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ORIGINAL PAPER

Kekuléan benzenoids

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Abstract A *Kekulé structure* for a benzenoid or a fullerene Γ is a set of edges K such that each vertex of Γ is incident with exactly one edge in K, i.e. a perfect matching. All fullerenes admit a Kekulé structure; however, this is not true for benzenoids. In this paper, we develop methods for deciding whether or not a given benzenoid admits a Kekulé structure by constructing Kekulé structures that have a high density of benzene rings. The *benzene rings* of the Kekulé structure K are the faces in Γ that have exactly three edges in K. The *Fries number* of Γ is the maximum number of benzene rings over all possible Kekulé structures for Γ and the set of benzene rings giving the Fries number is called a *Fries set*. The *Clar number* is the maximum number of independent benzene rings over all possible Kekulé structures for Γ and the set of benzene rings giving the Clar number is called a *Clar set*. Our method of constructing Kekulé structures for benzenoids generally gives good estimates for the Clar and Fries numbers, often the exact values.

Keywords Benzenoids · Graphene patches · Fullerenes · Conjugated 6-circuits · Benzene rings · Benzene faces · Fries number · Clar number · Kekulé structure

1 Introduction

A *benzenoid* $\Gamma = (V, E, F)$ is a plane graph with one distinguished face called the *outside face* and with all other faces hexagonal; in addition, we require that all vertices have degree 2 or 3 and that all vertices of degree 2 bound the outside face. For this

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paper, we will also assume that Γ is 2-connected or equivalently that the boundary of the outside face is an elementary circuit. Benzenoids are also called *hexagonal patches, hexagonal systems, benzenoid hydrocarbons, graphite patches and graphene patches* in the literature.

A *Kekulé structure* of a benzenoid or a fullerene Γ is a set of edges K of a perfect matching in Γ. All fullerenes admit a Kekulé structure, but benzenoids may or may not. A benzenoid that does admit a Kekulé structure is said to be *Kekuléan*. For a fullerene or a Kekuléan benzenoid Γ, let K denote a Kekulé structure and, for $i = 0, 1, 2, 3$, let $B_i(K)$ denote the set of faces in Γ that have i edges in K. The faces in $B_0(K)$ are called the *void faces* of K; the faces in $B_3(K)$ are called the *benzene rings* of K (also called *benzene faces* or *conjugated 6-circuits*). The *Fries number* of Γ is the maximum number of benzene rings over all possible Kekulé structures for Γ and the *Clar number* is the maximum number of independent benzene rings over all possible Kekulé structures for Γ.

For benzenoids, we adopt the convention that the term "face" will refer to the hexagonal faces unless it is specified to be the outside face. By the *boundary* of the benzenoid Γ we mean the boundary of the outside face. Since the number of faces of a plane graph with odd degree is even, the outside face of a benzenoid has even degree and hence every benzenoid is bipartite and the vertices have a unique vertex 2-coloring up to reversal of colors. We color our vertices black and white. Given a benzenoid we may project it onto Λ, the hexagonal tessellation of the plane, by simply tracing its boundary in Λ. Thus we may envision our benzenoid as a region (perhaps self-overlapping) of Λ. Up to a permutation of colors, Λ has a unique 2-coloring of its vertices (black and white), 3-coloring of its faces (red, blue and yellow) and 3-coloring of its edges (red, blue and yellow) that satisfies the following conditions:

(i) the color of an edge is different from the colors of the two faces it bounds;
(ii) red, blue and yellow faces are oriented clockwise around every degree-3 black vertex counterclockwise around every degree-3 white vertex;
(iii) and the edges are also oriented in this way (see Fig. 1).

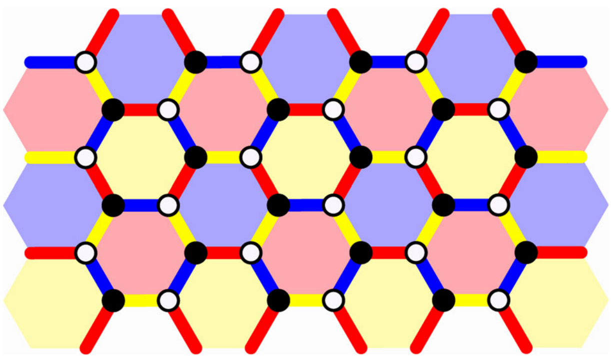


Fig. 1 A region of the hexagonal tessellation with the canonical coloring

We note that with this coloring scheme for Λ, each color class of edges is a perfect matching with the highest possible density of benzene rings. Specifically, choosing the red edges for our perfect matching, the red faces are all void faces while the blue and yellow faces are all benzene rings. Viewing a benzenoid as a region of Λ leads to the following observation:

