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Kekulé structures and the face independence number of a fullerene

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Abstract

We explore the relationship between Kekulé structures and maximum face independence sets in fullerenes: plane trivalent graphs with pentagonal and hexagonal faces. For the class of leap-frog fullerenes, we show that a maximum face independence set corresponds to a Kekulé structure with a maximum number of benzene rings and may be constructed by partitioning the pentagonal faces into pairs and 3-coloring the faces with the exception of a very few faces along paths joining paired pentagons. We also obtain some partial results for non-leap-frog fullerenes.

1. Introduction

Let $\Gamma = (V, E, F)$ be a fullerene: a trivalent plane graph with hexagonal and pentagonal faces. It follows directly from Euler's formula that a fullerene has exactly 12 pentagonal faces. These graph theoretic fullerenes are designed to model large carbon molecules: each vertex represents a carbon atom and the edges represent chemical bonds. Since a carbon atom has chemical valence 4, one edge at each of the graphs must represent a double chemical bond. A *Kekulé structure*, $K \subseteq E$, for $\Gamma = (V, E, F)$ is a perfect matching and the edges of the matching correspond to double bonds. It is convenient to use the Kekulé number, $k = |K|$, as a basic parameter for the fullerene Γ. Then we have $|V| = 2k$, $|E| = 3k$ and $|F| = k + 2$. The primary focus of this paper is the face independence number of a fullerene Γ which is, of course, the vertex independence number of the dual geodesic dome. We denote the face independence number of Γ by $\alpha^* = \alpha^*(\Gamma) = \alpha(\Gamma^*)$.

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Let $K \subseteq E$ be a Kekulé structure for the fullerene $\Gamma = (V, E, F)$. A face of Γ may have 0, 1, 2 or 3 of its bounding edges in K; we denote by $B_i(K)$ the set of faces that have exactly i of their bounding edges in K. The faces in $B_0(K)$ are called the *void faces* of K and the faces in $B_3(K)$ are called the *full faces* or *benzene-like faces* of K. We define $\kappa = \kappa(\Gamma)$, the *Fries number* [9] or *Kekulé parameter of* Γ, to be the maximum of the number of benzene-like faces over all Kekulé structures for Γ. Closely related to both of the parameters $\alpha^*(\Gamma)$ and $\kappa(\Gamma)$ is the *Clar number* [3] of the fullerene Γ. A set of benzene-like faces such that any two are pairwise disjoint is said to be *resonant*. The Clar number of Γ, $\gamma(\Gamma)$, is the size of the largest resonant set of benzene-like faces over all Kekulé structures for Γ or, equivalently, the largest independent set of benzene-like faces over all Kekulé structures for Γ.

This paper is devoted to computing or estimating the values of these parameters and to understanding the relationships between them. In the next section we prove some basic inequalities. Section 3 explores the class of fullerenes in which the exact values of α^*, κ and γ can be computed — the leap-frog fullerenes. These results for leap-frog fullerenes can best be understood in terms of face colorings, the topic of Section 4. The relationship between α^* and κ is the subject of Section 5. In Section 6, we develop methods for estimating these parameters and in the last section we draw some conclusions and discuss directions for further research.

2. Some basic lemmas

In a fullerene, at most one in three faces at any vertex can belong an independent face set. On the other hand, the hexagonal tessellation admits an independent face set with exactly one face at each vertex; take a color class of the obvious face 3-coloring. Since big regions of a large fullerene are regions of the hexagonal tessellation, we expect the face independence number of large fullerenes to be roughly $\frac{1}{3}|F| \sim \frac{k}{3}$. In our first lemma, we will prove that, in fact, $\alpha^*(\Gamma) \leq \frac{k}{3} + 2$. Anticipating that result, we say that an independent face set R is a *perfect* independent face set if $|R| = \alpha^*(\Gamma) = \frac{k}{3} + 2$.

Lemma 1. *Let $R \subseteq F$ be an independent face set of the fullerene $\Gamma = (V, E, F)$, let $p^*(R)$ be the number of pentagonal faces NOT in R and let $v^*(R)$ be the number of vertices NOT incident with a face in R. Then:*

(i) $|R| = \frac{k}{3} + 2 - \frac{p^*(R)+v^*(R)}{6}$;
(ii) $\alpha^*(\Gamma) \leq \frac{k}{3} + 2$, *with equality if and only if Γ admits a perfect independent face set;*
(iii) *R is a perfect independent face set if and only if $p^*(R) = v^*(R) = 0$.*

Proof. Let R, $p^*(R)$, $v^*(R)$ be as above and let $p(R)$ denote the number of pentagonal faces in R; then $p(R) + p^*(R) = 12$. Since Γ is trivalent, each vertex is incident with at most 1 face in R. The number of vertices incident with some face in R is then $6|R| - p(R) = 6|R| - 12 + p^*(R)$.
So, $6|R| - 12 + p^*(R) = |V| - v^*(R)$;
giving $6|R| = 2k + 12 - p^*(R) - v^*(R)$.
Dividing through by 6 gives Part (i); Parts (ii) and (iii) follow at once. □

Let $K \subseteq E$ be a Kekulé structure for the fullerene $\Gamma = (V, E, F)$. A face of Γ may have 0, 1, 2 or 3 of its bounding edges in K; we denote by $B_i(K)$ the set of faces that have exactly i of their bounding edges in K. The faces in $B_0(K)$ are called the *void faces* of K and the faces in $B_3(K)$ are called the *full faces* or *benzene-like faces* of K. We define $\kappa = \kappa(\Gamma)$, the *Kekulé parameter of* Γ, to be the maximum of the number of benzene-like faces over all Kekulé structures for Γ.

In our second lemma we will prove that $\kappa(\Gamma) \leq \frac{2k}{3}$. Anticipating that result, we say that a Kekulé structure $K \subseteq E$ is a *perfect* Kekulé structure if $|B_3(K)| = \frac{2k}{3}$.

Lemma 2. *Let $K \subseteq E$ be a Kekulé structure for the fullerene $\Gamma = (V, E, F)$ and, for $i = 0, 1, 2, 3$, let $B_i(K)$ denote the set of faces of Γ that have exactly i of their bounding edges in K. Then:*

(i) $|B_3(K)| = \frac{2k}{3} - \frac{|B_1(K)|+2|B_2(K)|}{3}$;
(ii) $\kappa(\Gamma) \leq \frac{2k}{3}$, *with equality if and only if Γ admits a perfect Kekulé structure;*
(iii) *K is a perfect Kekulé structure if and only if* $|B_1(K)| = |B_2(K)| = 0$.

