

The Structure of Fullerene Signatures

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ABSTRACT. This paper is devoted to developing the structure of fullerene signatures. These structure results are then used to construct a complete catalog of fullerenes with ten or more symmetries. These fullerenes fall into 112 families. The Coxeter fullerenes, obtained by subdividing the faces of the icosahedron, form the prototype family. Like the Coxeter families, each family in the catalog is a one, two, three or four parameter collection of labelings of a fixed planar graph on 12 vertices. The actual fullerenes are obtained by assigning positive integers to the parameters and filling in the faces of the plane graph with the regions from the hexagonal tessellation of the plane determined by the parameter values.

1. Introduction

By a fullerene, we mean a trivalent plane graph $\Gamma = (V, E, F)$ with only hexagonal and pentagonal faces. It follows easily from Euler's Formula that each fullerene has exactly 12 pentagonal faces. The simplest fullerene is the graph of the dodecahedron with 12 pentagonal faces and no hexagonal faces. It is frequently easier to work with the duals to the fullerenes: geodesic domes, i.e. triangulations of the sphere with vertices of degree 5 and 6. It is in this context that Goldberg[5], Caspar and Klug[1] and Coxeter[2] parameterized the geodesic domes/fullerenes that include the full rotational group of the icosahedron among their symmetries. In this paper we extend this work by giving a complete parameterization of all highly symmetric fullerenes. Specifically, we describe all fullerenes with ten or more symmetries.

The construction devised by Goldberg, Caspar and Klug and Coxeter starts with the icosahedron and then fills in each face with an equilateral triangular region from Λ , the triangular tessellation of the plane. In 1988, Fowler, Cremona and Steer [3] generalized this construction, filling in the faces of the icosahedron with triangular region from Λ that are not necessarily equilateral. Using their model, Fowler, Cremona and Steer generated all fullerenes with 4 or more symmetries and 256 or fewer atoms.

In [6], Graver also extended the Goldberg, Caspar and Klug and Coxeter construction. But, instead of keeping the icosahedral structure, a second feature of the

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Goldberg, Caspar and Klug and Coxeter construction was retained: the edges of the model all represent shortest distances between pentagons in the fullerene being modeled. The resulting model, called a signature, generally has fewer edges (as few as 11) and a simpler parameter structure than the triangulated model. There are no equations or inequalities for the parameters to satisfy; the parameters are simply independent positive or nonnegative integers. The cost of reducing the number of edges and simplifying the system of parameters is the larger number of cases that must be considered.

It is this author's hope that the ease of use of signature models will justify duplicating the results of Fowler, Cremona and Steer [3]. In particular the following features of a fullerene may be easily read from its signature, usually by inspection: its symmetry structure, the relative positions of its pentagons, whether or not it is a nanotube and whether or not it is a leapfrog fullerene.

We will rely heavily on some of the theorems and lemmas proved in [6]. For easy reference, we restate those results here, along with the necessary definitions. The main result of [6] is:

THEOREM 1.1. *A geodesic dome/fullerene is uniquely determined by its signature.*

A second result in that paper and the one that leads to this paper is:

THEOREM 1.2. *With the exception of one simple family of geodesic domes/fullerenes, the symmetry group of a geodesic dome/fullerene is isomorphic to the symmetry group of its signature.*

A key ingredient in our development is Λ , the triangular tessellation of the plane. We think of Λ as the infinite plane graph with all vertex degrees 6 and all face degrees 3. The automorphisms of this graph correspond the congruences of Λ as a geometric object in the plane: the translations, rotations, reflections and glide reflections that map Λ onto Λ . Two vertex sets of Λ are said to be *congruent* if there is an automorphism of Λ which maps one onto the other.

By a *segment* of Λ we simply mean a pair of vertices of Λ and we visualize a segment as the straight line segment joining the two vertices. To each segment which does not coincide with a "line" of the tessellation, we assign *Coxeter coordinates* (p, q) as follows: select one endpoint of the segment to be the origin; take the edge of the graph to the right of the straight line segment representing the segment as the unit vector in the p direction; take the edge of the graph to the left of the straight line segment as the unit vector in the q direction; finally assign to the segment the coordinates of its other endpoint in this coordinate system. If the segment coincides with a "line" of the tessellation, that segment is assigned the single Coxeter coordinate (p) , where p is the number of edges of Λ in the segment. The *length* of a segment σ with endpoints v and w is defined to be the distance between the endpoints in the graph Λ . It is denoted by $|\sigma|$ and one easily sees that $|\sigma| = p + q$, where (p, q) are its Coxeter coordinates.

Another important tool developed in [6] is the structure graph of a weighted graph. Let $\Phi = (V, E)$ be any graph with a set of edge weights, $\omega : E \rightarrow \mathbb{R}^+$. The *structure graph* of the weighted graph (Φ, ω) is the union of all shortest spanning trees of Φ .

Let $\Gamma = (V, E, F)$ be a geodesic dome and let P denote the set of the 12, degree 5 vertices of Γ . The first step in constructing the signature graph of Γ is to construct the complete graph on the vertex set P and assign to each edge $\{v, w\}$, $\omega_1(\{v, w\})$,

the distance between v and w , as vertices in Γ . This weighted graph is called the *first auxiliary graph* of Γ and is denoted by $(\mathcal{A}_1(\Gamma), \omega_1)$. The second step is to construct the structure graph of $\mathcal{A}_1(\Gamma)$. This graph is called the *second auxiliary graph* of Γ and is denoted by $\mathcal{A}_2(\Gamma)$. This graph, $\mathcal{A}_2(\Gamma)$, has a natural drawing on the sphere as an overlay of the drawing of Γ on the sphere. For each edge of $\mathcal{A}_2(\Gamma)$, there is a region of Γ containing it that is isomorphic to a region in Λ ; specifically, this region has no vertices of degree 5 in its interior. We have pictured such a region in Figure 1. In the figure, thin lines denote segments of lines of the lattice while the heavy line denotes the superimposed segment joining the two lattice points. The existence of this region permits us to identify each edge, $\{v, w\}$, of $\mathcal{A}_2(\Gamma)$ with a segment σ in Λ . And this identification enables us to assign Coxeter coordinates to each edge of $\mathcal{A}_2(\Gamma)$. If $\{v, w\}$ is an edge of $\mathcal{A}_2(\Gamma)$, σ its corresponding segment and (p, q) its Coxeter coordinates, we have $\omega_1(\{v, w\}) = |\sigma| = p + q$.

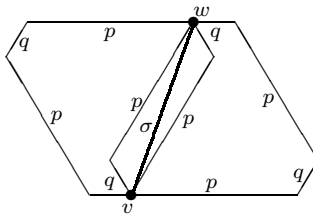


FIGURE 1.

While $\mathcal{A}_2(\Gamma)$ has a natural drawing in the plane, it may not be planar, i.e. it may admit crossing edges. To eliminate any crossings, we make a slight alteration in the weight function, replacing $\omega_1(\{v, w\})$ by $\omega_2(\{v, w\}) = \|\sigma\| = p + q + \frac{|p-q|}{p+q+1}$ which we call the *refined length* of σ . [If σ has the single Coxeter coordinate (p) , $\omega_2(\{v, w\}) = \|\sigma\| = p + \frac{p}{p+1}$.] The next step is to construct the structure graph of $(\mathcal{A}_2(\Gamma), \omega_2)$. This third graph also has a natural drawing on the sphere and it admits no crossings. The plane graph consisting of this third graph and its natural planar embedding is called the *signature graph* of Γ and is denoted by $\mathcal{S}(\Gamma)$. Each edge of $\mathcal{S}(\Gamma)$ may be identified with a line segment joining two vertices in Λ . This identification leads to a labeling system for the edges and angles of $\mathcal{S}(\Gamma)$. The signature graph of Γ along with this labeling is called the *signature* of Γ . To avoid confusion, we will henceforth refer to the edges of $\mathcal{S}(\Gamma)$ as segments leaving the term edge for the edges of Γ .

The results from [6] to which we will refer in this paper are listed using the numbering system from that paper which is distinct from the numbering system of these proceedings.

LEMMA 1.3. *Let Θ be the structure graph of the weighted graph Φ, ω .*

- (1) *If u, v, w are vertices of a 3-circuit in Φ with $\omega(\{u, v\}) < \omega(\{v, w\})$ and $\omega(\{u, v\}) < \omega(\{v, w\})$, then the edge $\{v, w\}$ is not in Θ .*
- (2) *The edges of Θ of maximum weight form an edge cut set for Θ .*
- (3) *If edges of Θ of maximum weight are deleted from Θ , then each of resulting components is the structure graph of the corresponding vertex induced weighted subgraph of Φ .*
- (4) *If Ω is any subgraph of Θ , then the edges of Ω of maximum weight form an edge cutset of Ω .*

LEMMA 1.4. *Let σ denote a segment in Λ with endpoints v and w and let (p, q) [or (p)] denote its Coxeter coordinates as computed from v .*

- (1) *The Coxeter coordinates of σ computed from w are also (p, q) [(p)].*
- (2) *p and q are positive integers [p is a positive integer].*
- (3) *$|\sigma| = p + q$ [$|\sigma| = p$].*
- (4) *The segments σ , with Coxeter coordinates (p, q) , and σ' , with Coxeter coordinates (p', q') , are congruent if and only if either $p' = p$ and $q' = q$ or $p' = q$ and $q' = p$. Furthermore, $p' = p$ and $q' = q$ if and only if σ' is the image of σ under a rotation or translation of the tessellation and $p' = q$ and $q' = p$ if and only if σ' is the image of σ under a reflection or glide reflection of the tessellation.*
- (5) *The segments σ , with Coxeter coordinate (p) , and σ' , with Coxeter coordinate (p') , are congruent if and only if $p' = p$. Furthermore, any two segments with coordinates (p) are images of one another under both a translation or rotation and a reflection or glide reflection.*

We are particularly interested in angles. Much of the information about an angle is coded in the Coxeter coordinates of its sides, but not all. Suppose that we have two segments forming an angle at a common endpoint v ; denote them, in clockwise order, by σ and σ' denoting their Coxeter coordinates by (p, q) and (p', q') , respectively. The missing information is the multiple of 60 degrees between the edge from v along which p is measured and the edge along which p' is measured. This multiple is easily seen to be the number of Λ edges from v which lie between the two segments. Hence, we define the *type* of the angle between two segments with a common endpoint v to be the number of edges from v which lie between the two segments. Segments with Coxeter coordinates of the form (p) coincide with an edge; in this case, the segment contributes $\frac{1}{2}$ to each of the types of the angles on either side of the segment.

LEMMA 1.5. *Consider segments and angles in Λ or a signature $\mathcal{S}(\Gamma)$.*

- (1) *Given segments α , β and γ in clockwise order around a common endpoint, the type of the angle between α and γ is the sum of the types of the angles between α and β and between β and γ .*
- (2) *Given segments $\sigma_1, \sigma_2, \dots, \sigma_n$ of Λ [of $\mathcal{S}(\Gamma)$] in cyclic order about a common endpoint, the sum of the types of the angles between consecutive segments is 6 [5].*
- (3) *Given an n -gon in Λ or a face in $\mathcal{S}(\Gamma)$ with angle types A_1, A_2, \dots, A_n , we have: $A_1 + \dots + A_n = 3n - 6$.*

As we construct signature graphs, we will be using both length functions for segments. The next lemma details the relationships between these two measures.

LEMMA 1.6. *For segments σ and σ' :*

- (1) $|\sigma| = \lfloor \|\sigma\| \rfloor$;
- (2) *if $\|\sigma\| = \|\sigma'\|$, then $|\sigma| = |\sigma'|$;*
- (3) *if $|\sigma| < |\sigma'|$, then $\|\sigma\| < \|\sigma'\|$;*
- (4) σ and σ' are congruent if and only if $\|\sigma\| = \|\sigma'\|$.

