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Resonance graphs of catacondensed even ring systems are median

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Abstract

Let G be a planar embedded 2-connected graph. Then the vertices of its resonance graph $R(G)$ are the 1-factors of G, two 1-factors being adjacent whenever their symmetric difference is a bounded face of G. For a class of graphs containing the chemically important catacondensed benzenoid graphs we show that the resonance graphs are median. In particular, if G belongs to this class, $R(G)$ has an isometric embedding into Q_f, where f is the number of bounded faces of G.

Keywords: Benzenoid graph; Median graph; Resonance graph; 1-factor; Z-transformation graph; Convex expansion

1. Introduction

Benzenoid hydrocarbons are composed of six-membered rings. Each pair of carbon atoms is connected by a single or a double bond. Double bonds in a single ring represent so called π-electrons. The distribution of π-electrons is represented by Kekulé structures. In Fig. 1(a) the three Kekulé structures of naphthalene are shown. Kekulé structures determine vertices of the resonance graphs. Two vertices are adjacent, if the corresponding Kekulé structures overlap in all double bonds except for the bonds in

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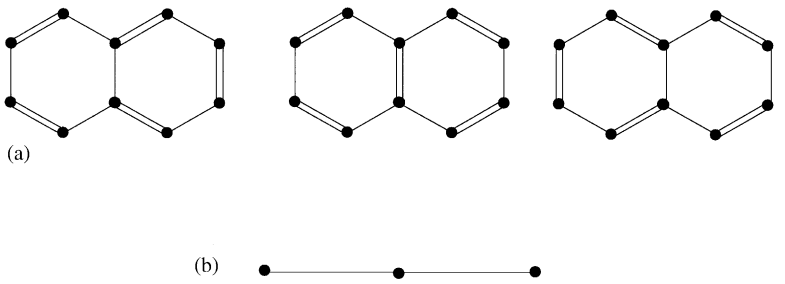

Fig. 1. Kekulé structures of naphthalene and its resonance graph.

a single ring. The resonance graph of naphthalene is the path on three vertices and is shown on Fig. 1(b).

The resonance energy is the energy gained by the delocalization of π-electrons. It can be derived from the number of Kekulé structures and the number of conjugated circuits, cf. [11]. It can also be calculated from the leading eigenvalue of the adjacency matrix of the resonance graph. Benzenoid hydrocarbons without Kekulé structures do exist, they are called non-Kekuléan. Though the problem to decide whether a benzenoid hydrocarbon has a Kekulé structure is easy from the algorithmic point of view (see [15]), there is no simple structure theorem distinguishing Kekuléan benzenoids from non-Kekuléan—see, for example, [12,13]. A more general problem is to determine the number of Kekulé structures of a benzenoid hydrocarbon, see [1,11,16,21,27]. For anyone, who is interested, there is an exhaustive bibliography on the enumeration of Kekulé structures in [11]. However, all catacondensed benzenoid hydrocarbons are Kekuléan, and so their resonance graphs are non-empty graphs.

Resonance graphs were under different names independently introduced by several chemists [6,7,9,10] and also by mathematicians. Zhang et al. [28] introduced them as Z-transformation graphs. They proved among others that the resonance graphs of Kekuléan benzenoid hydrocarbons are connected, bipartite, and that they are either a path or have girth 4. In [4] Chen and Zhang then proved that the resonance graph of a catacondensed benzenoid hydrocarbon has a Hamilton path.

The concept of the resonance graph was later rediscovered in [25,26]. In [26] a construction of the resonance graphs for some families of benzenoid compounds is outlined. In [25] Randić observed (due to a remark of Pisanski) that for some small examples constructed, the resonance graphs are median graphs. Our main result is a proof that even in a more general setting this is always the case, so especially for any catacondensed benzenoid hydrocarbon the resonance graph is a median graph. As the structure of median graphs is by now quite well understood, see [2,3,5,14,17,18,20,22,23], we hope that the present result can be used for some further insight into the resonance structure e.g. of benzenoid hydrocarbons. For instance, it follows from the proof of our theorem that if G is a catacondensed benzenoid graph with h hexagons then $R(G)$ can be isometrically embedded into the h dimensional hypercube.

2. Preliminaries

Benzenoid graphs are 2-connected subgraphs of the hexagonal (graphite) lattice so that every bounded face is a hexagon. If all vertices of a benzenoid graph B lie on its *perimeter*, then B is said to be *catacondensed*; otherwise it is *pericondensed*. For more information on these graphs see [11].