Proof. Adding up the number of edges of K in the boundary of each face, we get $|B_1(K)| + 2|B_2(K)| + 3|B_3(K)| = 2k$. Solving for $B_3(K)$ gives (i). Parts (ii) and (iii) follow at once from (i). □

What can we say about the Clar number? First of all, since a resonant set is an independent set, $\gamma \leq \alpha^*$. However, maximum independent face sets usually include many pentagons and resonant sets never include pentagons. Hence, we do not expect equality here. The best that we can say at this time is stated in the next lemma.

Lemma 3. *Let $C \subseteq F$ be a resonant face set of the fullerene $\Gamma = (V, E, F)$, and let $v^*(C)$ be the number of vertices NOT incident with a face in C. Then:*

(i) $|C| = \frac{k}{3} - \frac{v^*(C)}{6}$;
(ii) $\gamma(\Gamma) \leq \frac{k}{3}$.

Proof. Since C is an independent face set $|C| = \frac{k}{3} + 2 - \frac{p^*(C)+v^*(C)}{6}$. But, $p^*(C) = 12$, giving the result. □

3. Fullerenes with perfect face independent sets and perfect Kekulé structures

Lemma 4. *Let the fullerene $\Gamma = (V, E, F)$ be given. Then:*

(i) *The collection of void faces of a Kekulé structure for Γ is a face independent set of Γ.*
(ii) *The collection of void faces of a perfect Kekulé structure for Γ is a perfect face independent set of Γ.*
(iii) *Conversely, a perfect face independent set of Γ is the collection of void faces of some perfect Kekulé structure for Γ.*

Proof. (i) Let K be a Kekulé structure for $\Gamma = (V, E, F)$ and let F be a void face. Note that all of the edges that share exactly one vertex with F must belong to K; see Fig. 1. Hence, all of the faces that share a common boundary edge with F belong to $B_2(K)$ or $B_3(K)$ and no two void faces are adjacent.

(ii) Assume K is a perfect Kekulé structure. Then $B_1(K) = B_2(K) = \emptyset$. Let R be the independent collection of void faces for K. Since pentagons cannot be full, they must be void; hence, $p^*(R) = 0$. Next we note that, at each vertex, we have 2 full and one void face, see Fig. 2. Hence $v^*(R) = 0$. We conclude that $|R| = \frac{k}{3} + 2$.

(iii) Let R be the collection of faces of a perfect face independent set of Γ and let K be the collection of edges that do not bound a face in R. Let x be any vertex. Since $v^*(R) = 0$ there must be a face F $\in R$ with x as vertex, see Fig. 3. Let e be the edge containing x but not bounding

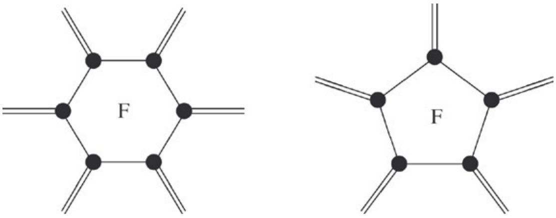

Fig. 1.

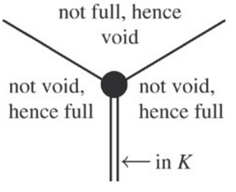

Fig. 2.

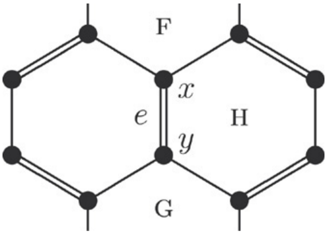

Fig. 3.

F and let y be the other endpoint of e. Since R is independent, the face $G \in R$ containing y cannot be either of the faces bounded by e. Hence e does not bound a face of R and must belong to K. So every vertex is incident with an edge in K. Furthermore, since two out of the three edges at any vertex bound a face in R, K is an independent edge set. We conclude that K is a Kekulé structure and, by the definition of K, the faces in R are all void faces of K.

Finally, let H be any face not in R. Since R is a maximum independent set, H must share a boundary edge with a face $F \in R$, see Fig. 3. Since F is void, the boundary edges on either side of the edge shared with F belong to K. Moving counterclockwise around H, let x be the leftmost vertex incident with both H and F and let y be the next vertex after x. Since R is a perfect face independent set, some face $G \in R$ contains y. Clearly $G \neq F$ and G shares an edge with H. Applying the above argument to G instead of F gives a third edge of H in K. We conclude that H is full. Hence K is a perfect Kekulé structure. □

Given a fullerene Γ, the leap-frog construction produces Γ^{ℓ}, a new fullerene, as follows. Draw a small hexagonal (pentagonal) face for Γ^{ℓ} inside each hexagonal (pentagonal) face of Γ, rotated by 30 (36) degrees (the faces bounded by the red edges in Fig. 4). Next connect the vertices of these new faces with edges that are "perpendicular bisectors" of the edges of Γ (the blue edges of the figure). One easily sees that Γ^{ℓ} has one hexagonal (pentagonal) face for each hexagonal (pentagonal) face of Γ and one additional hexagonal face for each vertex of Γ. Furthermore, the faces of Γ^{ℓ} that correspond to the faces of Γ, the red faces, form a perfect face independent

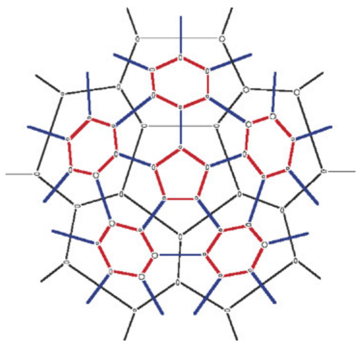

Fig. 4.

set while the edges between these faces, the blue edges, form the corresponding perfect Kekulé structure.

Starting with a fullerene Θ that has a perfect Kekulé structure, we construct a new fullerene Γ by placing a vertex in the center of each full face and joining two new vertices by an edge whenever their associated faces share an edge of the Kekulé structure. One may then check that $\Theta = \Gamma^{\ell}$. The details of this proof may be found in [7].

