, a 1-factor $f_+ \in \mathcal{F}(H; e_{n-1}, e+)$ is adjacent to a 1-factor $\overline{f_+} \in \mathcal{F}(H; e_{n-1}, \overline{e+})$ if the symmetric difference of f_+ and $\overline{f_+}$ is the edge set of A_+. Note that since $R(H)[\mathcal{F}(H; e_{n-1})]$ is connected and $\mathcal{F}(H; e_{n-1}, \overline{e+}) \neq \emptyset$, there exist at least one edge connecting a 1-factor from $\mathcal{F}(H; e_{n-1}, e+)$ with a 1-factor from $\mathcal{F}(H; e_{n-1}, \overline{e+})$. The discussion implies, that a vertex of $\mathcal{F}(H; e_{n-1}, e+)$ is adjacent to a vertex of $\mathcal{F}(H; e_{n-1}) \setminus \mathcal{F}(H; e_{n-1}, e+)$ if their joining edge belongs to the Θ-class corresponding to A_+.

(c) Both H_{e+} and H_{e-} differs K_2. Since $\mathcal{F}(H; e_{n-1}) = \mathcal{F}(H; e_{n-1}, e+) + \mathcal{F}(H; e_{n-1}, \overline{e+})$, a 1-factor $f_{+-} \in \mathcal{F}(H; e_{n-1}, e+, e-)$ is adjacent to a 1-factor $\overline{f_+} \in \mathcal{F}(H; e_{n-1}, \overline{e+})$ if the symmetric difference of f_{+-} and $\overline{f_+}$ is the edge set of A_+. Similarly, since $\mathcal{F}(H; e_{n-1}) = \mathcal{F}(H; e_{n-1}, e-) + \mathcal{F}(H; e_{n-1}, \overline{e-})$, a 1-factor $f_{+-} \in \mathcal{F}(H; e_{n-1}, e+, e-)$ is adjacent to a 1-factor $\overline{f_{e-}} \in \mathcal{F}(H; e_{n-1}, \overline{e-})$ if the symmetric difference of f_{+-} and $\overline{f_-}$ is the edge set of A_-. The discussion implies, that a vertex of $\mathcal{F}(H; e_{n-1}, e+, e-)$ is adjacent to a vertex of $\mathcal{F}(H; e_{n-1}) \setminus \mathcal{F}(H; e_{n-1}, e+, e-)$ if their joining edge belongs either to the Θ-class corresponding to A_+ or to the Θ-class corresponding to A_-, cf. Fig. 3 .

Let H be a subgraph of a graph G. Then ∂H is the set of all edges xy of G with $x \in H$ and $y \notin H$.

We say that Θ-classes E and F of a median graph G are *adjacent*, if there exist incident edges $e \in E$ and $f \in F$ such that e and f do not lie in a common 4-cycle. Note that a Θ-class E of a median graph G is *adjacent* to a Θ-class F ($\neq E$) of G if for $ab \in E$ the intersection of $\partial G[U_{ab}] \cup \partial G[U_{ba}]$ with F is not empty.

Proposition 2 *Let H be a catacondensed hexagonal graph and e an edge with ends of degree two with $|C_e| = n+1$, where $n \geq 1$. Let $E_1, E_2, \ldots, E_n, E_+, E_-$ denote the Θ-classes of $R(H)$ corresponding to $A_1, A_2, \ldots, A_n, A_+, A_-$, respectively. Then*

(i) E_1 is peripheral and adjacent exactly to E_2,

(ii) E_i is internal and adjacent exactly to E_{i-1} and E_{i+1}, $i = 2, 3, \ldots, n-1$,

(iii) E_n is peripheral and adjacent exactly to E_{n-1}, E_- and E_+.

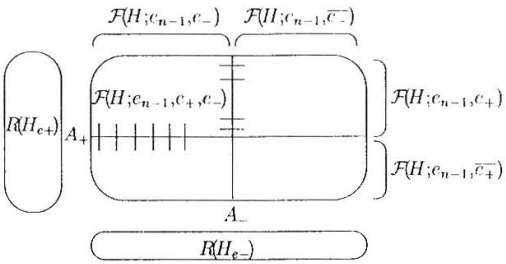

Figure 3: The structure of $\mathcal{F}(H;e_{n-1})$.

