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# The Structure of 4-Clusters in Fullerenes

Jennifer Edmond
*Syracuse University*

# Abstract

Fullerenes can be considered to be either molecules of pure carbon or the trivalent plane graphs with all hexagonal and (exactly 12) pentagonal faces that models these molecules. Since carbon atoms have valence 4 and our models have valence 3, the edges of a perfect matching are doubled to bring the valence up to 4 at each vertex. The edges in this perfect matching are called a Kekulé structure and the hexagonal faces bounded by three Kekulé edges are called benzene rings. A maximal independent (disjoint) set of benzene rings for a given Kekulé structure is called a Clar set, and the maximum possible size of a Clar set over all Kekulé structures is the Clar number of the fullerene. For any "patch" of hexagonal faces in the fullerene away from all pentagonal faces, there is a "perfect" Kekulé structure: a Kekulé structure for which the faces of an independent set of benzene rings are packed together as tightly as possible. Starting with such a patch and extending it as far as possible results in a "perfect" Kekulé structure except for isolated regions, called clusters, containing the pentagonal faces. It has been shown that clusters must contain even numbers of pentagonal faces. It has also been shown that the Kekulé structure of the patch can be extended into each of these clusters to give a full Kekulé structure. However, these Kekulé extensions will not admit as tightly packed benzene rings as in the patch external to the clusters. A basic problem in computing the Clar number of a fullerene is to make these extensions in a way that maximizes the number of benzene rings in each cluster. The simplest case, that of 2-clusters, has been completely solved. This thesis is devoted to developing a complete understanding of the Clar structures of 4-clusters.

# THE STRUCTURE OF 4-CLUSTERS IN FULLERENES

*By:*

JENNIFER J. EDMOND

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# Introduction

## 1.1 Introduction

### 1.1.1 Fullerenes

Fullerenes are molecules of pure carbon. We model these molecules using trivalent plane graphs $\Gamma = (V, E, F)$ in which all faces are pentagonal or hexagonal. We also use the term fullerene to denote the graphs used to represent these chemical structures. The vertices of a fullerene depict the carbon atoms and the edges at each vertex represent the bonds between the atom and its neighbors. With no pentagons, carbon forms graphene: sheets of the hexagonal tessellation formed purely by carbon. In order to close the molecule, pentagons are needed to give curvature to the structure. In fact, it follows directly from Euler's formula that in a fullerene, all but exactly 12 faces are hexagons.

**Theorem 1.1.1.** *Let $\Gamma = (V, E, F)$ be a trivalent plane graph such that all face boundaries have length 5 or 6. Then exactly 12 faces are pentagons.*

*Proof.* Euler's formula states that, for any finite connected planar graph, $|V| - |E| + |F| = 2$. $\Gamma$ satisfies this condition. In addition, $\Gamma$ is trivalent, thus we have the further condition that $2|E| = 3|V|$. Now let $P$ denote the set of pentagonal faces of $\Gamma$ and $H$

denote the set of hexagonal faces of $\Gamma$. Since all faces are hexagonal or pentagonal, $|F| = |P| + |H|$. Each face in $P$ contributes 5 edges to the set $E$ and each face in $H$ contributes 6 edges, but each edge is double counted; so, we have $|E| = \frac{1}{2}(5|P|+6|H|)$. Using this formula for $|E|$ as well as $|E| = \frac{3}{2}|V|$, we get $3|V| = 5|P|+6|H|$. Combining these with Euler's formula yields

$$\left(\frac{5}{3}|P| + \frac{6}{3}|H|\right) - \left(\frac{5}{2}|P| + \frac{6}{2}|H|\right) + \left(|P| + |H|\right) = 2,$$

or equivalently

$$\Big(10|P| + 12|H|\Big) - \Big(15|P| + 18|H|\Big) + \Big(6|P| + 6|H|\Big) = 12$$

Simplifying the expression gives us that $|P| = 12$. □

At times we consider the dual of a fullerene $\Gamma$, the geodesic dome $\Gamma^*$. The graph theoretic dual of a fullerene is a triangulation of the sphere in which 12 vertices have degree-5 and the remaining vertices have degree-6. For every pentagon, $P$, in a fullerene $\Gamma$, there is a corresponding degree-5 vertex, $P^*$, in $\Gamma^*$. By a *face path* between two pentagons in a fullerene, we look to the dual and consider the faces of $\Gamma$ identified with the vertices of a path between the corresponding degree-5 vertices. We say that two pentagons, $P$ and $Q$, are *neighbors* in $\Gamma$ if no other degree-5 vertices in $\Gamma^*$ lie on the shortest path between $P^*$ and $Q^*$. If we let $\Lambda$ be the hexagonal tessellation of the plane and $\Lambda^*$ be the triangular tessellation of the plane, then these tessellations form a framework upon which we can map our fullerene/geodesic dome structures. Just as a geodesic dome is the dual of a fullerene, $\Lambda^*$ is the dual of $\Lambda$.

Given two neighboring pentagons, $P$ and $Q$, we form a local coordinate system in $\Lambda^*$. See Figure 1.1. Pick $P^*$ as the origin and choose some ray from $P^*$ as the positive x-axis. We rotate this ray $60^\circ$ to form the positive y-axis. Rotate the axes about $P^*$ so

that $Q^*$ lies on the x-axis or interior to the first quadrant in this coordinate system. The unit length in this coordinate system is the edge length in $\Lambda^*$. For every pair of faces of $\Lambda$, we define a *segment* of $\Lambda$ to be the straight line segment in two-space joining the centers of the two faces. When we want to emphasize that the two faces $P$ and $Q$ are the pentagons connected by the segment we say the $PQ$ segment.

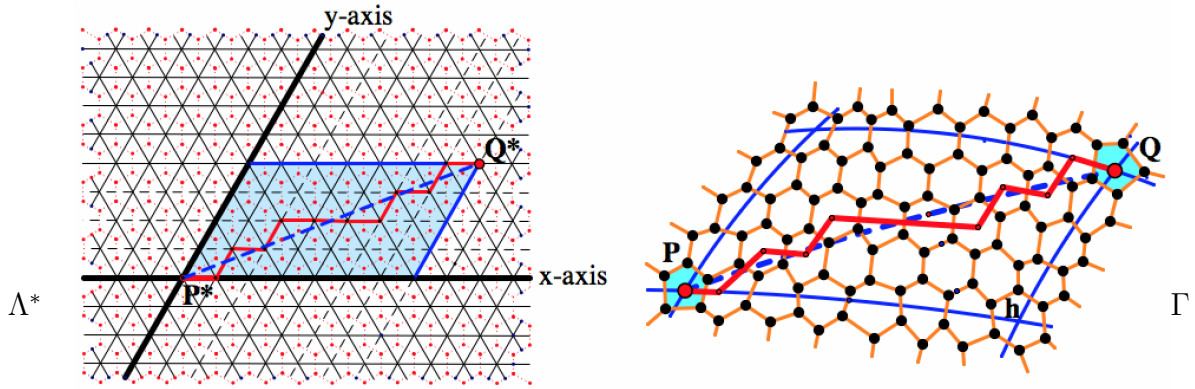



FIGURE 1.1: A $(7, 4)$-segment

The *coordinates* of a segment are the coordinates of $Q^*$ in this coordinate system. Practically, we take a path from one pentagon to the other traveling through the centers of hexagons with one left $120°$. One should note that the coordinates remain the same if the roles of $P$ and $Q$ are reversed; also, the coordinates are reversed for the segment joining $P$ and $Q$ in the mirror image of $\Gamma$. In the case when no turn is needed,$Q^*$ lies on the x-axis and the segment coordinates are of the form $(p, 0)$.

We often want to consider the *length* of a segment $\sigma$ with endpoints $P$ and $Q$. We define the length of $\sigma$, denoted $|\sigma|$, to be the distance between the endpoints in $\Lambda^*$. However, there are several ways to interpret this length. The first method is to consider the graph theoretic length and let $|\sigma| = p + q$ when $\sigma = (p, q)$. Using this definition of length, it is clear that there are many distinct coordinates that all have the same length. For example, $(2, 2)$ and $(4, 0)$ both have length four. This method doesn't take

geometric length into consideration as $(2,2)$ is shorter geometrically than $(4,0)$. To account for this segment length is defined in [1] as $|(p,q)| = p + q + \left|\frac{p-q}{p+q+1}\right|$. This way, segments are first divided into groups by graph theoretic distance and then within these groups are ordered by geometric distance.

For each segment there is an *coordinate path* . The coordinate path travels from one pentagon to the other directly through the centers of the hexagons used to determine the coordinates of the segment. In Figure 1.1 the segment is denoted by a dashed blue line in $\Gamma$ and the coordinate path between $P$ and $Q$ is denoted by two solid blue lines– the first of which initially leaves pentagon $P$ to the right of the segment and goes to the face labeled $h$ then the second segment travels from $h$ to $Q$. Notice that like all coordinate paths, these two segments intersect at a $120°$. For any segment there are two possible choices of coordinate paths. One in which you initially travel to the right of the segment and one in which you initially travel to left of the segment.

We say that two segments are *adjacent* if the segments share a common pentagon. Similarly, we say a set of segments, $\left\{P_1P_2,\ P_2P_3, ...,\ P_{n-1}P_n\right\}$, are mutually adjacent and thus form a *string*, if each segment is adjacent to two other segments with the possible exception of the first and last segments in the string, which could be adjacent to only one. If $P_1 = P_n$ then we say we have a *closed string* of segments. Figure 1.2 shows an open string of 3 segments. The segments are represented by the solid lines between pentagons while coordinate paths are indicated by the dotted lines.

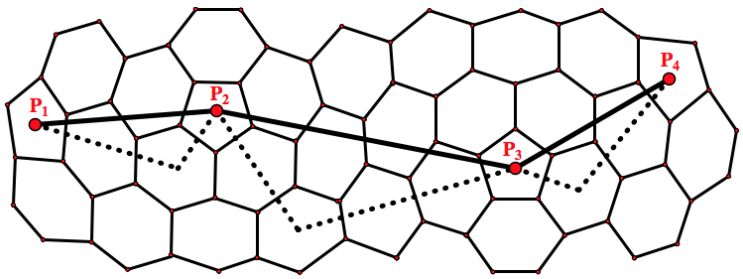
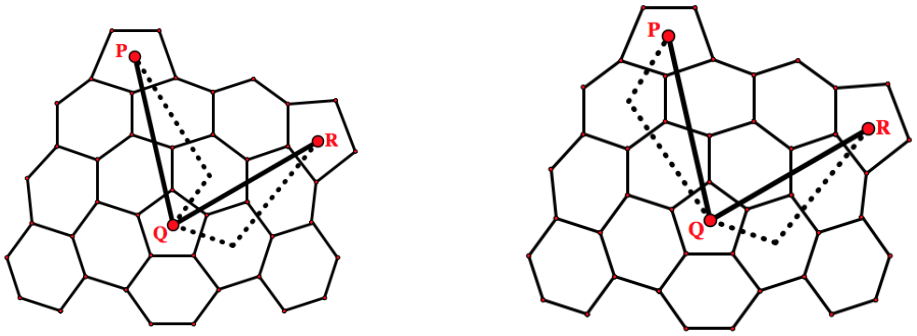



FIGURE 1.2: String of segments from $P_1$ to $P_4$ through $P_2$ and $P_3$

When traveling along a string of segments, we will usually choose a direction so that all coordinate paths lie on one side of the string as in Figure 1.2. In this case as we travel from $P_1$ to $P_4$ sequentially along the segments the coordinate paths all lie to the right of the segments.

For two adjacent segments, we define the angle between them to be $\theta \in \{0, 1, 2, 3, 4, 5\}$ where intuitively $\theta$ is the number of vertices of the pentagon that lie between the two coordinate paths. As we are measuring fullerene angles by counting vertices around a pentagon, it follows that the angles around any vertex in the graph of a fullerene sum to five.

In order to compute the measure of an angle, we choose the common pentagon as the starting point and we choose coordinate paths from that pentagon which both start to the right or both to the left. In Figure 1.3a we see that both sets of coordinate paths emanating from pentagon $Q$ lie to the right of the associated segments. There is one vertex of pentagon $Q$ between the two first legs of the coordinate paths indicating that the measure of $\angle Q$ is 1.




(A) Coordinate paths both on right side from Q

(B) Coordinate paths both on same side of string

FIGURE 1.3: Measuring Angle of Measure 1 from Coordinate Paths

In Figure 1.3b the coordinate paths are drawn on the right side of the segments when traveling first from pentagon $P$ and then from pentagon $Q$ and $\angle Q$ still has

measure 1. Although this can be a convenient way to draw coordinate paths and a method we will often employ, one must keep in mind that we can no longer merely count the vertices between these coordinate paths without first considering that one set of coordinate paths must be altered.

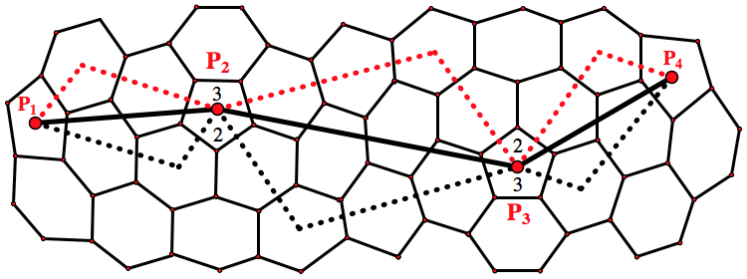



FIGURE 1.4: String of segments from $P_1$ to $P_4$ through $P_2$ and $P_3$

In Figure 1.4 we have included the missing coordinate paths from Figure 1.2. To determine the angles at pentagons $P_2$ and $P_3$ we count the number of vertices between a red coordinate path and a black coordinate path so that both lie to the right of the relevant segments or both lie to the left. All angle measures are shown in the figure.

Notice that this definition of angle measure is distinct from the geometric angle measure. Unless specifically stated we will consider angle measures to be the fullerene angle measure rather than the geometric measure of an angle. However as the first legs of coordinate paths emanating from a single pentagon are always separated by geometric angles of multiples of $60^\circ$ in the fullerene we can also compute angle measures by dividing the angle between the initial legs of coordinate paths by 60 so long as the coordinate paths are drawn appropriately.

### 1.1.2 Signature and Flat map

We now define an auxiliary graph in which the vertices represent the 12 pentagonal faces of $\Gamma$. The edges in this new graph correspond to segments joining neighboring

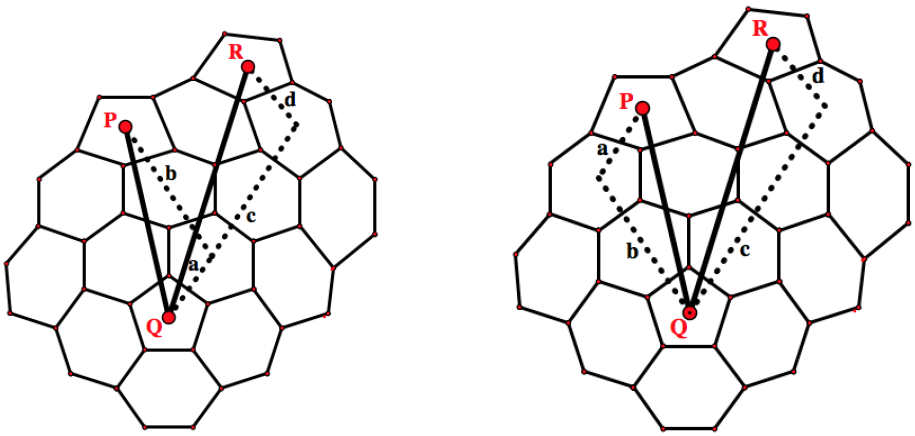
pentagons of $\Gamma$. Using the length formula, $|(p,q)| = p + q + \left|\frac{p-q}{p+q+1}\right|$, we assign weight to all of the edges in the auxiliary graph. The signature graph is the subgraph of the auxiliary graph that includes the edges that lie on some shortest spanning tree. We will often superimpose this signature graph onto the model of the fullerene. While the original auxiliary graph may not be planar, the signature graph always will be a plane graph. The *signature* of a fullerene is the labeled signature graph in which the edges are labeled with the coordinates, and angles between edges are labeled by the measure of the angles between adjacent segments. The signature uniquely determines the fullerene or corresponding geodesic dome, as is shown in [1] . Refer to the top left image in Figure 1.8 for an example of a signature. We denote the signature of a fullerene, $\Gamma$, to be $\mathscr{S}_\Gamma = (\Theta, \theta, c)$ in which $\Theta$ is the signature graph, $\theta$ is the function that represents the angle labels around each vertex and $c$ is the function that represents the coordinates of each segment.

From this point on we will simply use the graph theory length of segments $|(p,q)| = p + q$. The length formula,$|(p,q)| = p + q + \left|\frac{p-q}{p+q+1}\right|$, was needed to create a rigorous definition of the signature graph but for the remainder of our work the graph theory length will be sufficient.

A note that will be helpful in the following proof as well as many to come: when creating figures representing segments it is often useful to strategically choose which pentagon we choose as the initial pentagon so as to determine the correct side on which to construct the coordinate segments. When considering sets of more than two pentagons, it is often clearest in terms of visualization to construct the coordinate paths as a convex hull for the set. We defined the angle between two segments based on the choice that the common endpoint would be the initial pentagon for both coordinate paths. As such, when we sketch the set using coordinate paths that lie external to the set the angles appear to have been increased by 1. This was illustrated in Figure 1.3

for an angle of measure 1.

Our next lemma considers segments that have angles between them of measure 0 and how this affects the signature. In Figure 1.5 we see that for angles of measure 0, when the coordinate paths are drawn both emanating from pentagon $Q$ one set of coordinate paths coincide.




(A) Coordinate paths both on right side from Q

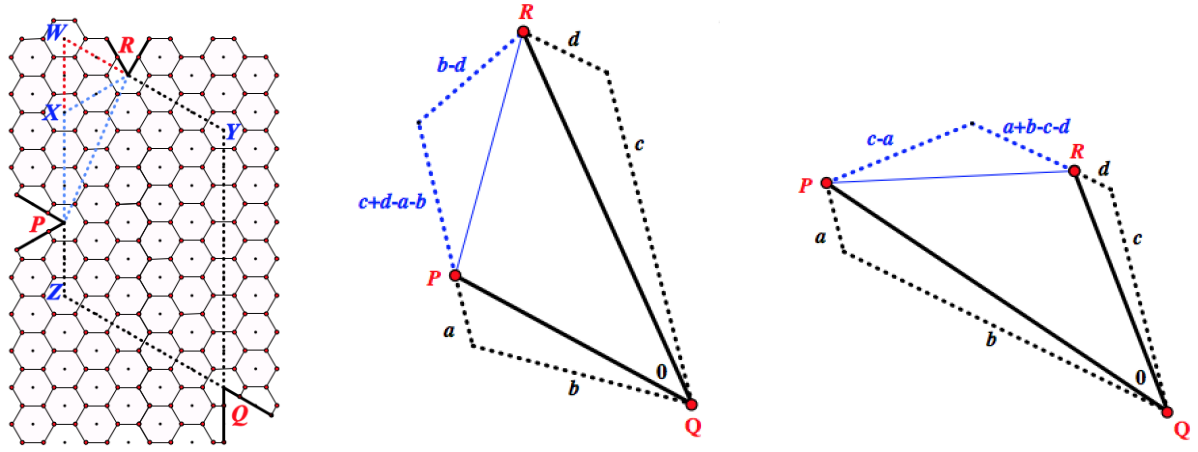
(B) Coordinate paths both on same side of string

FIGURE 1.5: Measuring Angle of Measure 0 from Coordinate Paths

**Lemma 1.1.2.** *Let $P, Q$ and $R$ be pentagonal faces in fullerene $\Gamma$ with signature $\mathscr{S}$. If angle $PQR$ has measure 0 then segment $RQ$ and segment $PQ$ cannot both be included in $\mathscr{S}$.*

*Proof.* Consider the triangular region formed by segments $PR$, $RQ$ and $PQ$. Let us say that segment $PQ$ has coordinates $(a, b)$ and segment $RQ$ has coordinates $(c, d)$. We first want to compute the coordinates of segment $PR$ in terms of $a, b, c$ and $d$. We have two distinct cases depending on whether segment $RQ$ or segment $PQ$ has greater length as shown in Figure 1.6.

Using the geometry of $\Lambda$, we easily compute the coordinates of segment $PR$. We illustrate this with a specific example as shown in Figure 1.6a. First note that $WYQZ$ is a parallelogram and $WXR$ is an equilateral triangle. The length of $WY$ is equal to




(A) Calculation Example (B) $c+d \geq a+b$ (C) $c+d < a+b$

FIGURE 1.6: Coordinates of non-included side across from angle of measure 0

the length of $ZQ$ which we know to be $b$ and the length of $RY$ is $d$, so we have that the length of $WR$ or equivalently $XR$ is $a-d$. Next consider that the length of $WZ$ is the equal to the length of $YQ$ which is $c$. The length of $WX$ is equal to the length of $XR$ which is $b-d$ and then length of $PZ$ is $a$. So $PX$ has length $c-a-(b-d) = c+d-a-b$.

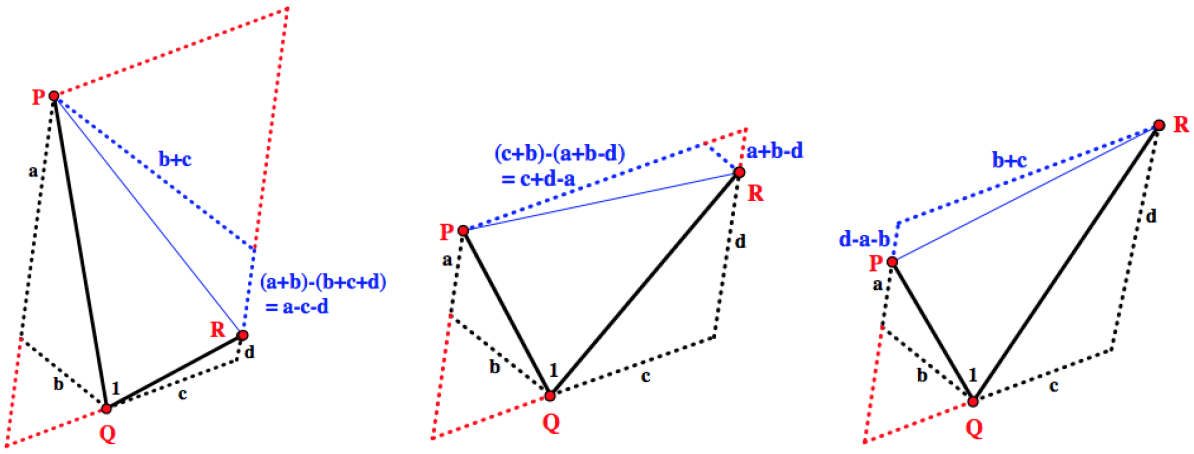
Thus in the case when $c+d \geq a+b$ as shown in Figure 1.6b we calculate that segment $PR$ has coordinates $(b-d,\ c+d-a-b)$ and hence we have length $c-a$. Notice that since segment $QR$ is in the signature, we have $c-a \geq c+d$ or equivalently $0 \geq a+d$ which is impossible.

Alternatively when $c+d < a+b$ as shown in Figure 1.6c, we similarly can compute that the length of segment $PR$ is $b-d$. In this case, consider that segment $PR$ must be longer than segment $PQ$ and hence $b-d \geq a+b$ or equivalently $0 \geq a+d$ which is again impossible. □

While it is possible for the signature graph of a fullerene to contain an angle of measure 1, the following lemma provides necessary conditions on the coordinates.

**Lemma 1.1.3.** *Let $P, Q$ and $R$ be pentagonal faces in fullerene $\Gamma$ with signature $\mathscr{S}$. If segment $PQ$ and segment $RQ$ given by coordinates $(a, b)$ and $(c, d)$ respectively are edges in $\mathscr{S}$ with angle $PQR$ having measure 1 then $c \geq a$ and $b \geq d$.*

*Proof.* We have two cases to consider. Namely when $d \geq a+b$ and when $d < a+b$. This second case breaks into two subcases: $d \leq a$ and $d > a$. All three cases are illustrated in Figure 1.7. The red dotted lines indicate the parallelogram and equilateral triangles used to compute the coordinates of segment $PR$ which is shown in blue.




(A) $a \geq d$ (B) $a + b \geq d$ and $d > a$ (C) $a + b \leq d$

FIGURE 1.7: Determining coordinates of segment opposite an angle of measure 1

If $a \geq d$, as shown in Figure 1.7a, we can use the parallelograms and equilateral triangles within the geometry of $\Lambda$ to easily compute that the coordinates of segment $PR$ are $(a - c - d, b + c)$. Thus the length of segment $PR$ is $a + b - d$. Since segment $PR$ is not included in signature we know it must have greater length than the lengths of either the segments $PQ$ or $QR$. Thus $a + b - d > a + b$ which is equivalent to $0 > d$ which is impossible since all coordinates have positive length. Thus, this case will never occur.

If $a < d$ but still with $a + b \geq d$ as shown in Figure 1.7b then segment $PR$ will have coordinates $(a + b - d, c + d - a)$ thus the segment will have length $b + c$. As above, it follows that $b + c \geq a + b$ since segment $PQ$ has length $a + b$ it follows directly that $c \geq a$. Segment $QS$ has length $c + d$ and hence $b + c \geq c + d$ so $b \geq d$.

Now when $d \geq a + b$ as shown in Figure 1.7c, we have the coordinates of $PR$ are $(b + c,\ d - a - b)$ and hence the $PR$ segment has length $c + d - a$. Since this segment is not included in the signature, it again must have length greater than segment $QR$ and hence $c + d - a \geq c + d$ or equivalently $a \leq 0$. This condition renders this case impossible. Hence we will never have a signature of this form when $d \geq a + b$.

Thus we have, for all possible cases, $c \geq a$ and $b \geq d$. □

Using the same calculations as shown in Figure 1.7 we can prove a related result about the angle measures between the segments connecting the three pentagons.

**Lemma 1.1.4.** *Let $P, Q$ and $R$ be pentagonal faces in fullerene $\Gamma$ with signature $\mathscr{S}$. If segments $PQ$ and $QR$ are included in $\mathscr{S}$ and angle $\angle PQR$ has measure 1 then $\angle QRP$ and $\angle RPQ$ must also have measure 1.*

*Proof.* It follows directly from the proof of Lemma 1.1.3 that the only coordinate structure giving a viable signature is the one shown in Figure 1.7b. Thus by the coordinate computations shown in Figure 1.7 we can see that all the angles in a 3-set must have measure 1.

□

To create a *flat map* of the fullerene in $\Lambda$, we cut along the segments that correspond to one of the shortest spanning trees and unfold the fullerene. It was shown in [1] that fullerenes can be unfolded in this manner without any overlap. An example of such a flat map is shown in Figure 1.8 along with the corresponding shortest spanning tree and the signature graph.

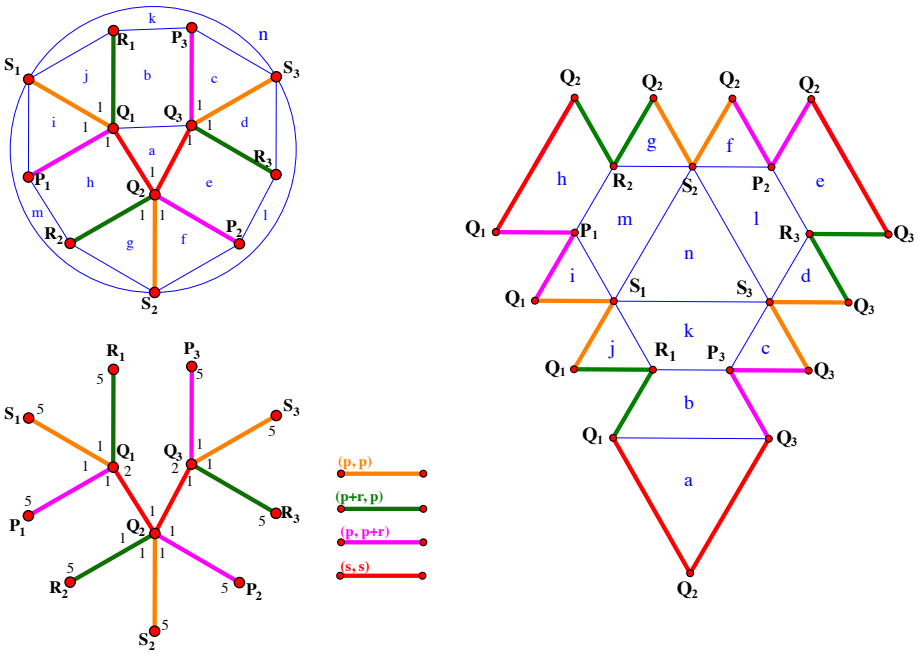



FIGURE 1.8: Arrowhead Fullerene Class. Top left: signature graph with auxiliary edges. Bottom left: signature graph of fullerene. Right: flat map of the fullerene.

Intuitively, we cut the fullerene along the spanning tree and flatten it out to the flat map. Hence, each edge of the tree will appear twice in the flat map corresponding to the edges of the flat map that are to be identified. Start cutting at $Q_2$ in the spanning tree shown in the upper left of Figure 1.8 and move to $Q_3$ with region $a$ on your left. Move on to $P_3$ with region $b$ on the left. At $P_3$ we have an angle of measure 5 so we move to the other side of the $P_3Q_3$ edge. Move along the other side of the edge with region $c$ on the left and we return to $Q_3$. We proceed in this way until the curve closes at $Q_1$. We now have the flat map shown in Figure 1.8. Now if we were to cut this flat map out of $\Lambda$ and make the identifications we would have a model of this fullerene.

### 1.1.3 Similarity

The signature gives us a unique representation for our fullerene. There are many important properties of fullerenes that are dependent on the parameters within the signature. In this subsection we show that, so long as we keep all these parameters in the same proportions, that the underlying structure of the fullerene will remain fixed.

Let $\Gamma_1$ and $\Gamma_2$ be two fullerenes and $\alpha \in \mathbb{Q}$. We say $\Gamma_1$ and $\Gamma_2$ are similar if the signature graphs are isomorphic with equal corresponding angles and the coordinates of the corresponding segments in the signature are proportional. More precisely, for every pair of corresponding segments, $(p_1, q_1)$ and $(p_2, q_2)$, we have $\frac{p_1}{p_2} = \frac{q_1}{q_2} = \alpha$, where $\alpha$ is the constant of proportionality. If the coordinates of the signature segments in a fullerene have no common divisors, then we say $\Gamma$ is *reduced.* Since all of the coordinates must be integers, it follows that all similar fullerenes are proportionally scaled versions of the reduced signature where the constant of proportionality is an integer. If we consider two non-reduced signatures, then the constant of proportionality can be a fixed rational constant, $\alpha$, given that scaling each coordinate by $\alpha$ yields integer coordinates. In Figure 1.9, we have taken the flat map of the reduced arrowhead fullerene with $p = s = 1$ and $r = 0$ (shown in black) and dilated its boundary by the factors of 2 (red) and 3 (blue). The center of the dilation is the red point in the center of the central hexagon.

Formally let $E$ be the euclidean plane and tessellate $E$ with hexagons to get $\Lambda$. Now let $X$ denote the set of all center points of the hexagons tessellating $E$. Let us set the unit length to be the fixed distance between centers of adjacent hexagons. Then our magnification constant $m \in \mathbb{Z}^+$ is a multiple of this unit length. We denote the dilation mapping that has magnification constant $m$ from origin $o \in X$ by $\delta_{o,m}$. If $f$ is a face in $\Lambda$ with center $r$, we adopt the convention that $\delta_{o,m}(f)$ is the face of $\Lambda$ with center $\delta_{o,m}(r)$.

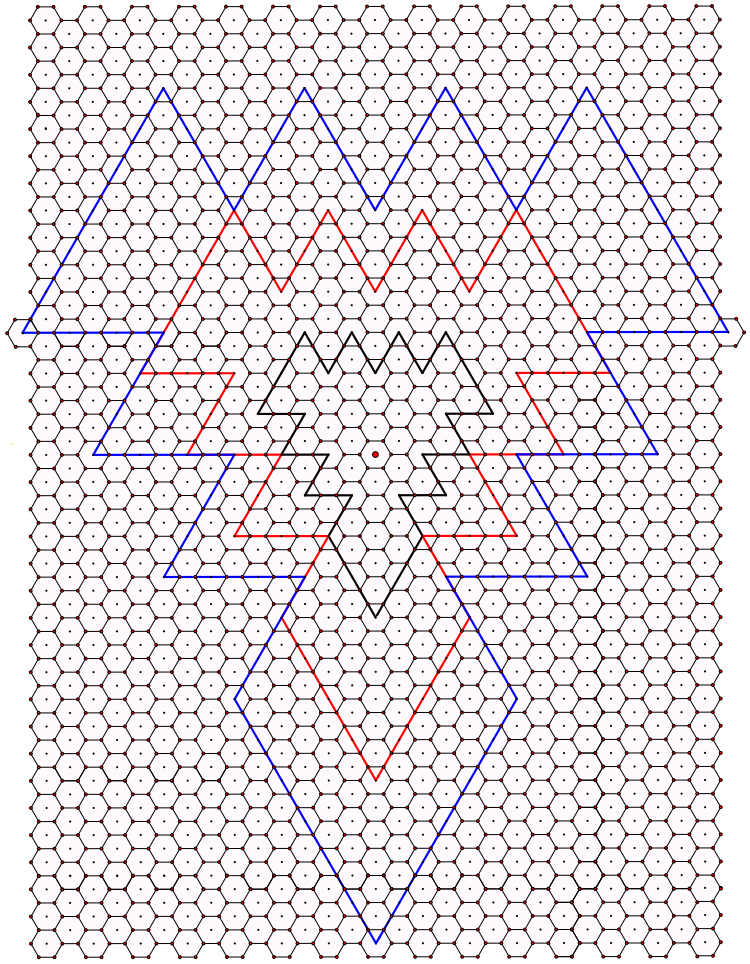


FIGURE 1.9: Dilating the flat map of arrowhead fullerene.

**Lemma 1.1.5.** *Let $o \in X$ be the center of a hexagon in $\Lambda$ and $m \in \mathbb{Z}^+$. $\delta_{o,m}(X) \subseteq X$ and, if $f$ and $g$ are hexagons joined by the segment with coordinates $(p, q)$, then the segment joining $\delta_{o,m}(f)$ and $\delta_{o,m}(g)$ has coordinates $(mp, mq)$.*

*Proof.* Consider the center, $r$, of an arbitrary face, $f$, in $\Lambda$. The segment connecting $o$ and $r$ has some coordinates $(p, q)$. $\delta_{o,m}(r) = r'$ for some $r' \in E$. By construction of the dilation we know that the segment connecting $o$ and $r'$ has coordinates $(mp, mq)$. As $ma$ and $mb$ are both integers then $(mp, mq)$ then $r' \in R$. Since we began with an

arbitrary face it follows that $\delta_{o,m}(X) \subseteq X$.

Now let $(p, q)$ be the coordinates of the segment that connects the centers of faces $f$ and $g$ and let $x$ be the center of the face at the turn of the coordinate path from $f$ to $g$. Now dilation with magnification $m$ maps any line segment with length $l$ onto a parallel line segment with length $ml$. Hence $\delta_{x,m}$ will map the coordinate path from $f$ to $g$ onto the coordinate path joining $\delta_{x,m}(f)$ to $\delta_{x,m}(g)$ and the length of the segments in this path will be $mp$ and $mq$. □

**Lemma 1.1.6.** *Let $o$ be the center of a hexagon in $\Lambda$. Dilating adjacent segments by an integer factor from $o$ yields adjacent segments with the same angle measure.*

*Proof.* Consider $\angle PQR$ and the coordinate paths of segments $QP$ and $QR$ starting to the right. The angle between the initial legs of these coordinate paths is preserved. Hence our fullerene angle measure is preserved. □

**Theorem 1.1.7.** *Let $\mathscr{S}$ be the signature of a reduced fullerene $\Gamma$. If all coordinates in $\mathscr{S}$ are multiplied by $m \in \mathbb{Z}$, then the resulting structure is the signature of a new fullerene, $m\Gamma$. Furthermore, the flat map of $m\Gamma$ is a scaled version of the flat map of $\Gamma$ so long as the flat maps are formed from corresponding spanning trees.*

*Proof.* Consider a spanning tree of $\Gamma$ with edge and angle labels. Scaling the spanning tree by multiplying all edge coordinates by $m$ yields a new labeled tree. We take a flat map of the original spanning tree, and using the two lemmas, we see that the image of the boundary of the flat map under dilation by $m$ corresponds to the dilated spanning tree. This shows that we do indeed have the flat map of a new fullerene $m\Gamma$.

□

### 1.1.4 Kekulé and Clar Structures

The graph theory model of a fullerene is trivalent corresponding to the three $\sigma$ bonds found in carbon molecules. However, carbon atoms actually have valence 4: three $\sigma$ bonds and a fourth $\pi$ bond. The $\pi$ bond at each atom is represented by doubling one of the edges leaving that vertex. There are many ways to select a perfect matching of the graph to represent the double bonds. In fullerenes, such perfect matchings are called *Kekulé structures*. It follows from Petersen's theorem [2] that every fullerene admits a Kekulé structure. We are interested in the hexagonal faces with three double bonds alternating around them and call these faces *benzene rings*. The maximum number of benzene rings over all Kekulé structures is called the *Fries number*. Of particular interest is the maximum number of independent (pairwise disjoint) benzene rings over all possible Kekulé structures. This number is the *Clar Number* of the fullerene and there is much indication that this number is directly related to the stability of the molecule as discussed in An Atlas of Fullerenes by P. W. Fowler and D. E. Manolopoulos [3] . We denote the Clar number $\gamma_\Gamma$ and the maximum number of independent benzene rings for a particular Kekulé structure, K, is $\gamma_\Gamma(K)$. Formally we define a *Clar Structure* to be $(C, A)$ where $C$ is a maximal set of independent benzene rings and $A$ is the set of Kekulé edges that do not bound any faces in $C$. A Clar structure that yields the Clar number is called a *maximum Clar Set*.

In general, we define a *patch* $\Pi = (V, E, F \cup \{f_0\})$ to be a plane graph such that all the vertices have degree 2 or 3 with all vertices of degree 2 lying on the boundary of the outside face $f_0$. In addition, we require that the boundary of $f_0$ is an elementary circuit. For convenience, we say that the faces of $\Pi$ are the internal faces F excluding $f_0$.

Any patch of the hexagonal tessellation admits a face 3-coloring which in turn yields an edge 3-coloring where each edge is colored with the color different from

the two colors of the two faces it bounds. This edge and face coloring is unique up to a permutation of the colors. We call this the *embedded coloring*. If you consider any face away from the boundary we see that the edge colors alternate around the perimeter.

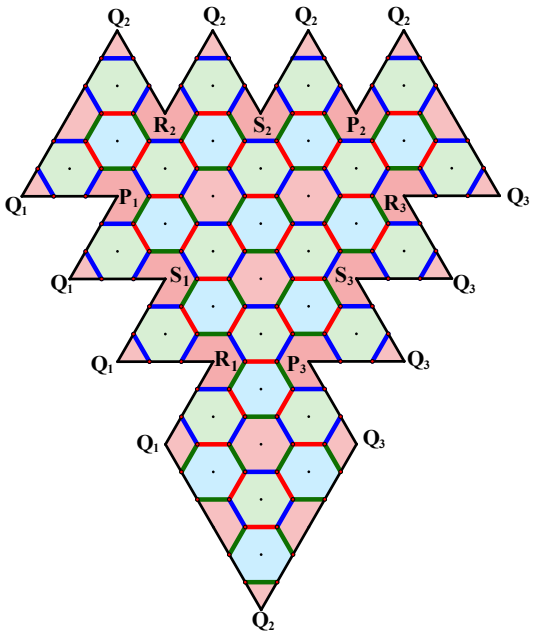



FIGURE 1.10: Embedded edge and face coloring of arrowhead fullerene

We extend this notion to the faces on the boundary and color their edges by extending and alternating the existing colors. For example, the edge between a red and a green face would be colored blue as illustrated in Figure 1.10. In general a flat map is not a patch since its boundary consists of segments that cut through the hexagonal faces. As a region in $\Lambda$ its faces and edges inherit this unique (up to permutation of colors) edge and face coloring of $\Lambda$. However, the coloring matches along some of the identified edges and not others.

We say a Kekulé structure is perfect in a region if there are the maximum number of benzene rings at each vertex, namely 2. The three embedded edge color classes each yield a distinct perfect Kekulé structure. To see this choose an edge color class to be the Kekulé structure, then the faces of the other two color classes form a set of benzene

rings of a Fries structure and the faces of either one of these color classes form the set of benzene rings of a Clar structure.

### 1.1.5 Clusters

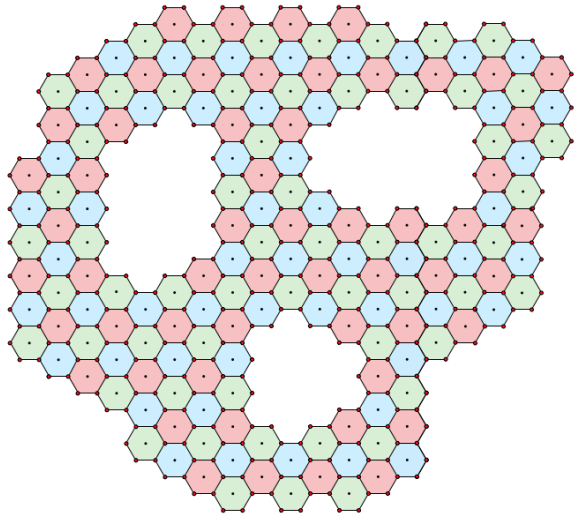


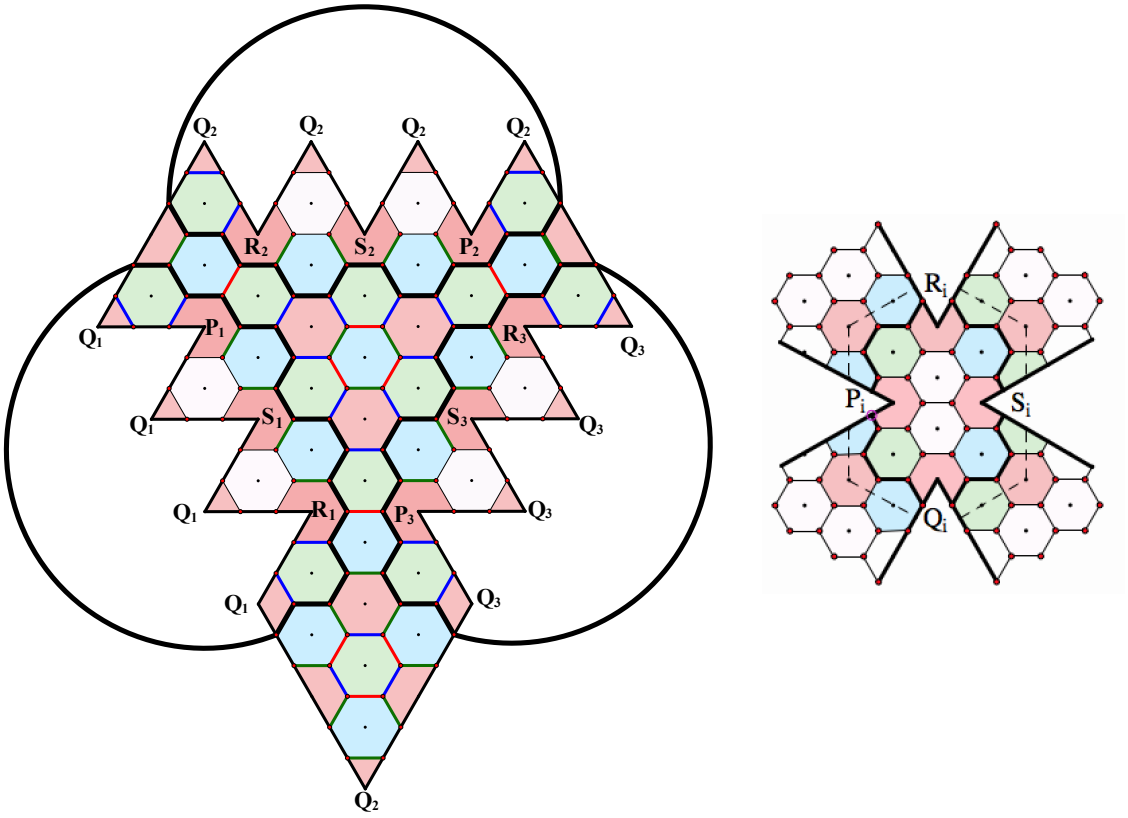
FIGURE 1.11: Ambient coloring around three removed clusters

A fullerene may be decomposed into *clusters* which we define to be sets of pentagons that when a set of faces of $\Gamma$ containing these pentagons is removed, we are left with a portion of the fullerene that can be perfectly 3-colored. We call the coloring outside these clusters the *ambient coloring*. Figure 1.11 shows a portion of $\Lambda$ with three clusters removed. This decomposition may not be unique and in that case we must consider each decomposition separately.

As removing clusters yields a perfectly colored portion of $\Lambda$, it must be that the Kekulé structure can extend throughout the faces we removed. As we will soon see, it follows that in order for this to hold, clusters must always contain an even number of pentagons.

Decomposition into six 2-clusters is well understood where an ambient coloring is fixed. However, up until this point, very little has been known about clusters of size

greater than two. The purpose of this thesis is to develop all the theory needed to completely understand 4-clusters.




(A) Ambient coloring with three 4-clusters removed

(B) Individual 4-cluster

FIGURE 1.12: Embedded edge and face coloring of arrowhead fullerene

If we consider the embedded coloring on the flat map shown in Figure 1.10, we see that in order for the ambient coloring to hold along the identified edges we may remove three 4-clusters as shown in Figure 1.12.

## 1.2 2-Clusters and Chains

For our purposes we want to choose regions of hexagons and pentagons from the flat map of the fullerene that are connected with no holes in which neighboring pentagons are on the boundary of $f_0$. Patches from the flat map can be embedded in the

hexagonal tessellation such that the centers of pentagons are centered on the centers of hexagonal faces in the tessellation with a $60^\circ$ wedge removed from the hexagon. Once embedded, the inherent 3-coloring of the tessellation gives a 3-coloring to the patch. This embedded coloring will not hold when the patch is removed from the embedding since we will necessarily have color incompatibilities around the pentagons. Thus it follows that there is no perfect 3-coloring of the entire fullerene which complicates finding the best Kekulé structures for a fullerene.

To see how the coloring is altered when we remove our patch from the tessellation, we select an edge-face 3-coloring for a patch and begin expanding the coloring throughout the entire fullerene. As the expansion wraps around a pentagon, we are forced to assign two adjacent faces the same color since there are an odd number of faces surrounding the pentagon. The edge between two adjacent faces of the same color leads to another face. Since this face already has two surrounding faces of incompatible color then either this face is a pentagon or there will be another pair of incompatible pentagons and thus these will lead to another edge and so on. This is illustrated in Figure 1.13. Hence, the incompatibility in coloring continues out from the pentagon along an alternating sequence of faces and edges which we call a *chain* starting with the pentagon and all face color incompatibilities occur at the edges of the chain. As long as all turns are sharp, the color of incompatibility remains the same. For the purpose of constructing Clar structure we restrict our attention to chains with one *color of incompatibility.* As we extend the face coloring throughout the fullerene, the chain continues to extend and only terminates in another pentagon. It is worth noting that chains are neither paths in the fullerene nor paths in the dual even though their structure behaves similarly to that of paths.

As an example of this coloring, the pentagon in the figure is colored red, hence the edges and other faces of the chain are also red. Blue and green face surround the red

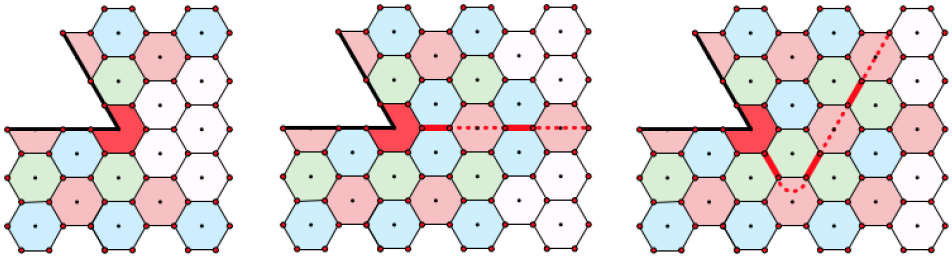


FIGURE 1.13: Building a chain from a pentagon.

pentagon so the direction in which the chain leaves the pentagon dictates whether the color of incompatibility is green or blue. Expanding the color throughout the fullerene results in a face 3-coloring where the incompatibilities all occur along six disjoint *pairing chains* that pair the 12 pentagons. As all incompatibilities occur along chains, it follows that away from the chains we have a proper edge-face 3-coloring.

Let $\Gamma = (V, E, F)$ be a fullerene and let $K$ denote any Kekulé structure. For any face $f$, an edge $e$ in $K$ is said to *exit* $f$ if it has exactly one endpoint on the boundary of $f$. Chains were first introduced in [4] and, formally, we define a chain as follows:

**Definition 1.2.1.** *A chain is an alternating sequence of faces and edges in* $\Gamma$, $\{f_0, e_1, f_1, \ldots, e_n, f_n\}$ *such that:*

1. *for all* $i$, $e_i$ *has exactly one endpoint in* $f_{i-1}$, *while the other endpoint is in* $f_i$;
2. *if* $f_i$ *is a hexagon, the endpoints of* $e_i$ *and* $e_{i+1}$ *are either opposite or adjacent around the boundary of* $f_i$;
3. *either* $f_n \neq f_0$ *which are two pentagons and all other faces are distinct hexagons in which case we say the chain is an open chain or* $f_0 = f_n$, *and all other faces on the chain are distinct hexagons in which case we say the chain is a closed chain.*

We now extend upon the properties of chains worked out in [5]. Consider two edges $e_i$ and $e_{i+1}$ that both exit the face $f_i$. We say that the chain continues directly through hexagon $f_i$, if $e_i$ and $e_{i+1}$ exit via vertices of $f_i$ that the minimum path between

them has length three. We say that the chain makes a sharp turn if $e_i$ and $e_{i+1}$ exit from adjacent vertices on $f_i$. Furthermore we can indicate the direction of the turn. We say the chain makes a sharp right (left) turn if $e_{i+1}$ follows $e_i$ in a counterclockwise (clockwise) direction about $f_i$ as the chain sequence progresses from $e_i$ to $e_{i+1}$. We define the *length* of a chain to be the index $n$. This is equivalent to the number of edges in the chain which is usually a more practical way to compute length when working with actual fullerenes.

Given a Kekulé structure, let $C$ be a disjoint set of benzene faces and let $A$ be the set of edges in the Kekulé structure that are not bounding a face in $C$. Recall that the maximum value for $|C|$ over all Kekulé structures gives us $\gamma_\Gamma$. Away from the chain where we have perfect coloring we have perfect Clar sets of faces and there are no Clar faces in the immediate neighborhood of the chain. The number of faces that we lose from the Clar structure, $2|A|$, along the chains is called *Clar deficit* for that Clar Structure.

