

Resonantly Equivalent Catacondensed Even Ring Systems

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Abstract

In this paper we generalize the binary coding procedure of perfect matchings from catacondensed benzenoid graphs to catacondensed even ring systems (also called CERS). Next, we study CERS with isomorphic resonance graphs. For this purpose, we define resonantly equivalent CERS. Finally, we investigate CERS whose resonance graphs are isomorphic to the resonance graphs of catacondensed benzenoid graphs. As a consequence we show that for each phenylene there exists a catacondensed benzenoid graph such that their resonance graphs are isomorphic.

1 Introduction

In the present paper we focus on a class of graphs called even ring systems. An *even ring system* is a simple bipartite 2-connected plane graph with all interior vertices of degree 3 and all boundary vertices of degree 2 or 3 [9]. If all inner faces of an even ring system are hexagons we obtain a well known class of molecular graphs named *benzenoid graphs* or *benzenoid systems* (see [7]). They represent aromatic hydrocarbon molecules composed of benzene rings. However, in the existing (both mathematical and chemical) literature, there is inconsistency in the terminology pertaining to benzenoid graphs, since in some literature it is assumed that a benzenoid graph can be embedded into the regular hexagonal lattice.

The *inner dual* of a given even ring system consists of vertices corresponding to inner faces of the system; two vertices are adjacent if and only if the corresponding faces have a

common edge. A *catacondensed even ring system* (short *CERS*) is an even ring system so that its inner dual is a tree T . An inner face of a CERS is called *terminal* if it corresponds to a vertex of degree one in T . The class of CERS contains chemically important structures called catacondensed benzenoid graphs as well as another class of interesting molecules named phenylenes: in particular, a *catacondensed benzenoid graph* B is a CERS where all inner faces are hexagons and if we add squares between all pairs of adjacent hexagons of B , the obtained graph is called a *phenylene*. There are also some other not so well known molecules that belong to even ring systems: for example, in [4] α -4-catafusenes were considered and in [11] cyclooctatetraenes.

The aromaticity of benzenoid hydrocarbon is the consequence of the delocalization of π -electrons, i.e. double bounds in the molecular orbitals and it is usually represented by Kekulé structures. The interaction between Kekulé structures is reflected in the resonance graph of a given molecular graph. Resonance graphs were independently introduced by chemists (El-Basil [1, 2], Gründler [6]), as well as by mathematicians, since a Kekulé structure is just a perfect matching of a given graph (Zhang, Guo, and Chen [16] used a term *Z-transformation graph*).

It was shown in [16] that the resonance graphs of benzenoid graphs are always connected, bipartite, and they are either a path or have girth 4. Later, some of these properties were obtained for all plane (elementary) bipartite graphs (for example, see [18]). Nowadays the structure of resonance graphs is well investigated for different families of graphs. Recently, some properties of resonance graphs or closely related concepts were established for benzenoid graphs [20, 21], fullerenes [5, 12, 15, 19], nanotubes [13, 14], and plane bipartite graphs [3].

For our purposes the most important result on resonance graphs was obtained in [9], where the authors proved that the resonance graph of a CERS belongs to the class of median graphs. This result led to an algorithm that assigns a unique and quite short binary code to every perfect matching of a catacondensed benzenoid graph [10]. Later, the binary coding of perfect matchings was generalized to any benzenoid graph [17]. For the computer-aided manipulation with the Kekulé structures a short representation of such a structure is very welcome. The possibility of storing a complete information on perfect matching by means of a short binary string is another asset that may become indispensable when dealing with graphs possessing many such matchings.

In the next section we present some basic notation and definitions. In section 3, the binary coding procedure of perfect matchings is generalized to all CERS. Moreover, CERS with isomorphic resonance graphs are studied in section 4. Finally, in section 5 the CERS whose resonance graphs are isomorphic to the resonance graphs of a catacondensed benzenoid graph are investigated.

2 Preliminaries

The *distance* $d_G(u, v)$ between vertices u and v of a graph G is defined as the usual shortest path distance. The distance between two edges e and f of G , denoted by $d_G(e, f)$ or shortly by $d(e, f)$, is defined as the distance between corresponding vertices in the line graph of G . Here we follow this convention because in this way the pair $(E(G), d)$ forms a metric space. On the other hand, for edges $e = ab$ and $f = xy$ of a graph G it is also legitimate to set $\widehat{d}_G(e, f) = \min\{d_G(a, x), d_G(a, y), d_G(b, x), d_G(b, y)\}$. Obviously, for $e \neq f$ it holds $d_G(e, f) = \widehat{d}_G(e, f) + 1$.

