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NANOSTRUCTURES OF FULLERENES

HIGHLY SYMMETRIC FULLERENES AND NANOTUBES

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Abstract: *The number of mathematically possible fullerenes and nanotubes grows rapidly with the number of atoms; there are over 2,500,000 possibilities on 100 or fewer atoms. However, the numbers with a high degree of symmetric are much smaller. In other words, given a fullerene or nanotube with a sufficiently rich symmetry group, the actual structure of the fullerene or nanotube is then uniquely determined by relatively few numerical parameters. The extreme example are the fullerenes with the full icosahedral automorphism group; each of these is determined by one numerical parameter.*

1. INTRODUCTION: FULLERENES WITH ICOSAHEDRAL SYMMETRY

The term fullerene is used here for both the trivalent plane graphs Γ with only hexagonal and pentagonal faces and the carbon molecule that they model. By a plane graph, we mean a decomposition of the sphere into regions called faces separated by boundary segments called edges. The points where the boundaries come together are called the vertices of the graph and the term "trivalent" means that three boundaries meet at each vertex. In modeling a carbon molecule, the vertices represent carbon atoms and the edges represent chemical bonds between atoms. It follows easily from Euler's Formula for plane graphs, that each fullerene has exactly 12 pentagonal faces. An example many people have seen but not recognized as a fullerene is the structure of a soccer ball; this fullerene has 60 atoms and is also referred to as the $\mathbf{C}_{60}$ carbon molecule. It was proposed that if carbon could exist in a form other than crystalline, diamond and graphite, then it would have the structure of this fullerene. The carbon atom tends to form hexagonal rings, which is it's most stable state. The pentagonal rings that carbon forms are much less stable. The simplest fullerene, also known as $\mathbf{C}_{20}$, is the graph of the dodecahedron with 12 pentagonal faces and no hexagonal faces. Without the presence of hexagonal rings to separate the pentagonal rings this structure is unstable. The first stable form discovered is the isomer of $\mathbf{C}_{60}$ in the soccer ball configuration. There are theoretically over 3,000 different ways that 60 carbon atoms can be arranged to form a carbon molecule, these are called isomers of $\mathbf{C}_{60}$, among them the soccer ball configuration is the only one in which no pentagons share an edge.

The simplest class of fullerens is based on the works of two mathematicians H. M. S. Coxeter [1] and M. Goldberg [4]. The Coxeter-Goldberg construction builds a particular class of fullerenes with icosehedral symmetry determined by just two parameters. These two parameters, as we will see, reveal a lot of information about this special class of fullerenes. Their construction uses the hexagonal tessallation of the plane to design these fullerenes. First, 20 congruent equilateral triangles are cut out of the hexagonal tessellation so the three verticies of the triangle are positioned at the centers of hexagonal faces. These equilateral triangles are placed on the faces of the icosehedron. The resulting polyhedron will have pentagonal faces centered on the 12 verticies of the icosehedron and hexagonal faces elsewhere.

The equilateral triangles corresponding to a face of the icosehedron in the Coxeter-Goldberg fullerenes are determined by two parameters (p, q), the "Coxeter coordinates" or simply the "coordinates" of the triangle's bounding segments. Once numerical values for the coordinates are chosen they define a unique fullerene in this infinite class of fullerenes. A *segment* in Λ, the hexagonal tessellation of the plane, is the straight line segment joining the centers of two hexagonal faces. A *straight segment* joins the centers of two hexagonal faces, but will be a perpendicular bisector of every edge it crosses. The coordinate of a straight segment is the single variable (p) where $p + 1$ is the number of hexagon centers on the segment. When it is not a straight segment a segment has coordinates (p, q). We obtain the parameters of the segment p and q by starting at one vertex of the segment and moving towards the other vertex through a straight segment that cuts through p hexagons, then turning left 60 degrees, through a straight segment of length q ending on the other vertex. Therefore, (p, q) defines the shortest two-leg path of two straight segments starting to the right of one endpoint of the segment and ending at the other endpoint.

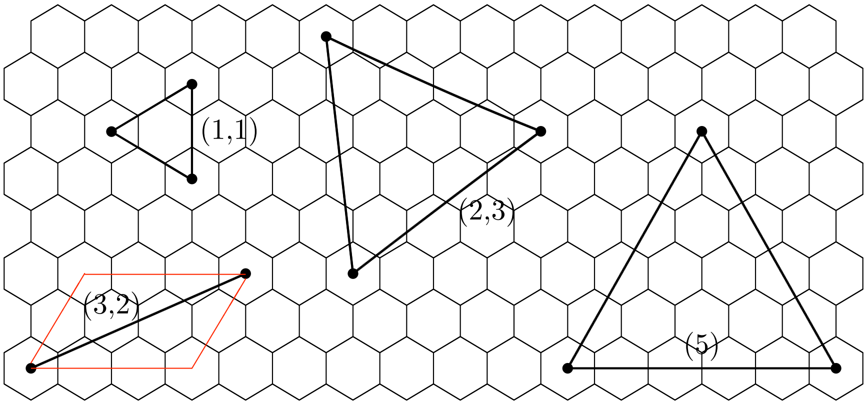


FIGURE 1. In the lower left hand corner of Figure 1 we have drawn a typical segment. The two red segments running perpendicular to the edges of Λ indicate how the coordinates are obtained.

The triangle in the upper left hand corner of Figure 1 has coordinates (1,1). If we place copies of this triangle on the faces of the icosehdron we will obtain the carbon molecule $\mathbf{C}_{60}$ in the soccer ball configuration. We illustrate the construction in Figure 2: the 12 pentagonal faces are black and the 20 hexagonal faces are white.

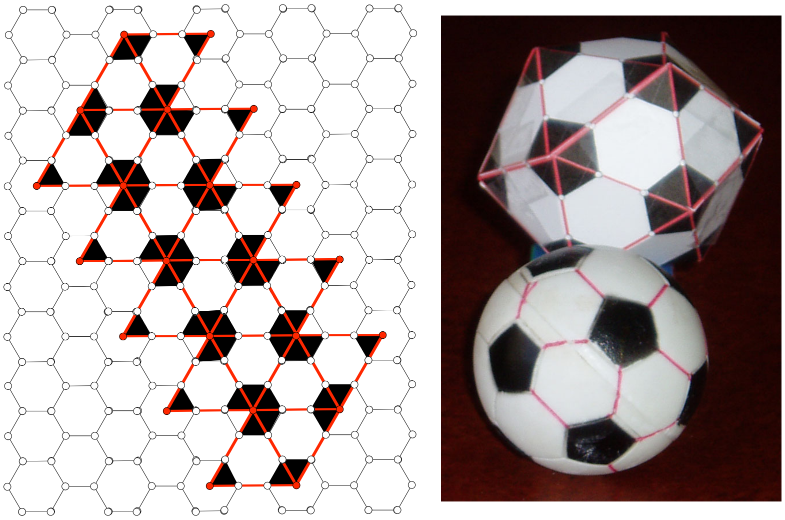


FIGURE 2. A flat map of $\mathbf{C}_{60}$, the folded icoshedral model and the soccer ball.

The class of Coxeter or icosahedral fullerenes have a high degree of symmetry due to the small number of parameters. The two types of symmetries we will discuss are direct, which are the rotations and opposite, the reflections and rotary - reflections. The equilateral triangle with coordinates (p, q) is clearly mapped onto itself by a 120° rotation. Hence, any rotation of the icosahedron gives a symmetry of the Coxeter fullerene. As for reflections, one easily sees that a (p, q) segment reflects into a (q, p) segment. The result is that Coxeter fullerenes defined by (p, q) will be preserved under the full icosahedral symmetry group if and only if $p = q$. In addition, the Coxeter fullerenes described by the single coordinate (p) will have full icosahedral symmetry.

