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# Totally Symmetric Kekulé Structures in Fullerene Graphs with Ten or More Symmetries

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**Abstract**

Graph theoretic fullerenes are designed to model large carbon molecules: each vertex represents a carbon atom and the edges represent chemical bonds. A totally symmetric Kekulé structure in a fullerene is a set of independent edges which is fixed by all symmetries of the fullerene.

It was suggested in a paper by S. J. Austin, J. Baker, P. W. Fowler, D. E. Manolopoulos and in a paper by K. M. Rogers and P. W. Fowler that molecules with totally symmetric Kekulé structures could have special physical and chemical properties. Starting from a catalog given by J.E.Graver, we study all graph theoretic fullerenes with at least ten symmetries and we establish exactly which of them have at least one totally symmetric Kekulé structure.

## 1 Introduction

By a *fullerene* we mean a trivalent plane graph $\Gamma = (V, E, F)$ with only hexagonal and pentagonal faces. Such graphs on $v$ vertices exist for all even $v \geq 24$ and for $v = 20$, [10]. 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 ones. See the monograph of Fowler and Manolopoulos [5] for more information.

The graph theoretic fullerenes are designed to model large carbon molecules: each vertex represents a carbon atom and the edges represent chemical bonds. Since a carbon atom has chemical valence 4, one edge at each vertex of the graph must represent a double chemical bond.

Graph theoretic fullerenes have achieved considerable interest since Kroto, Smalley and co-workers discovered the icoshaedral molecule $C_{60}$, [12] and through the analysis of the products obtained from the laser vaporizations of graphite, the mass spectroscopic evidence indicated that there would be numerous fullerenes with icosahedral symmetry, such as $C_{60}$, $C_{80}$, $C_{140}$, $C_{180}$, $C_{240}$, $C_{260}$, $C_{420}$, $C_{540}$, etc., [11], [4].

A *perfect matching* of $\Gamma$ is a set of independent edges (i.e., edges not shearing vertices) covering all vertices of $\Gamma$. In the chemical literature a perfect matching is often called a *Kekulé structure* and in the model of carbon molecules the edges of a perfect matching correspond to double bonds. A Kekulé structure is said to be *totally symmetric* if it is fixed by the full automorphism group of $\Gamma$.

Fullerenes generally have many Kekulé structures, but molecules with totally symmetric ones seem to have special physical and chemical properties, as suggested in [13] and [1]. For instance, $C_{60}$ has 12500 Kekulé structures, however it has been argued that $C_{60}$ is not aromatic in any traditional sense and that its special physical and chemical properties are compatible with the dominance of just one Kekulé structure: the only one of the 12500 to be totally symmetric (see [1] for more details). More precisely, the main idea in [13] is that any totally symmetric Kekulé structure could correspond to a minimum on the potential surface: for that reason, in the cited paper, a complete catalog of all fullerenes with at most 40 vertices which admit a totally symmetric Kekulé structure is obtained.

There is one class of fullerenes for which a totally symmetric Kekulé structure can always be found: the *leapfrog* fullerenes. A leapfrog fullerene $\Gamma^l$ is obtained by truncating the dual of a fullerene $\Gamma$. More precisely: draw a small hexagonal (pentagonal) face inside each hexagonal (pentagonal) face of $\Gamma$, rotate by 30 (36) degrees. Next connect the vertices of these new faces with edges which are perpendicular bisectors of the edges of $\Gamma$. Now delete all vertices and edges of $\Gamma$. The remaining graph is $\Gamma^l$. It is easy to check that the number of vertices of $\Gamma^l$ is three times the number of vertices of $\Gamma$. Moreover, the full automorphism group of $\Gamma^l$ coincides with that of $\Gamma$ and a totally symmetric Kekulé structure for $\Gamma^l$ is obtained by taking the drawn perpendicular bisectors.

It is straightforward that in a fullerene with trivial automorphism group each Kekulé structure is totally symmetric. On the other hand, it seems reasonable to have a few or no totally symmetric Kekulé structure in a fullerene with a significant automorphism group. Fullerenes with at least ten symmetries were studied, classified and listed in a complete catalog by J.E. Graver in [7], [8]. The aim of this paper is to discover which of these fullerenes admit at least one totally symmetric Kekulé structure. For brevity, we denote a totally symmetric Kekulé structure by TSKS.

