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RESONANCE GRAPHS OF CATACONDENSED BENZENOID GRAPHS ARE MEDIAN

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Resonance graphs of catacondensed benzenoid graphs are median

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Abstract

Let G be a benzenoid graph. Then the vertices of its resonance graph $R(G)$ are the 1-factors of G, two 1-factors being adjacent whenever one is obtained from the other by rotating the edges in a 6-cycle. We prove that the resonance graphs of catacondensed benzenoid graphs are median.

Key words: benzenoid graph, median graph, 1-factor, 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 the 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 a single ring. The resonance graph of the naphthalene is the path on three vertices and is shown on Fig.1(b).

The resonance energy is the energy needed for the delocalization of π-electrons. It can be derived from the number of Kekulé structures and the number of con-

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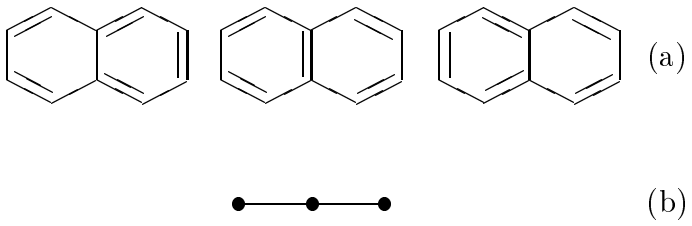

Fig. 1. Kekulé structures of the naphthalene and its resonance graph

jugated circuits, cf. [3]. It can also be calculated from the leading eigenvalue of the adjacency matrix of the resonance graph. Not all benzenoid hydrocarbons contain Kekulé structures, they are called non-Kekuléan. In some cases it is not trivial to decide, whether a given benzenoid hydrocarbon is non-Kekuléan or not, see, for example, [4,5]. A more general problem is to determine the number of Kekuléan structures of a benzenoid hydrocarbon, see [1,6,9,15].

Since all catacondensed benzenoid hydrocarbons are Kekuléan, their resonance graphs are nontrivial. A construction of the resonance graphs for some families of benzenoid compounds is outlined in [14]. Randić observed in [13] (due to a remark of Pisanski) that for some small examples constructed, the resonance graphs are median graphs. The main result of this note is a proof that this is always the case, that is, for any catacondensed benzenoid hydrocarbon, its resonance graph is a median graph. As the structure of median graphs is by now quite well understood, see [7,8,10,11], we hope that the present result can be used for some further insight into the resonance structure of benzenoid hydrocarbons.

2 Preliminaries

Benzenoid graphs are plane graphs representing benzenoid hydrocarbons. They are always considered as embedded into the hexagonal (graphite) lattice. All their hexagons are regular, mutually congruent. A benzenoid graph is always drawn so that some of its edges are vertical. If all vertices of a benzenoid graph B lie on its *circuit* (boundary), then B is said to be *catacondensed*; otherwise it is *pericondensed*. For more information on these graphs see [3].

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 hydrocarbon and the 1-factors of the corresponding benzenoid graph.

Let G be a benzenoid graph. Then the vertex set of the *resonance graph* $R(G)$ of G consists of 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 6-cycle. (A related concept was studied in [2], 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.2, where all the 1-factors of the benzenoid graph corresponding to a benzo[a]pyrene are shown as well as its resonance graph.