The signature $\mathcal{S}(\Gamma)$ of a fullerene Γ was defined in [11]. It is a labeled plane graph on 12 vertices. The vertices correspond to the 12 pentagonal faces of Γ. Vertices corresponding to pentagonal faces that are "near" one another are joined by edges and the edges are labeled by pairs of numbers called Coxeter coordinates. The signature is a generalization of Coxeter's description of the icosahedral fullerenes: the signature of an icosahedral fullerene has as the graph on 12 vertices the icosahedron and has the Coxeter coordinates (p, q) assigned to each edge.

The fact that leap-frog fullerenes admit a perfect Kekulé structure was proved in [5]. The connections between the independent face sets and Clar and Fries structure of a fullerene has been discussed in detail in [2,8,6]. In [12], it was proved that a fullerene is a leap-frog fullerene if and only if the two Coxeter coordinates are congruent mod 3, for every edge of its signature. For example, $\mathbf{C_{60}}$ with the soccer ball structure has as its signature the icosahedron with Coxeter coordinates (1, 1) assigned to each edge. In the following theorem, we summarize the above mentioned results relating perfect Kekulé structures, independent face sets and the Clar and Fries structures of a leap-frog fullerene.

Theorem 1. *Given a fullerene Γ, the following four statements are equivalent:*

(i) *Γ admits a perfect independent face set.*
(ii) *Γ admits a perfect Kekulé structure.*
(iii) *Γ is a leap-frog fullerene.*
(iv) *The Coxeter coordinates of each edge of the signature of Γ are congruent mod 3.*

We may take advantage of the special structure of leap-frog fullerenes to get a lower bound on the Clar number:

Theorem 2. *Let Γ^{ℓ} be the leap-frog fullerene obtained from the fullerene Γ. Then $\gamma(\Gamma^{\ell}) \geq \alpha(\Gamma)$.*

Proof. Consider the Kekulé structure associated with the construction of the leap-frog Γ^ℓ (the blue edges in Fig. 4). As we noted above the vertices of Γ correspond to the benzene-like faces of Γ^ℓ. Furthermore, two benzene-like faces of Γ^ℓ are adjacent if and only if the corresponding vertices in Γ are adjacent. Hence a maximum resonant face set for this Kekulé structure for Γ^ℓ corresponds to a maximum vertex independent set for Γ. □

A method for computing $\alpha(\Gamma)$ for any fullerene is given in [14] and, in that paper, the independence number is computed for the icosahedral fullerenes. Using those results, we have:

Corollary 3.1. *Let Γ^ℓ be the leap-frog fullerene from Γ and assume that Γ^ℓ has icosahedral symmetry. Then $\gamma(\Gamma) \geq \frac{k}{3} - 2(p + r)$.*

Proof. Let Γ^ℓ be the leap-frog fullerene from Γ and assume that Γ^ℓ has icosahedral symmetry with Coxeter coordinates $(p + r, p)$. Since, Γ^ℓ is a leap-frog fullerene, its Coxeter coordinates must be congruent mod 3; so r is a multiple of 3. It follows from Lemma 2.1 of [12] that Γ also has icosahedral symmetry and that its Coxeter coordinates are $(\frac{r}{3}, \frac{r}{3} + p)$. By Corollary 2.1 of [14], $\alpha(\Gamma) = 30(\frac{r}{3})^2 + 30(\frac{r}{3})p + 10p^2 - (6(\frac{r}{3}) + 2p) = \frac{10}{3}r^2 + 10rp + 10p^2 - 2(p + r)$. Finally, from [13], we have that, for Γ^ℓ, $k = 30p^2 + 30pr + 10r^2$. So $\frac{10}{3}r^2 + 10rp + 10p^2 = \frac{k}{3}$ and the result follows. □

4. Face colorings

Perhaps the best way to understand these parameters and results is to interpret them in terms of face colorings. In Fig. 5, we illustrate this with the icosahedral fullerene with Coxeter coordinates (10,7). We have 3-colored most of the faces of a region around two pentagonal faces. The uncolored faces all lie along a path of hexagonal faces joining the two pentagonal faces. We see that the red coloring actually matches across the dividing path, while the blue and yellow do not. This 3-coloring can be extended throughout the fullerene minus six paths joining pairs of pentagons, all of which are colored red. The pattern of red faces will match across these paths and the red faces form a perfect face independent set. The edges not bounding the red faces form a perfect Kekulé structure. The red faces are the void faces of this Kekulé structure and the blue, yellow and uncolored (white) faces are the benzene-like faces of this Kekulé structure. The set of blue faces and the set of yellow faces are both maximal resonant sets and hence yield lower bounds for the Clar number.

In Fig. 6, we illustrate just what goes wrong when the Coxeter coordinates of the signature edge joining the pentagonal faces are not congruent mod 3. Here, when the coloring is carried around the lower pentagonal face it no longer matches around the upper pentagonal face.

To better understand what is going on, consider a red, blue, yellow 3-coloring of the faces of a region of the hexagonal tessellation of the plane — look at the left hand region of Fig. 5 or 6. Going up a vertical line of hexagons the colors repeat in the order $b, y, r, b, y, r, \ldots$. If we rotate 60 degrees and look at the colors along the line of hexagonal faces, the colors repeat in the reverse order $b, r, y, b, r, y, \ldots$. Rotating another 60 degrees and we are back to a line of faces with the original pattern. Hence, as we rotate around the lower pentagonal face (an odd multiple of 60 degrees) the patterns along any line faces on the right are the reverse pattern along any parallel line on the left. These two patterns match only on every third hexagonal face, the ones with the same color as the pentagon. When we get to the top pentagonal face in either figure and try to close the coloring, we have rotated 10 times 60 degrees so the order of the pattern is the same from either side, $b, y, r, b, y, r, \ldots$ in the vertical direction, but the pattern may have

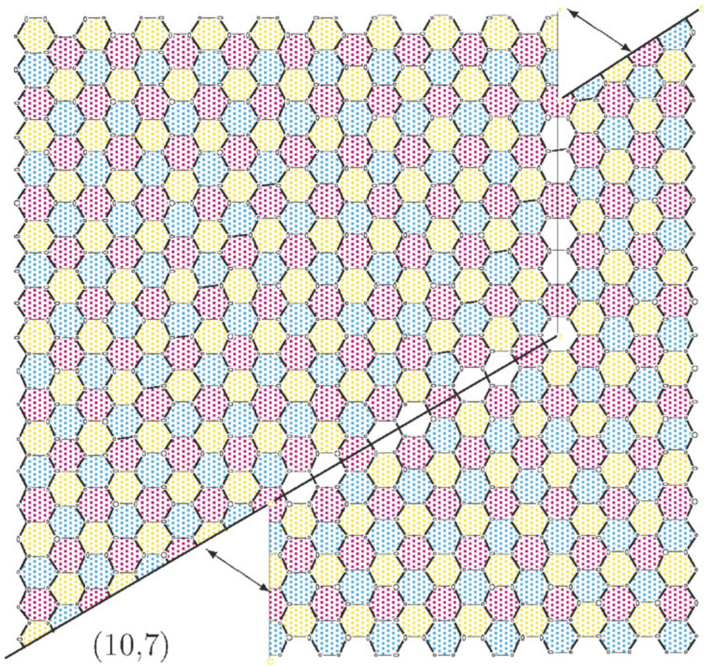

Fig. 5.