**Lemma 1.2.1.** *Let $K$ be a Kekulé structure for $\Gamma$, and let $\gamma_\Gamma(K)$ denote the size of the largest Clar set $C$ in $K$, then:*

$$\gamma_C(K) = \tfrac{1}{6}\left(|V| - 2\,|A|\right).$$

*Proof.* The faces in $C$ and the edges in $A$ cover every vertex exactly once. Hence, $6|C| + 2|A| = |V|$. Solving for $|C|$ yields the desired result. □

Thus using the notation of this previous lemma we have that:

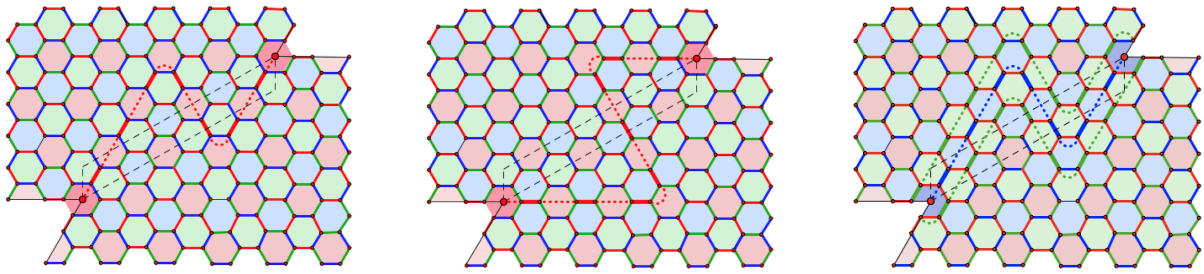
$$\gamma_\Gamma = \max_K \gamma_C(K)$$

Since we are trying to minimize the Clar deficit we will often choose to first try to pair the pentagons using the shortest chains possible as it is reasonable that these chains may contribute the least to the Clar deficit although this is not guaranteed to be

the case. Before we consider the shortest chain structures we first need to determine whether if it is possible for two pentagons to be paired by chains.

### 1.2.1 2-clusters

We start with the simplest possible case, namely when neighboring pentagons are isolated from other pentagons. For the time being, let us assume that there is a large patch of hexagons surrounding the pentagons such that there are no other pentagons near by. In the subsequent chapter we will develop tools to greatly reduce the necessary size of this patch. Using the embedded coloring we color the faces and edges. Now it is possible to join the pentagons by a *direct chain* contained completely within this patch if and only the two pentagons lie in the same color class in the embedded coloring. This happens exactly when the segment joining the pentagons has coordinates that are congruent modulo 3. In this case, the pentagons are said to be *chain available*. All chain available pentagons can be paired by three basic types of chains depending on which edge we choose to exit the initial pentagon. These three types of chains are illustrated in Figure 1.14. In this figure, the pentagons are chain available since the pentagons are connected by a segment with coordinates $(7, 1)$ which are congruent modulo 3.



(A) Type 1 (B) Type 2 (C) Type 3

FIGURE 1.14: Direct Chain types and their improper face 3-colorings

In Figure 1.14a the pentagons are paired with a *red-green chain*: the edges and faces of the chain are red and the improperly colored faces are green. We call it a *type 1* chain. Type 1 chains exit both pentagons within the parallelogram defined by its two coordinate paths. In Figure 1.14b we have a *red-blue chain* since the color of incompatibility is now blue. This is a *type 2* chain since it exits the paired pentagons outside of the coordinate parallelogram. Wrapping a chain in an addition chain as is shown in Figure 1.14c changes the primary color of the original type 1 chain. In this example, there is a green-blue chain surrounding the type 1 chain and so the red-green chain is converted to a blue-green chain. Nested pairs of chains such as these are said to be *type 3* chains.

In order to determine the way in which chains affect the Clar number. For each of the three chains in Figure 1.14 we can compute the contribution to $\delta_C(K)$ by doubling the length of the chain. We determine the color choices for the Kekulé structure and the Clar faces, by considering which color choices make sense for the fullerene as a whole. So we must consider all six possibilities.

If we choose the red edges as the edges in the Kekulé structure and the blue faces as the Clar faces then we we will use a type 1 chain since all blue faces are benzene rings and the edges that are not bounding a blue face are the 7 red edges on that chain. Therefore this chain contributes 7 to the Clar deficit and $\delta_C(K)$=14. We cannot choose a type 2 chain because in the immediate vicinity of this chain there are adjacent blue faces so the Clar faces would not be independent.

If again we choose the red edges as the Kekulé edges but instead choose the green faces to be the Clar faces then we must use a type 2 chain as the green faces in the type 1 chain are not independent. Thus we see that the 8 edges on the type 2 chain are the only Kekulé edges in this region that belong to the set $A$.

If the Kekulé structure consists of blue edges away from the paired pentagons and

the Clar faces are green, then again the 8 edges of the type 2 chain are the only Kekulé edges in this region that contribute to the set $A$.

Now if again the blue edges make up the Kekulé structure away from the chain and the red faces are chosen as the Clar faces, then we are forced to use the type 3 chain where the 7 edges on the blue pairing chain and 16 green edges on the encircling chain make up the contribution to $A$. Notice that whenever we must use Clar faces that are the same color as the primary color of the chain we must use a type 3 chain since the faces on the chain are not benzene rings. We wrap the chain in another chain so as to remove all Clar faces that are not benzene rings.

Finally, if we choose the green edges as the Kekulé edges and blue faces as the Clar faces then we will again use a type 1 chain which contributes 7 to the Clar deficit. Looking at the type 2 chains it is clear that the green edges do not form a perfect matching of region which discards the possibility of using a type 2 chain.

## 1.3 The Fullerene Project

Fullerenes can be organized into infinite classes that have similar arrangements of pentagonal faces. The Catalog of All Fullerenes with Ten or More Symmetries by J.E. Graver [6] outlines the infinite classes that possess especially high levels of symmetry. The Fullerene Project was a collaborative project started in 2016 involving undergraduates students, graduate students and faculty from Syracuse University, Massachusetts College of the Liberal Arts and the Graduate Workshop in Combinatorics that aimed to compute the Clar number for as many infinite class of fullerenes as possible. It was within the work of this project that we came to realize just how complex these calculations were and how much further theory was needed in our toolbox in order to tackle such problems.

Perhaps the simplest such class is that of the icosahedral fullerenes and so this was where the Fullerene Project began it's exploration. Icosahedral fullerenes are all obtained by constructing an equilateral triangle in the hexagonal tessellation with vertices at the centers of hexagons, cutting out 20 copies of this triangle and pasting them on the 20 faces of the icosahedron. Each such triangle can be identified by the coordinates of a segment corresponding to its side. This is illustrated in Figure 1.15. At every vertex of the icosahedron, five 60° wedges at the vertices of the triangle come together to form a pentagon and the sections of the hexagonal faces match along the edges.

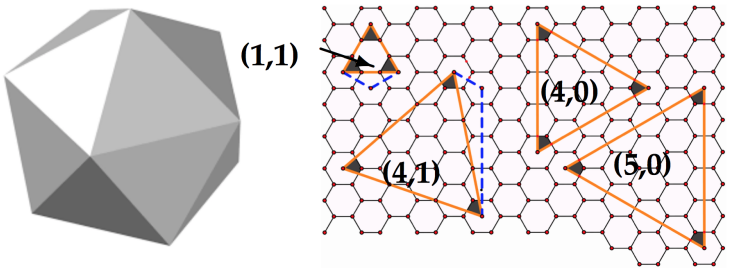



FIGURE 1.15: Icosahedral Fullerenes

Initially, we believed that such a simple fullerene would be an easy first case to solve before moving onto more complicated configurations. However, as work progressed it quickly became clear that the sheer number of possible chain configurations that needed to be checked was astronomical. Finding a reasonable lower bound was relatively easy using our existing results on direct chains. However, one of the most surprising results was the chain decomposition that gave this lower bound was not unique. In fact, many chain configurations of varying levels of complexity all resulted in the same Clar deficit.

We quickly realized that we simply did not have the tools to compute the chain length for chains that were intertwined. These chains wrapped around each other to create configurations that altered the primary colors of all chains involved. Thus we

had no way to confirm that there were no chain configurations that yielded a lesser deficit and the project came to a standstill.

Thinking that perhaps a case with a less symmetry would be more accessible, a research team at the Graduate Research Workshop in Combinatorics aimed to make progress on cuboctahedral fullerenes. However, after two weeks of delving deeply into the topic, we ran into the same road blocks as we did in the icosahedral case and very little progress was able to be made.

This thesis provides many of the initial tools necessary to begin actually having success computing the Clar number for infinite classes of fullerenes. As a natural next step we begin the study of 4-clusters; these structures prove to be much more complex than we ever predicted. By the conclusion of this work we will fully understand 4-clusters and use them to solve the first infinite class of fullerenes. Namely, we will compute the Clar number for the arrowhead fullerenes that we have used to illustrate the background concepts throughout this chapter, and these will be the first fully solved infinite classes of fullerenes.

# Chapter 2

# Wrap-Around Chains

## 2.1 Chain Length Equivalence Classes

When pairing the pentagons of a fullerene by chains we cannot always take the most direct path. Recall that as we defined the chain decomposition in Section 1.2, chains cannot cross one another. Hence, an existing chain structure can restrict a chain from taking the most direct route to the final pentagon. Clearly the minimal chain length will be different if a path must be taken that travels around other pentagons. Our first objective is to find the minimal chain lengths for all types of chains. To do so we consider them in two distinct cases. The first case considers direct chains where the chain can take the most direct route and need not wrap-around any intermediate pentagons. These were introduced in Section 1.2. In this section we study their structure in more detail. The second cases considers *wrap-around chains* where the chains must circumnavigate one or more intermediate pentagons in order to avoid crossing any chains.

### 2.1.1 Flipping Chains

If a chain makes no turns it is said to be a *straight chain*. In general though, the chains joining two pentagons may require sharp turns. At times it is simpler to consider

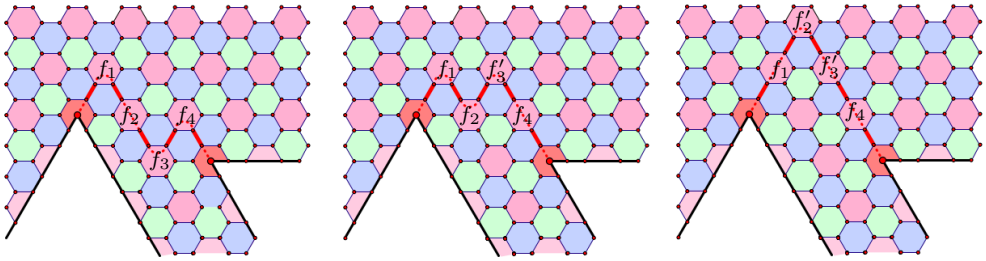



FIGURE 2.1: The chain in left image has been flipped twice to yield the chain on the right

chains with a minimal number of turns. So we use the action of *flipping* to reduce the numbers of sharp turns while still maintaining the length and color of incompatibility of the original chain. For the initial discussion of chains, we will assume that there are no additional pentagons in the vicinity of the two pentagons we wish to connect by a chain. In this way, we can be sure that as we are flipping our chains there will be no interference by additional pentagons. After developing this initial theory we will extend our notions to the more general situation when there may be nearby pentagons that we must consider.

We consider the chain $\{f_0, e_1, f_1, e_2, \ldots, e_n, f_n\}$ as one to be flipped. If $\{f_{i-1}, e_i, f_i, e_{i+1}, f_{i+1}\}$ is a portion of the chain which forms a parallelogram with $\{f_{i-1}, e_i', f_i', e_{i+1}', f_{i+1}\}$ where the sharp angles are at $f_i$ and $f_i'$ then

$$\{f_0, e_1, f_1, e_2, \ldots, f_{i-1}, e_i', f_i', e_{i+1}', f_{i+1}, \ldots, f_{n-1}e_n, f_n\}$$

is the flipped chain. See Figure 2.1. For every single flipping action we have an *inverse* flip that reverses a step. So if we begin with the chain segment $\{f_{i-1}, e_i', f_i', e_{i+1}', f_{i+1}\}$ then the image of the inverse flip is the chain segment $\{f_{i-1}, e_i, f_i, e_{i+1}, f_{i+1}\}$.

A chain with two consecutive right (left) turns can be *shortened* by constructing the chain that directly connects the face immediately before the first turn and the face directly after the second turn as long as there are no intervening pentagons to prevent

this. This is shown in Figure 2.2. Formally, consider the chain

$$\{f_0, e_1, f_1, e_2, \ldots, e_{i-1}, f_i, e_i, \ldots, e_{j-1}, f_j, e_j, \ldots, e_n, f_n\}$$

with sharp right (left) turns at both $f_i$ and at $f_j$ then we can shorten the chain to

$$\{f_0, e_1, f_1, e_2, \ldots, f_{i-1}, e'_{i-1}, f'_i, e'_i, \ldots, e'_{j-2}, f'_{j-2}, e'_{j-1}, \ldots, e'_{n-3}, f'_{n-3}\}$$

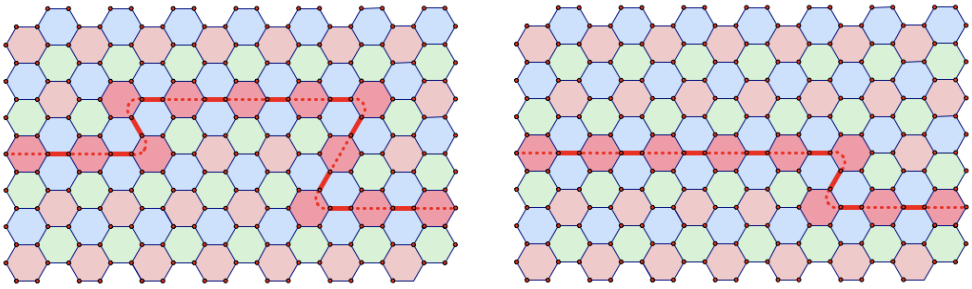


FIGURE 2.2: Shortening a chain with two consecutive right turns.

Shortening the chain in this manner shifts the indices by three and thus reduces the length of the chain by three. The shortened chain joins the original chain at the face originally labeled $f_{j+1}$; however, in the new labeling it is denoted $f_{j-2}$. Edges and faces that occur subsequently in the chain will all have indices reduced by three. Finally, it is worth noting that shortening the chain may yield a chain that still has consecutive right or left turns, in this case the process can be applied again. Each successive shortening of the chain will reduce the length by an additional three edges. A chain that consists of alternating left and right turns is said to be a *zig-zag chain*.

**Lemma 2.1.1.** *Fix two pentagons $P_1$ and $P_2$ and consider $\mathcal{C}$ to be the set of all $P_1 - P_2$ chains. The transitive closure of the flipping action is an equivalence relation on $\mathcal{C}$.*

*Proof.* Let $c_1$, $c_2$ and $c_3$ be three chains and let $c_i \sim c_j$ if and only if a finite sequence of flips starting at $c_i$ will lead to $c_j$ for $i, j \in \{1, 2, 3\}$.

The relation $\sim$ is reflexive since 0 flips yields $c_1 \sim c_1$.

The relation $\sim$ is a symmetric relation since if the inverse flips are performed in reverse order the original chain is retrieved.

Finally if $c_1 \sim c_2$ and $c_2 \sim c_3$ then $c_2$ can be achieved by flipping $c_1$ and $c_3$ can be achieved by a sequence of flips on $c_2$. Thus starting with $c_1$ and concatenating the two sequences of flipping actions results in the chain $c_3$ which indicates that $c_1 \sim c_3$ and the relation is transitive. As such, $\sim$ is an equivalence relation. □

**Lemma 2.1.2.** *Any zig-zag chain is equivalent to a chain with only one sharp turn.*

*Proof.* Consider a chain $\{f_0, e_1, f_1, e_2, \ldots, e_n, f_n\}$. Let $g_0 = f_0, g_1, g_2, \ldots, g_k = f_n$ be the set of initial and terminal faces as well as all faces in the chain where a turn occurs. Let $l_1, l_2, \ldots, l_{k-1}$ be the lengths of the straight chains such that $l_i$ for $i \in \{0, 1, \ldots, k-1\}$ is the length of the chain segment between $g_i$ and $g_{i+1}$. Let $T_i$ denote the turn at face $g_i$. If $k = 1$, and thus our chain only has one sharp turn, then we are done. If there is more than one consider $T_i$

If $T_i$ is a left hand turn then we flip the chain portion containing $T_i$ with $l_{i-1}$ left flips. This will yield a chain where the flipped portion of original chain is flush with the portion of chain entering the previous turn as is shown in the top right image in Figure 2.3. Now the $l_{i-2}$ will gain one in length as $l_i$ loses one in length and the length of $l_{i-1}$ remains fixed. We repeat this $l_i$ times so that $T_i$ has been replaced by a right hand turn.

If $T_i$ is not the first or last turn then there are two right turns on either side of $T_i$ which are eliminated as can be seen in the bottom right image in Figure 2.3. In the case where $T_i$ is the first or last turn in the chain then there is only one neighboring turn to eliminate and the edge leaving or entering respectively the pentagon is rotated left $120°$. In this way we see that any turn can be flipped away with a sequence of $l_{i-1} \cdot l_i$ flips.

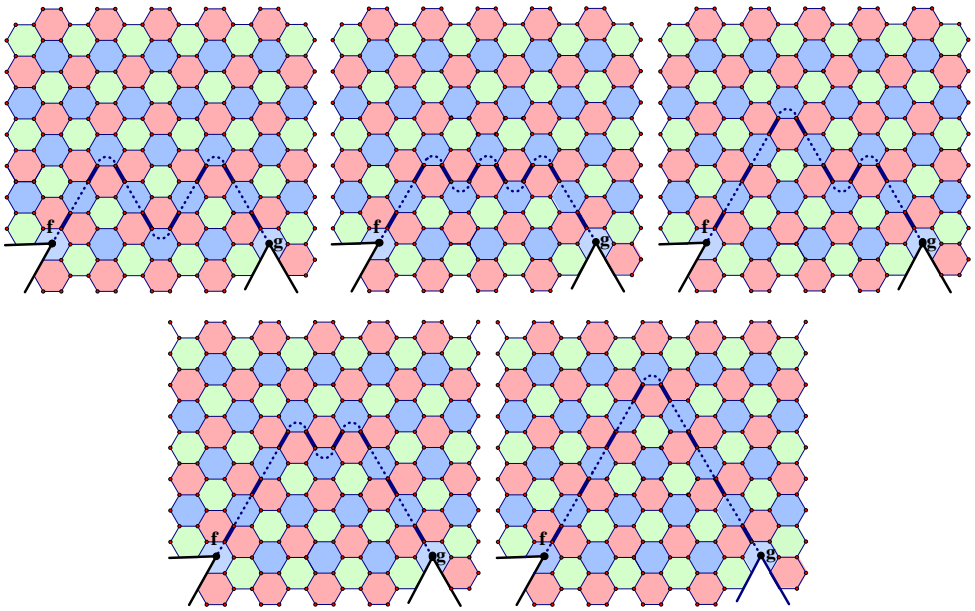



FIGURE 2.3: Flipping a zig-zag chain to a chain with a single turn

If we repeat this process and flip away all left hand turns then we will have a chain with one sharp right hand turn.

In the same manner we can flip away all right hand turns using right flips and $l_{i-1} \cdot l_i$ flips will flip the right hand turn and its two neighboring left hand turns (or a turn and a pentagon) into a single left hand turn.

□

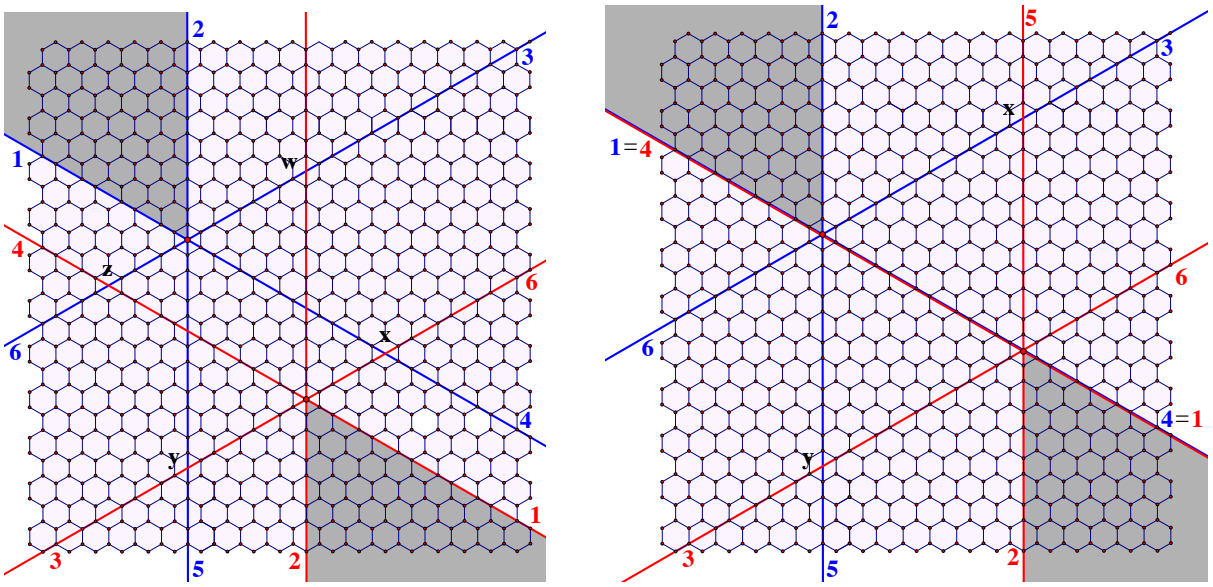
**Lemma 2.1.3.** *Equivalent chains are equivalent in length.*

*Proof.* Using the notation from the Lemma 2.1.2 we notice that each sequence of flips simply transfers chain length from $r_i$ to $r_{i-1}$ and from $l_i$ to $l_{i-1}$ and such neither $\Sigma_{i=1}^{n} r_i$ nor $\Sigma_{i=1}^{m} l_i$ changes. So the total chain length remains fixed. □

We now have that any zig-zag chain is equivalent to a chain with only one sharp turn. This gives us that there can be at most 5 chains with one sharp turn. One corresponding to each of the edges leaving the initial pentagon. Once we know which direction we exit the initial pentagon then the edge upon which the chain enters the

terminating pentagon is fixed since we will alway make a sharp turn towards the final pentagon. We now prove that only four of the five possible starting edges are possible.

**Lemma 2.1.4.** *There are at most four chains that have one turn connecting two pentagons in a fullerene.*




(A) Rays originating from pentagons (B) Two rays coincide

FIGURE 2.4: There exist at most four chains with a single sharp turn

*Proof.* Let $\Gamma$ be a fullerene and consider two chain-available pentagons in $\Gamma$. Consider the flat map of the $\Gamma$ embedded in the hexagonal tessellation. As each of the pentagons are represented by a hexagon, we can construct six "chain" rays each originating at the center of the face and extending through each of the six incident edges as in Figure 2.4a. If a red and blue ray intersect in a $60°$ angle, say at $x$, then the concatenation of the chain from the red pentagon to the hexagon at the intersection and the chain from this hexagon to the blue pentagon is a chain with a single sharp turn.

From each face there are two rays that never intersect the rays from the other pentagon. We identify these two rays at each hexagon so that the face becomes a pentagon and no zig-zag chain can exit along either of these rays.

So long as no rays coincide as in Figure 2.4a then we will have four points of intersection, $\{w, x, y, z\}$, and thus have four possible chains that contain exactly one sharp turn. In the case when two rays coincide as in Figure 2.4b we have two intersection points other than the overlapped rays and there is now an additional ray from each pentagon that does not intersect any others. In this case, namely when the coordinates of the segment connecting the pentagons are of the form $(p, p)$, we have two possible chains that have one sharp turn and one chain with no turns.

In all cases, there are no more than four chains connecting the two pentagons that have a single sharp turn. □

Just as we can flip a zig-zag chain in order to form a chain with only one sharp turn, we can also take a chain with one sharp turn and create an equivalent chain with many turns. In this way we can reduce the size of the patch containing the pair of pentagons and the chain connecting them. All equivalent chains will fall within the patches formed by the chain parallelograms shown in Figure 2.16 and we can make these patches even smaller by flipping them as close to the segment line as possible.

**Theorem 2.1.5.** *There are two equivalence classes of maximally shortened chains connecting pentagonal faces $P$ and $Q$ in the fullerene $\Gamma$. If the $P$ to $Q$ segment is given by coordinates $(p, q)$ then all the chains in one equivalence class have length $\max\{p, q\}$ and all the chains in the second class have length $p + q$.*

*Proof.* For any chain connecting $P$ and $Q$ we first shorten any double left or double right turns. We know by Lemma 2.1.4 that there are at most four chains that connect $P$ and $Q$ using exactly one sharp turn each. These chains form two parallelograms with pentagons on opposite obtuse corners. We will call them parallelogram 1 and parallelogram 2 as shown in Figure 2.5.

We know from Lemma 2.1.2 and Lemma 2.1.3 that if a zig-zag chain exits a pentagon along a side of a parallelogram then it will be equivalent to the chain that follows

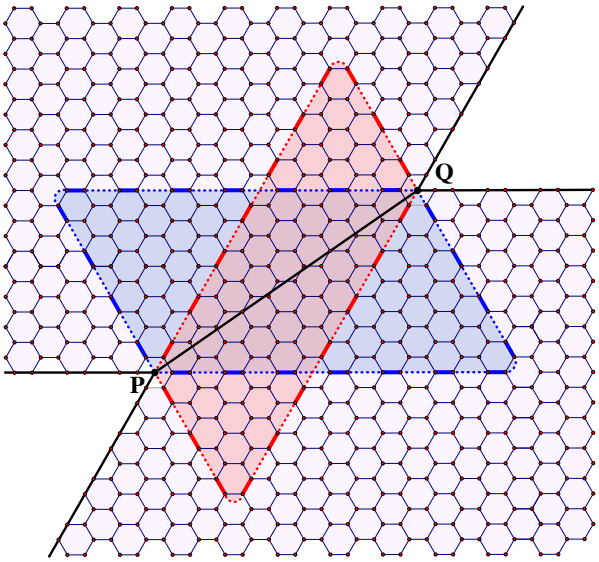
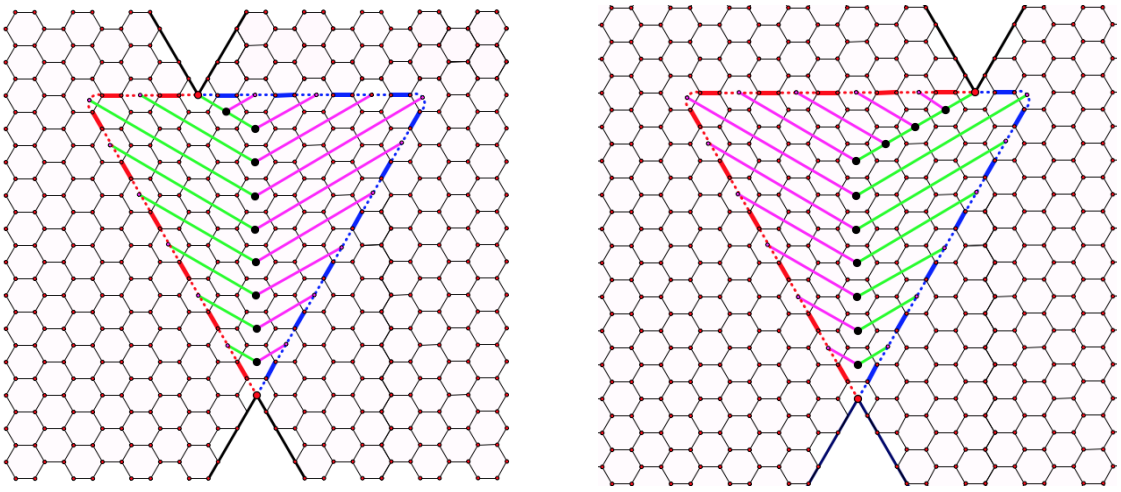



FIGURE 2.5: Parallelogram 1 is shown in red and Parallelogram 2 shown in blue.

the perimeter and thus will have the same length. It remains to show that the chains in parallelogram 1 correspond to chains of type 1 and have length $\max\{p, q\}$ and chains in parallelogram 2 correspond to chains of type 2 and have length $p + q$. In order to prove this, we construct a one-to-one correspondence between the faces in the chains making up the perimeter of the parallelograms and the faces in the coordinate paths.

We illustrate this bijection in the following way. To begin, we choose a pair of adjacent sides from each parallelogram that form an equilateral triangle. We choose the sides so that there is a pentagon on one vertex and the other pentagon is located on the opposite side. Beginning with the face that is the turning point in the coordinate path, we draw two segments joining this face with the center of a face on the chain forming the triangle. One segment coincides with the coordinate segment of minimum length and then we form the other by reflecting the first segment across the line coinciding with the coordinate segment of maximum length. Once we form the initial two segments, we use parallel segments originating from every face on the coordinate path as is shown in Figure 2.6.



(A) $p > q$ (B) $p < q$

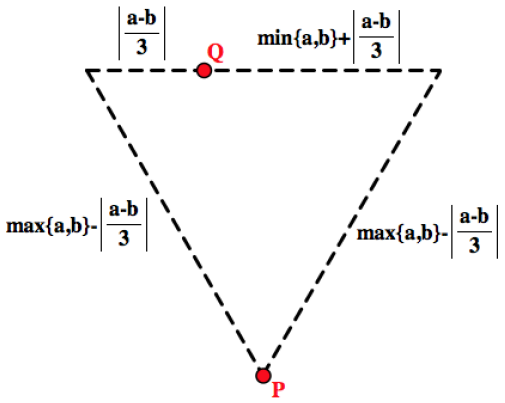
FIGURE 2.6: Finding chain lengths from the coordinate paths

This construction illustrates the one-to-one correspondence between faces on the coordinate path and faces on the type 2 chain shown using the pink segments in Figure 2.6. We have one more edge than hexagon on any chain but this additional edge is accounted for since there are $p + q - 1$ hexagons in a coordinate path. Hence chains of type 2 have length $p + q$. Similarly there is a bijection between faces on $\max\{p, q\}$ and the type 1 chain shown with the green segments in Figure 2.6. Therefore, any other zig-zag chain is equivalent to a chain of one of these two lengths. □

Further consideration of the equilateral triangles shown in Figure 2.6 leads us to an alternative argument as to why pentagons can be connected by a direct chain if and only if $p - q \equiv_3 0$. Take two chain-available pentagons and form the equilateral triangles as in Figure 2.6. The two sides leaving the initial pentagon both have length at most $p$ or equivalently the side length is $p - k$ where $k$ is a nonnegative integer less than $p$. This forces the third side to have length $q + 2k$. It follows that $p - k = q + 2k$ and solving for $k$ yields $k = \frac{p-q}{3}$. For $k$ to be an integer we must have that $p - q \equiv_3 0$. Conversely, if $p - q \equiv_3 0$ then $k$ will have integer length, and it will be possible to

construct chains as the boundary of the equilateral triangle. Thus we see that the pentagons are chain-available.

**Lemma 2.1.6.** *Let two pentagons, $P$ and $Q$, in a fullerene, $\Gamma$, be connected by a segment with coordinates $(a, b)$. Both types of direct chains can be constructed using at most two chain segments. The two chain segments in the type 1 chain have lengths $\max\{a, b\} - \left|\frac{a-b}{3}\right|$ and $\left|\frac{a-b}{3}\right|$. The type 2 chain has chain segments of length $\max\{a, b\} - \left|\frac{a-b}{3}\right|$ and $\min\{a, b\} + \left|\frac{a-b}{3}\right|$.*




*Proof.* The two chains with single sharp turns together form an equilateral triangle with a pentagon on one vertex and the other pentagon lying on the opposite side. As the type 1 chain has length $\max\{a, b\}$ the two chain segments leaving the initial pentagon both have length at most $\max\{a, b\}$ or equivalently the side length is $\max\{a, b\} - n$ where $n$ is a nonnegative integer less than $\max\{a, b\}$. Since the type 2 chain has length

$$a + b = \min\{a, b\} + \max\{a, b\}$$

We can compute the perimeter of the triangle in two ways. Either by considering the three sides of length $\max\{a, b\} - n$ or by summing the lengths of the two chains. This yields the following equality.

$$3\big[\max\{a, b\} - n\big] = \min\{a, b\} + \max\{a, b\} + \max\{a, b\}$$

In solving for $n$ we have $\max\{a,b\} - \min\{a,b\} = 3n$ or equivalently $n = \left|\frac{a-b}{3}\right|$. Notice that since the two pentagons are chain available, $n$ must be an integer and so we have $a - b \equiv_3 0$ and all chain segments have integer length. Thus the segments are in the proportions asserted in the lemma. □

We will now drop our assumption that there are no additional pentagons that interfere with any of chains within our equivalence classes of zig-zag chains. Without this assumption it may no longer be possible for every chain to be equivalent to a chain with a single sharp turn. Thus, the number of chains in an equivalence class may change depending on what pentagons lie in the vicinity. However, the number of equivalence classes will remain at two regardless.

## 2.2 The Length of U-Chains

Now we extend our consideration to chain-available pentagons $P$ and $R$ which cannot be paired by a direct chain. However, we assume that $P$ and $R$ can be paired by a chain that wraps around an intermediate pentagon $Q$. We call such a chain that wraps around a single intermediate pentagon a *u-chain*. Now we will not always be able to fully shorten our chains to be zig-zag chains. In fact, there will be times when we will extend our chains so that they reach around pentagon $Q$.

When we embed patches in the tessellation we inherit a perfect coloring for the patch and even though the coloring doesn't remain proper when removed from the embedding, it can still give us valuable information about the structure of the fullerene. Once the patch is embedded we can make computations in the tessellation rather than restricting ourselves to the hexagons in the flat map. Most importantly, the coordinates and corresponding segment lengths can be computed through wedges that would normally be removed when unfolding the fullerene into a flat map.

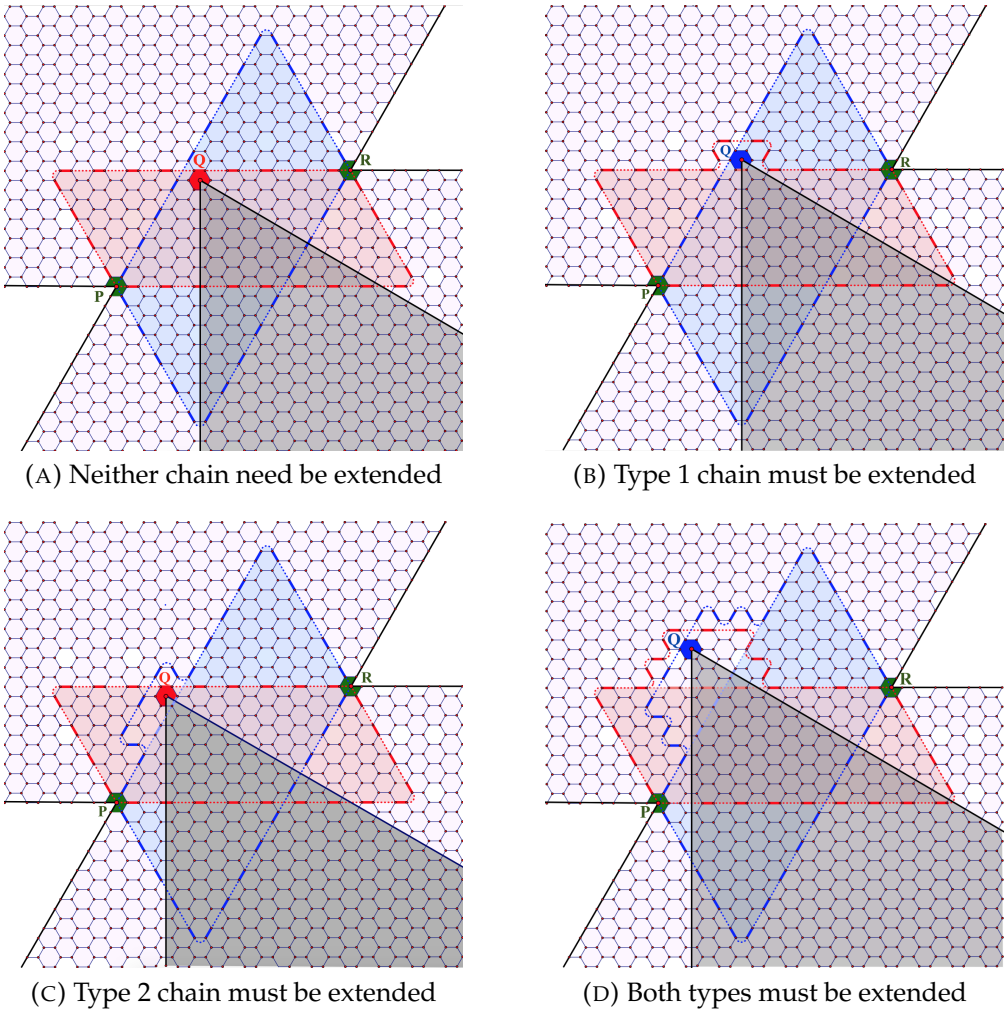
**Theorem 2.2.1.** *Consider a patch from the fullerene, $\Gamma$, and let $P$ and $Q$ in $\Gamma$ be two pentagons. If $P$ and $Q$ have the same color in the embedded coloring then the two pentagons can be connected by a chain entirely in the patch. Additionally, this occurs if and only if the coordinates, when computed in the embedding, are congruent modulo 3.*

*Proof.* We know that pentagons can be connected by chain if and only if the coordinates of the segment joining them in the tessellation are congruent modulo 3 or equivalently if and only if they are assigned the same color when embedded. Thus by embedding patches of a fullerene in the tessellation, we can see whether or not the inherited colors of the pentagons are the same and whether or not they can be connected by a chain in $\Lambda$. Now any chain in $\Lambda$ can be altered by inserting consecutive right (left) turns until the possibly lengthened chain lies entirely in the patch. □

To find the length of u-chains we consider the flat map of a fullerene embedded in the tessellation. We then construct the two parallelograms as we did in the case of direct chains. However, this time since the patches have been embedded in $\Lambda$, the parallelograms are formed across the wedges to be deleted.

In Figure 2.7, $P$ and $R$ are assigned to be green faces and so a u-chain joining them will have primary color green. The color of the parallelograms indicates the secondary color of the u-chain for chains exiting $P$ and $R$ along the edges of those parallelograms. If pentagon $Q$ lies inside the red parallelogram then some of the direct green-red chains from $P$ to $R$ will lie in this patch.

If the intermediate pentagon lies inside both parallelograms then there will be direct chains of both types joining $P$ and $R$ as shown in Figure 2.7a. If the intermediate pentagon lies inside one parallelogram and outside another then the length of the minimal chain leaving by one of those edges remains the same length as for direct chains and the other minimal chain will have to be extended to wrap-around the intermediate pentagon as shown Figure 2.7b and 2.7c. Finally if the the intermediate pentagon




(A) Neither chain need be extended

(B) Type 1 chain must be extended

(C) Type 2 chain must be extended

(D) Both types must be extended

FIGURE 2.7: The placement of intermediate pentagon dictates which chains need to be extended

is outside both parallelograms and the associated wedge crosses both parallelograms then each of the minimal chains will have to be extended as in Figure 2.7d.

In cases where we must extend the chain beyond the boundary of the parallelogram we push the chain away from the parallelogram boundary by adding consecutive left (right) turns. Shortening chains reduced the chain length by 3, and similarly each extension of the chain increases the length by 3. Considering Figure 2.7, we see that in Figure 2.7b, the chain with secondary color red has been extended once and the chain with secondary color blue not need be extended at all. Where as in Figure 2.7d

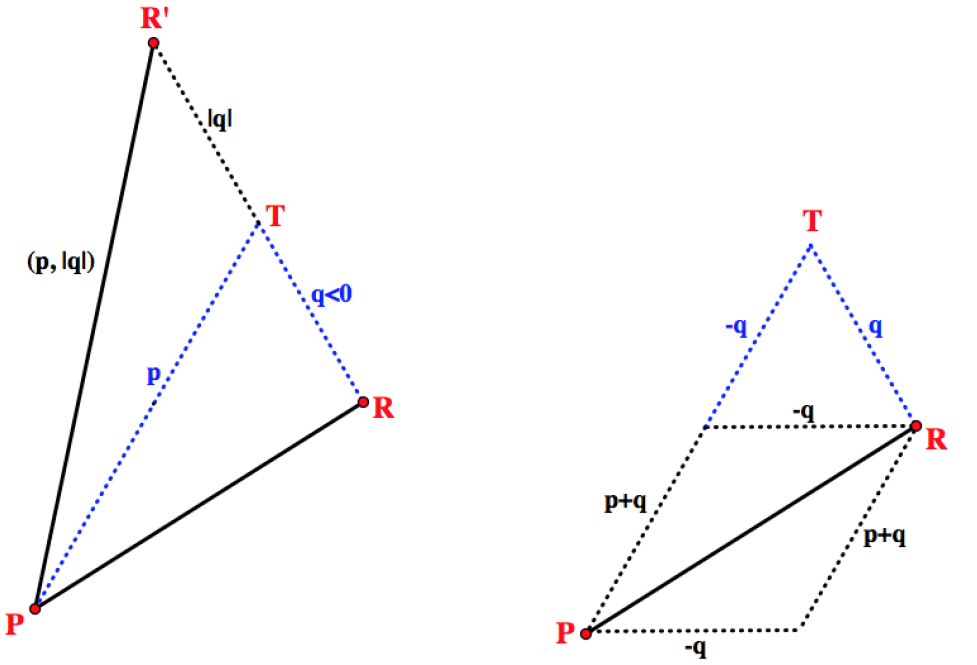
the chains with secondary color blue and red both required two extensions in order for the chain to wrap-around.

As we work towards a closed formula for the length of a u-chain, let us use consistent labeling for clarity of explanation. We name the pentagons on terminal ends of the u-chain $P$ and $R$ such that the chain is wrapping around pentagon $Q$. We say the intermediate $PQ$ and $QR$ segments have coordinates $(a, b)$ and $(c, d)$ respectively and furthermore the segment that travels through the wedge connecting the two paired pentagons $P$ and $R$ has coordinates $(p, q)$. $(a, b)$ and $(c, d)$ are the coordinates we know from $\Gamma$ and we need to compute the coordinates $(p, q)$ in $\Lambda$ from them. Lastly we denote the angle between the two intermediate segments by $\angle Q$. The base length of this $PR$ u-chain is computed from the coordinates $(p, q)$ in addition to any necessary extensions when $Q$ lies outside a parallelogram. The coordinates $(p, q)$ and the length of any required extensions will be dependent on the coordinates $(a, b)$ and $(c, d)$.

When computing the coordinates between two faces, $P$ and $R$, in $\Lambda$, we are striving to find two positive coordinates which, when formed at a geometric angle of 120°, connects faces $P$ and $R$. There are times in which our computations yield a coordinate with negative value indicating that the second coordinate is formed in the opposite direction and thus the angle between the two coordinate segments has geometric measure 60° rather than 120°. The following lemma will allow us to compute the actual coordinates from the calculated ones even when one value is negative.

**Lemma 2.2.2.** *Let $P$ and $R$ be faces in $\Lambda$ such that segment $PR$ has calculated coordinates $(p, q)$. If $q < 0$ then the coordinates for the segment are $(-q, p + q)$. Similarly if $p < 0$ the coordinates of the segment joing $P$ and $R$ have coordinates $(p + q, -p)$*

*Proof.* Let segment $PR$ have calculated coordinates $(p, q)$. If $q < 0$ then the orientation of the coordinate segment $q$ is reversed as shown in Figure 2.8a. The positive coordinates $(p, |q|)$ take us to $R'$ with a 120° left turn at $T$. Instead, with $q < 0$ we take a




(A) Positive vs negative $q$ (B) Constructing corrected coordinates

FIGURE 2.8: Correcting for negative coordinate

sharp right turn at $T$ to $R$. As coordinates are defined to be positive we rotate segment $TR$ 60° about $R$ so that it intersects segment $PT$ at an angle of 120°. The new segment satisfies the definition of coordinates and thus the coordinates of segment $PR$ are $(-q, p+q)$ as can be seen in Figure 2.8b.

The case when $p < 0$ is proved similarly. □

Now we return to our wrap-around problem pictured in Figure 2.7. Once we have determined the embedded coordinates of segment $PR$, we must determine whether or not a given chain must be extended to wrap-around $Q$. We know we have two equivalence classes for chains and that a chain must be extended if the intermediate pentagon lies outside the parallelograms joining $P$ and $R$ as shown in Figure 2.16. Hence, we now must find conditions on whether pentagon $Q$ lies inside or outside the red, or alternatively blue, parallelogram. Keep in mind that the color of the parallelogram need not only represent chains of a single type but rather indicate the secondary color

of the chain. In particular, if $p > q$ the blue parallelogram reflects type 1 chains and blue as the secondary color, however when $p \leq q$ the red parallelogram indicates type 1 chains and red is their secondary color.

The measure of $\angle Q$ determines the orientation of the coordinate segments $(a, b)$ and $(c, d)$ and forces pentagons $R$ to be within specific regions in respect to the location of pentagons $P$ and $Q$. Thus, the conditions that dictate when $Q$ lies within the parallelograms change based on the measure of $\angle Q$. These regions are shown in Figure 2.9.

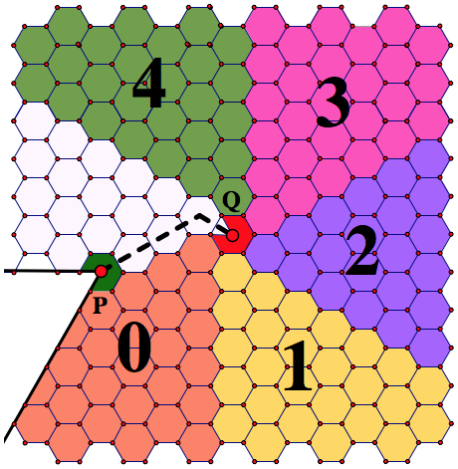
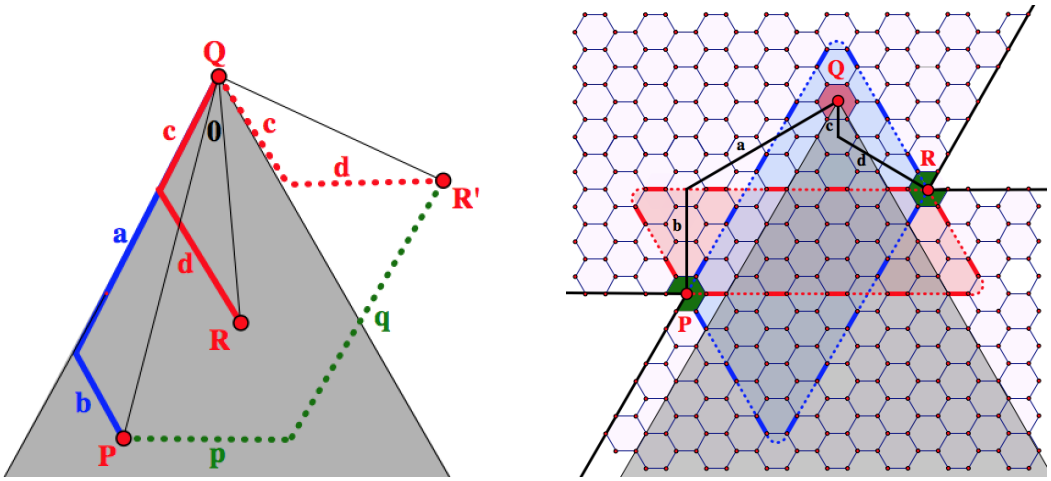



FIGURE 2.9: Regions representing location of $R$ for angles of different measures

The orange faces represent the possible locations on the fullerene of $R$ when $\angle Q = 0$ after $(c, d)$ has been rotated 60° to accommodate the open wedge from $Q$ counterclockwise from $P$. If $\angle Q = 1$, $\angle Q = 2$, $\angle Q = 3$ or $\angle Q = 4$ then $R$ lies in the yellow, purple, pink or green regions. Closing the wedge at $Q$, we see that $R$ in region 4 is the same as the case as $R$ in region 0–interchanging the role of $P$ and $R$. Similarly pentagon $R$ in region 3 is the same as the case $R$ in region 1. Thus we only need to consider cases in which $R$ lies within regions 0, 1 or 2.




(A) $\angle Q = 0$ on the fullerene (B) $\angle Q = 0$ in the tessellation

FIGURE 2.10: Determining chain length for u-chain around $Q$ when $\angle Q = 0$

Let us begin with the case in which $\angle Q = 0$ illustrated in Figure 2.10. In order to find the embedded coordinates $(p, q)$, we rotate segment $(c, d)$, 60° to $R'$ in $\Lambda$ and then compute the coordinates of segment $PR'$. Since this rotation comes from inserting a 60° wedge it does not matter whether we choose to rotate $R$ counterclockwise or alternatively we could rotate $P$ to some face $P'$ with a clockwise rotation. In either case we have expanded a 60° wedge at $Q$ and thus the new angle, which in either case we can call $PQR'$, has measure 1.

Since, with angle of measure 0, the coordinates lie along same initial path of faces, we always choose to rotate the point $P$ or $R$, whichever is larger, $a+b$ or $c+d$, so that we get a similar configuration shown in Figure 2.10b. Hence we assume that $a + b \geq c + d$. By considering parallel segments and the underlying geometry that is shown in Figure 2.10a we see that $(p, q)$ has the following coordinates.

$$(p, q) = \left\{ \begin{array}{lll} (c + d - b,\ a + b - c), & \text{for} & b < c + d \\ (a + d,\ b - c + d), & \text{for} & b \geq c + d \end{array} \right\}$$

As we have already justified Figure 2.10, whenever $a \geq b$, $Q$ will lie within the blue parallelogram in Figure 2.10b. When $a < b$ the chains with secondary color blue will have to be extended. Since both the coordinate path $c$ and $d$ travel in orientations away from the red parallelogram we see that there is no way for $Q$ to lie in the red parallelogram. As such a chain with red as the secondary color must be extended for any value of $c$ and $d$.

In Section 2.1.1 we considered the case where we could shorten a chain by removing two consecutive right (left) turns. We now wish to reverse this process and lengthen a chain to wrap-around a given face.

**Lemma 2.2.3.** *Given a chain $C$ and a face $Q$ not on the chain, we can extend the chain to wrap-around $Q$. If $P$ is on the chain with segment $PQ$ having coordinates $(a, b)$ where neither of the coordinate paths are perpendicular to the chain as pictured in Figure 2.11 then the shortest wrap-around chain is $3\lceil\frac{b-a}{3}\rceil$ longer than $C$. If $R$ is on the chain with segment $QR$ having coordinates $(c, d)$ where the $c$ coordinate path is perpendicular to the chain as pictured in Figure 2.11 then the shortest wrap-around chain is $3\lceil c + \frac{d-c}{3}\rceil$ longer than $C$.*

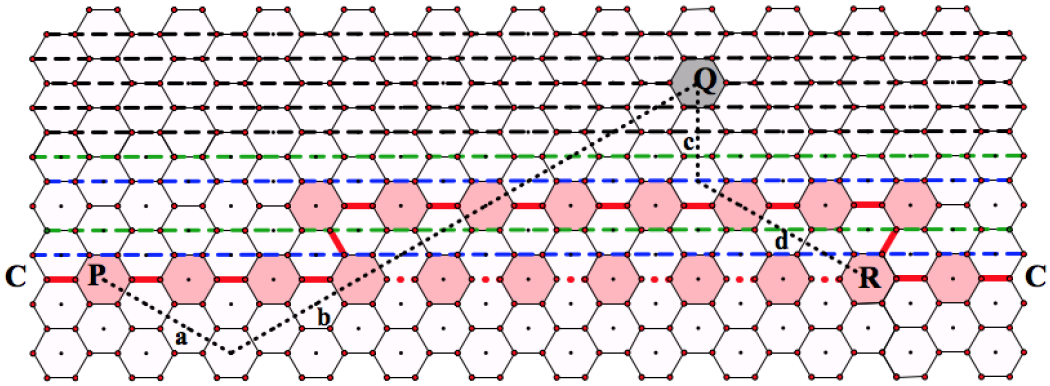



FIGURE 2.11: Extending chain $C$ around face $Q$

*Proof.* We have included all possible parallel chains between chain $C$ and pentagon $Q$. These chains are represented by the dashed lines in Figure 2.11. Assuming that the

secondary color of $C$ is blue, then the first chain level above $C$ is blue, the second level green, the third level red and the levels continue cyclically red, blue, green as we move toward $Q$.

