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The unfixed subgraph of a catacondensed hexagonal system obtained by fixing an alternating set

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We show that the unfixed subgraph of a catacondensed hexagonal system obtained by fixing an alternating set is either empty or its components are catacondensed hexagonal systems. Also, we provide some alternating sets for which this unfixed subgraph is empty. Finally, we prove that, in catacondensed hexagonal systems, the concept of a maximal M-resonant set, where M is a perfect matching, is equivalent to that of a maximal resonant set.

KEY WORDS: catacondensed hexagonal system, catacondensed benzenoid system, fixed edges, alternating set, resonant set

AMS subject classification: 05C90

1. Introduction

Let C be a cycle on the hexagonal lattice. Then the vertices and the edges lying on C and in the interior of C form a hexagonal system [1]. The vertices of a hexagonal system H are divided into external and internal. A vertex of H lying on the boundary of the exterior face of H is called an external vertex, otherwise, it is called an internal vertex. If a hexagonal system has no internal vertices, it said to be catacondensed, otherwise, it is pericondensed. A hexagonal system is to be placed on the plane so that a pair of edges of each hexagon lies in parallel with the vertical axis.

A perfect matching of a hexagon is called a sextet [2]. It is proper if the right vertical edge of the hexagon is in the perfect matching; otherwise, it is improper.

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Let H be a hexagonal system and P a non-empty set of hexagons. H-P denotes the subgraph of H obtained by deleting from H the vertices of the hexagons in P (together with their incident edges).

Let P be a non-empty set of hexagons of a hexagonal system H. Following Abeledo and Atkinson [3], we call P a set of mutually alternating hexagons of H (or simply an alternating set or a framed set) if there exists a perfect matching of H that contains a sextet of each hexagon in P. It can be seen that if P is an alternating set of H, then H-P is empty or has a perfect matching. An alternating set is maximal if it is not contained in a larger alternating set.

Let P be a non-empty set of hexagons of a hexagonal system H. Let M be a perfect matching of H. We call P an M-alternating set if the perfect matching M contains a sextet of each hexagon in P. It is clear that a non-empty set of hexagons P is alternating if and only if it is M-alternating for some perfect matching M. An M-alternating set is maximal if it is not contained in a larger M-alternating set. It is obvious that there is a unique maximal M-alternating set, namely, the set of all M-alternating hexagons.

Let P be a non-empty set of hexagons of a hexagonal system H. We call P a resonant set of H if the hexagons in P are pair-wise disjoint and there exists a perfect matching of H that contains a sextet of each hexagon in P [3] or equivalently [4] if the hexagons in P are pair-wise disjoint and H-P has a perfect matching or is empty. A resonant set is maximal if it is not contained in a larger resonant set.

Let P be a non-empty set of hexagons of a hexagonal system H. Let M be a perfect matching of H. We call P an M-resonant set if the hexagons in P are pair-wise disjoint and the perfect matching M contains a sextet of each hexagon in P. It is clear that a non-empty set of hexagons P is resonant if and only if it is M-resonant for some perfect matching M. An M-resonant set is maximal if it is not contained in a larger M-resonant set.

An edge of a graph H that has a perfect matching is said to be a fixed single (resp. fixed double) edge if it belongs to none (resp. all) perfect matchings of H. An edge is called fixed if it is either a fixed single edge or a fixed double edge.

Let H be a hexagonal system that has a perfect matching. Let P be an alternating set of H. Consider H-P. If H-P is nonempty, then it must possess at least one perfect matching. If H-P is empty, then the unfixed subgraph of H obtained by fixing P is the empty graph. In what follows we assume that H-P is nonempty, which is the non-trivial case. Some of the edges of H-P may be fixed (either double or single). Delete the fixed double edges of H-P (if any), together with their end vertices, and delete the fixed single edges of H-P (if any), without their end vertices. The remaining subgraph of H (possibly, an empty graph) is called the unfixed subgraph of H obtained by fixing P.

Let H be a hexagonal system that has a perfect matching. Let P be an alternating set of H. The definition of the unfixed subgraph of H obtained by fixing P can be reformulated as follows. Let M be a perfect matching of H that contains a sextet of each hexagon in P. Fix the hexagons in P as proper sextets or improper sextets as they are in M. Delete the fixed double edges of H together with their end vertices and delete the fixed single edges of H (without their end vertices). The remaining subgraph of H (possibly, an empty graph) is independent of the perfect matching M and we call it the unfixed subgraph of H obtained by fixing P.

We can relate this latter reformulation to literature, particularly, to Randić's fragmentation method [5]. Randić fixes an edge as a double edge or as a single edge. Generally, this results in the fixation of several other edges. Then the fixed double edges are deleted together with their end vertices and the fixed single edges are deleted without their end vertices. What is done here is that a collection of edges are fixed simultaneously (Randić fixes only one edge), some as double edges and others as single edges (the hexagons of the alternating set are fixed as sextets as appropriate). Then, as Randić does, the fixed double edges are deleted together with their end vertices and the fixed single edges are deleted without their end vertices.