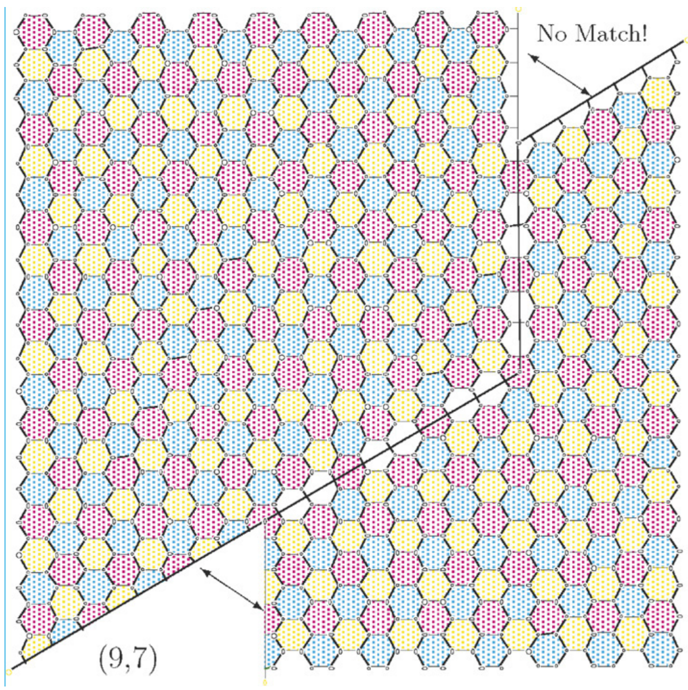

Fig. 6.

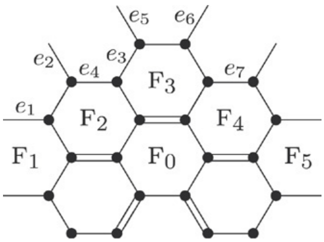

Fig. 7.

shifted. In the case that $p \equiv_3 q$, the top pentagon is assigned the same color from both sides, the same color as the lower pentagon, and the patterns match, as in Fig. 5; in the case that $p \not\equiv_3 q$ the patterns do not match at all, as in Fig. 6.

5. The relationship between the parameters α^* and κ

Let $\Gamma = (V, E, F)$ be a fullerene. A face independent set R for Γ is *maximum* if $|R| = \alpha^*(\Gamma)$ and a Kekulé structure K for Γ is *maximum* if $|K| = \kappa(\Gamma)$. In this section, we explore the relationship between maximum face independent sets and maximum Kekulé structures. We start with a result based on an extension of Lemma 3(i).

Theorem 3. *Let $\Gamma = (V, E, F)$ be a fullerene.*

(i) *If K is a maximum Kekulé structure for Γ, then there is a subset $H \subseteq B_1(K)$ with $|H| \geq \frac{1}{2}B_1(K)$ such that $H \cup B_0(K)$ is a face independent set for Γ.*
(ii) $\kappa(\Gamma) \leq 2\alpha^*(\Gamma) - 4$.

Proof. Let K be a maximum Kekulé structure for Γ. As we have already seen (in the proof of Lemma 4(i)) every face adjacent to a face in $B_0(K)$ belongs to $B_2(K) \cup B_3(K)$. Therefore, the union of $B_0(K)$ and any independent subset of $B_1(K)$ will be an independent face set for Γ. Let F_0 be a face in $B_1(K)$. In Fig. 7, we have pictured F_0, the edges of which contain vertices of F_0 and some of the faces near F_0. (A similar picture could be drawn if F_0 was a pentagon.) Note first that the bottom three faces adjacent to F_0 must all belong to $B_2(K) \cup B_3(K)$. (The bottom two if F_0 was a pentagon.) If $F_3 \in B_1(K)$, then edges e_4, e_5, e_6 and e_7 must all belong to K. Hence all of the faces bounding $F_0 \cup F_3$ belong to $B_2(K) \cup B_3(K)$.

Now suppose that $F_2 \in B_1(K)$. Then edges e_1, e_2 and e_3 must all belong to K. It follows that the top three faces bounding F_2 belong to $B_2(K) \cup B_3(K)$. By symmetry the same is true of F_4. It follows that F_0 is either adjacent to no other face in $B_1(K)$ or exactly one other face in $B_1(K)$ (F_2, F_3 or F_4) or exactly two other faces in $B_1(K)$ (F_2 and F_4). In the latter case, F_0 belongs to a path or circuit of faces from $B_1(K)$. In the case of a circuit, the faces alternate between being above and below the path consisting of the edges common to two of the faces in the circuit and the edges from K on the faces in the circuit. Hence such a circuit must be even in length. We conclude that the set of faces H, consisting of all "isolated" faces from $B_1(K)$, one face from each pair of faces from $B_1(K)$ and alternate faces from each path or circuit of faces from $B_1(K)$, is independent and have cardinality at least $\frac{1}{2}B_1(K)$.

Turning to (ii), we have by Lemma 2(i) that

$$\kappa(\Gamma) = \frac{2k}{3} - \frac{|B_1(K)| + 2|B_2(K)|}{3}.$$

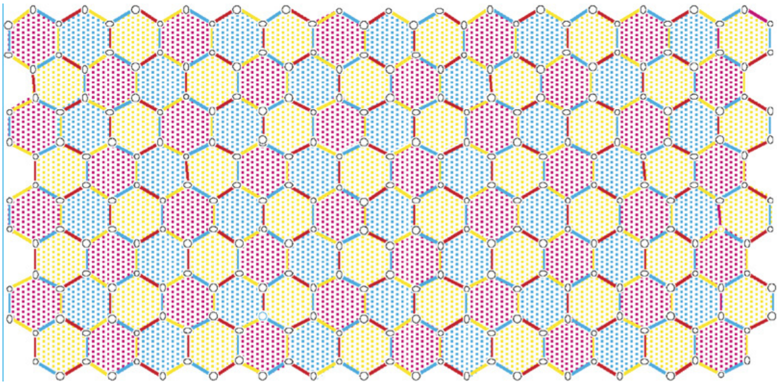

Fig. 8.

