communications in mathematical
match
and in computer chemistry

no. 49, September 2003
MATCDY (49) 99- 116 (2003)

ISSN 0340 - 6253

ON RESONANCE GRAPHS OF CATACONDENSED HEXAGONAL GRAPHS: STRUCTURE, CODING, AND HAMILTON PATH ALGORITHM

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(Received February 17, 2003)

Abstract. The vertex set of the resonance graph of a hexagonal 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. A decomposition theorem for the resonance graphs of catacondensed hexagonal graph is proved. The theorem intrinsically uses the Cartesian product of graphs. A canonical binary coding of 1-factors of catacondensed hexagonal graphs is also described. This coding together with the decomposition theorem leads to an algorithm that returns a Hamilton path of a catacondensed hexagonal graph.

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*Supported in part by the Ministry of Education, Science and Sport of Slovenia under the grant 0101-P-504.

1. INTRODUCTION

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. Hexagonal graphs are sometimes also called *fusenes*. They generalize *benzenoid graphs* that are defined as 2-connected subgraphs of the hexagonal lattice. A hexagonal graph G is *catacondensed* if any triple of hexagons of G has empty intersection, cf. Fig. 2.

Catacondensed hexagonal/benzenoid graphs form a well studied class of graphs. Among many different topics studied on this class of graphs we briefly mention counting the number of Kekulé structures [18, 19], the theory of elementary edge-cuts [9, 11], the Schultz index (or molecular topological index, MTI) [3] and the coding problem of Kekulé structures [12]. For more information on hexagonal graphs and related concepts we refer to the book [8].

Let G be a hexagonal graph. Then the vertex set of the resonance graph 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 phenanthrene is presented in Fig. 1.

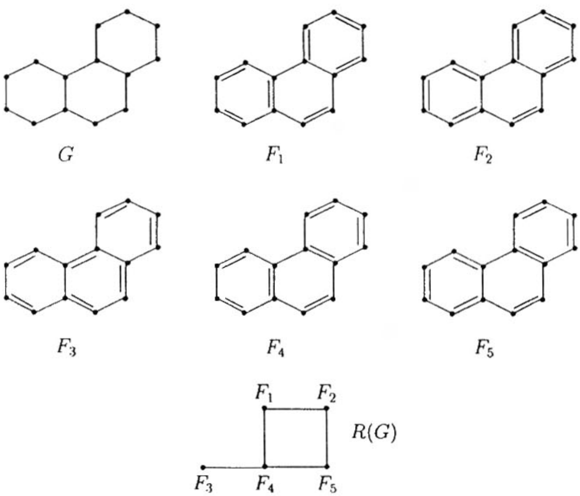


Figure 1: Phenanthrene G, 1-factors F_1, F_2, F_3, F_4, F_5 of G, and its resonance graph $R(G)$.

The concept of the resonance graph was introduced independently in mathematics (under the name Z-transformation graphs) by Zhang, Guo, and Chen [22] and in chemistry first by Gründler [6, 7] and later by El-Basil [4, 5] as well as by Randić with co-workers [16, 17]. In fact, the model appears to be very natural in chemistry, see the arguments from the introduction of [12] and references therein.

It turned out that resonance graphs of benzenoid/hexagonal graphs posses a lot of structure. Zhang, Guo, and Chen [22] proved that the resonance graph of a benzenoid graph with at least one 1-factor is connected, bipartite, and has, except in one special case, girth 4. Chen and Zhang [1] followed with a theorem asserting the resonance graph of a catacondensed benzenoid graph contains a Hamilton path, while in [15] it is established that the resonance graphs of the catacondensed benzenoid graphs belong to the class of median graphs. (In fact, the main result of the paper is slightly more general—it holds for the class of the so-called even ring systems.) The latter result turned out to be very useful, as it led (i) to an algorithm that assigns a unique and quite short binary code to every 1-factor of a catacondensed benzenoid graph [12] and (ii) to a simple method for determining the so-called Clar number of such graphs [14].

We also mention that the enumeration of benzenoid graphs whose resonance graphs have a vertex of degree one has been treated in [21]. The concept of the resonance graph has been extended (and studied) in [23, 24] in the natural way to plane bipartite graphs. For instance, in [23] it has been shown that the block graph of the resonance graph of a plane elementary bipartite graph is a path.

In this paper we closely examine the structure of the resonance graphs of hexagonal graphs. In the next section we give definitions and concepts needed in this paper. In particular we describe the Cartesian product of graphs that plays a crucial role in our main result. This result—decomposition theorem—is presented and illustrated with two examples in Section 3, while its proof is given in Section 4. We follow with a section describing a canonical binary coding of 1-factors of a catacondensed hexagonal graph. Combining this coding with the decomposition theorem an algorithm is presented in Section 6 that returns a Hamilton path of a catacondensed hexagonal graph. The paper is concluded with two open problems.