There are other convenient properties associated with the two parameters of the Coxeter fullerene. The formula p^2+pq+q^2 computes the total number of atoms in the equilateral triangle defined by (p, q). The formula counts each vertex on the boundary as $\frac{1}{2}$ an atom because they will be counted in two triangles. Since the icosehedron has 20 faces, it follows that the Coxeter fullerene (p, q) has $20(p^2+pq+q^2)$ atoms. For example, the soccer ball whose coordinates are $(1, 1)$ yields $20(1 + 1 + 1) = 60$ atoms. Once the number of atoms is known we can observe the relationship between the number of atoms a and the number of hexagons h. Counting the number of atoms around each face we obtain $6h + 5 \times 12 = 6(h + 10)$; however, since an atom belongs to three seperate faces of the fullerene every atom has been counted three times in this formula. Correcting for this, we have $a = 2h + 20$. We can check the example of the soccer ball where $a = 60$ and $h = 20$. A simple consequence of this formula is that all fullerenes have an even number of atoms.

The Coxeter fullerenes are a specific class with a great amount of symmetry. Fowler, Cremona and Steer [2] generalized Coxeter's construction to other triangulations of the sphere. In this paper we generalize Coxeter's construction to fullerenes that do not necessarily contain triangular regions between the pentagonal faces. Each fullerene is described as a planar graph on 12 vertices, which correspond to the 12 pentagonal faces. Transfering this graph to the hexagonal tessellation we place each vertex at the center of a hexagon. The edges between the vertices are labeled with coordinates, but the regions no longer need to be triangles. This approach permits grouping fullerenes into families where the edge labels are variables. The planar graph along with the variable edge labels defines what we call the signature of a family of fullerenes. The Coxeter fullerenes form a family of fullerenes where the signature graph is the icosehedron and each edge is labeled (p, q). Classifying the signature of a fullerene completely defines the symmetries of the particular fullerene. The fewer parameteres that are involved with describing the signature, the more symmetry this family of fullerenes will have. This paper will only focus on fullerenes that have at most four parameters.

2. FORMULAS, AREAS AND DISTANCE

It is frequently easier to work with the dual to the fullernes. The dual of a plane graph interchanges the roles of vertices and faces. The duals to the fullerenes have triangular faces and vertices of degree 5 and 6 and are usually called *geodesic domes*. They became of interest to biochemists in the 1960's. Many observed that under a microscope viruses had icosahedral symmetry and look like tiny geodesic domes. It was in the context of this class of viruses Coxeter developed his construction. We will discuss the particular uses of the dual which help provide means of obtaining information about the fullerene.

Knowing the number of atoms in a particular fullerene is essential; although, straight forward counting will not always be the easiest method to obtain this information. This is due to the fact that fullerenes can be quite large. Luckily, there is a way to extract the number of atoms of a specific fullerene by calculating its area. If we consider the dual tessellation of Λ, shown below in Figure 3 in red, then each face of the dual tessellation is a triangle and contains exactly one vertex. Similarly, each face of the dual of a fullerene will be a triangle and contain exactly one atom of that fullerene. If we assume that each of these basic triangles has area 1, then computing the area will yield the number of atoms in the fullerene. This approach to counting atoms consists of computing the area of the larger triangles and paralellograms that are pasted into the signature graph and then adding up those areas.

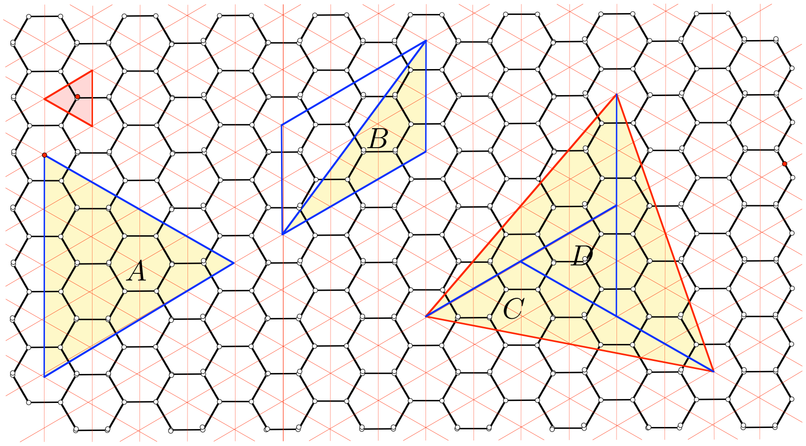


FIGURE 3. Area formulas for triangular regions.

One of the easiest regions to consider is an equilateral triangle, similar to triangle A in Figure 3; here the edges are straight segments, that are aligned with red grid lines of the dual triangular tessellation. Note that there will be n basic triangles along this edge of the grid line. Through a direct observaton we can see the number of basic triangles within a region of this type is $1+3+5+\cdots+2n-1$. This is the sum of the first n odd numbers, which is known to be simply n^2. We can demonstrate using triangle A that there are $1+3+5+7=16$ faces, hence it encloses 16 vertices. Now we consider a triangle having just 2 sides aligned with the dual tessellation, an example being triangle B in Figure 3. It is easy to compute the area of this region by considering the $r \times s$ parallelogram, where r and s correspond to the lengths of the sides aligned with the dual tessellation. The parallelogram will be comprised of rs smaller parallelograms, which in turn contain 2 basic triangles. We can conclude that the area of the parallelogram is $2rs$, leaving the triangle to have area rs, which was what we desired to find. For example if we look at triangle B, we see that it has area $3 \times 2 = 6$.

We now employ the area formulas of these two basic regions to compute the area of any arbitrary equilateral triangle whose edges have coordinates (p, q). Using the region on the right hand side of Figure 3 we will model this method. At the center, we have an aligned equilateral triangle with side coordinate $(p-q)$ (labeled D in the figure). This triangle is surrounded by three triangles with two aligned sides with coordinates (p) and (q) (labeled C in the figure). Summing the areas of these four triangles gives: $(p-q)^2 + 3pq = p^2 + pq + q^2$. For example the area of the red triangle to the right in Figure 3 is $4^2 + 4 \times 2 + 2^2 = 28$.

Another illustration of this decomposition method for developing formulas is to consider the general parallelogram with sides having coordinates

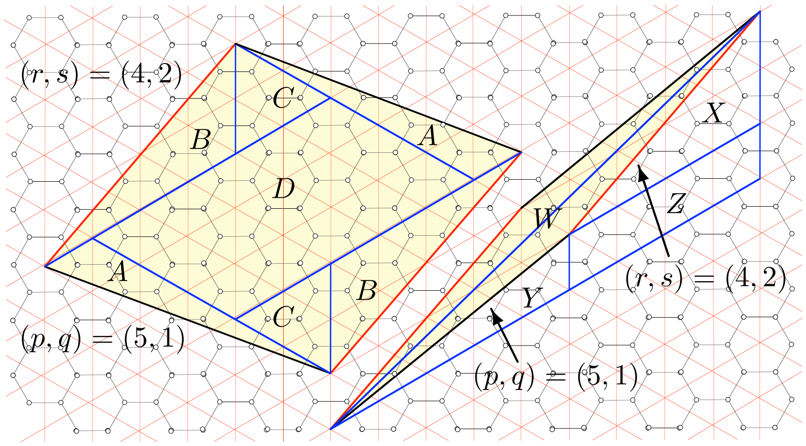


FIGURE 4. Area formulas for parallelograms.