Observation 1 *Let Γ be a benzenoid. We may choose a vertex 2-coloring (black and white), a face 3-coloring (red, blue and yellow) and an edge 3-coloring (red, blue and yellow) so that the color of an edge is different from the colors of the two faces it bounds, so that red, blue and yellow faces (edges) are oriented clockwise around every degree-3 black vertex and counterclockwise around every degree-3 white vertex and so that the edge colors alternate around each face. Furthermore, this coloring is uniquely determined by the colors of one degree-3 vertex and the faces or edges surrounding it.*

We call this *"the" canonical (vertex, edge and face) coloring* for the benzenoid Γ.

An obvious necessary condition for a benzenoid to be Kekuléan is that the numbers of black and white vertices are the same. However, this condition is far from sufficient. An algorithm to determine when a benzenoid is Kekuléan is given by Gutman and Cyvin in [1]. That algorithm was based on the theoretical results in the paper [5] by Sachs. In Sect. 2, we identify tighter necessary conditions that are encoded in the boundary vertex and face colorings. To verify the necessity of these conditions, we construct partial Kekulé structures for benzenoids that satisfy these additional conditions. Section 3 then considers just when such a partial Kekulé structure can be extended to a full Kekulé structure. In Sect. 4, we consider methods for verifying that a benzenoid is not Kekuléan and give sufficient conditions for a benzenoid to be Kekuléan. In Sect. 5 we will discuss the relationship between this approach and the approach in [5] and we include some observations about the Clar and Fries numbers of a benzenoid.

2 Necessary conditions on the boundary

By the *boundary* of a hexagonal face of Γ we mean the set of vertices and edges it shares with the outside face. The hexagonal faces that have non-empty boundaries are called *boundary faces.* If f is a boundary face, its boundary consists of one or more simple paths. These simple paths are called the *boundary segments* of Γ. For boundary segments of length 3 or 5, we pair adjacent degree-2 vertices; the edge joining paired vertices is called an *exposed edge*. The single degree-2 vertex on a bounding segment of length 2 is called an *exposed vertex*. The three degree-2 vertices on bounding segments of length 4 are partitioned into an *exposed edge* and an *exposed vertex*—in either order. Note that the color of the exposed vertex is the same for either choice. There are six exposed edges in the benzenoid pictured in Fig. 2; one is on a length-3 segment bounding a blue face, three are on length-4 segments bounding blue faces and two are on a single length-5 segment bounding a red face; there are ten exposed vertices on this benzenoid: two white and two black exposed vertices on blue

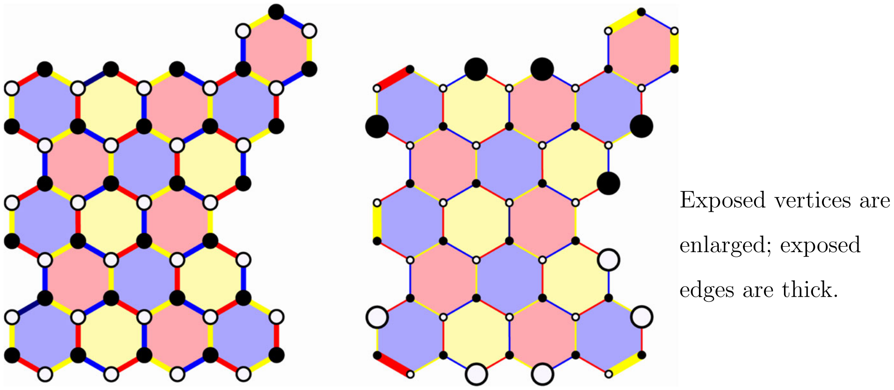


Fig. 2 A benzenoid with six exposed edges and ten exposed vertices

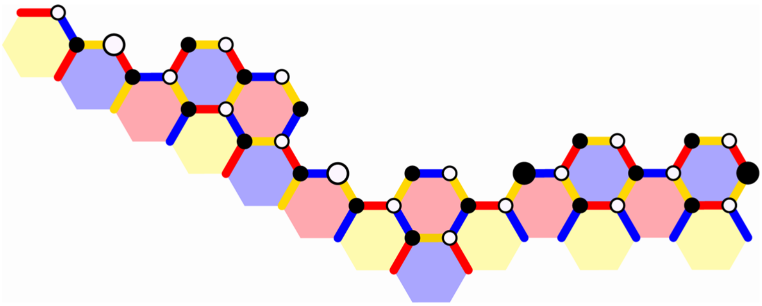


Fig. 3 A segment of the boundary of a benzenoid

faces, one white and one black exposed vertex on red faces and two white and two black exposed vertices on yellow faces.