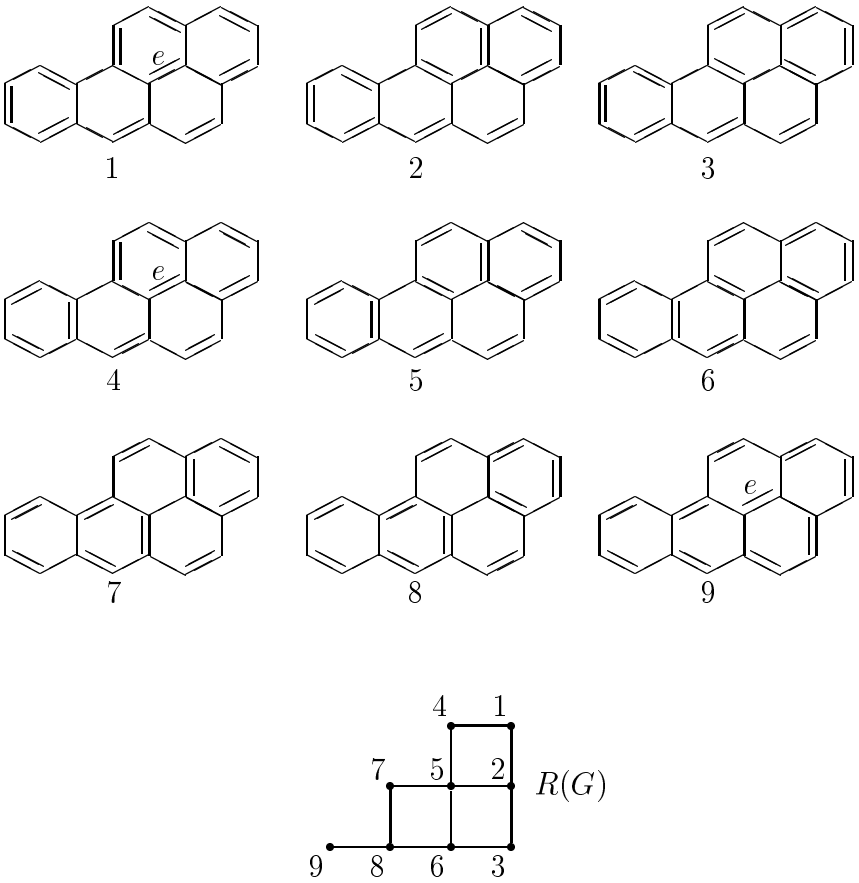

Fig. 2. A benzenoid graph and its resonance graph

If F_1 and F_2 are adjacent vertices of a resonance graph and A is the 6-cycle 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 of vertices of 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. By abuse of language we will also say that $X \subset V(G)$ is convex, if $G[X]$ induces a convex subgraph, where $G[X]$ denotes the subgraph of G induced by 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.

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 $\langle V_1 \rangle$ and $\langle V_2 \rangle$ 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 $v_1 v_2$.
(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 $v_1 u_1$ and $v_2 u_2$ whenever $v, u \in V_1 \cap V_2$ are adjacent in G.

The following result of Mulder [10,11] 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 $G \Box H$ of graphs G and H has the vertex set $V(G) \times V(H)$, and vertices (a, x) and (b, y) are adjacent in $G \Box H$ 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 $\mathcal{F}_e(G)$ be the set of 1-factors of G that contain e, and let $\mathcal{F}_{\overline{e}}(G)$ be the set of 1-factors of G that do not contain e.

Lemma 2 *Let G be a catacondensed benzenoid graph and let e be an edge on the circuit of G. Then the connected components of $R(G)[\mathcal{F}_e(G)]$ are convex in $R(G)$.*

PROOF. Suppose not and let F_1 and F_2 be vertices of a connected component of $R(G)[\mathcal{F}_e(G)]$, such that a shortest F_1, F_2-path P is not completely in $R(G)[\mathcal{F}_e(G)]$. Let F_1 and F_2 be as close as possible, so that we can assume that the neighbors F_1' of F_1 and F_2' of F_2 both belong to $R(G)[\mathcal{F}_{\overline{e}}(G)]$. It is possible that $F_1' = F_2'$. Note that $|F_1 \cap A| = 3$, for otherwise F_1 and F_1' would not be adjacent. Hence we also have $|F_1' \cap A| = 3$.

Case 1: Endpoints of e are of degree 2.
In this case we distinguish three subcases depending on the structure of F_1', see Fig.3.

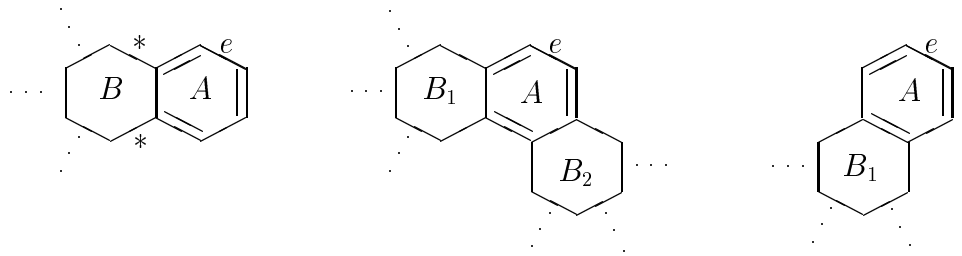

Fig. 3. Possible structures of F_1'

Case 1.a: e belongs to a pendant 6-cycle A and is on distance 1 to the neighboring 6-cycle B.