(p,q) and (r,s). There are two possibilities depending on the angles: these are illustrated in Figure 4. We will refer to the parallelogram on the left as a *wide parallelogram* and to the one on the right as a *narrow parallelogram*. Considering the leftmost vertex in the wide parallelogram we see that the p and r segments create a 60 degree angle, compared to the narrow where p and r are measured along the same line. The wide parallelogram may be decomposed into aligned triangles and an aligned parallelogram; the contributions to the area of the parallelogram are recorded on the left in the following table. Half of the narrow parallelogram W can be embedded in a larger aligned triangle T. The accounting here is given on the right in the table. Note that there is a smooth transition from narrow to wide: in the narrow case let $r \to 0$ and let $s = t$; in the wide case let $s \to 0$ and let $r = t$. Both formulas then agree on $2pt$ as the area.

Wide Parallelogram			**Narrow Parallelogram**		
Region(s)	*general*	*example*	*Region(s)*	*general*	*example*
$2A$	$2pq$	10	T	$(p+r)(q+s)$	27
$2B$	$2rs$	16	$-X$	$-rs$	-8
$2C$	$2s^2$	8	$-Y$	$-pq$	-5
D	$2(r+s-q)(p-s)$	30	$-Z$	$-2(qr)$	-8
Total	$2[(p+q)(r+s)-qr]$	64	$2 \times$ *Total*	$2(ps-qr)$	12

In our constructions we will use several polygonal regions that have reflective symmetry. In general, under a reflection or rotatory-reflection a segment with coordinates (p,q) will be mapped onto a segment with coordinates (q,p). Therefore a segment can be reflected onto itself if and only if it has coordinates of the form (p,p) or simply $(p) = (p,0) = (0,p)$. As we noted above in discussing the icosahedral case, equilateral triangles will have reflective symmetry only if their sides have coordinates (p,p) or (p). The wide and narrow parallelograms described above will be symmetric about their diagonals when $(r,s) = (q,p)$.

In Figure 5 we describe the other triangles and the quadrilaterals that have reflective symmetry; the axes of reflection are shown in red. The symmetric triangles with the same side parameters are either *tall* or *short*. This depends on whether the base angles are wide or narrow as we described above. We leave it for the interested reader to verify these area formulas using the appropriate decompositions.

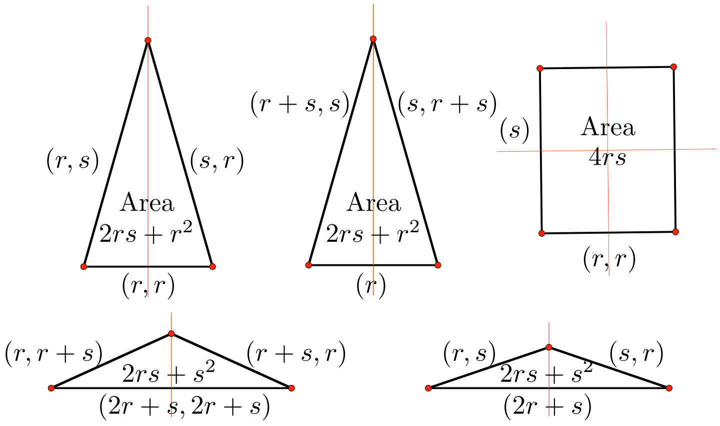


FIGURE 5. Area formulas for regions with reflective symmetry.

3. NANOTUBES

Included among the fullerenes are the nanotubes, which are relatively long tube-like structures. The tube is entirely composed of hexagonal faces and each cap contains exactly six pentagons. For our symmetric nanotubes, the caps must be identical and will have five or six pentagons at their bounding rims (the edge where the cap and the tube meet). The rim is uniquely determined by the coordinates of the bounding segments between pentagons. The nanotubes we will discuss have rotational symmetry about the axis of the tube. The rotation has order five or six depending on whether there is a hexagon or pentagon at the center of it's cap. The cylindrical part of the nanotube can be described by four parameters. We begin with the circumference parameter. Here we consider any hexagonal face and find the shortest path around the cylinder leading back to the hexagon. The coordinates of this path define the circumference parameters. The cylinder of the nanotube in Figure 6 has circumference parameters $(10, 5)$; its rim consists of 5 copies of the segment with parameters $(2, 1)$.

The next pair of parameters describe the length of the cylinder. We consider this to be the shortest distance between the centers of two pentagons - one on each rim. Here we do not mean distance in the geometric sense, but in the fullerene sense. The fullerene distance between two pentagons is described by the coordinates (p, q); this defines a path of hexagons of length

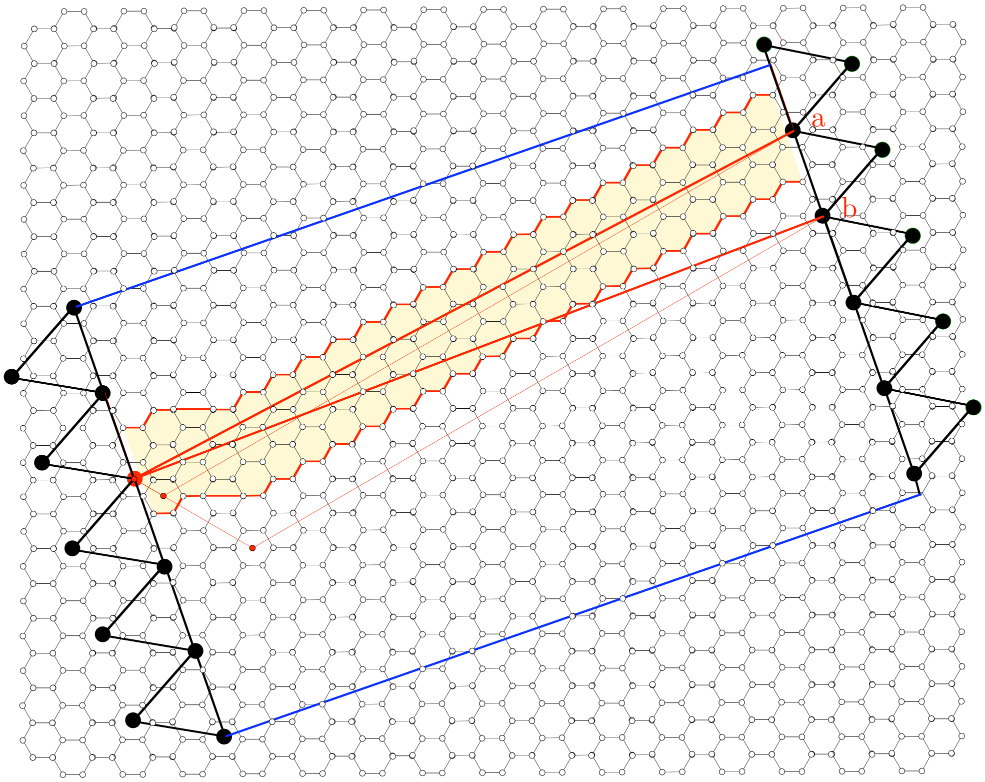


FIGURE 6. A nanotube with circumference parameters $(10, 5)$ and length parameters $(1, 21)$

$p + q$ linking the two faces. Once these parameters are known we can construct the nanotube from the hexagonal tessellation Λ. The construction consists of cutting out the region between two parallel lines and then identifying the boundary edges, Figure 6 exemplifies this. We can also use Figure 6 to illustrate the differences between geometric and fullerene distances. If we consider the pentagon corresponding to the red point on one rim, the pentagon on the other rim closest to it in geometric distance is labeled b. However, the coordinates of the segment joining these pentagons are $(4, 19)$, which makes the fullerene distance 23. Now consider the segment joining the red pentagon to the pentagon labeled a, it has coordinates $(1, 21)$ and its fullerene length is 22. Connecting each rim pentagon by a segment to its nearest neighbor on the other rim, divides the cylinder into parallelogram regions. In Figure 7, we have constructed a model of this nanotube.