Multiplying through by 3, replacing k by $|F| - 2 = \sum_0^3 |B_i(K)| - 2$ and simplifying gives:

$$3\kappa(\Gamma) = 2|B_0(K)| + |B_1(K)| + 2|B_3(K)| - 4.$$

But $|B_3(K)| = \kappa(\Gamma)$. So we have $\kappa(\Gamma) + 4 = 2|B_0(K)| + |B_1(K)|$. Finally, by the first part of this theorem, $\alpha^*(\Gamma) \geq |B_0(K)| + \frac{1}{2}|B_1(K)|$ and replacing $|B_0(K)| + \frac{1}{2}|B_1(K)|$ by $\frac{1}{2}\kappa(\Gamma) + 2$ gives $\frac{1}{2}\kappa(\Gamma) + 2 \leq \alpha^*(\Gamma)$ and the inequality we want. □

By Theorem 1, $\alpha^*(\Gamma) = \frac{k}{3} + 2 = \frac{1}{2}\kappa(\Gamma) + 2$, for a leap-frog fullerene Γ. In this case, the faces are partitioned into the maximum independent face set and the set of benzene-like faces and we have $\alpha^*(\Gamma) + \kappa(\Gamma) = k + 2$. If Γ is not a leap-frog fullerene, we have $\alpha^*(\Gamma) = \frac{1}{3}k + 2 - \epsilon_{\alpha^*}(\Gamma)$ and $\kappa(\Gamma) = \frac{2}{3}k + 2 - \epsilon_\kappa(\Gamma)$, where $\epsilon_{\alpha^*}(\Gamma) = \frac{p^*(R)+v^*(R)}{6}$ and $\epsilon_\kappa(\Gamma) = \frac{2k}{3} - \frac{|B_1(K)|+2|B_2(K)|}{3}$ for the appropriate sets R and K. So, $\alpha^*(\Gamma) + \kappa(\Gamma) = k + 2 - (\epsilon_\alpha + \epsilon_\kappa)$. Equality in Theorem 3(ii) is equivalent to the condition that $\epsilon_\alpha = \frac{1}{2}\epsilon_\kappa$. It would be interesting to know if these two parameters were always related to one another in this way. Even more interesting is the answer to the question: Is there always a maximum Kekulé structure K for a fullerene Γ so that the maximum independent set of faces in $B_0(K) \cup B_1(K)$ has cardinality $\alpha^*(\Gamma)$? What is needed is a method for computing these parameters for non-leap-frog fullerenes. A first step is to develop methods for estimating these two parameters in non-leap-frog fullerenes.

6. Estimating α^* and κ for a non-leap-frog fullerene

In this section, we sketch a method for computing lower bounds for α^* and κ of a non-leap-frog fullerene and the last section we will give an example.

Consider a patch of the hexagonal tessellation of the plane and properly 3-color its faces. The coloring is unique up to a permutation of the colors and induces a unique 3-coloring of the edges interior to the patch so that no edge bounds a face of the same color. Such a patch is pictured in Fig. 8. Interior to such a patch each face color class is locally a perfect face independent set and each edge color class is locally a perfect Kekulé structure.

Now think of a very large fullerene. Starting away from any pentagonal face, 3-color its faces and edges, extending this coloring as far as one can. What happens when one encounters a pentagon? As the coloring wraps around the pentagonal face, there is a mismatch along a polygonal path of hexagonal faces leaving the pentagonal face, as we saw in Figs. 5 and 6. Now think of connecting all of the pentagonal faces by a collection, a sort of “spanning tree”, of

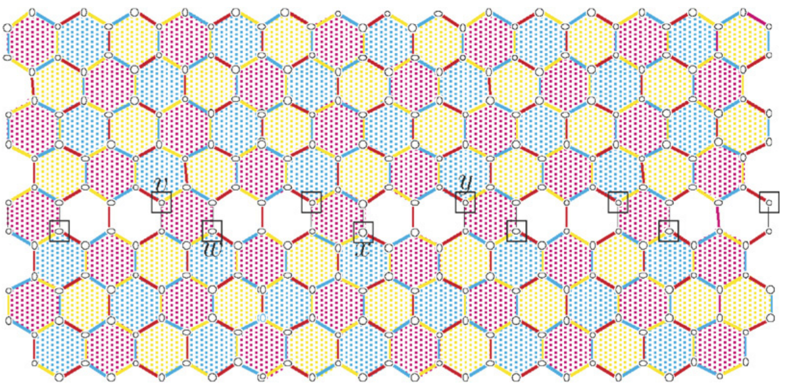

Fig. 9.

polygonal paths of hexagons, *(linear) fissures*. Using Figs. 5 and 6 as models, think of the fissure joining the two pentagonal faces in this region as one "edge" of this "spanning tree" and assume that a second fissure connects the upper pentagon to the remaining pentagons. Our face and edge 3-coloring will extend to all faces and edges not on this set of fissures. The mismatches along the fissures will be of two types: those where the orientations of the sequence of colors along the parallel direction differ across the fissure and those where the color orientations of parallel direction agree across the fissure; *orientation reversing* fissures and *orientation preserving* fissures, respectively. In our examples, the fissure joining the two pentagons is orientation reversing. As we saw there, one color matches through an orientation reversing fissure. The fissure connecting the upper pentagon to the remaining pentagons is orientation preserving. Here there are two possibilities: either all colors match and the fissure "disappears" or none of the colors match and all of the faces on the fissure must remain uncolored. In Fig. 5, the colors match and the fissure disappears while, in Fig. 6, the colors don't match and the entire fissure remains uncolored. After we complete the coloring and some fissures have disappeared, we are left with a "spanning forest" of linear fissures.