Theorem 1.1 implies that we may rebuild a geodesic dome from its signature and that that this can be done in essentially only one way. This boils down to filling in each face of the signature with a region from Λ that is consistent with the

segment and angle labels of that face. The natural approach to filling in the faces is to select a face of the signature and then simply reconstruct its boundary in Λ as prescribed by its segment and angle labels: denote the segments by $\sigma_1, \dots, \sigma_k$ in clockwise order around the face; draw a segment σ'_1 in Λ congruent to σ_1 ; draw in a segment σ'_2 congruent to σ_2 sharing an endpoint so that the angles between σ_1 and σ_2 and σ'_1 and σ'_2 have the same type; and so on. In [6], we showed that this “dead reckoning” approach worked.

If the Coxeter coordinates of the segments of the signature of a fullerene are replaced by compatible variable Coxeter coordinates, we have the signature for a family of fullerenes. The Goldberg, Caspar and Klug and Coxeter fullerenes form such a family: the signature graph is the icosahedron, the angle types are all 1 and the segment labels are all (p, q) or all (r) . The number of plane graphs on 12 vertices is finite and, to each such graph, the number of consistent assignments of types to the angles and variable Coxeter coordinates to the segments is finite. Hence a complete (finite) catalog of all families of fullerenes is theoretically possible. While constructing a catalog of all fullerenes is problematic, constructing catalogs of particular classes of fullerenes is certainly possible. In this paper we take that approach and construct a complete listing of all family signatures with certain symmetry structures. Specifically those with ten or more symmetries.

2. Signatures of leapfrog fullerenes

The leapfrog construction is most easily described for geodesic domes: a new vertex is added in the center of each triangle; the new vertices are joined by an edge to each of the old vertices of the triangle containing it and to its three neighboring new vertices; then all old edges are removed. A fullerene that can be constructed by the leapfrog method is called a *leapfrog fullerene*. The importance of leapfrog fullerenes results from the fact that they allow a very desirable arrangement of the double bonds. This is explained fully in [7]. The leapfrog construction on Λ results in a second copy of Λ which we denote by Λ' . Since the vertices of Λ are also vertices in Λ' , a segment in Λ is also a segment in Λ' . Hence such a segment has two sets of Coxeter coordinates, one as a segment in Λ and one as a segment in Λ' . The next lemma relates these coordinates.

LEMMA 2.1. *Let σ be a segment in Λ (or a Λ -region of a geodesic dome Γ) and let Λ' (or Γ') be the result of applying the leapfrog operation. Then the Coxeter coordinates of σ in Λ' (or Γ') are computed from the Coxeter coordinates of σ in Λ as follows:*

$$\frac{\Lambda \text{ coordinates}}{\Lambda' \text{ coordinates}} \left| \begin{array}{cccc} (p+r, p) & (p, p+r) & (p, p) & (r) \\ (r, r+3p) & (r+3p, r) & (3p) & (r, r) \end{array} \right.$$

PROOF. The graph Λ' (or the Λ -region Γ' containing σ) has a unique (up to a permutation of colors) vertex, 3-coloring and one easily checks that the old vertices from Λ form one of the color classes; see the first part of Figure 2. With this 3-coloring in mind, it is easy that a segment in Λ with a single Coxeter coordinate (r) (e.g. the heavy segment in the first part of the figure) will have Coxeter coordinates (r, r) in Λ' . Since a segment in Λ with Coxeter coordinates (p, q) is represented by the polygonal segment consisting of two segments with Coxeter coordinates (p) and (q) , we easily compute the function which converts the Coxeter coordinates of a segment in Λ to Coxeter coordinates of that same segment as a segment in Λ' . This

derivation is illustrated for the Coxeter coordinates $(p+r, p)$ in the second part of Figure 2. There the segment is represented by the dashed line; the lines of Λ are represented by heavy lines; the lines of Λ' are represented by thin lines; Coxeter coordinates and lengths in Λ are printed in large boldface while those in Λ' are printed in smaller italic. The remaining two cases follow by reflection or letting $r = 0$. \square

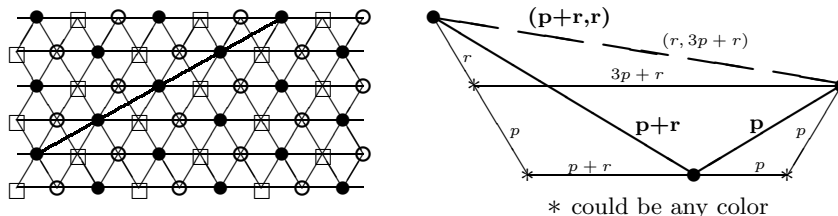


FIGURE 2.

Using our 3-colored model of Λ' , one easily checks that a segment of Λ' joins two vertices in the same color class if and only if the difference of its Coxeter coordinates is divisible by three; to be precise, if and only if its Coxeter coordinates are of the form $(3p+r, r)$, $(r, 3p+r)$, (p, p) or $(3r)$. We define the signature of a fullerene to be of *leapfrog type* if each of its segments has Coxeter coordinates of one of these four types.

THEOREM 2.2. *A fullerene is a leapfrog fullerene if and only if its signature is of leapfrog type.*

PROOF. Let $\mathcal{S}(\Gamma)$ be the signature of the geodesic dome Γ . It follows from the previous lemma that, if a fullerene is obtained by the leapfrog construction from another fullerene, then its signature is of leapfrog type. Now suppose that $\mathcal{S}(\Gamma)$ is of leapfrog type and apply the leapfrog construction to Γ to get Γ' . We may also apply the leapfrog construction to each face of $\mathcal{S}(\Gamma)$ to get a signature-like decomposition of Γ' . (Since the the leapfrog construction does not enlarge all lengths by the same factor the resulting decomposition may not be the actual signature of Γ' .) One feature of this signature-like decomposition of Γ' is that all of its individual coordinates are multiples of 3. Reducing all coordinates by this common factor of 3 results in a similar geodesic dome Γ^* . And one easily checks that applying the leapfrog construction to Γ^* yields Γ . \square

3. Angles and triangles

By Lemma 1.3(4), any face of the signature of a geodesic dome must have two sides of the same refined length which is greater than or equal to the refined length of the remaining sides. By Lemma 1.6(4), the longer two sides must be congruent segments. In Figure 3, we consider a small neighborhood of geodesic dome Γ about a vertex v of degree 5 - small enough so that all other vertices of degree 5 occur outside the neighborhood or on its boundary. Clearly there could be at most five segments with v as an endpoint and having Coxeter coordinates (p, q) (or (p)). If $p \neq q$, there could be up to five more with coordinates (q, p) . In the latter case, it is convenient to assume that $q > p$ and to replace q by $p+r$. In Figure 3, we illustrate this case with $p = 1$ and $r = 4$ by drawn in all ten of the possible segments.

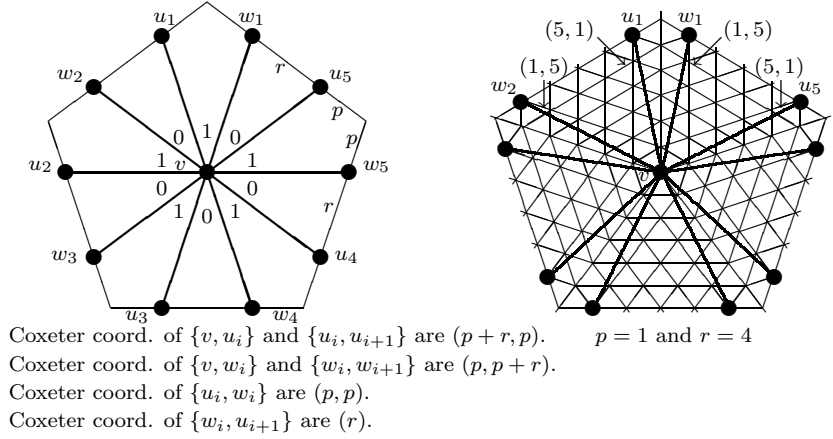


FIGURE 3.

By direct computation, we see that consecutive segments yield triangles of two types: moving counterclockwise about the common vertex v , a segment with Coxeter coordinates $(p, p+r)$ followed by a segment with Coxeter coordinates $(p+r, p)$ make an angle of type 1 at v and form an isosceles triangle whose third side has Coxeter coordinates (p, p) [e.g. $\Delta v, u_5, w_5$ in the figure] while a segment with Coxeter coordinates $(p+r, p)$ followed by a segment with Coxeter coordinates $(p, p+r)$ make an angle of type 0 at v and form an isosceles triangle whose third side has Coxeter coordinates (r) [e.g. $\Delta v, w_1, u_5$ in the figure]. Two consecutive segments with the same Coxeter coordinates make an angle of type 1 at v and form an equilateral triangle. The only other possibility that yields an angle of type 1 occurs when a segment with Coxeter coordinates $(p+r, p)$ is followed by the second segment with Coxeter coordinates $(p, p+r)$ (again moving counterclockwise). In this case, the Coxeter coordinates of joining the other endpoints of the segments are $(p+r, p+r)$ [$\Delta v, w_2, u_5$ in the figure]. Since the refined length of this third side is greater than the refined length of the congruent segments, no triangular face can occur using these congruent segments. This same argument excludes all pairs of segments subtending larger angles. We have proved:

LEMMA 3.1. *The only possibilities for a triangular face in the signature of a fullerene are described in Figure 4.*

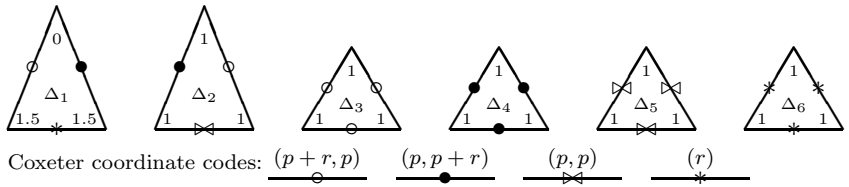


FIGURE 4.

Since the focus of this paper is the symmetries of signatures, we should identify the symmetries of these faces. All symmetries preserve angle types; an orientation preserving symmetry maps each segment onto a segment with the same Coxeter coordinates while an orientation reversing symmetry maps each segment onto a

segment with reversed Coxeter coordinates. Thus, the first two triangles in Figure 4 admit only the reflection through the vertical axis; the second two admit only rotations and each is reflected into the other; the last two admit all six of the symmetries of an equilateral triangle.

Next we turn our attention to angles between two segments of a signature but not part of a triangular face. We have pictured this configuration in Figure 5. In the figure α and β represent segments of the signature. We note that, if the angle type, T , is three or less, then the hexagonal regions of α and β overlap forming an enlarged region of Λ containing the triangle bounded by these segments and the segment indicated by the dashed line and labeled γ . This enable us to investigate this triangle as a triangle in Λ .

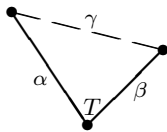


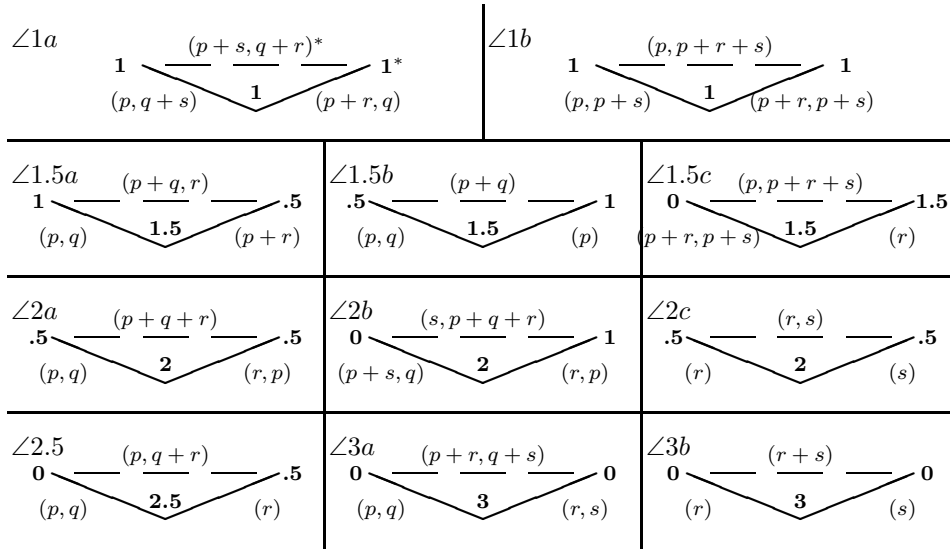
FIGURE 5.