Since $|F_1' \cap A| = 3$, F_1' does not contain edges on the two positions that are marked with stars on Fig.3(a). Therefore, an edge of the F_1', F_2'-subpath of P would correspond to a B-turn only if there would be another edge corresponding to an A-turn. Since the subpath is completely in $R(G)[\mathcal{F}_{\overline{e}}(G)]$ this is not possible. Hence P is not a shortest path, because the path which is defined by the same turns as P, except the first and the last A-turn, is an F_1, F_2-path (in $R(G)[\mathcal{F}_e(G)]$) which is shorter than P.

Case 1.b: e is on distance 1 to neighboring 6-cycles B_1 and B_2.

As in Case 1.a we infer that because $|F_1 \cap A| = 3$, no edge of P corresponds neither to a B_1-turn or to a B_2-turn. Thus, with the same argument we infer that P is not a shortest path.

Case 1.c: e belongs to a pendant 6-cycle A and is on distance 2 to the neighboring 6-cycle B_1.

Let $B_1, B_2, \ldots B_k$, $k \geq 1$, be the largest sequence of adjacent 6-cycles starting in B_1 that lie in a straight line. Note that unless G is a linear chain, the sequence will end up as it is shown on Fig.4.

If no edge of P corresponds to a B_i-turn ($1 \leq i \leq k$), then we can argue as before that P is not a shortest path. Hence let j be the largest index such that a B_j-turn was made. Then before the B_j-turn all the B_i-turns with $i < j$ must be performed. If $j < k$ then, in order to make the second A-turn, that is, to return to $R(G)[\mathcal{F}_e(G)]$, all the B_i-turns with $i = 1, 2, \ldots, j$ must be repeated. Therefore P cannot be a shortest path. Finally, if $j = k$, then, using the arguments of Case 1.a, we infer that for a neighboring 6-cycle C of B_k, which is different from B_{k-1} (if such a cycle exists), no C-turn is possible. But

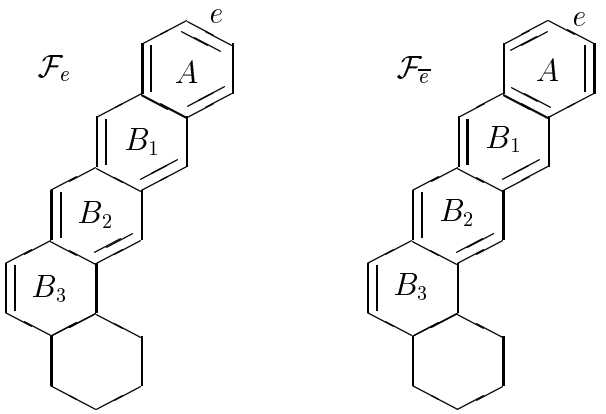

Fig. 4. Local straight line sequence

then again we infer again that P is not a shortest path.

Case 2: Endpoints of e have different degrees (that is, 2 and 3).

In this case we distinguish two subcases that are shown on Fig.5.

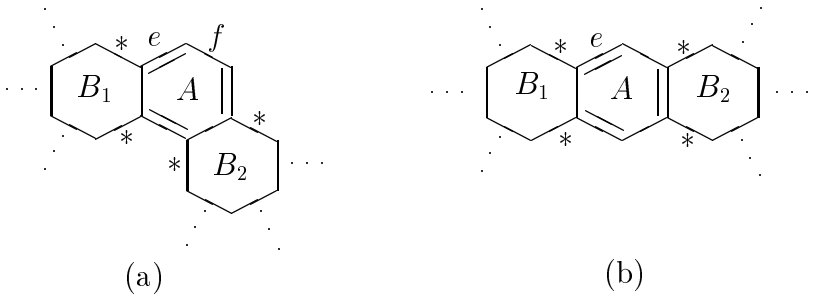

Fig. 5. Endpoints of the edge e are of degrees 2 and 3

Case 2.a: e is incident to an edge with both endpoints of degree 2.

Since $|F_1 \cap A| = 3$ and $|F_1' \cap A| = 3$, F_1' does not contain edges on four positions marked with stars on Fig.5(a). Let f be the edge of A as shown on the figure, and note that $f \in F_1'$. From Case 1.b we know that $R(G)[\mathcal{F}_f(G)]$ is a convex subgraph of $R(G)$. This means that a shortest path between F_1' and F_2' does not contain an edge corresponding to a B_1- or a B_2-turn. Thus, with the same argument as above, we find out that P is not a shortest path.

Case 2.b: e is not incident to an edge with both endpoints of degree 2.