In this paper we will discuss a more general class of graphs we will call *even ring systems*. An even ring system is a simple bipartite 2-connected planar graph embedded in the plane with all interior vertices of valency 3 and all boundary vertices of valency 2 or 3. So all the faces are of even size. Note that even when all faces are hexagons, the graph need not be a benzenoid, since it is not necessarily a subgraph of the hexagonal lattice. The subclass of graphs with all bounded faces hexagons is sometimes called *fusenes* in the chemical literature. A *catacondensed even ring system* (short *cers*) is an even ring system so that the inner dual is a tree. An example of a cers is depicted in Fig. 2. This class contains also other chemically interesting structures such as phenylenes and similar structures (see [19]), but catacondensed benzenoids are the by far most important subclass.

A *matching* of a graph G is a set of pairwise independent edges. A matching is *perfect* or a 1-*factor*, if it contains (covers) all the vertices of G. Clearly, there is a bijective correspondence between the Kekulé structures of a benzenoid and the 1-factors of the corresponding benzenoid graph. We will always depict perfect matchings in a graph by drawing the edges in the matchings as double edges.

Let G be a cers. Then the vertex set of the *resonance graph* $R(G)$ of G consists of all 1-factors of G, and two 1-factors are adjacent whenever one can be obtained from the other by rotating the edges of a single bounded face. In other words, two 1-factors are adjacent if their symmetric difference is the edge set of a bounded face of G. (A related concept was studied in [8], where vertices of an associated graph correspond to maximum matchings while two vertices are adjacent if for the corresponding matchings F_1 and F_2 we have $|F_1 - F_2| = 1$.) For an example see Fig. 3, where all the 1-factors of the benzenoid graph corresponding to benzo[a]pyrene are shown as well as its resonance graph.

First we will fix some notation:

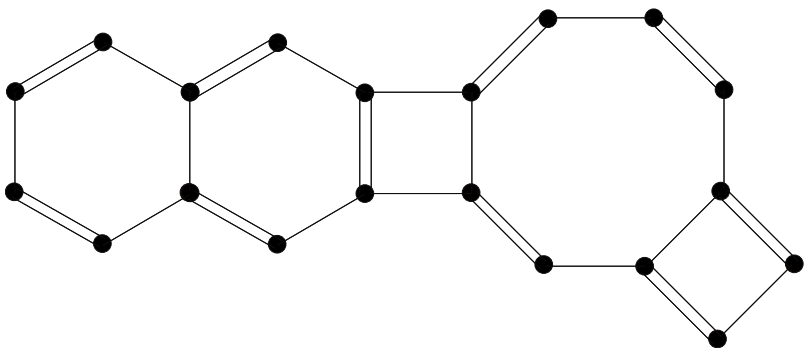

Fig. 2. An example of a cers with 4,6, and 8-sided faces and a perfect matching.

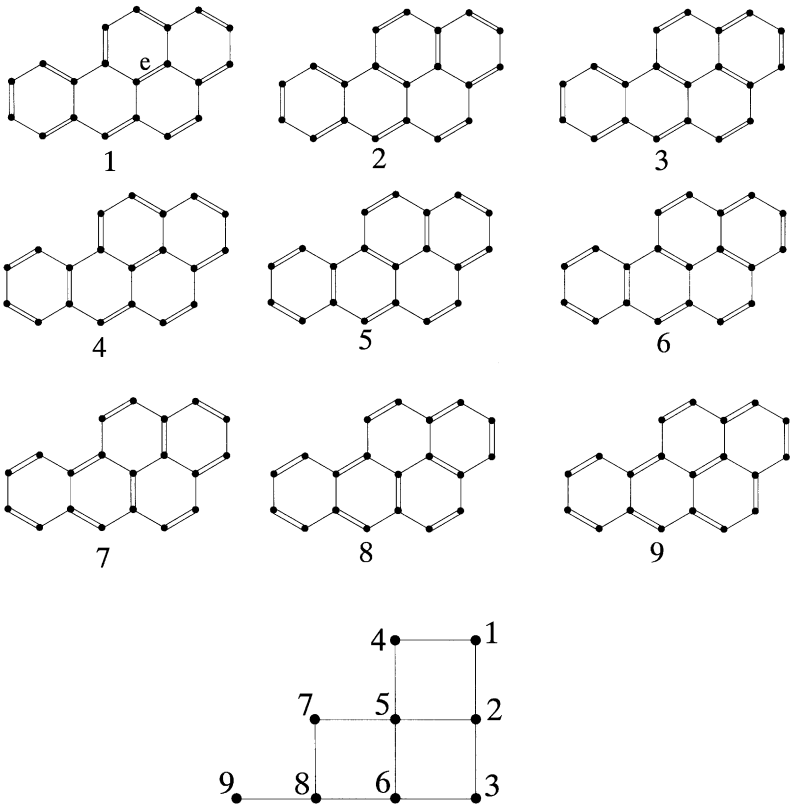

Fig. 3. A benzenoid graph and its resonance graph.