To better understand the construction of the partial matchings in the upcoming proof, we take a closer look at the sequence of boundary face colors. Based on the coloring convention described in Observation 1, we have:

Observation 2 *Let* $\Gamma = (V, E, F)$ *be a benzenoid with the canonical vertex and face colorings and let* f *be a boundary face.*

(i) If the boundary segment of f *has odd length, then one of the degree-3 endpoints of the boundary segment is white and the other is black; furthermore the boundary faces on either side of* f *have the same color.*
(ii) If the boundary segment of f *has even length, then either the degree-3 endpoints of the boundary segment are white and the exposed vertex on this face is black or the degree-3 endpoints of the boundary segment are black and the exposed vertex is white; furthermore the two adjacent boundary faces have different colors (Fig. 3).*

Lemma 1 *Let* $\Gamma = (V, E, F)$ *be a benzenoid. Then the number of white vertices equals the number of black vertices if and only if the number of white exposed vertices on red faces equals the number of black exposed vertices on red faces.*

Proof Observe that the red edges give a partial matching in which all degree-3 vertices are matched and all degree-2 vertices on blue and yellow faces are matched. The only unmatched vertices are the degree-2 vertices on red faces. If we add the exposed edges on red faces to this partial matching by red edges, the only unmatched vertices are the exposed vertices on red faces. Since the matched vertices are half black and half white, the total numbers of black and white vertices will be equal if and only if the number of white exposed vertices on red faces equals the number of black exposed vertices on red faces. □

The partial matching constructed in this proof is called the *red partial Kekulé structure* for Γ. Clearly, we could have stated and proved this result in terms of the blue or the yellow faces. Hence we have the following theorem:

Theorem 1 *Let* Γ *be a benzenoid. If any one of the conditions is satisfied, then they are all satisfied.*

(i) The number of white exposed vertices on red faces equals the number of black exposed vertices on red faces.
(ii) The number of white exposed vertices on blue faces equals the number of black exposed vertices on blue faces.
(iii) The number of white exposed vertices on yellow faces equals the number of black exposed vertices on yellow faces.
(iv) The number of white vertices equals the number of black vertices.

We will use the term *regular benzenoid* for those benzenoids that satisfy any one, and hence all, of the conditions in this theorem.

Corollary 1 *Let* Γ *be a benzenoid. If for any face color, the number of white exposed vertices on faces of that color is not equal to the number of black exposed vertices on faces of that color, then* Γ *is not Kekuléan.*

If for any color there are no exposed vertices on faces of that color, then the partial matching of that color is a complete matching, i.e. a Kekulé structure for Γ; hence:

Corollary 2 *Let* Γ *be a benzenoid. If for any face color, there are no exposed vertices on faces of that color,* Γ *is Kekuléan.*

The partial red, blue and yellow Kekulé structures for our basic example are portrayed in Fig. 4. It is natural to ask if any of these partial Kekulé structures could be altered to give a full Kekulé structure and, if so, how. To answer this question we turn to network flow theory.

3 Constructing a Kekulé structure

A standard approach to finding a maximal matching in a bipartite graph $\Gamma = (B \cup W, E)$ with the parts B (colored black) and W (colored white) is to set up a network flow: add a *source vertex* s connected to each black vertex and connect each white vertex to a new *sink vertex* t. The $s - B$ edges are directed from s to B and have

