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.

Key words: Hexagonal system, perfect matching, resonant set, alternating set, 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 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.

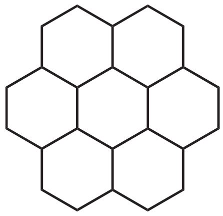

Fig. 1. Coronene.

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 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.

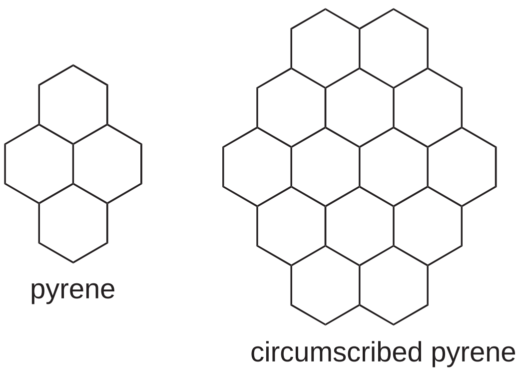

Fig. 2. Circumscribing.

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.*

An alternative formulation of this conjecture follows.

Conjecture 3.2 *Let H be a hexagonal system and P a maximal alternating set of H. Let M be a perfect matching of H that contains a perfect matching of each hexagon in P. For each maximum cardinality M-resonant set of H, S say, S is a maximum cardinality resonant set of H.*

Here, it is shown that this conjecture is false by providing an infinite sequence of normal hexagonal systems, each of which is a counterexample. In order to define this sequence, we recall the concept of an edge-join of two hexagonal systems [28].

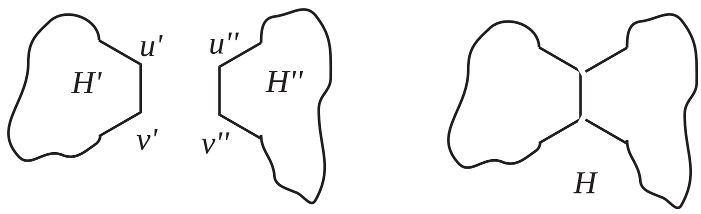

Fig. 3. An edge-join of two hexagonal systems.

Let H' and H'' be hexagonal systems. Let $u'v'$ ($u''v''$) be an edge of the boundary of the outer face of H' (H'') whose end-vertices are of degree two. Let H be the hexagonal system obtained by identifying u' with u'' and v' with v''. Then H is called an *edge-join* of H' and H''. Fig. 3 illustrates this concept.

Let H_n, $n \geq 1$, be the hexagonal system obtained from the amalgamation of n copies of circumscribed pyrene in a path-like fashion. Fig. 4 shows H_1 and H_2 and the construction of H_n should be clear for any $n \geq 3$. In fact, H_1 is circumscribed pyrene and for $n \geq 2$, H_n is an edge-join of H_{n-1} and H_1. The following results are needed to show that H_n, $n \geq 1$ is indeed an infinite sequence of normal hexagonal systems, each of which is a counterexample of Conjecture 3.1.

Lemma 3.3 *Let H be an edge-join of H' and H'', where H' and H'' are normal hexagonal systems. Let P be an alternating set of H. The hexagons of P that belong to H' constitute an alternating set of H' and the hexagons of P that belong to H'' constitute an alternating set of H''.*

PROOF. First note that each normal hexagonal system is Kekuléan, thus, it has an even number of vertices. Hence, each of H' and H'' has an even number of vertices. Let M be a perfect matching of H that contains a perfect matching of each hexagon in P. Let e be the edge in common between H' and H''. There are two possible cases. In one case, the end vertices of e are incident with distinct edges in M. Since both H' and H'' have an even number of vertices, both the distinct matched edges belong to H' or both of them belong to H''. In the other case, the end vertices of e are incident with the same edge in M, the edge e. In each case, it is not difficult to see that the result is true. $\square$