Proof. (i) and (ii) follow directly from the decomposition theorem and the discussion above. In order to prove (iii) note first that if H_{e+} (H_{e-}) $= K_2$ then E_+ (E_-) $= \emptyset$. We give the proof only for the case if both H_{e+} and H_{e-} differ K_2. Let $ab \in E_n$. Then (without loss of generality) $U_{ab} = W_{ab} = \mathcal{F}(H;e_n)$ and $U_{ba} = \mathcal{F}(H;e_{n-1},e+,e-)$. Therefore, $G[W_{ab}]$ is peripheral and $\partial G[U_{ab}] = F_{ab}$. From the discussion above it follows that in $\partial R(H)[\mathcal{F}(H;e_{n-1},e+,e-)]$ are only the edges of E_n, E_{n-1}, E_+ and E_-. Thus, the edges of E_n are adjacent only to the edges E_{n-1}, E_+ and E_-. □

The proposition is illustrated in Fig. 4 where the resonance graph of the graph from Fig. 2 is depicted. The Θ-classes $E_1,E_2,E_3,E_+,E_-,E_{+-}$, and E_{+-+} of $R(H)$ correspond to hexagons $A_1,A_2,A_3,A_+,A_-,A_{+-}$, and A_{+-+} of H, respectively.

Let G and G' be partial cubes and let E be a Θ-class of G. We define the set $E\Box G' := \{(u,x)(v,x);\ uv \in E,\ x \in V(G')\}$. For a Θ-class E' of G', $G'\Box E$ is defined analogously. It is well known that $E\Box G'$ forms a Θ-class in $G\Box G'$. Furthermore, each Θ-class of $G\Box G'$ is induced either by some E of G or by some E' of G'.

It is not difficult now to deduce the following lemma.

Lemma 3 *Let G and G' be median graphs and let E, F be Θ-classes of G and E' of G'. Then*

(i) $E\Box G'$ and $F\Box G'$ are adjacent in $G\Box G'$ if and only if E and F are adjacent Θ-classes of G,

(ii) $E\Box G'$ and $G\Box E'$ are not adjacent,

(iii) if E is peripheral (internal) then $E\Box G'$ is peripheral (internal).

Let G be a median graph. Then the definition of adjacency between two Θ-classes of G induces the graph with the vertex set consisting of all Θ-classes of G, two vertices

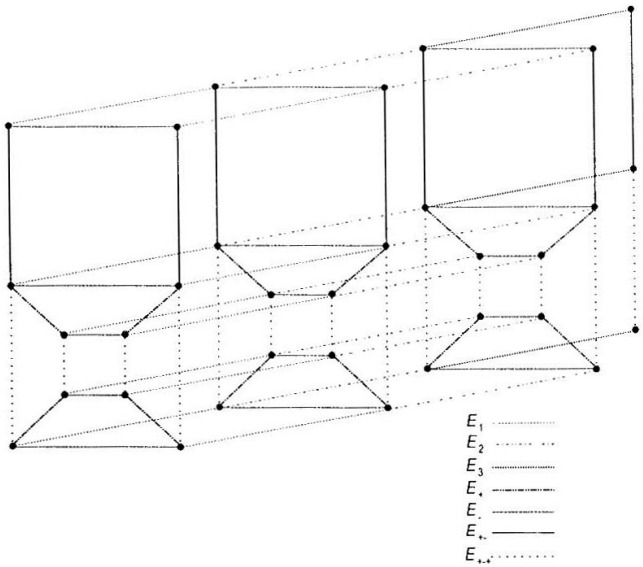

Figure 4: The resonance graph $R(H)$, cf. Fig. 2, with its Θ-classes.

being adjacent if the corresponding equivalence classes are adjacent. This graph will be denoted $T(G)$.

Theorem 4 *Let H be a catacondensed hexagonal graph. Then $T(R(H))$ is isomorphic to the inner dual of H. Moreover, a Θ-class of $R(H)$ is internal if and only if the corresponding hexagon is linearly connected.*

Proof. If H consists of a single hexagon, the theorem clearly holds. Assume that H contains at least two hexagons.

We will show that a Θ-class E of $R(H)$ is adjacent to E' of $R(H)$ if two corresponding hexagons A and A' are adjacent in H. In addition, we will show that E is internal, if and only if A is of degree two and linearly connected.

We distinguish four cases with respect to the position of A: (a) A is pendant, (b) A is angularly connected, (c) A is linearly connected, and (d) A is of degree three.

(a) Let e be the edge of A opposite to the join edge of A. By Proposition 2 (i) the corresponding Θ-class $E = E_1$ is adjacent exactly to E_2 and peripheral.