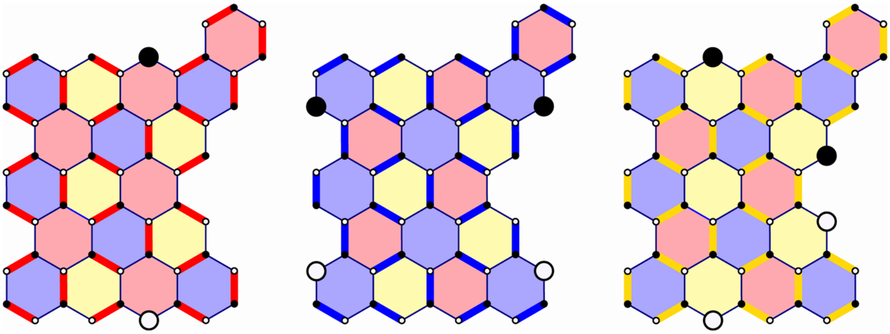


Fig. 4 Our basic example with partial red, blue, and yellow Kekulé structures

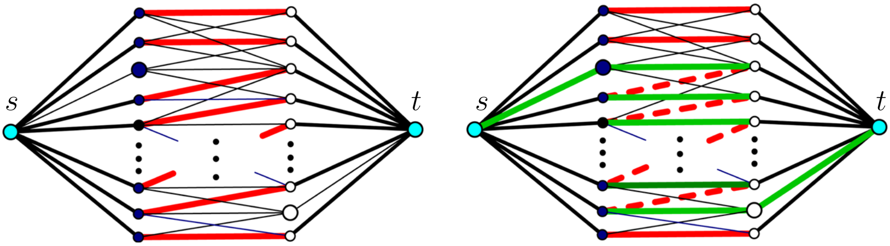


Fig. 5 A network flow

capacity 1; the $B - W$ edges (E) are directed from B to W and have infinite capacity; the $W - t$ edges are directed from W to t and have capacity 1. An integer flow in this network consists of edge-disjoint paths of length 3 from s to t with the middle edge corresponding to an edge of the partial matching; see the lefthand network in Fig. 5. If such a flow is not maximum, there exists an augmenting unit flow from the source to the sink. Such an augmenting unit flow consists of an unused edge from s to a black vertex, an alternating path of forward (thick green) edges (from black to white) and backward (dashed red) edges (from white to black) ending in a white vertex and the unused edge from that white vertex to the sink; see the righthand network in Fig. 5.

Starting with the red partial matching for our example, we have just one black vertex yet to match. On the left in Fig. 6 we have indicated the *alternating path* that represents a unit flow in the corresponding network; thus extending the red partial matching to the Kekulé structure for Γ shown on the right. We summarize this discussion in the next theorem.

Theorem 2 *Let* $\Gamma = (V, E, F)$ *be a Kekuléan benzenoid. Then there exists a collection of disjoint alternating paths that extends the red partial Kekulé structure to a full Kekulé structure for* Γ*; similarly the blue and yellow partial matchings may be extended to Kekulé structures for* Γ.

Proof Assume that Γ is Kekuléan. Let N denote the corresponding network, let k denote the integral flow in N that corresponds to a fixed Kekulé structure and let f denote the integral flow in N that corresponds to the red partial matching. The value of k is $\frac{1}{2}|V|$ and the value of f is $\frac{1}{2}|V| - m$, where m is the number of unmatched black

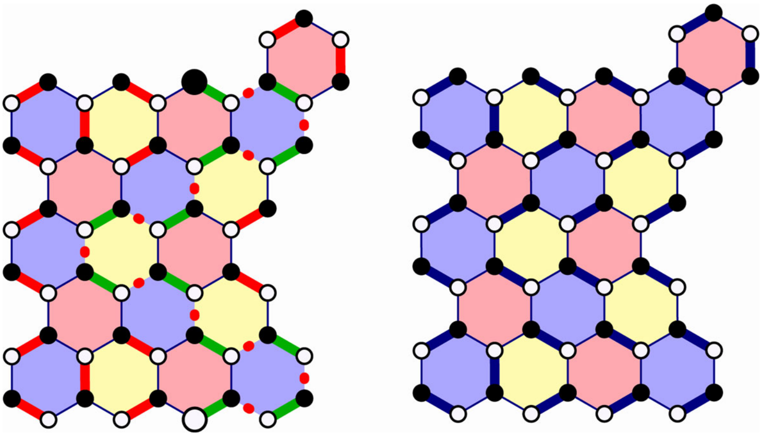


Fig. 6 An alternating path extending the partial red Kekulé structure to a perfect matching

(white) vertices. Then the flow $k - f$ is an integral flow of value m that decomposes into edge disjoint unit flows each joining an exposed black vertex on a red face to an exposed white vertex on a red face and possibly some circular unit flows. Ignoring the circular flows we have a collection of m edge-disjoint unit flows that extends the red partial matching to a Kekulé structure. □

Corollary 3 *Let* $\Gamma = (V, E, F)$ *be a regular benzenoid.*

(i) If any one of the red, blue or yellow partial matchings may be extended to a perfect matching for Γ*, then* Γ *is Kekuléan.*
(ii) If any one of the red, blue or yellow partial matchings fails to extend to a perfect matching for Γ*, then* Γ *is not Kekuléan.*

There are several cases in which it is easy to construct the required augmenting unit flows. To understand these we must take an even closer look at the coloring along the boundary.