The *hypercube* Q_n of dimension n is defined in the following way: all vertices of Q_n are presented as n -tuples $x_1x_2 \dots x_n$ where $x_i \in \{0, 1\}$ for each $i \in \{1, \dots, n\}$, and two vertices of Q_n are adjacent if the corresponding n -tuples differ in precisely one position. A subgraph H of a graph G is an *isometric subgraph* if for all $u, v \in V(H)$ it holds $d_H(u, v) = d_G(u, v)$. If a graph is isomorphic to an isometric subgraph of G , we say that it can be *isometrically embedded* in G . Any isometric subgraph of a hypercube is called a *partial cube*. Moreover, the notation $G[X]$ is used to denote the subgraph of G induced by the set X .

The *interval* $I(u, v)$ between vertices u and v consists of all vertices on a shortest path between u and v . A *median* of a triple of vertices u, v , and w is a vertex that lies in $I(u, v) \cap I(u, w) \cap I(v, w)$. A connected graph is a *median graph* if every triple of its vertices has a unique median. Basic results about median graphs can be found in [8]. It is well-known that every median graph is a partial cube.

A *1-factor* of a graph G is a spanning subgraph of G such that every vertex has degree one. The edge set of a 1-factor is called a *perfect matching* of G , which is a set of independent edges covering all vertices of G . In chemical literature, perfect matchings are known as Kekulé structures (see [7] for more details).

Let G be a CERS. We denote the edges lying on some face F of G by $E(F)$. The *resonance*

graph $R(G)$ is the graph whose vertices are the perfect matchings of G , and two perfect matchings M_1, M_2 are adjacent whenever their symmetric difference forms the edge set of exactly one inner face F of G , i.e. $M_1 \oplus M_2 = E(F)$. In such a case we say that M_1 can be obtained from M_2 by *rotating the edges* of F .

Finally, the Cartesian product $G \square H$ of graphs G and H has the vertex set $V(G) \times V(H)$, and vertices (a, x) and (b, y) are adjacent in $G \square H$ whenever $ab \in E(G)$ and $x = y$, or $a = b$ and $xy \in E(H)$.

3 Binary coding procedure of perfect matchings of CERS

In this section we generalize the binary coding of perfect matchings from catacondensed benzenoid graphs to CERS. For this purpose, some results from [9] are briefly repeated in the first part of the section.

Let G be a CERS. If F, F' are adjacent faces of G , then the two edges on the boundary of F that have exactly one vertex on the boundary of F' are called the *link* of F to F' . In [9] the authors proved the following proposition.

Proposition 3.1 [9] *Every CERS has a perfect matching and given a perfect matching M for every link either both edges or none belong to M .*

In that same paper the structure of the resonance graph of G was established and it was proved that the resonance graph can be isometrically embedded into the hypercube Q_n , where n is the number of inner faces of G . Let G be a CERS that is obtained from a CERS G' by attaching an inner face F over an edge e that belongs also to the inner face F' . Suppose that G' contains $n-1$ inner faces and that we have already embedded $R(G')$ into Q_{n-1} . We partition the perfect matchings of G into the sets $\mathcal{F}_e(G)$, $\mathcal{F}_e^{\bar{\ell}}(G)$, and $\mathcal{F}_e^{\ell}(G)$, accordingly to the presence or absence of edge e and link ℓ of F to F' . More precisely, $\mathcal{F}_e(G)$ is the set of perfect matchings of G that contain edge e , $\mathcal{F}_e^{\bar{\ell}}(G)$ is the set of perfect matchings of G that do not contain neither e nor link ℓ , and $\mathcal{F}_e^{\ell}(G)$ is the set of perfect matchings of G that do not contain edge e but contain link ℓ . Then $R(G)[\mathcal{F}_e(G) \cup \mathcal{F}_e^{\bar{\ell}}(G)]$ of $R(G)$ is isomorphic to $R(G')$ and also $R(G)[\mathcal{F}_e(G)]$ and $R(G)[\mathcal{F}_e^{\ell}(G)]$ are isomorphic. The resonance graph $R(G)$ can be embedded into $Q_n = Q_{n-1} \square K_2$ in such a way that the perfect matchings of $\mathcal{F}_e(G) \cup \mathcal{F}_e^{\bar{\ell}}(G)$ lie in one copy of Q_{n-1} , and the perfect matchings of

$\mathcal{F}_e^\ell(G)$ in the other copy, where perfect matchings of $\mathcal{F}_e(G)$ and $\mathcal{F}_e^\ell(G)$ are pairwise joined by an edge. For more details we refer to [9] or [10].