(b) Let e be the edge of A with ends of degree two. Then $|C_e| = n + 1 = 2$ and by Proposition 2 (iii) the corresponding Θ-class $E = E_1$ is peripheral and adjacent to E_+ and E_-.
(c) Note that in general we cannot find such an edge e that cut C_e involves A. However, the decomposition theorem implies the recursive procedure, starting on the edges $e+$ and $e-$, which can be repeated till A is engaged. We proceed by induction on the number of recursive steps r. Let e be an edge of H with ends of degree two. If $r = 0$, the case is settled by Proposition 2 (ii). For $r > 0$ assume without loss of generality that A is in H_{e+}. If $A = A_+$ then by Proposition 2 the corresponding Θ-class E is in H_{e+} peripheral and adjacent to exactly one Θ-class. Otherwise, E is internal in H_{e+} and adjacent to exactly two Θ-classes. From Lemma 3 follows that Θ-class $E \Box H_{e-}$ is either peripheral and adjacent in $H_{e+} \Box H_{e-}$ with exactly one Θ-class (if $A = A_+$) or internal and adjacent with two Θ-classes (if $A \neq A_+$). The decomposition theorem yields that the set of Θ-classes of $R(H)$ is made up of $E_1, E_2, \ldots, E_n$ as well as of the Θ-classes included in $H_{e+} \Box H_{e-}$. $E_1, E_2, \ldots, E_n$ are connected only among themselves with the exception of E_n which is connected also to E_+ and E_-. Therefore if $A = A_+$, then E is connected also with E_n and hence internal in $R(H)$ having exactly two adjacent Θ-classes. Otherwise, if $A \neq A_+$, then A is not adjacent with any of $E_1, E_2, \ldots, E_n$ and remains with only two neighbors.
(d) With induction on the number of recursive steps (analogous with c) we can show that E is peripheral and adjacent with exactly three Θ-classes.

Since we analyzed all possible positions of a hexagon in H, the proof is completed. $\Box$

A hexagonal chain with h hexagons is called a *linear chain* and denoted L_h if for $h = 1$ it consists of a single hexagon and for $h > 1$ all of its hexagons, apart from the two pendant ones, are linearly connected.

Before we state the main result, we recall the following lemma, cf. [9] and [10, Lemma 2.7]

Lemma 5 *If G is a median graph, then no edge in $\partial G[U_{ab}]$ is in relation Θ with any edge of $G[U_{ab}]$ for every edge ab of G.*

The following theorem characterizes the resonance graphs of catacondensed hexagonal graphs.

Theorem 6 *A median graph G is the resonance graph of a catacondensed hexagonal graph H if and only if $T(G)$ is a tree with maximum degree three, where vertices of degree three correspond to peripheral Θ-classes.*

Proof. In Theorem 4 we showed that $T(G)$ is isomorphic to the inner dual of H if G is the resonance graph of H. Moreover, it was established that every hexagon A of degree three corresponds to the peripheral Θ-class in G. Since the inner dual of H is a tree with maximum vertex degree three, this part of the proof is completed.

Let G be a median graph with every Θ-class of degree three being peripheral and with $T(G)$ being a tree with maximum vertex degree three. Note first that if G is isomorphic to P_h, then G is the resonance graph of the linear chain L_h. Suppose G is the graph with the least number of Θ-classes such that it is not the resonance graph of any catacondensed hexagonal graph. Since $T(G)$ is isomorphic to a tree, G contains at least one pendant Θ-class E. Let $ab \in E$ and let F be the Θ-class adjacent to E. Since E is pendant and adjacent only with F, we have $G[W_{ab}] = G[U_{ab}] \cong G[U_{ba}]$. Let G' be obtained by peripheral contraction with respect to U_{ab} (over the edges of E). Since G is median, by Lemma 5 the edges of U_{ab} and U_{ba} are not in relation Θ with the edges of E. Therefore the deletion of E affects only the neighborhood of F. Then $T(G')$ can be obtained simply by deleting E from $T(G)$. It follows that $T(G')$ is a tree with maximum vertex degree three with every Θ-class in G' of degree three being peripheral. Furthermore, from the assumption follows that G' is the resonance graph of some catacondensed hexagonal graph H'. Let A_F be the hexagon of H' corresponding to F and let $cd \in F$. Note that F is peripheral and of degree at most two in G'. We now distinguish three cases:

(i) F is of degree one in G' and $G[U_{cd}] = G[U_{ba}]$. Then A_F is pendant in H'. Let e be the edge opposite to the join edge of A_F.

(ii) F is of degree one in G' and $G[U_{cd}]$ a subgraph of $G[U_{ba}]$. Since F is of degree one, A_F is pendant in H'. Let e be the edge with ends of degree two that is not opposite to the join edge of A_F.

(iii) F is of degree two. Since F is peripheral then by Theorem 4 A_F is angularly connected in H'. Let e the only edge of A_F with ends of degree two in this case.