4. FULLERENE SYMMETRIES AND SYMMETRY GROUPS

This section will focus on the symmetry groups associated with fullerenes, the 28 possible groups are well known. A complete listing of them can be found in *An Atlas of Fullerenes* [3]. So far we have focused on the fullerenes with the most symmetries, those with icosahedral symmetry. While many

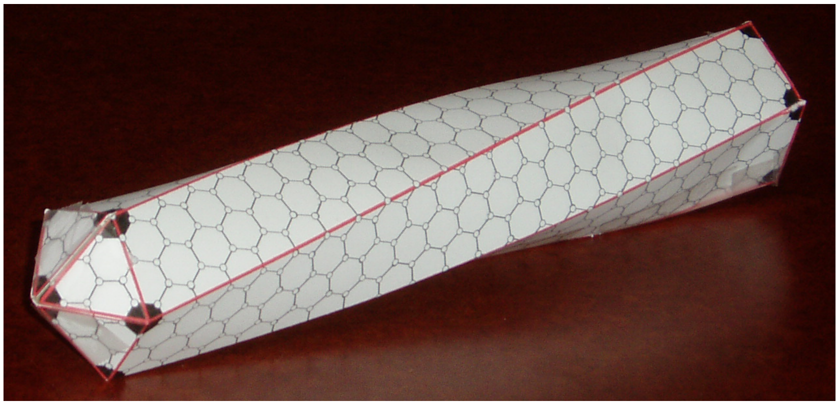


FIGURE 7. The equilateral triangular regions in the caps of this nanotube have coordinates $(2, 1)$ and the parallelogram sides of the cylinder have coordinates $(2, 1)$ and $(1, 21)$; giving a nanotube with 710 atoms.

of the smaller symmetry groups that we will consider are subgroups of the icosahedral group, not all of them are. Hence we start with a complete listing of all symmetries that a fullerene could admit.

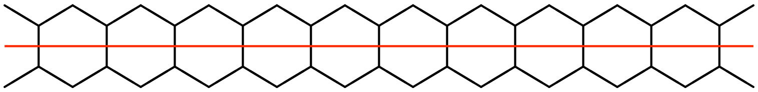
Possible rotation:

(i) rotations of order 6 with the axis of rotation passing through the centers of antipodal hexagonal faces,
(ii) rotations of order 5 with axis through the centers of antipodal pentagonal faces,
(iii) rotations of order 3 with axis through the centers of antipodal hexagonal faces or through antipodal vertices or through the center of a hexagonal face and a vertex,
(iv) rotations of order 2 with axis through the centers of antipodal hexagonal faces or through the centers of antipodal edges or through the center of an edge and the center of an opposite hexagonal face.

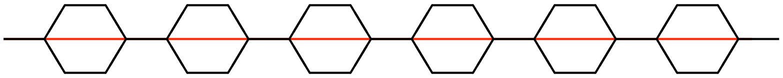
The plane of a reflection or of a rotary-reflection intersect the surface of the sphere in a circle - the circle of the reflection or rotary reflection. Since a reflection or a rotary-reflection interchanges the pentagonal faces on either side of the circle, there must be exactly the same number of pentagons on either side of the circle. When there are no pentagons on the circle there are six pentagons on each side and they form two identical nanotube caps.

Possible circles of reflection or of rotatory-reflection:

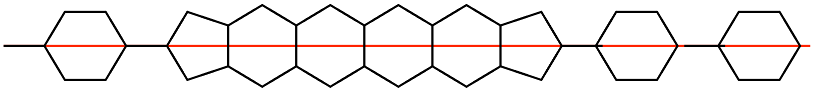
(i) a circle bisecting the faces in a circuit of faces around the center of a nanotube cap with circumference coordinates (p),



(ii) a circle bisecting the faces and containing the edges in a circuit of faces and edges around the center of a nanotube cap with circumference coordinates (p, p),

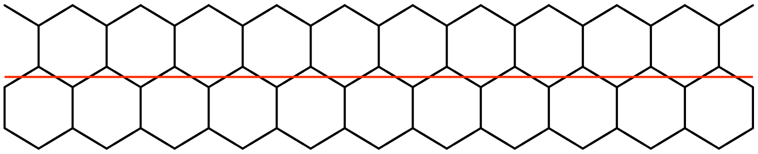


(iii) a circle that alternates between paths of the above two types with the transitions occurring at pentagonal faces.

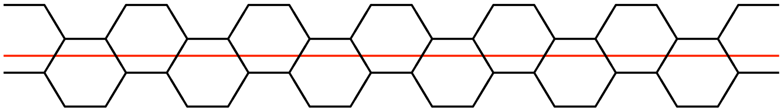


There are rotary-reflections where neither the reflection nor the rotation preserve symmerty. There are two cases where this can happen and they are obtained by slightly shifting circles (i) and (ii):

(iv) shifting circle (i) down or up slightly yields



(v) shifting circle (ii) down or up slightly yields



A region of a fullerene, a triangle or parallelogram, must be mapped to either a congruent region or onto itself. Hence we must understand the symmetries of these objects. Segments and parallelograms can be rotated 180 degrees about their midpoints and equilateral triangles can be rotated about their centers. Possible reflections are pictured in Figure 5.

5. Fullerenes with a rotation of order 5 or 6

Rotations of order five and six are very common among highly symmetric fullerenes. It is important to note that no fullerene has two distinct rotations of order 6 nor can it have a rotation of order 5 and 6 simultaneously. The case where there are two distinct rotations of order 5 generates the icosehedral symmetry. Therefore, we restrict our attention to fullerenes with exactly one rotation of order 5 or one rotation of order 6. As we will see these two cases are entirely parallel.

Let the center of the face f_0 be the center of a rotation of order 5 or 6 and consider the pentagonal faces that are its nearest neighbors. In a rotation of order 5 the maximum number of nearest neighbors is 10, and for a rotation of order 6 is 12. If we have 10 or 12 nearest pentagonal faces, they can only be arranged as pictured in Figure 8. To interpret this diagram, keep in mind that once values have been assigned to the parameters this diagram will be drawn on the hexagonal tessellation. The vertices of the diagram will be placed in the centers of hexagonal faces; the diagram will then be cut out along its outer edges. Folding along the internal edges and gluing together matching outer edges at each vertex will result in a closed polygon with pentagonal faces at its vertices. See Figure 9.

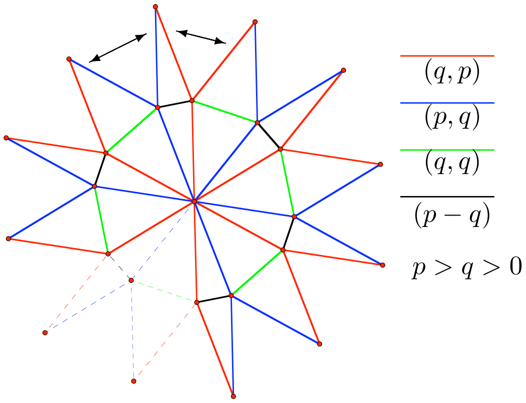


FIGURE 8. The pattern for a two parameter class of fullerenes with symmetry group D_{5h} (ignoring the dashed segments) or symmetry group D_{6h} (including the dashed segments).