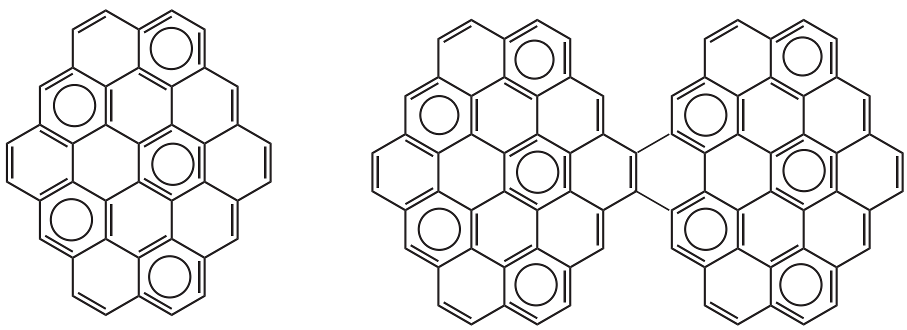

Fig. 4. Hexagonal systems H_1 and H_2 and their resonant sets Q_1 and Q_2.

Lemma 3.4 *Let H be an edge-join of H' and H'', where H' and H'' are normal hexagonal systems. Then H is a normal hexagonal system and $Cl(H) \leq Cl(H') + Cl(H'')$.*

PROOF. Let C' be the boundary of the outer face of H' and C'' be the boundary of the outer face of H''. Let M' be a perfect matching of H' such that C' is M'-alternating and let M'' be a perfect matching of H'' such that C'' is M''-alternating. The existence of M' and M'' follows from that both H' and H'' are normal hexagonal systems. Let C be the boundary of the outer face of H and let M_C be a perfect matching of C. It is not difficult to see that $M = (M' \setminus C') \cup (M'' \setminus C'') \cup M_C$ is a perfect matching of H such that C is M-alternating. Hence, H is a normal hexagonal system.

To prove the inequality, let P be a resonant set of H. Then P is an alternating set of H. By Lemma 3.3 the hexagons in P that belong to H' constitute an alternating set of H', P' say, whereas the hexagons in P that belong to H'' constitute an alternating set of H'', P'' say. Since P consists of pair-wise disjoint hexagons, so are P' and P'', thus, P' and P'' are resonant sets of H' and H'', respectively. It is obvious that $|P| = |P'| + |P''| \leq Cl(H') + Cl(H'')$. Since P is an arbitrary resonant set of H, $Cl(H) \leq Cl(H') + Cl(H'')$. $\square$

It is worth noting that a result analogous to Lemma 3.4 can be proven for Fries numbers.

Proposition 3.5 *For every $n \geq 1$, H_n is a normal hexagonal system.*

PROOF. The proof is by induction on n. Initial step: H_1 is a normal hexagonal system because there exists a perfect matching M of H_1, the one shown in Fig. 5, such that the boundary of the outer face of H_1 is M-alternating. Inductive step: Assume that H_n is a normal hexagonal system and we show that H_{n+1} is a normal hexagonal system, where $n \geq 1$. Recall that H_{n+1} is an edge-join of H_n and H_1. Hence by Lemma 3.4, H_{n+1} is a normal hexagonal system. $\square$

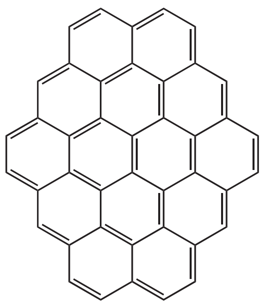

Fig. 5. H_1, circumscribed pyrene, is a normal hexagonal system.