As observed in [1], a trivial necessary condition for the existence of a TSKS in a fullerene is that each automorphism of order 3 has no fixed vertex. It is well known, see [13], that this condition is also sufficient for leapfrog fullerenes. Our aim is to prove that, except for a small number of instances, the condition is sufficient for each fullerene with at least ten symmetries. We can summarize our results in the following theorem (parameters and notations are referred to the catalog of [8]):

**Theorem 1.1.** *Except for all graphs in $\mathcal{P}_4 \cup \mathcal{P}_5$ with $r = 3$, $s = 1$ and $p$ even, for which a TSKS does not exist, a fullerene $\Gamma$ with at least ten symmetries has a totally symmetric Kekulé structure if and only if no order 3 symmetry of $\Gamma$ has a fixed vertex.*

The proof of the theorem above will be easily deduced by Propositions 3.3, 3.4, 3.5, 3.6, 3.7 in the following section 3.

## 2 Fullerenes and signatures

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. By dualization a planar embedding of the graph $\Gamma$ on the sphere is obtained. It is in this context that Goldberg [9], Caspar and Klug [2] and Coxeter [3] parameterized the geodesic domes/fullerenes that include the full rotational group of the icosahedron among their symmetries.

In [6], J. E. Graver extended the work of Coxeter presenting a classification scheme for all geodesic domes and fullerenes. To perform his contruction, Graver assigns to each fullerene/geodesic dome a $12-$vertex planar graph with edge and angle labels called the *signature* of $\Gamma$. The fullerene and its planar representation on the sphere can then be reconstituted from its signature in a manner which is proved in [6] to be unique.

To describe Graver's construction we must recall what *Coxeter coordinates* of segments and angles between segments are. Namely, let $\Lambda$ be a plane together with a regular hexagonal tesselation. Fix the center of each hexagon. By a *segment* in $\Lambda$ we mean a straight line segment that joins two centers. We assign Coxeter coordinates to a segment as follows: if it lies on a line perpendicular to hexagon edges, the single Coxeter coordinate $(p)$ is assigned, where $p+1$ is the number of centers of hexagons on the segment.

If not, take the first line to the right of the segment which is perpendicular to an hexagon edge to identify the first coordinate direction, then turn left with an angle of $60^o$ to find the second coordinate direction. The number $p+1$ (resp. $q+1$) of centers of hexagons we pass through in the first (resp. second) direction when connecting the two endpoints of the segment, give the Coxeter coordinates $(p,q)$ of the segment itself.

The type of an angle between two segments is the number of centers of the edges of the central hexagons between the segments. Segments which runs to successive centers contribute $1/2$ to each of the angle types on either side.

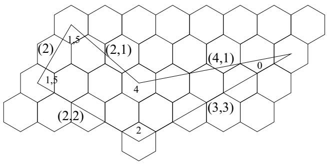


Figure 2.1: Coxeter coordinates

Essentially Graver's construction works as follows: denote by $\Lambda$ the plane with the hexagonal tessellation, take the signature of $\Gamma$, draw each face of the signature on $\Lambda$ putting each vertex of the face in the center of an hexagon of $\Lambda$ in such a way that the polygonal region of $\Lambda$ corresponding to that face is completely determined by the Coxeter coordinates which label edges of the face and by the types of angles between them. By gluing together the regions of $\Lambda$ corresponding to the faces of the signature, we reconstitute the geodesic dome and the graph model of $\Gamma$ together with its planar embedding on the sphere. The planar embedding of the signature on the sphere will be denoted by $S(\Gamma)$. Furthermore, in what follows we will denote by $\Lambda$ both the plane with the hexagonal tessellation, and the sphere with the tessellation into hexagons and pentagons inherited in the reconstruction of the geodesic dome from its signature.

To distinguish between edges of the graph $\Gamma$ and edges of $S(\Gamma)$, the latter are referred to as *segments*. Moreover, each vertex of the signature represents a pentagon in the fullerene being modeled and segments of $S(\Gamma)$ all represent shortest distances between pentagons. For each fullerene, the number of its vertices, faces and edges, and its symmetry structure are computed directly from its signature. By a symmetry of the signature we mean a symmetry of the underlying plane graph $S(\Gamma)$ 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. Since edge and angle labels around a face of $S(\Gamma)$ determine a unique region of $\Lambda$, each symmetry of the signature naturally induces a symmetry of the fullerene graph $\Gamma$ when looking at its model on the sphere.

It is proved in [6] that with one minor exception, a fullerene and its signature have the same symmetry group. The unique exception in which the two groups do not coincide is when the signature is either a path or a circuit with edge labels of the form $(p)$ or $(p,p)$ and the angle types are equal at each vertex. In this case both the identity and a reflexion of the sphere through the line or the circuit given on the sphere by $S(\Gamma)$ induce the identity on the signature graph.

In [7] J.E. Graver obtained results on the structure of fullerene signatures and constructed a complete catalog of fullerenes with ten or more symmetries. In [8] the complete catalog of their signatures is reported.