In this subcase we have a similar situation as in Case 1.b since a shortest path between F_1' and F_2' does not contain an edge with a B_1- or B_2-turn. Thus, again P is not a shortest path.

Case 3: Endpoints of e are of degree 3, see Fig.6.

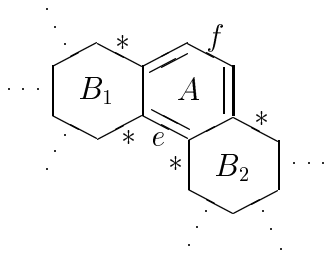

Fig. 6. Endpoints of the edge e are of degree 3

Let f be the edge of G as shown on Fig.6. Then by Case 1.b $R(G)[\mathcal{F}_f(G)]$ is a convex subgraph of $R(G)$, so we conclude again that P is not a shortest path. $\square$

We note here that for an arbitrary benzenoid graph G, $R(G)[\mathcal{F}_e(G)]$ need not be connected. Consider, for instance, the benzenoid graph from Fig.2 and the indicated edge e. The subgraph $R(G)[\mathcal{F}_e(G)]$ is induced by vertices 1,4, and 9, which is the disjoint union of K_2 and K_1.

Theorem 3 *The resonance graph of a catacondensed benzenoid graph is a median graph.*

PROOF. Let G be a catacondensed benzenoid graph with h hexagons and let $R(G)$ be the resonance graph of G. We proceed by induction on h.

If $h = 1$, that is, if $G = C_6$, then $R(G) = K_2$. Suppose now that $h > 1$. Let H be a pendant 6-cycle of G. Let e be the edge of H which lies in two 6-cycles of G and let G' be the graph which we obtain from G by removing H (but not ab). Then $R(G')$ is a median graph by the induction hypothesis.

Note that a 1-factor of $\mathcal{F}_{\overline{e}}(G)$ contains either two or three edges of H. We denote these 1-factors of G by $\mathcal{F}^2_{\overline{e}}(G)$ and $\mathcal{F}^3_{\overline{e}}(G)$, respectively. Then we can partition the 1-factors of G as

$$V(R(G)) = \mathcal{F}_e(G) + \mathcal{F}^2_{\overline{e}}(G) + \mathcal{F}^3_{\overline{e}}(G)\,.$$

There is a natural bijective correspondence between the 1-factors of $\mathcal{F}_e(G)$ and of $\mathcal{F}_e(G')$. In addition, a 1-factor from $\mathcal{F}^2_{\overline{e}}(G)$ corresponds to a unique 1-factor from $\mathcal{F}_{\overline{e}}(G')$. It follows that the subgraph $G_1 = R(G)[\mathcal{F}_e(G) + \mathcal{F}^2_{\overline{e}}(G)]$ of $R(G)$ is isomorphic to $R(G')$. Consider now a 1-factor F from $\mathcal{F}^3_{\overline{e}}(G)$. In $R(G)$ it is adjacent to a unique 1-factor $\overline{F}$ of G_1. We note next that two 1-factors F_1 and F_2 of $\mathcal{F}^3_{\overline{e}}(G)$ are adjacent if and only if the corresponding 1-factors $\overline{F_1}$ and $\overline{F_2}$ are adjacent. Therefore, $R(G)[\mathcal{F}_e(G)]$ and $R(G)[\mathcal{F}^3_{\overline{e}}(G)]$ are isomorphic and $R(G)[\mathcal{F}_e(G) + \mathcal{F}^3_{\overline{e}}(G)]$ is a subgraph of $R(G)$ isomorphic to $R(G)[\mathcal{F}_e(G)]\square K_2$.

By the above structure description it is an easy induction argument to show that $R(G')$ and $R(G)$ are connected. Moreover, the arguments of the proof of Lemma 2 can be used to infer that $R(G')[\mathcal{F}_e(G')]$ is a connected subgraph of $R(G')$. By Lemma 2 it is also convex. Therefore, by Mulder's convex expansion theorem the proof is complete. □

4 Concluding remarks

From the proof of Theorem 3 if follows not only that every resonance graph of a catacondensed benzenoid graph 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 pendant subgraph (called extremal subgraph in [12]). In general, it seems an interesting problem to characterize the resonance graphs of catacondensed benzenoid graphs among median graphs.

Randić [13] considered the question of embedding resonance graphs of catacondensed benzenoid graphs on a 3-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 3 also gives the following:

Proposition 4 *Let G be a catacondensed benzenoid graph with h hexagons. Then G can be isometrically embedded into Q_h.*

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