By Lemma 1.3(1), γ will not belong to the signature if its refined length is greater the refined lengths of both α and β . Suppose that the refined length of γ is less than or equal to the refined length of either α or β . Without loss of generality we may assume that $\|\beta\| \leq \|\alpha\|$ and that $\|\gamma\| \leq \|\alpha\|$. If the strict inequality holds in both cases, then, by Lemma 1.3(1), α could not belong to the signature. We conclude that either $\|\gamma\| = \|\alpha\|$ or $\|\beta\| = \|\alpha\|$. If $\|\beta\| < \|\alpha\|$, then $\|\gamma\| = \|\alpha\|$ and we have one of the triangles listed above. If $\|\beta\| = \|\alpha\|$ then we could have one of the triangles listed above with γ as its base. However, there is another possibility: γ does not belong to the signature because its endpoints are joined by a path of segments, each shorter than γ . Each of the triangles in Figure 4 gives rise to a family of n -sided faces obtained by replacing its shorter side by a path of $n - 2$ segments, each shorter than the replaced side.

LEMMA 3.2. *Let α and β be segments of the signature $\mathcal{S}(\Gamma)$ making an angle of type $T \leq 3$ and denote the segment joining the other endpoints of α and β by γ (whether it belongs to the signature or not). Then $T \neq \frac{1}{2}$ and exactly one of the following cases hold:*

- (1) $T = 0, 1, 1\frac{1}{2}$ and α , β and γ are the sides of one of the triangles described in Figure 4.
- (2) $T = 0, 1$, α and β are congruent and the largest sides of an n -gon obtained by replacing the remaining segment in one of the above triangles by a path of segments, each shorter than the replaced side.
- (3) $T = 1, 1\frac{1}{2}, 2, 2\frac{1}{2}, 3$ and we have one of the configurations pictured in Figure 6 or the reflection of one of those configurations.

PROOF. As we indicated above, the configuration pictured in Figure 5 lies entirely in a region of Γ that corresponds to a region of Λ . Hence we can draw our configurations and carry out our arguments in Λ . In view of the previous discussion, we may assume that $\|\gamma\| > \max\{\|\alpha\|, \|\beta\|\}$. One easily checks that, if $T = 0, \frac{1}{2}$, then $\|\gamma\| < \max\{\|\alpha\|, \|\beta\|\}$, contrary to our assumption. We start our discussion of



* The Coxeter coordinates of the dashed segment and the types of the remaining angles of the triangle it completes are listed across the top of each diagram.

FIGURE 6.

the remaining angle types $(1, 1\frac{1}{2}, 2, 2\frac{1}{2}, 3)$ by considering an angle of type 2. We have drawn such a configuration on the left in Figure 7. As in Figure 1, thin lines denote segments of lines of the lattice while heavy lines denote superimposed segments from the signature. In this drawing, we have assumed that $p > s$ where (p, q) and (r, s) are the Coxeter coordinates of α and β , respectively. It is easy to see that, in this case, γ has Coxeter coordinates $(p - s, q + r + s)$. In order to eliminate the inequality $p > s$, we make two substitutions: p for s and $p + s$ for p . This gives configuration $\angle 2b$ as it appears in Figure 6. Configuration $\angle 2a$ is obtained from configuration $\angle 2b$ by setting $s = 0$. The case $p < s$ (in the original notation) is just the reflection of configuration $\angle 2b$ and is not included. Finally the case in which α and β have single Coxeter coordinates is trivial and is pictured in the figure as configuration $\angle 2c$.

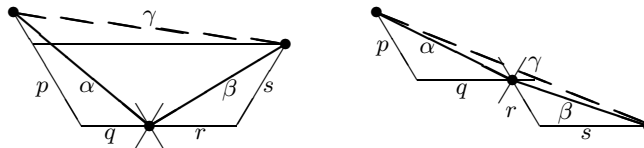


FIGURE 7.

The case of an angle of type $2\frac{1}{2}$ is straight forward. The case in which α has a pair of Coxeter coordinates while β has a single Coxeter coordinate is pictured as configuration $\angle 2.5$; the case in which β has a pair of Coxeter coordinates while α has a single Coxeter coordinate is its reflection and is not pictured. The case of two segments with two Coxeter coordinates making an angle of type 3 is pictured, on the right, in Figure 7 and recorded as configuration $\angle 3a$ in Figure 6 while the

case of two segments, each with one Coxeter coordinate, making an angle of type 3 is recorded as configuration $\angle 3b$. Again all computations are straight forward.

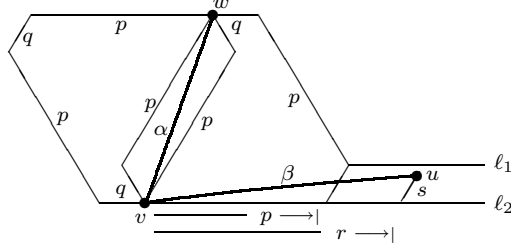


FIGURE 8.

This brings us to the case of two segments with two Coxeter coordinates making an angle of type 1 or type $1\frac{1}{2}$ such that the segment γ has longer refined length than both α and β . In Figure 8, we have drawn the hexagonal region about the segment α . The horizontal ray, ℓ_1 extending from the right hand vertex of the hexagon is the divide between those vertices closer to the vertex v and those closer to w . Hence u , the other endpoint of β , must lie on or below this ray. We have already noted that that u , being a degree 5 vertex, cannot lie in the hexagon and, if the angle type is 1, it must lie above the ray ℓ_2 . From this geometric argument, we conclude that $s \leq q$ while $r \geq p$. To eliminate these inequalities we make the following substitutions: $p + x$ for r , $q + y$ for q and q for s . With these substitutions we have $(p, q + y)$, $(p + x, q)$ and $(p + y, q + x)$ as the Coxeter coordinates of α , β and γ , respectively. In the figure we have pictured q as less than p . Were the picture drawn with $p \leq q$, same arguments would hold yielding the same conclusion. Hence, we proceed from this point algebraically with no assumptions on the relative sizes of p and q .

We have that the Coxeter coordinates of α , β and γ are $(p, q + y)$, $(p + x, q)$ and $(p + y, q + x)$ and that $x, y \geq 0$. If they are both positive than $|\gamma| > |\alpha|, |\beta|$ and by Lemma 1.6(3), $\|\gamma\| > \|\alpha\|, \|\beta\|$, as required. This case is pictured in Figure 6 as configuration $\angle 1a$. If both x and y were 0, we would have $\|\gamma\| = \|\alpha\| = \|\beta\|$, an excluded possibility. Assume that $y = 0$ and $x > 0$. Then $|\gamma| = |\beta| > |\alpha|$. So $\|\gamma\| > \|\alpha\|$. Requiring that $\|\gamma\| > \|\beta\|$ gives:

$$p + q + x + \frac{|(p - q) - x|}{p + q + x + 1} = \|\gamma\| > \|\beta\| = p + q + x + \frac{|(p - q) + x|}{p + q + x + 1}.$$

This implies $(p - q) < 0$ or $p < q$. Again, to eliminate the inequality, we replace q with $p + s$; replacing x with r gives configuration $\angle 1b$ in the figure. The case $x = 0$ and $y > 0$ leads to the reflection of configuration $\angle 1b$.

Finally, we turn to the case of angle type $1\frac{1}{2}$ (take u on ℓ_2 in Figure 8). We assume that α has Coxeter coordinates (p, q) while β has the single Coxeter coordinate (r) . The configurations in which α has the single Coxeter coordinate will be the reflections of the ones we construct under this assumption. There are three possibilities: $p < r$, $p = r$ and $p > r$. If $p < r$, we replace r by $p + r$. In this case, γ has Coxeter coordinates $(p + q, r)$ and it is clear that $|\gamma| > |\alpha|, |\beta|$. This case is recorded as configuration $\angle 1.5a$. If $p = r$, we replace r by p . In this case, γ has the single Coxeter coordinate $(p + q)$. Here $|\gamma| = |\alpha| > |\beta|$ and

$\|\gamma\| = p + q + \frac{p+q}{p+q+1} > p + q + \frac{|p-q|}{p+q+1} = \|\alpha\|$. This case is recorded as configuration $\angle 1.5b$. If $p > r$, we replace p by $p + r$. Here γ has Coxeter coordinates $(p, q + r)$ and again $|\gamma| = |\alpha| > |\beta|$. We require

$$p + q + r + \frac{|(p - q) - r|}{p + q + r + 1} = \|\gamma\| > \|\alpha\| = p + q + r + \frac{|(p - q) + r|}{p + q + r + 1}.$$

This implies $(p - q) < 0$ or $p < q$. To eliminate the inequality, we replace q by $p + s$ and get configuration $\angle 1.5c$. \square

4. Quadrilateral faces

We next consider quadrilateral faces. Quadrilateral faces, like all faces of a signature must have their longer two sides congruent. Furthermore, since the diagonals cannot belong to the signature, each diagonal along with two sides of the quadrilateral must form one of the configuration pictured in Figure 6. Quadrilateral signature faces are of two basic types: those with the longer congruent sides opposite (parallelograms and trapezoids) and those with the longer congruent sides adjacent (kites). To avoid duplication, faces with three or four congruent sides will be listed with the parallelograms and trapezoids and not with the kites.

LEMMA 4.1. *The only possibilities for a quadrilateral face in the signature of a fullerene are described in Figure 10 (kites) and Figure 12 (parallelograms and trapezoids).*

PROOF. We consider kites first. A prototype kite is pictured on the left in Figure 9. The sides are labeled 1 through 4; sides 1 and 2 are to be congruent and have refined length greater than the refined lengths of sides 3 and 4. The types of the angles are denoted by A, B, C and D ; the angle labeled A is called the apex angle. One of the diagonals is labeled δ_1 , the other will be denoted by δ_2 . Since either both of sides 1 and 2 have two Coxeter coordinates or both have one Coxeter coordinate, A is an integer.

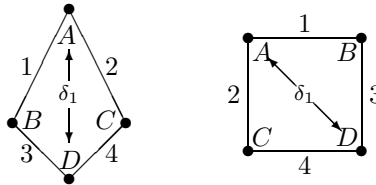


FIGURE 9.

Assume that $A = 0$. Then sides 1 and 2 must have Coxeter coordinates of the form $(p + x, p)$ and $(p, p + x)$, respectively. Thus the diagonal δ_2 of the kite has Coxeter coordinates (x) . The angles from Figure 6 with a single Coxeter coordinate for the third side are $\angle 1.5b, \angle 2a, \angle 3b$: $\angle 1.5b$ yields kite K_1 in Figure 10, $\angle 2a$ gives K_2 and the configuration from $\angle 3b$ has diagonal δ_1 too short.