# 3 Totally symmetric Kekulé structures

In this section we examine all the infinite families of fullerenes with ten or more symmetries encoded in [8] in order to discover which of them have at least one TSKS.

We will denote by $S(G)$ the symmetry group of $S(\Gamma)$ and by $G$ the symmetry group of $\Gamma$.

The image of a single point of the planar embedding $S(\Gamma)$ on $\Lambda$ under the action of $S(G)$ form an orbit of the action. We call a *fundamental domain* of $S(\Gamma)$ a subset of the points of $\Lambda$ which contain exactly one point from each of these orbits.

When speaking of an edge (respectively a vertex or a center) of $\Lambda$ we will mean an edge (respectively a vertex or a center) of an hexagon in the hexagonal tessellation.

When considering a closed region $T$ of $\Lambda$, we will say that a vertex $v$ of $\Lambda$ belongs to $T$

if $v$ is either in the interior or on the boundary of $T$. We also will say that a set of edges saturates a set of vertices if each vertex of the set is the end vertex of at least one edge.

A segment with Coxeter coordinates $(p)$, for some $p$, will be called a *central direction segment*, while a segment with Coxeter coordinates $(p, p)$ will be called an *edge direction segment*. In the same manner, a straight line on $\Lambda$ containing a central direction segment (resp. an edge direction segment) will be called a *central direction* (resp. an *edge direction*) *line*.

### 3.1 Fullerenes with symmetry group $I$,$I_h$, $T$, $T_d$ or $T_h$

We consider fullerenes which have either icosahedral or tetrahedral symmetries. In [1], the authors make the following remark: in order to have the existence of a TSKS, the number of atoms of the fullerene must be divisible by 12. Using the catalog of [8], which reveals the number of atoms for each fullerene together with the leapfrog condition on the parameters forming this number, we can check case by case all fullerenes with symmetry group $I$,$I_h$, $T$, $T_d$ or $T_h$. Easy counting, we verify that the number of atoms is divisible by 12 if and only if the leapfrog conditions on the parameters are verified. Therefore, the following Lemma 3.1 follows trivially:

**Lemma 3.1.** *A fullerene $\Gamma$ with a icosahedral or a tetrahedral symmetry group has a TSKS if and only if it is leapfrog.*

Furthermore, the following lemma holds:

**Lemma 3.2.** *Let $\Gamma$ be a leapfrog fullerene. No order 3 symmetry of $\Gamma$ has a fixed vertex.*

*Proof.* The order (i.e. the number of vertices) of a leapfrog fullerene $\Gamma$ is a multiple of 3 by the very definition of leapfrog fullerene. An automorphism of $\Gamma$ of order 3 with a fixed vertex is a rotation by an axis, so it has either 1 or 2 fixed vertices: in both cases the order of $\Gamma$ is not divisible by 3, a contradiction. □

Combining the previous considerations, we can claim that our main theorem holds at least for the subclasses of icosahedral and tetrahedral fullerenes.

**Proposition 3.3.** *A fullerene $\Gamma$ with a icosahedral or a tetrahedral symmetry group has a TSKS if and only if no order 3 symmetry of $\Gamma$ has a fixed vertex.*

## 3.2 Fullerenes with symmetry group $D_5$, $D_{5h}$, $D_{5d}$, $D_6$, $D_{6h}$ or $D_{6d}$

We consider fullerenes with at least ten symmetries and whose automorphism group admits either a rotation of order 6 or a rotation of order 5. For all these fullerene graphs the following holds:

**Proposition 3.4.** *No automorphism of order* 3 *fixes a vertex of the fullerene.*

*Proof.* This is obvious if the group is $D_5$, $D_{5h}$ or $D_{5d}$ since these groups do not contain an element of order 3. In all the other cases, one can easily check that the number of vertices of $\Gamma$ is a multiple of 3. Since a rotation of order 3 fixes at most two vertices and all the other vertices are divided into orbits of length 3, then the number of fixed vertices is necessarily zero. □

**Proposition 3.5.** *Each fullerene having full automorphism group* $D_6$*,* $D_{6h}$ *or* $D_{6d}$ *has a totally symmetric Kekulé structure.*

*Proof.* We consider the three cases $D_6$, $D_{6h}$ or $D_{6d}$ separately.

Suppose the symmetry group of $\Gamma$ to be the dihedral group $D_6$.