Proposition 3.6 *For every $n \geq 1$, $Cl(H_n) = 5n$.*

PROOF. It is clear that for every $n \geq 1$, Q_n is a resonant set of H_n, where Q_1 and Q_2 are shown in Fig. 4. Hence, for every $n \geq 1$, $Cl(H_n) \geq 5n$. It remains to show that for every $n \geq 1$, $Cl(H_n) \leq 5n$. The proof is by induction on n. Initial step: Consider the inner dual $D(H_1)$ of H_1 shown in Fig. 6. To simplify the notation let $G = D(H_1)$. Let $\alpha(G)$ denote the independence number of G. Clearly, $Cl(H_1) \leq \alpha(G)$. It is shown that $\alpha(G) \leq 5$. Let X be an independent set of vertices of G and let C be the boundary of the outer face of G, a 10-cycle. Since X is an independent set, it contains at most two vertices not lying on C. Let $i(X)$ be the number of vertices of X not lying on C. Case $i(X) = 0$: Since C is a 10-cycle, X has at most 5 vertices lying on C and $|X| \leq 5$. Case $i(X) = 1$: X has at most 4 vertices lying on C and $|X| \leq 5$. Case $i(X) = 2$: X has at most two vertices lying on C and $|X| \leq 4$. Hence $\alpha(G) \leq 5$ and $Cl(H_1) \leq 5$. Inductive step: Assume that $Cl(H_n) \leq 5n$ and we show that $Cl(H_{n+1}) \leq 5(n+1)$, where $n \geq 1$. Recall that H_{n+1} is an edge-join of H_n and H_1 and note that by Proposition 3.5, both H_n and H_1 are normal hexagonal systems. Hence, by Lemma 3.4, $Cl(H_{n+1}) \leq Cl(H_n) + Cl(H_1)$. The inductive assumption and the initial step imply that $Cl(H_n) + Cl(H_1) \leq 5n + 5 = 5(n+1)$. $\square$

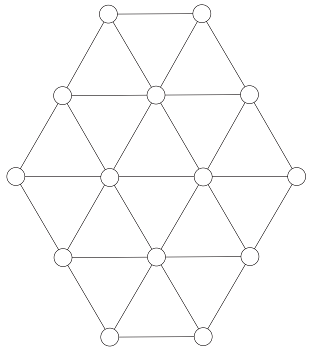

Fig. 6. The inner dual of H_1.

Proposition 3.7 *For every $n \geq 1$, there exists a maximal alternating set of H_n, P_n say, such that $|P_n| = 4n$.*

PROOF. It suffices to show that for every $n \geq 1$, P_n is a maximal alternating set of H_n, where P_1 and P_2 are shown in Fig. 7. The proof is by induction on n. Initial step: Fig. 7 shows that P_1 is an alternating set of H_1. There exists a unique perfect matching of H_1 that contains a perfect matching of each hexagon in P_1. Since only the (four) hexagons in P_1 are alternating in this (unique) perfect matching, P_1 is a maximal alternating set of H_1. Thus, the result is true for $n = 1$.

Inductive step: Assume that the result is true for n and we show that it is true for $n+1$, where $n \geq 1$. It is clear that P_{n+1} is an alternating set of H_{n+1}. For the sake of obtaining a contradiction, assume that P_{n+1} is not a maximal alternating set of H_{n+1}. Thus, P_{n+1} is contained in another alternating set of H_{n+1}, P say. Let h be a hexagon that belongs to P but does not belong to P_{n+1}. It is clear that $P_{n+1} \cup \{h\}$ is an alternating set of H_{n+1}. Recall that H_{n+1} is an edge-join of H_n and H_1 and note that by Lemma 3.5, H_n and H_1 are normal hexagonal systems. By Lemma 3.3, the hexagons of $P_{n+1} \cup \{h\}$ that belong to H_n constitute an alternating set of H_n, P' say, and the hexagons of $P_{n+1} \cup \{h\}$ that belong to H_1 constitute an alternating set of H_1, P'' say. The hexagon h belongs to either H_n or H_1. Case h belongs to H_n: Then $P' = P_n \cup \{h\}$ which contradicts the inductive assumption. Case h belongs to H_1: Then $P'' = P_1 \cup \{h\}$ which contradicts that P_1 is a maximal alternating set of H_1. $\square$

For every $n \geq 1$, the validity of H_n as a counterexample of Conjecture 3.1 follows from Propositions 3.6 and 3.7. This section is concluded with a related result, but before stating it, recall that we write

$$\lim_{n \to \infty} a_n = \infty,$$

where $\{a_n\}_{n=1}^{\infty}$ is an infinite sequence of real numbers such that for every $M > 0$, there exists an integer $n_0 \geq 1$ such that for every $n > n_0$, $a_n > M$.