If A,B are incident faces of a cers, then the two edges on the boundary of A that have exactly one vertex on the boundary of B are called the *link* of A to B.

For a cers G, we write $F(G)$ for its set of bounded faces and $s(A)$ denotes the number of vertices in the boundary of a face A. Note that in a cers the boundaries of faces are simple cycles.

The b-edges of a face are the edges that are in the intersection of the boundary of that face and the boundary of the cers. The set of b-edges of a face A is denoted by $b(A)$.

If F_1 and F_2 are adjacent vertices of a resonance graph and A is the face in which the 1-factors F_1 and F_2 differ, then we say that the edge F_1F_2 corresponds to an *A-turn*.

The *distance* $d_G(u,v)$ (or $d(u,v)$ for short) between vertices u and v of a graph G will be the usual shortest path distance. A subgraph H of a graph G is an *isometric* subgraph if $d_H(u,v)=d_G(u,v)$, for all $u,v\in V(H)$. The *interval* $I(u,v)$ between vertices u and v consists of all vertices on shortest paths between u and v. A subset $W\subseteq V(G)$ is *convex* if $I(u,v)\subseteq W$ for any $u,v\in W$. A *convex subgraph* is a subgraph induced

by a convex set. The notation $G[X]$ is used to denote the subgraph of G induced by the set X.

A *median* 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 [17].

Let $G=(V,E)$ be a graph, V_1 and V_2 subsets of V with nonempty intersection, and $V=V_1\cup V_2$. Suppose that $G[V_1]$ and $G[V_2]$ are isometric in G and that no vertex of $V_1\setminus V_2$ is adjacent to a vertex of $V_2\setminus V_1$. In addition, let $V_1\cap V_2$ be convex in G. Then the *convex expansion* of a graph G with respect to V_1 and V_2 is the graph obtained from G by the following procedure:

(i) replace each vertex $v\in V_1\cap V_2$ by vertices v_1, v_2 and insert the edge v_1v_2.
(ii) insert edges between v_1 and the neighbors of v in $V_1\setminus V_2$ as well as between v_2 and the neighbors of v in $V_2\setminus V_1$.
(iii) insert the edges v_1u_1 and v_2u_2 whenever $v,u\in V_1\cap V_2$ are adjacent in G.

The following result of Mulder [22,23] is the basic tool for the proof of our main result:

Theorem 1. *A graph G is a median graph if and only if G can be obtained from K_1 by a sequence of convex expansions.*

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 $xy\in E(H)$. Note that the Cartesian product of median graphs is again median.

3. Proof of the main result

For an edge e of a graph G let $\mathscr{F}_e(G)$ be the set of 1-factors of G that contain e, and let $\mathscr{F}_{\bar{e}}(G)$ be the set of 1-factors of G that do not contain e.

We will prove that for a cers G and an edge e on the boundary of G the connected components of $R(G)[\mathscr{F}_e(G)]$ as well as of $R(G)[\mathscr{F}_{\bar{e}}(G)]$ are convex.

This will be an easy consequence of the structural results we will prove first:

Proposition 2. *Every cers has a perfect matching and given a perfect matching M for every link either both edges or none belong to M.*

Proof. Since the boundary of a cers has even length, we can just take every second edge on the boundary. This gives a perfect matching.

For the second part suppose a perfect matching M contains exactly one edge of a link. Removing the two adjacent endpoints of the link, the cers falls into two connected components G_1 and G_2, both of even size. If G_1 is the part containing vertices adjacent to the link, we can just add the endpoint of that edge of the link that is in M to G_1 to obtain G_1'. The graph G_1' would have odd order, but M would induce a perfect matching on it, which is of course a contradiction.

Proposition 3. *Given a cers G and a perfect matching M of G. Then there is a face with all the links to it* **not** *contained in M.*

Proof. Assume there is no such face.

Since the 3 edges on the boundary of a face that are incident with the endvertices of a link in M cannot be contained in M, $f \in F(G)$ contains at most $s(f)/2-1$ edges of M in its boundary.