Any wrap-around chain must move up a multiple of three levels in order to stay in the same color class as $C$. In the figure, we illustrate extending the chain up three levels (the minimum possible) and see that the chain length is extended by three. If we extend the chain up another three levels the chain length will be extended by an additional three. Furthermore, we see that the length of the extended chain is increased by the number of levels we have to move up.

Coordinate paths of length $x$ perpendicular to the chain cross $2x$ levels; coordinate paths of length $x$ oblique to the chain cross $x$ levels. In our figure we see that coordinate path $c$ is perpendicular to chain $C$ while $a, b$ and $d$ are all oblique to chain $C$.

From $P$ to $Q$, we go down $a$ levels and then up $b$ levels to a net increase of $b - a$ levels. On the other hand, from $Q$ to $R$ we go down $2c$ levels and then down another $d$ levels for a total of $2c + d$ levels.

If $n$ is any positive integer, then the smallest multiple of 3 greater than or equal to $n$ is $3\lceil \frac{n}{3} \rceil$. So the minimum increases that bring us beyond the chain level including face $Q$ are $3\lceil \frac{b-a}{3} \rceil$ and $3\lceil \frac{2c+d}{3} \rceil$ =$3\lceil c + \frac{d-c}{3} \rceil$ □

This lemma allows us to compute the following formula table for the $PR$ u-chains when wrapping around $Q$ such that $\angle Q = 0$.

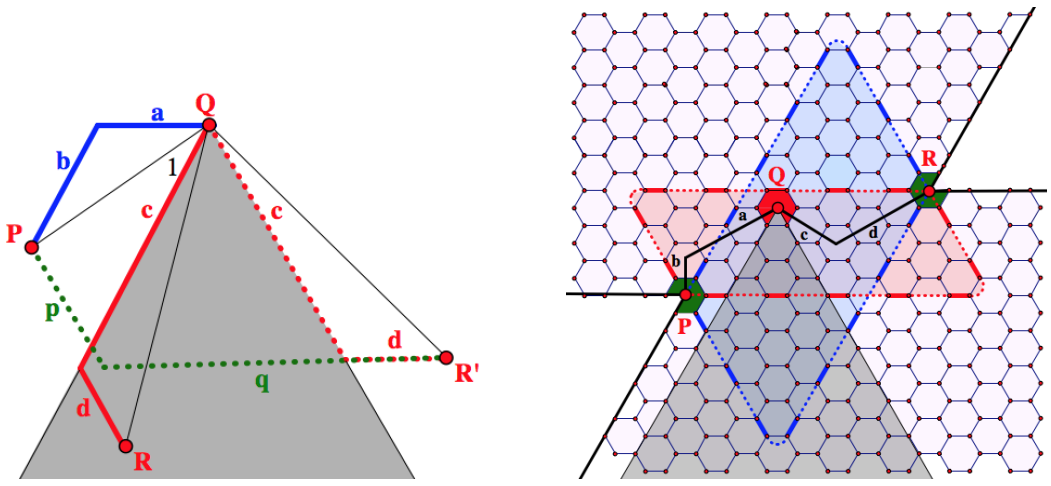
We will divide the table into two classes based on secondary color of the chain. Remember that when $p \leq q$ the red class will be type 1 chains and when $q < p$ the blue class will be type 1 chains.

| | | $a < b$ |
|---|---|---|
| $p \leq q$ | Type 1 | $\max\left\{d + \max\{c-b, a\},\ \lvert a+b-c\rvert\right\} + 3\left(c + \lceil \frac{d-c}{3} \rceil\right)$ |
| | Type 2 | $d + \min\{a, c-b\} + 3\lceil \frac{b-a}{3} \rceil$ |
| $p > q$ | Type 1 | $\max\left\{d + \max\{c-b, a\},\ \lvert a+b-c\rvert\right\} + 3\lceil \frac{b-a}{3} \rceil$ |
| | Type 2 | $d + \min\{a, c-b\} + 3\lceil \frac{b-a}{3} \rceil + 3\left(c + \lceil \frac{d-c}{3} \rceil\right)$ |

TABLE 2.1: u-chain lengths for $\angle Q = 0$ and $a < b$

| | | $a \geq b$ |
|---|---|---|
| $p \leq q$ | Type 1 | $\max\left\{d + \max\{c-b, a\},\ \lvert a+b-c\rvert\right\} + 3\left(c + \lceil \frac{d-c}{3} \rceil\right)$ |
| | Type 2 | $d + \min\{a, c-b\}$ |
| $p > q$ | Type 1 | $\max\left\{d + \max\{c-b, a\},\ \lvert a+b-c\rvert\right\}$ |
| | Type 2 | $d + \min\{a, c-b\} + 3\left(c + \lceil \frac{d-c}{3} \rceil\right)$ |

TABLE 2.2: u-chain lengths for $\angle Q = 0$ and $a \geq b$




(A) $\angle Q = 1$ on the fullerene (B) $\angle Q = 1$ in the tessellation

FIGURE 2.12: Determining chain length for u-chain around $Q$ when $\angle Q = 1$

Now let us move to the case where $\angle Q = 1$. To determine $p$ and $q$, we again expand a wedge at $Q$ by means of a 60° rotation to yield the following expressions for $(p, q)$. If the included angle between the two segments in the fullerene has angle measure 1 then opening a wedge, giving an angle of 2 in $\Lambda$, will result in the following embedded coordinates as shown in Figure 2.12a.

$$(p, q) = \left\{ \begin{array}{ll} (a + c + d,\ b - c), & \text{for} \quad b \geq c \\ (c - b,\ a + b + d), & \text{for} \quad b \leq c \end{array} \right\}$$

In this case $R$ must lie in the region of yellow faces shown in Figure 2.9. As before $Q$ will lie within the blue parallelogram whenever $a \geq b$ and, since $a$ and $b$ are oblique to the side of the parallelogram, the chain length will have to be extended by $3\lceil \frac{b-a}{3} \rceil$ whenever $b > a$. $Q$ will lie within the boundary of the red parallelogram whenever $d \geq c$ and the chain length will have to be extended by $3\lceil \frac{d-c}{3} \rceil$ whenever $c > d$. The following four tables give all possible u-chain lengths when $\angle Q = 1$.

| | | $a < b \quad \& \quad c \leq d$ |
|---|---|---|
| $p \leq q$ | Type 1 | $\max\left\{a + \min\{b, c\} + d,\ \lvert b - c\rvert\right\}$ |
| | Type 2 | $a + \max\{b, c\} + d + 3\lceil \frac{b-a}{3} \rceil$ |
| $p > q$ | Type 1 | $\max\left\{a + \min\{b, c\} + d,\ \lvert b - c\rvert\right\}) + 3\lceil \frac{b-a}{3} \rceil$ |
| | Type 2 | $a + \max\{b, c\} + d$ |

TABLE 2.3: u-chain lengths for $\angle Q = 1$, $a < b$ and $c \leq d$

| | | $a < b \quad \& \quad c > d$ |
|---|---|---|
| $p \leq q$ | Type 1 | $\max\left\{a + \min\{b, c\} + d,\ \lvert b - c\rvert\right\} + 3\lceil\frac{c-d}{3}\rceil$ |
| | Type 2 | $a + \max\{b, c\} + d + 3\lceil\frac{b-a}{3}\rceil$ |
| $p > q$ | Type 1 | $\max\left\{a + \min\{b, c\} + d,\ \lvert b - c\rvert\right\} + 3\lceil\frac{b-a}{3}\rceil$ |
| | Type 2 | $a + \max\{b, c\} + d + 3\lceil\frac{c-d}{3}\rceil$ |

TABLE 2.4: u-chain lengths for $\angle Q = 1$, $a < b$ and $c > d$

| | | $a \geq b \quad \& \quad c > d$ |
|---|---|---|
| $p \leq q$ | Type 1 | $\max\left\{a + \min\{b, c\} + d,\ \lvert b - c\rvert\right\} + 3\lceil\frac{c-d}{3}\rceil$ |
| | Type 2 | $a + \max\{b, c\} + d$ |
| $p > q$ | Type 1 | $\max\left\{a + \min\{b, c\} + d,\ \lvert b - c\rvert\right\}$ |
| | Type 2 | $a + \max\{b, c\} + d + 3\lceil\frac{c-d}{3}\rceil$ |

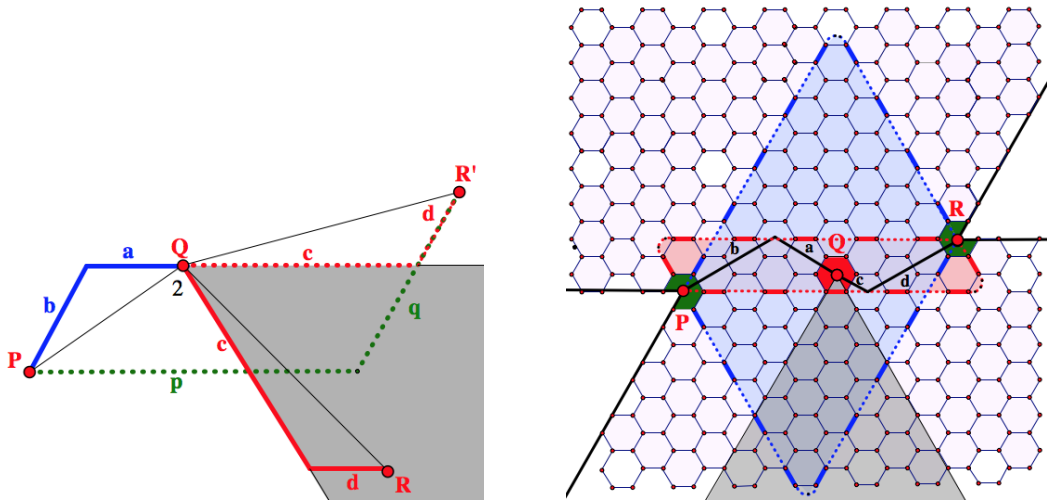
TABLE 2.5: u-chain lengths for $\angle Q = 1$, $a \geq b$ and $c > d$

| | | $a \geq b \quad \& \quad c \leq d$ |
|---|---|---|
| $p \leq q$ | Type 1 | $\max\left\{a + \min\{b, c\} + d,\ \lvert b - c\rvert\right\}$ |
| | Type 2 | $a + \max\{b, c\} + d$ |
| $p > q$ | Type 1 | $\max\left\{a + \min\{b, c\} + d,\ \lvert b - c\rvert\right\}$ |
| | Type 2 | $a + \max\{b, c\} + d$ |

TABLE 2.6: u-chain lengths for $\angle Q = 1$, $a \geq b$ and $c \leq d$

Lastly if the included angle in the fullerene has measure 2 as shown in Figure 2.13a then forming a wedge between the two segment yields the following embedded coordinates:

$$(p, q) = (a + c,\ b + d)$$




(A) $\angle Q = 2$ on the fullerene (B) $\angle Q = 2$ in the tessellation

FIGURE 2.13: Determining chain length for u-chain around $Q$ when $\angle Q = 2$

In this case $R$ must lie in the region of purple faces shown in Figure 2.9. As with the other cases, $Q$ will lie within the blue parallelogram whenever $a \geq b$ and the length of chains will blue as their secondary color will have to be extended by $3\lceil \frac{b-a}{3} \rceil$ whenever $b > a$. $Q$ will always lie within the boundary of the red parallelogram in this case and thus chains with red as their secondary color will never need to be extended.

| | | $a < b$ | $a \geq b$ |
|---|---|---|---|
| $p \leq q$ | Type 1 | $\max\{a+c,\ b+d\}$ | $\max\{a+c,\ b+d\}$ |
| | Type 2 | $a+b+c+d+3\lceil \frac{b-a}{3} \rceil$ | $a+b+c+d$ |
| $p > q$ | Type 1 | $\max\{a+c,\ b+d\} + 3\lceil \frac{b-a}{3} \rceil$ | $\max\{a+c,\ b+d\}$ |
| | Type 2 | $a+b+c+d$ | $a+b+c+d$ |

TABLE 2.7: u-chain lengths for $\angle Q = 2$

Combining the results for $(p, q)$ in each of the possible cases yields the following table outlining a sharp lower bound for the type 1 and type 2 chain lengths. This can

be useful if only a bound is needed and one does not want to consider all possible sub-cases.

| | Type 1 Lower Bound | Type 2 Lower Bound |
|---|---|---|
| $\angle Q = 0$ | $\max\left\{a + \min\{b, c\} + d,\ \lvert b - c\rvert\right\}$ | $a + \max\{b, c\} + d$ |
| $\angle Q = 1$ | $\max\left\{a + c,\ b + d\right\}$ | $a + b + c + d$ |
| $\angle Q = 2$ | $\max\left\{\min\{a, d\} + b + c,\ \lvert d - a\rvert\right\}$ | $\max\{a, d\} + b + c$ |

TABLE 2.8: Lower bound on length of U-chains

## 2.3 Wrapping Around Multiple Pentagons

Again we have two classes of chains. We must find the length of the shortest chain in each class. When we are wrapping around intermediate pentagons, the two classes are identified by their secondary color. When wrapping around more than one intermediate pentagon we must consider forming the chains in sections. To do so we choose an intermediate hexagon in the same color class as the original and terminating ends of the chain. We choose a hexagon of minimal distance from the second pentagon which is being wrapped around as the first intermediate pentagon can be treated as described in Section 2.2. The hexagon is chosen such that a chain from each pentagon leading to that hexagon need not wrap-around more than one intermediate pentagon. If there is more than one such hexagon we choose one arbitrarily. In this case the chains are handled separately and then joined. Once the hexagon has been chosen we can treat the two chains separately and construct the intermediate parallelograms to determine the minimal chain length of the chain sections. We then sum the minimal chain lengths to get the total minimal total chain length. It must be noted that some of the intermediate chains will have to be of type 1 and some of type 2 so as to ensure only sharp turns.

In lieu of finding what would be a very complicated closed formula for the extended wrap-around chains, we find a lower bound on the length of such a chain. These lower bounds are usually large enough to rule out these long chains when determining the minimal chain configuration and they are much simpler to compute than the actual length.

**Lemma 2.3.1.** *Let $\Gamma$ be a fullerene. Let $Q$ and $S$ be pentagons in $\Gamma$ such that the segment connecting them has coordinates congruent modulo 3. Let $R$ be a pentagon in $\Gamma$ such that $\angle QRS$ has external measure $\theta$ as illustrated in Figure 2.14 . Let $R'$ be a hexagon adjacent to pentagon $R$ such that both segments $QR'$ and $R'S$ have coordinates congruent modulo 3.*

*Then the type 1 chain pairing $Q$ and $R'$ and the type 1 chain pairing $R'$ and $S$ both have the same secondary color if $\theta$ is even and have different secondary colors if $\theta$ is odd.*

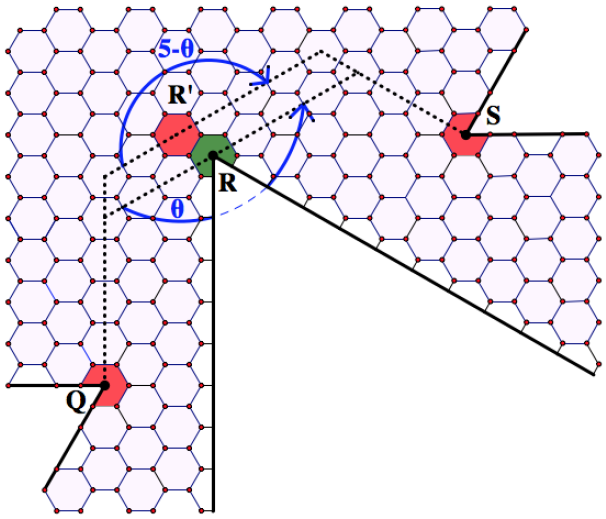
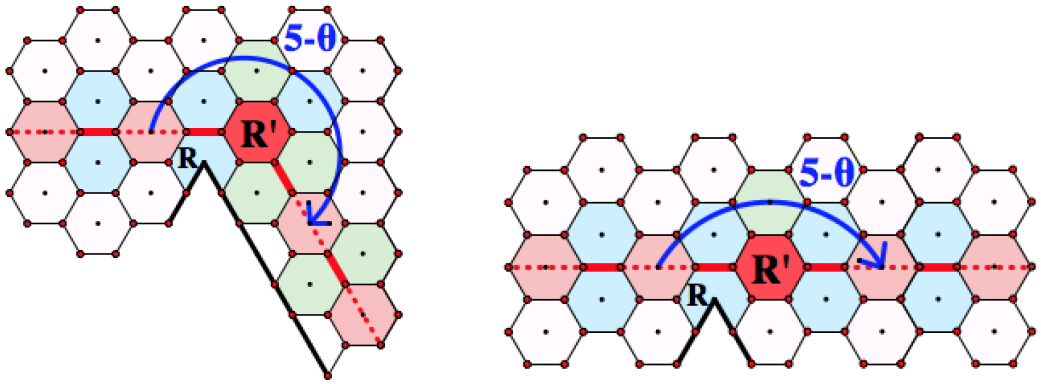



FIGURE 2.14: Wrapping around pentagon $R$ via hexagon $R'$

*Proof.* Due to the location of the removed wedge from $R$, it follows that the number of vertices of $R$ that lie outside $\angle QRS$ will be the same as the number of vertices of $R'$ that lies outside $\angle QR'S$. It follows that $\angle QRS$ and $\angle QR'S$ have the same exterior measure.

If the interior angle of $QRS$ has measure $\theta$ then the exterior angle of $QRS$ and equivalently $QR'S$ necessarily has measure $5 - \theta$. Hence, if the interior angle is even, then the exterior angle of $QR'S$ is odd and if the interior angle is odd then the exterior angle of $QR'S$ is even.

Since we assume an external coloring, the coloring of the exterior hexagons is fixed while the coloring of the interior hexagons is determined by which initial edge is used by the chain configuration. As we push the coloring in from the outside, the secondary color of the each chain will be determined by the color of the external face incident to the initial edge in the chain.




(A) Exterior angle of measure 4 (B) Exterior angle of measure 3

FIGURE 2.15: Secondary colors of chains depending on exterior angle measure

Hence, if the exterior angle has even measure then the first and last exterior hexagons between the two initial edges coming from $R'$ will be in distinct color classes and thus the secondary colors of the two possible chains will be distinct as illustrated in Figure 2.15a and if the exterior angle has odd measure then the first and last external hexagons will be the same color and thus we see that the type 1 chains will have the same secondary color as illustrated in Figure 2.15b.

Therefore the type 1 chain joining $Q$ and $R'$ and the type 1 chain joining $R'$ and $S$ both have the same secondary color if $\theta$ is even and have different secondary color if $\theta$

is odd . □

Notice that this result holds if both the $QR$ and the $RS$ segments have coordinates congruent modulo 3. In this case the two chains will not go to an nearby hexagon but rather will just meet at pentagon $R$.

**Theorem 2.3.2.** *Let $P_0$ and $P_n$ be two chain available pentagons with $P_1, ..., P_{n-1}$ be intermediate pentagons such that the segment connecting $P_i$ to $P_{i+1}$ has coordinates $(a_{i+1}, b_{i+1})$ for $i \in \{0, 1, ..., n-1\}$ and the internal angle between segment with coordinates $(a_i, b_i)$ and the segment with coordinate $(a_{i+1}, b_{i+1})$ is given by $\theta_i$. Then the length of any chain connecting $P_0$ to $P_n$ that wraps around each of the intermediate pentagons has length at least*

$$\Sigma_{i=1}^{n} \max\{a_i, b_i\} + \Sigma_{i \in I} \min\{a_i, b_i\}$$

*where $I = \{i \,|\{\theta_1, ..., \theta_i\}$ contains an odd number of angles with even measure$\}$ for one choice of secondary chain color or $I = \{i \,|\{\theta_1, ..., \theta_i\}$ contains an even number of angles with even measure or no such angles$\}$ for the alternative secondary color choice.*

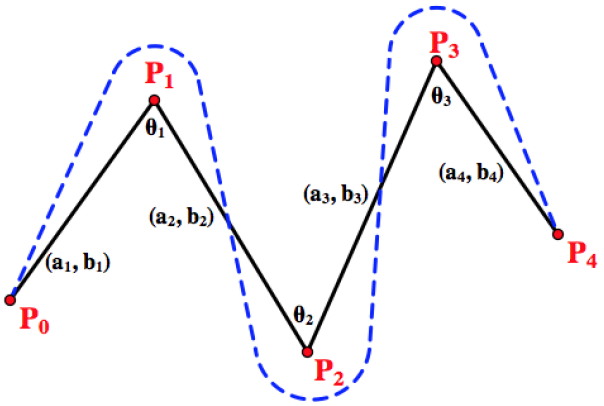



FIGURE 2.16: $P_0 - P_4$ chain wrapping around three intermediate pentagons

*Proof.* Consider the segment $(a_i, b_i)$. Notice that if $a_i \equiv_3 b_i$ then $P_{i-1}$ and $P_i$ are in the same color class and the minimum chain length between the two is $\max\{a_i, b_i\}$. If

$a_i - b_i \equiv_3 1$ then $a_i - (b_i + 1) \equiv_3 0$ and as such, the face reached by the segment with coordinates $(a_i, b_i + 1)$ will be in the same color class as $P_{i-1}$. The length of this chain will be at least $\max\{a_i, b_i + 1\}$.

Similarly if $a_i - b_i \equiv_3 2$ then $1 + a_i - b_i \equiv_3 0$ and as such, the face reached by the segment with coordinates $(1 + a_i, b_i)$ will be in the same color class as $P_{i-1}$. The length of this chain will be at least $\max\{a_i + 1, b_i\}$. In each of the three cases the chain length is at least $\max\{a_i, b_i\}$. Note that in each case we are extending the coordinates to a pentagon in the desired color class as opposed to shortening them. As such, we will always land on a face that is adjacent to the intermediate pentagon but outside the removed wedge from the embedding. It follows that we can sum over the segments connecting the pentagons to yield the desired result.

The entire wrap-around chain must have the same secondary color. As such some of our chain segments can be estimated by type 2 chains, and in these cases we also contribute the minimum of the coordinates to our chain length. From the previous lemma we conclude that wrapping around an angle of even measure will require us to change the chain type in order to keep the same secondary color. Wrapping around an angle of odd measure keeps the secondary color fixed.

Therefore, if we start with a type 1 chain segment, we begin by only summing the maximum coordinates until we reach the first angle of even measure. At this point we add the minimum coordinates and the maximum coordinates until the next angle of even measure. Now, we switch back to only summing the maximums. Continue on similarly. This is equivalent to adding on the minimum coordinate for all entries in the set $I = \{i \,|\{\theta_1, ..., \theta_i\}$ contains an odd number of angles with even measure$\}$.

Alternatively, if we begin with a type 2 chain segment, we start off adding both maximum and minimum coordinates until we reach the first angle of even measure. Then we do not add the minimum coordinates until the next angle of even measure or

equivalently $I = \{i \,|\{\theta_1, ..., \theta_i\}$ contains an even number of angles with even measure or no such angles$\}$.

It remains to be shown that no chain can be shorter. As we are wrapping around each of the intermediate pentagons, a minimal chain will pass as close to the intermediate pentagons as possible. If every intermediate pentagon is in the same color class as the initial and terminal pentagons then the shortest chain will travel directly through subsequent intermediate pentagons and so it follows that the chain could not be shorter than the sum of the chain segments connecting the pentagons.

If there is an intermediate pentagon not in the primary color class then any chain can be shortened until it passes through a face that is distance one from the intermediate pentagon. Furthermore by flipping the chains we can form a minimal chain that intersects any of the faces in the primary color class that are adjacent to the pentagon. Hence there is a minimal chain that passes through each of the faces used in our computation so there can be no chain of shorter length.

□

## 2.4 Color Configuration of 3-sets

**Theorem 2.4.1.** *Let $P$, $Q$ and $R$ be three pentagons in a fullerene $\Gamma$. If each of the segments between $P$, $Q$ and $R$ have coordinates that are congruent modulo 3 then there are three possible direct chains and three possible wrap-around chains. If only two of the three pentagons are joined by segments with coordinates that are congruent modulo 3 then the only possible chain is a direct chain between these two pentagons. Finally if none of the three segments joining the pentagons are congruent modulo 3 then we have three possible wrap-around chains and no direct chains can be formed.*

*Proof.* We know that if two pentagons are joined by a segment with coordinates congruent modulo 3 then the pentagons are chain available. It follows that a direct chain is possible between any two pentagons with such coordinates. Hence, if $P$, $Q$ and $R$ are all chain available we have three possible direct chains. In the second case, up to re-indexing we can say that that $P$ and $Q$ are joined by a segment with coordinates congruent modulo 3 and the segments between $R$ and either of the other two pentagons have coordinates not congruent modulo 3. In this case there is only one direct chain, namely the one connecting $P$ and $Q$. In the final case, if none of $P$, $Q$ and $R$ are joined by segments with coordinates congruent modulo 3 then no direct chains are possible.

Now we consider wrap-around chains. Without loss of generality let us assume we are trying to connect $P$ and $R$ by a chain wrapping around $Q$ and that $P$ is red. If we embed a flat map of the fullerene onto a three colored hexagonal tessellation then the pentagons that are chain available to $P$ are the red faces in the tessellation. However, closing the wedges in the flat map changes the color of the faces on one side of the wedge since there must necessarily be a chain leaving the intermediate pentagon and thus, this chain will interchange the two colors different from the color of $Q$. If $Q$ is a blue pentagon then $R$ will become green once the wedge is closed so long as the segment coordinates of $PR$ are not congruent modulo 3. Thus the chain available faces will now be those that are colored green.

Similarly, if $Q$ is a green face then $R$ will become blue, and so the chain available faces will be blue. If $Q$ is a red pentagon then the chain available faces will be red since the chain from $Q$ leaves the color red fixed.

Thus we see that in order for two pentagons to be connected by a wrap-around chain then either all three pentagons must be the same color or all three must be different. If all three pentagons are the same color then pairwise $P$, $Q$ and $R$ must be

joined by segments with coordinates that are congruent modulo 3. If all three pentagons are in distinct color classes then pairwise $P$, $Q$ and $R$ must be joined by segments in which none have coordinates congruent modulo 3. In either case we have three possible wrap-around chains. □

It is usually most practical to check whether pentagons are chain available by considering the coordinates of the segment connecting them. We know that two pentagons can be connected by a direct chain exactly when the associated coordinates are congruent modulo 3. We use the concepts presented from the previous theorem to prove a theorem relating the existence of wrap-around chains with the coordinates between the pentagons.

**Theorem 2.4.2.** *Let $P$, $Q$ and $R$ be three pentagons in a fullerene $\Gamma$. Let $P$ and $Q$ be connected by a segment with coordinates $(a, b)$ and $Q$ and $R$ be connected by a segment with coordinates $(c, d)$ such that $\angle PQR$ is given by $\theta$. Lastly let $P$ and $R$ be joined by a segment with coordinates $(l, m)$*

*If $\theta$ is even then $l - m \not\equiv_3 0$ so long as $(a - b) - (c - d) \equiv_3 0$ and $l - m \equiv_3 0$ so long as $(a - b) + (c - d) \equiv_3 0$. If $\theta$ is odd then $l - m \equiv_3 0$ so long as $(a - b) - (c - d) \equiv_3 0$ and $l - m \not\equiv_3 0$ so long as $(a - b) + (c - d) \equiv_3 0$.*

*Proof.* Rotations of $120^\circ$ in the hexagonal tessellation keep all three colors fixed and thus since the colors are fixed, the coordinates remain congruent modulo 3. Therefore, since angles of odd measure correspond to such rotations it suffices to check one angle of odd measure and one angle of even measure.

Let us begin with the case when $\theta \in \{1, 3\}$ and let us consider $\theta = 3$. Assume we have that $(c - d) + (a - b) \equiv_3 0$. If $d - c \equiv_3 0$ then we must have $b - a \equiv_3 0$ and thus we have two pairs of pentagons that are chain available and thus by the previous theorem all three pentagons must be able to be connected by direct chains. Similarly we get the same result if $b - a \equiv_3 0$.

Now assume both $d-c$ and $b-a$ are not congruent to 0.

For $\theta = 3$ the segment connecting $P$ and $R$ has coordinates $(l,m) = (a+d+c,\ b-c)$ when $b \geq c$ and $(l,m) = (c-b,\ a+b+d)$ when $c > b$. Notice that:

$$\begin{aligned} &[b-c] - [a+d+c] \equiv_3 0 \\ \iff\ &b - 2c - a - d \equiv_3 0 \\ \iff\ &(a-b) - (c-d) \equiv_3 0 \end{aligned}$$

If it happens that $l - m \equiv_3 0$ when $(a-b) - (c-d) \equiv_3 0$ and $d - c \not\equiv_3 0$ and $b - a \not\equiv_3 0$ then it follows that $l - m \not\equiv_3 0$ exactly when $(c-d) + (a-b) \equiv_3 0$. Similarly when $c > b$ and the coordinates are given by $(c-b, a+b+d)$ we have:

$$\begin{aligned} &[a+b+d] - [c-b] \equiv_3 0 \\ \iff\ &2b - c + a + d \equiv_3 0 \\ \iff\ &(c-d) - (a-b) \equiv_3 0 \end{aligned}$$

Similarly to above, we get that $l - m \not\equiv_3 0$ exactly when $(a-b) + (c-d) \equiv_3 0$. We have shown that for angles of even measure the condition $(a-b) + (c-d) \equiv_3 0$ yields that either all or none of the three segments have coordinates congruent modulo 3 to 0. Hence, by the previous theorem, the condition gives us that we can connect $P$ and $R$ using a wrap-around chain.

Now consider when $\theta \in \{0, 2, 4\}$. Similarly to above we consider just one of these angles as the others will be equivalent, so we consider $\theta = 2$. In this case the coordinates connecting $P$ and $R$ are $(l,m) = (a+c, b+d)$.

$$[b+d] - [a+c] \equiv_3 0 \iff (a-b) + (c-d) \equiv_3 0$$

If follows that if $d - c \not\equiv_3 0$ and $b - a \not\equiv_3 0$, $P$ and $R$ will not be chain available when $(a-b)-(c-d) \equiv_3 0$. If either $b-a \equiv_3 0$ or $d-c \equiv_3 0$ then the other must be congruent to 0 and so $l-m \equiv_3 0$ and $P$ and $R$ will be chain available. Hence when $(a-b)-(c-d) \equiv_3 0$ we have that the pentagons $P$ and $R$ can be paired by a wrap-around chain.

Finally, assume the equivalence classes of the coordinates of the segments joining the three pentagons are such that there can be a chain wrapping around $Q$. If $a-b \equiv_3 0$ and $c-d \equiv_3 0$ then $(a-b)-(c-d) \equiv_3 0$ holds trivially and if all are different we have $(a-b)-(c-d) \equiv_3 0$ by above. □

**Corollary.** *Let $P$, $Q$ and $R$ be three pentagons in a fullerene $\Gamma$. Let $P$ and $Q$ be connected by a segment with coordinates $(a,b)$ and $Q$ and $R$ be connected by a segment with coordinates $(c,d)$ such that the angle between $(a,b)$ and $(c,d)$ is given by $\theta$. A chain from $P$ to $R$ that wraps around $Q$ is possible if and only if $(a-b)-(c-d) \equiv_3 0$ when $\theta$ is even and $(a-b)+(c-d) \equiv_3 0$ when $\theta$ is odd.*

*Proof.* By Theorem 2.4.1 we know that $P$ and $R$ must be in different color classes in order for a wrap-around chain to exist. Theorem 2.4.2 gives us the desired conditions for this to occur. □

# Chapter 3

# 4-cluster Signature Configurations

In this chapter we begin our work examining sets of four pentagons that are isolated from the other pentagons in a fullerene. We will determine the conditions necessary to ensure that these pentagons can be joined by chains. Recall that in this case we call the 4-set of pentagons a 4-cluster.

## 3.1 The Geometry of the Hexagonal Tessellation

In this section we will explore some additional properties of the hexagonal tessellation, $\Lambda$, that provide a basic framework upon which we can build our theory on the 4-clusters we will be working with in this chapter.

We have spent much of Chapters 1 and 2 discussing the coordinates of segments between pentagons in a fullerene. However, equally as important as the coordinates between segments are the angles between adjacent segments. Thus, just as we discussed the implications of the relations between the coordinates themselves, we also need to discuss properties relating the angles between the segments. Recall that when we are considering the angles between segments in a fullerene we are concerned with fullerene angle measure rather than geometric angles. Therefore the first two results

of this chapter, verify that standard geometric properties regarding angles still hold with our alternate definition of angles.

**Theorem 3.1.1.** *Let $\{P, Q, R, S\}$ be a 4-set in a fullerene as oriented in Figure 3.1. Then $\angle PQS + \angle SQR = \angle PQR$.*

*Proof.* Construct segments $PQ$, $RQ$ and $SQ$ as well as their corresponding coordinate paths as shown in Figure 3.1. $\angle PQS$ is given by the number of vertices on pentagon $Q$ that lie between the first legs of the coordinate paths of $QS$ and $QP$ when traversed counterclockwise. Likewise $\angle RQS$ is given by the number of vertices on pentagon $Q$ that lie between the first legs of the coordinate paths of $QR$ and $QS$ when traversed counterclockwise. Since no vertices lie between segment $QS$ and itself, we see that $\angle PQS + \angle SQR = \angle PQR$ since it is equivalent to count the vertices when traversed from the first leg of the coordinate path of $RQ$ directly to the first leg of the coordinate path of $PQ$ or stopping at the first leg of the coordinate path of $QS$ on the way. □

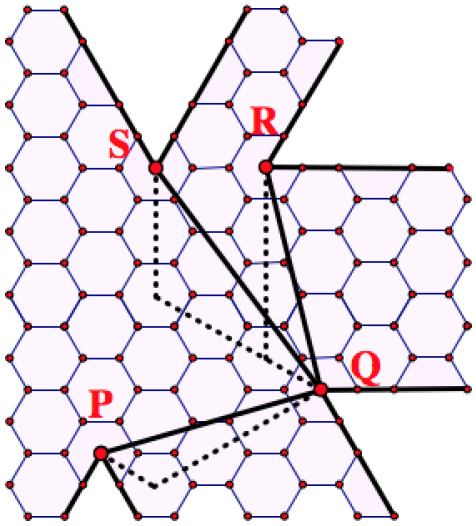



FIGURE 3.1: $\angle PQS + \angle SQR = \angle PQR$

Consider a subset of the pentagons in a fullerene and construct a planar circuit using the segments between neighboring pentagons. The following theorem allows us

to use a property similar to a geometric property of n-sided polygons in the Euclidean plane to determine the sum of the angles around the circuit. The proof is modeled off the geometric version of the theorem which relies on the angle addition formula to construct polygons with increasingly many sides.

**Theorem 3.1.2.** *The sum of the interior angle measures around the boundary of any n-set for* $n \leq 12$*in a fullerene is* $3(n-2)$.

*Proof.* We will proceed by way of induction. As means of a base case, we will prove the claim when $n = 3$.

Consider the flat map of 3-set $\{P, Q, R\}$ embedded in $\Lambda$ such that the removed wedges each point away from the 3-set. We construct a line, $l$, parallel to segment $RQ$ passing through the center of face $P$. We translate segment $QR$ onto $l$ forming segments $PR'$ and $PQ'$ as shown in Figure 3.2. Since we are taking the wedge to be external to the 3-set and the coordinate segments adjacent to pentagon $P$ are parallel, $\angle R'PQ'$ has measure 3 on the side opposite the removed wedge.

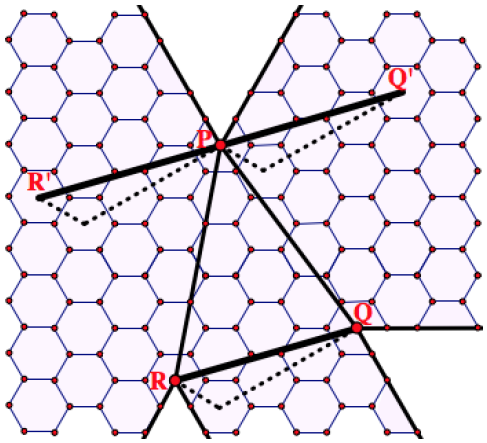



FIGURE 3.2: Sum of internal angles in a 3-set.

Since $PR'$ and $QR$ lie on parallel lines $\angle R'PR$ and $\angle PRQ$ have the same measure. Similarly, $PQ'$ and $QR$ lie on the same set of parallel lines and thus $\angle Q'PQ$ and $\angle PQR$

have the same measure. Finally, since $\angle R'PR + \angle RPQ + \angle Q'PQ = 3$ we have that $\angle PQR + \angle QRP + \angle RPQ = 3$ which proves the claim for the base case.

Assume the internal angle sum of an $k$-set is $3(k-2)$ and consider an arbitrary $(k+1)$-set. Construct a segment connecting the far ends of two adjacent segments dividing the $(k+1)$-set into a $k$-set and a 3-set where the two pentagons on the ends of the constructed segment are members of both sets. Since the internal angles of these two pentagon sets can be expressed as the sum of the internal angles in a 3-set, 3, and the sum of the angles in a $k$-set, $3(k-2)$, the angle sum of the $(k+1)$-set is just $3 + 3(k-2) = 3\big[(k+1)-2\big]$. Thus the claim holds for all $n \geq 3$.

□

When considering n-sets we often want to find relations about the coordinates as well as between the angles. The following lemma is particularly useful as it allows us to solve for individual coordinates in terms of the others.

**Lemma 3.1.3.** *Let $P, Q, R$ and $S$ be faces in $\Lambda$ such that $P$ and $S$ are on a line of hexagonal faces and $Q$ and $R$ are on a parallel line of faces. If segment $PQ$ has coordinates $(a, b)$ and segment $RS$ has coordinates $(e, f)$ such that none of the coordinate paths lie coincident with the parallel lines of faces then $a + b = e + f$.*

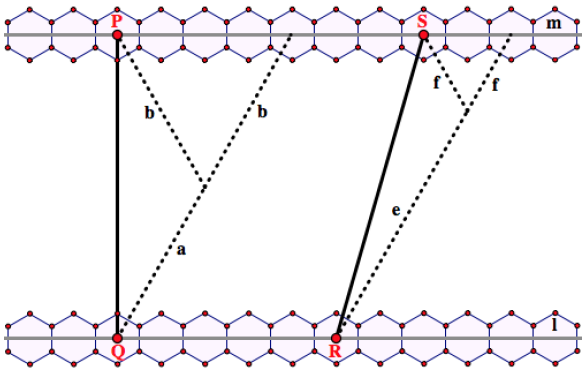



FIGURE 3.3: Segments between parallel lines have equal length

*Proof.* Construct two lines, $l$ and $m$, in $\Lambda$ such that $l$ passes through the centers of faces $Q$ and $R$ and $m$ passes through the centers of $P$ and $S$. Since $P$ and $S$ lie on a parallel line of hexagons to $Q$ and $R$ then $l$ and $m$ must be parallel lines.

Geometrically, coordinate segments $a$ and $e$ both lie at 60° to line $l$. Since $l$ and $m$ are parallel we extend coordinate segments $a$ and $e$ until they intersect with line $m$. Forming equilateral triangles with side length $b$ and $f$ respectively shows us that these extensions have length $a + b$ and $e + f$ respectively and so $a + b = e + f$. □

## 3.2 Requirements for Chain Availability

### 3.2.1 Color Configuration of 4-cluster

As we know, the sufficient and necessary conditions for the pentagons in a 2-cluster to be chain available can be interpreted in two equivalent ways. Either the coordinates of the segment connecting them must be congruent modulo 3 or alternatively when a patch of $\Lambda$ with the pentagons on the boundary is 3-colored, then the two pentagons are in the same color class. This is illustrated in Figure 3.4.

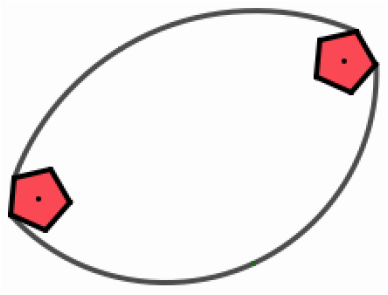


FIGURE 3.4: Two pentagons on the boundary of a patch that are in the same color class

In this chapter we will find conditions on the coordinates that ensure a 4-set is a 4-cluster. These conditions are significantly more involved than the conditions on a

2-cluster. Furthermore, in the case of 2-clusters we were ensured that the chain would remain within the patch. Within the case of 4-clusters, the chains may not necessarily be confined to the patches as we may have wrap-around chains that travel outside the patch. However, we assume that the clusters are isolated enough so as not to interfere with other chains in the remainder of the fullerene.

Before discussing coordinate conditions, we want to develop color conditions analogous to those of 2-clusters that will ensure that our 4-set is a cluster. The following table outlines all possible color configurations of a 4-set. Once we have outlined all possibilities we will determine which are 4-clusters and which are not.

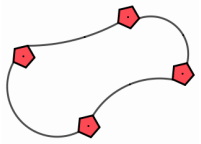
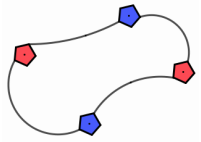
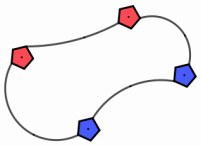
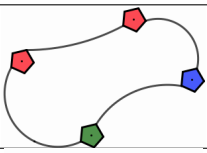
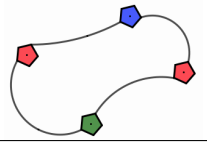
| **Colors Classes** | **Definition** | **Color Configuration** | **Example** |
|---|---|---|---|
| 1 | Monochromatic | All pentagons in same color class |  |
| 2 | Alternating | Colors alternating around boundary |  |
| 2 | Adjacent | Two adjacent same colored pairs |  |
| 3 | Single Adjacent | One adjacent pair same colored |  |
| 3 | Opposite | One opposite pair same colored |  |

TABLE 3.1: Possible color configurations of pentagons in a 4-set

In the next chapter we will delve into the intricacies and implications of the possible color configurations as well as precisely what it means to color a patch representing a 4-set. However, at this point we will restrict ourselves to merely determining which configurations are viable. In our next theorem we will prove that the only configurations that yield 4-clusters are those with monochromatic, adjacent or opposite configurations.

If we have two pairs of same colored pentagons then we have two distinct 2-clusters which, when combined as a 4-set, form a 4-cluster. When our 4-cluster factors into 2-clusters this way we say that the cluster has *adjacent configuration*. This also includes the special case in which all pentagons are colored the same color in which case we say that the cluster is *monochromatic*. If we do not specify we will assume that the two pairs of pentagons are in distinct color classes. It is worth noting from the start that just because a specific 4-cluster can be decomposed into two 2-clusters does not mean that the best chain configuration is two direct chains. We will discuss this in detail in Chapter 4.

Alternatively, another possible color configuration is to have one opposite pair of pentagons in the same color class and the other two are different colors. Namely an *opposite configuration*. We will show that these are the only two possible color configurations that yield a cluster.

Notice that the ordering of the pentagons and thus the color configurations class of a 4-set is not unique. We can choose a distinct patch that still has the same pentagons on the boundary but in a different order and thus the coloring may be different as shown in Figure 3.5. For each distinct boundary choice notice that the same colored pentagons can be joined by a u-chain that lies within the colored region, and the two pentagons assigned distinct colors can be paired by a chain the lies within the

uncolored region. In the next chapter we will discuss in full detail these chain configurations.

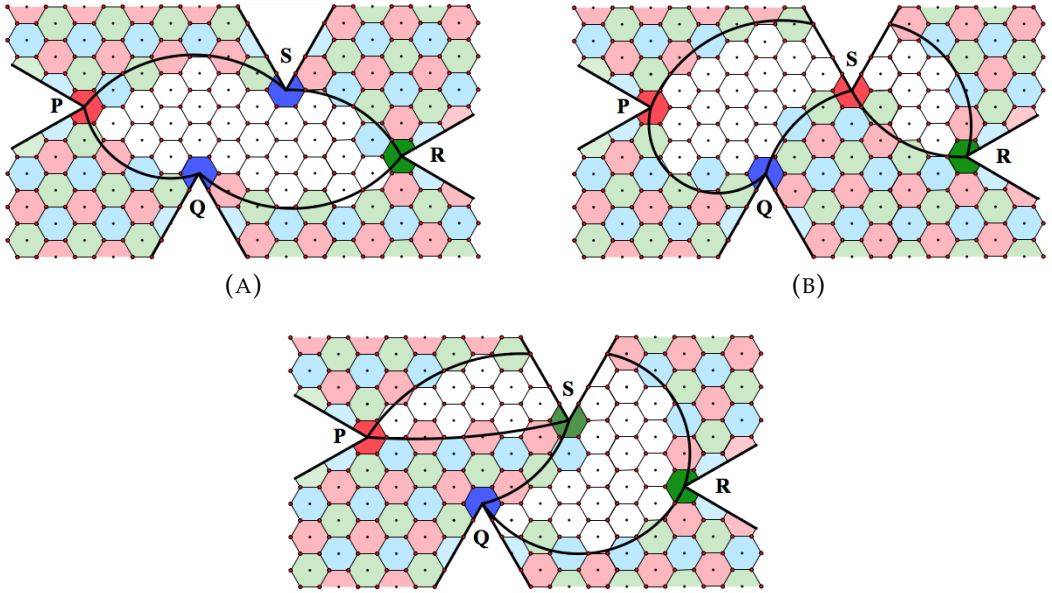



FIGURE 3.5: Distinct boundary choices for same 4-set

**Theorem 3.2.1.** *The only possible pentagon color configurations for a 4-cluster* $\{P, Q, R, S\}$ *are monochromatic, adjacent or opposite.*

*Proof.* In order for a 4-set to be a 4-cluster, a perfect coloring must extend through the annular neighborhood surrounding the cluster, passing the coordinate boundary and remain perfect within the interior except along the edges of the chains. If the coloring is consistent along the entirety of the boundary then we know it will be possible to pair the pentagons in the 4-set with chains and thus we will have a 4-cluster.

In order to describe what we mean by consistent we consider a perfect ambient coloring of patch of $\Lambda$ that we will be extending towards our 4-set. Up to permutation of colors we can, without loss of generality, say that the patch is colored as in the original configuration shown in Figure 3.6. As pentagons make a perfect coloring of the 4-set impossible, the 4-set will contain portions of the tessellation in which certain colors

are permuted. If we let $R$, $G$, $B$ represent the colors red, green and blue respectively, then Figure 3.6 shows the affects of permuting two colors and these transpositions are represented using cycle notation.

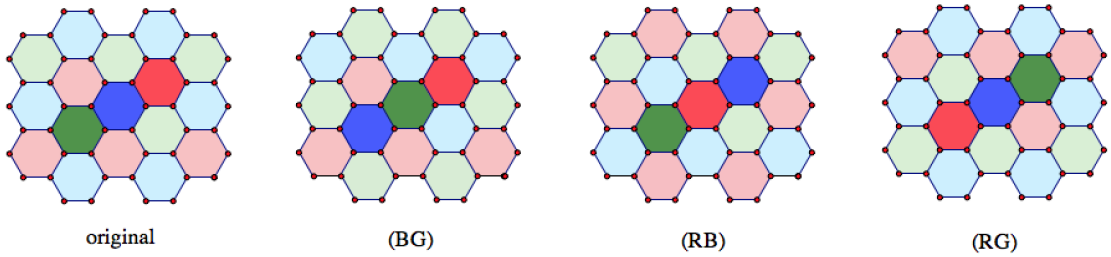
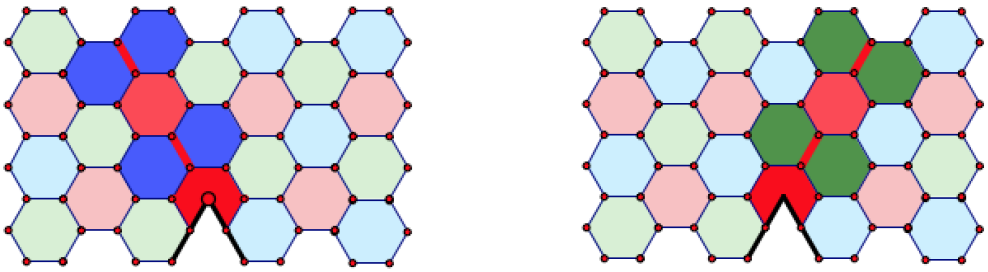



FIGURE 3.6: Examples of permuting colors in $\Lambda$

In tracing the boundary of our set we will encounter the four pentagons and each must be the end point of a chain if the set is to be a cluster. Say we encounter a red pentagon, then either we have a red-green chain or a red-blue chain emanating from this face. In either case, passing the chain permutes the green and blue color classes yielding the transposition (BG) as illustrated in Figure 3.7. The left edge of both



(A) Red Blue Chain (B) Red Green Chain

FIGURE 3.7: Passing a red pentagon permutes blue and green color classes

patches shown in Figure 3.7 matches the color configuration of the original colored tessellation in Figure 3.6. Then in passing either red primary chain to the right edge of the patch, the color configuration changes as blue and green faces are interchanged. It

follows that any time we pass a pentagon of some color, we permute the two remaining colors.

Now we must determine the possible color configurations of the pentagons that will ensure that the color configuration matches that of the original after passing all four pentagons in the 4-set. We do so by composing the permutations yielded by passing each pentagon consecutively along the boundary and determining which color configurations yield the identity.

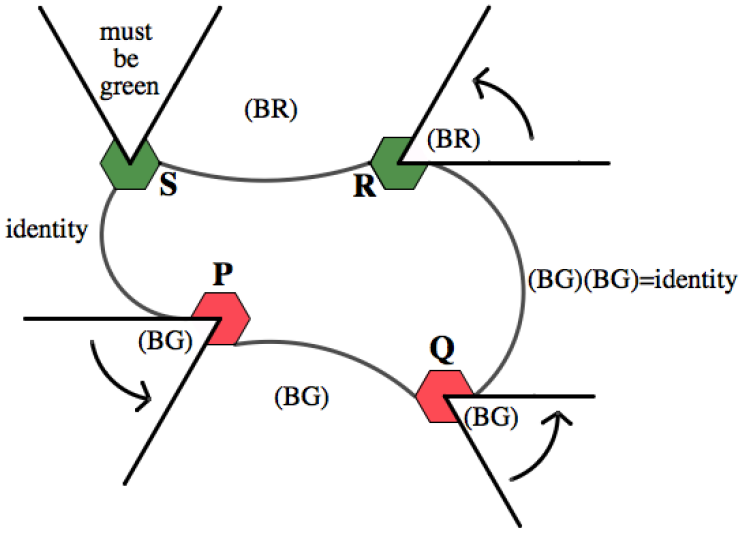



FIGURE 3.8: Color permutations around adjacent 4-cluster

By the pigeon hole principle we know that two of our four pentagons must be in the same color class. First assume we have a pair of adjacent pentagons that are in the same color class. An example of such a adjacent configuration is illustrated in Figure 3.8. In this example we have $P$ and $Q$ both colored red. As each transposition is its own inverse, passing through these two permutations consecutively yields the identity. Hence, the subsequent two pentagons must also be in one color class so as their associated permutations are self-inverse and thus the composition of the four permutations will yield the identity and an adjacent configuration.