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. If A and B are incident hexagons of a catacondensed hexagonal graph, then the two edges of A that have exactly one vertex on B are called the *link of A to B*.

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 that is not a benzenoid graph. Its hexagons A, B, and C are of degree two, tree, and one, respectively, while the edges f and g form the link of A to B.

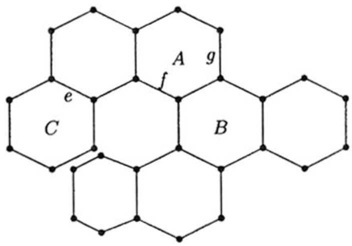


Figure 2: Catacondensed hexagonal graph G.

Let a hexagon A of a catacondensed hexagonal graph be adjacent to exactly two other hexagons. Then A possesses two vertices of degree 2. A is called *angularly connected*, if these two vertices are adjacent.

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 Djoković-Winkler [2, 20] relation Θ containing e, cf. [10].)

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. In addition, if $e_1, e_2, \ldots, e_n$ are fixed edges of G, let $\mathcal{F}(G; e_1, e_2, \ldots, e_n)$ denotes the set of those 1-factors of G that contain the fixed edges.

Let G be a hexagonal graph. Then the vertex set of the *resonance graph* $R(G)$ of G consists of all 1-factors of G, two 1-factors being adjacent whenever their symmetric difference is the edge set of a hexagon of G. We also set $R(K_2) = R(K_1) = K_1$.

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, if $a = b$ and $xy \in E(H)$. In Fig. 3 the Cartesian product of the path on 6 vertices P_6 and the claw graph $K_{1,3}$ is depicted.

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 $G_1 \Box G_2 \Box \cdots \Box G_k$.

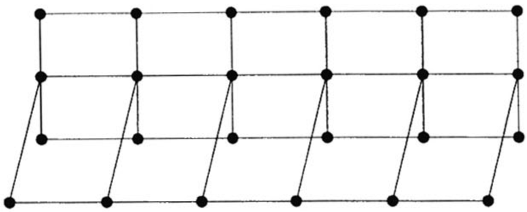


Figure 3: $P_6 \square K_{1,3}$

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 the complete graph on two vertices K_2.

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 $H \square K_2$.

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

3. DECOMPOSITION THEOREM

In this section we present our main theorem and illustrate it with a couple of examples. Before we state the result, some preparation is needed.

Let G be a catacondensed hexagonal graph and e the edge of G 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. We say that $e+$ and $e-$ are *the right and the left turn-edge* of C_e, respectively. Remove now from G the hexagons $A_1, \ldots, A_n$, except the turn-edges $e+$ and $e-$. Then the remaining graph consists of two connected components G_{e+} and G_{e-}, where $e+ \in G_{e+}$ and $e- \in G_{e-}$. Note that any of G_{e+} and G_{e-} is either a catacondensed hexagonal graph or a K_2. If G_{e+} is a catacondensed hexagonal graph, we repeat the described construction on G_{e+}, where the construction begins with $e+$. In this way we obtain two connected subgraph of G denoted G_{e++} and G_{e+-}. Similarly, if G_{e-} is a catacondensed hexagonal graph, then we repeat the construction on G_{e-}, starting with $e-$, to obtain connected subgraphs G_{e-+} and G_{e--}. In the case that $G_{e+} = K_2$ we set $G_{e++} = K_1$ and $G_{e+-} = K_1$, and if $G_{e-} = K_2$ we set $G_{e-+} = K_1$ and $G_{e--} = K_1$. These notations are illustrated in Fig. 4.

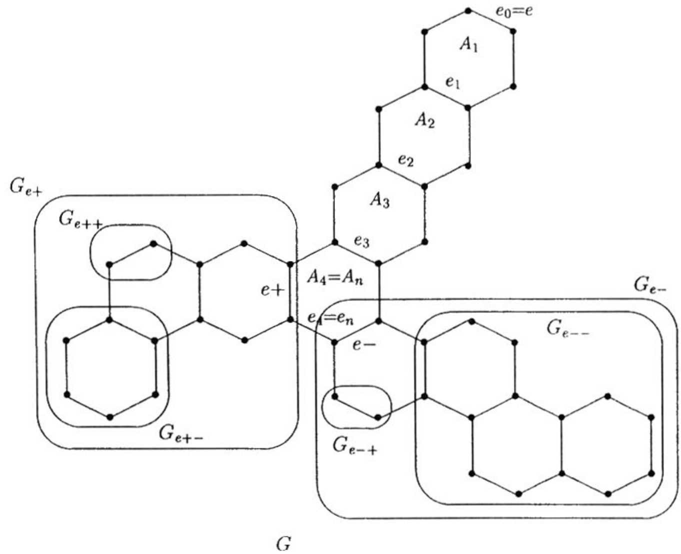


Figure 4: Subgraphs G_{e+}, G_{e-}, G_{e++}, G_{e+-}, G_{e-+}, G_{e--} of G.