Assume that $A = 1$ and that sides 1 and 2 have the same Coxeter coordinates. These kites are all formed by placing an equilateral triangle on top of each of the angles in Figure 6. We need only check the length of δ_1 . This check results in kites K_3 through K_{10} corresponding to the angles of types 1, 1.5 and 2. The angle of type 2.5 will have a short δ_1 unless $p > q$. This condition is incorporated in the

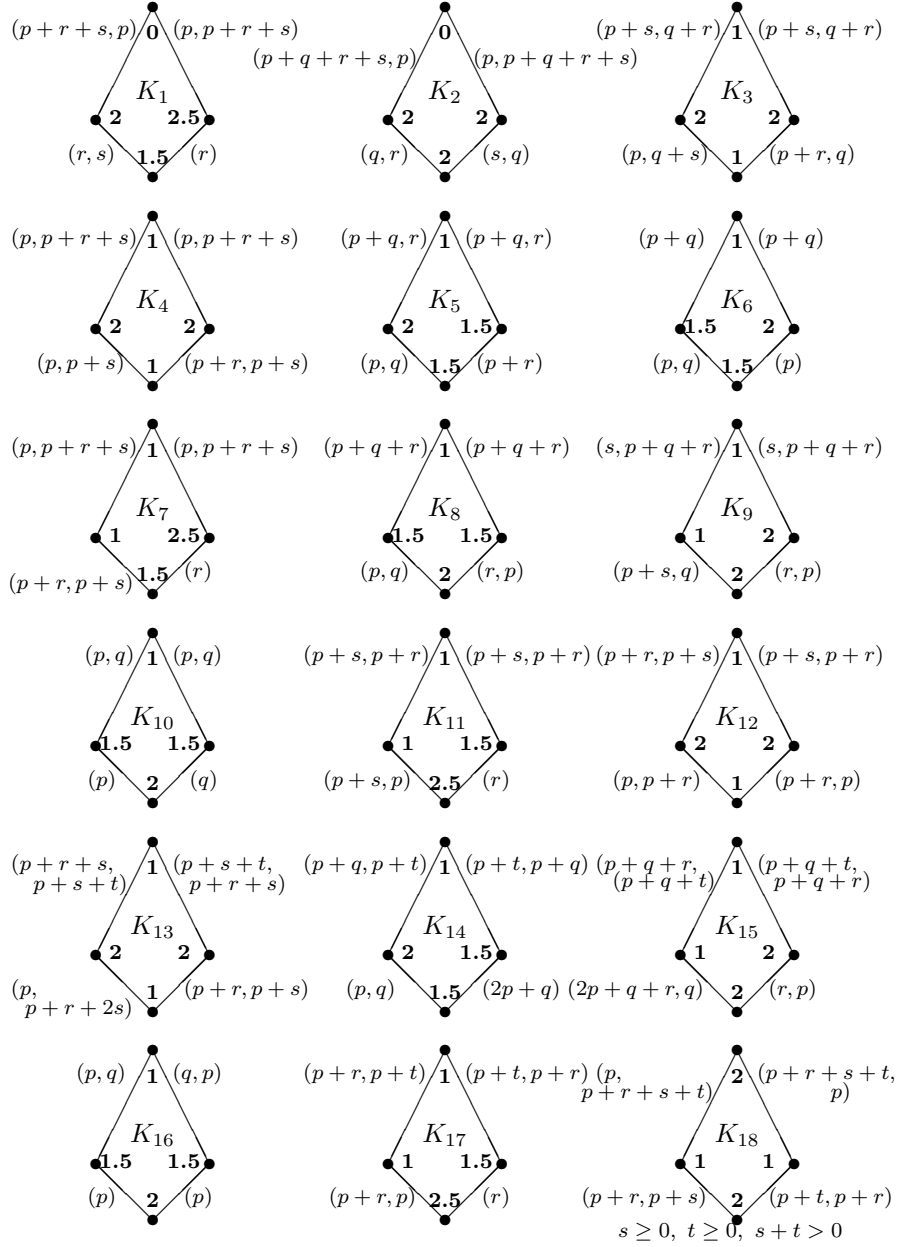


FIGURE 10.

parameters of kite K_{11} . Again the configurations from angles of type 3 have δ_1 too short.

Assume that $A = 1$ and that sides 1 and 2 have Coxeter coordinates of the form (x, y) and (y, x) respectively. Thus diagonal δ_2 has Coxeter coordinates (x, x) . The angles from Figure 6 which can have such double Coxeter coordinates for their

third side are $\angle 1a$, $\angle 1.5a$, $\angle 2b$, $\angle 2c$, $\angle 2.5$ and $\angle 3a$. We consider these options for D one at a time starting with $\angle 1a$. It is convenient to split this into two subcases: $q = p$ and $q \neq p$ or, by symmetry, $q > p$. If $q = p$, then $x = p+r$ and $s = r$. In order that side 1 have length greater than or equal to the length of side 3, we must have $y \geq p$. However if $y = p$, the configuration is also a parallelogram and we exclude that case from this listing. We let $y = p + s$ and this possibility is recorded as kite K_{12} in the figure. Now replace q by $p + w$. Then $p + s = x = q + r = p + r + w$, so $s = r + w$. Replacing s by $r + w$ and then w by s gives coordinates $(p, p + r + 2s)$ and $(p+r, p+s)$ for sides 3 and 4 and $x = p+r+s$. For the refined length of side 1 to be greater than or equal to the refined length of side 3, we must have $y > p + s$. Taking $y = p + s + t$ gives kite K_{13} . We turn next to the case of $\angle 1.5a$: clearly, $r = x = p + q$ and $y > p$. Writing y as $p + t$, we get kite K_{14} . In the case of $\angle 2b$, we have $s = x = p + q + r$ and $y = p + q + t > p + q$ giving K_{15} . In the case of $\angle 2c$, we have $s = x = r$ and $y > 0$ giving K_{16} after relabeling. Next consider the case $D = 2.5$. Here $p = x = q + r$. In order that δ_1 have refined length greater than or equal to the refined length of side 1, we must have $y > q$ or $y = q + t$. Replacing q with p gives kite K_{17} . Finally, if we take $D = 3$, δ_1 is too short, discounting this possibility.

Before proceeding, we note that, by straightforward computations, one can verify that the following result: if $D < A$ then one of sides 3 or 4 is longer than one of the sides 1 or 2. A second observation is that $A + D \leq 4$; this follows since $A + B + C + D = 6$ and $B \geq 1$ and $C \geq 1$. Assume then that $A = 2$ and that sides 1 and 2 have the same Coxeter coordinates and these coordinates are unequal. This can only occur when the angle at A is $\angle 2b$. It follows that the angle at D is also $\angle 2b$ oriented so that $B = C = 1$. And we have the left hand configuration in Figure 11. We have $s = y$ and $p + q + r = 3x + y$. Since side 1 is longer than side 3 and 4, we have $p + r \leq 2x + y$ and $p + q + s \leq 2x + y$; since $B = 1$, we have $x \leq p$ and $r \leq x + y$; and since $C = 1$, we have $q \leq x$ and $x + y \leq p + s$. This system has as its only solution $x = p = q$, $y = s$ and $r = p + s$. But then δ_1 also has coordinates $(p, p + s)$, eliminating this case. We turn to the case that $A = 2$ and that sides 1 and 2 have Coxeter coordinates of the form (x, y) and (y, x) respectively. In this the top and bottom angles must be of the form $\angle 2a$ resulting in the right hand configuration of Figure 11. Here we have $2x + y = u + v + w$, $x + y \geq u + v$ and $x + y \geq u + w$; since $B = 1$, we also have that $x \leq u$. Solving this system gives: $p = x$, $u = p + r$, $v = p + s$, and $w = p + t$, where $r > 0$, $s \geq 0$, $t \geq 0$ and $s + t > 0$. This is recorded as kite K_{18} and completes our discussion of kites.

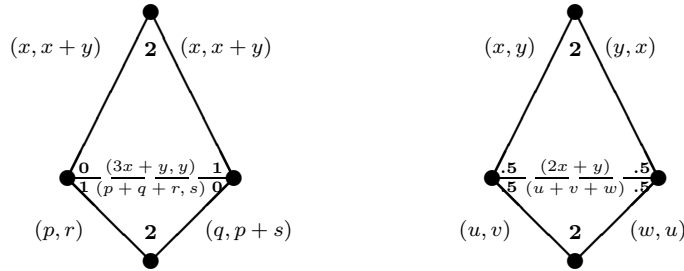


FIGURE 11.

We turn now to parallelograms and trapezoids. Picture our quadrilateral as drawn on the right in Figure 9 with longest, congruent sides vertical. One of the diagonals is labeled δ_1 , the other will be denoted by δ_2 . We have that $A + B + C + D = 6$; so, without loss of generality, we can insist that $C + D \leq 3$. Suppose that C is not an integer, then one of sides 2 or 4 has a single Coxeter coordinate while the other has two Coxeter coordinates. And, since sides 2 and 3 are congruent, the same must be true of sides 3 and 4. That is, if C is not an integer then neither is D or, simply stated, $C + D$ is an integer. Furthermore, by Lemma 3.2, none of A , B , C or D can be of type 0 or $\frac{1}{2}$. This leaves just three possibilities: $C = D = 1$, $C = D = 1.5$ and, up to symmetry, $C = 1$ while $D = 2$. We combine these three options with the three possibilities: the Coxeter coordinate of sides 2 and 3 are both (x) or are both (x, y) or are (x, y) and (y, x) , respectively. The result is nine cases.

Assume that sides 2 and 3 have the same Coxeter coordinate (x) . Since there is no angle of type 1 in Figure 6 with sides having a single Coxeter coordinate, the options $C = D = 1$ and $C = 1, D = 2$ cannot occur and we have $C = D = 1.5$. Let (y, z) be the Coxeter coordinates of the base (side 4). Drawing such a configuration in Λ , one sees at once that side 1 also has Coxeter coordinates (y, z) and $A = B = 1.5$. If one were to draw the configuration with Coxeter coordinates (y, z) for sides 2 and 3 and Coxeter coordinate (x) for side 4, the result is the same configuration on its side. Hence we consider both cases at the same time. That is we will consider this configuration without specifying which of the pairs of sides 1 and 4 or 2 and 3 is the longer. Without loss of generality we may assume that $y \geq z$; so let $y = p + t$ and $z = p$ where t is a nonnegative integer. The configuration will be acceptable if and only if the refined lengths of the diagonals are greater than the refined lengths of the sides. From Figure 6, that this requirement will be satisfied if and only if $x > t$. In other words, the parallelogram will be an acceptable face if and only if the single coordinate is greater than the difference of the coordinates in the pair. This parallelogram is pictured as Π_1 in Figure 12.

The only case remaining involving fractional angle types can be rotated so that side 1 has Coxeter coordinate (s) , sides 2 and 3 have Coxeter coordinates $(p+r, p)$ and $(p, p+r)$, respectively, and side 4 has Coxeter coordinate (x) . One easily sees that this configuration decomposes into a triangle of type Δ_1 and a parallelogram of type Π_1 from which we conclude that $x = r + s$. In order that the diagonals be longer than the sides, we must have $s > r$ and, in order that the sides are longer than the base, we must have $2p > s$. Thus the condition $2p > s > r$ must be satisfied. The resulting trapezoid is labeled T_1 in Figure 12. There are just four cases remaining: $C = D = 1$ or $C = 1$ while $D = 2$ combined with the Coxeter coordinate of sides 2 and 3 are both (x, y) or are (x, y) and (y, x) .

Assume that $C = D = 1$. Let the Coxeter coordinates of side 2 be (x, y) , the Coxeter coordinates of side 4 be (a, b) and the Coxeter coordinates of side 3 be (u, v) , where (u, v) is (x, y) or (y, x) . From Lemma 3.2, referring to Figure 6, we conclude that $x \leq a \leq u$ and $y \geq b \geq v$. Thus the choice $(u, v) = (x, y)$ results in an equilateral triangle and must be dismissed. So side 3 has coordinates (y, x) and the inequalities $x \leq a \leq y$ and $x \leq b \leq y$. Let $a = x + r$ and $b = x + s$. Since $x + y \geq a + b = 2x + r + s$, we may write $y = x + r + s + t$. It only remains to check whether any of the parameters r, s and t could be 0. Comparing the angle labeled D against $\angle 1a$ and $\angle 1b$ in Figure 6, we see that $s > 0$ and conclude, symmetry,

that $r > 0$. However the option $t = 0$ cannot be discounted. One easily computes the coordinates of side 1 to be (r, s) ; this trapezoid is listed as T_2 in Figure 12.

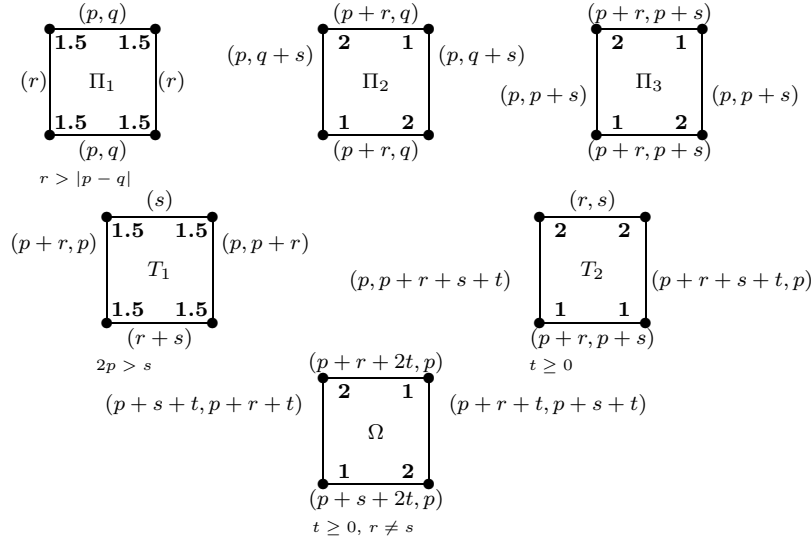


FIGURE 12.