The idea of edges fixed by fixing edges also appears in a paper by Hansen and Zheng [6].

In catacondensed hexagonal systems (excluding benzene, a single hexagon), one can distinguish between four types of hexagons [1,7]: (1) a hexagon adjacent to one hexagon, called terminal (T), (2) a hexagon adjacent to two hexagons in which the shared edges are parallel, called linearly annelated (L), (3) a hexagon adjacent to two hexagons in which the shared edges are not parallel, called angularly annelated (A), (4) a hexagon adjacent to three hexagons, called branched (B). It is clear that a T-hexagon is incident to a hexagon sequence of the form L^nY, where $n \geqslant 0$ and $Y \neq L$, an L- or an A-hexagon is incident to two hexagon sequences of the same form, and a B-hexagon is incident to three such sequences [1,7].

2. Results

Before stating the following algorithm, we recall that a catacondensed hexagonal system has perfect matchings and that each hexagon of a catacondensed hexagonal system is resonant [7]. More precisely, a catacondensed hexagonal system with h hexagons has at least $h+1$ perfect matchings [8].

Algorithm 1 [7]

Input: H, a catacondensed hexagonal system and R, a hexagon of H.

Output: U, the unfixed subgraph of H obtained by fixing the hexagon R.

Begin

Delete from H the hexagon R and all the (one, two or three) L^nY hexagon sequences incident to R($n \geqslant 0$, $Y \neq L$). U is the obtained subgraph.

End

Proposition 1 [7]. Algorithm 1 terminates and is correct.

Algorithm 2

Input: H, a catacondensed hexagonal system and P, an alternating set of H.
Output: U, the unfixed subgraph of H obtained by fixing P.

Begin

Initialization Step

Assign U = H. Associate a flag with each hexagon in P and set all the flags down.

Main Step

1. Pick a hexagon with a down flag from P and call it R. Delete from U the hexagon R and all the (one, two or three) L^nY hexagon sequences incident to R in H ($n \geqslant 0$, $Y \neq L$).
2. Assign U to its subgraph obtained in step 1 (which is possibly empty). Make the flag of R up. If an L-hexagon of a hexagon sequence in step 1 belongs to P, make its flag up. If a Y-hexagon of a hexagon sequence in step 1 belongs to P and is terminal, make its flag up.
3. If there exists a hexagon in P with a down flag, go to step 1, otherwise, stop (U is the unfixed subgraph of H obtained by fixing P).

End

Proposition 2. Algorithm 2 terminates and is correct.

Proof. That it terminates follows from the fact that P is finite and each application of the main step changes the status of at least one flag from down to up. Correctness follows from Proposition 1. □

Proposition 3. Let H be a catacondensed hexagonal system. Let P be an alternating set of H. Then the unfixed subgraph of H obtained by fixing P is either empty or its components are catacondensed hexagonal systems.

Proof. This follows from Algorithm 2. □

Proposition 4. Let H be a hexagonal system that has a perfect matching. Let P be an alternating set of H. The unfixed subgraph of H obtained by fixing P is empty if and only if H-P has a unique perfect matching or is empty.

Proof. Only if part:
Assume that the unfixed subgraph of H obtained by fixing P is empty.

P is an alternating set, so H-P has a perfect matching or is empty. It remains to show the uniqueness. Assume that H-P has more than one perfect matching. Then H-P has an alternating cycle and a non-fixed edge. Thus, the unfixed subgraph of H obtained by fixing P contains this non-fixed edge, hence, it is not empty, a contradiction.

If part:

Assume that H-P has a unique perfect matching or is empty.

If H-P is empty, then the unfixed subgraph of H obtained by fixing P is empty (by definition).

If H-P is not empty, then it has a unique perfect matching. The edges of this perfect matching are fixed double edges. Hence, the unfixed subgraph of H obtained by fixing P is empty. □

Corollary 5. Let H be a catacondensed hexagonal system. Let M be a perfect matching of H. Let P be a maximal M-resonant set. Then the unfixed subgraph of H obtained by fixing P is empty.

Proof. Fix the hexagons in P as proper sextets or improper sextets as they are in M. Assume that the unfixed subgraph of H obtained by fixing P is not empty. Then its components are catacondensed hexagonal systems (Proposition 3). M contains a perfect matching of these catacondensed hexagonal systems. This latter perfect matching contains a sextet of a hexagon, say of R [9]. $P \cup \{R\}$ is an M-resonant set that contains P as a proper subset, a contradiction. □

Corollary 6. Let H be a catacondensed hexagonal system. Let M be a perfect matching of H. Let P be a maximal M-resonant set. Then H-P has a unique perfect matching or is empty.

Remark. Corollary 5 and Corollary 6 are equivalent by Proposition 4.