Now we are ready to state:

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

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

Moreover,

(i) $Y = R(G_{e+}) \Box R(G_{e-})$ *and*

(ii) $X_1 = X = R(G_{e++}) \Box R(G_{e+-}) \Box R(G_{e-+}) \Box R(G_{e--})$.

Theorem 1 is proved in the next section, in the rest of this section we illustrate it with two examples. For the first example consider the graph G from Fig. 4. The construction of $R(G)$ is illustrated in Fig. 5. The graph $Y = R(G_{e+}) \square R(G_{e-})$ contains 40 vertices hence it is not drawn and therefore neither is $R(G)$. The black vertices present the vertices of X_1 that are expanded from Y.

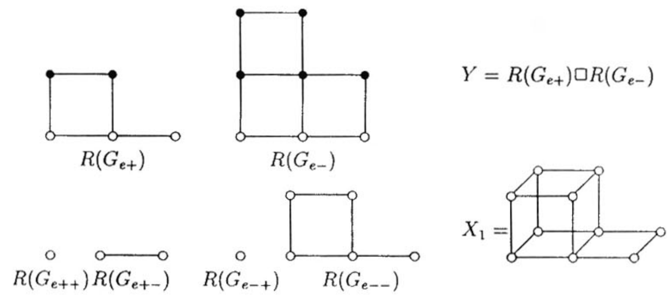


Figure 5: The decomposition theorem for the graph G of Fig. 4.

In the second example we consider the *starphene graphs* $HS_{j,k,l}$, $j, k, l \geq 1$, the definition of which should be clear from the example in Fig. 6. Let e be the edge of a pendant hexagon A corresponding to the parameter j opposite to the join edge of A, cf. Fig. 6. Then $|C_e| = j + 2$, $|C_{e+}| = k + 2$ and $|C_{e-}| = l + 2$.

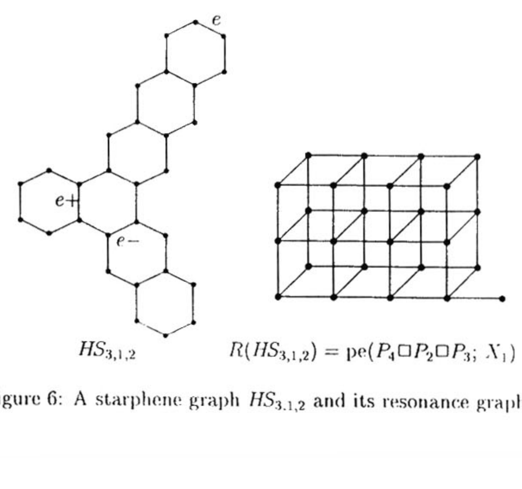


Figure 6: A starphene graph $HS_{3,1,2}$ and its resonance graph

Let $HS_{j,k,l}$ be a starphene graph and let edges e, $e+$, and $e-$ belong to the segments of length j, k, and l, respectively. Then $R(G_{e+}) = P_{k+1}$, $R(G_{e-}) = P_{l+1}$ and $n = j + 1$. The resonance graphs of components G_{e++}, G_{e+-}, G_{e-+}, G_{e--} are all isomorphic to the one vertex graph K_1. So, by the Theorem 1,

$$R(HS_{j,k,l}) = \mathrm{pe}(Y \Box P_n;\, X_1) = \mathrm{pe}(P_{j+1} \Box P_{k+1} \Box P_{l+1};\, X_1)\,,$$

where X_1 is the one vertex graph K_1. We will show in Section 5 how one determines the position of the peripheral expansion of X_1.

4. PROOF OF THE DECOMPOSITION THEOREM

We now prove Theorem 1 and begin with two lemmas. The first one is proved in [13] for the case of catacondensed benzenoid graphs. Analogous proof works for catacondensed hexagonal graphs, but to make the paper self-contained we repeat the argument.

Lemma 2 $R(G)[\mathcal{F}(G;e)] = R(G_{e+}) \Box R(G_{e-})$.