The symmetry groups of these fullerenes have order 20 or 24 with Schönflies symbol D_{5h} or D_{6h}. The 10 or 12 direct symmetries are the powers of the rotation by 60 degrees about the center of the figure and half turns with axes through the centers of the green and black edges. Half of the 10 or 12 opposite symmetries are composed of a reflection through the black-green circle (type (iii) in the list of possible axes of reflection) and one of the powers of the rotation by 60 degrees about the center of the figure. The other half are reflections through the planes containing the axis of the rotation by 60 degrees and the midpoint of a black or green edge. Using the fact that this fullerene is partitioned into symmetric (red-blue-green and red-blue-black) triangles allows us to easily compute the number of atoms. Referring to Figure 5 the number is $10(p^2+2pq)$, if the rotation has order 5, and $12(p^2+2pq)$, if the rotation has order 6. These fullerenes will have a very disk-like shape, particularly in the case of a rotation of order 6. In Figure 9 we have on the left the flat pattern for the simplest example of a fullerene in this class; $p=2$, $q=1$, giving a model for a isomer of C_{80}, on the right.

If there are not 10 or 12 pentagonal faces equidistant from the center of rotation, there are exactly 5 or 6, depending on the order of the rotation. It follows that the center of the rotation is also the center of a nanotube cap with individual rim segments having coordinates (p,q). Since the two caps must be identical the next nearest pentagonal faces must also lie on the other rim. Joining the endpoints of each segment on one rim to their

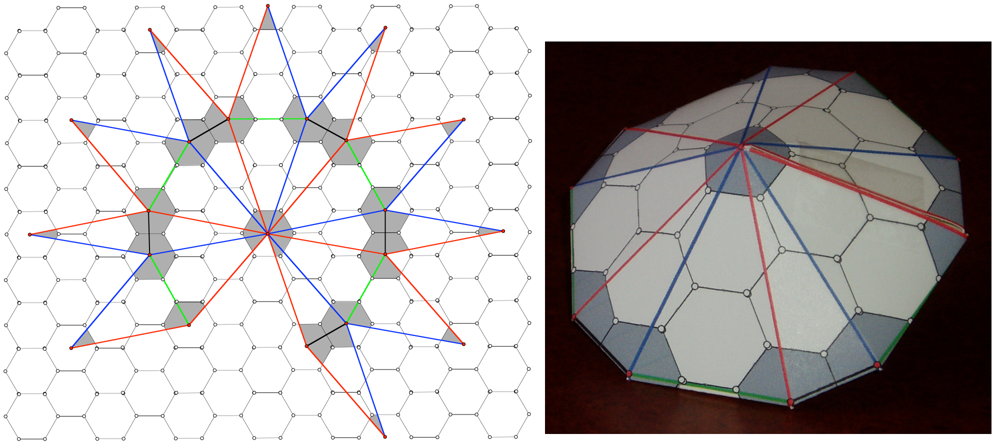


Figure 9. An isomer of C_{80} with symmetry group D_{5h}.

common neighbor on the opposite rim, shown in red and blue in Figure 10, forms a triangle with the (black) rim segment as a base. These triangles may then be paired to form parallelograms. This yields two cases depending on how close the two rings are, specifically on the type of parallelogram formed.

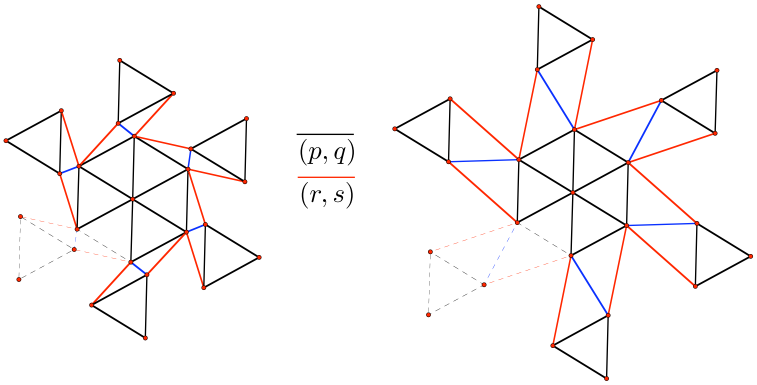


Figure 10. The basic structure of fullerenes admitting a rotation of order 5 (without the dashed segments) or a rotation of order 6 (including thedashed segments).

The segments on the rim have coordinates (p, q) where $p \geq q \geq 0$; if $q = 0$, then $p > 0$ and the segment has the single coordinate (p). Let (r, s) denote the coordinates of the (red) external segments of the parallelograms. In the case where the rims are close, causing the paralellograms to be narrow, we have the following constraints on r and s: $0 < r < p$, $p+q \geq r+s$ and either $s > q$ or $s = q$ and $r < q$. We might call these fullerenes “nanodisks.” The wider parallelogram arises when we have $0 < r \leq p+q$ with no restriction on s. In this case, we have a nanotube with the parameter s controlling its length. If the rotation is of order 5, $r = p$ and $s = q$ this reduces to the icosahedral fullerenes; hence we exclude that choice of parameters.

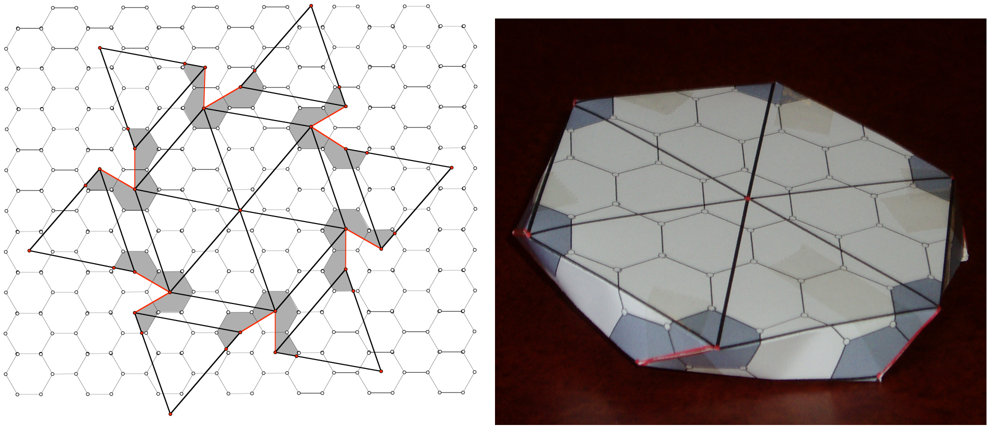


FIGURE 11. This nanodisk has parameters $p = 2$, $q = 1$, $r = 0$ and $s = 1$ giving a model for an isotope of $\mathbf{C}_{108}$ with symmetry group D_6.

In addition to the rotation of order 5 or 6 and its powers, these fullerenes admit half turns about the centers of the red and blue segments joining the rims. Opposite symmetries occur only in the special cases discussed below. So, in general these fullerenes are chiral and the symmetry group has Schönflies symbol D_5 or D_6. Each chiral fullerene in this class has a mirror image that is not included in the above description. To describe these mirror images directly, we simply reverse all coordinate pairs. In Figure 11, we have an example of a nanodisk with symmetry group D_6. A typical nanotube with symmetry group D_5 is modeled in Figure 7. In Figure 12 we include a second example from this class.