As a consequence of that decomposition structure the following result was also proved.

Theorem 3.2 [9] *The resonance graph of a CERS is a median graph.*

In [10] the algorithm of binary coding procedure for benzenoid graphs was presented. In this section the algorithm is generalized to an arbitrary CERS. Firstly, we need to generalize the concept of linear, kinky, and branched hexagons in a catacondensed benzenoid graph (see [7] for more details).

Definition 3.3 *Let F, F', F'' be three inner faces of a CERS such that F and F' have the common edge e and F', F'' have the common edge f . The triple (F, F', F'') is **regular** if the distance $d_G(e, f)$ is an even number and **irregular** otherwise. See Figure 1.*

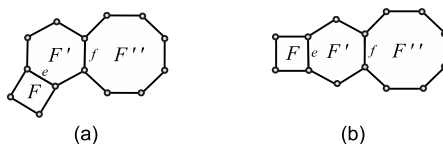


Figure 1. (a) Regular and (b) irregular triple (F, F', F'') of faces.

Let G be a CERS with n inner faces. Starting from an arbitrarily chosen terminal inner face F_1 we can assign consecutive numbers to each inner face to get the ordering F_1, F_2, \dots, F_n . Let T be an inner dual of CERS G which is a tree with n vertices. The pendant vertex of T , which corresponds to F_1 , is chosen as the root of this tree. The inner faces of G are then numbered such that F_i is a predecessor of F_j in T if and only if $i < j$. Such a numbering of inner faces is called *well-ordered* and can be obtained, for example, by the Depth-First Search algorithm (DFS) or by the Breadth-First Search algorithm (BFS).

Suppose that we have already obtained the binary coding for the perfect matchings of a graph composed of faces F_1, \dots, F_{k-1} and that we have obtained the set of binary strings S_{k-1} , $k \geq 3$. Let F_j be the face from the set $\{F_1, \dots, F_{k-1}\}$ that is adjacent to F_k . Moreover, define the face F_i as the face with the smallest index among all the adjacent inner faces of F_j . Then one can obtain S_k by choosing one of the next options:

- (a) if (F_i, F_j, F_k) is regular, we obtain S_k by inserting strings $x0$ (first two examples in Figure 2(a)) for each $x = x_1 \dots x_{k-1} \in S_{k-1}$ and inserting $x1$ (the last example in Figure 2(a)) for each x with $x_j = 0$.
- (b) if (F_i, F_j, F_k) is irregular, we obtain S_k by inserting strings $x0$ (first two examples in Figure 2(b)) for each $x = x_1 \dots x_{k-1} \in S_{k-1}$ and inserting $x1$ (the last example in Figure 2(b)) for each x with $x_j = 1$.

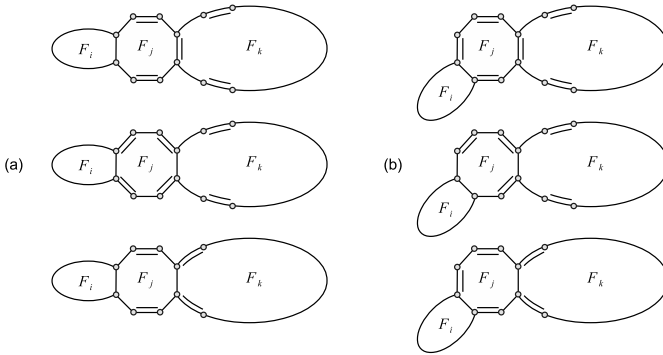


Figure 2. (a) Binary coding procedure in the regular and (b) in the irregular case.

From the above mentioned results we present the generalized version of the algorithm from [10]. For a greater transparency we mark $S_{k-1} := S$ and $S_k := S'$. For a CERS with two faces, F_1 and F_2 , we define the binary codes 00, 01, 10 for perfect matchings in the following way: code 00 represents the perfect matching that contains the common edge of F_1 and F_2 . Moreover, 01 represents the perfect matching obtained from 00 by rotating the edges in F_2 , and 10 is the remaining perfect matching. See Figure 3 for an example.