Proof. A 1-factor $F \in \mathcal{F}(G;e)$ is fixed on all the hexagons intersected by C_e except on the hexagon containing $e+$ and $e-$. If $G_{e+} = K_2$ (or $G_{e-} = K_2$) then $e+ \in F$ (or $e- \in F$). The edge e_n does not belong to F, for otherwise F cannot be extended to a 1-factor of G. If follows that, selecting a 1-factor F' of G_{e+} and a 1-factor F'' of G_{e-}, there is a unique way to extend it to a 1-factor from $\mathcal{F}(G;e)$. By the definition of the Cartesian product, the lemma follows easily. □

Lemma 3 $R(G)[\mathcal{F}(G;e,e+,e-)] = R(G_{e++}) \Box R(G_{e+-}) \Box R(G_{e-+}) \Box R(G_{e--})$.

Proof. A 1-factor F from $\mathcal{F}(G;e,e+,e-)$ is fixed on all hexagons intersected by C_e. Moreover, F is also fixed on all hexagons intersected by C_{e+}, except on the hexagon containing the turn-edges according to $e+$. Analogous conclusion holds for hexagons intersected by C_{e-}.

Using analogous arguments as in Lemma 2 it follows that, selecting 1-factors $F_1' \in \mathcal{F}(G_{e++})$, $F_1'' \in \mathcal{F}(G_{e+-})$, $F_2' \in \mathcal{F}(G_{e-+})$, and $F_2'' \in \mathcal{F}(G_{e--})$, there is a unique way to extend them to a 1-factor of $\mathcal{F}(G;e,e+,e-)$. The conclusion now follows by the definition of the Cartesian product. □

Using Lemma 2 and Lemma 3 we now prove Theorem 1. Note first that

$$\mathcal{F}(G) = \mathcal{F}(G;e_0) + \mathcal{F}(G;e_1) + \cdots + \mathcal{F}(G;e_n)\,, \tag{1}$$

that is, the sets of 1-factors $\mathcal{F}(G;e_i)$, $0 \le i \le n$, partition the set of all 1-factors of G.

Assume $n = 1$. Then $R(G)[\mathcal{F}(G;e_0)] = Y$ by Lemma 2, where $e = e_0$. Since $R(G)[\mathcal{F}(G;e_1)] = R(G)[\mathcal{F}(G;e_0,e+,e-)]$, Lemma 3 gives us $R(G)[\mathcal{F}(G;e_1)] = X_1$. Each 1-factor from $\mathcal{F}(G;e_1)$ is adjacent to exactly one 1-factor from $\mathcal{F}(G;e_0)$, since we have edges of the hexagon A_1 in their symmetric difference and thus

$$R(G) = R(G)[\mathcal{F}(G;e_0) + \mathcal{F}(G;e_1)] = \mathrm{pe}(\mathrm{Y}\Box\mathrm{P}_1;\ \mathrm{X}_1)\,.$$

Let $n = 2$. Then again $e = e_0$. Since 1-factors from $\mathcal{F}(G;e_0)$ and $\mathcal{F}(G;e_1)$ are fixed on the hexagon A_1, the corresponding resonance graphs are isomorphic. Hence by Lemma 2, $R(G)[\mathcal{F}(G;e_1)] = R(G)[\mathcal{F}(G;e_0)] = Y$. The rest of the proof now follows the same lines as in the case $n = 1$.

Suppose that $n \ge 3$. Then for $i = 1, 2, \ldots, n-2$, a 1-factor $F_i \in \mathcal{F}(G;e_i)$ is adjacent (in $R(G)$) to exactly one 1-factor $F_{i-1} \in \mathcal{F}(G;e_{i-1})$ and to exactly one 1-factor $F_{i+1} \in \mathcal{F}(G;e_{i+1})$. Moreover, F_{i-1} and F_{i+1} are the only 1-factors from $\mathcal{F}(G) \setminus \mathcal{F}(G;e_i)$ that are adjacent to F_i. So 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}, cf. Fig. 7.

Consider next a 1-factor $F_0 \in \mathcal{F}(G;e_0)$. It is adjacent to precisely one 1-factor $F_1 \in \mathcal{F}(G;e_1)$ and their symmetric difference is the edge set of A_1. Similarly, $F_{n-1} \in \mathcal{F}(G;e_{n-1})$ is in the resonance graph induced by the vertices from $\mathcal{F}(G) \setminus (\mathcal{F}(G;e_n) + \mathcal{F}(G;e_{n-1}))$ adjacent to exactly one 1-factor $F_{n-2} \in \mathcal{F}(G;e_{n-2})$, so that the edges of A_{n-2} form the symmetric difference of F_{n-1} and F_{n-2}.

