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Maximum cardinality resonant sets and maximal alternating sets of hexagonal systems

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ABSTRACT

It is shown that the Clar number can be arbitrarily larger than the cardinality of a maximal alternating set. In particular, a maximal alternating set of a hexagonal system need not contain a maximum cardinality resonant set, thus disproving a previously stated conjecture. It is known that maximum cardinality resonant sets and maximal alternating sets are canonical, but the proofs of these two theorems are analogous and lengthy. A new conjecture is proposed and it is shown that the validity of the conjecture allows short proofs of the aforementioned two results. The conjecture holds for catacondensed hexagonal systems and for all normal hexagonal systems up to ten hexagons. Also, it is shown that the Fries number can be arbitrarily larger than the Clar number.

1. Introduction

Perfect matchings play a meaningful role in mathematical chemistry and have been studied for many decades. Also, the topic received a lot of recent attention, in particular with respect to the fullerenes, see for instance [1–4]. The ongoing and recent interest in perfect matchings is specially true for hexagonal systems [5–10] since perfect matchings naturally model the so-called Kekulé structures of the corresponding benzenoid molecules.

In this paper, we are interested in both maximum cardinality resonant sets and maximal alternating sets of hexagonal systems (see Section 2 for all the definitions). In 1985, Zheng and Chen [11] proved that every maximum cardinality resonant set of a hexagonal system is canonical. (Gutman first proved the result for catacondensed hexagonal systems [12].) On the other hand, in 2006, more than two decades later, Salem and Abeledo [13] proved that every maximal alternating set of a hexagonal system is canonical. (Again, this was earlier proved in [14] for the case of catacondensed hexagonal systems.) The proof of this latter result replicates a lot of the ideas used in the proof of the earlier result.

So both – maximum cardinality resonant sets and maximal alternating sets – are canonical and the proofs of these results are analogous and in fact lengthy. This naturally leads to the question whether there is a connection between these two results. In an attempt to answer this question, a conjecture was put forward by one of the present authors [15] in the hope that if it is true, it can be combined with one of the two results to give a short and elegant proof of the other result. In Section 3, this conjecture is stated and an infinite sequence of hexagonal systems is given showing that it is false. The Clar numbers of these hexagonal systems are also computed which enables us to show that the Clar number can be arbitrarily larger than the cardinality of a maximal alternating set.

In Section 4, a weaker conjecture is proposed and its validity for catacondensed hexagonal systems is noted. It is shown that the validity of this weaker conjecture allows short proofs of the aforementioned two results. Section 5 explains the role of computer experiments in our work. In particular, algorithms for checking both conjectures are listed, the verification of

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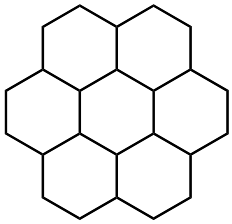

Fig. 1. Coronene.

the weaker conjecture for normal hexagonal systems up to ten hexagons is reported, and the smallest counterexample of the other conjecture is identified. Then, in Section 6, we relate the Clar number to the Fries number [16]. The latter number, as well as the Clar number, is associated with an optimization model for hexagonal systems and hence of relevance in chemical graph theory [17,18]. We present an infinite sequence of hexagonal systems to demonstrate that the Fries number of a hexagonal system can be arbitrary larger than its Clar number.

2. Preliminaries

A *hexagonal system* H is a 2-connected plane graph in which every inner face is a regular hexagon of side length one. A vertex of H lying on the boundary of the outer face of H is called an *external* vertex, otherwise, it is called an *internal* vertex. A hexagonal system having no internal vertices is called *catacondensed*, otherwise, it is called *pericondensed*. A hexagonal system that has a perfect matching is called a *Kekuléan* hexagonal system.

An edge of a graph that has a perfect matching is *fixed* if it belongs to all or none of the perfect matchings of the graph. A *normal* hexagonal system has a perfect matching but no fixed edges. A hexagonal system H is normal if and only if there exists a perfect matching M of H such that the boundary of the outer face of H, a cycle, is M-alternating [19]. It is clear that every catacondensed hexagonal system is normal. Fig. 1 presents a normal pericondensed hexagonal system.

Let P be a set of hexagons of a hexagonal system H. The subgraph of H obtained by deleting from H the vertices of the hexagons in P is denoted by $H - P$. It is clear that $H - P$ can be the empty graph.

Let P be a set of hexagons of a hexagonal system H. The set P is called an *alternating set* of H if there exists a perfect matching of H that contains a perfect matching of each hexagon in P. It is easy to see that if P is an alternating set of a hexagonal system H, then $H - P$ is empty or has a perfect matching [13,14]. The *Fries number* of a Kekuléan hexagonal system H [20] is the maximum of the cardinalities of all the alternating sets of H and is denoted by $Fr(H)$. An alternating set whose cardinality is the Fries number is called a *maximum cardinality* alternating set. An alternating set is *maximal* if it is not contained in another alternating set.

Let P be a set of hexagons of a hexagonal system H. The set P is called a *resonant set* of H [12,21] if the hexagons in P are pair-wise disjoint and $H - P$ has a perfect matching or is empty. (In the figures, resonant sets will be indicated with circles and alternating sets with filled circles.) Alternatively [17,18], P is 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 perfect matching of each hexagon in P. The *Clar number* of a Kekuléan hexagonal system H [22] is the maximum of the cardinalities of all the resonant sets of H and is denoted by $Cl(H)$. A resonant set whose cardinality is the Clar number is called a *maximum cardinality* resonant set. A resonant set is *maximal* if it is not contained in another resonant set.

Let P be a set of hexagons of a hexagonal system H. Let M be a perfect matching of H. The set P is called an *M-resonant set* of H [23] if the hexagons in P are pair-wise disjoint and the perfect matching M contains a perfect matching of each hexagon in P. An M-resonant set whose cardinality is the maximum of the cardinalities of all the M-resonant sets is called a *maximum cardinality* M-resonant set. For every perfect matching M of a hexagonal system H, there exists an M-alternating hexagon [24].

It is clear that a set of hexagons P is resonant if and only if it is M-resonant for some perfect matching M. However, the concept of a maximum cardinality resonant set and that of a maximum cardinality M-resonant set are not the same [23].

An alternating set P of a hexagonal system H satisfying $H - P$ is empty or has a unique perfect matching is called a *canonical* alternating set. This terminology is used in the literature for resonant sets only [25,26]. Here, its use is extended.

The *inner dual* of a hexagonal system H, denoted $D(H)$, is the plane dual of the hexagonal system with the vertex corresponding to the outer face deleted. A hexagonal system is *circumscribed* [27] if hexagons are added to edges of the boundary of the outer face and the subgraph of the inner dual induced by the vertices corresponding to the added hexagons is a cycle. For an illustration, Fig. 2 shows pyrene and circumscribed pyrene.

3. Infinite sequence of hexagonal systems

In this section we consider:

Conjecture 3.1 (*[15]*). *Let H be a hexagonal system and P a maximal alternating set of H. There exists a maximum cardinality resonant set of H contained in P.*