Since all edges of M lie in the boundary of some face, we have

$$|M| \leqslant \sum_{f\in F(G)} \left(\frac{s(f)}{2} - 1\right) = \sum_{f\in F(G)} \frac{s(f)}{2} - |F(G)|.$$

So at most $\sum_{f\in F(G)} s(f) - 2|F(G)|$ vertices can be matched. But since the inner dual of G is a tree, we have $|V| = \sum_{f\in F(G)} s(f) - 2|F(G)| + 2$. So M was not a perfect matching.

Proposition 4. *Given a cers G, a face $A \in F(G)$, and perfect matchings M, M'. Then there is a b-edge of A that is in exactly one of M, M' if and only if this is true for every b-edge of A.*

(*That is*: *M and M' either agree on all b-edges or differ on all b-edges of a face.*)

Proof. This can easily be shown by induction by observing that for any b-edge e the next b-edge f along the cycle has this property: If f is adjacent with e, this follows, since exactly one of e, f must be contained in every perfect matching. So if e is in exactly one of M, M', then f is also contained in exactly one of M, M' (in the other one to be exact). If there is a non-b-edge g in between, connecting the endpoints $u \in e, g$ and $v \in f, g$ of a link, then Proposition 2 ensures that either u and v are saturated by the link or none. So if e is contained in a matching M_0, then neither g nor the edges of the link are contained. So v must be saturated by f. If on the other hand e is not contained in M_0, then u is either saturated by g or by the link. In both cases v is also saturated and therefore f is also not in M. So if e is in exactly one of M, M', then f is also contained in exactly one of M, M' (in the same one to be exact).

Lemma 5. *Given a cers G and two perfect matchings M and M'. Then $d_{R(G)}(M, M') = |\mathrm{Diff}(M, M')|$ with $\mathrm{Diff}(M, M') := \{A \in F(G) \mid b(A) \cap M \neq b(A) \cap M'\}$.*

(*Especially*: *$R(G)$ is connected.*)

Proof. The fact that $d_{R(G)}(M, M') \geqslant |\mathrm{Diff}(M, M')|$ follows from the fact that for a face A edges in $b(A)$ can only change their belonging to the matching by an A-turn, so for each $A \in \mathrm{Diff}(M, M')$ there must be an edge corresponding to an A-turn in any path from M to M' in $R(G)$.

We prove $d_{R(G)}(M, M') \leqslant |\mathrm{Diff}(M, M')|$ by induction on $n = |\mathrm{Diff}(M, M')|$. We have $n = 0$ if and only if $M = M'$, so assume $n > 0$ and that for $n' < n$ the result has been shown.

Note that a link from a face not in $\mathrm{Diff}(M,M')$ to a face $A \in \mathrm{Diff}(M,M')$ cannot be in M or M', since it would imply that the neighboring edges in $b(A)$ are neither in M nor in M' and therefore—due to Proposition 4—$A \notin \mathrm{Diff}(M,M')$.

So M and M' induce perfect matchings on the subgraph G_0 induced by the vertices that belong to faces in $\mathrm{Diff}(M,M')$. Applying Proposition 3 to some component of G_0, we deduce that G_0 and (using also the note above) therefore also G contains a face $A \in \mathrm{Diff}(M,M')$ with all the links to it *not* contained in M. So we can turn A to obtain a matching M_1 at distance one from M and (due to Proposition 4) $|\mathrm{Diff}(M_1,M')| = n-1$. Induction completes the proof.

Corollary 6. *Let G be a cers and let e be an edge on the boundary of G. Then the connected components of $R(G)[\mathscr{F}_e(G)]$, resp. $R(G)[\mathscr{F}_{\bar{e}}(G)]$ are convex.*

Proof. Let A be a face so that $e \in b(A)$, $M,M' \in \mathscr{F}_e(G)$ (resp. $M,M' \in \mathscr{F}_{\bar{e}}(G)$). By Proposition 4, we have $A \notin \mathrm{Diff}(M,M')$. Since any path P between M and M' that contains a vertex M_0 not contained in the induced subgraph $\mathscr{F}_e(G)$ (resp. $\mathscr{F}_{\bar{e}}(G)$) must contain an edge that corresponds to an A-turn as well as A' turns for all $A' \in \mathrm{Diff}(M,M')$, it must have length $|P| > |\mathrm{Diff}(M,M')|$, so it is not a shortest path.