There are, of course, many different choices for such a "spanning forest" of linear fissures. Since each color class of faces is an independent face set, the largest color class of faces in any choice will give a lower bound for α^*. On the other hand, none of the edge color classes are Kekulé structures for the entire fullerene. To get a bound on κ, we must be able to amend one of these edge color classes to make it a Kekulé structure. In Figs. 9 and 10 we illustrate just how this can be done. Our first step is to extend the alternating edge colors around each hexagonal face on the boundary of the fissure and continue the edge coloring across the fissure for the color that matches across the fissure — if there is one. This has been done in Figs. 9 and 10. We note that at this point each edge color class is a partial matching. Next we select a color class and complete it to a perfect matching.

Suppose that we choose the blue edge color class to complete. No adjustment is necessary for any fissure through which the color blue passes. Now consider the fissure in Fig. 9. Here red passes through and blue does not. We have drawn squares around the vertices unmatched by the blue edges and we have done the same in Fig. 10. Starting at one pentagon, pair up consecutive unmatched vertices. Assuming that this pairing can be carried out throughout the spanning tree of fissures, we complete the blue matching as follows: if the vertices labeled v and w in Fig. 9 are paired, replace the black, blue, yellow path joining them by a blue, black, blue path: if the

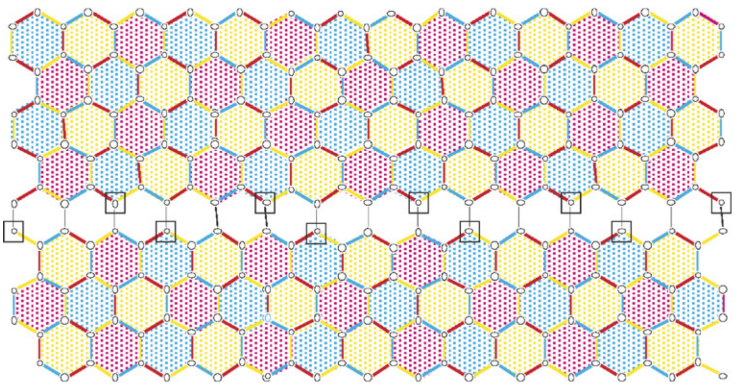

Fig. 10.

vertices labeled x and y in Fig. 9 are paired, replace the red, blue, red, blue, red path joining them by a blue, red, blue, red, blue path. A similar interchange can be made for any pairing along the fissure in Fig. 10.

Next we observe that the vertices and faces that contribute to the error terms $\epsilon_{\alpha^*}(\Gamma)$ and $\epsilon_\kappa(\Gamma)$ all lie on or are adjacent to these fissures and hence may be computed. To be specific assume that we have chosen the blue faces to be our independent face set and have altered the edge coloring along the fissure to make K, the collection of blue edges, a Kekulé structure. So we have $\epsilon_{\alpha^*}(\Gamma) = \frac{k}{3} + 2 - \frac{p^*(B)+v^*(B)}{6}$ and $\epsilon_\kappa(\Gamma) = \frac{2k}{3} - \frac{|B_1(K)|+2|B_2(K)|}{3}$. The non-blue pentagonal faces contributing to $p^*(B)$ occur at the endpoints of the fissures and the vertices not bounding to a blue face contributing to $p^*(B)$ must bound a white face and therefore lie along the fissure. Similarly, the faces in $B_1(K)$ and $B_2(K)$ are all on or adjacent to the fissures.

We illustrate the use of linear fissures in computing lower bounds for $\alpha^*(\Gamma)$ and $\kappa(\Gamma)$ in the case that Γ is a fullerene with icosahedral symmetry (see [4] or [10]). Let Γ be any fullerene with icosahedral symmetry given by the Coxeter coordinates (p, q). If $p \equiv_3 q$, then Γ is a leap-frog fullerene and has $\alpha^*(\Gamma) = \frac{k}{3} + 2$ and $\kappa(\Gamma) = \frac{2k}{3}$. Assume then that $p \not\equiv_3 q$ and, without loss of generality, that $p > q$. In Fig. 11, we have diagramed two adjacent icosahedral triangles of Γ. Observe that the Coxeter coordinates of the segment joining the "opposite" pentagons P_1 and P_4 are $(p - q, p + 2q)$ and therefore congruent mod 3. Now build a spanning tree of fissures starting with six linear fissures pairing up "opposite" pentagonal faces and connecting them up with five other linear fissures. Then the coloring will match across the five connecting fissures and they will all disappear. The result will be a spanning forest consisting of six disjoint linear fissures.

In Fig. 12, we illustrate such a set of six fissures. Since the Coxeter coordinates of the fissure are congruent mod 3, one of the colors will match across each fissure. However, it won't be the same color across all fissures. We "color" each fissure with the color that passes through it. Since p and q are not congruent mod 3, the pentagonal faces corresponding to the vertices of any triangle of the icosahedron not cut by a fissure must be assigned different colors. Hence, we may assume that P_1 is colored red, P_2 is colored blue and P_4 is colored yellow. As we observed above the colors of the adjacent pentagons are all forced: from the P_1–P_7 fissure, we have that P_7 is red. Similarly P_6 is yellow and P_{12} is blue. Since P_6 is yellow and P_2 is blue and the icosahedral triangle with vertices P_6, P_2 and P_3 is not cut by a fissure, we conclude that P_3 is red. Continuing in this way, we see that the coloring of the fissures in Fig. 12 is forced.

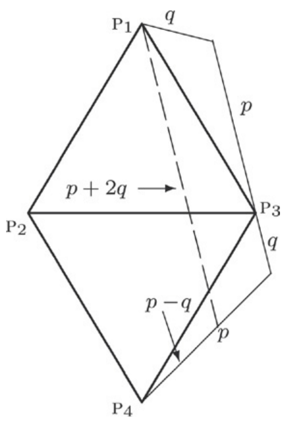

Fig. 11.

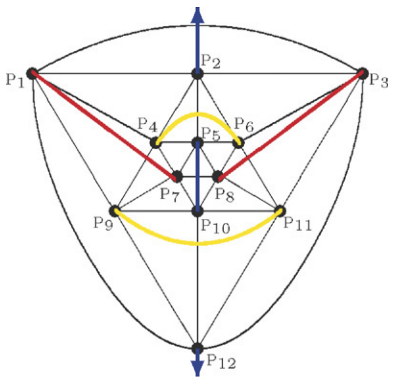

Fig. 12.