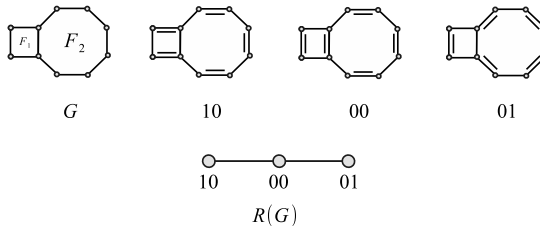


Figure 3. The graph G , the perfect matchings of G and the resonance graph $R(G)$.

Algorithm 1: Binary coding of perfect matchings of CERS

Input: Graph G well-ordered numbering of inner faces F_1, F_2, \dots, F_n

Output: Binary codes for all perfect matchings of a graph G

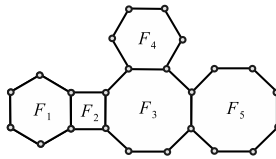
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1  $S := \{00, 01, 10\}$  for  $k = 3, \dots, n$  do
2    $S' := \emptyset$ 
3   set  $j \in \{1, \dots, k-1\}$  such that  $F_j F_k \in E(T)$ 
4    $i = \min\{l; F_l F_j \in E(T)\}$ 
5   if  $(F_i, F_j, F_k)$  is regular then
6     for each  $x \in S$  do
7        $S' := S' \cup \{x0\}$  if  $x_j = 0$  then
8          $S' := S' \cup \{x1\}$ 
9       end
10    end
11  else
12    for each  $x \in S$  do
13       $S' := S' \cup \{x0\}$  if  $x_j = 1$  then
14         $S' := S' \cup \{x1\}$ 
15      end
16    end
17  end
18   $S := S'$ 
19 end

```

It follows that this coding procedure results in an isometric embedding of the resonance graph of a CERS with n inner faces into a hypercube of dimension n . Therefore, two perfect matchings are adjacent in the resonance graph if and only if their codes differ in precisely one position and hence, we can easily construct the resonance graph from the set of binary codes of a CERS. Moreover, two CERS with the same sets of codes have isomorphic resonance graphs.

For an example, we use Algorithm 1 on the CERS G from Figure 4 and we denote its faces by F_1, \dots, F_5 . The resonance graphs obtained by Algorithm 1 are depicted in Figure 5. By G_k we denote the subgraph of G induced by the faces F_1, \dots, F_k , where $k \in \{2, 3, 4, 5\}$. Obviously, $G_5 = G$ and therefore, the last graph in Figure 5 is the resonance graph of G .



G

Figure 4. CERS G .

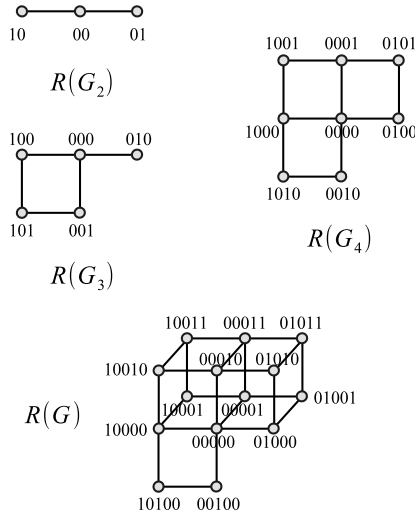


Figure 5. Resonance graphs $R(G_2)$, $R(G_3)$, $R(G_4)$, and $R(G)$ of graph G from Figure 4.

4 Resonantly equivalent CERS

In this section we investigate CERS with isomorphic resonance graphs. To describe such graphs, we define the following transformation. If G is a CERS with an inner face F and the outer face F_0 , then a connected component of the graph induced by the edges in $E(F) \cap E(F_0)$ is called a *boundary segment*.

Transformation 1. Let G be a CERS and P a boundary segment of G . A CERS G' is obtained from G by subdividing edges of P an even number of times or reversely, smoothing an even number of vertices of P (see Figure 6).

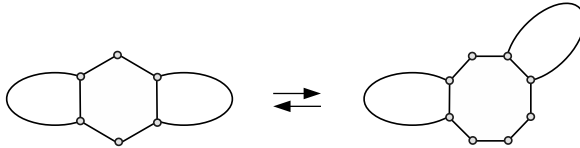


Figure 6. Subdividing (from left to right) and smoothing (from right to left) an even number of times.

Using the above transformation we define a new term which is essential for the rest of the paper.

Definition 4.1 Let G and H be two CERS. Then G is **resonantly equivalent** to H if G can be obtained from H by successively applying Transformation 1. In such a case we write $G \stackrel{R}{\sim} H$.

Resonantly equivalent CERS are shown in Figure 7

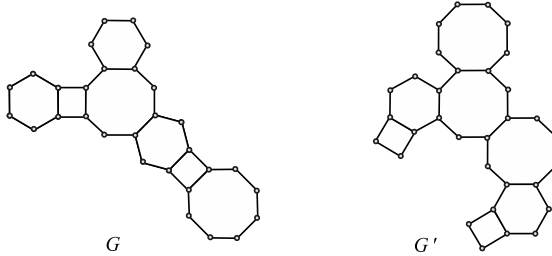


Figure 7. Resonantly equivalent CERS G and G' .