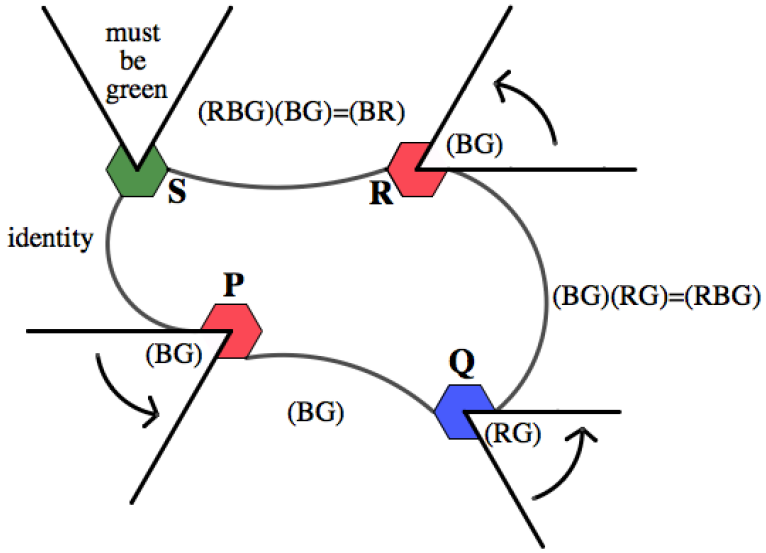



FIGURE 3.9: Color permutations around opposite 4-cluster

Now assume we have no pairs of adjacent same colored pentagons. Without loss of generality, let us say that pentagons $P$ and $R$ are in the same color class and pentagon $Q$ lies between $P$ and $R$ on the boundary. Up to permutation of colors let us say that $P$ and $R$ are red and that $Q$ is blue as is the example in Figure 3.9. Then, in tracing the boundary, we have the permutation $(BG)(RG)(BG) = (BR)$ after we pass pentagons $P$, $Q$ and $R$ and thus the final pentagon must be colored green in order for the composition of permutations to yield the identity. As such, we have an opposite configuration. □

## 3.3 Overview of Algebraic Method

In this section we give a second proof of Theorem 3.2.1. It is somewhat longer, however, it involves deriving some formulas that will be very useful later.

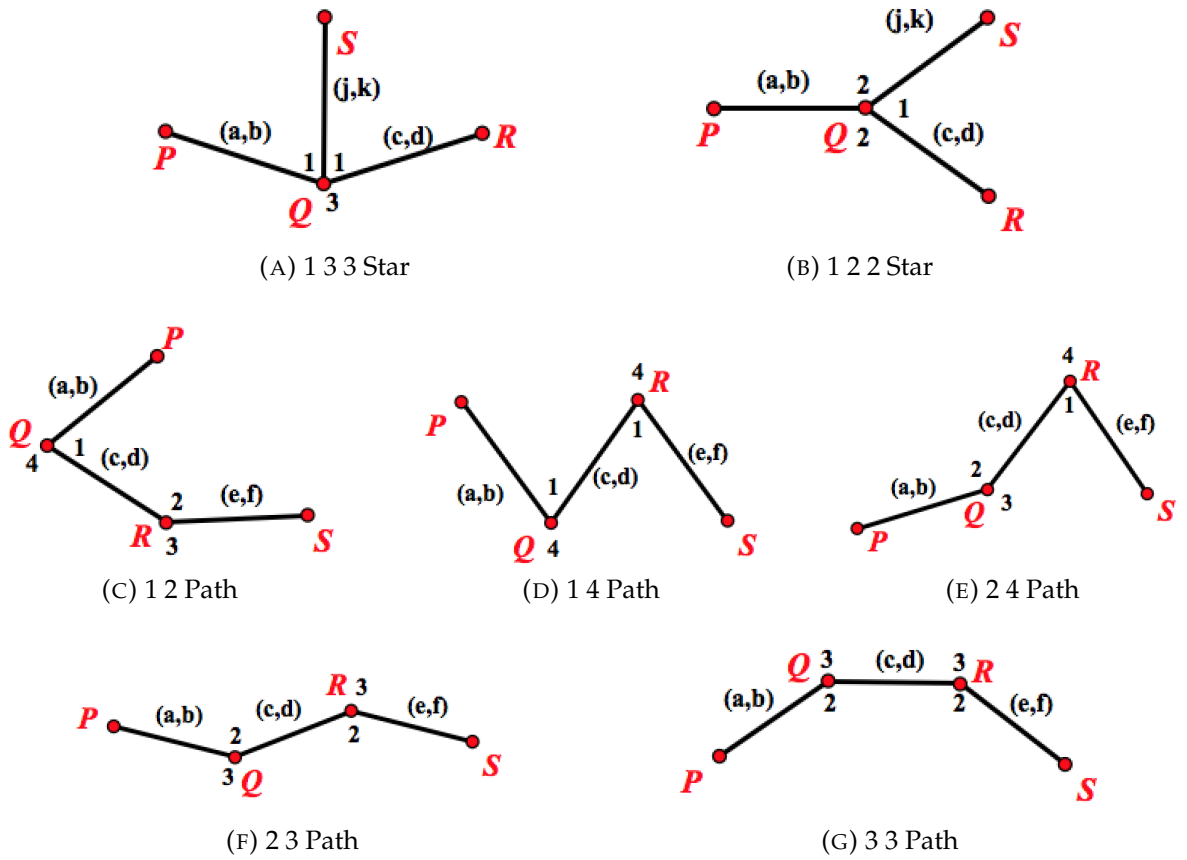
Consider four pentagons, $P, Q, R$ and $S$, of a 4-set in a fullerene. Consider $K_4$ constructed on the vertices $\{P, Q, R, S\}$ where the edges are the segments between vertices and each edge is weighted by the length of the respective segment. We can

uniquely describe the 4-set $\{P, Q, R, S\}$ by constructing the signature graph, $\mathscr{S}$, for these 4 pentagons in the fullerene. For the entirety of this discussion we say segment $PQ$ has coordinates $(a, b)$, segment $QR$ has coordinates $(c, d)$, segment $RS$ has coordinates $(e, f)$, segment $SP$ has coordinates $(g, h)$, segment $QS$ has coordinates $(j, k)$ and segment $PR$ has coordinates $(l, m)$. A shortest spanning tree on four vertices can either be a path of length three or a star with one vertex of degree 3 and three degree 1 vertices.

If $\mathscr{S}$ is a path graph we label the two degree 2 vertices $R$ and $Q$ and degree 1 vertices $P$ (adjacent to $Q$) and $S$ (adjacent to $R$) in reference to the pentagons the vertices represent. The signature also accounts for the angles at $Q$ and $R$, say $\theta_1$ and $\theta_2$ respectively. We can describe the 4-set by giving one angle at each pentagon so long as the chosen angles lie on the same side of the signature. We call sets of this type $\theta_1$ $\theta_2$ *path sets*. Since we could alternatively choose the angles on the other side of the signature, $\theta_1$ $\theta_2$ path sets are symmetric to $(5 - \theta_1)$ $(5 - \theta_2)$ path sets. For example a 3 1 path signature is isomorphic to a 2 4 path signature. Additionally, reversing the order of the angles results in an isomorphic signature up to relabeling. Coupling this with the fact that we cannot have angles of measure 0 occurring in the signature, as shown in Chapter 1, we have five non isomorphic path signatures.

If $\mathscr{S}$ is a star graph then we label the degree 3 vertex $Q$. Since the angles around pentagon $Q$ must sum to 5 with no angles of measure 0 we have two nonisomorphic options for the angle configuration. Namely two angles of measure 1 and one of measure 3 or one of measure 1 and two of measure 2. This leads to seven non-isomorphic signature configurations shown in Figure 3.10.

For any signature configuration we determine a patch that contains the 4-set in which all four pentagons lie on the boundary and coordinate paths between adjacent




(A) 1 3 3 Star (B) 1 2 2 Star

(C) 1 2 Path (D) 1 4 Path (E) 2 4 Path

(F) 2 3 Path (G) 3 3 Path

FIGURE 3.10: Non-isomorphic Signature Graphs of 4-sets

pentagons form the boundary. To choose such a patch we consider all possible coordinate paths connecting pairs of pentagons in our 4-set and choose the outermost coordinate segments and all contained faces.

We define the *boundary* of an n-set to be the n pentagons of the set as well as the faces on the circuit of coordinate segments in sequential counterclockwise order connecting the pentagons. The boundary of a possible 4-set is illustrated Figure 3.11. In this example, $a = g = 1$, $b = c = d = e = 2$, $f = h = 3$. In order to uniquely describe the boundary of a set we must also account for the angles between the segments. We say the *angle configuration* of the boundary is the internal angle measures listed in counterclockwise order using cycle notation. By Theorem 3.2, in order for the circuit to close,

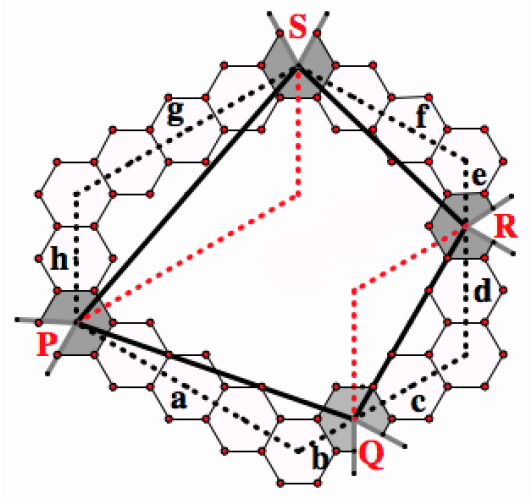



FIGURE 3.11: Boundary of a 4-set

the four angle measures must sum to $3(4-2) = 6$.

Given the angle and segment parameters of the signature configuration there is a segment that wraps around the entirety of the set. We call this the *boundary segment* and we are able to compute the boundary segment's coordinates which we call the *boundary coordinates*. In order to compute the boundary coordinates we unwind all the individual segments between adjacent pentagons on the boundary of the set. This process is shown in Figure 3.12.

First we rotate segment $SP$ 60° to segment $SP'$. We know that 60° rotations in $\Lambda$ take centers of faces to centers of faces so $P'$ represents a new hexagonal face in $\Lambda$. Then we rotate the concatenated segment string $RS$ and $SP'$ 60° so that $S$ rotates to $S'$ and $P'$ rotates to $P''$. Finally, we rotate the resulting string of segments so that $R$ is rotated to $R'$, $S'$ is rotated to $S''$, and $P''$ is rotated to $P'''$. The boundary segment is the segment from $P$ to $P'''$ shown as the blue dashed line in Figure 3.12. The boundary coordinates will be the coordinates associated with the boundary segment.

Boundary coordinates are of particular interest since the relationship between the two coordinates determines whether or not the pentagons in the set are a cluster. If

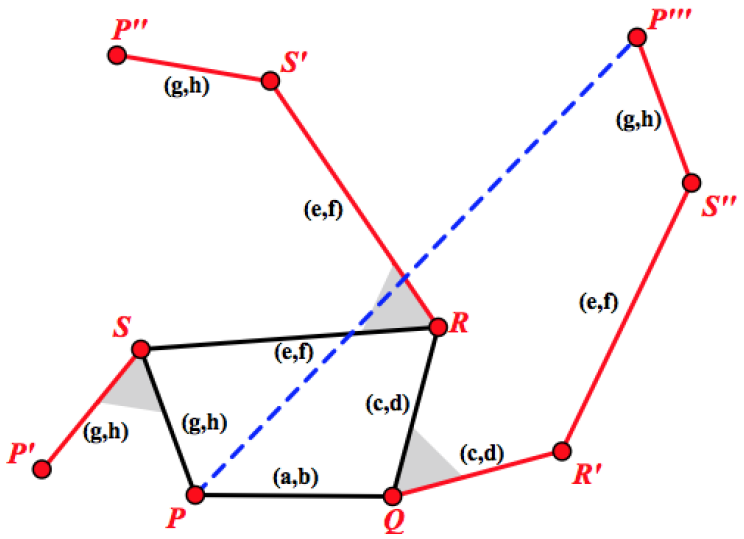



FIGURE 3.12: Unwinding segments in 4-set to find boundary segment

the coordinates of the boundary are congruent module 3, then we know the contained pentagons are a cluster and are able to be connected by chains that need not wrap-around any pentagons external to our 4-set. In this case these four pentagons can be isolated as a unit, all pentagons will be able to be paired by chains and the 4-set is a 4-cluster as defined in Section 1.1.5.

**Lemma 3.3.1.** *Let the boundary of a patch in $\Lambda$ have boundary coordinates $(x, y)$ then the pentagons contained in the patch are chain available if and only if $x - y \equiv_3 0$.*

*Proof.* First assume that $y \geq 0$. Then if $x - y \equiv_3 0$ we know that around the boundary there is no incompatibilities in the coloring. Hence the color incompatibilities are resolved by chains pairing the pentagons within the set. No chains are required to pair a pentagon within the set with one outside the set, otherwise the coloring around the boundary would have the incompatibility of the chain.

If $y < 0$ then we have the coordinates $(-y, x+y)$. Now $(x+y)-(-y) = x+2y \equiv_0 x-y$. Hence the coordinates $x$ and $y$ are congruent modulo 3 if and only if the coordinates

$-y$ and $x + y$ are equivalent modulo 3. Thus we see that the same condition holds regardless of the parity of $y$. □

In this section, we use $\mathscr{S}$ and boundary coordinates to find conditions used to determine whether or not a 4-set with given signature graph is a 4-cluster. To do so, we pair the property of boundary coordinate congruency with the fact that the coordinates of one segment in the boundary are uniquely determined by the coordinates of the other three segments and the angles defining the cluster. Each case is proved similarly so we begin by giving an conceptual overview of the method.

The angles along the boundary determine the orientation of each segment in the embedded tessellation in addition to the orientation of the coordinate paths. The sum of the coordinates of any segment connecting parallel lines of hexagons in the tessellation will always be equal by Lemma 3.1.3. We couple this fact with the underlying structure of the 4-set, which is fixed by the boundary angles, to find two pairs of parallel coordinate paths. Between the parallel sets we find two unique coordinate paths to connect them. We can set the sum of these coordinates equal to each other and solve for the coordinates of one segment based on the coordinates of the other three.

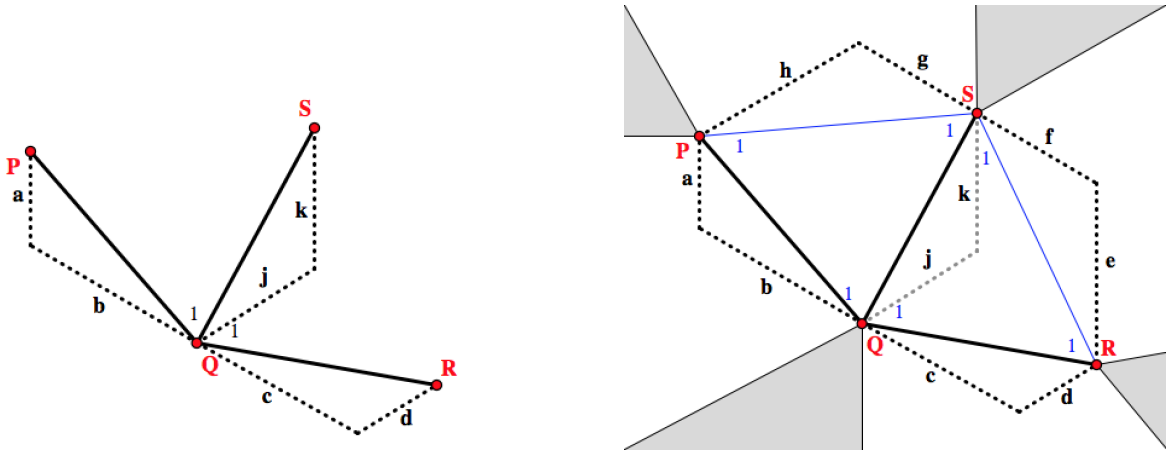
The other piece of information that we need for the following calculations is the boundary coordinates of the 4-set. If we were to consider the 4-set as the cap on a tube then the boundary segment is the segment that would form the circumference of the tube with minimal radius that would not interfere with the 4-set as a cap.

## 3.4 Star Signatures

### 3.4.1 1 1 3 star signature

Consider a 4-set with labeled pentagons, $P,\ Q,\ R$ and $S$, such that a shortest spanning tree consists of one degree 3 vertex at pentagon $Q$ as shown in Figure 3.13a. We begin

by considering the case when $\angle PQS$ and $\angle SQR$ both have measure 1. This forces $\angle PQR$ to have measure 3 in order that the angles around the pentagon sum to 5. We call this signature configuration a 1 1 3 star and when the pentagons in the set are chain available we say that $\{P, Q, R, S\}$ is a 1 1 3 star cluster; the configuration is shown below. Figure 3.13b also includes ancillary segments and coordinates which we will use in further calculations regarding 4-sets of this configuration.




(A) Signature graph of a 1 1 3 star set

(B) Coordinate and angle structure of 1 1 3 star set

FIGURE 3.13: Structure of a 1 1 3 Star Set

**Lemma 3.4.1.** *Every 4-set represented by a 1 1 3 star signature graph, has an ordered boundary angle configuration of (1 2 1 2).*

*Proof.* By Lemma 6.11a all the angles in the boundary of the 3-set $\{Q, R, S\}$ must have measure 1 since angle $RQS$ has measure 1 and is included in the signature. Similarly all the angles in the boundary of $\{P, Q, S\}$ must also have measure 1. By identifying the $SQ$ segment on the boundary of two the 3-sets, the boundary of the resulting 4-set has two angles of measure 2 each separated by angles of measure 1 as we see in Figure 3.13b.

□

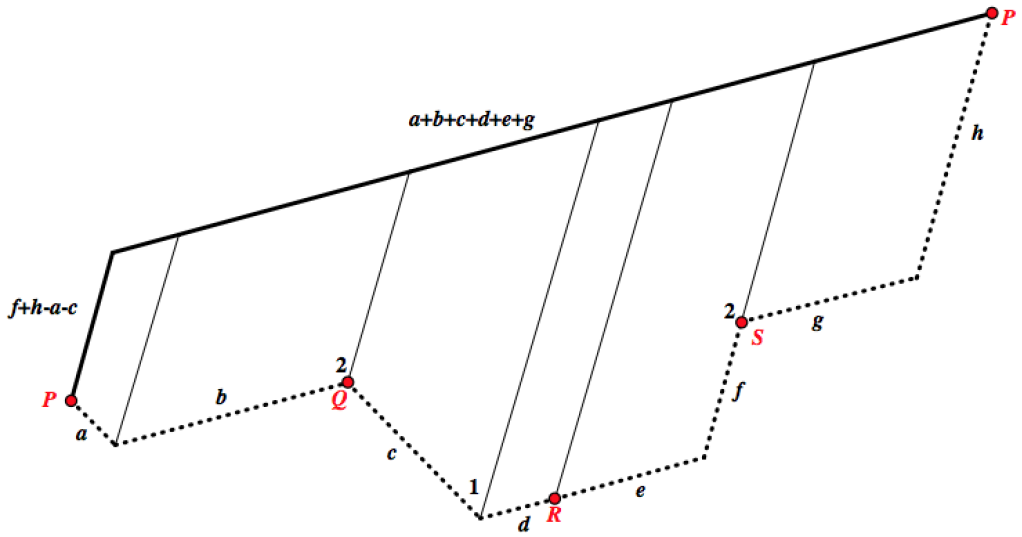



FIGURE 3.14: Unwound boundary of (1 2 1 2) 4-set

**Lemma 3.4.2.** *If a 4-set, $\{P, Q, R, S\}$, has an ordered boundary angle configuration of (1 2 1 2) then the unwound boundary segment has coordinates*

$$(b + d + e + f + g + h,\ a + c - f - h) \text{ when } a + c > f + h$$

*and alternatively the boundary segment has coordinates*

$$(f + h - a - c,\ a + b + c + d + e + g)) \text{ when } a + c \leq f + h$$

*Proof.* Starting at pentagon $P$ and working counterclockwise around the boundary, we form the boundary segment by closing the wedges shown in Figure 3.13b. By unwinding the coordinate paths of the boundary in this way and embedding the new path in hexagonal tessellation, we calculate the coordinates between the initial pentagon and it's second identified location in the tessellation. If the second coordinate is negative we rewrite the coordinates using Lemma 2.2.2.

The unwound boundary of the patch is shown in Figure 3.14 and we calculate, that the boundary coordinates are given by

$$(a+b+c+d+e+g,\ f+h-a-c)$$

Now if $a+c > f+h$ we use Lemma 2.2.2 to see that the other possible set of coordinates is given by:

$$(a+c-f-h,\ b+d+e+f+g+h)$$

□

**Theorem 3.4.3.** *If a 4-set $\{P,Q,R,S\}$ is represented by a 1 1 3 star signature graph then $\{P,Q,R,S\}$ is a 4-cluster if any only if $(a-b)+(j-k)+(c-d) \equiv_3 0$.*

*Proof.* We label the signature and underlying coordinate structure as in Figure 3.13b. In order to prove sufficient and necessary conditions for $\{P,Q,R,S\}$ to be a 4-cluster, we will prove necessary and sufficient conditions to guarantee that the boundary coordinates are congruent modulo 3. In this configuration the coordinate paths labeled $h$ and $j$ in Figure 3.13b are parallel so by Lemma 3.1.3, $g+k=a+b$. In addition, $b$ and $g$ are parallel giving us $h+a=j+k$. Thus we have that $g=a+b-k$ and $h=j+k-a$. We can similarly calculate that $e=j+k-d$ since $c$ and $f$ are parallel and $f=c+d-j$ since $k$ and $d$ are parallel.

From Lemma 3.4.2 we know that the boundary segment has two possible sets of boundary coordinates. Namely, $(b+d+e+f+g+h,\ a+c-f-h)$ if $a+c>f+h$ and $(f+h-a-c,\ a+b+c+d+e+g)$ if $a+c \leq f+h$. By Lemma 3.3.1 we know that $\{P,Q,R,S\}$ is a 4 cluster exactly when the difference of one possible set of coordinates is congruent to 0.

For this 4-set configuration we will show that $[b+d+e+f+g+h]-[a+c-f-h] \equiv_3 0$. Substituting in our expressions for $g$, $h$, $e$ and $f$ yields the following chain of equivalenct conditions for $\{P, Q, R, S\}$ to be a 4-cluster.

$$
\begin{aligned}
&[b+d+e+f+g+h]-[a+c-f-h] \equiv_3 0 \\
&\iff b-a+d-c+e+2f+g+2h \equiv_3 0 \\
&\iff b-a+d-c+e-f+g-h \equiv_3 0 \\
&\iff b-a+d-c+[j+k-d]-[c+d-j]+[a+b-k]-[j+k-a] \equiv_3 0 \\
&\iff 2b+a-2c-d+j-k \equiv_3 0 \\
&\iff (a-b)+(c-d)+(j-k) \equiv_3 0
\end{aligned}
$$

□

### 3.4.2 1 2 2 Star Cluster

The other possible signature graph with a degree 3 vertex at pentagon $Q$ is shown in Figure 3.15. We consider the case when angle $PQS$ has measure 2 and angle $SQR$ has measure 1 which forces angle $PQR$ to have measure 2. We call this signature configuration a 1 2 2 star signature and when $\{P, Q, R, S\}$ are chain available we call it a 1 2 2 star cluster. For this case, as well as all the remaining ones, we will use a method similar to that of the 1 1 3 star cluster but will combine all the preliminary lemmas as well as the main result into one theorem for each case.

Remember that angles are measured between the first legs of coordinate paths. So from now on we will not put in the segment lines unless the segments are in the signature graph of the 4-cluster. Furthermore, recall that if coordinate paths lie on opposite sides of the two adjacent segments then we divide the geometric angle by 60°

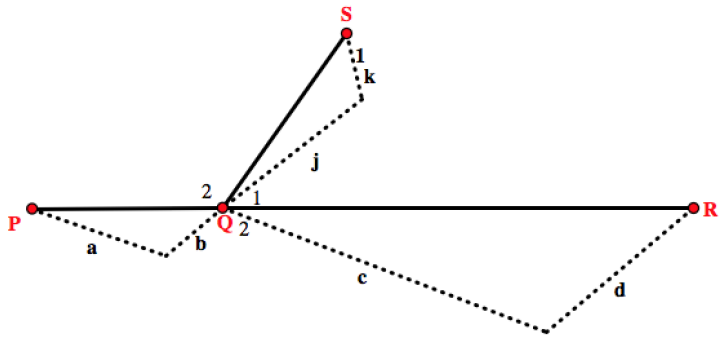


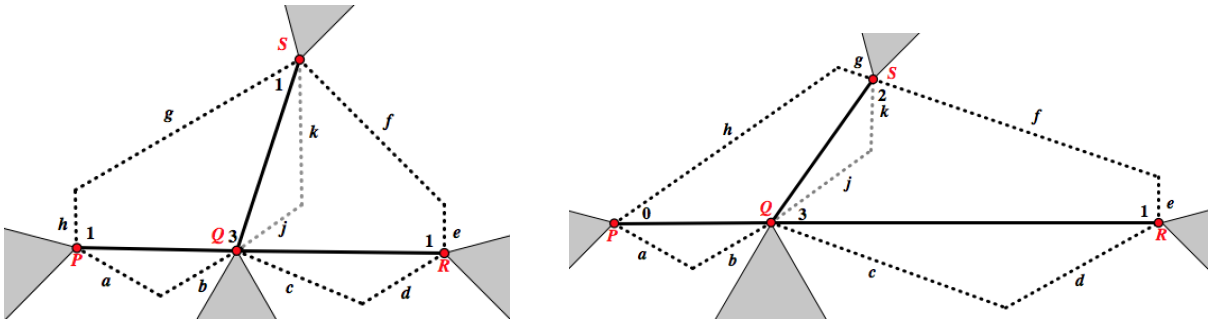

FIGURE 3.15: Signature graph of a 1 2 2 star set

to get the fullerene angle measure and if the two coordinate paths lie on the same side of two segments we divide by 60° and subtract 1 to get the fullerene angle measure.

**Theorem 3.4.4.** *A 4-set with the signature of a 1 2 2 star labeled as above is a 4-cluster if and only if* $(a-b)+(j-k)+(d-c) \equiv_3 0$.

*Proof.* By Lemma 6.11a all the angles in the boundary of the $QRS$ set must have measure 1 since angle $RQS$ has measure 1 and is included in the signature. We have no such restriction on the angles in the 3-set $\{P, Q, S\}$ so we must consider both possible angle configurations. For each we will find the boundary coordinates and find the conditions that ensure that these coordinates are congruent. The angles in triangle $PQS$ must have measures 0, 1 and 2. By identifying the $SQ$ segment of the boundaries, the boundary of the resulting 4-set either has ordered boundary angles of measure (1 3 1 1) or (0 3 1 2) as we see in Figure 3.16.

First consider the case where the boundary angles are given by (1 3 1 1) as shown in Figure 3.16a. Considering the underlying coordinate structure of a 4-set of this type we have that the coordinate paths $g$ and $b$ are parallel which gives us that $h = k - a$ by Lemma 3.1.3. In addition, $h$ and $k$ are parallel giving us $g = a + b + j$. Similarly we see that $e = k + j - d$ since $f$ and $c$ are parallel and $f = c + d - j$ since $k$ and $e$ are parallel.




(A) Boundary angles (1 3 1 1) (B) Boundary angles (0 3 1 2)

FIGURE 3.16: Underlying coordinate structure and internal triangless of a 1 2 2 star set

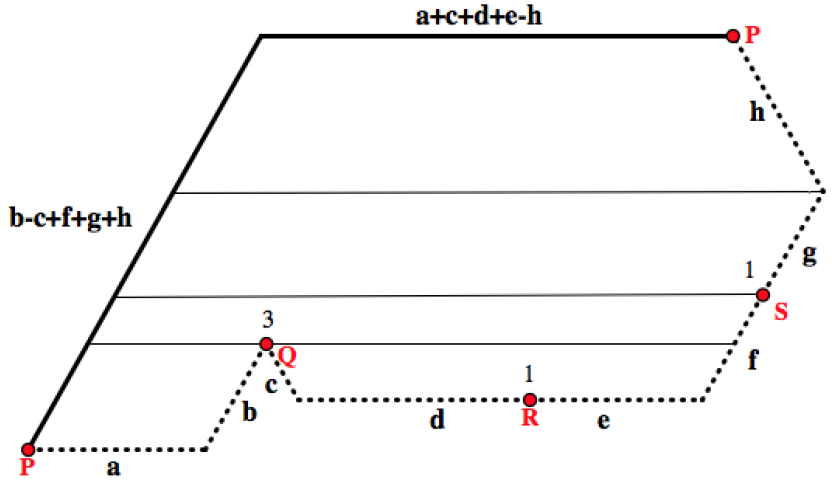



FIGURE 3.17: Unwound boundary of (1 3 1 1) 4-set

By unwinding the coordinate paths of the boundary we find that the boundary segment has the following coordinates when $h < a + c + d + e$:

$$(a + c + d + e - h,\ b - c + f + g + h)$$

Thus by Lemma 2.2.2 when $h \geq a + c + d + e$ the boundary coordinates are given by

$$(b - c + f + g + h,\ a + b + d + e + f + g)$$

By Lemma 3.3.1 we know that $\{P, Q, R, S\}$ is a 4 cluster exactly when the difference of one of these possible sets of coordinates is congruent to 0.

This 4-set configuration will be a 4-cluster if and only if $[b-c+f+g+h]-[a+c+d+e-h] \equiv_3 0$. Substituting in our expressions for $g$, $h$, $e$ and $f$ yields the following chain of equivalence necessary and sufficient conditions for $\{P, Q, R, S\}$ to be a 4-cluster.

$$
\begin{aligned}
&[b-c+f+g+h]-[a+c+d+e-h] \equiv_3 0 \\
&\iff -a+b-2c-d-e+f+g+2h \equiv_3 0 \\
&\iff -a+b-2c-d-[k+j-d]+[c+d-j]+[a+b+j]-[k-a] \equiv_3 0 \\
&\iff a+2b-2c+d-j-2k \equiv_3 0 \\
&\iff (a-b)+(d-c)+(k-j) \equiv_3 0
\end{aligned}
$$

Now we consider the case where the boundary angles are (0 3 1 2) as shown in Figure 3.16b. In this case, by considering parallel sets of coordinate paths we have that $g = a-k$ since $b$ and $h$ are parallel, $h = b+j+k$ since $g$ and $a$ are parallel, $e = k+j-d$ since $f$ and $c$ are parallel and $f = c+d-j$ since $k$ and $e$ are parallel.

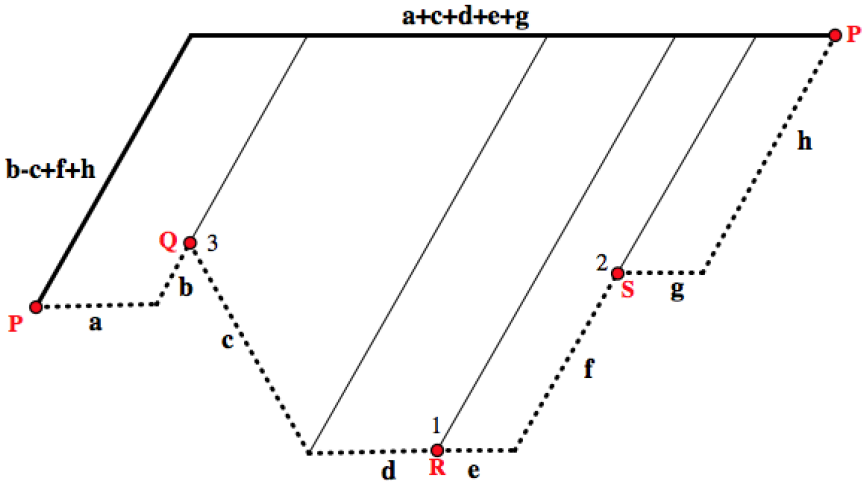



FIGURE 3.18: Unwound boundary of (0 3 1 2) 4-set

By unwinding the coordinate paths of the boundary we find that the boundary segment has the following coordinates when $c < b + f + h$:

$$(a + c + d + e + g,\ b - c + f + h)$$

Thus by Lemma 2.2.2 when $c \geq b + f + h$ the boundary coordinates are given by

$$(-b + c - f - h,\ a + b + d + e + f + g + h)$$

By Lemma 3.3.1 we know that $\{P, Q, R, S\}$ is a 4 cluster exactly when the difference of one of these possible sets of coordinates is congruent to 0.

This 4-set configuration will be a 4-cluster if and only if $[b - c + f + h] - [a + c + d + e + g] \equiv_3 0$. Substituting in our expressions for $g$, $h$, $e$ and $f$ yields the following chain of equivalence necessary and sufficient conditions for $\{P, Q, R, S\}$ to be a 4-cluster.

$$\begin{aligned}
&[b - c + f + h] - [a + c + d + e + g] \equiv_3 0 \\
&\iff -a + b - 2c - d - e + f - g + h \equiv_3 0 \\
&\iff -a + b - 2c - d - [k + j - d] + [c + d - j] - [a - k] + [b + j + k] \equiv_3 0 \\
&\iff -2a + 2b - c + d - j + k \equiv_3 0 \\
&\iff (a - b) + (d - c) + (k - j) \equiv_3 0
\end{aligned}$$

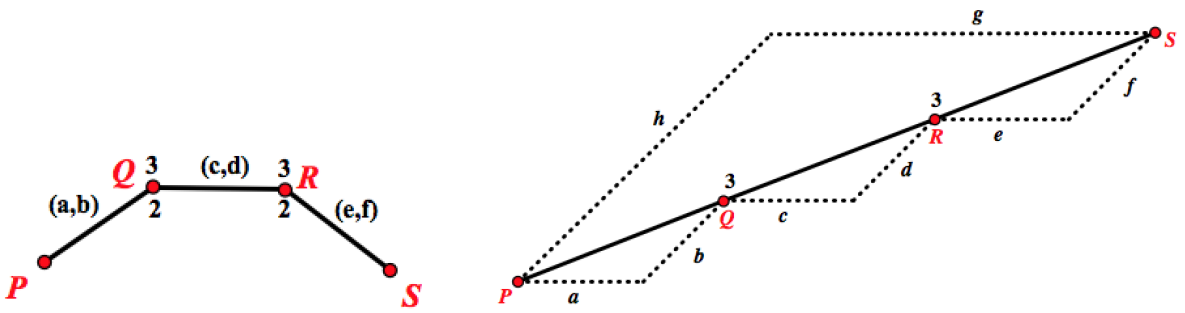
Hence, since the claim holds for both possible sets of boundary angles, all 1 2 2 star sets are 4-clusters exactly when $(a - b) + (d - c) + (k - j) \equiv_3 0$. □

## 3.5 Path Signatures

Now we consider signatures in the form of a path. We will prove that, for any 4-set with a path signature, if the sum of these two angle measures is even then the 4 set is a cluster if and only if $a - b \equiv_3 f - e$ and if the sum of these two angle measures is odd then the 4 set is a cluster if and only if $a - b \equiv_3 e - f$.

### 3.5.1 3 3 path signature

First we consider the signature graph with two included angles of measure 3. This configuration is symmetric to a 2 2 path signature. The signature graph for this configuration is shown in Figure 3.19a.




(A) 3 3 Path Signature (B) Boundary angle configuration (0 3 3 0)

FIGURE 3.19: Underlying coordinate structure of 3 3 path set with boundary configuration (0 3 3 0)

**Lemma 3.5.1.** *If a 4-set $\{P, Q, R, S\}$ is represented by a 3 3 path signature graph then $\{P, Q, R, S\}$ is a 4-cluster if and only if $(a - b) + (e - f) \equiv_3 0$*

*Proof.* We begin by forming a patch so that the two angles of measure 3 lie internal to the patch. Since the boundary angles must sum to 6 we know that the remaining two internal angles must both have measure 0. Thus we have boundary angle configuration (0 3 3 0) for any 4-set with this signature. Three of the boundary segments are

given by the segments in the signature and the fourth segment is given by $(g, h)$. The underlying boundary coordinate structure is shown along with the signature in Figure 3.19b.

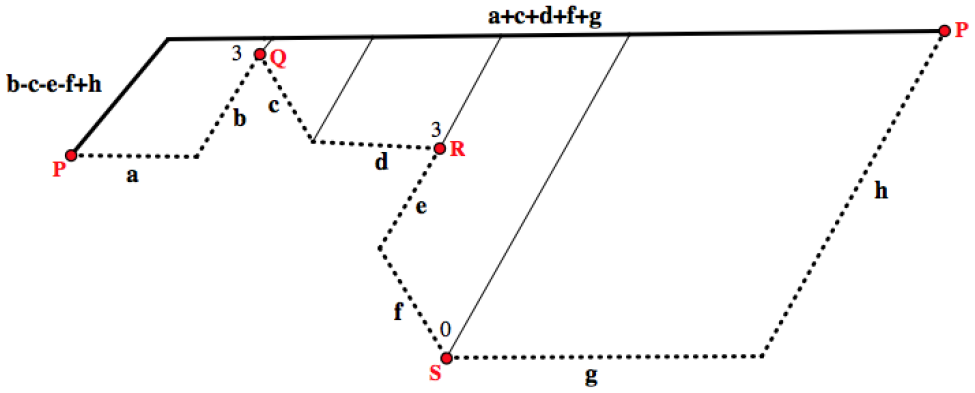



FIGURE 3.20: Unwound boundary of (0 3 3 0) 4-set

In the underlying coordinate structure of a 4-set with boundary angles (0 3 3 0), $f$ and $h$ are parallel which gives us that $g = a + c + e$. In addition, $a$ and $g$ are parallel giving us $h = b + d + f$. By unwinding the coordinate paths of the boundary we find that the boundary segment has the following coordinates when $b + h \geq c + e + f$:

$$(a + c + d + f + g,\ b - c - e - f + h)$$

By Lemma 2.2.2 we know that $b + h < c + e + f$ yields boundary coordinates given by

$$(-b + c + e + f - h,\ a + b + d - e + g + h)$$

Additionally, by Lemma 3.3.1 we know that $\{P, Q, R, S\}$ is a 4 cluster exactly when the difference of one of these possible sets of coordinates is congruent to 0.

This 4-set configuration will be a 4-cluster if and only if $[b - c - e - f + h] - [a + c + d + f + g] \equiv_3 0$. Substituting in our expressions for $g$ and $h$ yields the following chain

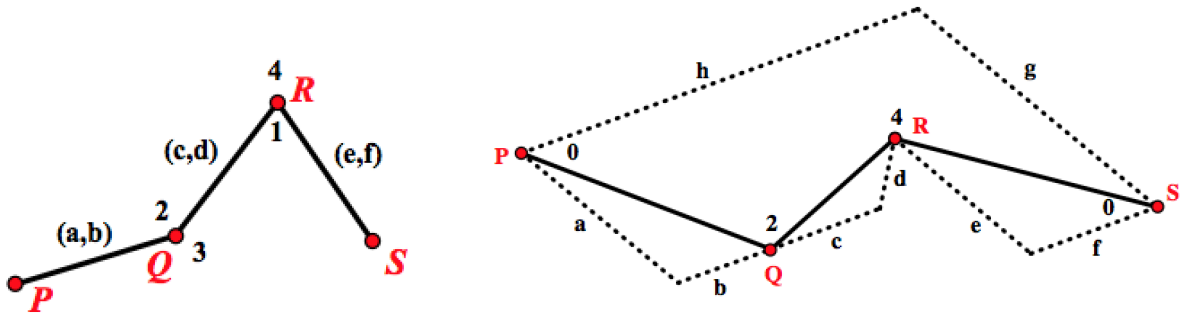
of equivalence necessary and sufficient conditions for $\{P, Q, R, S\}$ to be a 4-cluster.

$$
\begin{aligned}
&[b-c-e-f+h]-[a+c+d+f+g] \equiv_3 0 \\
&\qquad \iff b-c-e-f+b+d+f-a-c-d-f-a-c-e \equiv_3 0 \\
&\qquad \iff 2b-2a-3c-f-2e \equiv_3 0 \\
&\qquad \iff (a-b)+(e-f) \equiv_3 0
\end{aligned}
$$

□

### 3.5.2 2 4 path signature

Now consider the signature graph with two included angles of measure 2 and 4. This is symmetric to a path signature graph with internal angles of 3 and 1. This signature graph is shown in Figure 3.21a




(A) 2 4 Path Signature (B) Boundary angle configuration (0 2 4 0)

FIGURE 3.21: Underlying coordinate structure of 2 4 path set with boundary configuration (0 2 4 0)

**Lemma 3.5.2.** *If a 4-set $\{P, Q, R, S\}$ is represented by a 2 4 path signature graph then $\{P, Q, R, S\}$ is a 4-cluster if and only if $(a-b)+(e-f) \equiv_3 0$*

*Proof.* Form a patch so that the angles of measure 2 and 4 lie internal to the patch. Since the boundary angles must sum to 6 we again know that the remain two internal angles must both have measure 0. The underlying coordinate structure is shown along with the signature graph in Figure 3.21b.

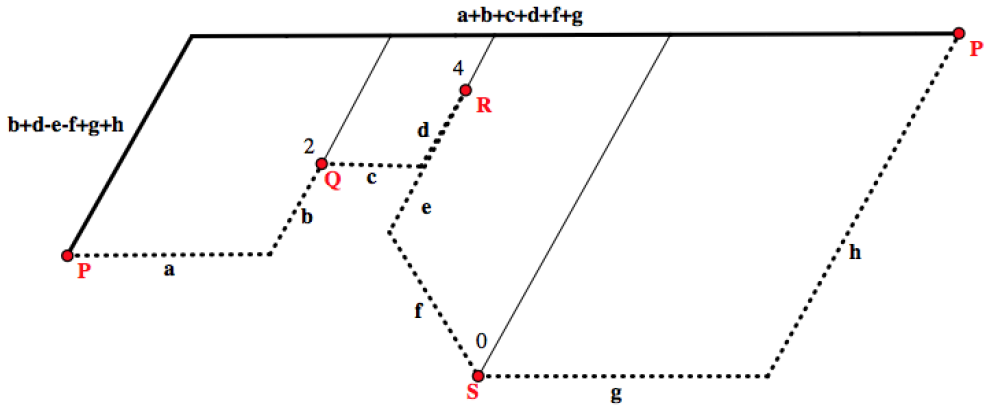



FIGURE 3.22: Underlying coordinate structure 2 4 path set with boundary configuration (0 2 4 0)

In the underlying coordinate structure of a patch with boundary angles of measure (0 2 4 0), $f$ and $h$ are parallel which gives us that $g = a - d + e$. In addition, $a$ and $g$ are parallel giving us $h = b + c + d + f$.

By unwinding the coordinate paths of the boundary we find that the boundary segment has the following coordinates when $e + f < b + d + h$:

$$(a + c + f + g,\ b + d - e - f + h)$$

. By Lemma 2.2.2 we know that $e + f \geq b + d + h$ yields boundary coordinates given by

$$(-b - d + e + f - h,\ a + b + c + d - e + g + h)$$

Additionally, by Lemma 3.3.1 we know that $\{P, Q, R, S\}$ is a 4 cluster exactly when the difference of one of these possible sets of coordinates is congruent to 0.

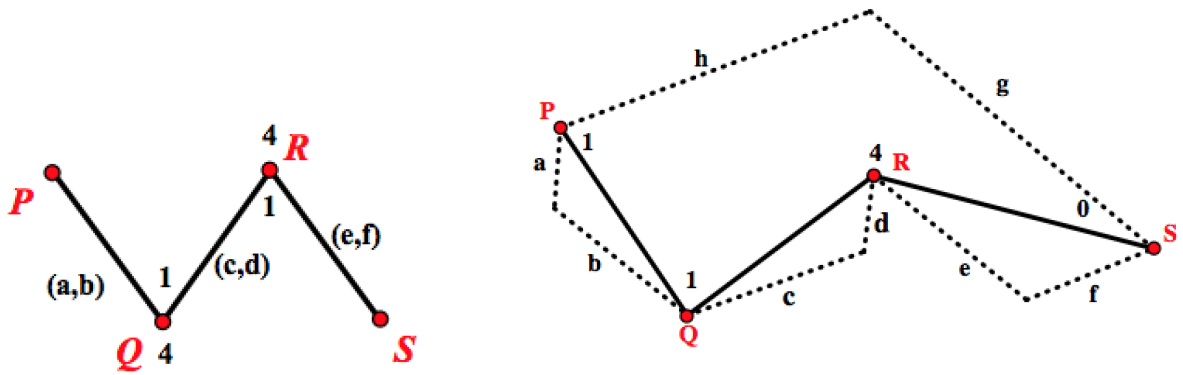
This 4-set configuration will be a 4-cluster if and only if $[b+d-e-f+h]-[a+c+f+g] \equiv_3 0$. Substituting in our expressions for $g$ and $h$ yields the following chain of equivalence necessary and sufficient conditions for $\{P,Q,R,S\}$ to be a 4-cluster.

$$
\begin{aligned}
&[b+d-e-f+h]-[a+c+f+g] \equiv_3 0 \\
&\qquad \iff b+d-e-f+b+c+d+f-a-c-f-a+d-e \equiv_3 0 \\
&\qquad \iff 2b-2a+3d-f-2e \equiv_3 0 \\
&\qquad \iff (a-b)+(e-f) \equiv_3 0
\end{aligned}
$$

□

### 3.5.3 1 4 path signature

Now consider the signature graph with two included angles of measure 1 and 4. This is another self symmetric configuration. This signature graph is shown in Figure 3.23a.




(A) 1 4 Path Signature (B) Boundary angle configuration (1 1 4 0)

FIGURE 3.23: Underlying coordinate structure of 1 4 path set with boundary configuration (1 1 4 0)

**Lemma 3.5.3.** *If a 4-set $\{P,Q,R,S\}$ is represented by a 1 4 path signature graph then $\{P,Q,R,S\}$ is a 4-cluster if any only if $(a-b)+(f-e) \equiv_3 0$*

*Proof.* Form a patch so that the angles of measure 1 and 4 lie internal to the patch. We know that since a measure of angle 1 is found in the signature, the other angles in the triangle, when we construct the side opposite the included angle, will both have measure 1. Therefore the angle on the boundary at pentagon $P$ will have measure at least 1. Since the boundary angles must sum to 6, we now must have that the angle at pentagon $R$ has measure 0 and we have a boundary of angle configuration (0 1 1 4). The underlying coordinate structure is shown along with the signature graph in Figure 3.23b

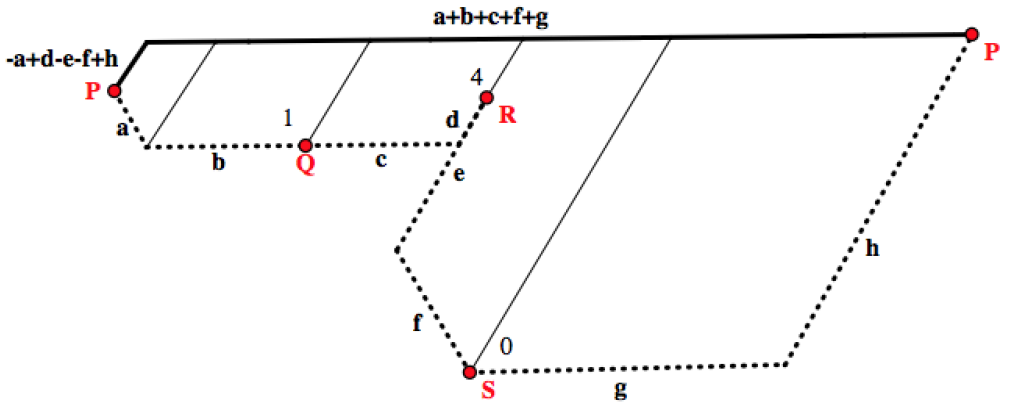



FIGURE 3.24: Unwound boundary of (1 1 4 0) 4-set

In the underlying coordinate structure of a 4-set with boundary angles (1 1 4 0), $b$ and $g$ are parallel which gives us that $h = c+d+f-a$. In addition, $h$ and $f$ are parallel giving us $g = e + b + a - d$. By unwinding the coordinate paths of the boundary we find that the boundary segment has the following coordinates when $e + g \geq b + c + d$:

$$(a + b + c + f + g,\ -a + d - e - f + h)$$

By Lemma 2.2.2 we know that $e + g < b + c + d$ yields boundary coordinates given by

$$(a - d + e + f - h,\ b + c + d - e + g + h)$$

Additionally, by Lemma 3.3.1 we know that $\{P, Q, R, S\}$ is a 4 cluster exactly when the difference of one of these possible sets of coordinates is congruent to 0.

This 4-set configuration will be a 4-cluster if and only if $[-a+d-e-f+h]-[a+b+c+f+g] \equiv_3 0$. Substituting in our expressions for $g$ and $h$ yields the following chain of equivalence necessary and sufficient conditions for $\{P, Q, R, S\}$ to be a 4-cluster.

$$
\begin{aligned}
&[-a+d-e-f+h]-[a+b+c+f+g] \equiv_3 0 \\
&\iff -2a-b-c+d-e-2f-g+h \equiv_3 0 \\
&\iff a-b-c+d-e+f-[e+b+a-d]+[c+d+f-a] \equiv_3 0 \\
&\iff -a-2b+3d-2e+2f \equiv_3 0 \\
&\iff (b-a)+(e-f) \equiv_3 0
\end{aligned}
$$

□

### 3.5.4 2 3 path signature

Now consider the signature graph with two included angles of measure 2 and 3. This is the final self symmetric signature form. This signature graph is shown in Figure 3.25

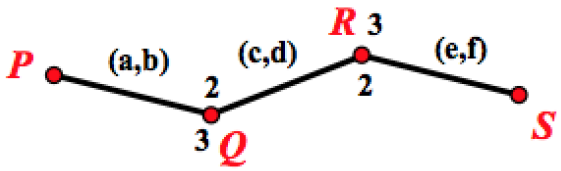
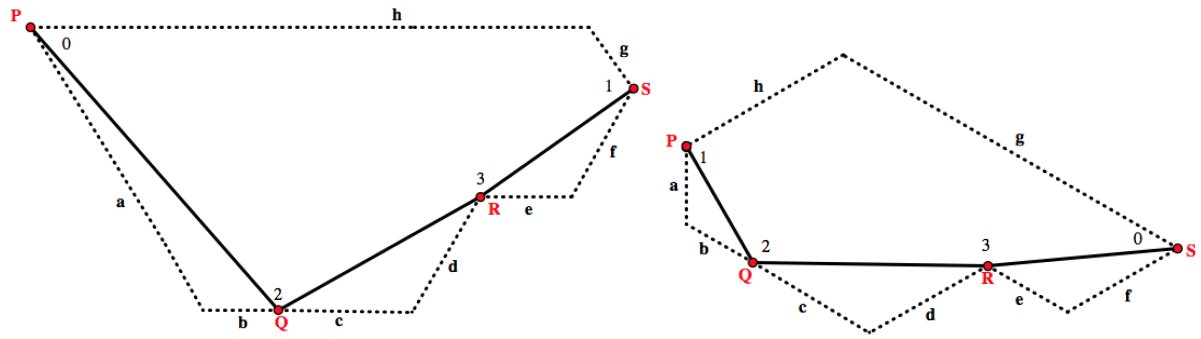



FIGURE 3.25: 2 3 path signature

**Lemma 3.5.4.** *If a 4-set $\{P, Q, R, S\}$ is represented by a 2 3 path signature graph then $\{P, Q, R, S\}$ is a 4-cluster if any only if $(a-b)+(f-e) \equiv_3 0$*




(A) Boundary angle configuration (0 2 3 1) (B) Boundary angle configuration (1 2 3 0)

FIGURE 3.26: Two possible boundary angle configuration for 2 3 path signature

*Proof.* Form a patch so that the angles of measure 2 and 3 lie internal to the patch. Since the boundary angles must sum to 6 we know that one of the remaining angles must have measure 1 and the other have measure 0. We check the two possible configurations separately. The underlying coordinate structure of both cases are shown along with the signature graph in Figure 3.30

First let us consider the case shown in Figure 3.26a. In this case the boundary angles are (0 2 3 1). In the underlying structure, $b$ and $h$ are parallel which gives us that $g = a - d - f$. In addition, $a$ and $g$ are parallel giving us $h = b + c + e + d + f$. By unwinding the coordinate paths of the boundary we find that the boundary segment has the following coordinates when $e < b + d + h$:

$$(a + c + e + f + g,\ b + d - e + h)$$

By Lemma 2.2.2 we know that $e \geq b + d + h$ yields boundary coordinates given by

$$(-b - d + e - h,\ a + b + c + d + f + g + h)$$

Additionally, by Lemma 3.3.1 we know that $\{P, Q, R, S\}$ is a 4 cluster exactly when the difference of one of these possible sets of coordinates is congruent to 0.