In Fig. 13 we give a detailed view of the red fissure joining P_1 and P_7 for the case $(p, q) = (10, 5)$. By symmetry we see that the three face color classes all have the same cardinality — our lower bound on α^*. So let's select blue. We could compute the contribution to $\frac{p^*(B)+v^*(B)}{6}$ for each red and yellow fissure to get our bound. However, because of the symmetry, there is a short cut. The formula for the number of vertices gives $|V| = 20(10^2 + 5 \times 5 + 5^2) = 3500$ (see [13]). Hence $k = 1750$ and $|F| = 1752$. There are 16 white (uncolored) faces in each fissure for a total of 96 white faces and 1656 colored faces. Then, by symmetry, there are 552 blue faces. Compare this with the upper bound on α^*, $\frac{k}{3} + 2 = 585\frac{1}{3}$. There is no shortcut to computing the error for K consisting of the adjusted blue edges. The computation is a bit tedious but straightforward and yields a bound of 1036 for κ. Compare this with $\frac{2k}{3} = 1166\frac{2}{3}$.

In [14], the author showed that the exact value of the vertex independence number was always given by such a set of six linear fissures. But it turns out not to be true for the face independence number! Consider a spanning tree of the icosahedron and replace its edges by the corresponding linear fissures. If we selected the right tree, just two of the fissures will disappear leaving three paths of length three each. The corresponding path in the dual would have length $3(p+q)$. As we saw above, the longer the total length of the fissures, the more white faces we are likely to have.

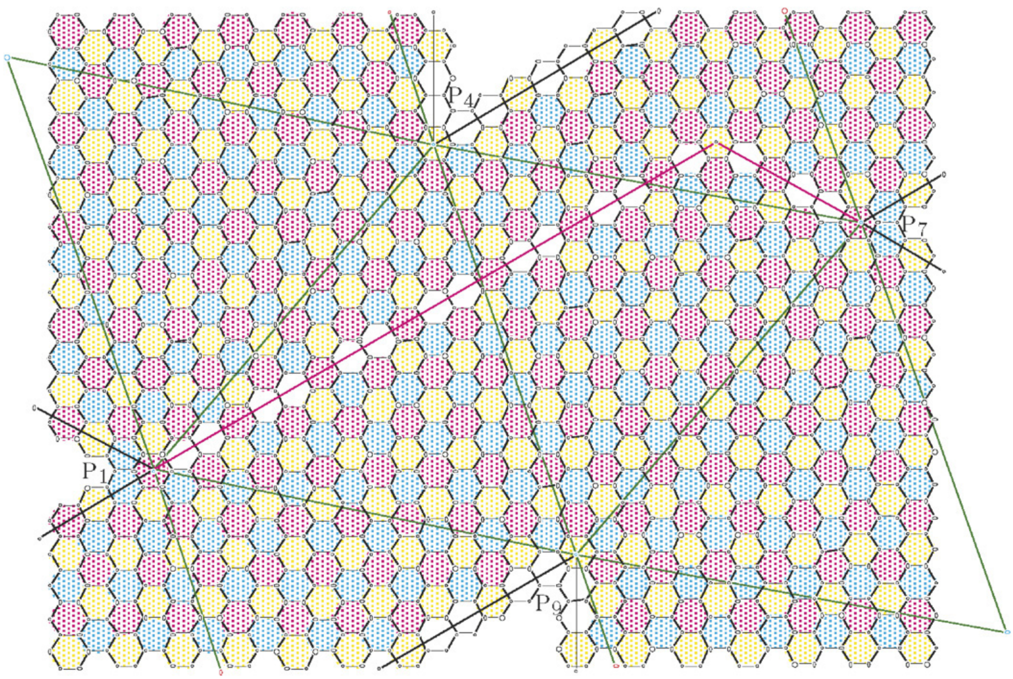

Fig. 13.

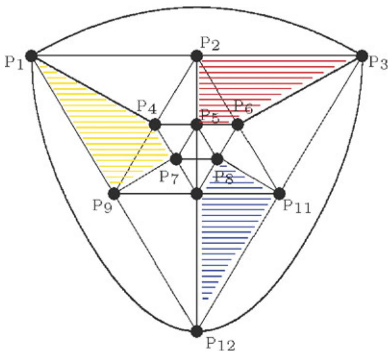

Fig. 14.

Hence, we may try to connect the four pentagons on a path with a shorter configuration using two Steiner points. We have pictured one of these “quadrilateral fissures” in Fig. 15. It has one red pentagon, one blue pentagon and two yellow pentagons. Identifying it with the two yellow pentagons; we call it a “yellow quadrilateral fissure”. It turns out that this decomposition yields one quadrilateral fissure of each color, as pictured in Fig. 14.

By symmetry, the lower bound on α^* given by this configuration is easily computed by counting the white faces ($3 \times 24 = 72$), subtracting from the total number of faces, (1752) and divide by 3 to get $\frac{1752-72}{3} = 560$. Compare this with the bound of 552 given by the linear

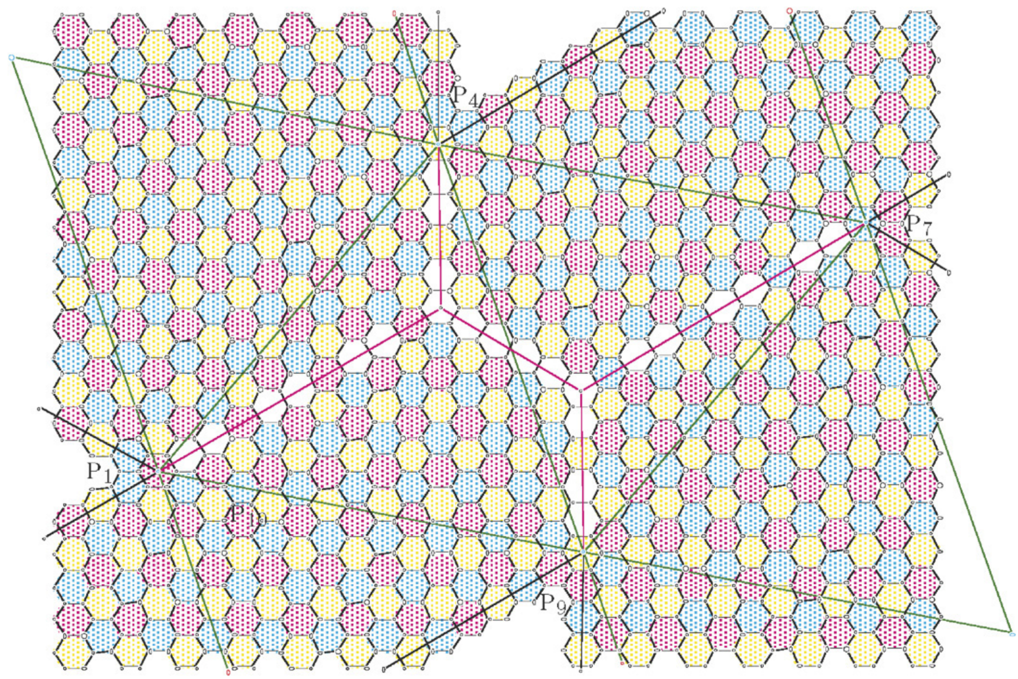

Fig. 15.

fissures. The lower bound on κ given by this collection of quadrilateral fissures is 1062 compared with 1036 given by the linear fissures.