Using the triangle and parallelogram formulas we have that the number of atoms in a nanodisk is 10 or 12 times $(p^2+pq+q^2+ps-qr)$. In a nanotube is there are 10 or 12 times $(p^2 + pq + q^2 + pr + (p + q)s)$ atoms. Observe that this number grows linearly in s, *the nanotube length parameter*.

Reflections are possible only if $q = p$ or $q = 0$. There is an additional condition on the alignment of the two rims, which can be broken down into two cases. In one case the two rims will match, each pentagon on one rim will be directly across from its unique nearest neighboring pentagonal face on the other rim. In the second case the two rims will be rotated with respect to one another and each each pentagon face will be equidistant from two pentagonal faces on the other rim. See Figure 13.

If the rims are matching, the parallelogram faces are really rectangles of the type pictured in Figure 5. The coordinates of the form (r, r) for the black edges and (s) for the red edges or the reverse (r) for the black edges and (s, s) for the red edges. See the left hand diagram in Figure 13. In both cases, these are nanotubes. The centers for the half turns are the

FIGURE 12. The Callaway golf balls are manufactured with a hexagonal pattern instead of the traditional dimples. Hence, they model fullerenes and must include 12 pentagons. This ball has parameters $p = 6$, $q = 0$, $r = 5$ and $s = 0$ giving a model of $\mathbf{C}_{660}$ with symmetry group D_5. The number of atoms converts to 342 "dimples" - 330 hexagons and 12 pentagons. An interesting related paper on golf ball symmetry [7] is listed in the references.

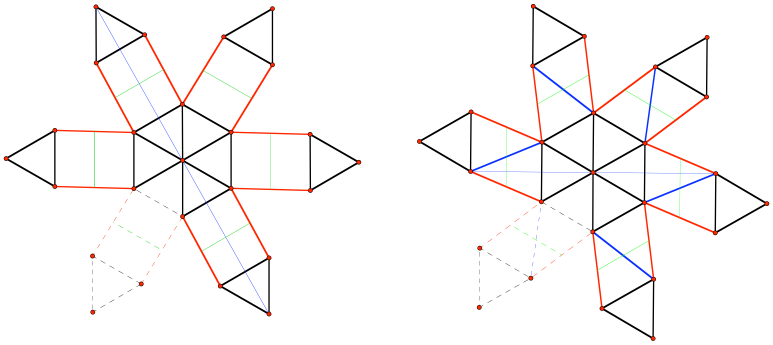


FIGURE 13. The basic structure of fullerenes admitting a rotation of order 5 (without the dashed segments) or a rotation of order 6 (including the dashed segments) along with reflections.

midpoints of the sides of the rectangles and the centers of the rectangles themselves. The circles that pass through the centers of the rotation of order 5 or 6 and the center of a half turn (representative shown in blue) are the circles of reflections in the symmetry group. In addition, there is the reflection through the circle that passes through all of the centers of the half turns (shown in green). The rotatory-reflections obtained by composing this reflection with the powers of the rotation of order 5 or 6 complete the list of symmetries. This group has order 20 or 24 with Schönflies symbol D_{5h} or D_{6h}. The number of atoms is easily computed to be 10 or 12 times $(3r^2 + 2rs)$ when the black edges have coordinates (r, r) and 10 or 12 times

$(r^2 + 2rs)$ when the black edges have the coordinate (r). An example with symmetry group D_{5h} is pictured on the left in Figure 14.

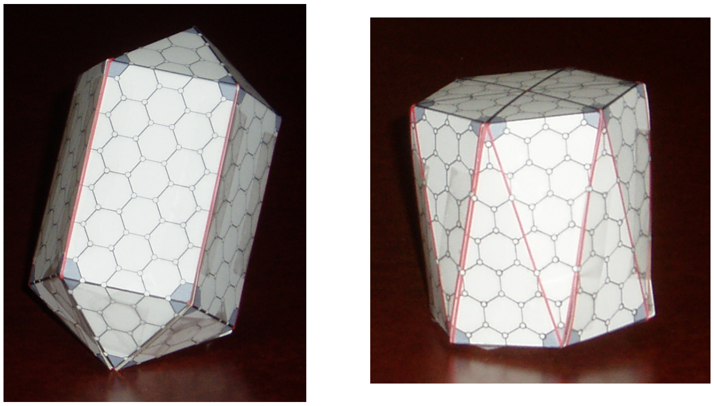


FIGURE 14. The left hand model of an isotope of $\mathbf{C}_{360}$ has symmetry group D_{5h}; the right hand model also of an isotope of $\mathbf{C}_{360}$ has symmetry group D_{6d}.

The second case for the nanodisks are when the rims are shifted, the triangles with a red side, a blue side and black base have reflective symmetry interchanging the red and blue sides (see the right hand diagram in Figure 13). In this case, the axes of reflections that pass through the centers of the rotation of order 5 or 6 are the circles that also pass through a pentagonal face on one of the rims (a representative is shown in blue). The remaining opposite symmetries are all rotatory-reflections consisting of the composition of this reflection with a rotation of an odd multiple of 30 degrees about the main axis. These symmetry groups have Schönflies symbol D_{5d} or D_{6d}. The right hand model in Figure 14 has symmetry group D_{6d}. This class includes both nanotubes and nanodisks. There are four distinct patterns of edge parameters depending on which of the four triangles from Figure 5 are used to construct the sides; they are listed in the following table.

black	*red*	*blue*	*type*	*# of atoms*
(r, r)	(r, s)	(s, r)	*nanotube*	$[20 \textit{ or } 24](2r^2 + rs)$
(r)	$(r + s, s)$	$(s, r + s)$	*nanotube*	$[20 \textit{ or } 24](r^2 + rs)$
$(2r + s, 2r + s)$	$(r, r + s)$	$(r + s, r)$	*nanodisk*	$[20 \textit{ or } 24](6r^2 + 7rs + 2s^2)$
$(2r + s)$	(r, s)	(s, r)	*nanodisk*	$[20 \textit{ or } 24](2r^2 + 3rs + s^2)$

6. FULLERENES WITH TETRAHEDRAL SYMMETRY

Fullerenes with tetrahedral symmetry are quite different than the fullerenes previously mentioned. We will discuss the rotational and reflective symmetries separately. Beginning with the rotational symmetries we see that this class of fullerenes will have four distinct axes in a rotation of order 3. Connecting the centers of the images of pentagonal faces closest to a center of order 3 rotation yields an equilateral triangle (shown in black in Figure 15). The other center of that rotation also yields a triangle (shown in red).

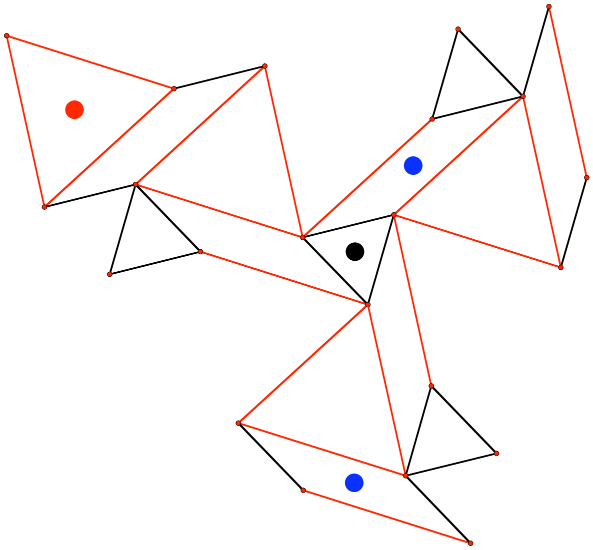


FIGURE 15. The basic structure of fullerenes with tetrahedral symmetry.