Take an hexagon $\Sigma$ on $\Lambda$ whose vertices are vertices of $S(\Gamma)$ and which is fixed by an order 6 rotation of $G(S)$. More precisely, looking at the catalog, if $\Gamma$ is one of the fullerenes in a family $\mathcal{D}_i$, $i = 5, \ldots 13$, take the hexagon $\Sigma$ whose vertices are alternated vertices on the circuit representing the signature, otherwise, if $\Gamma$ is not a fullerene in such a family, take as $\Sigma$ the internal hexagonal face of the signature (or equivalently the external one). Except for the fullerenes in $\mathcal{D}_{12}$, a fundamental domain $\mathcal{W}$ of $S(\Gamma)$ is individuated by a quadrilateral face with the following vertices: the center $C$ of the chosen hexagon (i.e. the unique point of the hexagon fixed by the rotation), two consecutive vertices of $\Sigma$, say $A$ and $B$, a vertex $D$ of $S(\Gamma)$ connected by a segment of $S(\Gamma)$ to both $A$ and $B$, if it exists, or connected to $A$ by a segment of $S(\Gamma)$ and not on $\Sigma$.

When $\Gamma \in \mathcal{D}_{12}$, a fundamental domain $\mathcal{W}$ for $S(\Gamma)$ is individuated by a triangle of $\Lambda$ with vertices $A$, $B$, $C$, where $C$ is the center of $\Sigma$ and $A$ and $B$ are consecutive vertices of $\Sigma$ (see Figure 3.1).

In this particular case, take the set $F$ of all edges of $\Lambda$ whose direction is orthogonal to $AB$ and having at least one vertex inside the triangle $\mathcal{W}$. When we look at the planar embedding of $\Gamma$ on the sphere, $F$ is a set of independent edges of $\Gamma$ and the orbit of $F$ induced by the action of $D_6$ on $\mathcal{W}$ gives a TSKS for $\Gamma$ (see Figure 3.1).

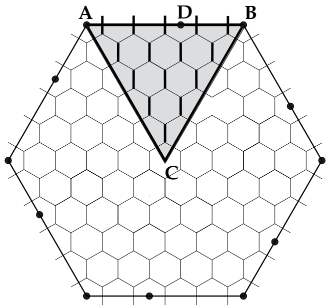


Figure 3.1

Now go back to $\Gamma \notin \mathcal{D}_{12}$.

The triangle $ABC$ is equilateral and its edges have either Coxeter coordinates $(p)$, $p > 0$, or $(p, q)$, $p, q > 0$. If either $p$ is odd in the first case, or both $p$ and $q$ are odd in the latter, the middle point of at least one of the segments $AD$ or $BD$ is the middle point of an edge of $\Lambda$. In fact, in both cases, the middle point $M$ of $AB$ lies on an edge of $\Lambda$, now let $P$ and $Q$ be the middle points of $AD$ and $BD$ respectively, obviously $QM$ and $PA$ are parallel in the plane $\Lambda$ and with the same length, as $A$ is a center of $\Lambda$ and $M$ is not, necessarily $P$ and $Q$ cannot both be center of $\Lambda$.

Suppose $AB$ to have Coxeter coordinates $(p, q)$. From each vertex of $\Sigma$, draw the central direction lines of $\Lambda$ thus forming two regular hexagons inside $\Sigma$. The edges of these hexagons are segments of Coxeter coordinates $(p)$, respectively $(q)$. Without loss of generality. we suppose $(p)$ even in the case in which at least one of $p$ and $q$ is even. We denote by $\Sigma_1$ the hexagon with side of length $p$ .

If $AB$ has Coxeter coordinates $(p)$, set $\Sigma_1 = \Sigma$.

We thus have the following possibilities: the edges of $\Sigma_1$ are segments with even coordinates $(p)$ or the edges of $\Sigma_1$ are segments of odd coordinates $(p)$. The latter occurs when either $AB$ has coordinates $(p, q)$ with both $p$ and $q$ odd, or $AB$ has coordinate $(p)$ with $p$ odd.

Suppose $\Sigma \neq \Sigma_1$ (see Figure 3.2 when $p$ is even and Figure 3.3 when $p$ is odd).

Let $\mathcal{T}$ be the triangle $A'B'C$, where $A'$ and $B'$ are consecutive vertices of $\Sigma_1$ such that $B'$ is inside the triangle $ABC$ while $A'$ is outside. Without loss of generality, suppose $AC$ to cross $\mathcal{T}$. A fundamental domain $\mathcal{W}'$ for $S(\Gamma)$ is individuated by taking the quadrilateral $BCAD$ and substituting the triangle $CB'B$ with the triangle $CA'A$.

Suppose $p$ is even.