Remark 4.2 Relation $\stackrel{R}{\sim}$ is an equivalence relation on the set of all CERS. If G and H are resonantly equivalent, then both graphs have the same number of faces which differ only in lengths of its boundary segments.

The following lemma is needed for the main result of this section.

Lemma 4.3 Let G and H be resonantly equivalent CERS and let F_1, F_2, F_3 be three inner faces of G such that F_1, F_2 have a common edge and F_2, F_3 have a common edge. If we denote by F'_1, F'_2, F'_3 the corresponding faces of H , respectively, then the triple (F_1, F_2, F_3) is regular if and only if the triple (F'_1, F'_2, F'_3) is regular.

Proof. Let $e \in E(F_1) \cap E(F_2)$, $f \in E(F_2) \cap E(F_3)$, $e' \in E(F'_1) \cap E(F'_2)$ and let $f' \in E(F'_2) \cap E(F'_3)$. Obviously, by the definition of Transformation 1 it holds that $d_G(e, f)$ is an even number if and only if $d_H(e', f')$ is an even number. Therefore, the triple (F_1, F_2, F_3) is regular if and only if (F'_1, F'_2, F'_3) is regular. ■

Theorem 4.4 Let G and H be two CERS. If G and H are resonantly equivalent, then the resonance graph $R(G)$ is isomorphic to the resonance graph $R(H)$.

Proof. Let F_1, \dots, F_n be a well-ordered numbering of inner faces of G . Moreover, let F'_1, \dots, F'_n be the corresponding faces of graph H . We prove the theorem by using

induction on the number of faces. Let $G_k, H_k, k \in \{1, \dots, n\}$, be the graphs induced by the faces F_1, \dots, F_k and F'_1, \dots, F'_k , respectively. Obviously, the resonance graphs $R(G_2), R(H_2)$ are both isomorphic to the path P_2 and therefore isomorphic to each other. Suppose that we have already proved that for some $k \geq 3$ the sets of codes S_{k-1} and S'_{k-1} are the same (and therefore, $R(G_{k-1})$ is isomorphic to $R(H_{k-1})$). Let F_j be the face of G_k from the set $\{F_1, \dots, F_{k-1}\}$ that is adjacent to F_k . Moreover, define the face F_i as the face with the smallest index among all the adjacent inner faces of F_j . We define F'_j and F'_i from H_k in the same way. By Lemma 4.3 it follows that (F_i, F_j, F_k) is regular if and only if (F'_i, F'_j, F'_k) is regular. Therefore, by using Algorithm 1 we obtain that $S_k = S'_k$. Hence, $R(G_k)$ is isomorphic to $R(H_k)$.

By induction we obtain $R(G) = R(G_n) \cong R(H_n) = R(H)$ and the proof is complete. ■

5 Catacondensed benzenoid graphs and CERS with isomorphic resonance graphs

Definition 5.1 A CERS G is called **normal** if the following conditions hold:

- (i) any inner face is adjacent to at most three other inner faces,
- (ii) if an inner face F is adjacent to three other distinct inner faces F_1, F_2, F_3 , then all the triples $(F_1, F, F_2), (F_1, F, F_3)$, and (F_2, F, F_3) are regular.

Theorem 5.2 If G is a CERS, then G is normal if and only if G is resonantly equivalent to a catacondensed benzenoid graph.

Proof. Let G be a normal CERS. To obtain a catacondensed benzenoid graph G' , we successively replace all the inner faces of G by hexagons in the following way: when considering a particular inner face F we perform Transformation 1 on boundary segments of F such that F becomes a hexagon (note that this can be done since G is a normal CERS). Obviously, G and G' are resonantly equivalent.