7. Comments and conclusions

It is probably true that the exact values of α^* and κ will be given by some system of fissures. However, that has yet to be proved and, in view of this last example, the fissures may turn out to be quite complicated and very different from one class of fullerene to another. Nevertheless, fissures yield very easy-to-compute lower bounds for α^*.

Lemma 5. *Let $\Gamma = (V, E, F)$ be a fullerene and suppose that it admits a system of fissures with w uncolored faces. Then $\alpha^* \geq \frac{|F|-w}{3}$.*

Consider any family of fullerenes and select a spanning tree of its signature. Now construct a corresponding set of eleven linear fissures. The number of hexagonal faces along these fissures grows linearly in the parameters of the signature while the number of faces grows quadratically in these parameters. Hence, α^* will also grow quadratically or the error term will grow as the square root of the number of faces.

Lemma 6. *Consider the class of fullerenes with a fixed signature $\mathcal{S}$. Then, for this class of fullerenes, there is a constant s such that*

$$\alpha^*(\Gamma) \geq \frac{|F|}{3} - s\sqrt{|F|},$$

for any fullerene $\Gamma = (V, E, F)$ in this class.

We illustrate these results with the class of Icosahedral fullerenes. Referring to [13], we see that the icosahedral fullerene with Coxeter parameters $(p+r, p)$ has $|V| = 60p^2+60pr+20r^2$. Hence $|F| = 30p^2+30pr+10r^2+2$. Of course we are only interested here in the non-leap-frog case, that is when $p+r$ and p are not congruent mod 3 or, when $p = 0$, r is not congruent to 0 mod 3. Now consider the six linear fissures described in the last section. They have Coxeter coordinates $(3p+r, r)$ and, by direct computation, the number of uncolored face w is given by $12p+8r-8$ when $r \equiv_3 1$ and $12p+8r-10$ when $r \equiv_3 2$. One easily checks that $\frac{64}{10}|F| \geq w^2$, for all possible values of the parameters p and r (both are nonnegative integers with at least one positive). Hence:

Theorem 4. *For any icosahedral fullerene $\Gamma = (V, E, F)$,*

$$\alpha^*(\Gamma) \geq \frac{|F|}{3} - \frac{4\sqrt{10}}{15}\sqrt{|F|}.$$

A slightly smaller value for s can be obtained using quadrilateral fissures. But the computations involve several cases and are rather tedious. It is clear that much work remains to be done.

- Results similar to those in this section could be proved for κ. But without the "shortcut" afforded by simply counting uncolored faces, the proof may be rather complex.
- Two pentagons can be joined by a single linear fissure if and only if the Coxeter coordinates of a path joining them are congruent mod 3. What are the necessary and sufficient conditions for a grouping of 4 pentagons to admit a quadrilateral fissure?
- Are there examples where hexagonal fissures would be best?
- On the theoretical side it would be very nice to have proof that α^* and κ will always be given by a system of fissures.
- Exactly how are α^*, κ and γ related?
- Can one find another inequality going in the opposite direction from the one in Theorem 3(ii)?
- Perhaps the linear programming approach developed by Hansen and Zheng [15], [1] can be adapted to fullerenes and used to prove that the lower bounds for κ and γ given by a set of fissures are indeed optimal.

References

[1] H. Abeledo, G. Atkinson, The Clar and Fries problems for benzeoid hydrocarbon are linear programs, in: DIMACS, vol. 51, Amer. Math. Soc., Providence, RI, 2000, pp. 1–8.

[2] S.J. Auston, P.W. Fowler, P. Hansen, D.E. Manolopoulos, M. Zheng, Fullerene isomers of $\mathbf{C_{60}}$: Kekul=E9 counts versus stability, Chem. Phys. Lett. 228 (1994) 478–484.

[3] E. Clar, The Aromatic Sextet, John Wiley & Sons, London, 1972.

[4] H.S.M Coxeter, Virus macromolecules and geodesic domes, in: J.C. Butcher (Ed.), A Spectrum of Mathematics, Oxford Univ. Press, 1971, pp. 98–107.

[5] P.W. Fowler, Localized models and leapfrog structures of fullerenes, J. Chem. Soc. Perkin 2 (1992) 145–146.

[6] P.W. Fowler, A. Ceulemans, Electron deficiency of the fullerenes, J. Phys. Chem. 99 (1995) 508–510.

[7] P.W. Fowler, D.E. Manolopoulos, An Atlas of Fullerenes, Clarenden Press, Oxford, 1995.

[8] P.W. Fowler, T. Pisanski, Leapfrog fullerenes and Clar polyhedra, J. Chem. Soc. Faraday 90 (1994) 2865–2871.

[9] K. Fries, Über byclische verbindungen und ihren vergleich mit dem naphtalin, Ann. Chem. 454 (1927) 121–324.

[10] M. Goldberg, A class of multi-symmetric polyhedra, Tohoku Math. J. 43 (1937) 104–108.

[11] J.E. Graver, Encoding fullerenes and geodesic domes, SIAM. J. Discrete Math. 17 (4) (2004) 596–614.

[12] J.E. Graver, The structure of fullerene signatures, in: DIMACS Series in Discrete Mathematics and Theoretical Computer Science, vol. 69, AMS, 2005, pp. 137–166.

[13] J.E. Graver, A catalog of fullerenes with 10 or more symmetries, in: DIMACS Series in Discrete Mathematics and Theoretical Computer Science, vol. 69, AMS, 2005, pp. 167–188.
[14] J.E. Graver, The independence number of fullerenes and benzenoids, European J. Combin. (6) (2006) 850–863.
[15] P. Hansen, M. Zheng, The Clar number of a benzeoid hydrocarbon and linear programming, J. Math. Chem. 15 (1994) 93–107.