For $i = 0, 1, \ldots, n-1$, any 1-factor from $\mathcal{F}(G;e_i)$ is fixed on hexagons $A_1, A_2, \ldots, A_{n-1}$. Thus the resonance graphs induced by the sets $\mathcal{F}(G;e_i)$, $i = 0, 1, \ldots, n-1$, are all isomorphic. Hence Lemma 2 yields

$$R(G)[\mathcal{F}(G;e_i)] = R(G_{e+})\Box R(G_{e-})\,,\quad i = 0, 1, \ldots, n-1\,.$$

From the above considerations we conclude that

$$R(G)[\mathcal{F}(G;e_0) + \mathcal{F}(G;e_1) + \ldots + \mathcal{F}(G;e_{n-1})] = R(G_{e+})\Box R(G_{e-})\Box P_n = Y\Box P_n\,. \qquad (2)$$

Consider now a 1-factor $F_n \in \mathcal{F}(G;e_n)$. It is adjacent to exactly one 1-factor F from $\mathcal{F}(G;e_0) + \mathcal{F}(G;e_1) + \ldots + \mathcal{F}(G;e_{n-1})$. The 1-factor F belongs to $\mathcal{F}(G;e_{n-1})$ and the symmetric difference of F_n and F is the edge set of A_n, cf. Fig 7. Since F_n is fixed exactly on the same hexagons as an arbitrary 1-factor from $\mathcal{F}(G;e_{n-1},e+,e-)$, we infer that

$$R(G)[\mathcal{F}(G;e_n)] = R(G)[\mathcal{F}(G;e_{n-1},e+,e-)]\,. \qquad (3)$$

By (1),

$$R(G) = R(G)[\mathcal{F}(G;e_0) + \mathcal{F}(G;e_1) + \ldots + \mathcal{F}(G;e_n)]\,,$$

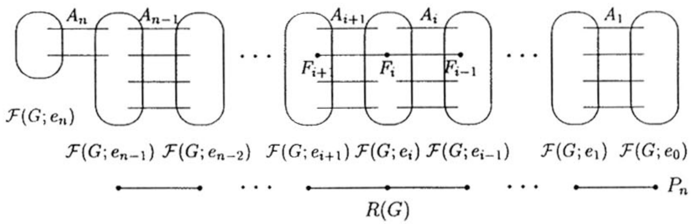


Figure 7: Decomposition of $R(G)$.

hence combining this equality with (2) and (3) we get

$$R(G) = \mathrm{pe}(Y \square P_n;\ R(G)[\mathcal{F}(G; e_{n-1}, e+, e-)]) . \tag{4}$$

Finally, a 1-factor from $\mathcal{F}(G; e_{n-1}, e+, e-)$ is fixed on the same hexagons as a 1-factor from $\mathcal{F}(G; e_0, e+, e-)$, thus the corresponding resonance graphs are isomorphic. Hence, using Lemma 3, where $e_0 = e$, we have

$$R(G)[\mathcal{F}(G; e_{n-1}, e+, e-)] = R(G_{e++}) \square R(G_{e+-}) \square R(G_{e-+}) \square R(G_{e--}) = X_1$$

so the theorem is established by plugging the last equality into (4). □

We conclude the section by noting that Theorem 1 can be generalized to any edge belonging to the cut C_e, except the edge incident with edges $e+$ and $e-$.

5. CANONICAL BINARY CODING

We have already mentioned that in [12] an algorithm is given by means of which to every 1-factor of a catacondensed benzenoid graph (with h hexagons) a binary code (of length h) is assigned. The algorithm is based on the results from [13, 15] where it is proved that the resonance graph $R(G)$ of a catacondensed benzenoid graph G can be isometrically embedded into the h-dimensional hypercube Q_h, where h is the number of hexagons of G. Moreover, it is not difficult to see that the same approach can be applied to catacondensed hexagonal graphs as well.

In this section we first summarize the basis of the above algorithm. Furthermore, since the role of the digits in the coding algorithm can vary, we describe a procedure that gives the so-called canonical coding. This coding will then be applied in the next section to the Hamilton path problem.

Let A be a pendant hexagon of a catacondensed hexagonal graph G. Let G' be the graph obtained from G by removing A (but not the join edge). Suppose that G' contains $h-1$ hexagons and that we have already embedded $R(G')$ into Q_{h-1}. Let $S(G')$ be the set of the binary strings of length $h-1$ corresponding to the embedding of $R(G')$. In order to establish the embedding of G we distinguish three cases with respect to the corresponding 1-factors as shown in Fig. 8.

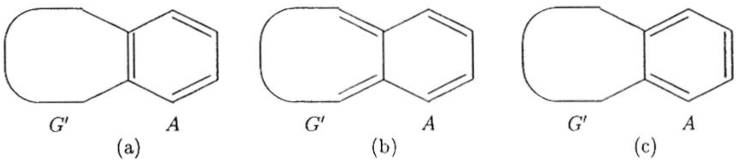


Figure 8: Possible intersections of a 1-factor with A.