Let $F_1$ be a set of independent edges of $\Lambda$ constructed as follows: let $M_1$, $M_2$, $M_3$ be the middle points of $A'B'$, $B'C$, $A'C$ respectively, draw the lines connecting $M_1$ with $M_2$ and $M_1$ with $M_3$ and set in $F_1$ all the edges of $\Lambda$ which are orthogonal to $A'B'$ and saturating the vertices of the quadrilateral $CM_2M_1M_3$, together with all the edges of $\Lambda$ orthogonal to $B'C$ (resp. $A'C$) and saturating the vertices of $M_1M_2B'$ (resp. $M_1M_3A'$). Now let $F_2$ be a set of independent edges of $\Lambda$ which are neither orthogonal to $AA'$ nor to $A'B$ and saturating the vertices of $BA'AD$. Set $F = F_1 \cup F_2$. The orbit of $F$ induced by the action of $D_6$ on $\mathcal{W}'$ gives a TSKS for $\Gamma$ (see Figure 3.2).

Suppose $p$ is odd.

If $p > 1$, take the vertices of $\Lambda$, say $A''$ and $B''$ on $CA'$ and $CB'$ respectively, in such a way that $A''B''$ has Coxeter coordinates $(p-1)$. Proceed with the triangle $CA''B''$ as done above for the triangle $A'B'C$ when $p$ was supposed to be even, and construct a set $F_1$ of independent edges saturating the vertices of $CA''B''$. These edges do not cross $A''B''$ and an odd number of vertices of $\Lambda$ is inside the quadrilateral $B'B''A''A'$. For what observed at the beginning of our proof, at least one of the segments $BD$ or $AD$ (say $BD$) has its middle point on the middle point of an edge $f$ of $\Lambda$. Choose an alternating path $\mathcal{Z}$ on the edges of $\Lambda$ inside $\mathcal{W}'$ and which connects $f$ with an edge $e$ crossing $A'B'$. Pair the vertices inside $B'B''A''A'$ which are not on $e$, to obtain an independent set $F_4$ of edges of $\Lambda$. Set $F_3 = F_1 \cup F_4 \cup \{e\}$.

If $p = 1$ simply set $F_3 = \{e\}$.

Let $F_2$ be a set of independent edges of $\Lambda$ which are neither orthogonal to $A'B$ nor to $A'A$ and saturating the vertices of $BA'AD$. If no edge in $F_2$ shares a vertex with $e$ set $F = F_2 \cup F_3$. Otherwise let $\bar{F}_2 = (F_2 - \mathcal{Z}) \cup (\mathcal{Z} - F_2)$ and set $F = \bar{F}_2 \cup F_3$. The orbit of $F$ induced by the action of $D_6$ on $\mathcal{W}'$ gives a TSKS for $\Gamma$ (see Figure 3.3).

Finally, if $\Sigma = \Sigma_1$, repeat the previous constructions simply taking $A' = A$, $B' = B$ and $\mathcal{W} = \mathcal{W}'$.

Suppose the symmetry group of $\Gamma$ to be the dihedral group $D_{6d}$.

Take an hexagon $\Sigma$ on the plane $\Lambda$ whose vertices are vertices of $S(\Gamma)$ and which is fixed by a rotation of $G(S)$ of order 6. More precisely, looking at the catalog, if $\Gamma$ is one of the fullerenes in $\mathcal{F}_i$, $i \in 1, 2, 4, 5$, take as $\Sigma$ the internal hexagonal face of the signature (or equivalently the external one) and observe that each edge of $\Sigma$ is either a central direction

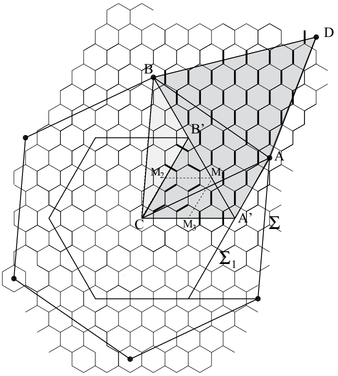


Figure 3.2

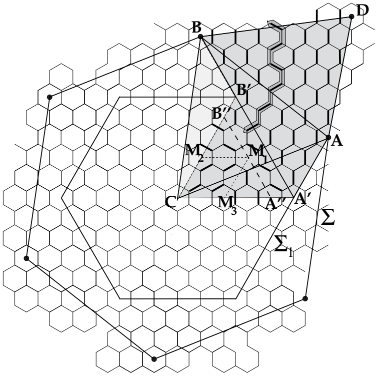


Figure 3.3

segment or an edge direction segment according to whether $i = 1, 4$ or $i = 2, 5$. If $\Gamma$ is one of the fullerenes in $\mathcal{D}_i$, $i \in 2, 3, 4$ take the hexagon $\Sigma$ whose vertices are alternated vertices on the circuit representing the signature. Also in these cases the edges of $\Sigma$ are either central direction segments or edge direction segments.