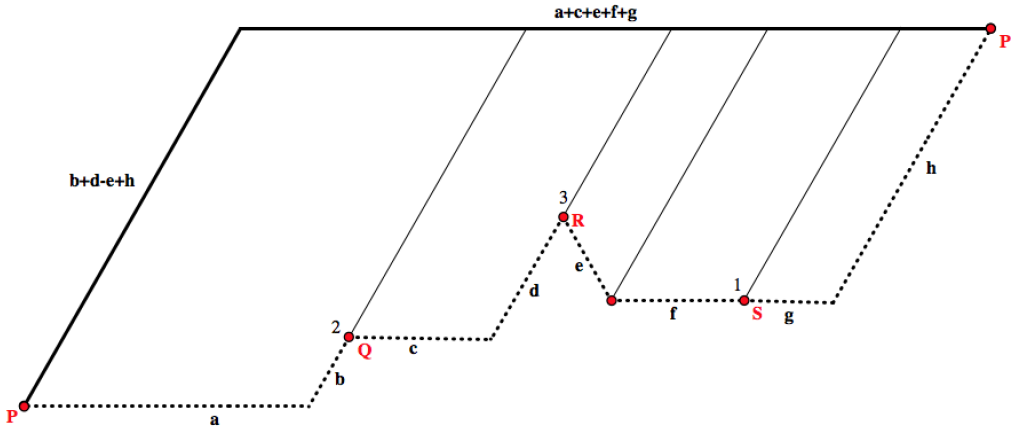



FIGURE 3.27: Unwound boundary of (0 2 3 1) 4-set

This 4-set configuration will be a 4-cluster if and only if $[b+d-e+h]-[a+c+e+f+g] \equiv_3 0$. Substituting in our expressions for $g$ and $h$ yields the following chain of equivalence necessary and sufficient conditions for $\{P, Q, R, S\}$ to be a 4-cluster.

$$
\begin{aligned}
&[b+d-e+h]-[a+c+e+f+g] \equiv_3 0 \\
&\quad \iff -a+b-c+d-2e-f-g+h \equiv_3 0 \\
&\quad \iff -a+b-c+d-2e-f-[a-d-f]+[b+c+e+d+f] \equiv_3 0 \\
&\quad \iff -2a+2b+3d+2e+f \equiv_3 0 \\
&\quad \iff (b-a)+(e-f) \equiv_3 0
\end{aligned}
$$

Alternatively, consider the angles are in the configuration (1 2 3 0) as shown in Figure 3.26b. In the underlying coordinate structure $f$ and $h$ are parallel which gives us that $g = a+b+c+e$. In addition, $b$ and $g$ are parallel giving us $h = d+f-a$. By unwinding the coordinate paths of the boundary we find that the boundary segment has the following coordinates when $e < b+d+g+h$:

$$(a+c+e+f-h,\ b+d-e+g+h)$$

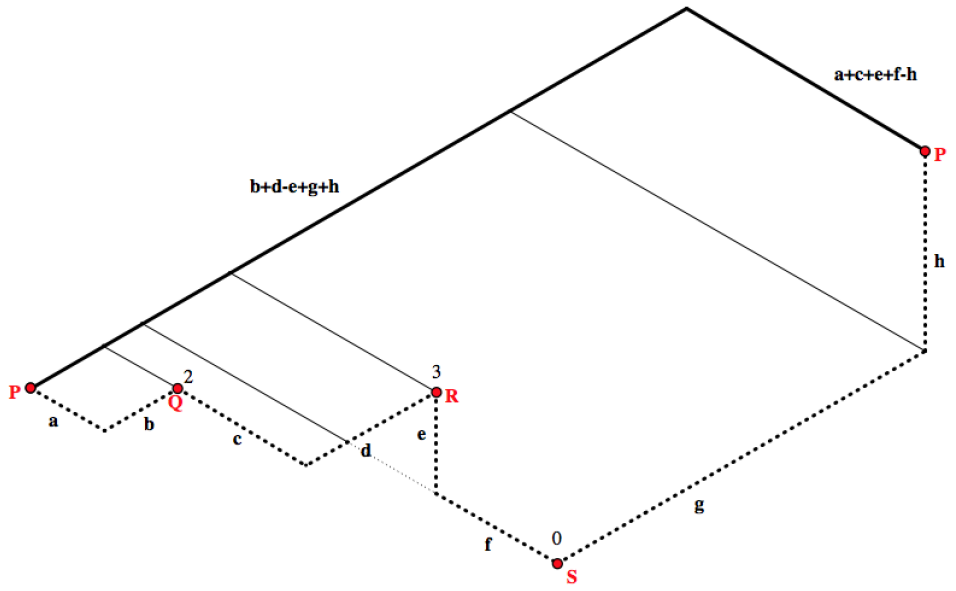



FIGURE 3.28: Unwound boundary of (1 2 3 0) 4-set

By Lemma 2.2.2 we know that $e \geq b+d+g+h$ yields boundary coordinates given by

$$(-b-d+e-g-h,\ a+b+c+d+f+g)$$

Additionally, by Lemma 3.3.1 we know that $\{P,Q,R,S\}$ is a 4 cluster exactly when the difference of one of these possible sets of coordinates is congruent to 0.

This 4-set configuration will be a 4-cluster if and only if $[a+b+c+d+f+g]-[-b-d+e-g-h] \equiv_3 0$ . Substituting in our expressions for $g$ and $h$ yields the following chain of equivalence necessary and sufficient conditions for $\{P,Q,R,S\}$ to be a 4-cluster.

$$[b+d-e+g+h]-[a+c+e+f-h] \equiv_3 0$$

$$\iff -a+b-c+d-2e-f+g+2h \equiv_3 0$$

$$\iff -a+b-c+d+e-f+[a+b+c+e]-[d+f-a] \equiv_3 0$$

$$\iff (a-b)+(f-e) \equiv_3 0$$

Again we have the relation that $\{P, Q, R, Q\}$ is a cluster if $(a - b) + (f - e) \equiv_3 0$ so the claim holds for all 2 3 path sets.

□

### 3.5.5 1 2 path signature

Our final case to consider is the signature path graph with two included angles of measure 1 and 2. This signature form is symmetric when the two included angles are 4 and 3. However, it is worth noting that in forming a patch there is no way to close the boundary if the angle 4 and 3 are chosen to be internal to the patch since they exceed the angle measure bound of 6. This signature graph is shown in Figure 3.29

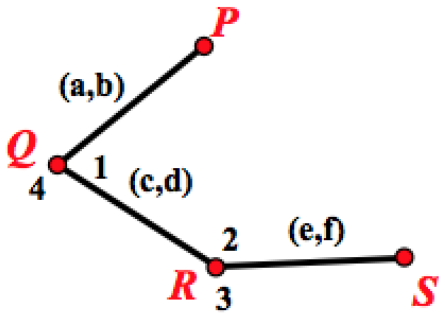
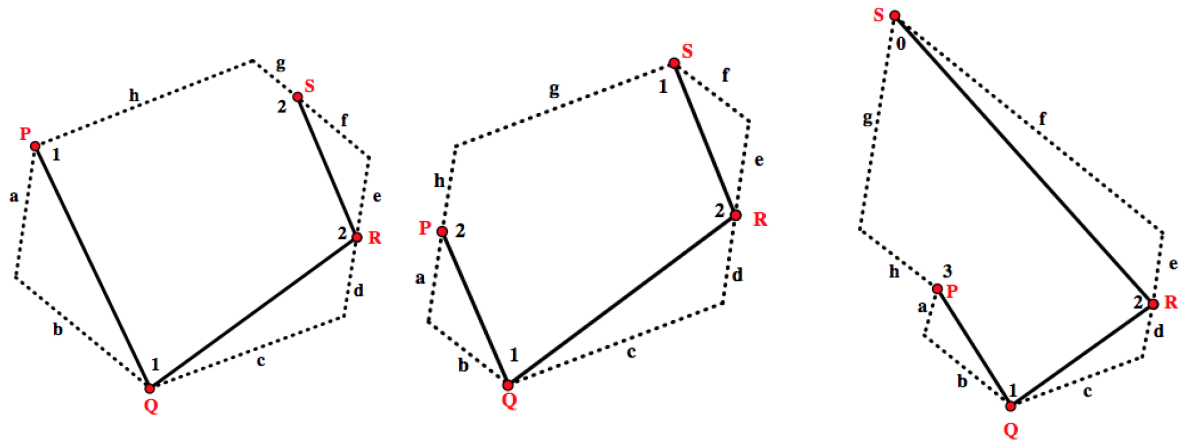



FIGURE 3.29: 1 2 path signature

**Lemma 3.5.5.** *If a 4-set $\{P, Q, R, S\}$ is represented by a 1 2 path signature graph then $\{P, Q, R, S\}$ is a 4-cluster if and only if $(a - b) + (f - e) \equiv_3 0$*

*Proof.* Form a patch so that the angles of measure 2 and 3 lie internal to the patch. Since the boundary angles must sum to 6 we know that one of the remaining angles must have measure 1 and 2 or measure 0 and 3. Since we have an angle 1 included in the signature we know that it will not lie adjacent to an angle 0 in the signature. Thus we have three possible configurations, namely with angle configurations (1 1 2 2 ), (2 1 2 1) and (3 1 2 0). We will work through the three cases separately.




(A) Boundary angle configuration (1 1 2 2 )

(B) Boundary angle configuration (2 1 2 1)

(C) Boundary angle configuration (3 1 2 0)

FIGURE 3.30: Two possible boundary angle configuration for 2 3 path signature

We begin with the case in Figure 3.30a.

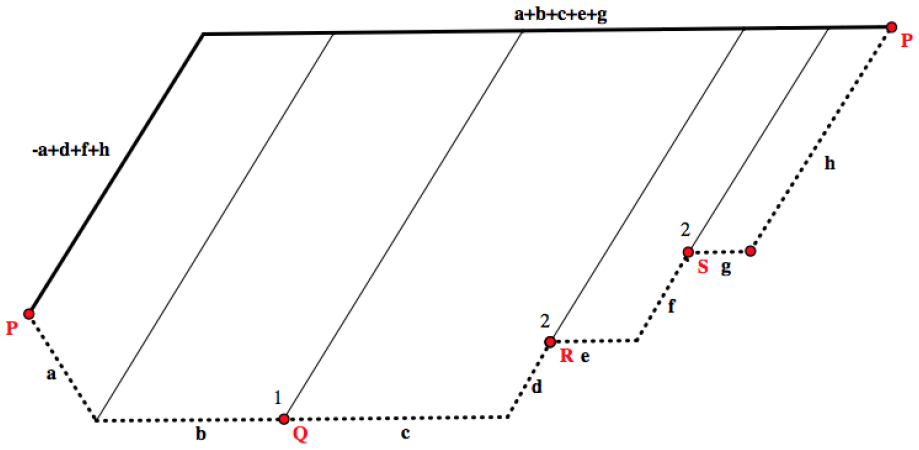



FIGURE 3.31: Unwound boundary of (1 1 2 2) 4-set

In the underlying coordinate structure of a cluster with boundary angles (1 1 2 2), coordinate paths $c$ and $h$ are parallel which gives us that $g = a+b-d-e-f$. In addition, $b$ and $g$ are parallel giving us $h = e + d + c - a$. By unwinding the coordinate paths of the boundary we find that the boundary segment has the following coordinates when

$a < d + f + h$:

$$(a + b + c + e + g,\ d + f + h - a)$$

By Lemma 2.2.2 we know that $a \geq d + f + h$ yields boundary coordinates given by

$$(a - d - f - h,\ b + c + d + e + f + g + h)$$

Additionally, by Lemma 3.3.1 we know that $\{P, Q, R, S\}$ is a 4 cluster exactly when the difference of one of these possible sets of coordinates is congruent to 0.

This 4-set configuration will be a 4-cluster if and only if $[d + f + h - a] - [a + b + c + e + g] \equiv_3 0$. Substituting in our expressions for $g$ and $h$ yields the following chain of equivalence necessary and sufficient conditions for $\{P, Q, R, S\}$ to be a 4-cluster.

$$\begin{aligned}
&[d + f + h - a] - [a + b + c + e + g] \equiv_3 0 \\
&\quad \iff -2a - b - c + d - e + f - g + h \equiv_3 0 \\
&\quad \iff -2a - b - c + d - e + f - [a + b - d - e - f] + [e + d + c - a] \equiv_3 0 \\
&\quad \iff (a - b) + (f - e) \equiv_3 0
\end{aligned}$$

This proves the lemma for the boundary angle configuration (1 1 2 2).

Now we move to the case with boundary angles of (2 1 2 1) shown in Figure 3.30b. In the underlying coordinate structure of a cluster with boundary angles (2 1 2 1), coordinate paths $c$ and $g$ are parallel which gives us that $h = f + e + d - a - b$. In addition, $d$ and $h$ are parallel giving us $g = b + c - f$. First we consider the case when $a < d + f + g + h$ in which the coordinates are given by:

$$(a + b + c + e - h,\ -a + d + f + g + h)$$

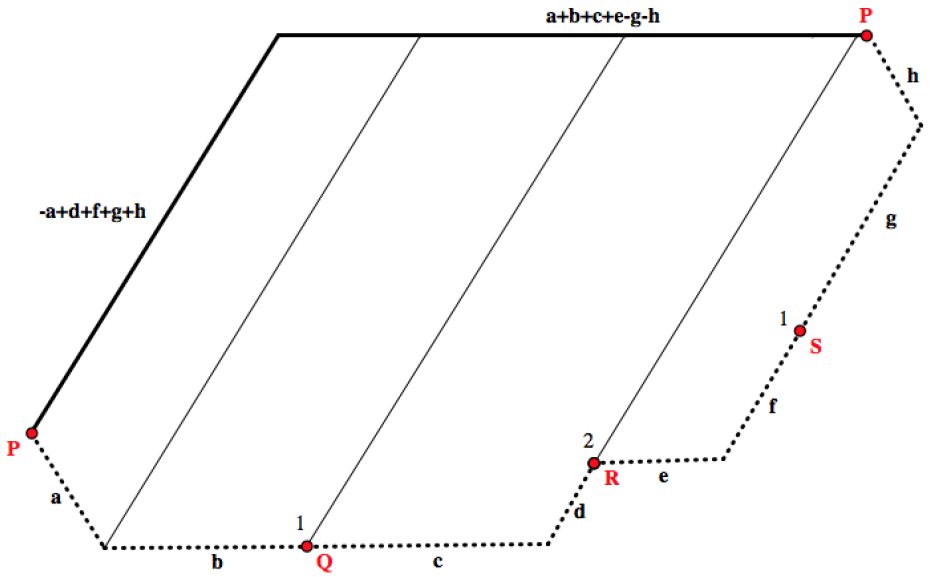



FIGURE 3.32: Unwound boundary of (2 1 2 1) 4-set

By Lemma 2.2.2 we know that $a + c \leq f + h$ yields boundary coordinates given by

$$(d + f + g + h - a,\ b + c + d + e + g)$$

Additionally, by Lemma 3.3.1 we know that $\{P, Q, R, S\}$ is a 4 cluster exactly when the difference of one of these possible sets of coordinates is congruent to 0.

This 4-set configuration will be a 4-cluster if and only if $[d+f+g+h-a]-[a+b+c+e-h] \equiv_3 0$ . Substituting in our expressions for $g$ and $h$ yields the following chain of equivalence necessary and sufficient conditions for $\{P, Q, R, S\}$ to be a 4-cluster.

$$[d + f + g + h - a] - [a + b + c + e - h] \equiv_3 0$$

$$\iff -2a - b - c + d - e + f + g + 2h \equiv_3 0$$

$$\iff a - b + d - c + f - e + [b + c - f] - [f + e + d - a - b] \equiv_3 0$$

$$\iff 2a - 2b - 2e - f \equiv_3 0$$

$$\iff (a - b) + (f - e) \equiv_3 0$$

This proves the lemma for the boundary angle configuration (2 1 2 1).

Now we move to the case with boundary angles of (0 3 1 2) shown in Figure 3.30c. In the underlying coordinate structure of this 4-set configuration $d$ and $g$ are parallel which gives us that $h = f - b - c$. In addition, $f$ and $b$ are parallel giving us $g = e + d + c - a$. First we consider the case in which $a \leq d + g + f$ and the coordinates are given by:

$$(a + b + c + e - g - h,\ -a + d + g + f)$$

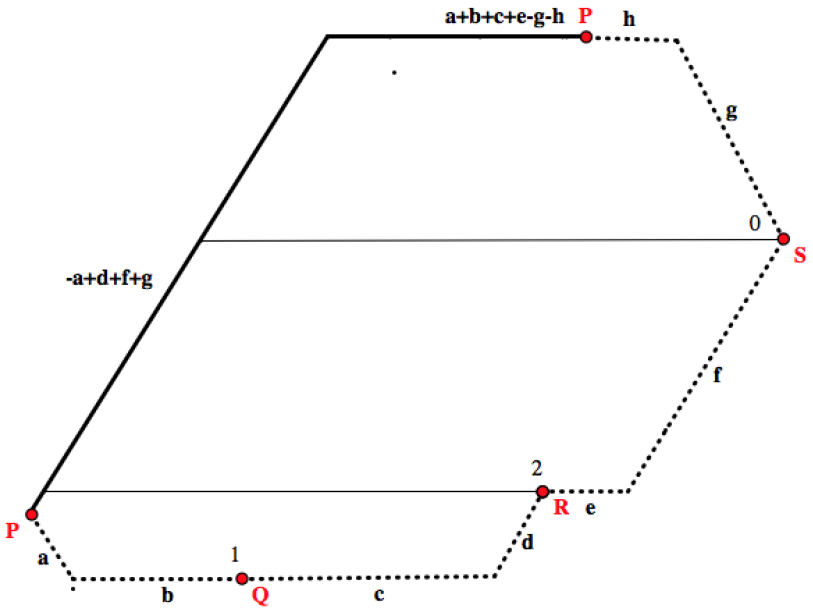



FIGURE 3.33: Unwound boundary of (3 1 2 0) 4-set

By Lemma 2.2.2 we know that $a > d + g + f$ yields boundary coordinates given by

$$(a - d - f - g,\ b + c + d + e + f - h)$$

Additionally, by Lemma 3.3.1 we know that $\{P, Q, R, S\}$ is a 4 cluster exactly when the difference of one of these possible sets of coordinates is congruent to 0.

This 4-set configuration will be a 4-cluster if and only if $[b+c+d+e+f-h]-[a-d-f-g] \equiv_3 0$. Substituting in our expressions for $g$ and $h$ yields the following chain of equivalence necessary and sufficient conditions for $\{P, Q, R, S\}$ to be a 4-cluster.

$$
\begin{aligned}
&[-a+d+g+f]-[a+b+c+e-g-h] \equiv_3 0 \\
&\qquad \iff -2a-b-c+d-e+f+2g+h \equiv_3 0 \\
&\qquad \iff -2a-b-c+d-e+f-[e+d+c-a]+[f-b-c] \equiv_3 0 \\
&\qquad \iff (a-b)+(f-e) \equiv_3 0
\end{aligned}
$$

This proves the lemma for the boundary angle configuration (0 3 1 2). □

**Theorem 3.5.6.** *Consider a 4-set, $P,\ Q,\ R,\ S$, with path signature including two angles $\theta_1$ at pentagon $Q$ and $\theta_2$ at pentagon $R$. If $\theta_1+\theta_2$ is odd then the 4 set is a cluster if and only if $a-b \equiv_3 e-f$. If $\theta_1+\theta_2$ is even then the 4 set is cluster if and only if $a-b \equiv_3 f-e$.*

*Proof.* Follows directly from the previous results. □

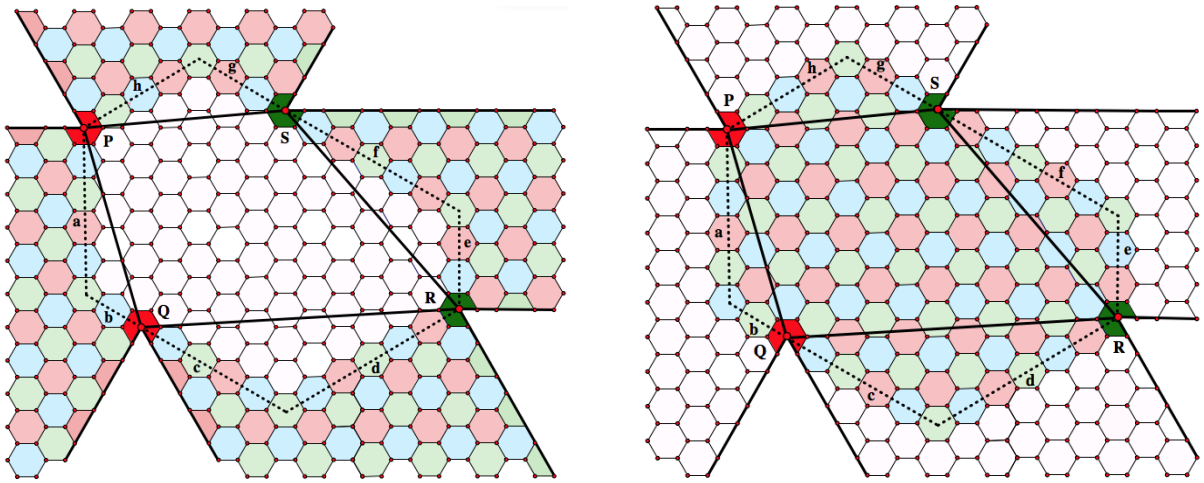
# Chapter 4

# 4-Cluster Chain Configurations

## 4.1 Internal and External Perimeter Color Assignments

In the previous chapter we found algebraic and color configuration conditions on the coordinates that ensured a 4-set of pentagons was a 4-cluster. Before we can delve deeper into the theory of coloring a 4-cluster we must consider precisely what it means to color the pentagons in a 4-cluster. In a 2-cluster isolated from the other pentagons of the fullerene, the color of the pentagons is fixed by the ambient coloring. This simplicity is lost when coloring the pentagons of a 4-set.

Once we have more than three pentagons in a cluster, there are two ways in which we can assign colors to the faces forming the perimeter of a patch in a fullerene. The two methods are distinguished by which faces of $\Lambda$ are chosen to determine the color of the perimeter of the patch. Either we push the coloring in from the ambient coloring of the faces external to the patch or we extend the coloring out towards the perimeter from faces internal to the patch. We call the two methods *external coloring* and *internal coloring* respectively and they are illustrated for a 4-cluster with an adjacent configuration in Figures 4.1 and 4.2. Note that external coloring is well defined only if the 4-set is a cluster while inside coloring is always defined.

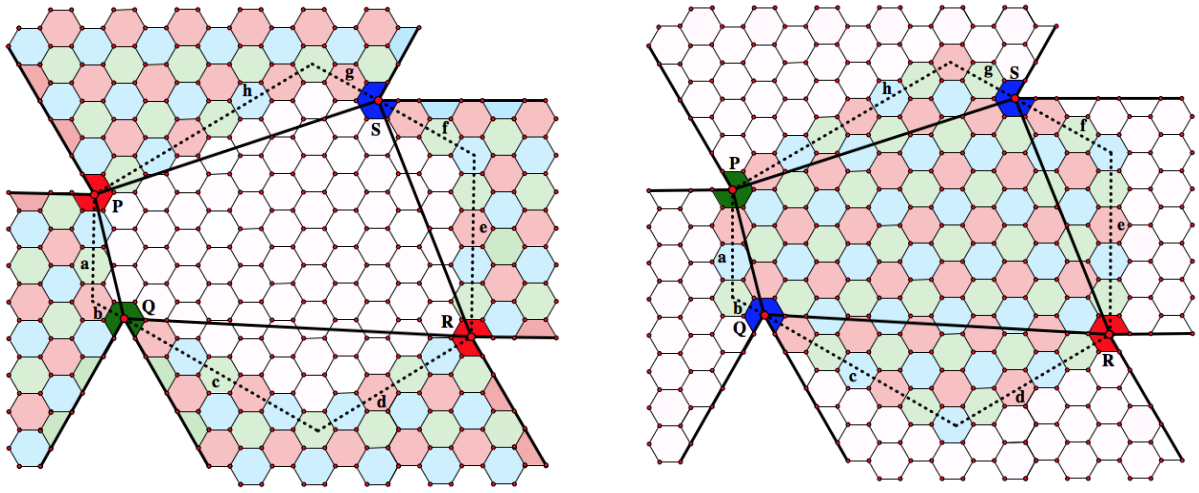



(A) External Perimeter Coloring (B) Internal Perimeter Coloring

FIGURE 4.1: External vs. Internal Coloring of an adjacent 4-cluster with angle configuration 1 2 1 2

Once we decompose our fullerene into three distinct 4-clusters and we must consider all the possible clusters in the fullerene. In doing so, the coloring of each cluster must match with the ambient coloring of the rest of the fullerene regardless of whether the cluster is colored externally or internally. As such, generally it makes the most sense to assume the ambient coloring has been fixed and hence, when not specified, we assume external coloring.

Figure 4.1 shows us an example of a 4-cluster with adjacent color configuration that has been colored both internally and externally while Figure 4.2 shows us an example of a 4-cluster with opposite color configuration colored internally and externally. Notice that although the colors of the boundary pentagons are the same for either method of coloring in Figure 4.1, in Figure 4.2 the color classes of the pentagons change depending on the coloring method. For this reason, it is important that we distinguish the coloring method used and that we set it as a standard for this work that the perimeter is colored externally. However, whether colored internally or externally we still have an opposite color configuration. In the subsequent subsections we will




(A) External Perimeter Coloring (B) Internal Perimeter Coloring

FIGURE 4.2: External vs. Internal Coloring of an opposite 4-cluster with angle configuration 1 2 1 2

further discuss the implications of the different methods of coloring the pentagons.

## 4.2 Algebraic Relations of Adjacent and Monochromatic Color Configurations

Now let us consider specifically 4-clusters with two pairs of same colored adjacent pentagons. If these two pairs are in different color classes we know this to be an adjacent configuration and if these pairs are both in the same color class the configuration is known to be monochromatic. For the purposes of this section it is not necessary to separate these into two distinct cases, rather we think of them as two possibilities within one larger case.

If we are considering a 4-set $\{P, Q, R, S\}$ with segment labels as in Chapter 3, either pentagons $P$ and $Q$ are in one color class and pentagons $R$ and $S$ are in one color class or alternatively pentagons $P$ and $S$ are in one class and pentagons $Q$ and $R$ are in

the same color class. Clusters have this configuration with pentagons $P$ and $Q$ in one color class when $a - b \equiv_3 0$ and $e - f \equiv_3 0$ or with pentagons $Q$ and $R$ in one class when $c - d \equiv_3 0$ and $g - h \equiv_3 0$. When all four are equivalent to 0 is when we have monochromatic clusters.

A 4-set with an adjacent color configuration will clearly always yield a 4-cluster as the pairs of pentagons in the same color class can be connected by direct chains. The following lemma shows that if we have one pair of adjacent pentagons in the same color class and we know the 4-set to be a cluster then the cluster conditions from the previous chapter forces the other two pentagons to be in the same color class.

**Lemma 4.2.1.** *If $a - b \equiv_3 0$ or $c - d \equiv_3 0$ in a 4-cluster $\{P, Q, R, S\}$, then the cluster has an adjacent color configuration*

*Proof.* If $a-b \equiv_3 0$ or $c-d \equiv_3 0$ then we have a pair of adjacent same colored pentagons. Then by Theorem 3.2.1 we know that the other pair of pentagons must be the same color and hence if $a - b \equiv_3 0$ or $c - d \equiv_3 0$ then $e - f \equiv_3 0$ or $g - h \equiv_3 0$ respectively. This proves an adjacent color configuration. □

**Lemma 4.2.2.** *If $a - b \equiv_3 0$ and $c - d \equiv_3 0$ in a 4-cluster $\{P, Q, R, S\}$, then the cluster is monochromatic.*

*Proof.* By Lemma 4.2.1 we know that the cluster has an adjacent configuration. Since $a - b \equiv_3 0$ and $c - d \equiv_3 0$, both pairs must be in the same color class yielding a monochromatic configuration. □

## 4.3 Algebraic Relations of Opposite Configurations

Let us now consider clusters with an opposite configuration. More precisely, a cluster $\{P, Q, R, S\}$ in which the pentagons are assigned all three colors and either pentagons

$P$ and $R$ are in one color class and pentagons $Q$ and $S$ are assigned the two remaining colors or alternatively pentagons $Q$ and $S$ are in one class and pentagons $P$ and $R$ are assigned the two remaining colors. Notice that by the Lemma 4.2.1 we are ensured that it is always a nonadjacent pair of pentagons that are in the same color class since with one adjacent pair of same colored pentagons we are guaranteed to have an adjacent color configuration and hence the pentagons would not achieve all three color possibilities.

**Lemma 4.3.1.** *If $\{P, Q, R, S\}$ is a 4-cluster with $a - b \not\equiv_3 0$ and $c - d \not\equiv_3 0$ then the cluster has opposite configuration.*

*Proof.* Since $a - b \not\equiv_3 0$ and $c - d \not\equiv_3 0$ we know from Lemma 4.2.1 that $e - f \not\equiv_3 0$ and $g - h \not\equiv_3 0$. By the pidgeon hole principle at least two of the pentagons must be in the same color class. It must be an opposite pair of pentagons since none of $(a, b)$, $(c, d)$, $(e, f)$ or $(g, h)$ are congruent coordinates. Since the 4-set is a cluster we know that they must be able to be connected by chains. Thus if we connect the pair of same colored pentagons by a direct chain then the chain connecting the remaining two pentagons must be a wrap-around chain, thus by Theorem 2.4.1 the remaining two must be in different color classes. So the cluster is of opposite configuration. □

Using these lemmas we are able to easily give an alternate proof that these are the only two possible color configurations that guarantee our 4-set is a 4-cluster.

**Theorem 4.3.2.** *There are only two possible color configurations of the pentagons in a 4-cluster up to permutation of the three color classes.*

*Proof.* We have already proved that two non-isomorphic color configurations exist for a 4-cluster. It remains to be shown that no further color configuration options exist. Consider that a cluster has opposite configuration exactly when neither $a - b \equiv_3 0$ nor $c - d \equiv_3 0$ and has adjacent configuration if we have either $a - b \equiv_3 0$ or $c - d \equiv_3 0$.

Since this exhausts all possibilities, these are all possible color configurations for a 4-cluster. □

Given any cluster with opposite configuration, the pair of pentagons that lie in the same color class depends on whether we choose to color the perimeter internally or externally. Look back to Figure 4.2 to see this illustrated. We know in this configuration we cannot have two direct chains. Our most basic configuration will be one direct chain and one u-chain wrapping around one end or other of the direct chain. When colored externally, the u-chain lies external to the pentagon it wraps around and thus alters the initial color of the intermediate pentagon while the endpoints of the u-chain are faces in the same color class. Hence, in the initial external coloring of an opposite cluster it is the pentagons connected by the u-chain that are in the same color class. If we had chosen an internal coloring then the pentagons connected by the direct chain would be in the same color class since the direct chain is internal to the cluster. The other two pentagons will be in two distinct color classes since, once the direct chain is formed, they will lie on opposite sides of a chain which reverses the colors. We know these pentagons cannot be in the same color class as the primary color of the direct chain since then we would have an adjacent pair of same colored pentagons.

Physically coloring the perimeter of a cluster in a fullerene can be quite tedious, so we use the simple relation on signature coordinates in the following lemma in order to determine which diagonal pair is in the same color class for opposite clusters.

**Lemma 4.3.3.** *Given 4-cluster $\{P, Q, R, S\}$ with opposite configuration, pentagons $P$ and $R$ can be connected with u-chain if angle $Q$ has odd measure and $(a - b) + (c - d) \equiv_3 0$ or angle $Q$ is even and $(a - b) - (c - d) \equiv_3 0$. Otherwise $Q$ and $S$ can be connected by a u-chain.*

*Proof.* Follows directly from Corollary 2.4. □

## 4.4 4-Cluster Chain Configurations

Recall that for our main goal in this body of work is to fully understand 4-clusters. This includes finding a closed formula for the Clar deficit for any 4-cluster. Specifically this means we must find the chain configuration with minimal total chain length given that the primary and secondary colors in both of the chains in a 4-cluster are constrained to two color classes.

In the case where a 4-cluster has an adjacent color configuration, we know we are able to pair the pentagons using two direct chains. Since this is not possible for 4-clusters with an opposite color configuration, we will be forced to use at least one wrap-around chain when pairing the pentagons in an opposite 4-cluster. We will see that wrap-around chains such as these may be necessary for constructing chain configurations for any 4-clusters.

Although these configurations with wrap-around chains are essential for the construction of any chain configuration for opposite clusters, they may also come into play when considering clusters with adjacent configuration. Depending on the chosen color for the Clar faces, the associated wrap-around configuration for adjacent configurations may at times yield the minimal Clar structure for clusters with adjacent configurations.

By wrapping around various pentagons it is possible to form a chain between any pair of the four pentagons of a cluster regardless of how they are arranged. Once we have paired two pentagons in a cluster, it must be possible to connect the remaining pentagons by a chain as shown in the following lemma.

**Lemma 4.4.1.** *If two pentagons in a 4-cluster have been paired by a chain, then there exists a chain pairing the remaining two pentagons.*

*Proof.* Since the four pentagons are part of a 4-cluster, we know that there is an ambient coloring surrounding a patch containing all four pentagons. Furthermore, the two pentagons that can be paired by a chain are a 2-cluster within the confines of the 4-cluster. Thus we see that there is an ambient coloring surrounding just these two pentagons within the ambient coloring surrounding the 4-cluster. Hence this ambient coloring extends through the remaining two pentagons and so they must also be able to be paired by a chain. □

As we begin to explore the chain configurations of 4-clusters we first examine what happens to the colors of pentagons as we alter the underlying configuration of the pentagons. Once we have an initial set of configurations for some 4-cluster, we will gradually shift the pentagon arrangements–moving one pentagon at a time–to create different configurations while keeping the original chains intact.

The key property to keep in mind when translating faces within $\Lambda$ is that when a chain of some primary color is formed, the remaining two color classes are permuted as one moves across the chain. Thus, we sometimes think of a chain as dividing a large patch into two individual patches since the coloring is distinct in the two portions. Consider a 4-cluster with external coloring as shown in Figure 4.3. As this is an external coloring, the interior of the patch is initially uncolored.

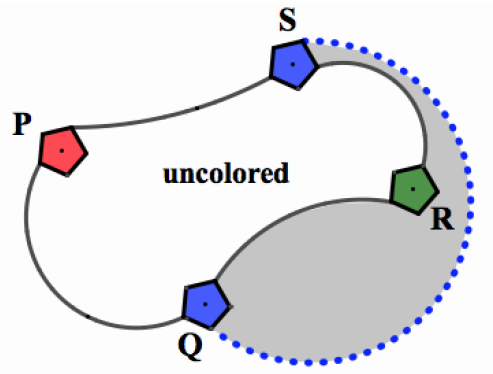



FIGURE 4.3: Chain between blue pentagons subdivides initial patch into two distinct patches.

If we have a u-chain like the one connecting the blue pentagons, then the coloring of the portion of $\Lambda$ that lies outside the patch but within the u-chain has been altered from the coloring of the remainder of the fullerene. In our example, this region has been shaded grey. In this region red and green are interchanged and thus, before the blue pentagons are paired by a chain, pentagon $R$ is colored green even though it can be joined by a direct chain to pentagon $P$. Furthermore, this new coloring matches the fixed external coloring as it is extended around $Q$ and $S$. Hence, $P$ and $R$ form a red 2-cluster.

If we translate a pentagon from within the confines of the u-chain to outside the u-chain, then the initial coloring of that pentagon will be altered. For example, if we push pentagon $P$ in Figure 4.3 past the end points of the blue chain, it will be permuted to a green face. Similarly if we push pentagon $R$ past the end points of the blue chain it will become a red face since it will no longer lie within the boundary of the u-chain. Note that once two pentagons have been paired they may be pushed around without altering the primary color of the chain.

To see all possible chain configurations for any 4-cluster we first note that there are three distinct ways to partition the four pentagons into two pairs. We choose one pair from each partition and connect these pentagons with a chain that wraps the other additional pentagons as necessary. To construct the second chain, we either wrap-around one end of the first chain or wrap-around the other end, yielding two distinct configurations. The six configurations for one such 4-cluster are illustrated in Figure 4.4.

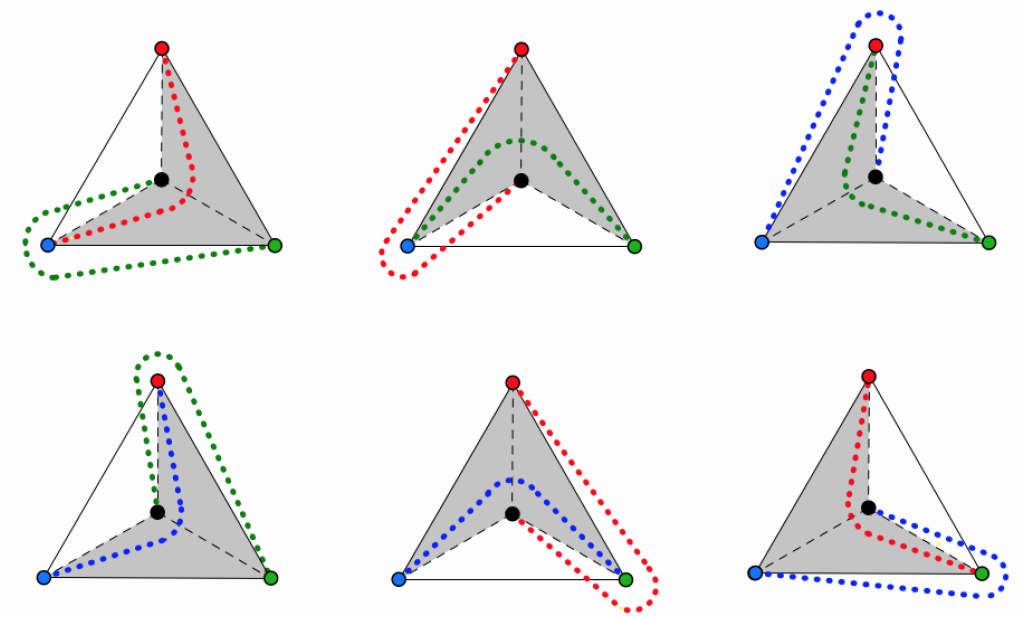
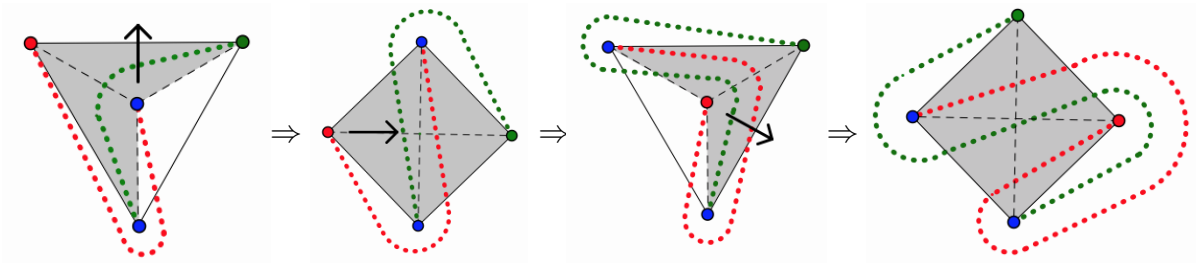


FIGURE 4.4: Chain configurations on a concave 4-cluster with opposite configuration

Figure 4.4 shows pairs of configurations in three columns. Each column represents an initial pairing of two pentagons and the two rows represent the alternate ways to form the second chain. The vertices representing the pentagons are colored to indicate the initial external perimeter coloring of the respective pentagons and the dotted lines represent the chains, the colors of which indicate the chain's primary color. As we are only indicating the primary color we must keep in mind that we may need different types of these chains so as to use the appropriate secondary color of the chain. We may even change the primary color if necessary by constructing a type 3 chain. Additionally, notice that when we wrap around a different pentagon, the primary color of the chains is altered. Thus we see that we have various methods of changing the primary color of the chains in a 4-cluster where as in a 2-cluster we were only able to change the primary color by constructing type 3 chains. All of these different methods will be considered in the following chapters.

The pentagons in this cluster are positioned in order to best illustrate the six possible chain configurations. However, as the pentagons are shifted throughout the tessellation the chain configurations can look much more complicated. To help understand the possible configurations, we initially view the pentagons in our 4-set as the vertices of a quadrilateral and we separate these into a classes of concave and convex quadrilaterals. This distinction does not alter the color configuration possibilities of the cluster nor does it change the chain configuration possibilities as we will soon show. However, it will make the transition between classes more straightforward and so for the time being we will consider the cases separately. For example, the underlying configuration of the 4-cluster in Figure 4.4 has opposite coloring and a concave quadrilateral.



(A) Concave Opposite (B) Convex Opposite (C) Concave Adjacent (D) Convex Opposite

FIGURE 4.5: Moving between chain configurations by moving pentagons

Although the basic chain construction remains fixed for any orientation of pentagons in a 4-cluster, the locations of the pentagons can affect the complexities of the chains within the configuration. The process of moving pentagons to yield all possible chain configurations is illustrated in Figure 4.5. First consider one of the 4-clusters from Figure 4.4. This 4-cluster will have a concave configuration with an opposite external coloring. Moving the pentagon that lies inside the convex hull to a position outside the center will not change its initial color if we move it between two pentagons

in opposite color classes as shown in the transition from Figure 4.5a to Figure 4.5b. We now have a convex 4-cluster still with an opposite color configuration.

In continuing to alter our configuration, we now move a pentagon to the center to create a concave 4-cluster. We have two non-isomorphic choices for which pentagon to move in the subsequent step. Either we move a pentagon from the pair of same colored pentagons or one of the uniquely colored ones. We need to consider the cases separately. First we choose to push in one of the pentagons from the pair of same colored pentagons. These pentagons lie in the same patch of the tessellation and thus the color configuration remains unchanged as the pentagon gets pushed towards the center. Hence, we are still in an opposite configuration as we have one pair of pentagons in the same color class and one pair in the opposite remaining color classes and we see that we have returned to the case in Figure 4.5a

Alternatively if we push one of the other pentagons to the center, then eventually we will push it past the end points of two same colored pentagons and the color of the shifted pentagon will be reversed. In this case we end up pushing the red pentagon to the center of the cluster and we end up with two pairs of pentagons–one pair green and the other blue–in Figure 4.5c. However, we would have had similar results had we chosen to move the green pentagon. In that case we would have ended up with a red pair of pentagons and a blue pair.

Once our 4-cluster has an adjacent color configuration, changing the location of the two pairs of pentagons does not change the initial colors so long as each pair remains in a distinct region of the hexagonal tessellation. As such, moving the internal green pentagon outside the convex hull will not change any initial pentagon colors since the pentagon will stay in the same uninterrupted patch of $\Lambda$ as shown in Figure 4.5d. We have now found all configuration options since we have formed concave and convex configurations for opposite and adjacent color configurations.

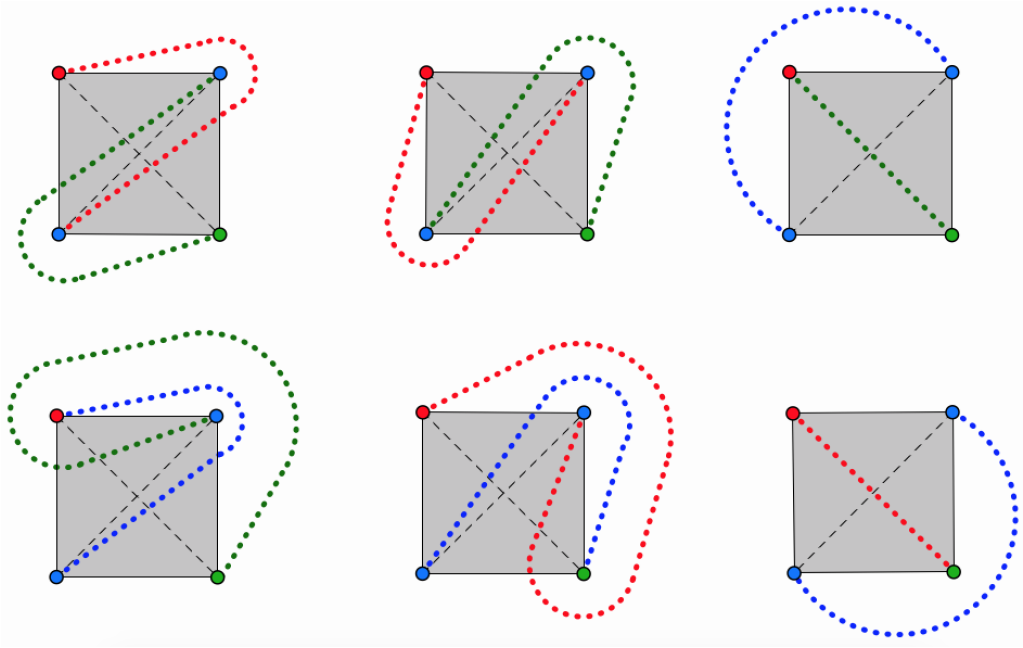


FIGURE 4.6: Chain configurations on a convex 4-cluster with opposite configuration

Since any configuration can be altered in this way we get six analogous configurations for any possible configuration of 4-cluster. We perform the first step of the process shown in Figure 4.5 for each of the chain configurations Figure 4.4 to get the six possible non-isomorphic configurations for a convex cluster with an opposite external coloring. These configurations are shown in Figure 4.6.

We give names to each of the configurations based on the types of chains used within the configurations. The two rightmost configurations consist of one direct chain and one u-chain and thus are called *Single u-chain configurations* . The remaining two on the top row consist of two u-chains giving them the name *double u-chain configuration*. Finally the remaining two configurations have one u-chain and then a second wrap-around chain that spirals around one end of the u-chain. We call these configurations *spiral configurations*.

Inspection shows that each of the configurations in Figure 4.6 is the same as the corresponding configuration in Figure 4.4 with the center pentagon shifted out between

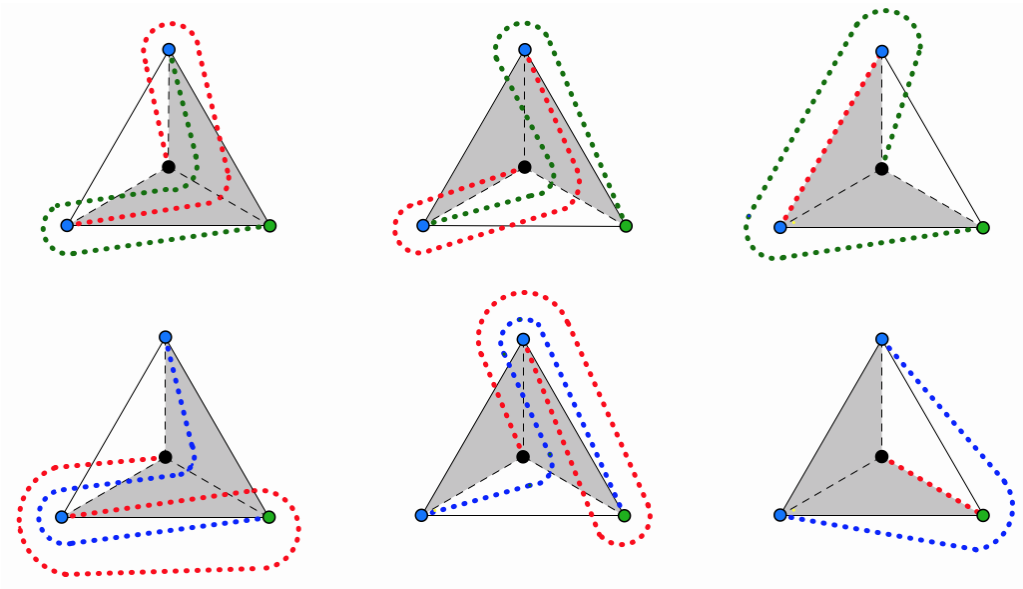


FIGURE 4.7: Chain configurations on a concave 4-cluster with adjacent configuration

the red and green pentagons until the cluster has convex perimeter.

From here we alter our configuration to have a convex adjacent color configuration as in the second step described above. In this case we shift the red pentagon between the two blue pentagons to the interior of the triangle formed by the two blue pentagons and the one green one. The set of chain configurations is shown in Figure 4.7.

Our final possible configuration of pentagons leads us to a convex adjacent configuration as we push the internal pentagon until the configuration is convex. This is shown in Figure 4.8. Again we give names to our configurations. In this case the rightmost configurations which correspond to the single u-chain configurations from the opposite configurations are called *Single wrap configurations* since the wrapped chains now wrap-around multiple configurations so they are no longer technically u-chains. The remaining configurations are all *spiral configurations*.

We have thus found all viable wrap-around chain configurations for 4-clusters.