Corollary 3.8 *There exists an infinite sequence (H_n, P_n), $n \geq 1$, where H_n is a normal hexagonal system and P_n is a maximal alternating set of H_n, such that*

$$\lim_{n\to\infty} Cl(H_n) - |P_n| = \infty \,.$$

PROOF. The result follows from Propositions 3.5, 3.6, and 3.7. □

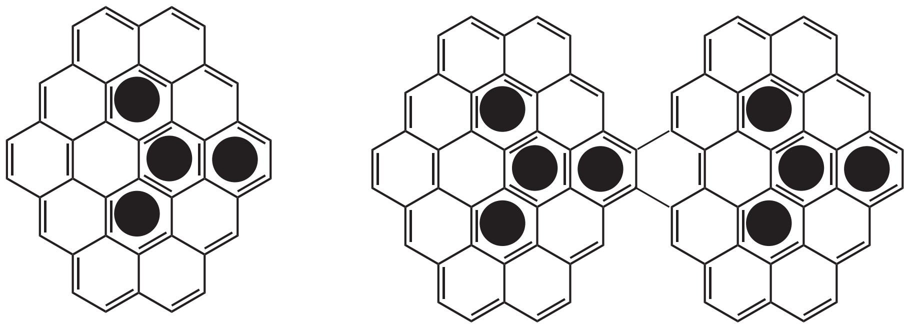

Fig. 7. Hexagonal systems H_1 and H_2 and their alternating sets P_1 and P_2.

4 New conjecture and its corollaries

We now propose:

Conjecture 4.1 *Let H be a hexagonal system and P a maximal alternating set of H. Let M be a perfect matching of H that contains a perfect matching of each hexagon in P. For each maximum cardinality M-resonant set of H, S say, S is a canonical resonant set of H.*

We first observe that Conjecture 4.1 holds for catacondensed hexagonal systems. The proof of this fact follows from Corollary 6 in [14]. We next demonstrate that, assuming the validity of Conjecture 4.1, the following two theorems (mentioned earlier) have short proofs.

Theorem 4.2 ([11,12]) *Let H be a hexagonal system and P a maximum cardinality resonant set of H. Then P is a canonical resonant set.*

PROOF. It can be easily seen that P is contained in a maximal alternating set of H, A say. Let M be a perfect matching of H that contains a perfect matching of each hexagon in A. It is clear that P is a maximum cardinality

M-resonant set of H. Hence, by Conjecture 4.1, P is a canonical resonant set of H. $\square$

Theorem 4.3 ([13,14]) *Let H be a hexagonal system and P a maximal alternating set of H. Then P is a canonical alternating set.*

PROOF. Assume that P is not a canonical alternating set. Then $H - P$ has more than one perfect matching. Let M_1 and M_2 be two perfect matchings of $H - P$. Let M be a perfect matching of H that contains a perfect matching of each hexagon in P. By Conjecture 4.1, the set P contains a canonical resonant set, S say. Let $M_{P \setminus S}$ be the edges of M that belong to some hexagon of P but not to any hexagon of S. It is not difficult to see that $M_1 \cup M_{P\setminus S}$ and $M_2 \cup M_{P\setminus S}$ are two perfect matchings of $H - S$, a contradiction. $\square$

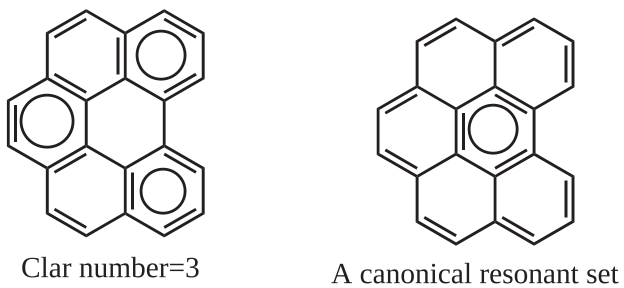

Fig. 8. Benzo[*ghi*]perylene. Conjecture 4.1 is weaker than Conjecture 3.2.