A fundamental domain $\mathcal{W}$ for $S(\Gamma)$ is individuated by a triangle $BCD$ obtained as follows: $C$ is the center of the chosen hexagon (i.e. the unique point of the hexagon fixed by the rotation), $A$ and $B$ are consecutive vertices of $\Sigma$ and $D$ is a vertex of $S(\Gamma)$ which is adjacent in $S(\Gamma)$ to both $A$ and $B$. If the segment $AB$ is a central direction segment, let $F$ be the set of independent edges of $\Lambda$ which are orthogonal to $AB$ and which saturates the vertices of the triangle $BCD$. If the segment $AB$ is an edge direction segment, let $F$ be the set of independent edges of $\Lambda$ which are parallel to $BC$ and saturating the vertices of the triangle $BCD$.

The orbit of $F$ induced by the action of $D_{6d}$ on $\mathcal{W}$ gives a TSKS for $\Gamma$ (see Figure 3.4).

Suppose the symmetry group of $\Gamma$ to be the dihedral group $D_{6h}$.

This group contains a reflection by a plane which exchanges the northern and the southern hemisphere of the geodesic dome. In order to be preserved by this involution, the edges of a TSKS lies on the equator or are perpendicular to it in the planar representation $\Lambda$.

Suppose $\Gamma$ to be in $\mathcal{E}_i$, $\;i = 1, 2$. Denote by $\Sigma$ the internal hexagonal face of $S(\Gamma)$.

A fundamental domain $\mathcal{W}$ for $S(\Gamma)$ is individuated by a quadrilateral $ABCD$ obtained

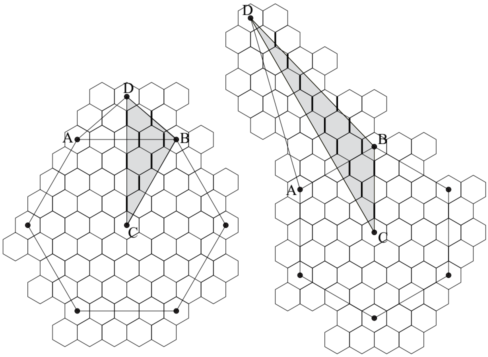


Figure 3.4

as follows: $C$ is the center of the chosen hexagon (i.e. the unique point of the hexagon which fixed by the rotation), $B$ and $B'$ are consecutive vertices of $\Sigma$, $A$ is the middle point of the segment of $S(\Gamma)$ containing $B$ and not lying on the hexagon, $D$ is a point on the equator such that the line $CD$ is perpendicular to $BB'$ on the plane $\Lambda$.

If $\Gamma$ is a fullerene of $\mathcal{E}_2$, let $F$ be the set of all the independent edges of $\Gamma$ perpendicular to the equator and which saturates the vertices of $\mathcal{W}$.

If $\Gamma$ is a fullerene of $\mathcal{E}_1$, let $E$ be a point on $CD$ which is the center of an hexagon of $\Lambda$ adjacent to the hexagon of the tessellation containing $D$. Let $F_1$, respectively $F_2$, be the set of all the independent edges of $\Gamma$ parallel to the equator, respectively to $BC$, and which saturates the vertices of the triangle $DEA$, respectively of the quadrilateral $CBAE$. Set $F = F_1 \cup F_2$.

In all the above cases, the orbit of $F$ induced by the action of $D_{6h}$ on $\mathcal{W}$ gives a TSKS for $\Gamma$ (see Figure 3.5).

Now suppose $\Gamma$ to be in $\mathcal{D}_1$. Let $C$ be the center of the circuit representing $S(\Gamma)$. Let $M_1$ and $M_2$ be the middle points of two consecutive segments of $S(\Gamma)$ with common vertex $A$. Without loss in generality, we can choose $M_1$ and $M_2$ in such a way that the edges of $\Gamma$ with a point on $AM_1$ lie on the circuit, while those with a point on $AM_2$ are perpendicular to it. Therefore all the edges of $\Gamma$ with a point on $CM_2$ are parallel to $CM_2$, while those with a point on $CM_1$ are perpendicular to $CM_1$. A fundamental domain $\mathcal{W}$ for $S(\Gamma)$ is individuated by the quadrilateral $CM_1AM_2$.

Let $E$ be a point on $CM_1$ and the center of an hexagon of $\Lambda$ adjacent to the hexagon of the tessellation containing $M_1$.