The corresponding set of strings of length h is obtained by concatenating 0 to each $x \in S(G')$ if (a) or (b) is the case, and by concatenating 1 to each $x \in S(G')$ if (c) is the case. In other words, we add 1 if there is the link of A to the neighboring hexagon and 0 if the link is not present. Since G' is a catacondensed hexagonal graph, the method can be applied as a recursive procedure repeated until a single hexagon remains. The two 1-factors of a single hexagon are shown in Fig. 9. Their set of strings consists of digits 0 and 1, where 1 pertains to the 1-factor on the left-hand side and 0 to the 1-factor at the right-hand side. We call the above coding of 1-factors of G the *canonical coding*.

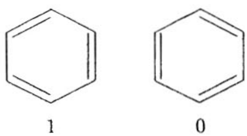


Figure 9: 1-factors and codes of a hexagon.

To see the benefits of the canonical coding consider the *linear chain* L_h with h hexagons. Let e be the edge of L_h as shown in Fig. 10, and let $e = e_0, e_1, \ldots, e_n$ be the consecutive edges of the cut C_e. It is straightforward to conclude that 1^i0^{h-i} is the canonical code of the 1-factor containing e_i, where 1^i0^{h-i} denotes the string obtained by concatenating the string of i ones with the string of $h-i$ zeros. In Fig. 10 these observations are illustrated on the linear chain L_4. In conclusion, the number of ones in the canonical code corresponds to the index of the edge e_i, and the coding returns

$$000\ldots00,\ 100\ldots00,\ 110\ldots00,\ \ldots,\ 111\ldots10,\ 111\ldots11.$$

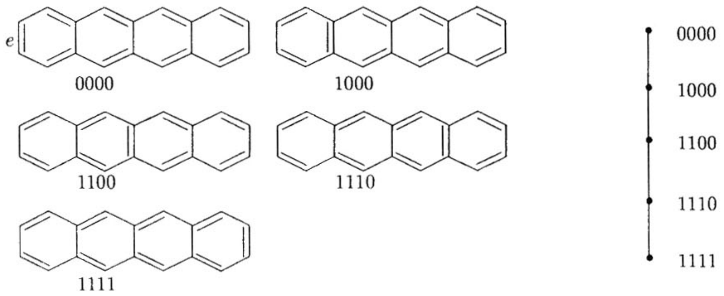


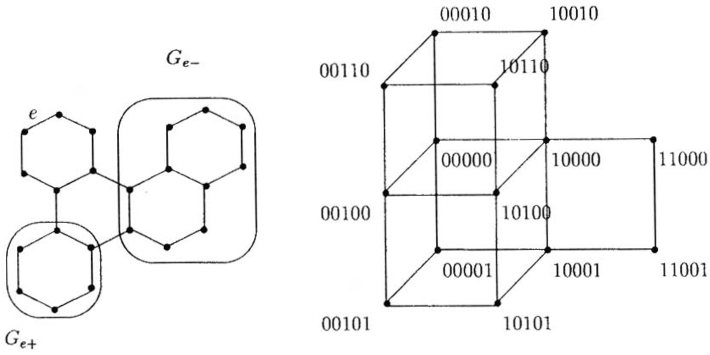
Figure 10: 1-factors and codes of four linear hexagons.

The situation for a (general) catacondensed hexagonal graph G is more involved. Recall first that the sets of 1-factors $\mathcal{F}(G;e_i)$, $0 \le i \le n$, partition the set of all 1-factors of G. Furthermore, by Theorem 1, $R(G)[\mathcal{F}(G;e_i)] = Y$, $0 \le i \le n-1$. Thus, if y is the canonical code of a vertex of Y, then the corresponding vertex in $\mathcal{F}(G;e_i)$, $0 \le i \le n-1$, is coded with $1^i0^{n-i}y$. Moreover, since $Y = R(G_{e+})\Box R(G_{e-})$, the set of codes of Y consists of strings $y = y_+y_-$, where y_+ and y_- are the canonical codes of vertices of $R(G_{e+})$ and $R(G_{e-})$, respectively.

Loosely speaking, the code $x = 1^i0^{n-i}y_+y_-$ of a vertex of $\mathcal{F}(G;e_i)$, $0 \le i \le n-1$, (a vertex in a copy of Y in terms of Theorem 1) is composed of three parts: the substring 1^i0^{n-i} defines a position of a copy of Y in $Y\Box P_n$, while the substrings y_+ and y_- define a contribution of $R(G_{e+})$ and $R(G_{e-})$.