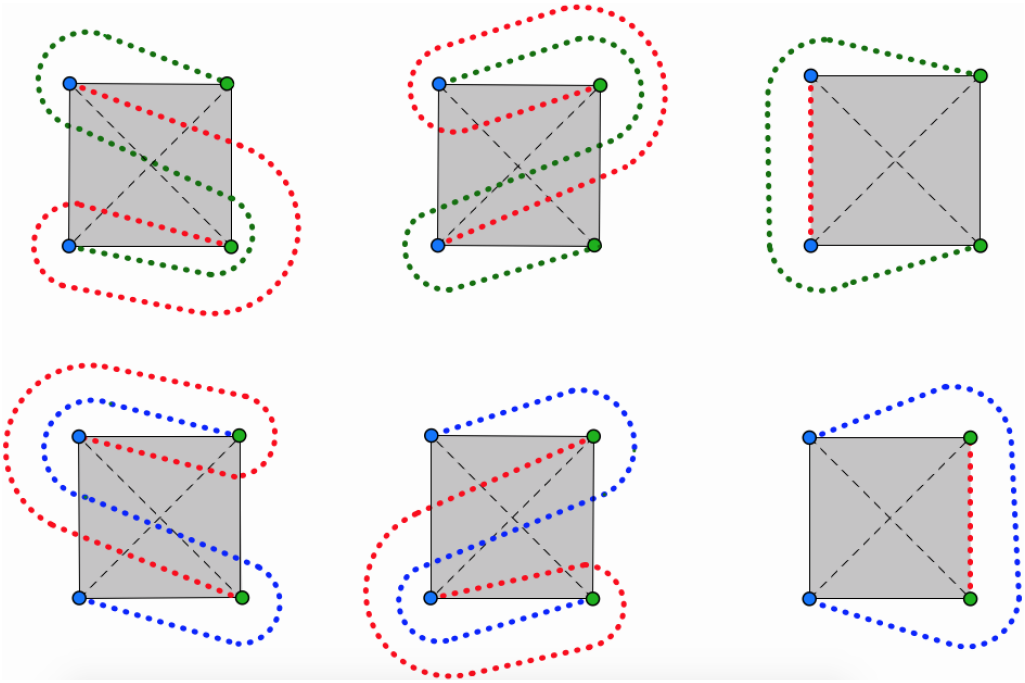
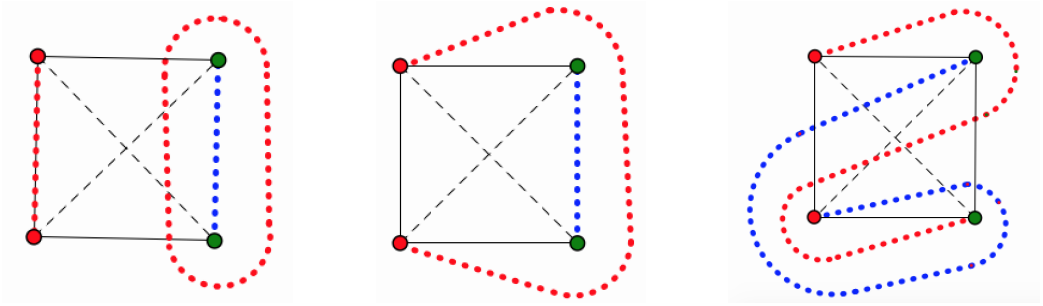


FIGURE 4.8: Chain configurations on a convex 4-cluster with adjacent configuration

## 4.5 Length of Chain Configurations

Examining the six possible chain configurations for a particular 4-cluster we see that the chains in some of the configurations wrap around fewer intermediate pentagons. For example, in Figure 4.9, we have three possible configurations for a 4-cluster that have an adjacent color configuration where the initial external coloring of the pentagons are red and green. Each of the chains in these configurations avoid using green as their primary color.

In Figure 4.9a we have the direct chain configuration that decomposes into two 2-clusters and in order to avoid using green as a primary color, the direct chain between the two green pentagons is forced to be a type 3 chain. In Figure 4.9b we have one direct chain of either type 1 or 2 depending on which option avoids green as it's secondary color and one chain that wraps around the entirety of the direct chain. In Chapter 6 we will discuss in full detail the conditions that determine which of these



(A) Two direct chains

(B) Direct and wrap-around chains

(C) Two wrap-around chains

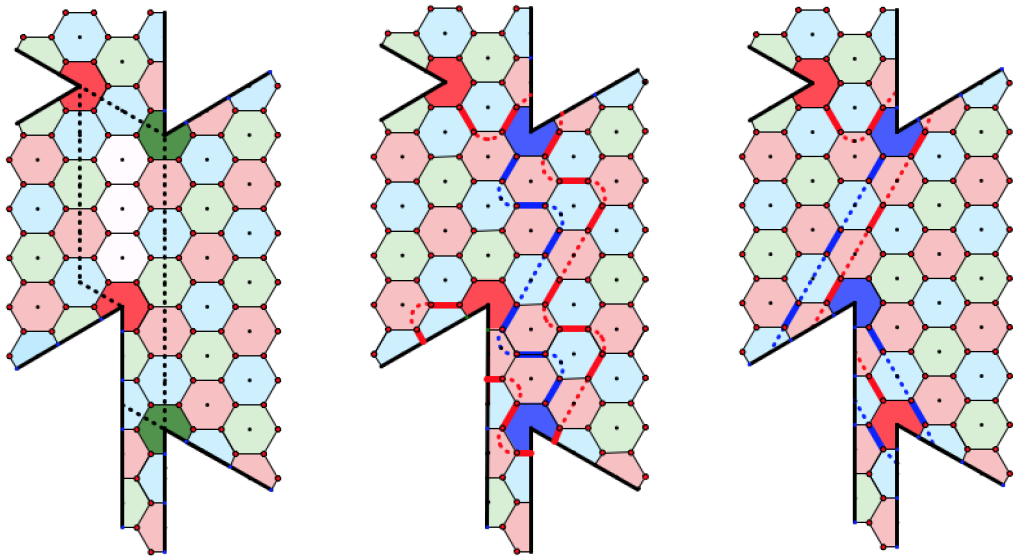
FIGURE 4.9: Three possible chain configurations for green Clar faces

configurations yields the lesser Clar deficit.

The last possible configuration is shown in Figure 4.9c and upon initial inspection it would appear that this configuration should never yield a minimal chain deficit as it's chains wrap around so many additional intermediate pentagons. However, this is not the case. If the chain length were in a metric space then wrap-around chains between two pentagons would always be longer than a direct chain through adjacent faces. However, chain length does not follow the triangle inequality so at times making a convoluted configuration that wraps around many pentagons may be shorter in chain length that the simpler alternative.

Figure 4.10 shows a counterexample that illustrates this surprising consequence. In Figure 4.10a the initial external coloring of a 4-cluster is shown. For this 4-cluster we see that the red pentagons are connected by a segment with coordinates $(4, 1)$ and the green pentagons are connected by a segments with coordinates $(6, 0)$. The direct chain configuration with one type 1 and one type 3 chain will thus have length $4+3(6)+2 = 24$ since we will have one type 1 chain and one type 3 chain.

In Figure 4.10b we see the construction of wrap-around chain configuration shown in Figure 4.9b. For the specific 4-cluster in our example this configuration yields a Clar deficit of 19. However, when we look at the configuration in Figure 4.10c which



(A) External coloring (B) Total chain length 19 (C) Total chain length 12

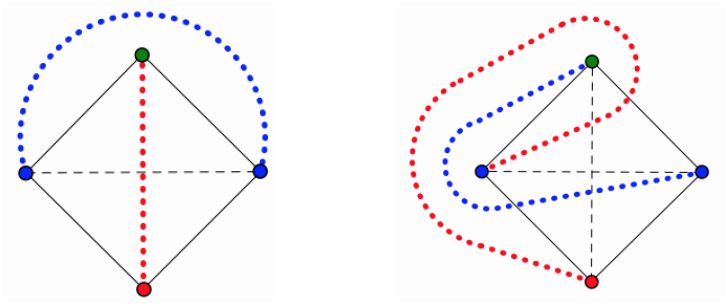
FIGURE 4.10: Comparing configurations for 4-cluster with adjacent color configuration

corresponds to the spiral configuration in Figure 4.9c, we get a Clar deficit for this cluster of 12 which is shorter than either other configuration possibility.

We can construct a similar counterexample for a 4-cluster with an opposite configuration as the opposite configurations are just translations of particular pentagons within an adjacent configuration. In this case, if our external perimeter coloring has two blue pentagons and one each of red and green, we have two chain configuration possibilities that avoid using green as a primary coloring. Namely a single u-chain configuration as shown in Figure 4.11a or a a spiral configuration as illustrated in Figure 4.11b.

The following configuration with external coloring shown in Figure 4.12a is a counterexample where the spiral chain configuration in Figure 4.11b yields the least Clar deficit rather than the single u-chain configuration.

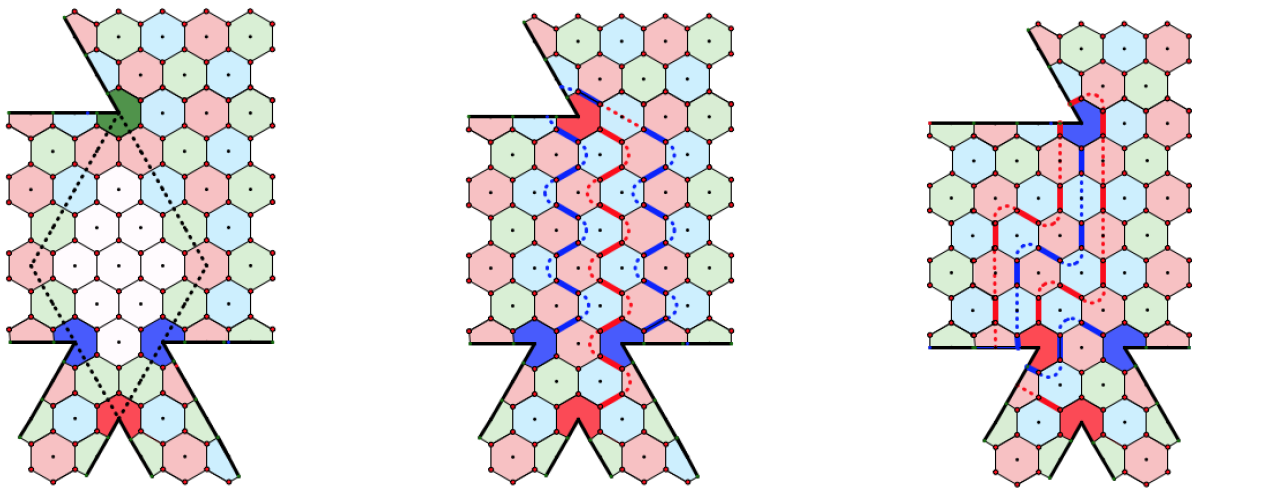
To avoid the color green from the primary and secondary color of the two chains in



(A) Two direct chains (B) Two wrap-around chains

FIGURE 4.11: Three possible chain configurations for green Clar faces

Figure 4.12b both the u-chain and the direct chain must be type 2 which greatly extends their length. In this case the combined length of the two chains is 21. However the u-chain and the spiral chain in spiral configuration of Figure 4.12c can both avoid the color green while being type 1 chains and this is enough to make this configuration shorter. The total length of the spiral configuration is 18.



(A) External coloring (B) Total chain length 21 (C) Total chain length 18

FIGURE 4.12: Comparing configurations for 4-cluster with opposite color configuration

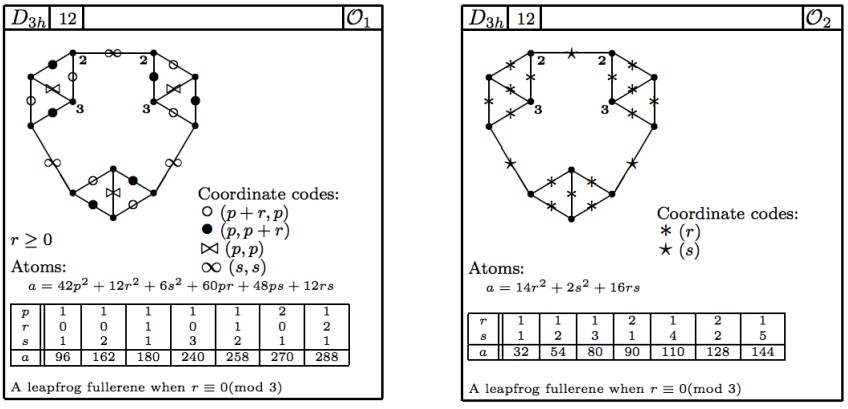
These examples show us that any of the chain configurations for a cluster may be the configuration that yields the minimal Clar structure. It all depends on the relative locations of the pentagons within the structure of the specific fullerene.

# Chapter 5

# Infinite Classes of Arrowhead Fullerenes

## 5.1 Infinite Classes of Arrowhead Fullerenes

Fullerenes can be organized into infinite classes that all have similar arrangements of pentagonal faces. From the infinite classes with high levels of symmetry, we choose to focus our study on the arrowhead classes of fullerenes used to illustrate the preliminary concepts in Chapter 1. We choose these particular classes since they have an underlying structure that is conducive to utilizing the theory of 4-clusters developed in this thesis.




| $p$ | 1 | 1 | 1 | 1 | 1 | 2 | 1 |
|---|---|---|---|---|---|---|---|
| $r$ | 0 | 0 | 1 | 0 | 1 | 0 | 2 |
| $s$ | 1 | 2 | 1 | 3 | 2 | 1 | 1 |
| $a$ | 96 | 162 | 180 | 240 | 258 | 270 | 288 |

| $r$ | 1 | 1 | 1 | 2 | 1 | 2 | 1 |
|---|---|---|---|---|---|---|---|
| $s$ | 1 | 2 | 3 | 1 | 4 | 2 | 5 |
| $a$ | 32 | 54 | 80 | 90 | 110 | 128 | 144 |

FIGURE 5.1: Infinite Classes $\mathcal{O}_1$ and $\mathcal{O}_2$ Reprinted from Ref. [6] with permission

In this chapter, we will investigate the Clar deficit for the two infinite arrowhead classes shown in Figure 5.1. We begin by finding a closed formula for the Clar number for fullerenes in $\mathcal{O}_1$. Once we have our desired formula for $\mathcal{O}_1$, we move on to examine $\mathcal{O}_2$. Due to the more complicated underlying structure of this class we will not find a closed formula for the Clar deficit of fullerenes in $\mathcal{O}_2$. To do so would require a full understanding of larger clusters. However, we will find the deficit for each of the three 4-clusters and combine them to compute a lower bound on the Clar deficit for the entire fullerene. This bound will be sharp when the clusters are far enough apart.

## 5.2 $\mathcal{O}_1$

In the description of the class shown in Figure 5.1, some relevant segments representing neighboring pentagons are not included. Thus, we begin by adding edges to the graph in Figure 5.1 to get the auxiliary graph of $\mathcal{O}_1$ shown in Figure 5.2. Here, as in Figure 5.1, the vertices represent the pentagonal faces of $\mathcal{O}_1$ and the edges in this new graph correspond to segments joining neighboring pentagons of $\mathcal{O}_1$.

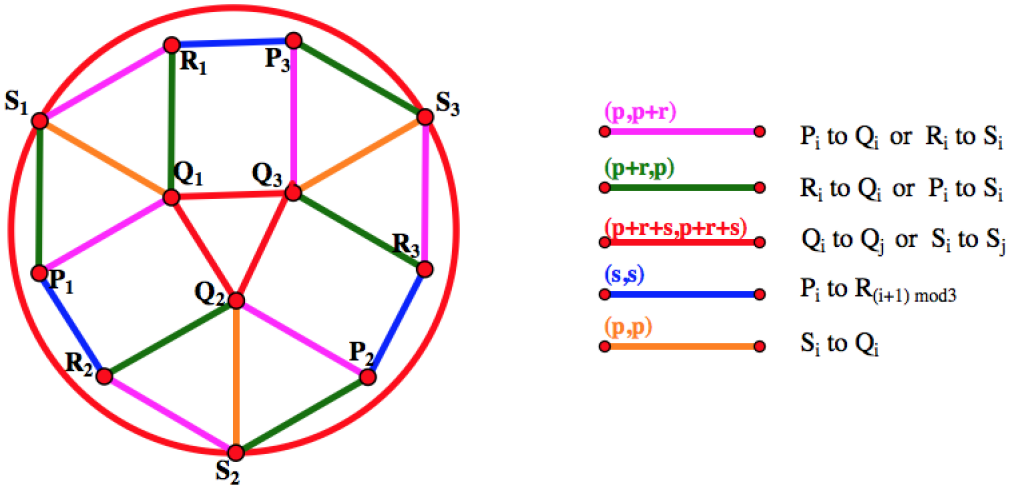



FIGURE 5.2: Segment Structure of $\mathcal{O}_1$

Fullerenes in this infinite class decompose into three distinct 4-clusters $\{P_i, Q_i, R_i, S_i\}$ for $i = 1, 2, 3$. Before we dive into these 4-clusters in detail, it will be helpful to determine a benchmark configuration that will form a Clar structure for any fullerene in this class. By computing the associated Clar deficit, we will be able to compare our future results to this benchmark deficit so as to be able to disregard configurations that yield a deficit greater than this lower bound.

### 5.2.1 Benchmark Configuration

The pentagons in $\mathcal{O}_1$ all lie within two color classes. Notice that the coordinates of the red and orange segments shown in Figure 5.2 are congruent modulo 3 regardless of the values of $p, r$ or $s$. Therefore, all pentagons in the set $\{Q_1, Q_2, Q_3, S_1, S_2, S_3, \}$ are in one color class.

Similarly the coordinates of the segments represented by the blue edges in Figure 5.2 are congruent modulo 3. However, this is not enough to conclude that all pentagons in the set $\{R_1, R_2, R_3, P_1, P_2, P_3, \}$ are in the same color class. To determine this fact, we need to consider additional segments joining pentagons in the set $\{R_1, R_2, R_3, P_1, P_2, P_3, \}$ that are not included in our auxiliary graph. Let us consider another auxiliary subgraph on just these six pentagons. This auxiliary subgraph is shown in Figure 5.3 with segment coordinates given. Now we see that the turquoise, brown and pink edges are given by coordinates which all clearly congruent modulo 3 and thus all pentagons in $\{R_1, R_2, R_3, P_1, P_2, P_3, \}$ are in the same color class.

The color classes of the two sets of pentagons need not be distinct. The color classes will be distinct when $r \not\equiv_3 0$ and, in this case, $\mathcal{O}_1$ decomposes into two sets of chain available pentagons. When $r \equiv_3 0$, all pentagons will be assigned the same color and, in this case, all pentagons in the fullerene will be pairwise chain available.

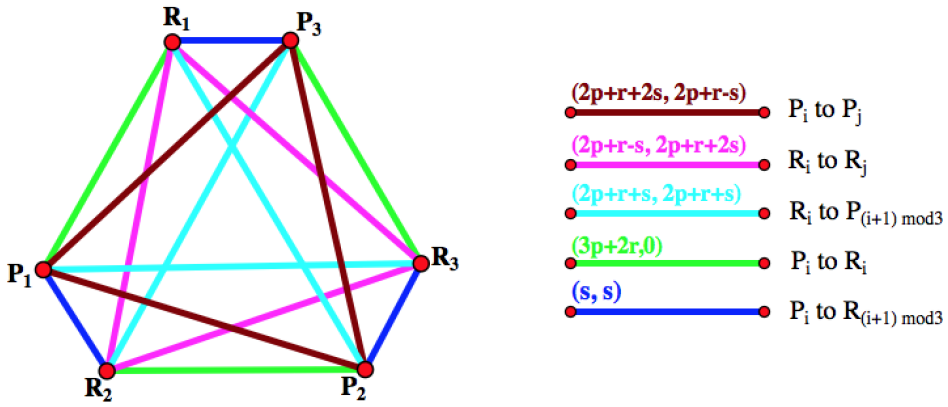



FIGURE 5.3: Segment coordinates between pentagons in $\{R_1, R_2, R_3, P_1, P_2, P_3, \}$

For our benchmark configuration, we decompose the pentagons in $\mathcal{O}_1$ into six 2-clusters using the edges given by coordinates $(p, p)$ and $(s, s)$. With the associated chains between these pentagons we compute a lower bound on the Clar deficit for $\mathcal{O}_1$.

Without loss of generality, we assume that a direct chain from $Q_1$ to $S_1$ has primary color red and secondary color blue. It follows that all chains from $Q_i$ to $S_i$ will have primary color red. There are only two possibilities for the secondary color of these three chains. By symmetry, two chains having one secondary color and one having the other color is not possible so all three chains must have the same secondary color.

In addition to our chains from $Q_i$ to $S_i$ for $i = 1, 2, 3$, we also connect pentagons $P_i$ and $R_{i+1\text{mod}3}$ by direct chains. To determine the colors of such chains we first use Figure 5.4 to determine the primary color of the pentagons $P_i$ and $R_i$ given that $Q_i$ and $R_i$ are red. By similarity these patterns will hold for each congruency class on the parameter $r$: $r \equiv_3 0$, $r \equiv_3 1$, and $r \equiv_3 2$. This gives us equivalence classes on the color structure of each 4-cluster for each value of $r$ when considered modulo 3. When $r \equiv_3 0$, $P_i$ and $R_i$ will be assigned the color red, when $r \equiv_3 1$, $P_i$ and $R_i$ will be assigned the color green and when $r \equiv_3 2$, $P_i$ and $R_i$ will be blue.

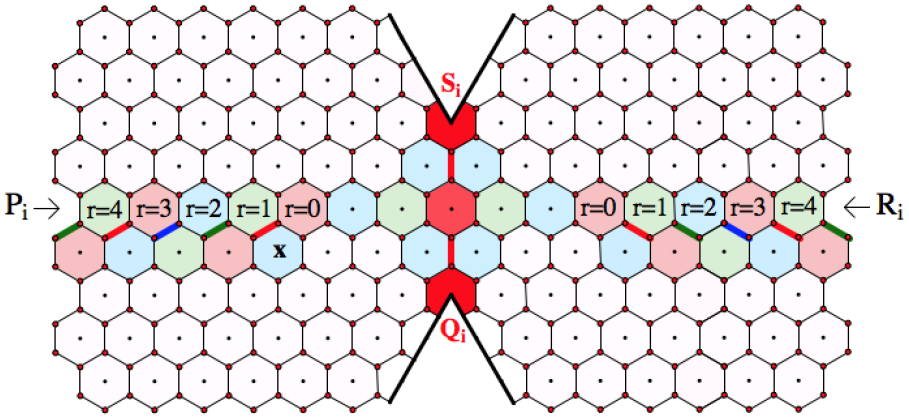
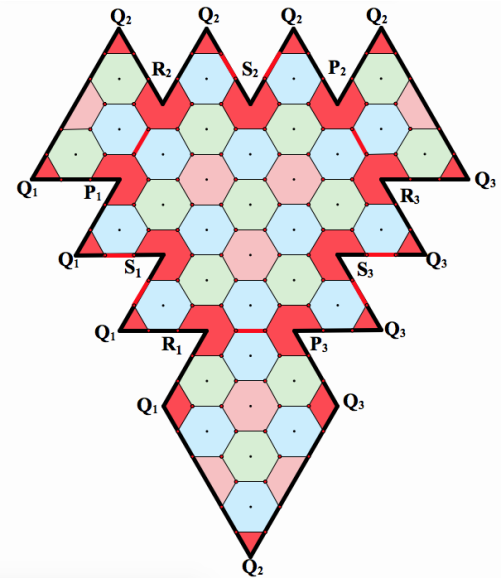



FIGURE 5.4: Illustrating Colors of Pentagon $P_i$ and $R_i$

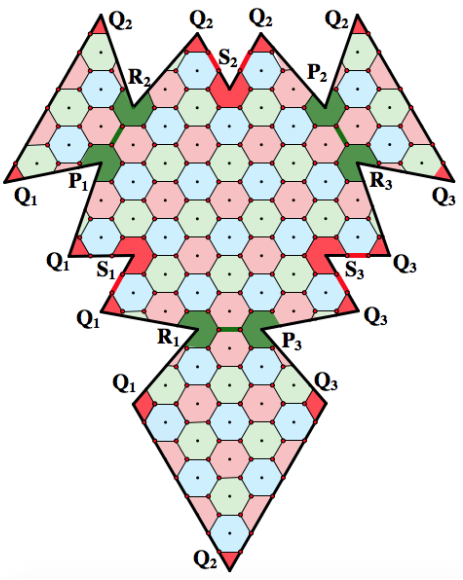
We know from the underlying structure of this class of fullerenes that the internal angle between the segments given by the green and blue edges in Figure 5.2 has measure 2. This piece of information allows us to determine the secondary color of the direct type 1 $P_iR_{i+1 \mod 3}$ chain. The secondary color will be given by the color of the hexagon that lies between and below the pentagon and the face one unit away from the $Q_iS_i$ chain in Figure 5.4. The color of the hexagon that lies one unit farther along the path will be altered since it will lie directly adjacent to an edge in the chain.

To illustrate we consider an example in which $r = 0$. In this case, all pentagons in fullerene will be in the same color class. By the above method the secondary color of the $P_iR_{i+1}$ chain is determined by the blue face labeled with an $x$ in Figure 5.4. Hence, we get that when $r \equiv_3 0$ the secondary color will be blue giving us that all direct type 1 chains in this configuration will have primary color red and secondary color blue as shown in Figure 5.5a.

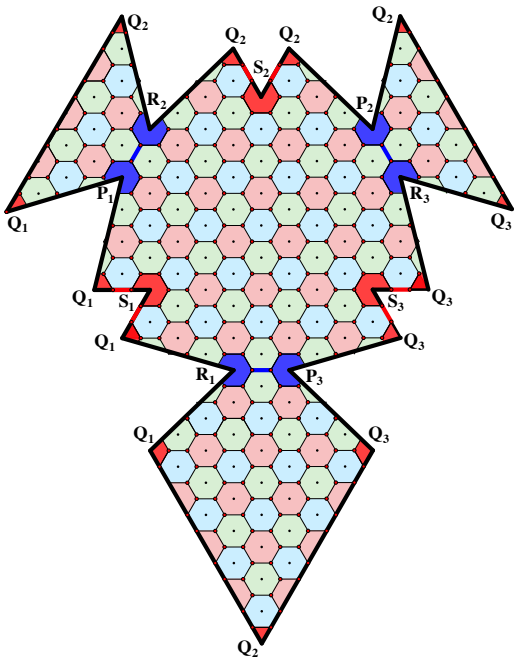
When $r \not\equiv_3 0$, the primary and secondary colors will be distinct between the two classes of chains. Using Figure 5.4, we can determine that when $r \equiv_3 1$ the $(s, s)$ chains will all have primary color green and secondary color red. An example of such a fullerene in the class with these parameters and type 1 chains is shown in Figure 5.5b.




(A) $\mathcal{O}_1$ with $s = p = 1$ and $r = 0$




(B) $\mathcal{O}_1$ with $s = p = 1$ and $r = 1$




(C) $\mathcal{O}_1$ with $s = p = 1$ and $r = 2$

FIGURE 5.5: Benchmark Configuration for each congruency class of $r$

On the other hand if $r \equiv_3 2$, then the $(s, s)$ chains have primary color blue and secondary color green. An example of fullerene with such parameters and all type 1

direct chains drawn is shown in Figure 5.5c.

For each congruency class of $r$ and each choice of Clar color, we compute the total Clar deficit by determining the number and length of each type of chain needed. For example, if $r \equiv_3 0$ and we use green Clar faces than we can use six type 1 chains–three of length $p$ and three of length $s$–yielding a Clar deficit of $3p + 3s$. If we use blue Clar faces then we use six type 2 chains–three of length $2p$ and three of length $2s$–yielding a Clar deficit of $6p + 6s$. Finally, if we use red Clar faces then we must use six type 3 chains–three of length $3p + 2$ and three of length $3s + 2$. This yields a Clar deficit of $9p+9s+12$. Hence the minimal Clar deficit is $3p+3s$ when we use this chain structure.

| Equivalence Class of $r$ | $r \equiv_3 0$ | $r \equiv_3 1$ | $r \equiv_3 2$ |
|---|---|---|---|
| $(s, s)$ Type 1 chain color | Red Blue | Green Red | Blue Green |
| **Clar Color** | **Clar Deficit** | | |
| Blue Clar Faces | $6p + 6s$ | $6p + 3s$ | $6p + 9s + 6$ |
| Red Clar Faces | $9p + 9s + 12$ | $9p + 6s + 6$ | $9p + 3s + 6$ |
| Green Clar Faces | $3p + 3s$ | $3p + 9s + 6$ | $3p + 6s$ |

TABLE 5.1: Total Clar Deficit assuming type 1 chain for $(p, p)$ segments is Red Blue

For $r \equiv_3 1$ and $r \equiv_3 2$, we similarly compute the Clar deficit for each choice of Clar color. In these cases, we will have to use a combination of type 1, type 2 and type 3 chains for any choice of Clar color so as to ensure that the configuration avoids the Clar color in both the primary and secondary color of each chain. The Clar deficit for all possible cases are outlined in the Table 5.1.

If $r \equiv_3 1$, the minimal Clar deficit is $6p + 3s$ so long as $p \leq 2s + 2$ and otherwise the minimal clar deficit is $3p + 9s + 6$. If $r \equiv_3 2$, the minimal Clar deficit is $3p + 6s$ so long as $s \leq 2p + 2$ and otherwise the minimal clar deficit is $9p + 3s + 6$. We will use these values as bench marks when considering alternate chain configurations. If the total length of the chains in a subset of any future chain configuration yields a value larger

than these given deficits, then we no longer need to consider the new configuration as a candidate for the minimal Clar structure.

We summarize what we have just proved in the following lemma for ease of later reference.

**Lemma 5.2.1.** *If $\Gamma$ is a $\mathcal{O}_1$ fullerene then the Clar deficit is at most:*

$$\begin{cases} 3p+3s & \text{when } r \equiv_3 0 \\ 6p+3s & \text{when } r \equiv_3 1 \text{ and } p \leq 2s+2 \\ 3p+9s+6 & \text{when } r \equiv_3 1 \text{ and } p > 2s+2 \\ 3p+6s & \text{when } r \equiv_3 2 \text{ and } s \leq 2p+2 \\ 9p+3s+6 & \text{when } r \equiv_3 2 \text{ and } s > 2p+2 \end{cases}$$

### 5.2.2 $\mathcal{O}_1$ 4-Clusters

For this infinite class of fullerenes, we have a clear opportunity to decompose the set of pentagonal faces into three congruent 4-sets $\{P_i, Q_i, R_i, S_i\}$ for $i = 1, 2, 3$. One of these isomorphic sets is shown in Figure 5.19 with both the segments and the corresponding coordinate paths. We use our theory of 4-sets in order to understand these individual sets more completely before combining the three sets to compute the Clar deficit for the fullerene as a whole. In order to determine whether these sets are clusters for all possible equivalence classes on the parameter $r$, we first consider the signature graph on these four vertices.

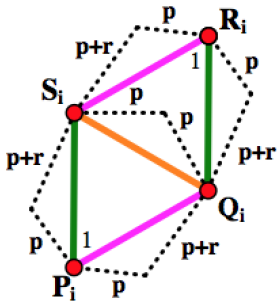



FIGURE 5.6: 4-set $\{P_i, Q_i, R_i, S_i\}$

**Lemma 5.2.2.** *For $i = 1, 2, 3$, the 4-set $\{P_i, Q_i, R_i, S_i\}$ in $\mathcal{O}_1$ will have a 1 1 3 star signature.*

*Proof.* The segment connecting $P_i$ and $R_i$ has coordinates $(3p + 2r, 0)$. The length of segment $Q_iS_i$ which has coordinates $(p, p)$ is clearly less than the length of the remaining segments in the auxiliary graph of the set, namely the segments with coordinates $(p + r, p)$, $(p, p + r)$ or $(3p + 2r, 0)$. So any shortest spanning tree of the auxiliary graph on $\{P_i, Q_i, R_i, S_i\}$ will necessarily include the segment $Q_iS_i$.

$(3p+2r, 0)$ is the segment with longest length and the remaining segments all have equal length. So we choose any of the two others to form the signature. Without loss of generality, we can choose to use segments $P_iQ_i$, $R_iQ_i$ and $S_iQ_i$ to form the edges of the signature graph. We know from the underlying structure of $\mathcal{O}_1$ that $\angle P_iQ_iR_i$ has external measure 3 giving us that the signature of set $\{P_i, Q_i, R_i, S_i\}$ has the form of a 1 1 3 star. □

**Lemma 5.2.3.** *Each 4-set $\{P_i, Q_i, R_i, S_i\}$ in $\mathcal{O}_1$ will be a 4-cluster for any value of $r$ or $p$.*

*Proof.* In order for these 4-sets to be classified as 4-clusters, we know from Lemma 3.4.3 that $(a - b) + (c - d) + (j - k) \equiv_3 0$. In the context of these sets, we have $a = d = p + r$ while $b = c = j = k = p$ for each of the sets. Making the appropriate substitutions yields the sufficient and necessary condition:

$$(p + r - p) + (p - (p + r)) + (p - p) = 0$$

Hence, $\{P_i, Q_i, R_i, S_i\}$ is always a 4-cluster. □

Clearly when $r \equiv_3 0$ our 4-clusters will be monochromatic. When $r \not\equiv_3 0$, we will have clusters in an opposite configuration by Lemma 4.3.1. Since these 4-sets are clusters, we can completely avoid using the parameter $s$ in calculating the Clar deficit. This will be useful when $s$ is large in comparison to $p$, that is when the clusters lie far apart.

For any 4-cluster, we know we have six chain configurations to consider. Two configurations with a direct chain and a u-chain which we call the single u-chain configuration, two configurations using two u-chains which we call the double u-chain configuration and two configurations with a single u-chain and a spiral wrap around chain which we call a spiral configuration. Due to the high level of symmetry in these clusters, each pair of similar configurations will have the same chain length even if the chains lie in distinct color classes.

**Single U-Chain Configuration**

As we did for the benchmark configuration, let us begin by assuming that we are connecting pentagons $Q_i$ and $S_i$ by a chain with primary color red and secondary color blue where the primary color red is determined from the initial coloring of the pentagons surrounding pentagon $Q_i$. We can connect pentagons $P_i$ and $R_i$ by a u-chain wrapping around $Q_i$ or $S_i$. An example of a fully colored single u-chain configuration in which we wrap around pentagon $S_i$ is shown in Figure 5.7.

Due to the symmetry, the direction of wrapping does not change the length of the u-chain. However, the direction does change the primary color of the $Q_iS_i$ chain. If we use a u-chain that wraps around pentagon $Q_i$, then we we will be altering the colors of the pentagons directly surround this pentagon. This change in coloring will emanate out altering the primary color of the $Q_iS_i$ chain. Where before it was a red-blue chain

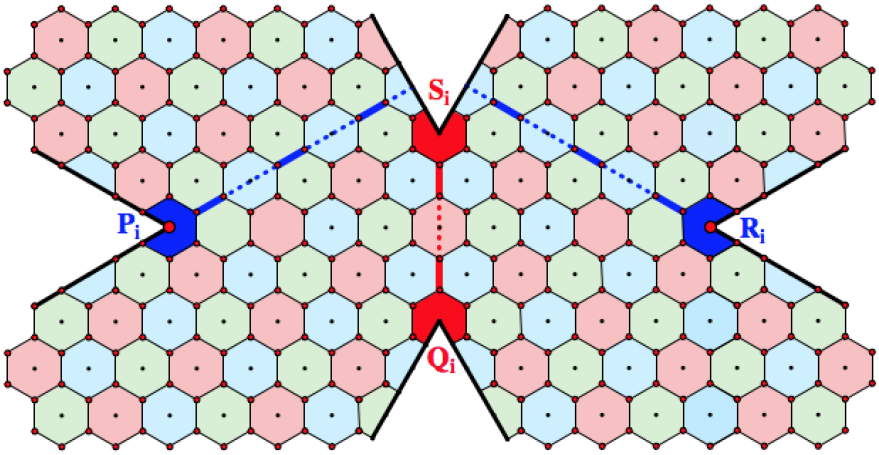



FIGURE 5.7: Possible Type 1 Chain Configuration of 4-Cluster with $p = 2$ and $r = 2$

it will now be a green blue chain and thus we can use this configuration if the Clar structure is chosen to use faces that have been assigned the color green. An example of such a configuration is shown in Figure 5.8.

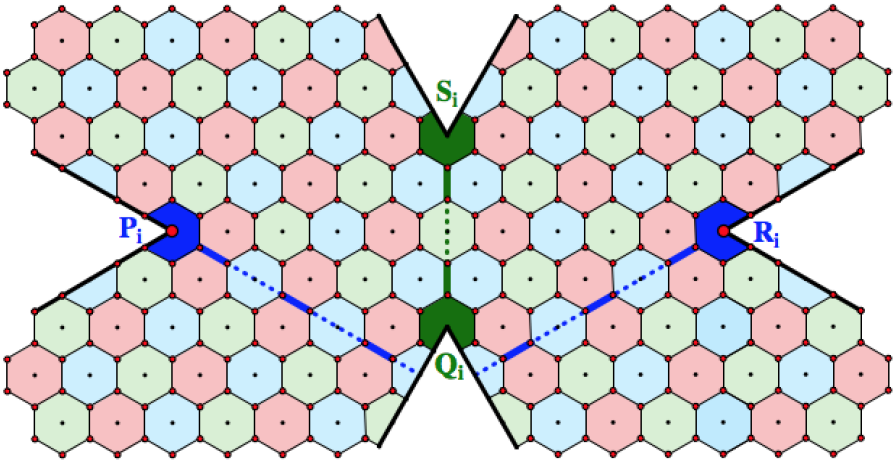



FIGURE 5.8: Possible Type 1 Chain Configuration of 4-Cluster with $p = 2$ and $r = 2$

The direct chain between $Q_i$ and $S_i$ will have length $p$, if we use a type 1 chain, and length $2p$, if we use a type 2 chain. Referring to Table 2.7 and noting that $p + r \geq p$, we calculate that the type 1 u-chain between $P_i$ and $R_i$ has length $2p + r$ and the type 2 u-chain will have length $4p + 2r$. We can use such a configuration so long as the Clar

faces are not chosen to be the primary color of the u-chain. Note that if the Clar color is chosen to be red, then we would wrap the u-chain around pentagon $Q_i$ and if the Clar color is chosen to be green we wrap around pentagon $S_i$. If the Clar color is chosen to be blue we can wrap either direction.

The secondary colors of the type 1 u-chains are determined from a different face in the configuration than those of the the direct chains in the benchmark configuration. This time the secondary color is dictated by the color assigned to the face one unit previous in the path from the direct chain between $Q_i$ and $S_i$ as shown in Figure 5.9. For example, if $r = 1$ and we are wrapping around pentagon $S_i$ then the secondary color of the u-chain would be dictated by the color of the hexagon labeled $x$ and if we are wrapping around pentagon $Q_i$ then the color is dictated by the color of the hexagon labeled $y$. In both cases, the secondary color is red.

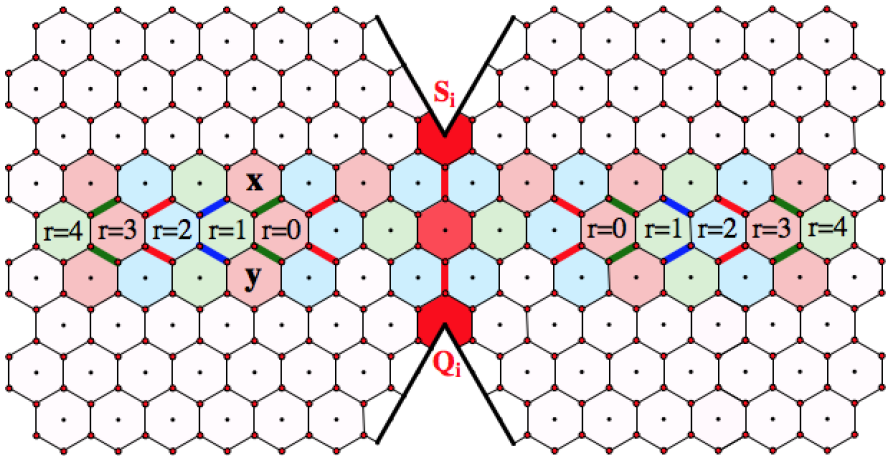



FIGURE 5.9: Illustrating Chain Colors of u-chain between $P_i$ and $R_i$

In this configuration, when $r \equiv_3 0$, both chains have primary color red and secondary color blue. So we can use two type 1 chains giving us a Clar deficit for the cluster of $3p + r$. If $r \equiv_3 1$, the u-chain has primary color green and secondary color red so we can use a type 1 u-chain and type 2 direct chain giving us a Clar deficit $4p + r$. If $r \equiv_3 2$, the u-chain has primary color blue and secondary color green so

we can use a type 1 direct chain and type 2 u-chain giving us a Clar deficit $5p + 2r$. The cluster shown in Figure 5.7 was an example with such parameters. The two type 1 chains shown in Figure 5.7 will not be a valid configuration for any choice of Clar color. Hence, to use green Clar faces we construct the wrap around chain as a type 2 chain as shown in Figure 5.10 so that both chains avoid using the color green as either primary or secondary color.

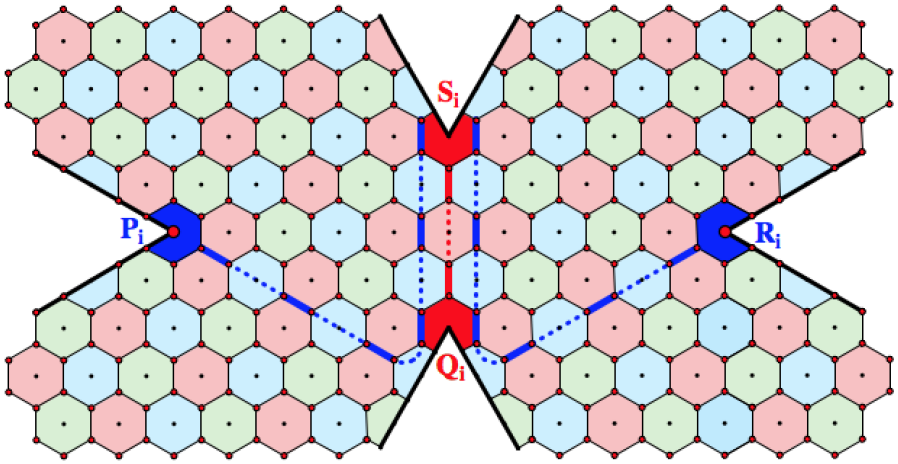



FIGURE 5.10: Type 1 direct chain and type 2 u-chain

We summarize these results in the following lemma.

**Lemma 5.2.4.** *If $\Gamma$ is a $\mathcal{O}_1$ fullerene then the total chain length for a 4-cluster $\{P_i, Q_i, S_i, R_i\}$ in $\Gamma$ is at most:*

$$\begin{cases} 3p + r & \text{when } r \equiv_3 0 \\ 4p + r & \text{when } r \equiv_3 1 \\ 5p + 2r & \text{when } r \equiv_3 2 \end{cases}$$

### Spiral Configuration

Next we consider the spiral configuration in which we have one u-chain and one chain that spirals around the u-chain. Since all clusters are isomorphic and always lie in the same color class, we will never be forced to eliminate any certain color. As a result,

we can use the Clar color that creates the most efficient chain decomposition for one cluster and then use this configuration for each of the others. Notice that neither the spiral configuration nor the single u-chain configuration allows us to eliminate the primary color of the u-chains in the single u-chain configuration.

Just as Figure 5.10 illustrated a configuration that would be compatible with using green as the color of the Clar faces, Figure 5.11 gives the other possible configuration that avoids using green faces. In this case we still have a single u-chain but instead of a direct chain we are forced to use a chain that spirals around the u-chain.

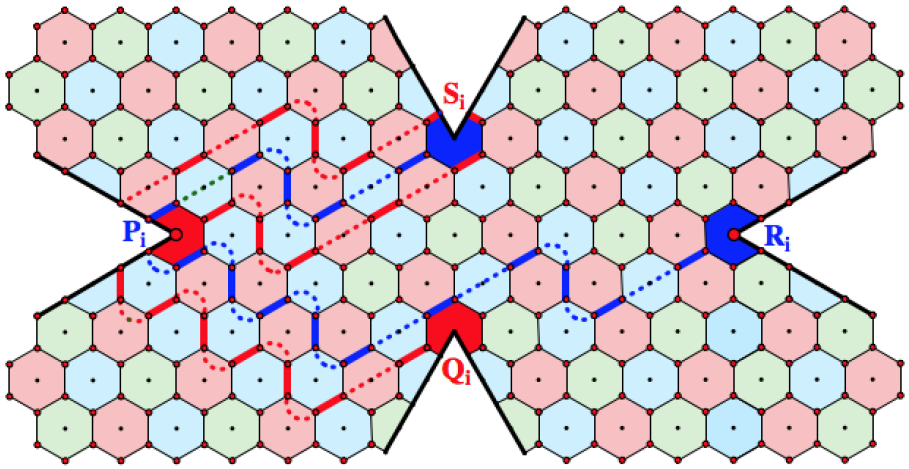



FIGURE 5.11: Type 2

Although in Chapter 4 we showed using a counterexample that the configuration in Figure 5.11 is not necessarily always longer than the configuration shown in Figure 5.10, we will show that for the 4-clusters in $\mathcal{O}_1$ this configuration will always yield total chain length greater than that of the chains in a single u-chain configuration.

**Lemma 5.2.5.** *The total chain length of a spiral chain configuration for a 4-cluster in $\mathcal{O}_1$ will be at least $5p + 4r$.*

*Proof.* To prove this claim we will find a lower bound on the spiral configuration. First will use Table 2.2 to find the length of the u-chain in the configuration. This u-chain

connects pentagons $R_i$ and $S_i$ and wraps around pentagon $P_i$ such that $\angle R_iP_iS_i = 0$. Segment $R_iP_i$ has coordinates $(3p + r, 0)$, segment $P_iS_i$ has coordinates $(p, p + r)$ and segment $R_iS_i$, once a 60° wedge has been opened at pentagon $P_i$, has coordinates $(2p + r, 2p + r)$.

Thus the length of the type 1 u-chain is

$$\max\{p + r + \max\{p, 3p + r\},\ |3p + r - p|\} + 3\left(p + \left\lceil \frac{p + r - p}{3} \right\rceil\right) = 7p + 2r + 3\left\lceil \frac{r}{3} \right\rceil$$

.

The length of the type 2 u-chain is $p + r + \min\{3p + r, p\} = 2p + r$. It is clear that the type 2 chain will always yield a shorter chain length so we will use this length in our lower bound.

Now we will use Theorem 2.3.2 to find a lower bound on the length of the spiral chain. This chain begins at pentagon $Q_i$, wraps around pentagon $P_i$ with an angle of measure 1 and then around pentagon $S_i$ at an angle of measure 0 back to pentagon $P_i$. In the notation of Theorem 2.3.2 this gives us $(a_1, b_1) = (p, p + r)$, $(a_2, b_2) = (p + r, p)$ and $(a_3, b_3) = (p + r, p)$ with $I = \{1, 2\}$ for one chain type and $I = \varnothing$ for the other chain type. Since the lower bound is given by

$$\Sigma_{i=1}^{n} \max\{a_i, b_i\} + \Sigma_{i \in I} \min\{a_i, b_i\}$$

clearly $I = \varnothing$ will give a smaller lower bound. Thus we get that a lower bound of $3(p + r)$.

Combining this with the lower bound on the u-chain yields a lower bond on the total length of $5p + 4r$. □

Referring to Lemma 5.2.6, we see that $5p + 4r$ is longer than any of the total chain lengths of any single u-chain configuration. Thus we do not need to consider this

configuration as it will never yield the minimal Clar deficit.

### Double U-Chain Configuration

Now we want to consider the double u-chain configuration. One example of such a configuration is shown in Figure 5.12. The benefit of this configuration in a more general setting is that it allows more control over the primary color of the u-chains than with the single u-chain configuration or the spiral configuration.

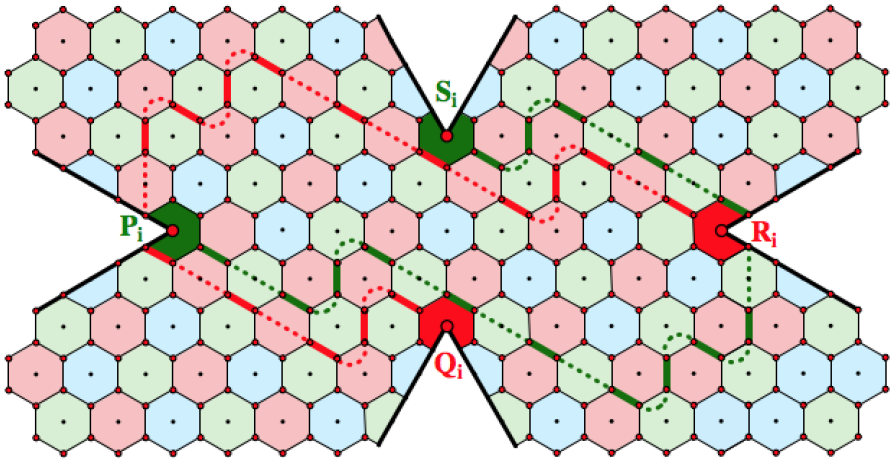



FIGURE 5.12: Double u-Chain Configuration of 4-Cluster with $p = 2$ and $r = 2$

Precisely the double u-chain configuration includes one u-chain from $P_i$ to $Q_i$ around $S_i$ and one u-chain from $S_i$ to $R_i$ around $Q_i$. Alternatively we can use two chains $R_i$ to $Q_i$ around $S_i$ and one from $P_i$ to $S_i$ around $Q_i$ but again due to symmetry these will have equivalent chain lengths. So let us choose the second option.

Looking back to our formula for the length of u-chains in Chapter 2, the 4-clusters in this infinite class have parameters $a = p$, $b = p + r$, $c = 2p + 2r$ and $d = 0$. As such, $p + r \geq p$, $3p + 2r \geq 0$ and we are wrapping around a pentagon associated with angle measure 1 so we appeal to Table 2.5. As a result, we calculate that a type 1 chain will

have length:

$$\max\{p + \min\left\{p + r, 3p + 2r\right\} + 0, |(p + r) - (p)|\right\} + 3\left\lceil \frac{3p + 2r}{3} \right\rceil = 5p + r + 3\left\lceil \frac{2}{3}r \right\rceil$$

We will need two such chains for this configuration so the Clar deficit for this configuration will be doubled. Thus by Lemma 5.2.6, we see that the Clar deficit from this configuration will always be greater than any of the deficits from a single u-chain configuration and hence the double u-chain configuration will never yield a minimal Clar deficit. We rule it out as a result.

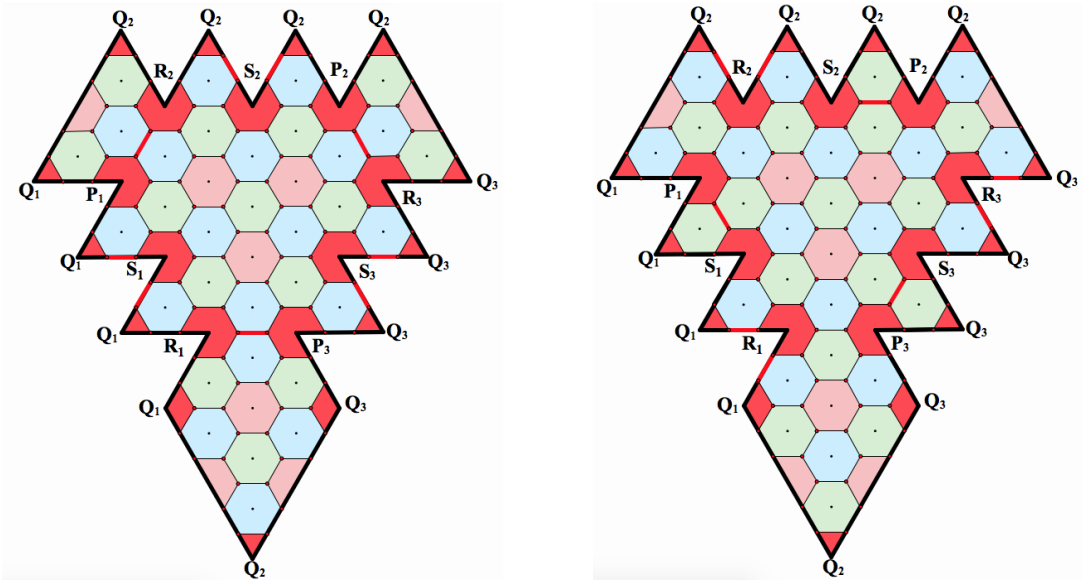
**Fully Monochromatic Configuration**

If $r \equiv_3 0$ then all pentagons in the fullerene will be chain available. Still we must pair all pentagons in a way that yields the least Clar deficit but we have further possibilities of chain available pairs of pentagons than when $r \equiv_3 1$ or $r \equiv_3 2$. Without loss of generality, let us say that all four pentagons are red. Two examples of chain configurations for a fullerene in $\mathcal{O}_1$ are shown in Figure 5.13.