We now assume that $C = 1$, $D = 2$ and sides 2 and 3 have Coxeter coordinates (x, y) . Let (a, b) denote the coordinates of the base, side 4. This configuration is a parallelogram in Λ ; so, side 1 also has coordinates (a, b) , $A = 2$ and $B = 1$. Consulting angles of type 1 in Figure 6, we see that there are just two options for these coordinates resulting in two parallelograms, Π_2 and Π_3 in Figure 12. As with Π_1 , we need not specify which pair of sides is the longer in Π_2 .

We are now down to the last option: $C = 1$, $D = 2$ and sides 2 and 3 have Coxeter coordinates of the form (x, y) and (y, x) , respectively. Using the coordinates from $\angle 1a$, we let sides 2 and 3 have Coxeter coordinates $(a, c+d)$ and $(c+d, a)$ while side 4 has Coxeter coordinates $(a+b, c)$. Since we insist that sides 2 and 3 be the longer sides, we also have $a+c+d \geq a+b+c$ or $d \geq b$. So we replace d by $b+d$; The coordinates of sides 2 and 3 are now $(a, c+b+d)$ and $(c+b+d, a)$. Using these parameters, we compute the coordinates of side 1 to be $(c+2b+d, c)$ and note that angle type A is 2. To insure that side 1 has refined length less than that of sides 2 and 3, we must have that $a > c+b$. At this point we note that, if we permit $b = 0$, we have the case of $\angle 1b$. Thus by permitting $b = 0$, we cover all possibilities. Returning to the inequality $a > c+b$, we let $a = c+b+e$. After substituting this expression for a throughout, we make the following change of variables to get the rather distorted “trapezoid” listed as Ω in Figure 12: $p = c$, $r = d$, $s = e$ and $t = b$. Finally we note that, if we select $r = s$, then we actually have a parallelogram; hence we exclude this possibility. \square

5. The symmetry groups of fullerenes

By a symmetry of a signature we mean a symmetry of the underlying plane graph that maps angles onto angles of the same type and segments onto congruent segments; specifically, if the underlying plane graph symmetry is orientation preserving, all segments must be mapped onto segments with the same Coxeter coordinates while, if the underlying plane graph symmetry is orientation reversing, all Coxeter coordinates must be reversed. Theorem 2 of [6] states that, with one minor exception that does not concern us here, a fullerene and its signature have the same symmetry group. In [4] Fowler and Manolopoulos show that there only 28 fullerene symmetry groups and, therefore, only 28 symmetry groups for the signatures of the fullerenes. In investigating just which signatures are attached to a given symmetry group, it useful to consider which subgroups can occur as vertex, segment and face stabilizers in the symmetry group of the signature of a fullerene.

LEMMA 5.1. *Below is a complete list of the possible vertex, segment and face stabilizers in the symmetry group of the signature of a fullerene.*

- (1) **Vertex stabilizers:** *the identity, the group generated by a single reflection, the rotation group of order 5 or the dihedral group of order 5.*
- (2) **Segment stabilizers:** *the identity, the identity and the half-turn about the center of the segment. and, if Coxeter coordinates of the form (p, p) or (r) , the identity and the reflection through the center of the segment and perpendicular to it, the identity and the reflection through the segment itself, all four of these symmetries.*
- (3) **Face stabilizers:** *the rotation group of order k or the dihedral group of order $2k$ where $k = 1, 2, 3, 6$*

PROOF. Let $\mathcal{S}(\Gamma) = (V, E, F)$ be the signature of a fullerene/geodesic dome and consider the stabilizer of a vertex v . Consider a segment σ of the signature joining v to some other vertex w . Any non trivial rotation in the stabilizer of v must map σ onto some other segment at v with the same Coxeter coordinates. In view of Figure 3, any such rotation must have order 5 and all 5 segments at v with the same Coxeter coordinates as σ must belong to $\mathcal{S}(\Gamma)$. The only reflections which leave v fixed are those which interchange the 5 segments at v with the same Coxeter coordinates as σ and 5 segments at v with the Coxeter coordinates of σ reversed. Hence there are just four possibilities for the stabilizer of a vertex: the identity, the group generated by a single reflection, the rotation group of order 5 or the dihedral group of order 5.

The possible segment stabilizers are the same for all planar graphs: the identity; the 2-element groups containing the identity and one of the reflection with axis containing the segment, the reflection with axis perpendicular to the segment or the half-turn about the center of the segment; the group of order 4 containing all of these. Note, if the segment has Coxeter coordinates (p, q) , with $p \neq q$, then its stabilizer contains no reflections.

Consider a face of $\mathcal{S}(\Gamma)$ that admits a rotation of order k . Then the number of bounding segments is a multiple m of k . Hence we may label the bounding segments cyclically: $\sigma_1, \dots, \sigma_m, \sigma_{m+1}, \dots, \sigma_{2m}, \dots, \sigma_{km}, \sigma_{km+1} = \sigma_1$. Let A_i be the type of the angle formed by σ_i and σ_{i+1} . If necessary, replace the initial the rotation of order k by one of its powers so that it maps σ_1 onto σ_{m+1} . Since σ_1 and σ_{m+1} are congruent, the number of times between σ_1 onto σ_{m+1} that Coxeter coordinates

change between 1 to 2 coordinates must be even. Hence $A_1 + A_2 + \dots + A_m$ must be an integer. We also have that $k(A_1 + A_2 + \dots + A_m) = A_1 + A_2 + \dots + A_{km} = 3mk - 6$. We conclude that $3m - \frac{6}{k}$ must be an integer and k divides 6. \square

6. Atoms and areas

We wish to compute the number of atoms in a fullerene which is also the number of faces in the dual geodesic dome. Assuming all faces of Λ have area 1, it is also the total area of the geodesic dome. So, we start with a set of area formulas for large triangles. These are easy to compute using simple geometric arguments in Λ . In Table 1, we list the formulas for the areas of triangles having sides σ and τ with Coxeter coordinates (p, q) and (r, s) or (r) , respectively, forming a clockwise angle from σ to τ of type A .

TABLE 1.

$A = 1$	$(p + q)(r + s) - ps$	$=$	$pr + qr + qs$
$A = 1.5$	$(p + q)r$	$=$	$pr + qr$
$A = 2$	$(p + q)(r + s) - qr$	$=$	$pr + ps + qs$
$A = 2.5$	$p(q + r)$	$=$	$pq + pr$
$A = 3$	$ps - qr$		

To compute the area of any face, we triangulate that face and add the areas of the triangles in the decomposition; the results are listed in Table 2.

7. Constructing the catalog

7.1. Icosahedral symmetry. These fullerenes were characterized by Coxeter [2]. In our catalog, they are grouped into three families labeled \mathcal{A}_1 and \mathcal{A}_2 with symmetry group I_h and \mathcal{A}_3 with symmetry group I . If the symmetry group of a signature admits no reflections, as in the case \mathcal{A}_3 , the catalog entry represents the signature presented and its reflection.

7.2. Tetrahedral symmetry. By Lemma 5.1, the center of a rotation of order 3 must be a face: a triangle, a hexagon, a nonagon or a dodecagon. Actually, the axis of a rotation of order 3 must join the centers of two such faces. In sorting out the possibilities, the following formula is helpful:

$$(7.1) \quad \sum_{i=3}^{\infty} (i - 2)f_i = 20,$$

where f_i is the number of faces that are i -gons. This formula is obtained by combining the formula for the total number of faces, $\sum_{i=3}^{\infty} f_i = f$, the formula for twice the number of segments, $\sum_{i=3}^{\infty} if_i = 2e$ and Euler's formula, $v - e + f = 2$, with $v = 12$.

Signatures of fullerenes with tetrahedral symmetry must have four distinct axes of order 3 rotations; giving rise to eight distinct faces admitting rotations of order 3. From the above formula, it is clear that all eight faces cannot be hexagonal, nonagonal and dodecagonal. Hence one 3-rotation must be centered in a triangle. But each axis of rotation can be transformed onto any other. Hence each axis of rotation must have at least one triangular face. Thus our graph has at least 4 triangular faces and 4 k -gons as faces where $k = 3, 6, 9, 12$. The cases $k = 9$ and 12

TABLE 2.

Δ_1	$a = 2pr + r^2$
Δ_2	$a = 3p^2 + 2pr$
Δ_3	$a = 3p^2 + 3pr + r^2$
Δ_4	$a = 3p^2 + 3pr + r^2$
Δ_5	$a = 3p^2$
Δ_6	$a = r^2$
K_1	$a = 2r^2 + s^2 + 3rs + 2p(r + s)$
K_2	$a = 2q^2 + r^2 + s^2 + 3qr + 3qs + 2rs + 2p(q + r + s)$
K_3	$a = 2p^2 + 2q^2 + r^2 + s^2 + 2pq + 2pr + 3ps + 3qr + 2qs + 2rs$
K_4	$a = 6p^2 + r^2 + 2s^2 + 5pr + 6ps + 3rs$
K_5	$a = 2p^2 + q^2 + r^2 + 3pq + 2pr2qr$
K_6	$a = 2p^2 + q^2 + 3pq$
K_7	$a = 3p^2 + 2r^2 + s^2 + 5pr + 3ps + 3rs$
K_8	$a = 2p^2 + q^2 + r^2 + 3pq + 3pr + 2qr$
K_9	$a = 2p^2 + q^2 + r^2 + s^2 + 3pq + 3pr + 2ps + 2qr + qs + 2rs$
K_{10}	$a = p^2 + q^2 + 2pq$
K_{11}	$a = 4p^2 + r^2 + s^2 + 4pr + 4ps + 2rs$
K_{12}	$a = 6p^2 + 2r^2 + 8pr + 2s(p + r)$
K_{13}	$a = 6p^2 + 2r^2 + r^2 + 5s^2 + 8pr + 11ps + 7rs + 2t(p + r + s)$
K_{14}	$a = 5p^2 + 2q^2 + 7pq + 2t(p + q)$
K_{15}	$a = 5p^2 + 3q^2 + 2r^2 + 8pq + 7pr + 6qr + 2t(p + q + r)$
K_{16}	$a = 2p^2 + 2pq$
K_{17}	$a = 4p^2 + 2r^2 + 6pr + 2t(p + r)$
K_{18}	$a = 2p^2 + 2r^2 + s^2 + t^2 + 8pr + 5ps + 5pt + 3rs + 3rt + 2st$
Π_1	$a = 2r(p + q)$
Π_2	$a = 2(p^2 + q^2 + pq + pr + ps + qr + qs + rs)$
Π_3	$a = 2(3p^2 + s^2 + 2pr + 3ps + rs)$
T_1	$a = r^2 + 2pr + 4ps + 2rs)$
T_2	$a = 3p^2 + 2r^2 + 2s^2 + 5pr + 5ps + 2pt + 4rs + 2rt + 2st)$
Ω	$a = 6p^2 + r^2 + s^2 + 8t^2 + 5pr + 5ps + 14pt + 2rs + 6rt + 6st)$

are immediately excluded by the above formula. And, if $k = 6$, the formula tells us that the graph has exactly 4 triangular and 4 hexagonal faces. It is easy to check that there is only one such graph on 12 vertices with tetrahedral symmetry, the truncated tetrahedron. It is pictured in Figure 13 as graph C .

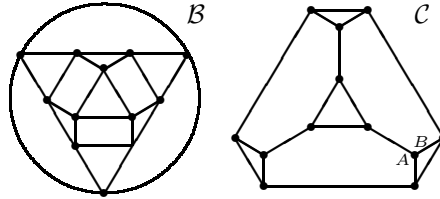


FIGURE 13.