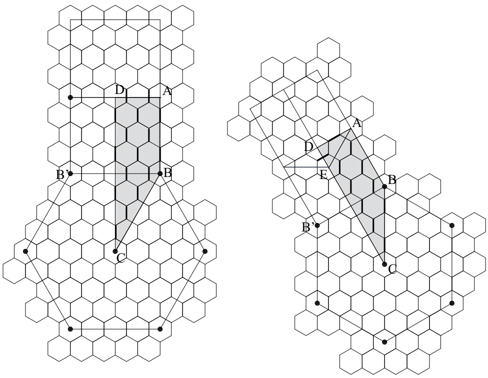


Figure 3.5

Let $F_1$, respectively $F_2$, be the set of all the independent edges of $\Gamma$ parallel to $AM_1$, respectively to $CM_2$, and saturating the vertices of the triangle $EM_1A$, respectively of the quadrilateral $CEAM_2$. Set $F = F_1 \cup F_2$.

In all the above cases, the orbit of $F$ induced by the action of $D_{6h}$ on $\mathcal{W}$ gives a TSKS for $\Gamma$ (see Figure 3.6).

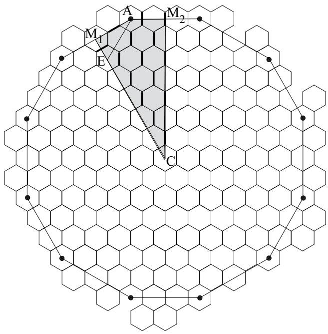


Figure 3.6

□

**Proposition 3.6.** *Each fullerene having full automorphism group $D_5$, $D_{5h}$, $D_{5d}$ has a totally symmetric Kekulé structure.*

*Proof.* First of all, we prove that the signature of a fullerene $\Gamma'$ with an order 5 rotation in its automorphism group can be reconstructed from the signature of a fullerene $\Gamma$ admitting a rotation of order 6. Further we observe that a TSKS for $\Gamma'$ can be obtained from a TSKS for $\Gamma$.

Let $S(\Gamma)$ be a signature admitting a rotation of order 6. Follow the proof of Proposition 3.5 together with its notations. Let $C$ and $C'$ be the antipodal points on the sphere which are fixed by the rotation. Add the two points $C$ and $C'$ to $S(\Gamma)$.

When $S(\Gamma)$ is a 12−gon, draw all segments joining alternatively $C$ with the vertices of the 12−gon of the signature, together with all segments joining $C'$ with the remaining vertices on the 12−gon.

If $S(\Gamma)$ is not a 12−gon, follow the notation of Proposition 3.5 and take the hexagon $\Sigma$ (with center $C$) together with the external face of $S(\Gamma)$, i.e. an hexagon $\Sigma'$ with center $C'$, and draw all segments joining $C$ with a vertex of $\Sigma$, together with all segments joining $C'$ with a vertex of $\Sigma'$.

Starting from the fundamental domain $\mathcal{W}$ exhibited in the proof of Proposition 3.5, we construct on the sphere a connected region $\bar{\mathcal{W}}$ which is a fundamental domain for the group generated by the rotation.

More precisely, when $D_6$ is the full automorphism group of $\Gamma$, we set $\bar{\mathcal{W}} = \mathcal{W} \cup \mathcal{W}_1$ where $\mathcal{W}_1$ is obtained by applying to $\mathcal{W}$ a reflection of $D_6$ in such a way that $\mathcal{W}$ and $\mathcal{W}_1$ share the edge $AD$ ($AB$ if the family is $\mathcal{D}_{12}$).

When $D_{6d}$ is the full automorphism group of $\Gamma$, we set $\bar{\mathcal{W}} = \mathcal{W} \cup \mathcal{W}_1 \cup \mathcal{W}_2$. Where $\mathcal{W}_1$ is obtained from $\mathcal{W}$ by the reflection fixing $CD$, and $\mathcal{W}_2$ is obtained by applying an element of $D_{6d}$ to $\mathcal{W} \cup \mathcal{W}_1$ in such a way that $\mathcal{W}_2$ and $\mathcal{W} \cup \mathcal{W}_1$ share the edge $BD$.

When $D_{6h}$ is the full automorphism group of $\Gamma$, we set $\bar{\mathcal{W}} = \mathcal{W} \cup \mathcal{W}_1 \cup \mathcal{W}_2$. Where $\mathcal{W}_1$ is obtained from $\mathcal{W}$ by the reflection fixing $CM_1$, and $\mathcal{W}_2$ is obtained by the reflection fixing the equator, i.e. the 12−gon of $S(\Gamma)$.