We note here that for an arbitrary benzenoid graph G, $R(G)[\mathscr{F}_e(G)]$ need not be connected. Consider, for instance, the benzenoid graph from Fig. 3 and the indicated edge e. The subgraph $R(G)[\mathscr{F}_e(G)]$ is induced by vertices 1,4, and 9, which is the disjoint union of K_2 and K_1.

Theorem 7. *The resonance graph of a cers is a median graph.*

Proof. Let G be a cers with h bounded faces and let $R(G)$ be the resonance graph of G. We proceed by induction on h.

If $h=1$, that is, if $G=C_n$ for some even n, then $R(G)=K_2$. Suppose now that $h>1$. Let H be a face corresponding to a leaf of the inner dual of G. Let e be the edge of H which lies in two bounded faces of G and let G' be the graph which we obtain from G by removing those vertices and edges that are incident only with H. Then $R(G')$ is a median graph by the induction hypothesis.

Note that a 1-factor that is a vertex of $\mathscr{F}_{\bar{e}}(G)$ either contains the link of H to its neighboring face (we denote this set of vertices by $\mathscr{F}_{\bar{e}}^{l}(G)$) or not ($\mathscr{F}_{\bar{e}}^{\bar{l}}(G)$). Then we can partition the 1-factors of G as

$$V(R(G)) = \mathscr{F}_e(G) \cup \mathscr{F}_{\bar{e}}^{l}(G) \cup \mathscr{F}_{\bar{e}}^{\bar{l}}(G).$$

There is a natural bijective correspondence between the 1-factors of $\mathscr{F}_e(G)$ and of $\mathscr{F}_e(G')$. In addition, there is a bijection from the 1-factors of $\mathscr{F}_{\bar{e}}^{\bar{l}}(G)$ to those from $\mathscr{F}_{\bar{e}}(G')$. It follows that the subgraph $G_1 = R(G)[\mathscr{F}_e(G) \cup \mathscr{F}_{\bar{e}}^{\bar{l}}(G)]$ of $R(G)$ is isomorphic to $R(G')$. Consider now a 1-factor F from $\mathscr{F}_{\bar{e}}^{l}(G)$. In $R(G)$ it is adjacent to a unique 1-factor $\bar{F}$ of $\mathscr{F}_e(G)$. Mapping F to $\bar{F}$ defines a bijection from $\mathscr{F}_{\bar{e}}^{l}(G)$ to $\mathscr{F}_e(G)$. We note next that two 1-factors F_1 and F_2 of $\mathscr{F}_{\bar{e}}^{l}(G)$ are adjacent if and

only if the corresponding 1-factors $\bar{F}_1$ and $\bar{F}_2$ are adjacent. Therefore, $R(G)[\mathscr{F}_e(G)]$ and $R(G)[\mathscr{F}_{\bar{e}}^I(G)]$ are isomorphic and $R(G)[\mathscr{F}_e(G) \cup \mathscr{F}_{\bar{e}}^I(G)]$ is a subgraph of $R(G)$ isomorphic to $R(G)[\mathscr{F}_e(G)] \,\square\, K_2$.

By Lemma 5 $R(G')$ and $R(G)$ are connected. Moreover, the arguments used in the proof can be applied to infer that $R(G')[\mathscr{F}_e(G')]$ is a connected subgraph of $R(G')$. By Corollary 6 it is also convex. Therefore, by Mulder's convex expansion theorem applied to $R(G')$ with V_1, V_2 corresponding to $F_e(G)$ and $F_e(G) \cup \mathscr{F}_{\bar{e}}^I(G)$ the proof is complete. □

4. Concluding remarks

From the proof of Theorem 7 if follows not only that every resonance graph of a cers is median, but also that it can be obtained by an expansion procedure in which at every step an expansion is done with respect to the so-called peripheral subgraph (called extremal subgraph in [24]). In general, it seems an interesting problem to characterize the resonance graphs of catacondensed even ring systems or especially catacondensed benzenoid graphs among median graphs. In particular, we know by the result of [4] that the later ones are median graphs with Hamilton paths.

Randić [25] considered the question of embedding resonance graphs of catacondensed benzenoid graphs on a three-dimensional Cartesian coordinate grid. On the other hand, it is well-known that a median graph G provides an isometric embedding into a hypercube Q_n, i.e., G is isomorphic to an isometric subgraph of Q_n. Since in addition each step of the convex expansion procedure increases the dimension of a hypercube into which the median graph is embeddable by one, the proof of Theorem 7 also gives the following:

Proposition 8. *Let G be a cers with h bounded faces. Then $R(G)$ can be isometrically embedded into Q_h.*

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