The only other option is that all faces admitting an order 3 rotation are triangles. So, in this case we have at least 8 triangular faces. One possibility is that all

faces are triangular and we have the icosahedron. If there are face which are not triangles these must be permuted by these rotations of order three. It is not too difficult to see that, if there is a k -face, then it cannot share segments with both of the triangles containing the center of a rotation. It follows that there are at least 6 k -faces. Thus, by the above formula, the only other option is a plane graph with 8 triangular faces and 6 quadrilateral faces. Again, it is easy to check that there is only one such graph on 12 vertices with tetrahedral symmetry, the cuboctahedron. It is pictured in Figure 13 as graph B .

We start by considering signatures based on the icosahedron. If the signature admits rotations of order 3 about two faces sharing a common segment, it follows easily that it admits rotations of order 3 about each face resulting in an icosahedral group. Since the icosahedron does not have 8 faces no two of which share a vertex, we must have two faces sharing a vertex (but not an segment) both of which contain a center of rotation of order 3. These two faces must be equilateral triangles. Since the common vertex has degree 5 there must be one triangle that shares an segment with each of these. Once the Coxeter coordinates of that triangle are identified, the Coxeter coordinates of the remaining segments of the two triangular centers of rotation can be filled in and then, by symmetry, the Coxeter coordinates of all segments are forced. This connecting triangle must be of one of the six types listed in Figure 4. However, this connecting triangle cannot have the same Coxeter coordinates assigned to all of its segments as that would result in a signature with Icosahedral symmetry. Thus, triangles Δ_1 and Δ_2 are the only ones we can use here. Each has three orientations giving six possibilities. Four of these choices are pictured in Figure 14; the remaining two cases are obtained by reflecting each of the last two selections in the figure.

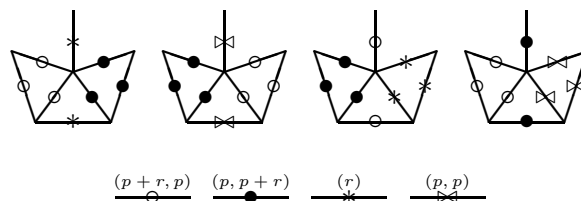


FIGURE 14.

Since the first two pictures admit the reflection through their central vertical axes and since these reflections extend to reflections of the entire signature, the symmetry group of the resulting signature is either T_h or T_d . The signatures corresponding to the first and second pictures in the figure are labeled \mathcal{A}_8 and \mathcal{A}_9 in the catalog. Once the signature is constructed, one easily checks that their common symmetry group is T_h . The third and fourth choices and their reflections do not admit opposite symmetries and have symmetry group T . The reflection of the third is recorded as \mathcal{A}_{10} and reflection of the fourth is recorded as \mathcal{A}_{11} in the catalog.

Next, we turn our attention to the cuboctahedron, graph \mathcal{B} . This graph has 48 symmetries many of which cannot be a symmetry of the signature of a fullerene. In particular, we have seen that the rotations of order 4 about the centers of opposite quadrilaterals cannot be a symmetry of the signature of a fullerene. The subgroup of direct symmetries will be T only if the rotations of order 3 about axes through

the centers of opposite triangles and the rotations of order 2 about axes through the centers of opposite quadrilaterals belong to the symmetry group. Thus the triangles must be equilateral and the quadrilaterals must be parallelograms. It follows that the entire structure of the signature is determined once the parallelogram is selected. All possible parallelogram faces are pictured in Figure 12.

Parallelogram Π_2 admits reflections through the diagonal of the parallelogram when $p = q$ and $r = s$; this signature family is labeled \mathcal{B}_1 and has symmetry group T_h . Parallelogram Π_1 with $p = q$ admits reflections through the sides of the parallelogram; the resulting signature, listed as \mathcal{B}_2 , has T_d as symmetry group. The remaining cases, Π_2 with $p \neq q$ or $r \neq s$, Π_1 with $p \neq q$ and Π_3 all yield signatures with T as symmetry group. The first option is split into two cases: $q > p$ and $q = p$ with $s > r$; with a change of variables, these yield signatures \mathcal{B}_3 and \mathcal{B}_4 respectively. The remaining two cases are listed in the catalog as \mathcal{B}_5 and \mathcal{B}_6 respectively.

Finally, we consider the truncated tetrahedron, \mathcal{C} . The symmetry group of this graph is T_d . Its rotational subgroup T has the obvious two segment orbits and three angle orbits. Since the triangles must be equilateral their angles must all have type 1. So a signature will be determined by assigning Coxeter coordinates to the segments in each of these two segment orbits and by selecting the two angle types labeled A and B in Figure 13. Since the sum of the angle types at a vertex is 5, $A + B = 4$. If the symmetry group is T_d , all of the segments must have Coxeter coordinates of the form (p, p) or (r) and $A = B = 2$. This gives two families \mathcal{C}_1 and \mathcal{C}_2 in the catalog. The remaining possible labelings all yield a signatures with symmetry group T . When $A = B = 2$, we must choose Coxeter coordinates to destroy the reflective symmetry. This cannot be done with single Coxeter coordinates; but, it can be done in two different ways with pairs of Coxeter coordinates, \mathcal{C}_3 and \mathcal{C}_4 . In constructing the remaining signatures, the only restrictions on the coordinates are those necessary to force the chords of the hexagonal faces to be too long be included in the signature, i.e. the restrictions listed in Figure 6. The result is seven more families based on the graph \mathcal{C} . The choices, conditions and catalog names are pictured in Figure 15.

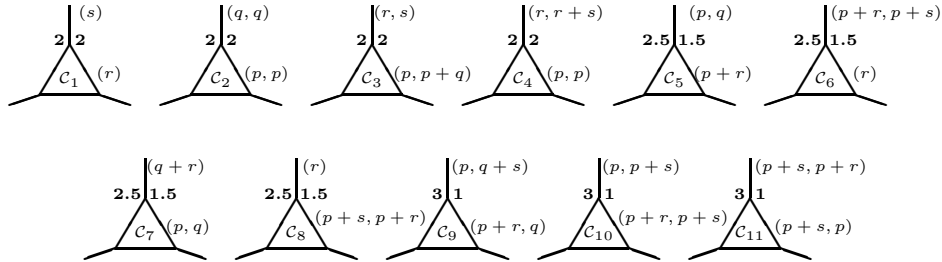


FIGURE 15.

7.3. Signatures admitting rotations of order 5 or 6. Let $\mathcal{S}(\Gamma) = (V, E, F)$ be the signature of a geodesic dome/fullerene and assume that $\text{Aut}(\mathcal{S}(\Gamma))$ admits a rotation of order 5. As stated in Lemma 5.1, this rotation must belong to the stabilizer of a vertex v . Let σ_0 be the of the segment joining v to some other vertex w_0 and let σ_i and w_i , for $i = 1, \dots, 4$, be the images of σ_0 and w_0 under i iterations

of this rotation. Without loss of generality we may assume that σ_i and w_i are in order clockwise around v . Now suppose that τ is any other segment with v as endpoint; we may assume that τ lies between σ_0 and σ_1 . By Lemma 3.2i, we have that τ cannot make an angle of type $\frac{1}{2}$ with either σ_0 or σ_1 and can make an angle of type 0 with one of them only if it is congruent to them, i.e. only if the Coxeter coordinates of τ are the reverse of the Coxeter coordinates of σ_0 . In this case, the images of τ under the rotation also belong to the signature. We conclude that v has degree 5 or 10.

By including “construction” segments, we may give a parallel treatment for the classification of signatures admitting rotations of order 6. The center of a rotation of order 6 must be the center of a face. Since the rotations of Λ of order 6 all are centered at vertices, we may add a vertex, v , of degree 6 to the signature $\mathcal{S}(\Gamma)$ at the center of the center of the rotation. As above, let σ_0 be the of the segment joining v to a vertex w_0 on the bounding circuit of the face and closest to the center v ; let σ_i and w_i , for $i = 1, \dots, 5$, be the images of σ_0 and w_0 under i iterations of this rotation. Without loss of generality we may assume that σ_i and w_i are in order clockwise around v . Now suppose that τ is the segment joining v to some other vertex on the boundary of the face and that τ has the same refined length as the σ_i . Then τ is congruent to the σ_i and we add to the signature the images of τ under the rotation. Thus the added vertex v , has degree 6 or 12.

7.3.1. *Rotation of order 5 with v of degree 10.* We have accounted for 11 of the vertices and the 12th can only be the other center v' of the rotation. This signature appears as family \mathcal{G}_1 in the catalog and has symmetry group D_{5h} .

7.3.2. *Rotation of order 6 with v of degree 12.* In this case, the face containing the center of rotation is a 12-gon. Furthermore, all of the vertices are equidistant from the center of the face. This is possible only if we have the configuration in Λ similar to the configuration in Figure 3 but with a vertex of degree 12 at the center. Deleting the construction vertex and segments, we have that the signature consists of a 12-gon with the Coxeter coordinates of the segments alternating between (r) and (p, p) around the faces and with each angle labeled $2\frac{1}{2}$. The symmetry group of this signature is D_{6d} : As a 12-circuit with alternately labeled segments it has the dihedral group of order 12 as its symmetry group. But as a plane graph with two distinct faces, each symmetry of the 12-circuit corresponds to two symmetries of the plane graph. For example the identity and the reflection through the circuit (interchanging the faces) leave the circuit fixed. Similarly, the half-turns about lines joining the centers of opposite segments interchanges the two faces while the reflection with this axis does not. This signature is listed as \mathcal{D}_1 in the catalog.

From now on we assume that v , as well as the other center of the rotation v' , has degree 5 (or 6) and that $\sigma_0, \dots, \sigma_4, (\sigma_5)$ have the same Coxeter coordinates. The segments τ_i joining w_i to w_{i+1} , indices read mod 5 (or mod 6), could belong to the signature. If they do not, we add them as construction segments. Thus v is surrounded by 5 (or 6) equilateral triangles. We note that no vertex of the signature could lie inside or on the bounding segments of these triangles as such vertices would be closer to v than the w_i . Now let w'_0 be one of the remaining vertices that is closest to w_0 and hence joined to it by a segment γ_0 . Let $w'_1, \dots, w'_4, (w'_5)$ and $\gamma_1, \dots, \gamma_4, (\gamma_5)$ denote the images of w'_0 and γ_0 under the rotation. Let A and B denote the types of the angles between γ_i and both τ_{i-1} and τ_i . See the left hand drawing in Figure 16. Since the triangles are equilateral, their angle types are

all 1. Thus, the sum of the angle types at the vertex w_i is $A + B + 2 = 5$ giving $A + B = 3$. From this, we conclude that $w'_1, \dots, w'_4, (w'_5)$ are indeed distinct and that γ_i, τ_{i-1} and γ_{i-1} are three sides of a parallelogram. Let τ'_{i-1} denote the fourth side. Now $\tau'_0, \dots, \tau'_4, (\tau'_5)$ form a regular pentagon (hexagon) mapped onto itself by the rotation. Thus, its center is fixed by the rotation and must be v' . Let σ'_i denote the segment of the signature (or the construction segment) joining v' to w'_i , for all i . Since the triangles at v' must be equilateral and, since τ'_i and τ_i are opposite sides of a parallelogram, all of the $\sigma_i, \sigma'_i, \tau_i$ and τ'_i have the same Coxeter coordinates. Finally, let δ_0 denote shorter diagonal of the $\gamma_1, \tau_0, \gamma_0, \tau'_0$ parallelogram (arbitrarily choose one, if the diagonals have equal length) then fill in the δ_i by rotating δ_0 . Note that choosing the other diagonal yields the same graph but with the γ and δ labels interchanged. Also note that this graph is a triangulation and the shortest distances between the vertices are all represented by segments in this triangulation.

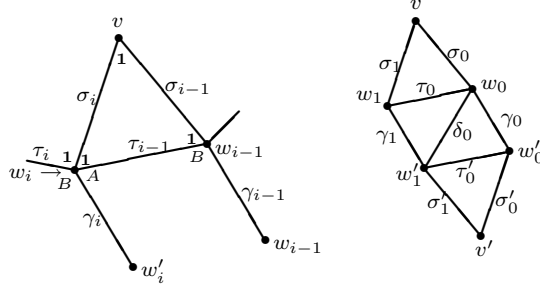


FIGURE 16.