To determine the code of a vertex in $\mathcal{F}(G;e_n)$ note first that it starts with n 1's. In addition, since by Theorem 1 $\mathcal{F}(G;e_n) = X = \mathcal{F}(G;e_{n-1},e+,e-)$, it follows that the rest of the digits are composed of two substrings that start with 0: the first is the code of a vertex of $R(G_{e+})$ and the second is the code of a vertex of $R(G_{e-})$. More formally, if x is the code of a vertex of $\mathcal{F}(G;e_n)$, then $x = 1^nab$, where a (b) is a code of a vertex of $R(G_{e+})$ ($R(G_{e-})$) with 0 in the first place.

We are now ready to present the procedure LABELS, which assigns canonical codes to the vertices of $R(G)$. The procedure starts the computation at an edge with ends of degree two, which is passed to the procedure as the parameter e.



$$Q_2 = \{00, 10\}$$

$$Q_+ = \{0, 1\}$$

$$Q_- = \{00, 01, 10\}$$

$$Q_Y = \{000, 001, 010, 100, 101, 110\}$$

$$Q_X = \{11000, 11001\}$$

Figure 11: Canonical coding of the vertices of $R(G)$.

Procedure LABELS(G, e, Q);

begin

1. **if** $G = K_2$ **then begin** $Q := \emptyset$; **exit**(LABELS); **end**;
2. Determine: G_{e+}, G_{e-}, and $|C_e| = n + 1$;
3. $Q_n := \{1^i 0^{n-i};\ 0 \le i \le n - 1\}$;
4. LABELS(G_{e+}, $e+$, Q_+); LABELS(G_{e-}, $e-$, Q_-);
5. $Q_Y := \{y_+ y_-;\ y_+ \in Q_+ \text{ and } y_- \in Q_-\}$;
6. $Q_{Y\square P} := \{py;\ p \in Q_n \text{ and } y \in Q_Y\}$;
7. $Q_X := \{1^n ab;\ a = 0u \in Q_+ \text{ and } b = 0v \in Q_-\}$;
8. $Q := Q_{Y\square P} + Q_X$;

end.

The procedure is illustrated in Fig. 11. Line 1 checks whether the graph G equals an edge. If it does, then the procedure returns the empty set in Q. Line 2 computes the number of edges in C_e and determines the connected components G_{e+} and G_{e-}. Line 3 computes the prefixes of the codes needed in copies of Y. Line 4 contains two recursive calls which compute the codes of the vertices of the connected components G_{e+} and G_{e-}, starting at the edges $e+$ and $e-$, respectively. Line 5 calculates the substrings which are in common for the corresponding vertices in the copies of Y, while Line 6 gives the prefixes to the codes of the vertices of each copy of Y. Finally, the codes for vertices in $\mathcal{F}(G; e_n)$ are computed in Line 7 and then merged with the codes of $Y \Box P_n$ in Line 8.

6. ALGORITHM FOR HAMILTON PATHS

As already mentioned, Chen and Zhang [1] proved that the resonance graph of a catacondensed benzenoid graph has a Hamilton path. In fact, the inductive proof of the main theorem of [1] gives an implicit construction of a Hamilton path. In our terminology, it is shown that there exists a zigzag Hamilton path among the copies of Y, as well as a Hamilton path among the vertices inside a copy of Y.

In this section we present an algorithm HAMILTON PATH that for a (slightly) more general class of catacondensed hexagonal graphs returns such a path. The algorithm intrinsically uses the canonical coding in order to list the vertices in a Hamilton path.

In the rest we assume that the sets of strings are represented as linked lists, that is, strings $Q_1, Q_2, \ldots, Q_{|Q|}$ are in the linked list $Q = (Q_1, Q_2, \ldots, Q_{|Q|})$ arranged in a linear order. Let procedure APPEND(A,B) appends the linked list B to the linked list A.

The procedure COMBINE plays a crucial role in providing a zigzag path among the vertices. The procedure computes from the set of strings A and B the set of strings $C = \{ab;\ a \in A \text{ and } b \in B\}$. However, the order of the strings in C is of great importance now. The procedure has the additional parameter n which is needed to provide the proper order of the strings in C.

```
Procedure COMBINE(A,B,n,C);
  begin
   C := ∅;
   for i := 1 to |A| do
     if ODD(i + n) then
       for j := 1 to |B| do APPEND(C, (A_i B_j));
     else
       for j := |B| downto 1 do APPEND(C, (A_i B_j));
  end.
```