Remark 4.4 *Fig. 8 shows that there exists a canonical resonant set that is not a maximum cardinality resonant set. This fact, coupled with Theorem 4.2, shows that Conjecture 4.1 is weaker than the (false) Conjecture 3.2.*

5 Computer experiments

Two algorithms were designed and implemented in order to check Conjecture 3.1 and Conjecture 4.1 for each normal hexagonal system. The algorithm for checking Conjecture 3.1 is presented in Fig. 9. The (unique) smallest counterexample of Conjecture 3.1 found using the algorithm is presented in Fig. 10. It has six hexagons. Conjecture 4.1 was checked using the algorithm presented in Fig. 11. However, no counterexample was found among all normal hexagonal systems with up to ten hexagons. This gives some support for Conjecture 4.1. Hexagonal systems could be produced using the generating algorithm presented in [29,30]. The enumeration of perfect matchings was commenced using the algorithms presented in [31,32].

```
Input: a normal hexagonal system H
Output: true or false

 1. Enumerate all perfect matchings of H.
 2. Find all maximal alternating sets.
 3. Find all maximum cardinality resonant sets.
 4. Check whether for every maximal alternating set P, there
    exists a maximum cardinality resonant set contained in P.
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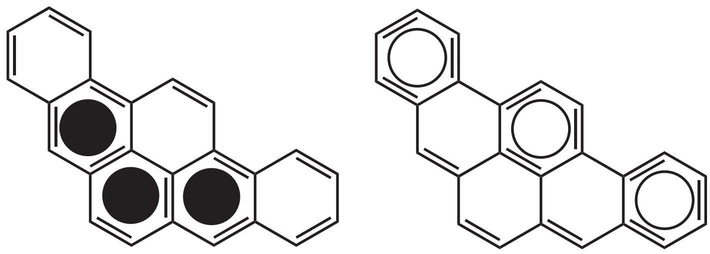
Fig. 9. Algorithm for checking Conjecture 3.1.



A maximal alternating set

The unique maximum cardinality resonant set

Fig. 10. The smallest counterexample of Conjecture 3.1.

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Input: a normal hexagonal system H
Output: true or false

 1. Enumerate all perfect matchings of H.
 2. Find all maximal alternating sets.
 3. For each maximal alternating set P
   3.1. Find a perfect matching M of H that contains
        a perfect matching of each hexagon in P.
   3.2. Find all maximum cardinality M-resonant sets.
   3.3. Check that each of these later sets is canonical.
```

Fig. 11. Algorithm for checking Conjecture 4.1.

6 The Fries number versus the Clar number

It is clear that $Fr(H) \geq Cl(H)$ for an arbitrary Kekuléan hexagonal system H. In this section we show that the difference $Fr(H) - Cl(H)$ can be arbitrarily large. More precisely, we prove the following:

Theorem 6.1 *There exists an infinite sequence of normal hexagonal systems B_n, $n \geq 0$, such that*

$$\lim_{n\to\infty} (Fr(B_n) - Cl(B_n)) = \infty\,.$$

Let B_n, $n \geq 0$, be the sequence where B_0 is benzo[a]coronene and for $n \geq 1$, B_n is an edge-join of B_{n-1} and naphthalene as shown in Fig. 13. In another terminology, for $n \geq 1$, B_n is an edge join of B_0 and the zigzag fibonacene Z_{2n} [33]. Fig. 12 proves that B_0 is normal (since the outer cycle is alternating). Z_{2n} is normal as well being a catacondensed hexagonal system. Hence, by Lemma 3.4, for every $n \geq 0$, B_n is a normal hexagonal system.

The two results below give the Clar numbers and the Fries numbers of B_n, $n \geq 0$, and they prove Theorem 6.1 immediately.

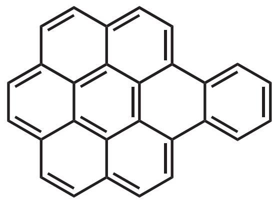

Fig. 12. Benzo[a]coronene is a normal hexagonal system.