On the right in Figure 16, we have pictured one “wedge” joining v and v' . The entire triangulation consists of 5 or 6 of these wedges glued together to form a sphere. Once we decide which segments in one of the wedges actually belong to the signature, we can simply rotate those segments to get the signature. By the way that we constructed this “super signature,” we know that the σ_i and the σ'_i always belong in the case of a rotation of order 5 and never belong in the case of a rotation of order 6 and we know that the γ_i always belong. Applying Lemma 1.3(1), we see that there are only three possibilities: the τ_i, τ'_i and δ_i all belong; the τ_i and τ'_i belong, but not the δ_i ; the δ_i belong, but not the τ_i and τ'_i . In all three cases, we note that the half-turn about the centers of the parallelograms must also belong to the symmetry group.

7.3.3. *The τ_i, τ'_i and δ_i all belong.* In this case, when the rotation has order 5, the underlying graph is the icosahedron and, when the rotation has order 6, the underlying plane graph is graph \mathcal{F} pictured in Figure 17. The symmetry group of graph \mathcal{F} is D_{6d} and the subgroup of the icosahedral group which fix or interchange the vertices v and v' is D_{5d} . For both graphs, the entire signature is forced once the triangle with sides τ_0, δ_0 and γ_1 has been identified. To do this we select a triangle from Figure 4 and select an orientation. If we select Δ_1 and orient it so that τ_0 is its base, the resulting signature admits reflections resulting in symmetry group D_{6d} or D_{5d} . These signatures are listed as \mathcal{F}_4 and \mathcal{A}_4 the other two orientations result in signatures that do not admit reflections but are reflections of one another: signatures \mathcal{F}_6 and \mathcal{A}_6 with symmetry groups D_6 and D_5 , respectively. Similarly,

triangle Δ_2 gives \mathcal{F}_5 with symmetry group D_{6d} , \mathcal{A}_5 with symmetry group D_{5d} , \mathcal{F}_7 with symmetry group D_6 and \mathcal{A}_7 with symmetry group D_5 . Triangles Δ_3 through Δ_6 result in icosahedral symmetry in the case of a 5-fold rotation. However, In the case of the rotation of order 6, filling in graph \mathcal{F} with Δ_3 and Δ_4 give signatures without reflective symmetries that reflect into one another. They are denoted by \mathcal{F}_3 under the group D_6 . Δ_5 and Δ_6 give distinct signatures with group D_{6d} and they are listed as \mathcal{F}_2 and \mathcal{F}_1 in the catalog.

7.3.4. *The τ_i and τ'_i belong, but not the δ_i .* If δ_0 does not belong to the signature $\mathcal{S}(\Gamma)$, the face bounded by the segments $\tau_0, \gamma_0, \tau'_0$ and γ_1 must be a parallelogram. The options are listed in Figure 12. If we are considering rotations of order 6, the underlying graph is labeled \mathcal{E} in Figure 17; if we are considering rotations of order 5, the underlying graph is the one labeled \mathcal{H} . The symmetry group of the graph \mathcal{E} is D_{6h} ; the symmetry group of \mathcal{H} is D_{5h} . We only get the full symmetry groups when the parallelogram admits reflections through its sides and the only parallelogram admitting such reflection is Π_1 with $p = q$. The two orientations of this parallelogram yield Families \mathcal{E}_1 and \mathcal{E}_2 with symmetry group D_{6h} and Families \mathcal{H}_1 and \mathcal{H}_2 with symmetry group D_{5h} . The parallelogram Π_2 has the same form in either orientation; the corresponding families are recorded as \mathcal{E}_3 and \mathcal{H}_3 with symmetry groups D_6 and D_5 , respectively. The two orientations of parallelogram Π_3 yield \mathcal{E}_4 and \mathcal{E}_5 , with symmetry group D_6 , and \mathcal{H}_4 and \mathcal{H}_5 , with symmetry group D_5 . Finally, the two orientations of parallelogram Π_1 with $q > p$ yield \mathcal{E}_6 and \mathcal{E}_7 , with symmetry group D_6 , and \mathcal{H}_6 and \mathcal{H}_7 , with symmetry group D_5 .

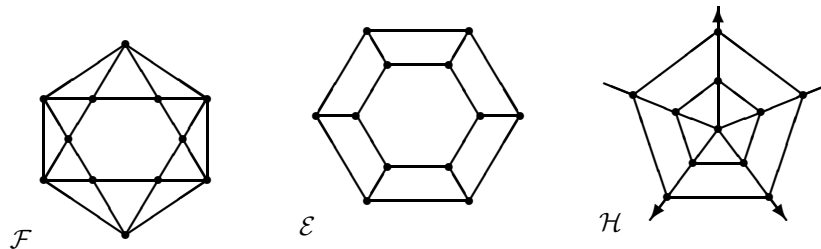


FIGURE 17.

7.3.5. *The δ_i belong, but not τ_i and τ'_i .* With τ_i and τ'_i deleted, we have kites as pictured on the left in Figure 18. The 5 (or 6) kites about v dovetail with the 5 (or 6) kites about v' . In the case of a rotation of order 5, the signature graph is a new

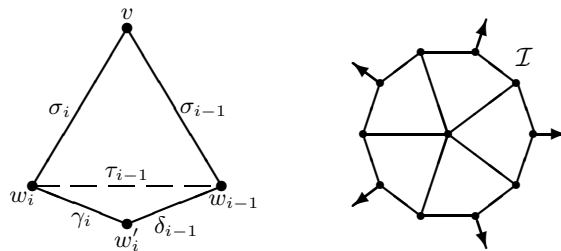


FIGURE 18.

graph labeled \mathcal{I} and pictured on the right in Figure 18. In the case of a rotation of order 6, the constructions and vertices are deleted leaving a dodecagon. Referring to Figure 10, we have that kites K_3 through K_{11} give rise to these signatures. In the case of a rotation of order 6, we are able to coalesce two of the cases. The resulting signatures are listed in the Table 3.

TABLE 3.

<i>Kite</i>	<i>Conditions</i>	D_6	D_5
K_3	$p = q, r = s$	\mathcal{D}_2	\mathcal{I}_1
K_8	$r = q$	\mathcal{D}_3	\mathcal{I}_2
K_{10}	$p = q$	\mathcal{D}_4	\mathcal{I}_3
K_3	$q > p$	\mathcal{D}_5	\mathcal{I}_4
K_3	$q = p \ \& \ s > r$	\mathcal{D}_6	\mathcal{I}_5
K_4		\mathcal{D}_7	\mathcal{I}_6
K_5		\mathcal{D}_8	\mathcal{I}_7
K_6		"	\mathcal{I}_8
K_7		\mathcal{D}_9	\mathcal{I}_9
K_8	$r \neq q$	\mathcal{D}_{10}	\mathcal{I}_{10}
K_9		\mathcal{D}_{12}	\mathcal{I}_{11}
K_{10}	$p \neq q$	\mathcal{D}_{12}	\mathcal{I}_{12}
K_{11}		\mathcal{D}_{13}	\mathcal{I}_{13}

7.4. Signatures with symmetry group D_{3d} or D_{3h} . Let Γ have symmetry group D_{3d} or D_{3h} . Then G , the dihedral group of order 6, is a subgroup the symmetry group of $\mathcal{S}(\Gamma)$. The orbits of this subgroup acting on the vertex set of $\mathcal{S}(\Gamma)$ consist of either three or six vertices. Hence we either have four orbits of three vertices each, two orbits of six vertices each or two orbits of three vertices each and one orbit of six vertices. By Lemma 5.1, the rotation of order 3 three must be about the center of a face. Let u and u' denote the two face centers on the axis of rotation. Note that the entire symmetry group is generated by the dihedral subgroup G and one reflection that interchanges u and u' . If that reflection is the reflection through the plane that is the perpendicular bisector of the segment uu' , we have D_{3h} ; if it is the reflection through the midpoint of this segment, we have D_{3d} . Thus, once we work out the structure in the ‘‘northern hemisphere’’, the structure in ‘‘southern hemisphere’’ will be the same. Furthermore, the relative position of the two hemispheres will determine whether the signature has symmetry group D_{3d} or D_{3h} .

We start by considering the case of four orbits. Let v_1, v_2 and v_3 be the vertices of the orbit that is closest to u ; if two orbits have their vertices equally close to u , arbitrarily select one. Let w_1, w_2 and w_3 be the vertices of the next closest orbit. The v 's may be connected to the w 's in just two basic ways forming the two ‘‘caps’’ C_1 and C_2 pictured in Figure 19. In order to maintain dihedral symmetry, the angle types in cap C_1 are determined and there just two choices for the Coxeter coordinates of the segments leading to caps C_{1a} and C_{1b} in Figure 20. The angles are fixed in cap C_2 once the angle type A is identified. There are six options that admit dihedral symmetry, C_{2a} and C_{2f} in Figure 20. Two options that are not included are variations on C_{2f} : regular hexagons with Coxeter coordinate (x, x) or

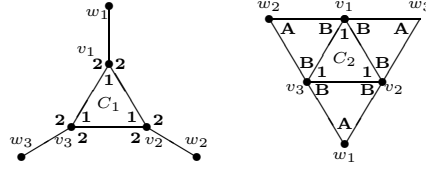


FIGURE 19.

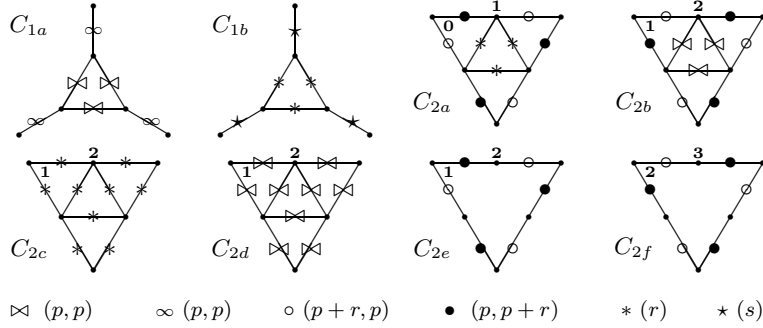


FIGURE 20.

(x). These admit a rotation of order six which cannot be removed by connecting the caps.

First we consider signatures with D_{3h} symmetry. To produce such a signature from a cap, we reflect it through the equatorial plane and connect nearest neighbors by segments with Coxeter coordinates that reflect into themselves. Caps C_{1a} and C_{1b} yield signatures \mathcal{J}_1 and \mathcal{J}_2 , respectively. Caps C_{2a} through C_{2d} yield signatures \mathcal{K}_1 through \mathcal{K}_4 , respectively. Cap C_{2e} gives signature \mathcal{L}_1 and cap C_{2f} gives signature \mathcal{E}_8 .

We turn now to signatures made from these caps but having D_{3d} as symmetry group. Reflecting C_{1a} or C_{1b} through the center of the sphere and connecting nearest neighbors result in graphs with two triangular faces at the poles and six interlocking pentagonal faces around the equator. Typical pentagonal faces are pictured in Figure 21. The two segments making the angle labeled A (or B) must reflect into one another; hence, angle types A and B must be integers. Clearly, $A \neq 0$. If $A = 1$, then the coordinates of the segments $\{w_1, w'_3\}$ and $\{w_2, w'_3\}$ must be $(p, r + s)$ and $(r + s, p)$, respectively. This signature is listed as \mathcal{P}_1 . Note that the segment joining v_1 and v_2 will belong to the signature only if $r \leq s$. When $A = 2$, then the coordinates of the segments $\{w_1, w'_3\}$ and $\{w_2, w'_3\}$ must be simply $(r + s)$ giving signature \mathcal{P}_2 . Again, the segment joining v_1 and v_2 will belong to the signature as long as $r \leq s$. Let $A = 3$; then the angles at w_1 and w_2 have type 1. By assumption, the segment joining v_1 and w_1 has length less than or equal to the length of the segment joining v_1 and w'_3 . However, equality would result in an icosahedral signature with all coordinates equal to (s, s) ; so, we conclude that the segment joining v_1 and w'_3 cannot belong to the signature. Referring then to $\angle 1a$ and $\angle 1b$ in Figure 6 and using a bit of algebra, we may relabel the segments so that the segment from w_1 to w'_3 has coordinates $(p + r + s, p)$, the segment from v_1 to w_1 has coordinates $(p + s, p + s)$ and the segment from v_1 to v_2 has coordinates

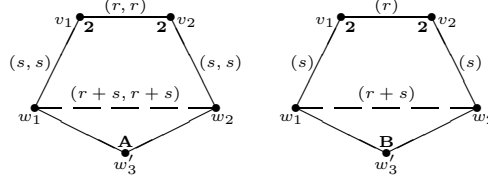


FIGURE 21.