Corollary 7. Let H be a catacondensed hexagonal system. Let P be a maximal resonant set. Then the unfixed subgraph of H obtained by fixing P is empty.

Proof. Let M be a perfect matching of H that contains a sextet of each hexagon in P. P is a maximal M-resonant set. Use Corollary 5. □

Corollary 8 [4]. Let H be a catacondensed hexagonal system. Let P be a maximal resonant set. Then H-P has a unique perfect matching or is empty.

Remark. Corollary 7 and Corollary 8 are equivalent by Proposition 4.

The following four corollaries can be proved using proof techniques similar to those used in proving the above four corollaries, respectively.

Corollary 9. Let H be a catacondensed hexagonal system. Let M be a perfect matching of H. Let P be the set of all M-alternating hexagons. Then the unfixed subgraph of H obtained by fixing P is empty.

Corollary 10. Let H be a catacondensed hexagonal system. Let M be a perfect matching of H. Let P be the set of all M-alternating hexagons. Then H-P has a unique perfect matching or is empty.

Corollary 11. Let H be a catacondensed hexagonal system. Let P be a maximal alternating set. Then the unfixed subgraph of H obtained by fixing P is empty.

Corollary 12. Let H be a catacondensed hexagonal system. Let P be a maximal alternating set. Then H-P has a unique perfect matching or is empty.

Proposition 13. Let H be a catacondensed hexagonal system. Let M be a perfect matching of H. Let P be a maximal M-resonant set. Then P is a maximal resonant set.

Proof. Suppose that P is not a maximal resonant set. Then there exists a resonant set that contains P as a proper subset, say P ∪ {R}, where R is a hexagon of H (without loss of generality). Let M′ be a perfect matching of H that contains a sextet of each hexagon in P ∪ {R}. M′ contains a perfect matching of H-P. This perfect matching of H-P contains a sextet of R, hence, H-P has more than one perfect matching, a contradiction (Corollary 6). □

Remark. Proposition 3 and Corollaries 5–10 cannot be extended to pericondensed hexagonal systems. This can be seen from figure 1, where a pericondensed hexagonal system is shown and P = {R} is an alternating set (Proposition 3 fails), a maximal resonant set (Corollaries 5–8 fail) and the set of all M-alternating hexagons (Corollaries 9–10 fail). On the other hand, Corollaries 11–12 may be extended to pericondensed hexagonal systems [10]. That Corollary 8 cannot be extended to pericondensed hexagonal systems was also mentioned in [4].

Proposition 13 cannot be extended to pericondensed hexagonal systems. This can be seen from figure 2, where a pericondensed hexagonal system is shown together with a perfect matching M and P = $\{R_1\}$ is a maximal M-resonant set.

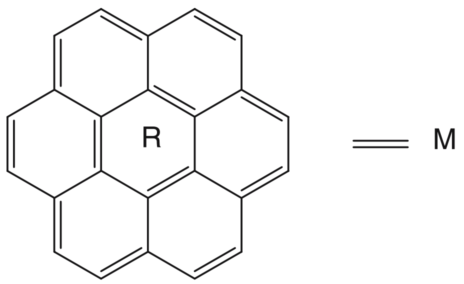

Figure 1. A pericondensed hexagonal system (coronene).

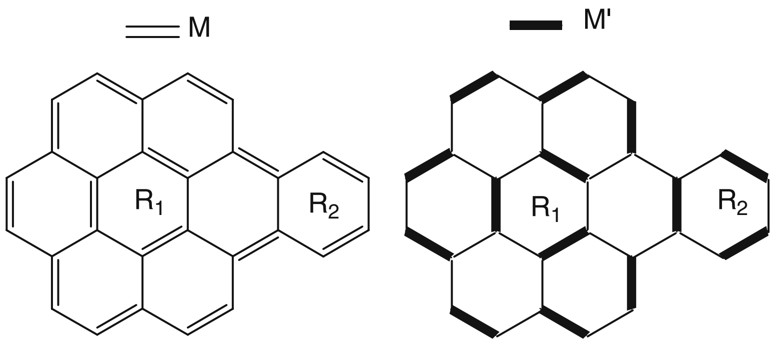

Figure 2. A pericondensed hexagonal system (benzo[a]coronene).

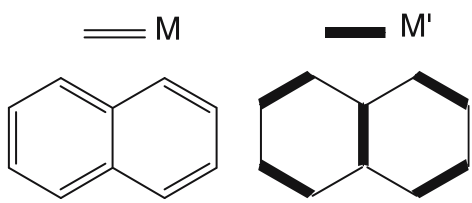

Figure 3. A catacondensed hexagonal system (naphthalene).

Remark. Let H be a hexagonal system (catacondensed or pericondensed), M a perfect matching of H, and P the set of all M-alternating hexagons. Then P is not necessarily a maximal alternating set. See figure 2 (a pericondensed hexagonal system) and figure 3 (a catacondensed hexagonal system).

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