Lemma 2 *Let* $\Gamma = (V, E, F)$ *be a benzenoid with the canonical vertex and face colorings. In the sequence of exposed vertices clockwise around the boundary* $\{v_1, \ldots, v_k\}$*, let* f_i *denote the boundary face containing the exposed vertex* v_i*.*

(i) Between v_i *and* v_{i+1} *the faces alternate between two colors.*
(ii) If v_i *and* v_{i+1} *have the same color,* f_i *and* f_{i+1} *have different colors.*
(iii) If v_i *and* v_{i+1} *have different colors,* f_i *and* f_{i+1} *have the same color.*
(iv) If v_i *and* v_{i+1} *have different colors, then the edges of boundary segment between them alternate between edges that belong to the partial Kekulé structure of the color common to the faces* f_i *and* f_{i+1} *and those that do not.*

Proof The reader may wish to refer to Fig. 3.

(i) The faces between v_i and v_{i+1} have no exposed vertices and hence have odd boundary segments. By Observation 2(i), the faces on either side of each of these faces have the same color. Hence these faces alternate in color.

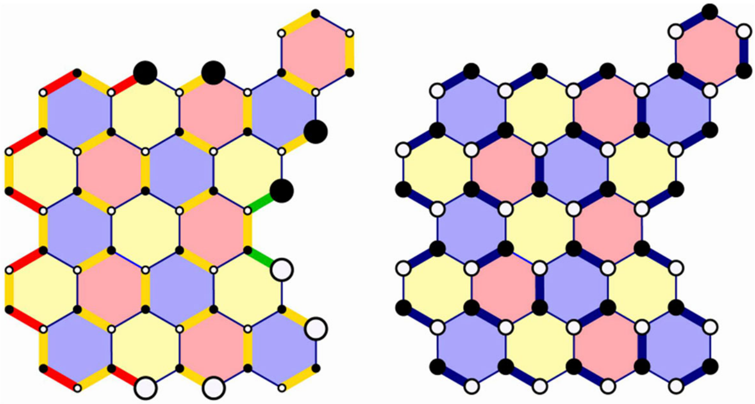


Fig. 7 Boundary segments between exposed vertices on yellow faces

(ii) By Observation 2(ii) the degree-3 vertices on the bounding segment of f_j have the same color and that color is different from the color of v_j. Hence if v_i and v_{i+1} have the same color then the degree-3 vertices of the boundary path joining f_i to f_{i+1} have the same color. Therefore that boundary path has even length. Since it consists of the odd boundary segments of the intervening faces there must be an even number of these faces and, since they are alternating in color, f_i to f_{i+1} are assigned different colors.

(iii) A similar argument proves this part.

(iv) Assume that f_i and f_{i+1} are yellow and that the faces between them alternate between yellow and red and consider the boundary path between v_i and v_{i+1}. The edges at a degree-3 vertex on this path that do not lie on the path are all assigned the color blue. Hence the edges on this path alternate between red edges and edges of the yellow partial Kekulé structure. See Fig. 7. □

Combining the contrapositive of (ii) and (iv) of this lemma gives:

Theorem 3 *Let $\Gamma = (V, E, F)$ be a benzenoid and consider the partial Kekulé structure for one of the face colors. If v and w are exposed vertices on faces of this color and they are consecutive (among all exposed vertices) on the boundary, then they have different colors and the boundary segment joining them is the alternating path of a unit augmenting flow.*

Corollary 4 *Let $\Gamma = (V, E, F)$ be a benzenoid. If for any face color class the corresponding exposed vertices can be split into pairs that are consecutive on the boundary, Γ is Kekuléan.*

We illustrate this result with a slight variation on our basic example. Here the two black exposed vertices on yellow faces are consecutive with the two white exposed vertices on yellow faces and the alternating paths along the boundary are the augmenting paths needed to extend the yellow partial Kekulé structure to a complete Kekulé structure.

Given a regular benzenoid, a straight forward case by case consideration shows that when the total number of exposed vertices is small enough either there are no exposed vertices on faces for one of the colors or the exposed vertices on faces for one of the colors may be split into pairs that are consecutive on the boundary. Specifically:

Corollary 5 *A regular benzenoid with eight or fewer exposed vertices is Kekuléan.*

Proof Let Γ be a regular benzenoid with eight or fewer exposed vertices. If one color class of faces has no exposed vertices Γ is Kekuléan. Hence we may assume without loss of generality that Γ has two black and two white exposed vertices on red faces and one black and one white exposed vertex on blue faces and one black and one white exposed vertex on yellow faces. Now there must be at least two black-white pairs of consecutive exposed vertices. If either pair is blue or yellow, Γ is Kekuléan. Otherwise both pairs are red and Γ is Kekuléan. □