The configuration shown in Figure 5.13a is the configuration from Figure 5.5 that yields our benchmark Clar deficit which for this configuration is $3s + 3p$.

We also have the possible configuration with a direct chain and a wrap around chain as discussed in the previous section. In that case, we had a calculated Clar deficit of $3p + r$. Now we need to consider the configuration in which we use two direct chains within each cluster. Such a configuration is only possible when $r \equiv_3 0$

To form a direct chain configuration for these 1 1 3 star 4-clusters, we must choose two independent pairs of pentagons. Notice that since the segment connecting $P_i$ and $R_i$ has coordinates $(3p + 2r, 0)$ there is no circumstance when choosing a chain connecting $P_i$ and $R_i$ will be the shortest option. We have already fully discussed the results of choosing a direct chain from $Q_i$ to $S_i$.




(A) Benchmark Configuration (B) Chain Confined within Clusters

FIGURE 5.13: Possible Type 1 Chain Configurations when $r \equiv_3 0$

We are left with the options to either choose to construct a $P_iQ_i$ and $R_iS_i$ pair of chains or to join $P_iS_i$ and $Q_iR_i$ as in Figure 5.13b. Due to the symmetry of $\mathcal{O}_1$ either option will yield two isomorphic pairs of chains. So, without loss of generality, we pair pentagons $P_i$ and $S_i$ and additionally $Q_i$ and $R_i$ .

These two direct chains do not have the same secondary color. Since $\angle P_iQ_iR_i$ and $\angle P_iS_iR_i$ both have measure 2, it follows from Lemma 2.3.1 that the $P_iQ_i$ and $Q_iR_i$ type 1 chains have the same secondary color as do the $P_iS_i$ and $R_iS_i$ type 1 chains. Furthermore, since $\angle Q_iR_iS_i$ has measure 1, the $Q_iR_i$ and $R_iS_i$ type 1 chains must have distinct secondary colors. As a result, if the $P_iQ_i$ and $Q_iR_i$ type 1 chains have a secondary chain color of blue then the $P_iS_i$ and $R_iS_i$ type 1 chains must have secondary color green. As the two pairs of pentagons in the chain configuration must be independent, the type 1 direct chains formed by any independent set of pentagon pairs will always have distinct secondary colors.

If we choose blue Clar faces, then the chain containing pentagon $P_i$ will be constructed as a type 1 chain while the chain containing pentagon $R_i$ will be constructed as a type 2 chain. Similarly, if we take the Clar faces to be green, we still need to use both a type 1 and a type 2 chain. This time the type 2 chain contains pentagon $P_i$ and the type 1 chain must contain pentagon $R_i$.

For red Clar faces we must change the primary colors of the chains. We have already considered the option where we use two u-chains and determined that this will not yield a minimal option. The other possibility is to use two type 3 chains.

The formulas for computing the Clar deficit for each of the three color classes is given in the following table:

TABLE 5.2: Clar Deficit for 4-cluster within $\mathcal{O}_1$ with $r \equiv_3 0$

| Clar Faces | Clar Deficit | Chain Structure |
|---|---|---|
| Red | $6p + 6r + 4$ | two type 3's |
| Blue | $3p + 2r$ | type 1 & type 2's |
| Green | $3p + 2r$ | type 1 & type 2's |

The most efficient option is when we use blue or green Clar faces, and we get a Clar deficit for the cluster of $3p + 2r$. However, referring to Lemma 5.2.6, the deficit for the single u-chain configuration was at most $3p + r$. It may be a bit surprising that a direct chain and a u-chain yields a shorter chain configuration than one with two direct chains. However, notice that in this configuration with two direct chains one chain was forced to be type 2 whereas in the configuration using one direct chain and one u-chain we were able to use only type 1 chains.

### Combining all 4-Clusters

Therefore, we have that the minimal Clar deficit when decomposing these fullerenes into three 4-clusters is given by using a single u-chain decomposition for each of the

4-clusters. Hence, we simply multiply the Clar deficit for the minimal Clar structure from the single u-chain configuration by 3 to get the total Clar deficit for the fullerene. By Lemma 5.2.6, we compute that the Clar deficit over the entire fullerene is given by $3(3p+r) = 9p+3r$ when $r \equiv_3 0$, $3(4p+r) = 12p+3r$ when $r \equiv_3 1$ and $3(5p+2r) = 15p+6r$ when $r \equiv_3 2$.

We summarize these results in the following lemma for ease of reference in future sections.

**Lemma 5.2.6.** *If $\Gamma$ is a $\mathcal{O}_1$ fullerene then the Clar deficit for $\Gamma$ is at most:*

$$\begin{cases} 9p + 3r & \text{when } r \equiv_3 0 \\ 12p + 3r & \text{when } r \equiv_3 1 \\ 15p + 6r & \text{when } r \equiv_3 2 \end{cases}$$

## 5.3 Other Possible Chain Decompositions

We have found the best configuration given that we constrain our chains to be within the 4-clusters. However, we have only considered one possible configuration that includes chains between the clusters. We need to consider configurations other than our benchmark configuration to make sure the benchmark is, in fact, the most efficient option among such decompositions.

Once we form a chain between pentagons in distinct 4-clusters, the Clar deficit will necessarily depend on both the parameters $s$ and $p$. In joining two pentagons in distinct clusters, these clusters are left with three unpaired pentagons in each set. Hence, if we have one chain leaving a cluster, we must have at least two chains leaving that cluster and at most one chain remaining internal to the 4-clusters.

Let us return to our consideration of the two pentagon color classes in $\mathcal{O}_1$. First consider the subset of vertices $\{Q_1, Q_2, Q_3, S_1, S_2, S_3, \}$. As all pentagons in this set

are in the same color class, our auxiliary graph of chain available pentagons is the complete graph $K_6$ as shown in Figure 5.14.

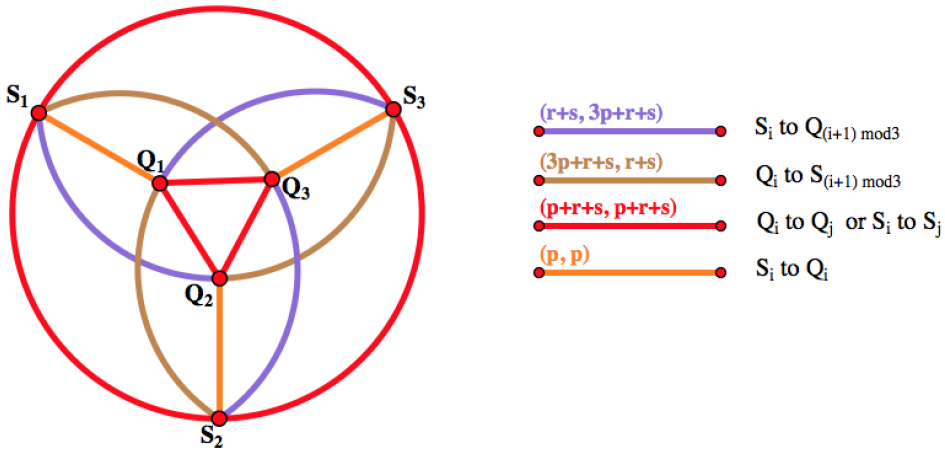
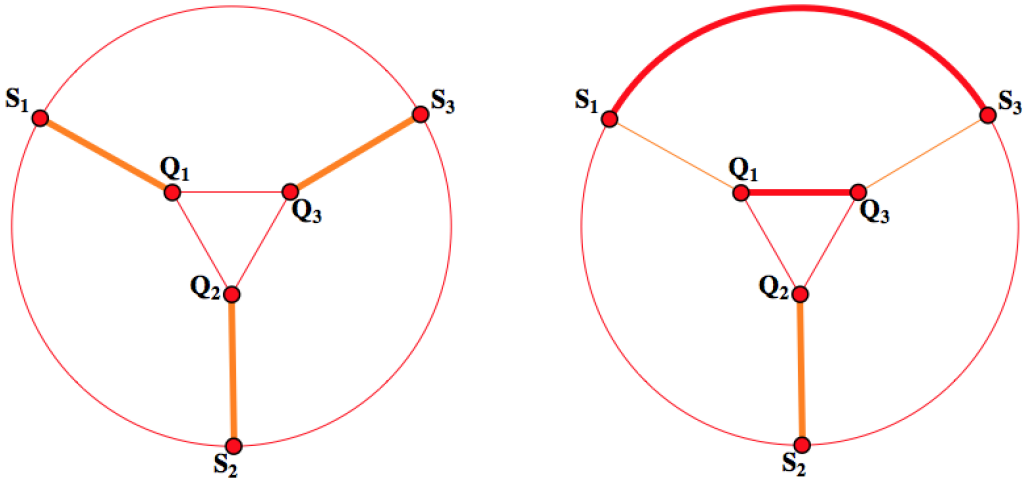



FIGURE 5.14: Segment lengths between neighboring pentagons in $\{Q_1, Q_2, Q_3, S_1, S_2, S_3, \}$

Notice that the orange edges have coordinates $(p, p)$. For each of the other segments, with the exception of the red segments, the maximum coordinate is at least $2p$. Hence, even if we are forced to use a type 2 chain to connect pentagons $S_i$ to $Q_i$ the chain will still be shorter than a type 1 chain corresponding to the the other segments. Thus, we see that we can disregard the lavender and brown edges.

Once we disregard these edges we are left with only two perfect matchings as shown in Figure 5.15.

We want to determine conditions that will indicate which matching in Figure 5.15 yields the chain configuration with the least Clar deficit. Let us assume that we are able to use all type 1 chains for the configuration in Figure 5.15b in order to find the lower bound on the length of such a chain configuration. Additionally notice that angle $S_1Q_1Q_3$ has angle measure 2. Thus, by Lemma 2.3.1, the chain from $S_1$ to $Q_1$ and the chain joining $Q_1$ and $Q_3$ will have the same secondary colors. Similarly the chain from $S_1$ to $S_3$ will also have the same secondary color. Hence, if the coloring allows us




(A) 1st Perfect Matching Option (B) 2nd Perfect Matching Option

FIGURE 5.15: Possible perfect matchings of auxiliary graph on $\{Q_1, Q_2, Q_3, S_1, S_2, S_3, \}$

to use all type 1 chains in the configuration shown in Figure 5.15b then we can use all type 1 chains in the configuration shown in Figure 5.15a. If we were to use all type 1 chains in the configuration in Figure 5.15a then we get a Clar deficit of $3p$. However, for the configuration shown in Figure 5.15b, we get a lower bound given by

$$\max\{p, p\} + \max\{p + r + s, p + r + s\} + \max\{p + r + s, p + r + s\}$$

This yields $p + p + r + s + p + r + s = 3p + 2r + 2s$. As such, the configuration using all orange edges will always be the most efficient option.

Now let us move on to consider the graph on the vertices $\{R_1, R_2, R_3, P_1, P_2, P_3, \}$. Again using edges to connect neighboring vertices between these pentagons yields a graph isomorphic to $K_6$ labeled with the corresponding coordinates between neighboring pentagons as shown in Figure 5.16.

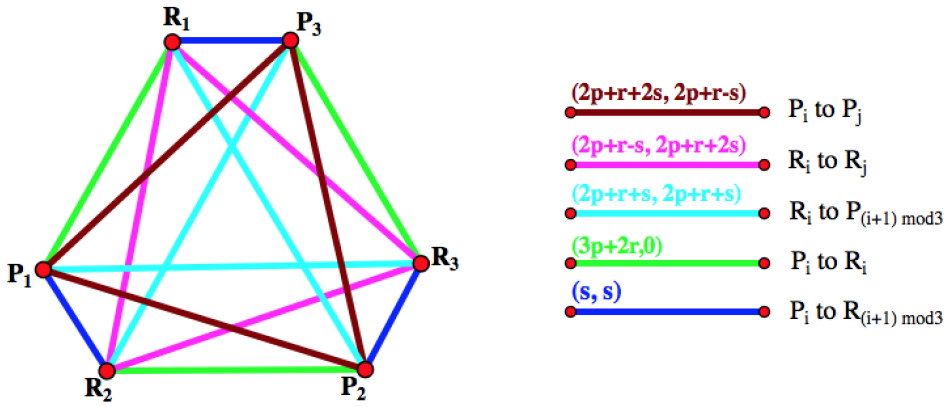
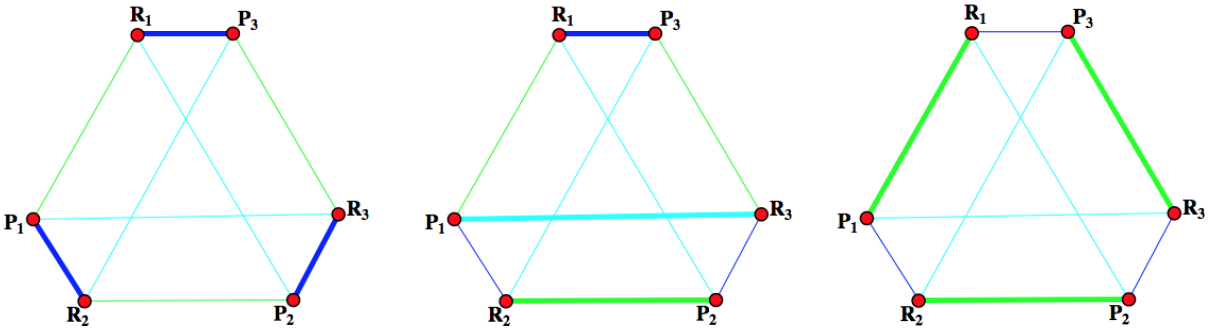



FIGURE 5.16: Segment coordinates between neighboring pentagons in $\{R_1, R_2, R_3, P_1, P_2, P_3, \}$

First note that we will never need to use chains associated with pink or brown edges since both have a maximum coordinate larger than the sum of the coordinates $(s, s)$. Once we eliminate those edges we are now left with three possible perfect matchings on the remaining edges for the set $\{R_1, R_2, R_3, P_1, P_2, P_3, \}$ as shown in Figure 5.17.




(A) 1st Perfect Matching Option (B) 2nd Perfect Matching Option (C) 3rd Perfect Matching Option

FIGURE 5.17: Possible perfect matchings of auxiliary graph on $\{R_1, R_2, R_3, P_1, P_2, P_3, \}$

Notice that since we are only considering direct chains, the green edges do not have coordinates congruent modulo 3 when $r \not\equiv_3 0$. However, we know that these pentagons are chain available when the chains are chosen to be u-chains. Once we

incorporate in the remaining pentagons the coordinates associated with the green edge changes to $(2p + r, 2p + r)$ as it is now a u-chain.

Using the matching in Figure 5.17a along with our matching from Figure 5.15a yields the benchmark configuration. Using the matching in Figure 5.17c along with our matching from Figure 5.15a yields the configuration that constrains the chains to the three 4-clusters. We are left with the configuration in Figure 5.17b.

The Clar deficit for the configuration in Figure 5.17b is at least

$$\max\{s, s\} + \max\{2p + r, 2p + r\} + \max\{2p + r + s, 2p + r + s\} = 4p + 2r + 2s$$

Combining this with the configuration in Figure 5.17a yields a minimal Clar deficit of $7p + 2r + 2s$. This is a larger deficit than the deficit in the benchmark configuration for any equivalence class of $r$.

## 5.4 Clar Deficit for $\mathcal{O}_1$

All that remains to do is to combine our results into a table outlining the Clar deficit and Clar number for all possible cases. Recall from Chapter 1 that the Clar number of a fullerene is given by $\frac{1}{6}(|V| - 2|A|)$ where $|A|$ denotes the Clar deficit. Furthermore, $|V|$ is given by the number of atoms in the carbon structure. Referring to Figure 5.1, we see that for a fullerene in $\mathcal{O}_1$, $|V| = 42p^2 + 12r^2 + 6s^2 + 60pr + 48ps + 12rs$. For any equivalence class of $r$ we have that the benchmark configuration will yield the least Clar deficit when $s \leq 2p + r$ and otherwise we use our cluster configuration. However, within the benchmark configuration we have that the minimal Clar deficit is dependent on further relations between $s$ and $p$.

Table 5.3 gives us the Clar deficit and Clar number for each equivalence class of $r$.

| Equivalence Class of $r$ | Parameter Conditions | Clar Deficit | Clar Number |
|---|---|---|---|
| $r \equiv_3 0$ | $s \leq 2p + r$ | $3p + 3s$ | $\frac{1}{6}\|V\| - (p + s)$ |
| | $s > 2p + r$ | $9p + 3r$ | $\frac{1}{6}\|V\| - (3p + r)$ |
| $r \equiv_3 1$ | $s < 0.5p - 1$ | $3p + 9s + 6$ | $\frac{1}{6}\|V\| - (p + 3s + 2)$ |
| | $0.5p - 1 \leq s \leq 2p + r$ | $6p + 3s$ | $\frac{1}{6}\|V\| - (2p + s)$ |
| | $s > 2p + r$ | $12p + 3r$ | $\frac{1}{6}\|V\| - (4p + r)$ |
| $r \equiv_3 2$ | $s < 2p + 2$ | $9p + 3s + 6$ | $\frac{1}{6}\|V\| - (3p + s + 2)$ |
| | $2p + 2 \leq s \leq 2p + r$ | $3p + 6s$ | $\frac{1}{6}\|V\| - (p + 2s)$ |
| | $s > 2p + r$ | $15p + 6r$ | $\frac{1}{6}\|V\| - (5p + 2r)$ |

TABLE 5.3: Clar Deficit and Clar Number of $\mathcal{O}_1$

## 5.5 $\mathcal{O}_2$

We now move onto considering another class of arrowhead fullerenes, $\mathcal{O}_2$. Let us look at the underlying auxiliary graph on neighboring pentagons for $\mathcal{O}_2$ as shown in Figure 5.18. Notice that since all the included segments have a second coordinate of 0 the segments will all lie directly along a coordinate path. Thus, any pair of pentagons that is of distance two segments apart with an angle of measure 2 between them will be connected by a segment with the first coordinate given by the non-zero coordinate of one segment and the second coordinate given by the non-zero coordinate of the other segment. For example the coordinates of the segment between $R_1$ and $Q_2$ will be $(r, r + s)$ as noted in Figure 5.18.

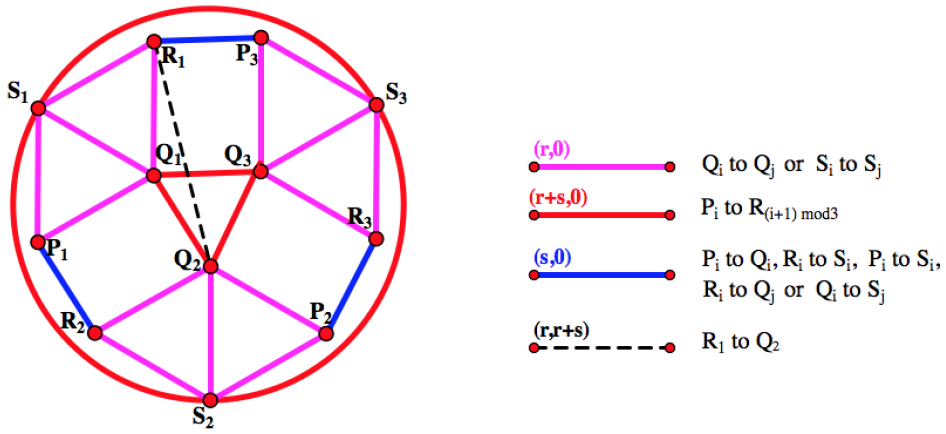



FIGURE 5.18: Segment Structure of $\mathcal{O}_2$

For the configuration in $\mathcal{O}_2$ there is no obvious benchmark configuration so we will move directly to considering the 4-sets $\{P_i, Q_i, R_i, S_i\}$.

### 5.5.1 $\mathcal{O}_2$ 4-Clusters

For this infinite class of fullerenes, we again have a clear opportunity to decompose the set of pentagonal faces into three congruent 4-sets $\{P_i, Q_i, R_i, S_i\}$ for $i = 1, 2, 3$. One of these isomorphic sets is shown in Figure 5.19 with all segments. The pink edges lie along coordinate paths due to the structure of the segments in this class. Since these 4-sets have the same underlying angle configuration and all pink segments have the same length, the clusters will have a 1 1 3 star signature, as in the clusters for in $\mathcal{O}_1$

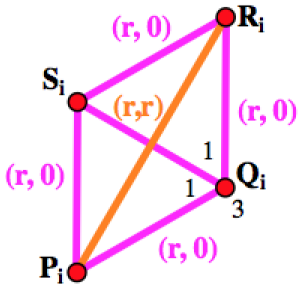



FIGURE 5.19: 4-set $\{P_i, Q_i, R_i, S_i\}$

**Lemma 5.5.1.** *For $i = 1, 2, 3$, the 4-set $\{P_i, Q_i, R_i, S_i\}$ in $\mathcal{O}_2$ will have a 1 1 3 star signature.*

*Proof.* The segment connecting $P_i$ and $R_i$ has coordinates $(r, r)$ which is clearly the longest and so will not appear in any shortest spanning tree of $\{P_i, Q_i, R_i, S_i\}$. Since all other segments have the same length we can choose any three to form the shortest spanning tree so long as they do not form a triangle. Without loss of generality, we can choose to use segments $P_iQ_i$, $R_iQ_i$ and $S_iQ_i$ to form the edges of the signature graph. We know from the underlying structure of $\mathcal{O}_2$ shown in Figure 5.1 that $\angle P_iQ_iR_i$ has external measure 3 giving us that the signature of set $\{P_i, Q_i, R_i, S_i\}$ has the form of a 1 1 3 star. □

**Lemma 5.5.2.** *Each 4-set $\{P_i, Q_i, R_i, S_i\}$ in $\mathcal{O}_2$ will be a 4-cluster for any value of $r$.*

*Proof.* In order for these 4-sets to be classified as 4-clusters we know from Lemma 3.4.3 that $(a - b) + (c - d) + (j - k) \equiv_3 0$. In the context of these sets we have $a = c = j = r$ while $b = d = k = p$ for each of the sets. Making the appropriate substitutions yields the sufficient and necessary condition

$$(r) + (r) + (r) = 3r \equiv_3 0$$

which holds for any value of $r$ hence $\{P_i, Q_i, R_i, S_i\}$ is always a 4-cluster. □

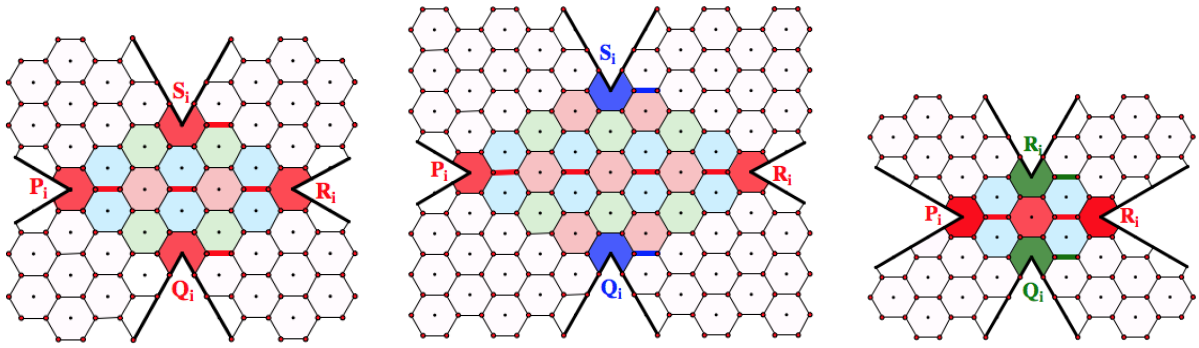
The deficits calculated in this section will hold so long as $s$ is large, and thus, the clusters are far apart.

When $r \not\equiv_3 0$, we will have clusters in an opposite configuration by Lemma 4.3.1. Again we will consider the three possible wrap around chain configurations for these clusters. When $r \equiv_3 0$ our 4-clusters will be monochromatic. Even though we can use the theory discussed in subsection 5.2.2 to find a total chain length for such configurations, we must still check that the possible wrap around configurations do not yield a lesser total chain length for monochromatic clusters.

### Single U-chain Configuration

The $P_iR_i$ segment has coodinates $(r, r)$ so we can form a direct chain between these two pentagons. Let us begin by assuming that we are connecting pentagons $P_i$ and $R_i$ by a chain with primary color red and secondary color blue where the primary color red is determined from the initial coloring of the pentagons surrounding pentagon $P_i$. Let us say the face directly below pentagon $P_i$ in our figures is initially colored green. We can connect pentagons $Q_i$ and $S_i$ by a u-chain wrapping around $P_i$ or $R_i$. Due to the symmetry in this class, the direction of wrapping will not change the length of the u-chain. However, the direction will change the colors of the $P_iR_i$ chain and the secondary color of the u-chain.

Due to the symmetry in these clusters, we need only determine the secondary colors of the u-chains for one example in each equivalence class of $r$ and then by similarity these secondary colors will hold for all possible choices of $r$ within the respective equivalence class. This is an example of a cluster in which the type 2 u-chain will not necessarily be longer than than the type 1 u-chain.




(A) $r \equiv_3 0$ (B) $r \equiv_3 1$ (C) $r \equiv_3 2$

FIGURE 5.20: Determining the secondary colors of u-chains in $\mathcal{O}_2$

Figure 5.20 shows an example of a 4-cluster in $\mathcal{O}_2$ for each possible equivalence class of $r$, and highlights the edges that will be used in the type 2 u-chain if we wrap

around pentagon $R_i$. In each case, the initial edges of the type 2 u-chain that wraps around $R_i$ in our figures use initial edges parallel to the $P_iR_i$ chain. The color of the face one step closer to the $P_iR_i$ chain will determine the secondary color of the type 2 u-chain. Thus, when $r \equiv_3 0$, we see the primary color is red and the secondary color is green. When $r \equiv_3 1$, we see the primary color is blue and the secondary color is red. Finally, when $r \equiv_3 2$, we see the primary color is green and the secondary color is blue. Notice that wrapping around pentagon $P_i$ will permute the secondary colors of the u-chain since we will be changing the primary color of the direct chain.

The direct chain between $Q_i$ and $S_i$ will have length $r$ if we use a type 1 chain and length $2r$ if we use a type 2 chain. Referring to Table 2.5 and noting that $r \geq 0$ we calculate that the type 1 u-chain between $Q_i$ and $S_i$ has length $r + 3\lceil \frac{r}{3} \rceil$, and the type 2 u-chain will have length $2r$. We can use such a configuration so long as the Clar faces are not chosen to be the primary color of the u-chain.

**Double U-chain Configuration**

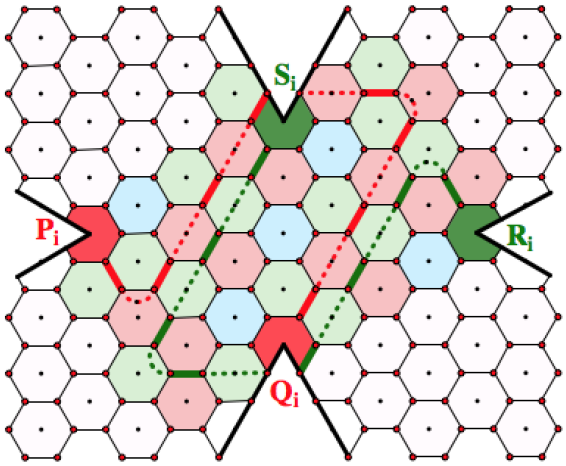
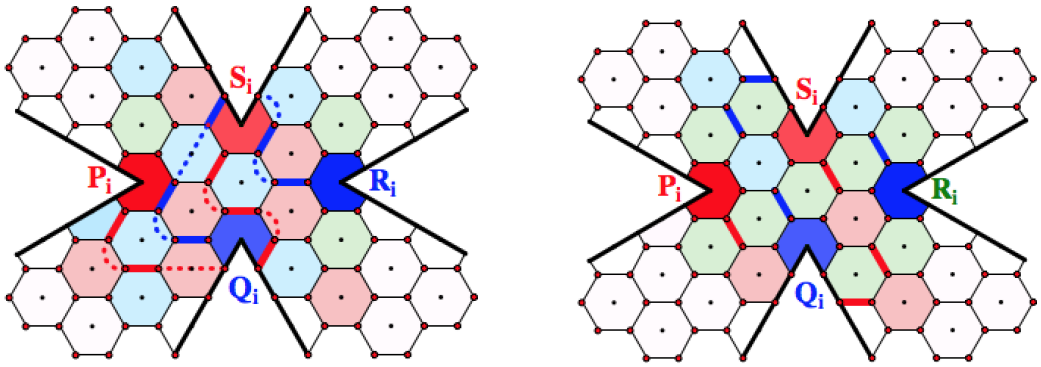



FIGURE 5.21: Double type 2 u-chain configuration of 4-cluster with $r = 4$

Specifically the double u-chain configuration includes one u-chain from $P_i$ to $Q_i$

around $S_i$ and one u-chain from $S_i$ to $R_i$ around $Q_i$. An example of such a configuration is shown in Figure 5.21. Alternatively, we can use two u-chains $R_i$ to $Q_i$ around $S_i$ and one from $P_i$ to $S_i$ around $Q_i$ but again due to symmetry these will have equivalent chain lengths. So let us choose the first option as we did in the case of $\mathcal{O}_1$.

Since $r \geq 0$ and we are wrapping around a pentagon associated with angle measure 1, the wrap around chains in this configuration have the same length as the u-chains in the single u-chain configuration. Namely, the type 1 u-chains have length $r + 3\lceil \frac{r}{3} \rceil$ and the type 2 u-chains have length $2r$. In Figure 5.22 we show the configuration for an example of such a cluster with $r = 2$ using two type 1 u-chains and using two type 2 u-chains.




(A) Two type 1 u-chains (B) Two type 2 u-chains

FIGURE 5.22: Configuration of 4-cluster in $\mathcal{O}_2$ with two u-chains

### Minimal Total Chain Length for 4-cluster in $\mathcal{O}_2$

Now we consider each of the equivalence classes for $r$ to determine the Clar deficit for each case. We assume here that we will be either using a direct configuration, single u-chain or double u-chain configuration. In the next section, we will show that the spiral configuration never yields a lesser Clar deficit.

For these 4-clusters when $r \equiv_3 0$, if we were to use a single u-chain configuration both the type 1 direct chain and the type 1 u-chain have primary color red and secondary color blue. So if the Clar color is chosen to be green we can use two type 1 chains giving us a clar deficit of $2r + 3\lceil \frac{r}{3} \rceil$. However, we can do better than this by appealing to subsection 5.2.2 which discussed fully monochromatic 1 1 3 star 4-clusters. Since the clusters in both $\mathcal{O}_1$ and $\mathcal{O}_2$ have the same angle configurations, we will still not be able to choose two type 1 direct chains between pairs of pentagons. Hence, for either blue or green Clar faces we will need a type 1 and a type 2 direct chain. For direct chains between pentagons with segment coordinates $(r, 0)$, both type 1 and type 2 chains will have length $r$ which gives us a total Clar deficit for the 4-cluster of $2r$. Since $2r \leq 2r + 3\lceil \frac{r}{3} \rceil$ for any value of $r$, this will necessarily give us the minimal Clar deficit for either choice of Clar color. In the monochromatic case, if we must choose red as our Clar color we will be forced to use two type 3 direct chains giving us a Clar deficit of $6r + 4$.

TABLE 5.4: Clar deficit for 4-cluster within $\mathcal{O}_2$ with $r \equiv_3 0$

| **Clar Faces** | **Clar Deficit** | **Chain Structure** |
|---|---|---|
| Red | $6r + 4$ | two type 3 direct chains |
| Blue | $2r$ | type 1 & type 2 direct chains |
| Green | $2r$ | type 1 & type 2 direct chains |

If $r \equiv_3 1$, the type 2 u-chain has primary color blue and secondary color red so if the Clar color is chosen to be green we can use a type 1 direct chain and type 2 u-chain giving us a Clar deficit $3r$. If the Clar color is chosen to be red, then we must wrap around pentagon $P_i$ which interchanges the colors red and green. Thus, the direct chain will now have primary color green and the secondary color will be unchanged. The secondary color of the u-chain will now be green. Hence, we will still be able to use a type 2 u-chain and a type 1 direct chain giving us a Clar deficit of $3r$. If we

must choose blue as the color of the Clar faces, we may use two type 2 u-chains in the double u-chain configuration giving us a Clar deficit of 4r.

TABLE 5.5: Clar deficit for 4-cluster within $\mathcal{O}_2$ with $r \equiv_3 1$

| Clar Faces | Clar Deficit | Chain Structure |
|---|---|---|
| Red | $3r$ | type 2 u-chain & type 1 direct chain |
| Blue | $4r$ | two type 2 u-chains |
| Green | $3r$ | type 2 u-chain & type 1 direct chain |

Finally we will consider the case when $r \equiv_3 2$. Now the type 1 u-chain has primary color green and secondary color red. If we choose red as the Clar color, then we will wrap our u-chain around $P_i$ to eliminate red as a primary chain color. Now our direct type 1 chain has primary color blue and secondary color red and the type 2 u-chain has primary color green and secondary color red. To use red as the Clar color, we will use a type 2 u-chain and a type 1 direct chain giving a deficit of $3r + 3\lceil \frac{r}{3} \rceil$. Notice that since $r \equiv_3 2$, we have that $\lceil \frac{r}{3} \rceil = \frac{r+1}{3}$. We can thus simplify our formula for total chain length to $3r + 3\lceil \frac{r}{3} \rceil = 4r + 1$

If we choose blue as the Clar color, we will wrap the u-chain around pentagon $R_i$, and again must use a type 1 u-chain and type 2 direct chain giving us a Clar deficit $3r + 3\lceil \frac{r}{3} \rceil = 4r + 1$. Finally, if we choose green as our Clar color, we must use a double u-chain configuration. In this case to eliminate the green faces from the chain, we have to use two type 1 u-chains giving us a Clar deficit of $2r + 6\lceil \frac{r}{3} \rceil$ or equivalently $4r + 2$.

These results are outlined in the following table:

TABLE 5.6: Clar deficit for 4-cluster within $\mathcal{O}_2$ with $r \equiv_3 2$

| Clar Faces | Clar Deficit | Chain Structure |
|---|---|---|
| Red | $4r + 1$ | type 2 u-chain & type 1 direct chain |
| Blue | $4r + 1$ | type 1 u-chain & type 2 direct chain |
| Green | $4r + 2$ | two type 1 u-chains |

In each of these clusters, we have three choices of Clar color. If we choose the Clar color to be the primary color of the $Q_i$ $S_i$ u-chain then we will have to use a double u-chain configuration and will end up with one possible value for the Clar deficit. On the other hand, if we choose one of the remaining two colors then the chain configuration will be symmetric no matter which color we wish to eliminate from the faces making up the Clar structure. So for either choice of Clar color, we get the same Clar deficit. In all cases, choosing a Clar color that is distinct from the primary color of the $Q_i$ $S_i$ u-chain will yield a smaller Clar deficit. So when possible we will avoid such a choice for the color of the Clar face.

**Spiral Configuration**

Again we need to confirm that the spiral configuration is not going to yield a more efficient chain structure for the 4-clusters in $\mathcal{O}_2$.

**Lemma 5.5.3.** *The total chain length of a spiral configuration for a 4-cluster in $\mathcal{O}_2$ will be at least $5r$.*

*Proof.* In this case, we will have a u-chain from $Q_i$ to $R_i$ around pentagon $S_i$ such that $\angle Q_i S_i R_i$ has measure 1. This chain will have the same length as the u-chains in the single u-chain configuration. Thus, we have a type 1 chain with length $r + 3\lceil \frac{r}{3} \rceil$ and the type 2 chain will have length $2r$. Hence, our lower bound on the u-chain will be $2r$.

In finding the lower bound on the spiral chain, we note that the spiral starts at pentagon $P_i$, wraps around pentagon $S_i$ with a measure of angle 2 and then around pentagon $R_i$ with an angle of measure 0 and then back to pentagon $S_i$. All relevant segments have coordinates $(r, 0)$. Since the minimum coordinate in all cases is 0, the lower bound will be

$$\Sigma_{i=1}^{n} \max\{a_i, b_i\} = 3r$$

for any ordering of angle measures.

This gives us a lower bound of $5r$ for the entire configuration. □

Considering all the possible chain lengths outlined in the table above, we see that the longest total chain length is when $r \equiv_3 2$. This spiral configuration is only viable for red or blue Clar faces so we compare our lower bound to $4r + 1$. $4r + 1 \leq 5r$ as long as $r \geq 1$. Since this upper bound was when $r \equiv_3 2$, we have $r \geq 2$ and so all possible configurations are more efficient than the spiral configuration. Thus, we need not consider this configuration further.

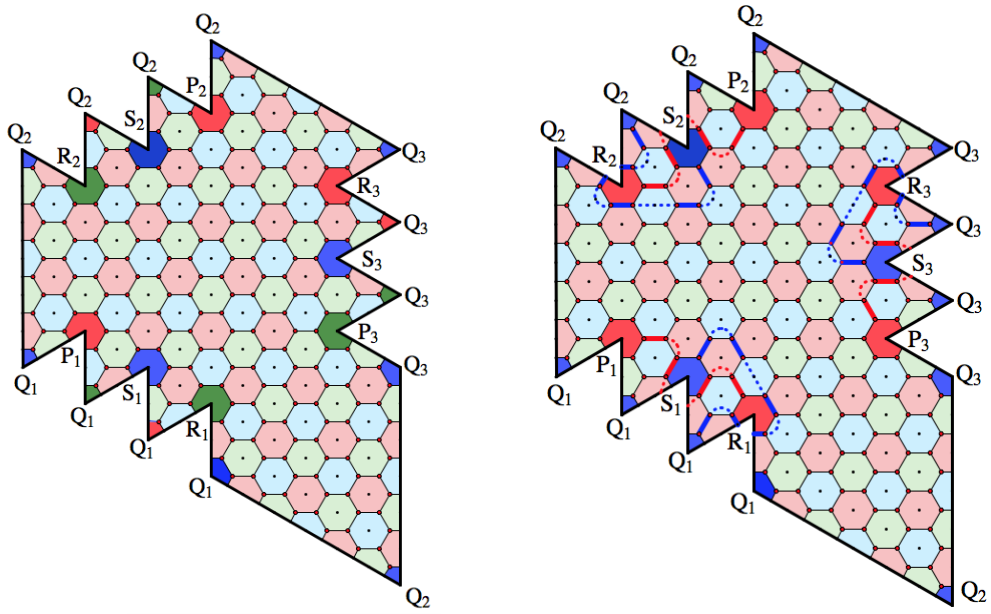
### 5.5.2 Combining the three 4-clusters

Now we need consider the three 4-clusters simultaneously in order to determine the Clar deficit for a fullerene in this class.

Since the three 4-clusters will not necessarily all be identically colored, we need to determine more than just the cheapest Clar deficit for any choice Clar color. Rather, we need to find the Clar deficit for any choice of Clar color so that, when we consider the Clar color for the entire fullerene, we will be able to choose the configuration for each cluster that minimizes the Clar deficit for the entirety of $\mathcal{O}_2$.

First recall that the coordinates between $S_i$ and $S_j$ for $i \neq j$ are given by $(r + s, 0)$ as shown in Figure 5.18. Hence, if $r + s \equiv_3 0$ then $\{S_1, S_2, S_3\}$ will be in the same color class. In this case, we can use a single u-chain configuration for each cluster without being forced to use the primary color of the u-chain as the Clar color for any of the clusters.

An example of such an arrowhead fullerene from $\mathcal{O}_2$ is shown in Figure 5.23. Figure 5.23a shows the flat map embedded in $\Lambda$, and we see that the coloring along the boundary of the flat map does not match up along all associated sides. In this coloring $\{S_1, S_2, S_3\}$ are colored blue so if we choose red or green as the Clar color, we




(A) Flat map of $\mathcal{O}_2$ embedded in $\Lambda$ before chains are formed

(B) Identical configurations for each 4-cluster

FIGURE 5.23: Clar Structure for $\mathcal{O}_2$ with $r + s \equiv_3 0$ with $r = 2$

can choose identical chain configurations for the three 4-clusters. The configuration for our example shown in Figure 5.23b, uses green as the color of the Clar faces. We see that once the six chains are constructed, the coloring matches on the boundary and throughout the flat map with the exception of along the chains. Since we can use the same configuration for each 4-cluster, the Clar deficit can be calculated as three times the minimal Clar deficit for an individual cluster in the appropriate equivalence class of $r$.

Referring to Figure 5.1, we see that $|V| = 14r^2 + 2s^2 + 16rs$. Thus, we can use the computations for the Clar deficit to additionally compute the Clar number for each equivalence class of $r$. Our calculated lower bound on Clar deficit and associated upper bound on Clar number for such fullerenes in $\mathcal{O}_2$ are outlined in Table 5.7.

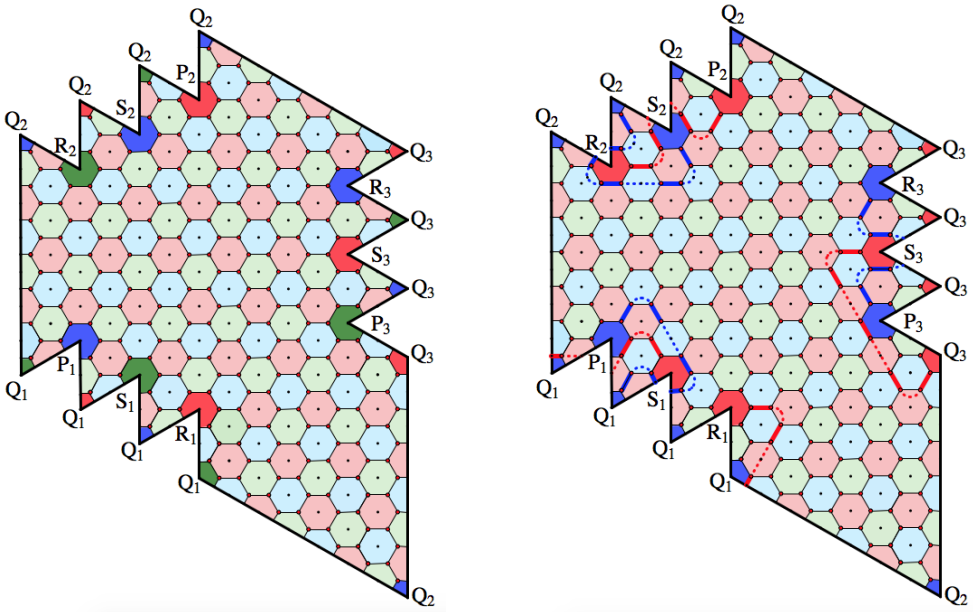
For the fullerene in Figure 5.23b, we have $r = 2$. According to Table 5.7 we should have a Clar deficit of $12(2) + 3 = 27$ which we can verify simply by counting the total

TABLE 5.7: Clar Deficit and Clar Number for entirety of $\mathcal{O}_2$ with $r+s \equiv_3 0$

| **Equivalence Class of $r$** | **Clar Deficit** | **Clar Number** |
|---|---|---|
| $r \equiv_3 0$ | $6r$ | $\frac{1}{6}\|V\| - 2r$ |
| $r \equiv_3 1$ | $9r$ | $\frac{1}{6}\|V\| - 3r$ |
| $r \equiv_3 2$ | $12r + 3$ | $\frac{1}{6}\|V\| - (4r + 1)$ |

chain length in Figure 5.23b.

In the cases when $r + s \not\equiv_3 0$, then $\{S_1, S_2, S_3\}$ are each in distinct color classes and so any choice of Clar color will be the color of $S_i$ for some $i \in \{1, 2, 3\}$. An example of such an arrowhead fullerene embedded in $\Lambda$ is shown in Figure 5.24a.




(A) Flat map of $\mathcal{O}_2$ embedded in $\Lambda$ before chains

(B) Distinct configurations for each 4-cluster

FIGURE 5.24: Clar Structure for $\mathcal{O}_2$ with $r + s \not\equiv_3 0$ with $r = 2$

Since each $S_i$ for $i \in \{1, 2, 3\}$ is in a distinct color class, we cannot use the same configurations for each of the 4-clusters. This is illustrated by our example in Figure 5.24b. $\{P_1, Q_1, R_1, S_1\}$ and $\{P_2, Q_2, R_2, S_2\}$ use single u-chains configurations and

$\{P_3, Q_3, R_3, S_3\}$ uses a spiral configuration. Even though we can choose to use a configuration that yields a minimal deficit for two of the clusters, we will always need to use the configuration yielding a greater deficit for one of the three 4-clusters. The Clar deficit and Clar number for the entire fullerene are outlined in the following table:

TABLE 5.8: Clar Deficit and Clar Number for entirety of $\mathcal{O}_2$ with $r+s \not\equiv_3 0$

| **Equivalence Class of** $r$ | **Clar Deficit** | **Clar Number** |
|---|---|---|
| $r \equiv_3 0$ | $10r + 4$ | $\frac{1}{6}(\|V\| - (20r + 8))$ |
| $r \equiv_3 1$ | $10r$ | $\frac{1}{6}(\|V\| - 20r)$ |
| $r \equiv_3 2$ | $12r + 4$ | $\frac{1}{6}(\|V\| - (24r + 8))$ |

We have not considered configurations involving chains that join pentagons in distinct 4-clusters so the values in Tables 5.7 and 5.8 only give us a lower bound on the Clar deficit for $\mathcal{O}_2$. This is turn gives us an upper bound on the Clar number. However, all of these deficits are independent of the parameter $s$. Thus, for large values of $s$, when these 4-clusters are very isolated from each other, this bound will be sharp.

# Chapter 6

# Clar Deficit for 4-Clusters with Adjacent Configuration

Although we discussed adjacent configurations in Chapter 4, we restricted our in depth attention to the opposite configurations since that was all we needed for Chapter 5. We will now take a closer look at adjacent 4-clusters such as the one removed from the ambient coloring as shown in Figure 6.1.

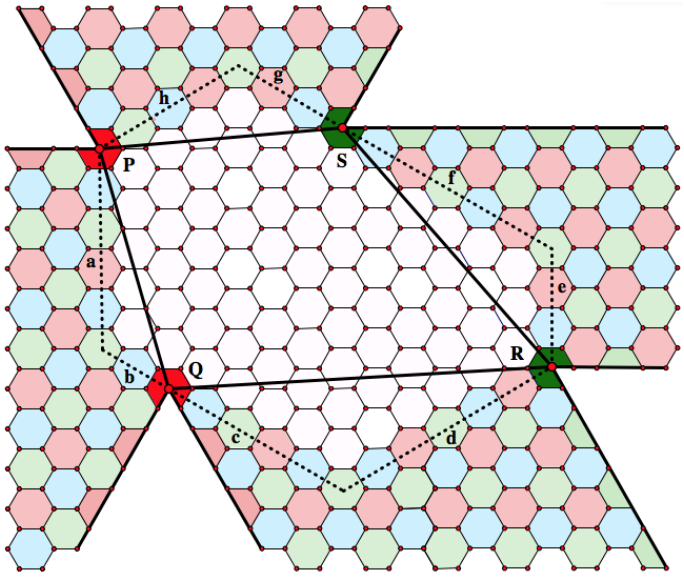



FIGURE 6.1: Externally colored adjacent 4-Cluster

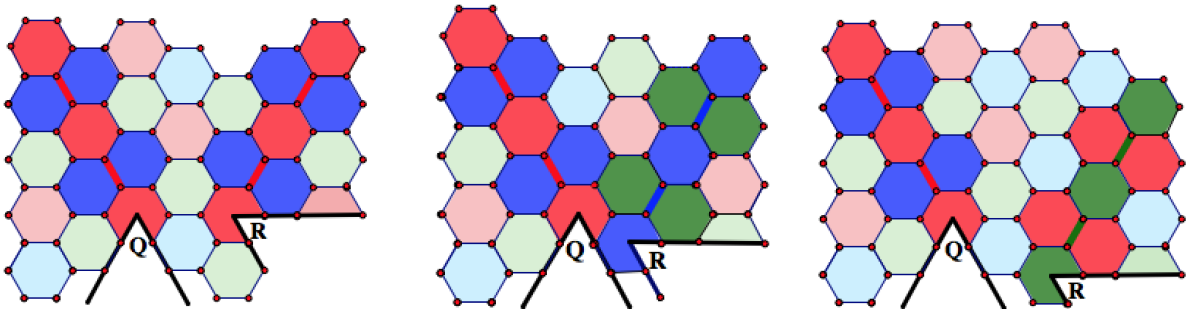
In this chapter we will study in depth the chain configurations for such 4-clusters.

Either $a - b \equiv_3 0$ or $c - d \equiv_3 0$ for all adjacent 4-clusters. Let us label our cluster as shown in Figure 6.1 with $a - b \equiv_3 0$. We know that 4-sets with such configurations are always clusters since they decompose into two 2-clusters using two direct chains between same colored pentagons. However, it remains to be shown what the maximal Clar structure is for such sets.

## 6.1 Primary and Secondary Colors of Chains in Adjacent 4-Clusters

The following theorem allows us to determine the primary and secondary color of the $RS$ type 1 chain given that pentagons $P$ and $Q$ are paired by a type 1 chain with primary color red and secondary color blue. Up to permutation of colors and pentagon labels, this covers all cases of adjacent configurations.

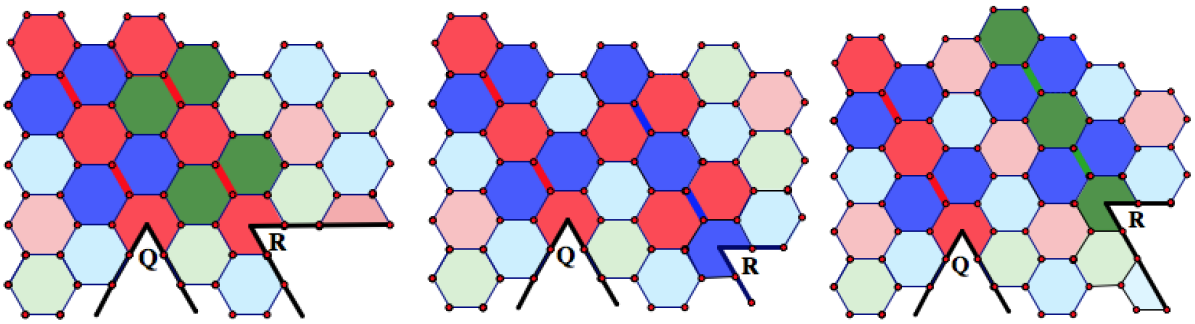
Figures 6.2 and 6.3 give examples of chain segments emanating from pentagons $Q$ and $R$. With these simple examples it is easy to find consistent color arrangements and to find the primary and secondary colors of the chain from $R$ based on the colors of the chain from $Q$ and the relation of the coordinates of segment $QR$. Theorem 6.1.1 shows that the color patterns are dependent on the parity of $\angle Q$ and $\angle R$.