$(p+r, p+r)$. The latter segment will belong only if $r \leq s$. This case is recorded as \mathcal{P}_3 .

Turning to the second cap, we can let $B = 0$. Then the coordinates of the segments $\{w_1, w'_3\}$ and $\{w_2, w'_3\}$ must be $(p, p+r+s)$ and $(p+r+s, p)$, respectively, and we have signature \mathcal{P}_4 . If $B = 1$, then the coordinates of the segments $\{w_1, w'_3\}$ and $\{w_2, w'_3\}$ must be simply $(r+s)$ and we have signature \mathcal{P}_5 . Assume that $B = 2$ and let the segments $\{w_1, w'_3\}$ and $\{w_2, w'_3\}$ have coordinates (p, q) and (q, p) , respectively. We then have the equality $p+2q = r+s$. In order to avoid this rather complicated equality, we split it apart into three cases: $s \geq 2q$, $2q > s \geq q$ and $q > s$. In the first case, we replace s with $2q+t$, where t can take on the value 0. It then follows that $p = r+t$. This case, with a change of variables, yields signature \mathcal{P}_6 . Next, we replace s by $x+2t$ and q by $x+t$, where again $t = 0$ is a possibility. In this case, $r = p+x$. Replacing x by the now free s and t by the now free r , we have \mathcal{P}_7 . Finally, we let $q = s+t$. Then $r = p+s+2t$. In this case, the segments joining the v 's won't belong to the signature which is recorded as \mathcal{Q}_1 , with t replaced by r .

Reflecting C_2 through the center of the sphere and connecting nearest neighbors results in a graph with eight triangular faces, four around each center of rotation, and six interlocking kites around the equator. The kites must have bilateral symmetry. Consulting Figure 10, we identify the candidates as: kite K_2 with $r = s$; kite K_8 with $r = q$; kite K_{12} (has K_3 with $q = p$ and $r = s$ as a special case); kite K_{16} (has K_{10} with $q = p$ as a special case); ; kite K_{18} with $s = t$. Since kites that are also parallelograms are listed among the parallelograms, we check Figure 12 and include Π_2 with $q = p$ and $r = s$; this is the same as kite K_{12} with $t = 0$. In Figure 22, we have drawn three of the interlocking kites and labeled the angle types A, B, C and D . There two equations that must be satisfied: the sum around a quadrilateral face must be 6 ($A+2B+C=6$) while the sum around a vertex must be 5 ($D+2B+C=6$). We conclude that $A = D+1$. From this equation the options available for the faces we see that the possible values $A = 1, 2$, $B = 1, 1.5, 2$, $C = 0, 1, 2$ and $D = 0, 1$.

We next turn to the case of two orbits of three vertices each connected to a central orbit of six vertices. The six vertices of the central orbit must form a hexagon that is mapped into itself by the reflections through the centers of opposite segments. Hence, the coordinates of the segments are either of the form (p, p) or (r) and all of the angles have the same type. But this hexagon is also mapped into itself by the reflection through the plane of the hexagon or the reflection through the center of the hexagon. In either case types of the angles inside the hexagon must be the same as the types of the angles outside. Hence all angle types are 2.5 and the coordinates of the segments alternate between (p, p) and (r) . It then follows that

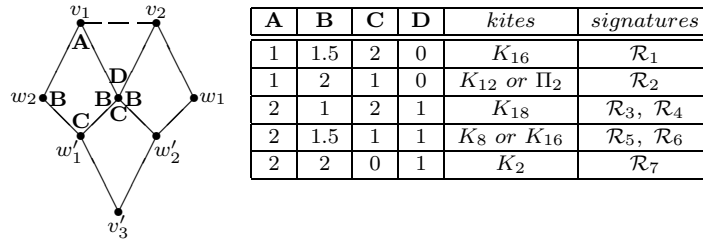


FIGURE 22.

this hexagon is not mapped into itself by the reflection through its center. Thus, this configuration will always have D_{3h} as symmetry group.

The orbit of three vertices on one side of this central circuit can be connected to it in basically only one way. We have pictured this in Figure 23. The signature is completed by reflection the v 's and the segments connecting them through the plane of the outer circuit. Referring to Figure 23, we note that there are four equations among the angle types: $A + 2C = 3$, $A + 2B = 4$, $C + D = 2.5$ and $2B + 2D = 6$. Since A must be an integer less than or equal to 3, we have just the four solutions listed in the table includes in the figure. Depending on these angle types the segments labeled x, y and z and their images may or may not belong to the signature; and, when $A \geq 2$, the segments joining v_i and v'_i may belong.

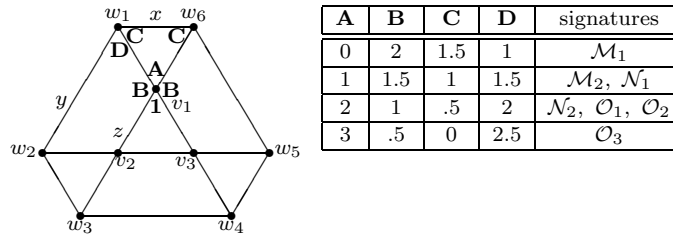


FIGURE 23.

Consider first the case $A = 0$. In this case, the triangle with apex v_1 and base on the hexagon is Δ_1 and we may assign Coxeter coordinates $(p, p + r)$ and $(p + r, p)$ to its sides in the obvious way and (r) to its base - which does belong to the signature. The side the quadrilaterals also have coordinates $(p, p + r)$ and $(p + r, p)$; segment z then has coordinates (s, s) and y has coordinates $(p + s, p + s)$. If $r \geq 2s$, segment y belongs to the signature and the quadrilaterals are trapezoids with prototype T_2 ; if $r < 2s$, segment y does not belong to the signature. These two options are recorded as the single signature \mathcal{M}_1 in the catalog.

Consider $A = 1$ next. This has two subcases. First, assume the triangle with apex v_1 and base on the hexagon is Δ_2 or Δ_5 and we assign Coxeter coordinates $(p, p + r)$ and $(p + r, p)$ to its sides in the obvious way and (p, p) to its base, noting that $r = 0$ is a possibility. The sides the quadrilaterals also have coordinates $(p, p + r)$ and $(p + r, p)$; segment z then has coordinate (s) and y has coordinates $(r + s)$. If $s < 2p$, segment y belongs to the signature; and the quadrilaterals are

trapezoids with prototype T_1 ; if $s \geq 2p$, segment y does not belong to the signature. These two options are recorded as the single signature \mathcal{M}_2 in the catalog. Next suppose that the triangle with apex at v_1 is equilateral with sides having Coxeter coordinates (r) . Then both segments y and z have coordinates (p, p) and must belong to the signature. This signature is recorded as \mathcal{M}_3 in the catalog. Now assume the triangle with apex v_1 and base on the hexagon is not a face, i.e. x does not belong. Then the Coxeter coordinates of its sides are $(p, p+r)$ and $(p+r, p)$ in the reverse order and its, not included, base has coordinates $(p+r, p+r)$. The side the quadrilaterals also have coordinates $(p, p+r)$ and $(p+r, p)$; segment z then has coordinate $(r+s)$ and y has coordinates (s) . If $s < 2p$, segment z belongs to the signature; and the quadrilaterals are trapezoids with prototype T_1 ; if $s \geq 2p$, segment z does not belong to the signature. These two options are recorded as the single signature \mathcal{N}_1 in the catalog.

Next assume $A = 2$. Clearly, x does not belong to the signature; but the segment joining v_1 and v'_1 could belong. If we let the v_1, w_1 -segment have coordinates $(p+r, p)$, then the v_1, v'_1 -segment won't belong. If we let y have coordinates (s, s) , z will have coordinates $(p+s, p+s)$. This give signature \mathcal{N}_2 and z will not belong if $2s > r$. Now let the v_1, w_1 -segment have coordinates $(p+r, p)$, where $r = 0$ is a possibility. Then the v_1, v'_1 -segment will belong to the signature and have Coxeter coordinates (p, p) . If we let y have coordinates (s, s) , z will have coordinates $(p+r+s, p+r+s)$ and will not belong. The result is signature \mathcal{O}_1 . The next possibility to consider is assigning the coordinate (r) to the segments joining the $v's$ and $w's$ and (s) to segment y ; this is recorded as \mathcal{O}_2 . Finally, let $A = 3$. Then $C = 0$ and the v_1, w_1 -segment must have coordinates $(p+r, p)$. Then the v_1, v'_1 -segment will belong to the signature and have Coxeter coordinates (r) . We let y have coordinate (s) and note that z will not belong to this signature, \mathcal{O}_3 .

The last configuration to consider is the one in which we have two orbits of six vertices each. Again the reflections through the centers of the segments of the hexagon associated with an orbit must be symmetries of the signature and force the angles to be equal and the segments to have coordinates of the form (p, p) or (r) . Since this hexagon can be drawn in Λ , all of the angles are of type 2. It follows that the coordinates of the segments alternate between (p, p) and $(p+r, p+r)$, cap C_a , or between (r) and $(r+s)$, cap C_b . (If all coordinates were the same, the orbit admits a rotation of order 6 that cannot be destroyed by connecting the two orbits.) If we reflect cap C_a through the equatorial plane, the nearest neighbors are joined by a segment with coordinate (s) and we have signature \mathcal{E}_9 ; if we reflect cap C_b through the equatorial plane, the nearest neighbors are joined by a segment with coordinate (p, p) and we have signature \mathcal{E}_{10} .

If we reflect cap C_a through the center of the sphere, the nearest neighbors are joined by a segment with coordinates (q, r) and (r, q) consistent with trapezoid T_2 . If $q \geq 2p+r$, we do have trapezoidal faces, if $q < 2p+r$, the segments with coordinates $(p+r, p+r)$ do not belong to the signature. Both possibilities are represented in signature \mathcal{E}_{11} . If we reflect cap C_b through the center of the sphere, the nearest neighbors may be joined by a segment with coordinates $(p, p+r)$ and $(p+r, p)$ consistent with trapezoid T_1 . If $2p > s$, we do have trapezoidal faces, if $2p \leq s$, the segments with coordinate $(r+s)$ do not belong to the signature. Both possibilities are represented in signature \mathcal{E}_{12} . The remaining possibility is when

nearest neighbors are joined by segments with coordinate (r) - letting $p = 0$ in the previous case. The resulting signature is recorded as \mathcal{D}_{14} .

References

- [1] D. L. D. Caspar and A. Klug, *Viruses, nucleic acids and cancer*, 17th Anderson Symposium, Williams & Wilkins, Baltimore, 1963.
- [2] H. S. M. Coxeter, Virus macromolecules and geodesic domes, in (J. C. Butcher, ed.), *A Spectrum of Mathematics*, Oxford Univ. Press, 1971, 98–107.
- [3] P. W. Fowler, J. E. Cremona, and J. I. Steer, Systematics of bonding in non-icosahedral carbon clusters, *Theor. Chim. Acta* **73** (1988), 1–26.
- [4] P. W. Fowler and D. E. Manolopoulos, *An Atlas of Fullerenes*, Clarendon Press, Oxford, 1995.
- [5] M. Goldberg, A class of multi-symmetric polyhedra, *Tohoku Math. J.* **43** (1939), 104–108.
- [6] J. E. Graver, Encoding Fullerenes and Geodesic Domes, *SIAM J. Discrete Math.* **17**(4) (2004), 596–614.
- [7] D. E. Manolopoulos, D. R. Woodall, and P. W. Fowler, Electronic Stability of Fullerenes: Eigenvalue Theorems for Leapfrog Carbon Clusters, *J. Chem. Soc. Faraday Trans.* **88**(17) (1992), 2427–2435.

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