For the other direction, suppose that G is resonantly equivalent to a catacondensed benzenoid graph G' . Therefore, G can be obtained from G' by successively applying Transformation 1. Since this transformation preserves the number of adjacent inner faces of some inner face, it follows that any inner face of G is adjacent to at most three inner faces. Moreover, let F be an inner face of G that is adjacent to three other inner faces

F_1, F_2, F_3 . Let H, H_1, H_2, H_3 be the hexagons in G' that correspond to F, F_1, F_2, F_3 , respectively. Since H is branched, the triples (H_1, H, H_2) , (H_1, H, H_3) , (H_2, H, H_3) are all regular. Therefore, by Lemma 4.3 all the triples (F_1, F, F_2) , (F_1, F, F_3) , (F_2, F, F_3) are regular. Hence, we have proved that G is normal. ■

Theorem 5.3 *If G is a normal CERS, then the resonance graph $R(G)$ is isomorphic to the resonance graph of some catacondensed benzenoid graph.*

Proof. Let G be a normal CERS and let G' be the catacondensed benzenoid graph obtained in the same way as in the proof of Theorem 5.2. Since G is resonantly equivalent to G' , by Theorem 4.4 the resonance graph $R(G)$ is isomorphic to the resonance graph $R(G')$ and the proof is complete. ■

Obviously, phenylenes are normal CERS and therefore, we obtain the following result.

Corollary 5.4 *For any phenylene B' there exists a catacondensed benzenoid graph B such that the resonance graph $R(B')$ is isomorphic to the resonance graph $R(B)$.*

In Figure 8 two resonantly equivalent graphs are depicted. Therefore their resonance graphs are isomorphic.

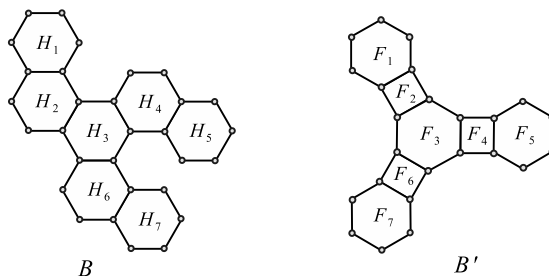


Figure 8. Resonantly equivalent benzenoid graph B and phenylene B' .

However, there are some CERS for which the resonance graphs are not isomorphic to the resonance graph of some catacondensed benzenoid graph. In the following example we show a CERS in which any inner face is adjacent to at most three other inner faces, but it has an irregular triple of faces. We show that the resonance graph of such CERS is not the resonance graph of a catacondensed benzenoid graph. For this purpose, the following theorem will be used.

Theorem 5.5 [16] *Let G be a benzenoid graph with a perfect matching that can be embedded into the regular hexagonal lattice. Further, let V_1 be the set of vertices of degree one in $R(G)$. If $R(G)$ is not a path, then it is a graph of girth 4 and $R(G) - V_1$ is 2-connected.*

Note that the previous theorem was proved in [16] only for benzenoid graphs that can be embedded into the regular hexagonal lattice. However, the same proof can be used for all catacondensed benzenoid graphs.

Example 5.6 *Let G be a CERS depicted in Figure 9. The resonance graph $R(G)$ is constructed from the perfect matchings also shown in the same figure. Let H be the subgraph obtained from $R(G)$ by removing the (unique) vertex of degree one. Obviously, H contains a cut vertex and therefore, it is not 2-connected. Hence, by Theorem 5.5, $R(G)$ can not be the resonance graph of some catacondensed benzenoid graph.*

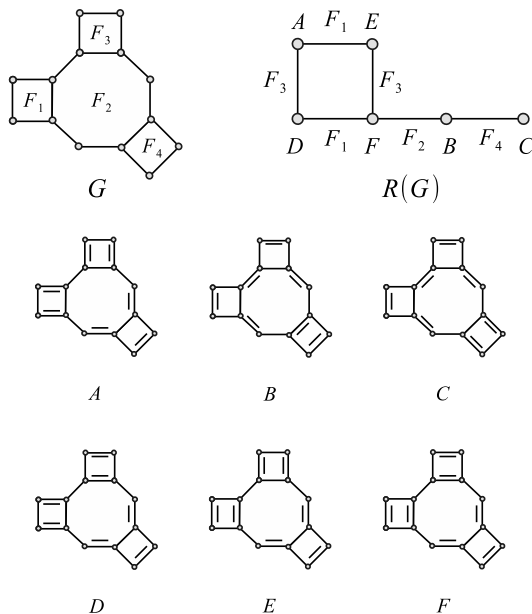


Figure 9. Graph G with its perfect matchings and the resonance graph.

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