4 Non-Kekuléan benzenoids

Let $\Gamma = (V, E, F)$ be a regular benzenoid and let $N = (\Gamma, s, t)$ be the corresponding network. We have already described the integer flows in N and noted that, if Γ admits a Kekulé structure, then the value of a maximum flow in N is $\frac{1}{2}|V|$. In order to exploit the Max-flow Min-cut Theorem, we need to understand how the cuts in N are manifested in Γ. An arbitrary cut in N is simply a partition of the vertices with s in one set called the *top set* and t in the *bottom set*. The capacity is then the sum of the capacities of the edges directed from a vertex in the top set to a vertex in the bottom set. If the cut includes a black vertex in the top set joined to a white vertex in the bottom set, the capacity of the cut is infinite. It is natural to restrict our attention to cuts with finite capacity. Because of the simple structure of the corresponding network and the fact that Γ is planar the cuts are easy to describe. In Fig. 8, we have illustrated a cut with finite capacity.

For a finite cut, the capacity of the cut is the number of white vertices above the cut, W_{above}, plus B_{below}, the number of black vertices below the cut. Since $B_{below} = \frac{1}{2}|V| - B_{above}$, the capacity of the cut is $\frac{1}{2}|V| + W_{above} - B_{above}$. The following lemma then follows at once from the Max-flow Min-cut Theorem.

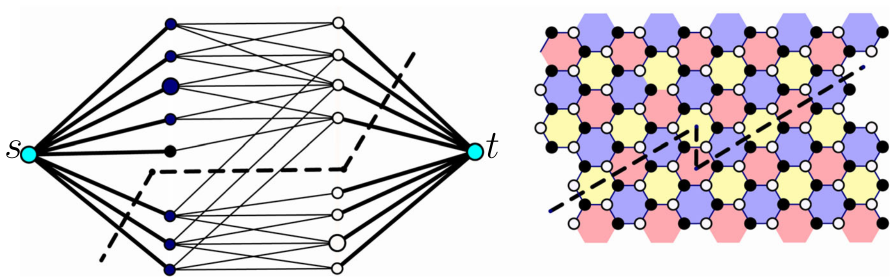


Fig. 8 A finite cut in Γ

Lemma 3 *Let* $\Gamma = (V, E, F)$ *be a regular benzenoid.* Γ *will admit a Kekulé structure if and only if for every cut* $W_{above} \geq B_{above}$.

We need to take a closer look at the structure of cuts. The cut pictured in Fig. 8 illustrates the basic features. First we may think of the cut as the set of edges of a dual path; as we move along this path the white endpoints must all be on one side, the *top side*, and the black end points on the *bottom side*. One easily sees that this forces the cut (dual path) to be a "zig-zag": having entered a face through an edge one must exit through the opposite edge or one of the adjacent edges. The cut we have pictured cuts across from the outside face to the outside face on the other side. But such a zig-zag path could be a closed circuit. Consider such a circuit and assume that the top side is the inside of the circuit. Now consider Θ, the subgraph spanned by the vertices on the inside. Every black vertex in Θ has degree 3 while some of the white vertices have degree 3, those bounding the cut have degree less than 3. It follows at once that $W_{above} > B_{above}$. Similarly if the bottom is inside $B_{below} > W_{below}$ implying $W_{above} > B_{above}$ in this case too. Hence there is no need to consider these dual circuits or *trivial cuts*, and the lemma may be restated:

Lemma 4 *Let* $\Gamma = (V, E, F)$ *be a regular benzenoid.* Γ *will admit a Kekulé structure if and only if for every non-trivial cut* $W_{above} \geq B_{above}$.

Now consider a non-trivial cut in Γ and consider the red partial matching. B_{above} consists of the black exposed vertices above the cut on red faces plus the black vertices above the cut that are matched by a red edge to a white vertex above the cut. W_{above} consists of the white exposed vertices above the cut on red faces plus the white vertices above the cut that are matched by a red edge to a black vertex above the cut plus the white endpoints of the red edges in the cut. Hence $W_{above} \geq B_{above}$ if and only if the number of white exposed vertices above the cut on red faces plus the number of red edges in the cut is greater than or equal to the number of black exposed vertices above the cut on red faces. We have

Theorem 4 *Let* $\Gamma = (V, E, F)$ *be a regular benzenoid.* Γ *will admit a Kekulé structure if and only if for every non-trivial cut the number of white exposed vertices above the cut on red (blue or yellow) faces plus the number of edges of the red (blue or yellow) partial Kekulé structure in the cut is greater than or equal to the number of black exposed vertices above the cut on red (blue or yellow) faces.*

We illustrate this result in Fig. 9.