We can now present the procedure HAMILTON PATH that returns a Hamilton path of $R(G)$ for a catacondensed hexagonal graph G.

```
Procedure HAMILTON PATH(G, e, Q);
  begin
  1. if G = K_2 then begin Q := ∅; Exit(HAMILTON PATH); end;
  2. Determine: G_{e+}, G_{e-}, and |C_e| = n + 1;
  3. Q_n := (0^n, 10^{n-1}, 110^{n-2}, ..., 1^{n-1}0);
  4. HAMILTON PATH(G_{e+}, e+, Q_+); HAMILTON PATH(G_{e-}, e+, Q_-);
  5. COMBINE(Q_+,Q_-,0,Q_Y);
  6. COMBINE(Q_n,Q_Y,n,Q_{Y□P});
  7. For each y+ ∈ Q_+ do
       if y+ = 0a then APPEND(A,(1^n y+));
  8. For each y- ∈ Q_- do
       if y- = 0b then APPEND(B,(y-));
  9. COMBINE(A,B,0,Q_X);
 10. APPEND(Q_{Y□P},Q_X); Q := Q_{Y□P};
  end.
```

Since the codes in lists Q_n, Q_Y, $Q_{Y\square P}$, Q_X, and Q computed by HAMILTON PATH correspond to the codes in the sets determined in Lines 3, 5, 6, 7, and 8 of LABELS, it is straightforward to see that HAMILTON PATH computes the set of canonical codes Q to the vertices of the catacondensed hexagonal graph G.

In order to prove that the procedure finds a Hamilton path in $R(G)$, we have to show that two consecutive strings in Q differs in exactly one bit. We proceed by induction on the number of recursive calls.

If $G = K_2$, the assertion is clear. Assume then $G \neq K_2$. To prove the claim note first that $Q = Y_0, Y_1, \ldots, Y_{n-1}, Y_n$, where the strings in Y_i form the set of codes of all vertices in $\mathcal{F}(G;e_i)$. We will show first that Y_i admits a Hamilton path in $\mathcal{F}(G;e_i)$. Line 6 yields that the strings in Y_i have the same prefix 1^i0^{n-i}. Therefore, it suffices to show that two consecutive codes in Q_Y differs in exactly one bit.

The codes of Q_Y are computed in Line 5 by combining codes of Q_+ and Q_-. By the induction hypothesis the codes of $Q_+ = (a_1, a_2, \ldots, a_s)$ as well as the codes of $Q_- = (b_1, b_2, \ldots, b_t)$ form Hamilton paths. It follows that two consecutive codes a_ib_j and a_ib_{j+1} composed within the i-th run of the main for loop obviously differ in exactly one bit. To complete the proof for the codes in Q_Y consider the last code computed in the i-th run of the main for loop a_ib_t (or a_ib_1) and the first code computed in the $(i+1)$-st run of the main for loop $a_{i+1}b_t$ (or $a_{i+1}b_1$).

That $Y_0, Y_1, \ldots, Y_{n-1}$ as well as strings in Q_X form Hamilton paths is proved analogously as above. We are left to prove that the last code in Y_{n-1} denoted v and the first code in Q_X denoted u differ in exactly one bit. Note that $u = 1^n0a0b$. In order to prove $v = 1^{n-1}00a0b$ we infer that v is formed in the n-th run of the main for loop of COMBINE. Since $2n$ is even, $v = 1^{n-1}0a_1b_1$. Moreover, a_1 (b_1) is the first vertex in Q_+ (Q_-), therefore obviously starts with 0 and the proof is complete.

To conclude the section consider the graph of Fig. 11. The procedure HAMILTON GRAPH returns

$$\begin{aligned}
Q_+ &= (0,\ 1),\\
Q_- &= (01,\ 00,\ 10),\\
Q_Y &= (001,\ 000,\ 010,\ 110,\ 100,\ 101),\\
Q_{Y\Box P} &= (00001,\ 00000,\ 00010,\ 00110,\ 00100,\ 00101,\\
&\quad\ 10101,\ 10100,\ 10110,\ 10010,\ 10000,\ 10001),\\
Q_X &= (11001,\ 11000),
\end{aligned}$$

and the obtained Hamilton path is then obtained by appending Q_X to $Q_{Y\Box P}$.

7. TWO PROBLEMS

In this paper we have recursively described the structure of the resonance graphs of catacondensed hexagonal graphs. It would be nice to obtain an explicit characterization of these graphs. Since they are median graphs, we ask the following question.

Problem 1 *Which additional characteristic properties must a median graph possess in order to be the resonance graphs of a catacondensed hexagonal graph?*

Let G be the resonance graph of a catacondensed hexagonal graph. Since G is a median graph and hence bipartite, the order of G must be even if G contains a Hamilton cycle. Let $\delta(G)$ denotes the smallest degree of G. Then we state:

Problem 2 *Is it true that $R(G)$ contains a Hamilton cycle if and only if $R(G)$ is of even order and $\delta(R(G)) \geq 2$?*

ACKNOWLEDGMENT

We are grateful to Tomaž Pisanski for his interest in our work.

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