(A) $c - d \equiv_3 0$, Red-Blue (B) $c - d \equiv_3 1$, Blue-Green (C) $c - d \equiv_3 2$, Green-Red

FIGURE 6.2: Example of type 1 chains when $\angle Q = 2$ and $\angle R = 2$

Examples of type 1 chains when both $\angle Q$ and $\angle R$ are even are shown in Figure 6.2. The type 1 chains need not be in this exact orientation but, with these parity classes, the primary and secondary colors will remain the same. Examples of of type 1 chains when $\angle Q$ is even and $\angle R$ is odd are shown in Figure 6.3.




(A) $c - d \equiv_3 0$, Red-Green (B) $c - d \equiv_3 1$, Blue-Red (C) $c - d \equiv_3 2$, Green-Blue

FIGURE 6.3: Example of type 1 chains when $\angle Q = 2$ and $\angle R = 1$

**Theorem 6.1.1.** *Given a 4-cluster with an adjacent configuration such that pentagons $P$ and $Q$ are connected by a red-blue type 1 chain and the segment connecting $R$ and $Q$ has coordinates $(c, d)$, then $R$ and $S$ can be paired by a type 1 chain with primary and secondary colors as outlined in the following table:*

| | $\angle Q$ odd | | |
|---|---|---|---|
| | $c - d \equiv_3 0$ | $c - d \equiv_3 1$ | $c - d \equiv_3 2$ |
| $\angle R$ even | Red-Green | Green-Blue | Blue-Red |
| $\angle R$ odd | Red-Blue | Green-Red | Blue-Green |

| | $\angle Q$ even | | |
|---|---|---|---|
| | $c - d \equiv_3 0$ | $c - d \equiv_3 1$ | $c - d \equiv_3 2$ |
| $\angle R$ even | Red-Blue | Blue-Green | Green-Red |
| $\angle R$ odd | Red-Green | Blue-Red | Green-Blue |

*Proof.* First, we determine the primary color of the $R - S$ chain by considering the relation between coordinates $c$ and $d$ as well as the parity of $\angle Q$. The color of pentagon $R$ will be the primary color of the $RS$ chain. The permutation representing translating from pentagon $Q$ to $R$ is given by $(RBG)^{c-d}$ when $\angle Q$ is odd and $(RGB)^{c-d}$ when $\angle Q$ is even. This is easily verified by considering that when $c - d = 1$ and $\angle Q = 0$ then $R$ is a blue face that is part of the red-blue chain emanating from pentagon $Q$. Rotating by an angle of even measure will lands us on another blue face and then by similarity the permutation remains the same whenever $c - d$ is in the same equivalence class. If we rotate by an angle of odd measure then $c - d \equiv_3 2$ will yield $R$ being a blue face. It follows that $R$ will be colored according to the Table 6.1.

| | $c - d \equiv_3 0$ | $c - d \equiv_3 1$ | $c - d \equiv_3 2$ |
|---|---|---|---|
| $\angle Q$ even | Red | Green | Blue |
| $\angle Q$ odd | Red | Blue | Green |

TABLE 6.1: Primary Color of $RS$ chain

The secondary color of the type 1 $RS$ chain is determined by the orientation of it's coordinate parallelogram, as it is this orientation that dictates which edge initiates the chain. The secondary color is also dependent on the primary color of the chain. Thus, to determine the color of the type 1 chain connecting $R$ and $S$, we must know the color of the pentagons and the orientation of the coordinate parallelogram connecting them. We will rotate and translate the $PQ$ chain until it lies coincident with the initial edge of the $RS$ chain to see the effects on the secondary color.

First we rotate about the center of face $Q$ an angle of measure $\angle Q$. This rotation yields the permutation $(GB)^{\angle Q}$. If $\angle Q$ is even, then the colors remain fixed but if $\angle Q$ is odd this rotation permutes blue and green while red remains fixed. Now we must translate to pentagon $R$ using the permutation above and lastly we rotate about the

center of pentagon $R$ an angle of measure $\angle R$. Again if $\angle R$ is even the color classes are fixed and if $\angle R$ is odd we permute the two colors distinct from the color of $R$. The composition of the three permutations are shown in the following tables: one for each possible color of $R$.

| **R red** | $\angle R$ odd | $\angle R$ even |
|---|---|---|
| $\angle Q$ odd | $(GB)(GB) = I$ | $(GB)$ |
| $\angle Q$ even | $(GB)$ | $I$ |

TABLE 6.2: Composition of permutations when primary color of $RS$ chain is red

Recall that any time $c - d \equiv_3 0$, we will have that the primary color of the $RS$ chain will be red. In this case we see that if $\angle Q + \angle R$ is even then the secondary color will be unchanged from the secondary color of the $PQ$ chain and thus, be blue. If $\angle Q + \angle R$ is odd then the secondary color will be green as we are left with the green blue permutation.

| **R green** | $\angle R$ odd | $\angle R$ even |
|---|---|---|
| $\angle Q$ odd | $(RB)(RGB)(GB) = (GBR)$ | $(RGB)(GB) = (GR)$ |
| $\angle Q$ even | $(RB)(RGB) = (GR)$ | $(GBR)$ |

TABLE 6.3: Composition of permutations when primary color of $RS$ chain is green

Recall that the primary color of the $R - S$ chain will be green if $\angle Q$ is odd and $c - d \equiv_3 1$ or if $\angle Q$ is even and $c - d \equiv_3 2$. In this case when the primary color is known to be green, we see that, if $\angle Q + \angle R$ is odd, we must permute the colors of the $PQ$ chain according to $(GR)$ and thus, our secondary color will be blue. Similarly the secondary color will be red if $\angle Q + \angle R$ is even.

| **R blue** | $\angle R$ odd | $\angle R$ even |
|---|---|---|
| $\angle Q$ odd | $(GR)(RBG)(GB) = (GRB)$ | $(RBG)(GB) = (RB)$ |
| $\angle Q$ even | $(GR)(RBG) = (RB)$ | $(GRB)$ |

TABLE 6.4: Composition of permutations when primary color of $R - S$ chain is blue

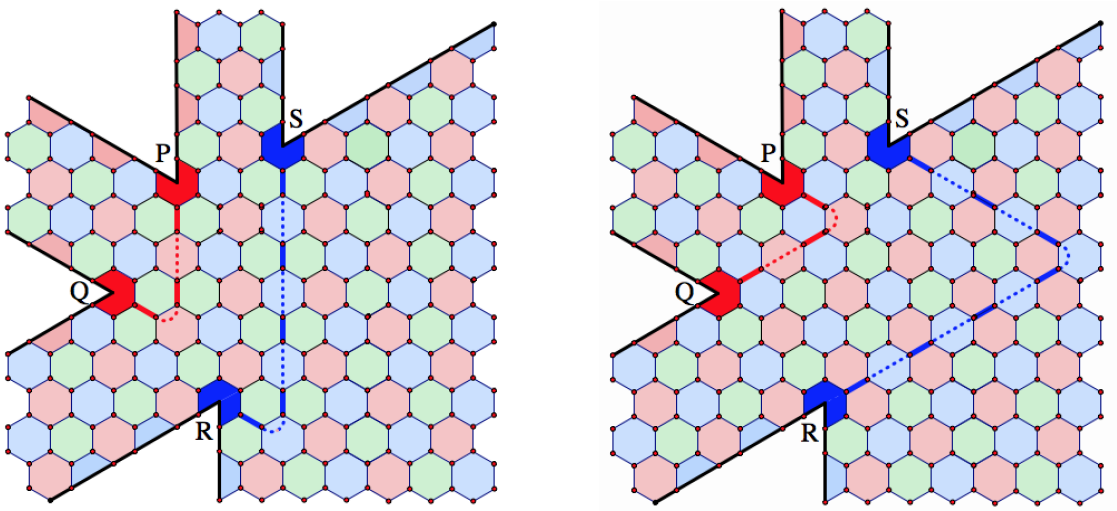
Recall that the primary color of the $RS$ chain will be blue if $\angle Q$ is odd and $c-d \equiv_3 2$ or if $\angle Q$ is even and $c - d \equiv_3 1$. In this case when the primary color is known to be blue, we see that, if $\angle Q + \angle R$ is odd, the secondary color will be red and if $\angle Q + \angle R$ is even then the secondary color will be green.

Combining all these cases yields the results given in the statement of the theorem.

□

## 6.2 Comparing Direct Chain Configurations and Single Wrap Configurations

For any adjacent configuration, we always have the option of using a direct chain configuration which reduces the 4-cluster into two individual 2-clusters. This is an especially useful option when the chosen color for the Clar faces is not one of the primary colors of the two original chains. We will begin by considering the example shown in Figure 6.4. Take particular note that $P$ and $Q$ lie along a single coordinate path. This indicates that the second coordinate of the segment joining them is 0. Having such pairs of pentagons in a configuration creates an additional level of subtly in determining angle measures and orientation of chain types. However, all our previously discussed methods and rules still hold.




(A) Two type 1 chains (B) Two type 2 chains

FIGURE 6.4: Direct configuration for adjacent 4-cluster using green Clar faces.

The $PQ$ type 1 chain, shown in Figure 6.4a, has primary color red and secondary color green. To apply the results of Theorem 6.1.1, we must use a permutation of green and blue since our type 1 chain has secondary color green. With this permutation, we determine that the $RS$ chain will have primary color blue and secondary color green since $\angle Q$ has measure 2, $\angle R$ has measure 1 and $c - d \equiv_3 2$. The two type 1 chains are shown in Figure 6.4a.

If the Clar faces are chosen from the ambient coloring to be green then there is no need to change the primary color of either chain. We can treat the two 2-clusters $\{P, Q\}$ and $\{R, S\}$ separately by forming two type 2 chains in order to avoid the color green from both the primary and secondary color in either chain. The two type 2 chains are shown in Figure 6.4b.

However, due to the other clusters in a fullerene, there are cases in which the Clar color must be chosen to be the primary color of one of the chains. For instance, in the case of Figure 6.4b, if we had chosen to use red faces for our Clar color then we will need to change the primary color of the red-blue chain. We can change the primary

color in one of two ways. One option is to construct a type 1 chain and a type 3 chain as shown in Figure 6.5. In this case we have made the $PQ$ chain a type 3 chain and the $RS$ chain a type 1 chain eliminating all red faces from either chain.

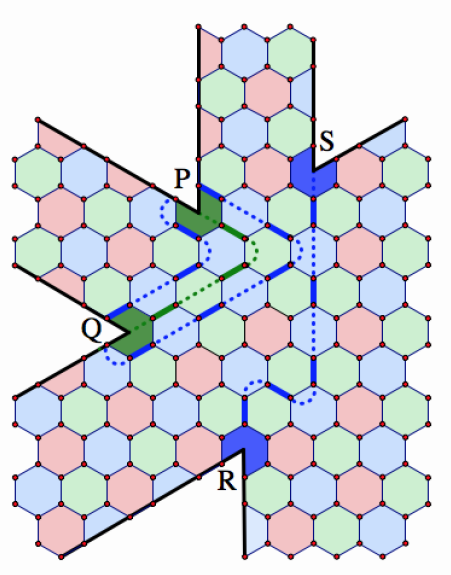
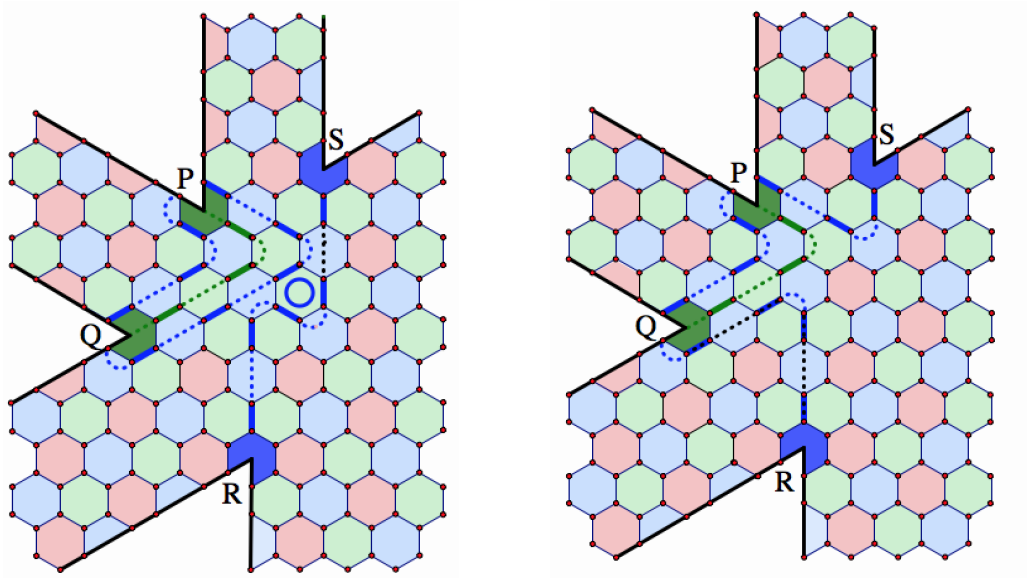



FIGURE 6.5: Type 1 and type 3 direct chains

Alternatively, we form a single wrap configuration, as discussed in Chapter 4. To do so, we take the pair of pentagons of which we ultimately want to change the primary color and construct a type 1 direct chain. Instead of another direct chain, we wrap the second chain around the entirety of the first chain. This wrap around chain changes the primary color of the initial chain and can be also be constructed in such a way that both chains avoid the color class to be chosen as the Clar color. As we have two options, we must determine which configuration yields the minimal Clar deficit in any scenario.

The following series of operations will determine which configuration gives the minimal Clar deficit.

1. Construct a type 3 chain in order to change the primary color of the direct chain with primary color matching that of the Clar faces.




(A) Direct configuration yields additional benzene ring

(B) Wrap around configuration yields minimal Clar deficit of 13

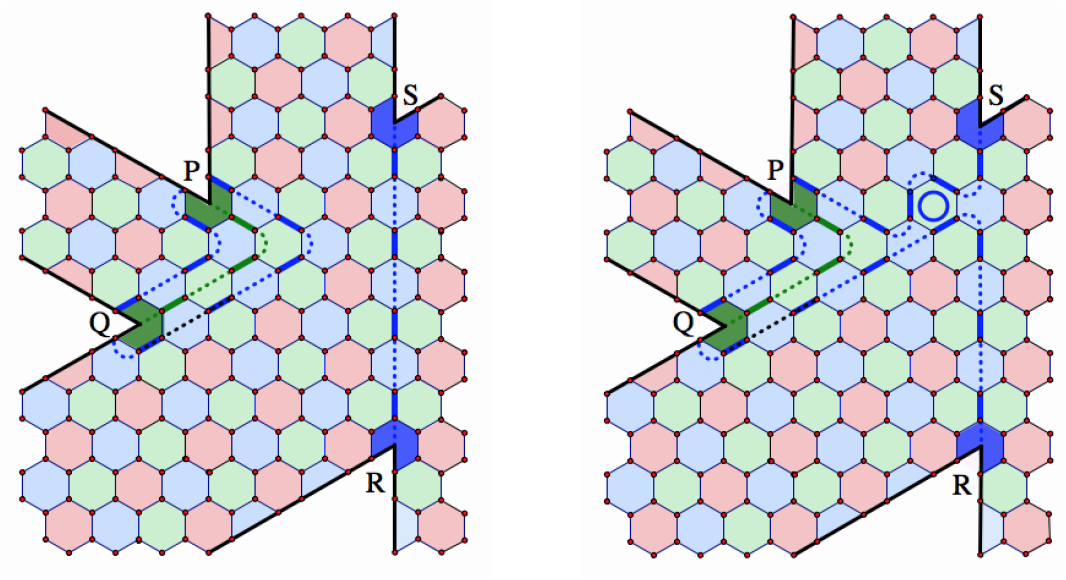
FIGURE 6.6: Comparing direct configuration and wrap around configuration in adjacent 4-cluster

2. Pair the remaining two pentagons with a type 1 or 2 chain–this choice is forced since only one will avoid the color of the Clar faces.

3. Using the flipping action construct equivalent chains that are as close together as possible. For example we flip the type 1 chain in Figure 6.5 to get the chain configuration in Figure 6.6a.

4. If, in doing so, additional benzene Rings are formed between the two chains, as they are in Figure 6.6, then the configuration can be reduced and thus does not give the minimal Clar deficit. In removing the edges from the additional benzene ring, we are left with a single wrap configuration as shown in Figure 6.6b.

5. If no additional benzene Rings are formed then the cheaper configuration is the direct configuration.




(A) Direct configuration yields minimal Clar deficit of 15

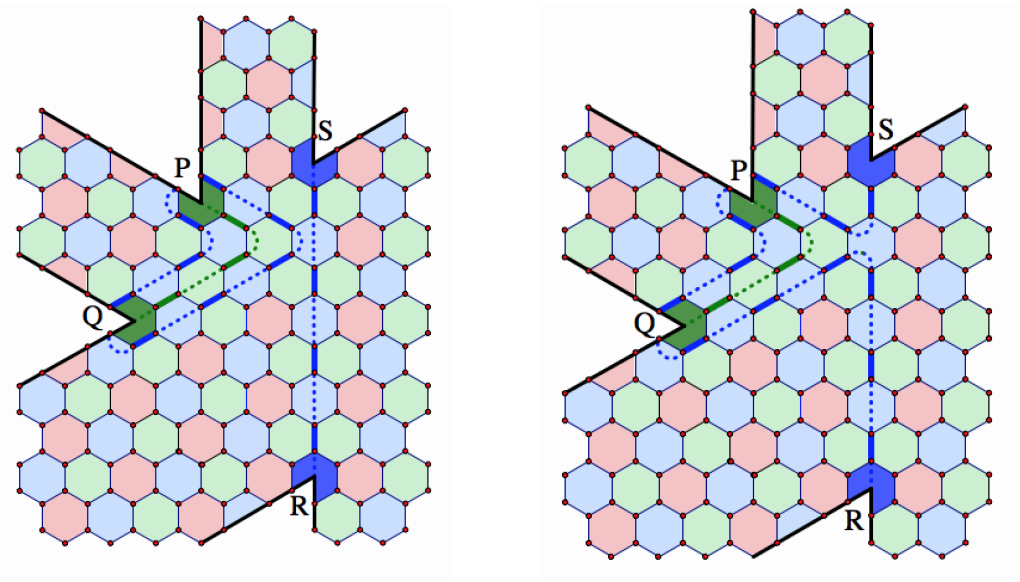
(B) Wrap around configuration contains additional benzene ring

FIGURE 6.7: 4-cluster in which constructing type 3 direct chain yields least Clar deficit

Another example of such a configuration is illustrated in Figure 6.7. In this case, there are no possible flipping operations that can move the two chains closer together and no additional benzene rings have been formed. It follows that the configuration shown in Figure 6.7a is the best possible configuration. Notice that if we force ourselves to use a single wrap configuration as in Figure 6.7b and push the chains together we will create an additional benzene ring. Removing this benzene ring from the configuration leaves us with the direct configurations that we desired. This shows us that we can either start with a direct chain configuration or a wrap around configuration and by performing the above actions always get to the cheapest configuration. However, we will choose to start with a direct configuration due to the ease of computing the total chain length of two distinct direct chains.

There are also configurations of pentagons that lead to no additional pentagons regardless of which initial configuration is chosen. In these cases, the chains pass so

close to one another that the same set of edges can be viewed as either configuration as illustrated in Figure 6.8.

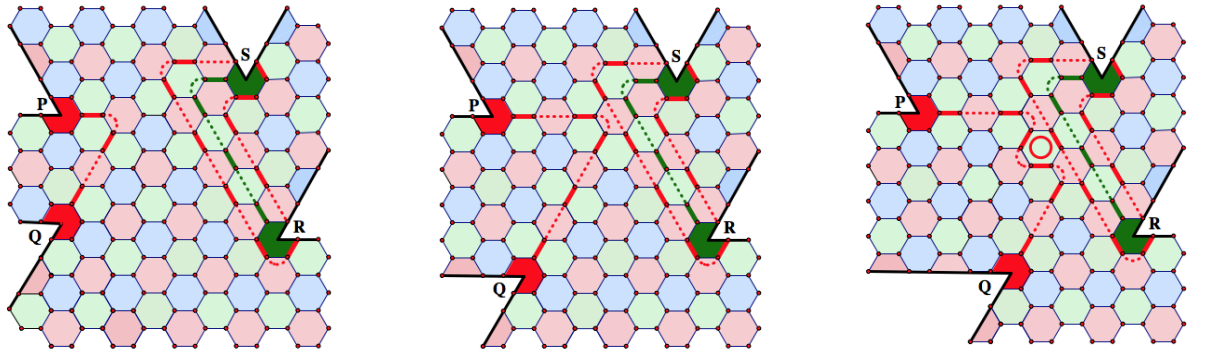



(A) Direct Configuration (B) Wrap around configuration

FIGURE 6.8: Comparing direct configuration and wrap around configuration in adjacent 4-cluster

Of course, we get similar cases when we wish to use blue as our Clar color. In this case we will make the blue chain a type 3 chain or wrap the red chain around the entirety of the blue chain. Figure 6.9 shows the three possibilities for when we must eliminate the color blue from our chains.

In Figure 6.9a, the formation of the two direct chains are far enough apart so that no additional benzene rings are formed and the direct configuration yields the least Clar deficit. In Figure 6.9b the two direct chains are just close enough together that either configuration will yield the same deficit. Finally, in Figure 6.9c the direct chains are so close together that an additional benzene ring is formed and the single wrap configuration yields the most efficient Clar deficit. In the subsequent sections we explore in depth the case in which blue is chosen to be the Clar color.




(A) Direct configuration yields the least Clar deficit

(B) Both configurations yield equal deficit

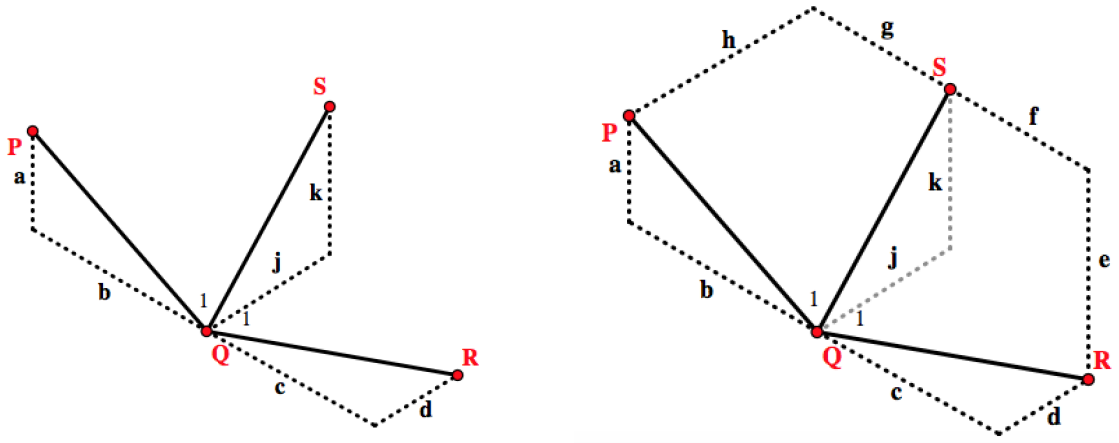
(C) Single wrap configuration yields the least Clar deficit

FIGURE 6.9: Configurations when Clar color chosen to be blue

## 6.3 Determining Intersection Bound for 1 1 3 Star Cluster

Once we fix the signature type of the cluster we can say even more about the total chain length of each configuration. Each of the 4-clusters that arose naturally in the arrowhead fullerenes had a 1 1 3 star signature configuration in the opposite or monochromatic color configuration. Thus, through our discussion of these specific infinite classes, we gained insight on how to approach clusters when faced with these color configurations. However, in the course of our analysis we did not have the opportunity to look deeply at 4-clusters that possess a strictly adjacent configuration. The rest of this chapter will be devoted to these specific 4-clusters, namely the ones in which $a - b \equiv_3 0$ or $c - d \equiv_3 0$.

As we have in the previous chapters, we will define our 4-clusters by the pentagons in the set $\{P, Q, R, S\}$ and use the same convention in labeling the coordinates of segments between neighboring pentagons as shown in Figure 6.10. Due to the symmetry of 4-clusters with a 1 1 3 star configuration we can choose either $a-b \equiv_3 0$ or $c-d \equiv_3 0$ with no loss of generality. We choose $a - b \equiv_3 0$ for this discussion. We must keep in mind that our end goal for this section is a closed formula giving the total chain length for whichever chain configuration is the most efficient.




(A) Signature graph of a 1 1 3 star set (B) Coordinate structure of 1 1 3 star set

FIGURE 6.10: Structure of a 1 1 3 Star Set

Recall from Lemma 3.4.3 that a 4-set with a 1 1 3 star signature is a 4-cluster if and only if $(a-b)+(c-d)+(j-k) \equiv_3 0$. We have several non-isomorphic coordinate conditions to consider if we wish to consider all possible 1 1 3 star 4-clusters. Fixing pentagon $P$ to be red in the ambient coloring of $\Lambda$ allows the coordinate relations to dictate the external color configuration of the remaining pentagons in the 4-cluster.

All possible combinations of congruency classes for the pairs of coordinates pairing neighboring pentagons in a 1 1 3 star 4-cluster and the associated color possibilities up to permutation of colors are outlined in Table 6.5. Included are the associated classes of color configurations for each set as well as the infinite class in which such a cluster was studied in Chapter 5.

Intuitively, if the type 3 and type 1 or type 2 chains in a direct configuration do not come close to each other, even when constructed as tight as possible, then no additional benzene rings will be formed. Thus, to compute the desired formula, we need to find a relation based upon the parameters in the perimeter of the 4-cluster that tells us whether or not additional benzene rings will be formed.

In order for additional benzene rings to be formed, the direct chains have to come

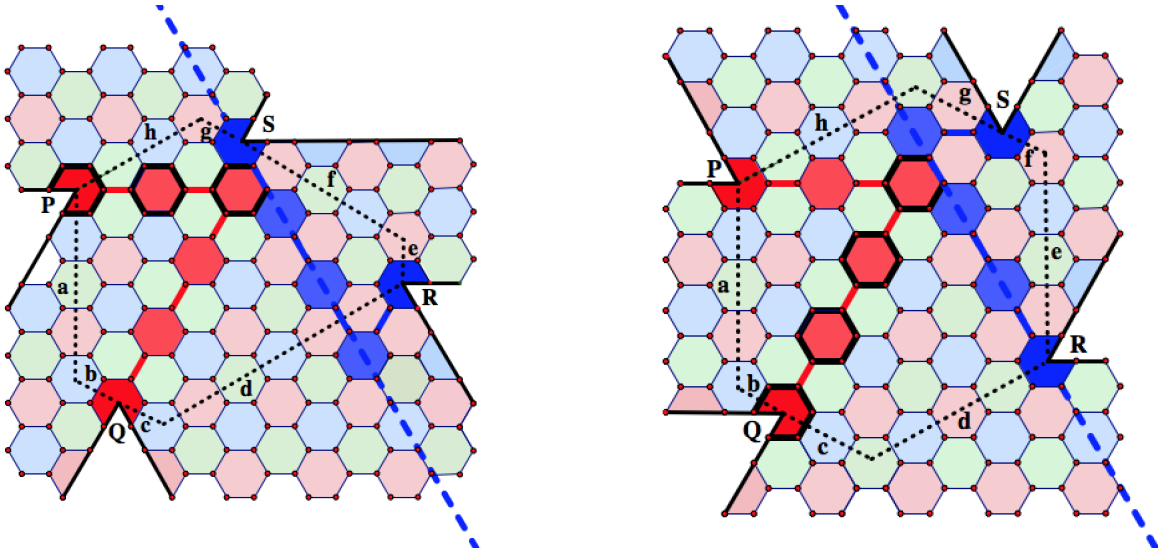
TABLE 6.5: Nonisomorphic Coordinate Cases for 1 1 3 Star Cluster

| **a-b** | **j-k** | **c-d** | **P** | **Q** | **R** | **S** | Color Configuration | Infinite Class |
|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | Red | Red | Red | Red | Monochromatic | $\mathcal{O}_1$ & $\mathcal{O}_2$ |
| 0 | 1 | 2 | Red | Red | Blue | Blue | Adjacent | Neither |
| 0 | 2 | 1 | Red | Red | Green | Green | Adjacent | Neither |
| 1 | 0 | 2 | Red | Blue | Green | Blue | Opposite | $\mathcal{O}_1$ |
| 1 | 1 | 1 | Red | Blue | Red | Green | Opposite | $\mathcal{O}_2$ |
| 1 | 2 | 0 | Red | Blue | Blue | Red | Adjacent | Neither |
| 2 | 0 | 1 | Red | Green | Blue | Green | Opposite | $\mathcal{O}_1$ |
| 2 | 1 | 0 | Red | Green | Green | Red | Adjacent | Neither |
| 2 | 2 | 2 | Red | Green | Red | Blue | Opposite | $\mathcal{O}_2$ |

close enough to one another that they will intersect unless there are multiple sharp turns. Equivalently we see that the direct configuration will give the minimal Clar deficit so long as the two chains do not intersect when constructed with at most one sharp turn in any orientation. To find algebraic conditions on which configuration is most efficient we need to rigorously develop a technique that will tell when the two direct chains will intersect. To do so, we need to find the bound on intersecting length as well as the length of the chain segment that is in danger of exceeding it.

In Figure 6.11, we see two cases in which the type 3 chain and the type 2 chain come just as close as possible without intersecting. We see that when $e \leq f$ as in Figure 6.11a, we extend the $RS$ chain segment incident with pentagon $S$ and if $e > f$ as in Figure 6.11b, we extend the $RS$ chain segment incident with pentagon $R$ so that we are always extending the chain that is geometrically closer to the $PQ$ chain. The extensions are indicated by the dashed blue line. These relations will hold for all 1 1 3 star clusters.

The set of pentagons, $\{P, Q\}$, gives us the initial face to calculate the chain length




(A) $e \leq f$ (B) $e > f$

FIGURE 6.11: Calculating chain length between pentagon and extended chain

to the extended chain. The straight chain segment from this face to the extended chain is the chain segment length we are striving to find.

For example, in Figure 6.11a the bound is given by the maximum chain length from pentagon $P$ to the segment of the extended chain that has been marked with the blue dashed line–the chain emanating from pentagon $S$. In this case, the bound is 2 and the chain segment from pentagon $P$ has exactly this length. We can easily see that if the chain segment from $P$ was longer the two would intersect.

We could have reasonably chosen pentagon $Q$ to give the other endpoint of our bound rather than pentagon $P$. In this case we would have gotten a bound on the intersection of 3. However, to build our algebraic conditions from the signature parameters used in the previous chapters, it is convenient to have a set of perimeter coordinates that travels from the initial pentagon to a face on the extended chain. Therefore, if we are trying not to intersect the chain segment emanating from pentagon $S$, then we compute our bounding length as maximal straight chain from pentagon $P$ to this chain

segment. Thus, since $P$ and $S$ are adjacent we know one set of coordinates between the pentagon and extended chain is given by $(g, h)$.

On the other hand, if we use the extended chain segment incident with $R$ as our bounding chain then we will choose pentagon $Q$ as our endpoint and a set of coordinates from $Q$ to the extended chain segment is given by $(c, d)$. For example, in Figure 6.11b, we use the bound given by the maximum chain length from pentagon $Q$ to the extended chain segment marked with the blue dashed line. This time the extended chain segment emanates from pentagon $R$. In this case, the bound is 3 and the chain segment from pentagon $Q$ with primary color red has exactly this length.

Notice that we have yet to find a general formula that gives the bound. This is the first time we have had to calculate a chain length between a face and another chain rather than between two faces. Thus, finding this bound in general is more complicated than it initially sounds.

## 6.4 Algebraic Conditions Determining Most Efficient Configurations

Since pentagons $P$ and $Q$ are in a different color class than the primary color of the extended chain, the coordinates from either pentagon to a face on the extended chain will never be congruent modulo 3. However, we still use the coordinates from $P$ or $Q$ to a face on the extended chain in our computations.

We know that a segment with coordinates in the form $(p, p)$ correspond to a straight chain segment of length $p$. It follows that if a segment has coordinates in the form $(p, p-1)$, then the maximum chain length of a corresponding chain segment has length $p - 1$. The example in Figure 6.11 specifically has $g - h \equiv_3 c - d \equiv_3 1$. The coordinates of a segment from $P$ or $Q$ to any face on the extended chain must also be congruent

modulo 3 to 1. As such, there exists a face on the extended chain with coordinates from the initial pentagon in the form $(p, p-1)$. This gives us a bound of $p-1$. However, an expression for $p$ dependent on the parameters of our cluster remains to be found.

First let's focus on the case when $e \leq f$. Hence, we know that one set of coordinates from pentagon $P$ to the extended chain is given by $(g, h)$. In this case, we seek an expression for such a $p$ in terms of $g$ and $h$.

Notice that decreasing $h$ by 1 requires extending $g$ by 2 in order to stay on the same chain line and to keep the relation between the coordinates fixed. Similarly if we increase $h$ by 1, then we must decrease $g$ by 2. Thus, for any integer $n$, all coordinates from pentagon $P$ to the extended chain line will have form $(g+2n,\ h-n)$. Our bound on the intersecting length will be $h-n$ for the value of $n$ that makes the coordinates $(g+2n,\ h-n)$ be in the form of $(p, p-1)$ for some $p$. It follows that we need to find $n$ so that $(g+2n)-(h-n)=1$. Solving for $n$ gives us $n=\frac{h-g+1}{3}$. Therefore the chain length across, and our intersecting bound, will be $h-n=3-\frac{3-1+1}{3}=2$ in this example or generally

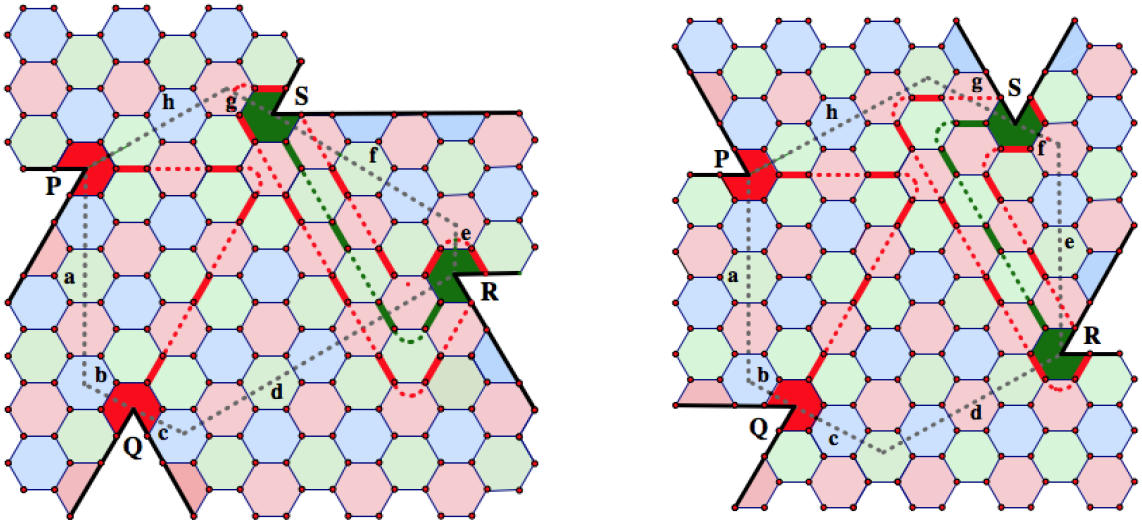
$$h-n=\frac{2h+g-1}{3}$$

When $e>f$, we want to find the bound on chain length that will guarantee that we don't intersect the chain segment from pentagon $R$ and hence are concerned with the coordinates given by $(c,\ d)$. This time as we decrease $d$ by 1 we must increase $c$ by 2 to stay on the same chain line. Using the same method as above, we find that $n=\frac{d-c+1}{3}$. So our bounding chain length, will be given by $d-n=4-\frac{4-2+1}{3}=3$ in this example or generally

$$c-n=\frac{2d+c-1}{3}$$

In both examples shown in Figure 6.11, we see that the $PQ$ type 2 chain achieves these bounds without crossing the $RS$ chain. In Figure 6.12 we construct the type 3

chains for the configurations in Figure 6.11 and see that these the chains come just as close as possible without creating additional benzene rings.




(A) $e \leq f$ (B) $e > f$

FIGURE 6.12: Configuration as two independent 2-clusters

Using Lemma 2.1.6, we calculate that the chain segment of the red-green chain incident with pentagon $P$ has length $\min\{a, b\} + \left|\frac{a-b}{3}\right|$ and the chain segment of the red-green chain that is incident with pentagon $Q$ has length $\max\{a, b\} - \left|\frac{a-b}{3}\right|$.

Thus we see that if $e \leq f$, then the direct configuration will yield the least Clar deficit when

$$\min\{a, b\} + \left|\frac{a-b}{3}\right| \leq \frac{2h+g-1}{3}$$

or equivalently

$$3\min\{a, b\} + \left|a-b\right| = 3\min\{a, b\} + \max\{a, b\} - \min\{a, b\} \leq 2h+g-1$$

which we can simplify to

$$\min\{a, b\} + a + b \leq 2h+g-1$$

On the other hand, if $\min\{a,b\}+a+b > 2h+g-1$ then we get one additional benzene ring for each edge length that the type 2 chain crosses the extended chain. Equivalently, we get $\left(\min\{a,b\}+\left|\frac{a-b}{3}\right|\right)-\left(\frac{2h+g-1}{3}\right)$ additional benzene rings.

If $e > f$ then the direct configuration is optimal when

$$\max\{a,b\}-\left|\frac{a-b}{3}\right| \leq \frac{2d+c-1}{3}$$

or equivalently

$$3\max\{a,b\}+\min\{a,b\}-\max\{a,b\} \leq 2d+c-1$$

which we can simplify to

$$\max\{a,b\}+a+b \leq 2d+c-1$$

Again, if $\max\{a,b\}+a+b > 2d+c-1$ we get $\Big(\max\{a,b\}+a+b\Big)-\Big(2d+c-1\Big)$ additional benzene rings.

When additional benzene rings are formed then the single wrap configuration yields a lesser Clar deficit. To find the expression for the total chain length we begin by computing the length as interpreted as two distinct direct chains–in this case a type 2 and a type 3 chain. This is easily computed using our theory of 2-clusters.

Hence, when $e \leq f$ the total chain length of the two direct chains is $a+b$ for the type 2 chain joining $P$ and $Q$ and $3(\max\{e,f\})+2$ for the type 3 chain joining $R$ and $S$. If additionally we have $\min\{a,b\}+\left|\frac{a-b}{3}\right| > \frac{2h+g-1}{3}$ then we must subtract $3(\min\{a,b\}+\left|\frac{a-b}{3}\right|-\frac{2h+g-1}{3})$ from the total chain length to remove the three edges

from every additional benzene ring. Hence, our total chain length in this scenario is

$$a + b + 3(\max\{e, f\}) + 2 - 3\Big(\min\{a, b\} + \Big|\frac{a-b}{3}\Big| - \frac{2h+g-1}{3}\Big)$$

We can simplify our expression by noticing the following relation:

$$\begin{aligned} a + b - |a - b| &= \Big[\max\{a, b\} + \min\{a, b\}\Big] - \Big[\max\{a, b\} - \min\{a, b\}\Big] \\ &= 2\min\{a, b\} \end{aligned}$$

This equivalence along with the fact that we are in the case when $e \leq f$ allows us to rewrite our expression for chain length in the following way:

$$\begin{aligned} & a + b + 3(\max\{e, f\}) + 2 - 3\Big(\min\{a, b\} + \Big|\frac{a-b}{3}\Big| - \frac{2h+g-1}{3}\Big) \\ &= a + b - |a - b| - 3\min\{a, b\} + 3\max\{e, f\} + 2h + g + 1 \\ &= 2\min\{a, b\} - 3\min\{a, b\} + 3\max\{e, f\} + 2h + g + 1 \\ &= 1 + 3\max\{e, f\} + 2h + g - \min\{a, b\} \\ &= 1 + 3f + 2h + g - \min\{a, b\} \end{aligned}$$

Similarly if we have $e > f$ and $\max\{a, b\} - \left|\frac{a-b}{3}\right| > \frac{2d+c-1}{3}$ then the direct chain configuration will yield additional benzene rings and when computing the Clar deficit, we subtract $3\Big(\max\{a, b\} - \left|\frac{a-b}{3}\right| - \frac{2h+g-1}{3}\Big)$ from the total direct chain configuration to get a final chain length of

$$a + b + 3(\max\{e, f\}) + 2 - 3\Big(\max\{a, b\} - \Big|\frac{a-b}{3}\Big| - \frac{2h+g-1}{3}\Big)$$

or using the same simplification as above we see this is equivalent to a final chain length of

$$1 + 3e + 2d + c - \max\{a, b\}$$

We have thus found a closed formula for the Clar number where the Clar faces are chosen to be blue for a 4-cluster with an underlying signature in the form of a 1 1 3 star when $c - d \equiv_3 1$. The Clar deficit for all cases is given by:

TABLE 6.6: Clar Deficit for adjacent 1 1 3 Star Cluster with $c - d \equiv_3 1$

| **Clar Deficit** | **Conditions** |
|---|---|
| $a + b + 3f + 2$ | $e \leq f$ and $\min\{a, b\} + a + b \leq 2h + g - 1$ |
| $1 + 3f + 2h + g - \min\{a, b\}$ | $e \leq f$ and $\min\{a, b\} + a + b > 2h + g - 1$ |
| $a + b + 3e + 2$ | $e > f$ and $\max\{a, b\} + a + b \leq 2d + c - 1$ |
| $1 + 3e + 2d + c - \max\{a, b\}$ | $e > f$ and $\max\{a, b\} + a + b > 2d + c - 1$ |

We can use similar methods to find the Clar deficit for adjacent 4-clusters with different underlying signature conditions and for 1 1 3 star clusters when $c - d \equiv_3 2$.

# Chapter 7

# Future Work

## 7.1 Future Work

Recall from Chapter 1, that a flat map for a given fullerene is formed from a signature graph. There may be several non-isomorphic signature graphs so there may be several distinct candidates for the flat map for any particular fullerene.

If the flat map is cut from a perfectly 3-colored region of $\Lambda$, then it will inherit this unique edge and face coloring (up to permutation of colors). The inherited coloring may match along some of the identified edges but not all. This is where we will now focus our attention. The portion of the flat map that includes identified edges with consistent 3-coloring corresponds to the region of hexagons that can be perfectly colored using the ambient coloring. This naturally decomposes the fullerene into clusters as the coloring remains perfect outside these clusters. Different flat maps may decompose the same fullerene into different sets of clusters, and we must consider all possible cases.

The next endeavor in this work is to find the cluster decomposition directly from the signature of a fullerene rather than constructing and coloring the flat map. By tracing along the edges of the signature as we did in creating the flat map, we can determine associated color transpositions at each vertex. These transpositions will be

dependent on the angle at the vertex as well as the coordinates of the segment. By composing these transpositions as we move along adjacent segments, we will be able determine the 3-coloring of any region of hexagons within the fullerene. Thus, by finding the color configuration for regions adjacent to identified edges, we will be able to tell when the colors match and when there will be a discrepancy. This technique will give us the cluster decomposition without having to construct the physical flat map.

Once this process is formalized, a future area of research will be to determine patterns in the signature structure that will indicate when clusters of different sizes will arise. By these means, we will determine the natural cluster decomposition for various classes of fullerenes. With the level of complication of 4-clusters now apparent, we know that developing analogous theory for clusters of size at least 6 will be even more complicated. Before diving into such a line of work, it is prudent to verify that fullerenes will actually decompose into clusters of these larger sizes. Specifically we want to make sure that large clusters will not always decompose into smaller clusters.

6-clusters are of particular interest since fullerenes that decompose into two 6-clusters will be structures classified as carbon nanotubes. Carbon nanotubes, sometimes referred to as carbon threads, can be very long and constructed to have very strong material properties. Signatures of such fullerenes will have two components of six vertices connected by an isthmus.

This isthmus corresponds to the length of the tube and the two components will represent the nanocaps. As the isthmus may be very long the structures will have the most stability when the 6-sets forming the nanocaps are 6-clusters. Thus, in considering the cases of two 6-clusters, we will have a signature graph consisting of two distinct components each consisting of sets of five edges on the six vertices. We wish

to know the fullerene structure that will lead to these caps being clusters in themselves as well as whether these 6-clusters will always decompose into 2- and 4-clusters. From here we can use the theory developed in this thesis as well as any further theory needed on 6-clusters to fully understand nanotubes.

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# Index

# JENNIFER EDMOND

Mathematics Deptartment ◇ Syracuse University ◇ Syracuse, NY 13244-1150
(315) · 857 · 7007 ◇ jledmond@syr.edu

## EDUCATION

**Syracuse University** *May 2018*
*Syracuse, New York*
Ph.D. in Mathematics
Current GPA: 3.92

**Syracuse University** *May 2015*
*Syracuse, New York*
M.S. in Mathematics
Overall GPA: 3.9

**Goucher College,** *May 2011*
*Baltimore, Maryland*
B.A. in Mathematics
Minor in Physics & Studio Art
Overall GPA: 3.93

**Monteverde Institute** *June 2010*
*Monteverde, Costa Rica*
Intensive study of Spanish language, environmental sustainability and development of Costa Rican society.

## RESEARCH INTERESTS

Graph theory and combinatorics especially chemical graph theory, carbon nanostructures and fullerenes.

## TEACHING EXPERIENCE

**Primary Instructor** January 2014 - May 2018
*Syracuse University* Syracuse, NY
Responsible for planning lessons, writing and grading exams and quizzes as well as assisting students with homework and course concerns.
- Calculus II for the Life Sciences *Spring 2014, Spring 2016, Spring 2018*
- Calculus I for the Life Sciences *Fall 2017*
- Calculus I *Fall 2015, Spring 2017*
- Calculus III *Fall 2016*

**Recitation Leader** August 2012 - May 2014
*Syracuse University* Syracuse, NY
Responsible for planning lessons, writing and grading exams and quizzes .
Business Mathematics *Fall 2012*
Introduction to Statistics *Spring 2013, Fall 2014*

**Grader** January 2008 - May 2011, Spring 2016
*Goucher College* Baltimore, MD
*Syracuse Unversity* Syracuse NY
Graded for classes including statistics, partial differential equation and calculus courses.

**Supplemental Instruction Leader** September 2007 - May 2011
*Goucher College Academic Center for Excellence* Baltimore, MD
Ran weekly sessions for both mathematics and phyics classes covering additional material and answering questions.

**Peer Mentor** June 2009 - August 2009
*Education Opportunity Program, Summer Bridge* Baltimore, MD
Led three-hour tutoring sessions daily for students who needed additional support prior to entering college.

## PUBLICATIONS

*Injective choosability of subcubic planar graphs with girth 6* (with B. Brimkov, R. Lazar, B. Lidick, K. Messerschmidt, S. Walker) Discrete Mathematics. **340** (2017) 2538-2549

*Similarity and a Duality for Fullerenes* (with J. Graver) Symmetry. **7** (2015) 2047-2061

*Transmission Holograms - A Three-Dimensional Examination.* Verge. **6** (2009)

## CONFERENCE TALKS

**CSD 7: Computational Methods for Carbon Nanostructure Research** *July 21, 2015*
Virginia Commonwealth University
*Similarity and a New Definition of Duality for Fullerenes.*

**Center for Undergraduate Research in Mathematics Conference** *March 19, 2010*
Brigham Young University
*Follow the Food Feeding Function: A Biomathematical Look at Gastric Emptying.*

**MathFest 2009** August 8, 2009
Portland
*Follow the Food Feeding Function: A Biomathematical Look at Gastric Emptying.*
Awarded AMS/ASA award for presentation.

**Landmark Conference Research Symposium** *July 22, 2009*
Susquehanna University
*Follow the Food Feeding Function: A Biomathematical Look at Gastric Emptying.*

**Summer Research Symposium** *July 16, 2009*
Goucher College
*Follow the Food Feeding Function: A Biomathematical Look at Gastric Emptying.*

## AWARDS AND ACCOMPLISHMENTS

**Donald E. Kibbey Prize in Mathematics** *April 2018*
The Donald Kibbey Prize for outstanding work in mathematics is awarded, usually annually, for excellence in the Ph.D. program and/or for an excellent doctoral dissertation.

**Outstanding Teaching Assistant** *April 2016*
Awarded to the top 4% of all Teaching Assistants campus-wide. Recognizes Teaching Assistants who have made distinguished contributions to Syracuse University by demonstrating excellence in significant instructional capacities

**Syracuse University Graduate Fellowship** *August 2011-May 2018*
Consists of a stipend and a full-tuition scholarship. Includes a year of fellowship followed by two years of teaching assistantship followed by a fourth year of fellowship support and two more years of teaching assistantship. Awarded annually to one incoming graduate student in each department.

**Goucher College Dean Scholar** *September 2007-May 2011*
Full tuition scholarship for four years of study at Goucher College; awarded to 10 students a year.

**The Marian M. Torrey Prize** *May 2011*
Awarded to senior mathematics major selected by the department for excellent records, firm grasp of subject matter, creative imagination, incisive thinking, and ability to present ideas clearly. Includes monetary award of $3000.

**Mathematics Writing Award** *May 2009, May 2011*
Awarded to a student who has demonstrated excellence in the exposition of mathematics. Includes monetary award of $100.

**Goucher Senior Leadership Service Award** *May 2011*
Awarded to senior students who demonstrated commitment to community service.

**The Pearl Davis Leavitt Prize** *June 2008, June 2009, June 2010*
Awarded to mathematics major, other than a graduating senior, who has exhibited meritorious achievement in mathematics. Includes monetary award of $300.

**Eleanor Spencer Grant** *June 2010*
Wrote a proposal and earned grant to complete a research project abroad in the visual arts culminating in a formal exhibition. Awarded $5000 for a rock-climbing photography project in the Lofoten Islands in Norway.

**Innovation Grant** *November 2010*
Wrote a proposal and received grant to install clotheslines in every laundry room on campus.

**Goldwater Scholar** Honorable Mention *April 2009*
Awarded to select highly qualified scientists, mathematicians and engineers in undergraduate studies who intend to pursue careers in research.

## LEADERSHIP POSITIONS

**Mathematics Graduate Organization** President *May 2015- May 2016*
*Syracuse University, Syracuse, NY*
Planned annual department picnic and annual mathematics conference which is run entirely by graduate students and is supported by the American Mathematical Society.

**Pi Mu Epsilon** President *May 2008- May 2011*
*Goucher College, Baltimore, MD*
Ran induction ceremonies and organized events for mathematics department.

**Mathematics and Computer Science Club** President *September 2008- May 2011*
*Goucher College, Baltimore, MD*
Led many events throughout the year including organizing alumni dinner and awards ceremony.

**Verge Magazine** Reviewer *September 2008- May 2011*
*Goucher College, Baltimore, MD*
Reviewed articles for peer-reviewed journal.

**Physics Club** Secretary *September 2007-June 2008*
*Goucher College, Baltimore, MD*
Led monthly astronomy nights using the school observatory and telescopes.

**Agricultural Co-op** President, Treasurer, Member *September 2008-May 2011*
*Goucher College, Baltimore, MD*
Cultivated herbs and vegetables to sell to dining halls and organized the composting of all food scraps from the food services on campus.

## MEMBERSHIPS

American Women in Mathematics *September 2007-present*
American Mathematical Society *September 2009-present*
Pi Mu Epsilon *September 2008-present*