In this type of symmetry the axes of order 3 rotations are rotated into one another, this gives 4 black triangles and 4 red triangles connecting with six (red-black) parallelograms. The symmetry group in the chiral case has order 12. There are four 120 degree rotations and four 240 degree rotations about the centers of the black/red triangles. We have indicated one such center and its paired center with black and red dots in Figure 15. The center of opposite parallelograms give three half-turns; one pair of half-turn centers is indicated by blue dots in the figure. The parameters on the black and red edges are independent. We use (p, q) for the black edges and (r, s) for the red edges. With this assignment, the parameters assigned to the parallelograms match the parameters in Figure 4. Using this information the number of atoms are given by $4(p^2+pq+q^2)+4(r^2+rs+s^2)$, then adding either 6 times the area $2(ps-qr)$ if the parallelograms are narrow and $2[(p+q)(r+s)-qr]$ if they are wide. A chiral fullerene with tetrahedral symmetry is pictured in Figure 16.

Now we will discuss the reflective symmetries of the tetrahedral fullerenes. There are two distinct configurations that admit reflective symmetries; these are pictured in Figure 17. Typical centers of rotation are indicated as before. The coordinates for the left hand diagram are (p, p) for the black edges and (s) for the red edges. Now these parallelograms are of the type pictured in Figure 5. The number of atoms is given by $4(3p^2) + 4(s^2) + 6(4ps) = 12p^2 + 24ps + 4s^2$. We can see the blue line is a circle of a reflection - there are six such circles. The green line is a circle of a rotary-reflection of 90 degrees about the axis through the blue centers - there are 6 of these. The exact location and type of circle in a rotary-reflection depends on the

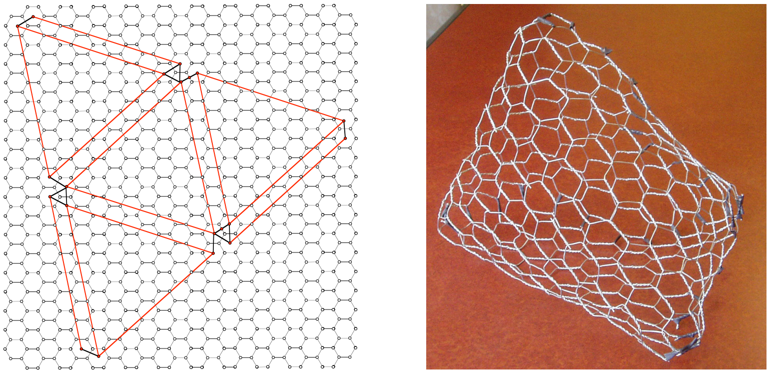


FIGURE 16. This model is chiral and has tetrahedral symmetry Its parameters are $p = 1$, $q = 0$, $r = 7$ and $s = 2$ and the parallelogram is wide giving a model for an isotope of $\mathbf{C}_{380}$.

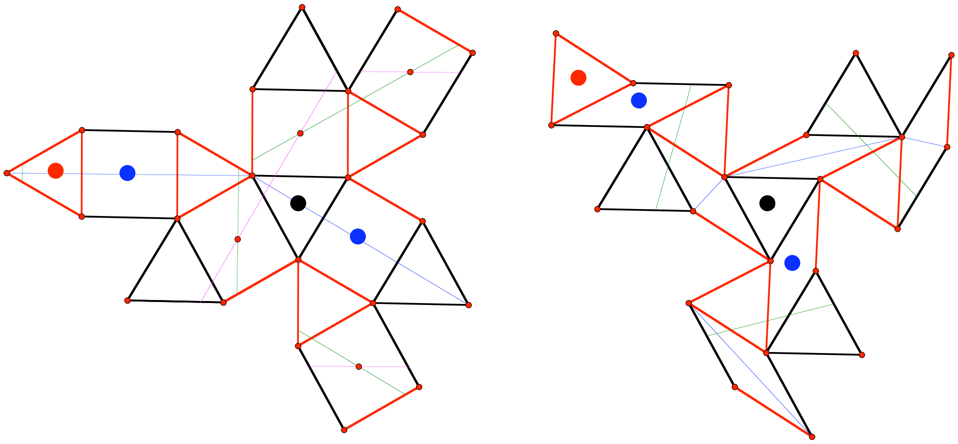


FIGURE 17. Basic structure of tetrahedral fullerenes with reflective symmetry.

relative values of p and s. In fact, in many cases these rotary-reflections will map two distinct circles into themselves. If $s \geq p$, there is a circle of a rotary-reflection of type (i) or (iv) (in green); if $s \leq 3p$, there is another circle of type (ii) or (v) for the same rotary-reflection (in purple). The Schönflies symbol for the symmetry group of this class of tetrahedral fullerenes is T_d.

To calculate the number of atoms we use the coordinates for the right hand figure which are (p, q) for the black edges and (q, p) for the red edges. The number is $8(p^2 + pq + q^2)$ and we add either $6(2p^2 + 4pq)$ when the parallelograms are wide parallelograms or $6(2p^2 - 2q^2)$ in the case or narrow parallelograms. We can easily simplify this to $20p^2 + 32pq + 8q^2$ atoms in the wide case and $20p^2 + 8pq - 4q^2$ atoms in the narrow case. Turning to the symmetry structure, the blue line is a circle of a reflection - there are three such circles. The green line is the circle of a rotary-reflection of 60, 180 and 270 degrees about the axis through the red and black centers. Since

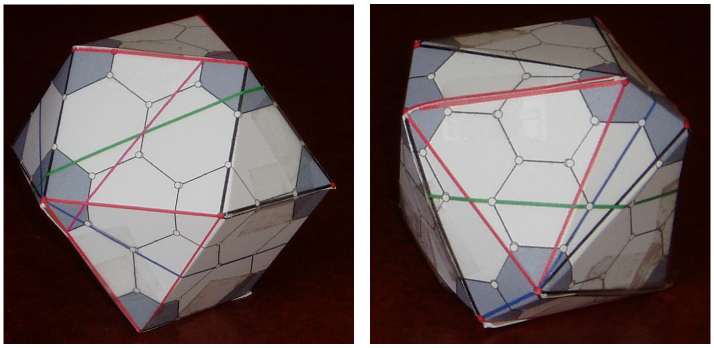


FIGURE 18. The left hand model of an isotope of $\mathbf{C}_{76}$ has symmetry group T_d; the right hand model of an isotope of $\mathbf{C}_{92}$ has symmetry group T_h. This last model along with nanotube model in Figure 7 illustrates that quadrilateral faces of a folded paper model may be twisted or bent.

the 180 degree rotary-reflection about all four axes give the same symmetry - the reflection through the center of the fullerene, there are $2 \times 4 + 1$ or nine distinct rotary-reflections. The Schönflies symbol for the symmetry group of this class of tetrahedral fullerenes is T_h.

7. SUMMARY AND A FEW ADDITIONAL CLASSES

In the following table we summarize the classes of fullerenes that we have constructed above.