Our basic example appears on the left. One easily checks that the conditions are satisfied for red and yellow: there is one black exposed vertex on a red face above the cut, no white exposed vertices on red faces above the cut and one red edge in the cut; there are two black exposed vertices on yellow faces above the cut, no exposed white vertices on yellow faces above the cut and two yellow edges in the cut. However, there are two black exposed vertices on blue faces above the cut, no exposed white vertices on blue faces above the cut but only one blue edge in the cut. The explanation is that while the exposed edge on the cut is colored yellow, it is nevertheless in the blue partial Kekulé structure.

5 Comments

The constructions in papers [1–3] and [5]can be easily understood in the framework we have set up here. The edges of a benzenoid fall into three parallel classes and we may orient the benzenoid so that the edges of any one of the parallel classes are vertical; see Fig. 10. This set of vertical edges is then a partial matching. The vertices unmatched by this partial matching are degree-2 vertices pointing up, *peaks*, or degree-2 vertices pointing down, *valleys*. All peaks will be in one color class (black in the following example) while all valleys are in the other color class. Therefore a benzenoid will be regular if and only if in any orientation the number of peaks equals the number of valleys. A system of disjoint peak to valley paths corresponds to a set of augmenting unit flows. The surprising feature of this approach is: if there is no perfect matching then there is a simple horizontal cut that demonstrates this—one need not check zig-zag cuts. This fact leads to linear-time algorithms for checking if a benzenoid is Kekuléan or not.

While the approach based on parallel classes as partial matchings and the approach based on color classes as partial matchings both yield a Kekulé structure, if one exists, or show that none exists, there are several features that distinguish them. If you simply want to know whether a given benzenoid is Kekuléan, you can't beat the peaks and