By the decomposition theorem the edge e in all three cases induces the decomposition with Y isomorphic to $G[U_{ba}]$. Let H be a catacondensed hexagonal graph which we obtain from H' by appending a new hexagon to A_F at the edge e. The resonance graph of H can be obtained by peripheral extension of G' with respect to Y. Since the obtained graph is isomorphic to G, the contradiction proves the claim. □

4. RECOGNITION ALGORITHM

Theorem 6 conveys that a median graph G is the resonance graph of a catacondensed hexagonal graph H if the Θ-classes of G form a tree of maximum vertex degree three where

the Θ-classes of degree three are peripheral. The theorem is not only a characterization of the resonance graphs of catacondensed hexagonal graphs, it is also practical from an algorithmic point of view.

Let $d(v)$ denotes the degree of the vertex v.

Procedure RESONANCE(G);

1. **if** G is K_2 **then** ACCEPT.
2. **if** G **not** a median graph **then** REJECT.
3. Form a totaly disconnected graph T with the vertices being the Θ-classes of G.
4. **for** each Θ-class E of G **do**
   4.1 Determine the corresponding sets U_{ab} and U_{ba}.
   4.2 For any edge uv of $\partial G[U_{ab}]$ and $\partial G[U_{ba}]$ do
   if uv belongs to Θ-class F **then** make E and F adjacent in T.
   4.3 Determine whether E is internal or peripheral.
   4.4 **if** $d(E) = 0$ **or** $d(E) > 3$ **then** REJECT.
   4.5 **if** $d(E) = 3$ **and** E internal **then** REJECT.
5. **if** T is a tree **then** ACCEPT **else** REJECT.

Theorem 7 *RESONANCE correctly recognizes resonance graphs in $O(mn)$ time.*

Proof. It is clear that the algorithm determines $T(G)$ and checks if it is isomorphic to a tree such that the degree of any vertex does not exceed three. In addition, it checks if every Θ-class with three neighbors is peripheral. Thus by Theorem 6 the algorithm is correct.

Concerning the time complexity, we invoke [10, Algorithm 2.3] for Step 2 and Step 4.1. The algorithm recognizes median graph in $O(mn)$ time. Moreover, it also determines all Θ-classes of G and for each Θ-class the corresponding sets U_{ab} and U_{ba}.

For Step 4.2 we can perform a check for every edge uv in constant time with the appropriate data structure. Note also that inserting an edge in a graph can also be done in constant time. Therefore the time complexity of this step is $O(m)$.

E is peripheral if one of the corresponding $\partial G[U_{ab}] \setminus E$ or $\partial G[U_{ba}] \setminus E$ is empty. Therefore Step 4.3 clearly does not violate the desired time bound as well as Steps 4.4. and 4.5. For Step 5 note that one can check in $O(m)$ time whether T is a tree. Thus, the overall complexity of the algorithm is $O(mn)$ and the proof is completed. □

The Fibonacci cubes are for $n \geq 1$ defined as follows. The vertex set of Γ_n is the set of all binary strings $b_1 b_2 \ldots b_n$ containing no two consecutive ones. Two vertices are adjacent in Γ_n if they differ in precisely one bit.

A catacondensed hexagonal graph H with h hexagons is called a *fibonaccene* if for $h = 1$ it consists of a single hexagon and for $h > 1$ all of its hexagons, apart from the two pendant ones, are angularly connected. It was proved in [14] that the resonance graph of a fibonaccene with h hexagons is isomorphic to the Fibonacci cube Γ_h. Note that the benzo[c]phenanthrene (see Fig. 1) is a fibonaccene with four hexagons, hence its resonance graph is isomorphic to Γ_4.

Theorem 8 *A median graph G is Γ_h if and only if every Θ-class in G is peripheral and $T(G)$ is isomorphic to P_h.*

Proof. The Fibonacci cube Γ_h is isomorphic to the resonance graphs of a fibonaccene with h hexagons. All hexagons in fibonaccene, apart the pendant ones, are angularly connected (and of the degree two). Therefore, by Theorem 6, all Θ-classes are peripheral and $T(G)$ is isomorphic to P_n. □

Theorem 9 *Fibonacci cubes can be recognized in $O(mn)$ time.*

Proof. Modify RESONANCE as follows. Let Step 4.3 rejects G if E is internal. Let Step 4.4 rejects G if $d(E) = 0$ or $d(E) > 2$. Omit Step 4.5. Let Step 5 rejects G if T is not isomorphic to P_h. From Theorem 9 it follows that the modified algorithm correctly recognizes the Fibonacci cubes. Moreover, it is straightforward to see that the modified steps can be implemented to run within the $O(mn)$ time. □

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