Proposition 6.2 *For every $n \geq 0$, $Cl(B_n) = 4 + n$.*

PROOF. It is clear that for every $n \geq 0$, the set of circled hexagons shown in Fig. 13 is a resonant set of cardinality $4+n$. Hence, for every $n \geq 0$, $Cl(B_n) \geq 4 + n$. It remains to show that for every $n \geq 0$, $Cl(B_n) \leq 4 + n$. The proof is by induction on n. Initial step: In B_0, benzo[a]coronene, the central hexagon of the coronene subgraph cannot belong to a maximum cardinality resonant set and such a set cannot contain more than three of the remaining hexagons in the coronene subgraph. Hence, $Cl(B_0) \leq 4$. Induction step: Assume that $Cl(B_n) \leq 4 + n$, then we show that $Cl(B_{n+1}) \leq 4 + (n + 1)$, where $n \geq 0$. Recall that B_{n+1} is an edge join of B_n and naphthalene. It is easily verified that the Clar number of naphthalene is one. Hence, by Lemma 3.4, $Cl(B_{n+1}) \leq Cl(B_n) + 1$, which completes the induction step. $\square$

Proposition 6.3 *For every $n \geq 0$, $Fr(B_n) = 7 + 2n$.*

PROOF. For each $n \geq 0$, there exists a perfect matching, M_n say, of B_n that contains a perfect matching of each hexagon in B_n other than the central hexagon of the coronene subgraph. Fig. 13 depicts the perfect matchings M_n for $n = 0, 1, 2, 3$. Hence, for each $n \geq 0$, the set of all the hexagons other than the central hexagon of the coronene subgraph is an alternating set of B_n. Thus, for each $n \geq 0$, $Fr(B_n) \geq 7 + 2n$. For the sake of obtaining a contradiction, assume that $Fr(B_n) > 7+2n$. Then the set of all the hexagons in B_n, $\mathcal{F}_n$ say, is an alternating set of B_n. The subgraph of the inner dual of B_n induced by the vertices corresponding to the alternating set $\mathcal{F}_n$ is bipartite [23]. Obviously,

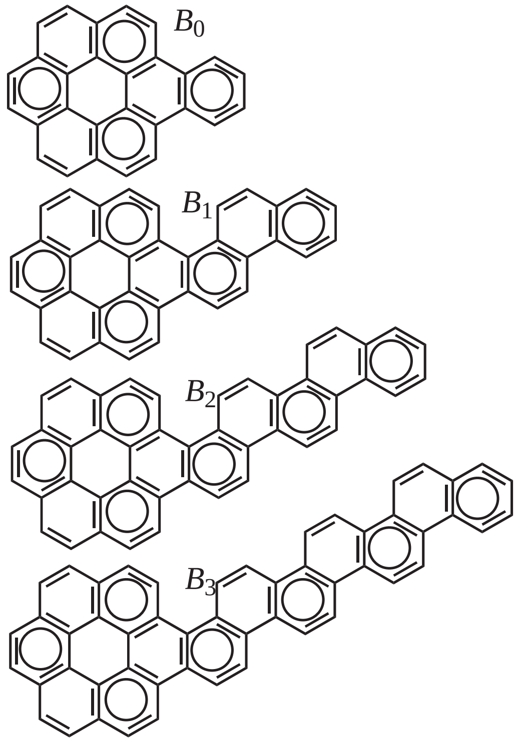

Fig. 13. Hexagonal systems B_n, $n = 0, 1, 2, 3$, and their resonant sets.

this subgraph is the inner dual of B_n, a pericondensed hexagonal system, hence, it contains a triangle, a contradiction. $\square$

7 Concluding remarks

The paper is concluded with the following related result:

Proposition 7.1 *Let H be a hexagonal system and let P be a canonical resonant set of H. Then P is a maximal resonant set of H.*

PROOF. Assume that P is contained in another resonant set, P' say. There exists a hexagon, R' say, that belongs to P' but does not belong to P. Let M be a perfect matching of H that contains a perfect matching of each hexagon in P'. Let $E_{M,P}$ be the set of edges of M that belong to some hexagon of P. It is clear that R' is contained in $H - P$ and $M \setminus E_{M,P}$ is a perfect matching of $H - P$ that contains a perfect matching of R'. Hence, $H - P$ has more than one perfect matching, a contradiction. $\square$

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