Symmetry Group	*Numberof Parameters*	*type*	*General Pattern*	*Example*
$I_h(120)$	1	*icosahedral*	*Figure*2	*Figure*2
$I(60)$	2	*chiral icosahedral*	*not shown*	*not shown*
$T_h(24)$	4	*tetrahedral*	*Figure* 17	*Figure* 18
$T_d(24)$	4	*tetrahedral*	*Figure* 17	*Figure* 18
$D_{6h}(24)$	2	*nanodisk*	*Figure* 8	*not shown*
$D_{6h}(24)$	4	*nanotube*	*Figure* 13	*not shown*
$D_{6d}(24)$	4	*nanotube*	*Figure* 13	*Figure* 14
$D_{5h}(20)$	2	*nanodisk*	*Figure* 8	*Figure* 9
$D_{5h}(20)$	4	*nanotube*	*Figure* 13	*Figure* 14
$D_{5d}(20)$	4	*nanotube*	*Figure* 13	*not shown*
$T(24)$	4	*chiral tetrahedral*	*Figure* 15	*Figure* 16
$D_6(12)$	4	*chiral nanodisk*	*Figure* 10	*Figure* 11
$D_6(12)$	4	*chiral nanotube*	*Figure* 10	*not shown*
$D_5(10)$	4	*chiral nanodisk*	*Figure* 10	*not shown*
$D_5(10)$	4	*chiral nanotube*	*Figure* 10	*Figures* 7 & 12

There are several other 4-parameter classes of fullerenes; these have symmetry groups D_{3h} and D_{3d}. Constructing them can be quite tedious. The interested reader may consult [6] for a complete listing of these classes. We close this paper with a few examples of fullerenes with these symmetry structures.

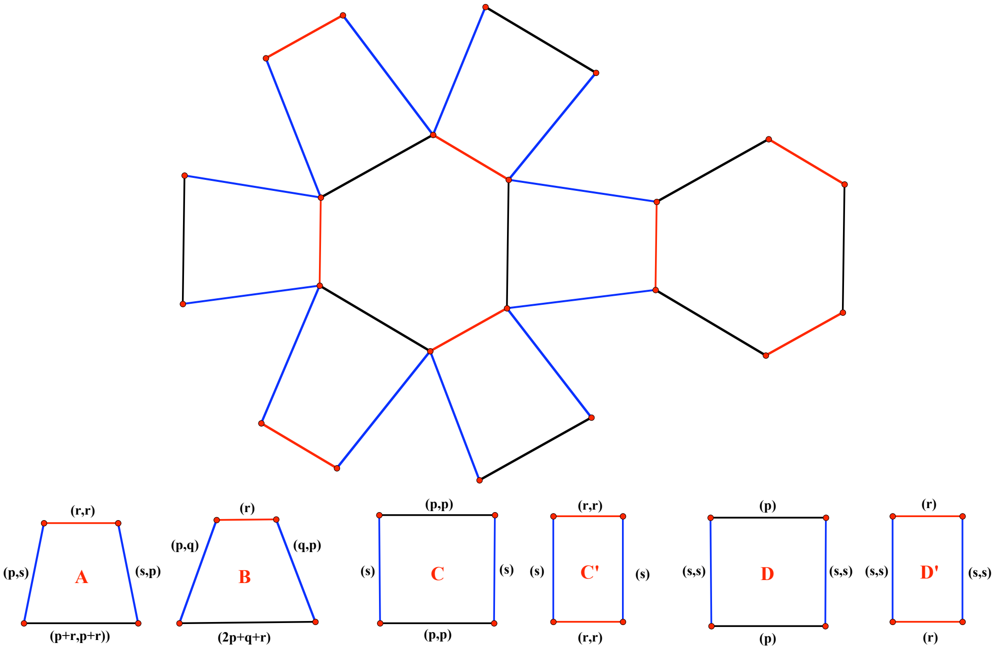


Figure 19. This is one basic structure for fullerenes with D_{3h} or D_{3d} symmetry: two semi-regular hexagons connected by quadrilaterals. We describe just 4 of the several patterns using this structure. In types A and *B*, the hexagons are skew and the quadrilaterals are trapezoids - the group is D_{3d}. In types C and D (or C' and D') the hexagons match and the quadrilaterals are rectangles alternating in width - the group is D_{3h}. Types A, C and D are nanotubes with *s* as the nanotube parameter; type *B* is a nonodisk.

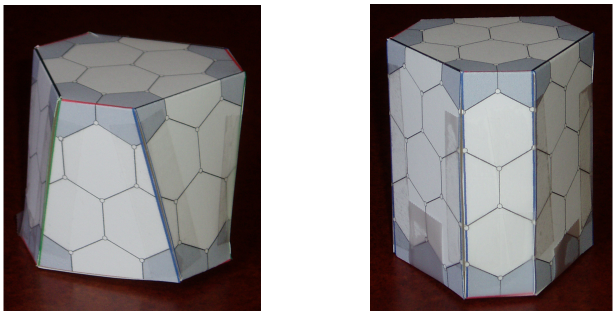


Figure 20. The left hand model of an isotope of $\mathbf{C}_{116}$ has symmetry group D_{3d}; the right hand model of an isotope of $\mathbf{C}_{98}$ has symmetry group D_{3h}.

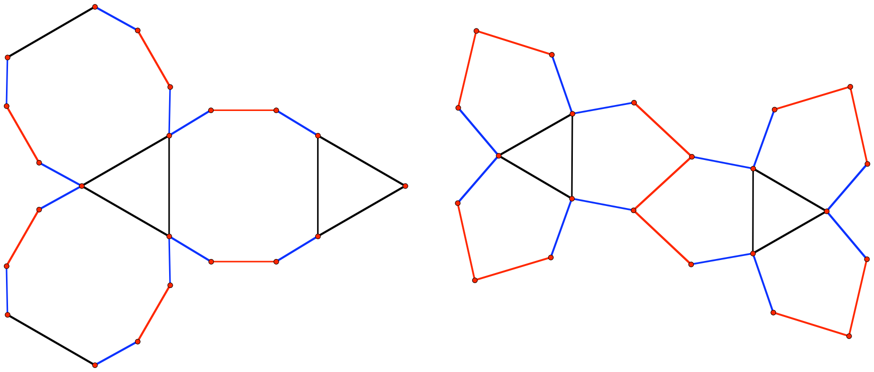


Figure 21. Here are two more basic structures for fullerenes with D_{3h} symmetry (on the left) or D_{3d} symmetry (on the right). The first pattern always yields a nanotube. With certain selection of parameters the second also yields a nanotube.

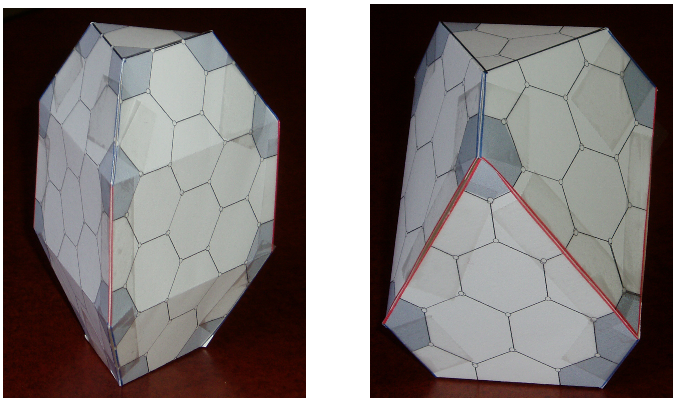


Figure 22. The left hand model of an isotope of $\mathbf{C}_{108}$ has symmetry group D_{3h}; the right hand model of an isotope of $\mathbf{C}_{92}$ has symmetry group D_{3d}.

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