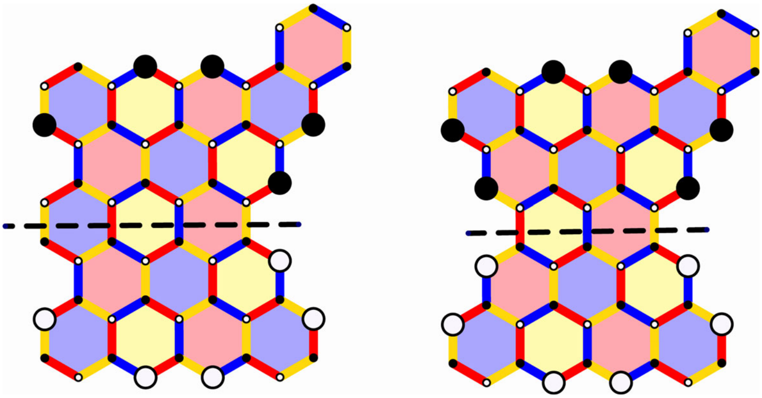


Fig. 9 An illustration of Theorem 4

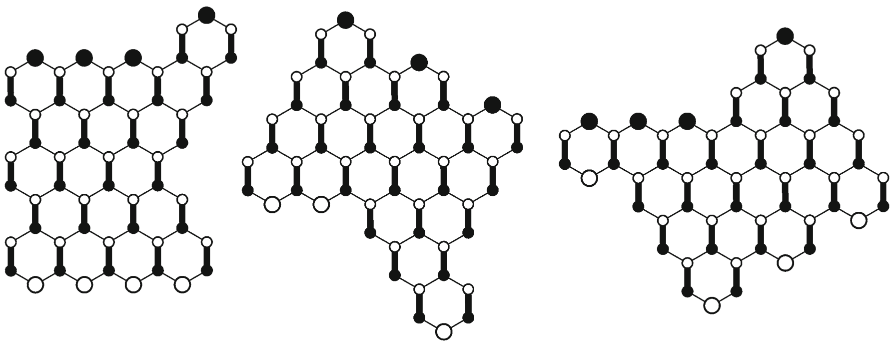


Fig. 10 A partial matching with the peaks and valleys approach

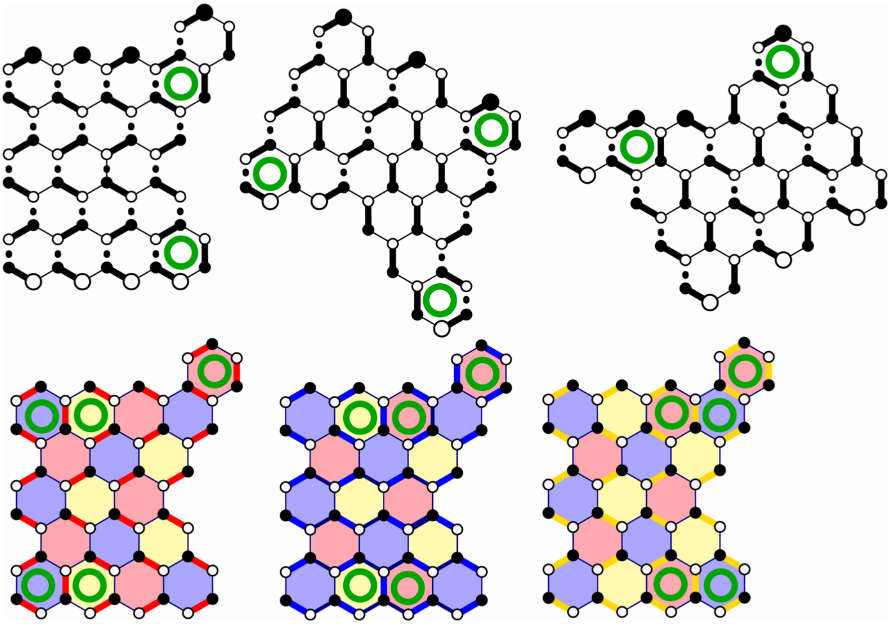


Fig. 11 Kekulé structures based on parallel classes and based on color classes

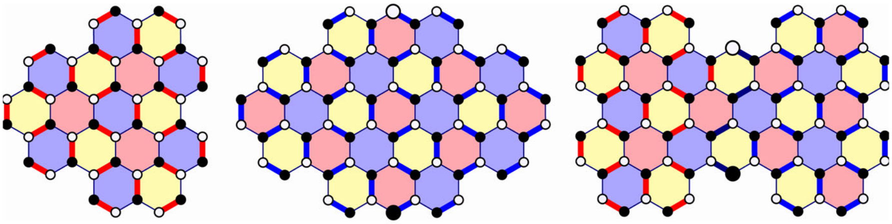
valleys approach. However, if you wish to actually construct a Kekulé structure for a given benzenoid, the color class approach has several advantages.

First, there are generally fewer, frequently far fewer, exposed vertices than there are peaks and valleys. To see this note that every degree-2 vertex on the boundary is a peak or valley in some orientation, while no degree-2 vertex on an odd boundary segment and only one degree-2 vertex on an even boundary segment can be an exposed vertex. It follows that the partial matchings based on color classes need fewer augmenting paths than do the parallel class partial matchings.

Second, the approach based on color classes usually gives Kekulé structures with more, often significantly more, benzene rings. In Fig. 11, the parallel classes give at most three benzene rings. Each of the three color class partial matchings extend to a Kekulé structure with 5 benzene rings, three of which are independent. The Fries number of this benzenoid is five and its Clar number is three.

The big advantage of constructing Kekulé structures based on color classes is that one can then exercise some control over the Fries and Clar numbers as one designs Kekuléan benzenoids. The paper [4] is devoted to a study of those benzenoids without exposed vertices. In that paper it was shown that:

(i) The boundary faces alternate between faces in the two larger color classes; the third *interior* color class of faces is smaller than the other two.
(ii) Taking the faces of the interior (smallest) color class as the void faces gives the unique Kekulé structure that yields the Fries number.
(iii) The unique Fries set consists of the union of the two largest color classes.



Fries # 13, Blue and Yellow faces; Clar # 7, Blue faces.

Fries # 17, Red & Yellow faces; with yellow void, Red & Blue faces. Clar # 9, Red faces in both cases.

Fries # 20, 12 Yellow faces, 4 Blue faces on the left and 4 Red faces on the right. Clar # 12, Yellow faces.

Fig. 12 Benzenoids with Kekulé structures giving the Fries number and Clar number

(iv) The Clar set(s) is always a subset of this unique Fries set, very often simply the largest color class.

A simple example of a benzenoid with no exposed vertices is included on the left in Fig. 12. In that figure we have included two examples of benzenoids with one pair of exposed vertices. The center benzenoid was designed to have two totally disjoint Kekulé structures that give two distinct Fries sets. With the blue faces void, the yellow and red faces form a Fries set and the set of red faces is a Clar set; with the yellow faces void (not shown), the blue and red faces form a Fries set and again the set of red faces is a Clar set. The right hand benzenoid demonstrates that when a benzenoid has "lobes" the optimal Kekulé structure may involve different color matchings on different lobes.

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