Now delete all the points of the sphere which are internal to $\bar{\mathcal{W}}$ and identify the points on the boundary using the order 6 rotation. We thus obtain the signature graph $S(\Gamma')$ of a fullerene admitting a rotation of order 5. More precisely, there is a correspondence between fullerenes with a rotation of order 6 and fullerenes with a rotation of order 5. This correspondence is provided in the following table:

| | | |
|---|---|---|
| $\mathcal{E}_i$ | $\mathcal{H}_i$ | $i = 1, 2, 3, 4, 5, 6, 7$ |
| $\mathcal{D}_i$ | $\mathcal{I}_{i-1}$ | $i = 2, 3, 4, 5, 6, 7$ |
| $\mathcal{D}_8$ | $\mathcal{I}_7/\mathcal{I}_8$ | |
| $\mathcal{D}_i$ | $\mathcal{I}_i$ | $i = 9, 10, 11, 12, 13$ |
| $\mathcal{D}_1$ | $\mathcal{G}_1$ | |
| $\mathcal{A}_i$ | $\mathcal{F}_i$ | $i = 4, 5, 6, 7$ |
| $\mathcal{A}_i$ | $\mathcal{F}_i$ | $i = 1, 2, 3$ $*$ |

$*$: Note that the full automorphism groups for families $\mathcal{A}_i$ $(i = 1, 2, 3)$ are not $D_6, D_{6d}$ nor $D_{6h}$.

It is also obvious that the fundamental domain $\mathcal{W}$ of $S(\Gamma)$ is a fundamental domain for $S(\Gamma')$ itself. Therefore, the existence of a TSKS in the first case, see Proposition 3.5, naturally extends to the existence of a TSKS in the second one. □

## 3.3 Fullerenes with symmetry group $D_{3h}$ or $D_{3d}$

In this section, we will prove the following Proposition:

**Proposition 3.7.** *Except for all graphs in $\mathcal{P}_4 \cup \mathcal{P}_5$, with $r = 3$, $s = 1$ and $p$ even, each fullerene preserved by either a $D_{3h}$ or $D_{3d}$ symmetry group has a totally symmetric Kekulé structure if and only if each automorphism of order 3 does not fix any vertex.*

First of all observe that all fullerene graphs of the family $\mathcal{K}_4$ are leapfrog, and so a TSKS always exists in this case. Moreover, the requested condition of Proposition 3.7 is assured.

For the other families to be considered, one of the main tool used in the construction of a TSKS is the decomposition of a fundamental domain into internal disjoint regions: a set of representatives for the edges of a TSKS is obtained by fixing a suitable direction for each region, and then taking the union of all the edges saturating the vertices of the region and parallel to the associated direction.

The families covered by a construction of this type are presented in the first table below. In some cases this approach must be slightly modified. Namely, for the remaining families presented in the second table below, a direction for each region is chosen, together with all edges in that direction saturating the maximum number of vertices of the region. Some edges are then deleted or added in a suitable manner, in order to obtain, by the union of the selected edges in each region, a set of representatives for the edges of a TSKS.

In all these cases, the automorphism group contains an order 3 rotation, say $\alpha$. This rotation fixes either two vertices of $\Gamma$ or the centers of two hexagons of $\Lambda$, it depends upon the values assigned to the Coxeter coordinates. Obviously the points fixed (vertices or centers) correspond in the reflection exchanging the northern with the southern hemisphere. Since we are looking for the existence of a TSKS, in all these families, we will focus our attention on those Coxeter coordinates for which $\alpha$ fixes the centers, $C$ and $C'$, of two hexagons.

In the following two tables, we refer to the parameters contained in the catalog of [8] and report the necessary conditions to be satisfied to be sure that $\alpha$ fixes the centers of two hexagons. Our constructions below will respect the conditions on the parameters. If no condition is reported in the tables, then each value for the parameters of [8] is permitted. Without loss in generality, we will denote by $C$ be the center of the signature graph $S(\Gamma)$ represented on the plane.

The constructions that we will provide, do not work in the sporadic cases $\mathcal{P}_4$, with $r = 3$, $s = 1$ and $p$ even, and $\mathcal{P}_5$ with $r = 3$, $s = 1$, even if the Coxeter coordinates respect the necessary condition for $C$ to be the center of an hexagon. These cases will be treated in the last paragraph. Here the non-existence of a TSKS will be proved.

| | | |
|---|---|---|
| $D_{3h}$ | $\mathcal{K}_2, \mathcal{L}_1$ | |
| $D_{3d}$ | $\mathcal{P}_1$, $\mathcal{P}_2$,$\mathcal{P}_3$,$\mathcal{R}_3$,$\mathcal{R}_4$,$\mathcal{R}_5$, $\mathcal{R}_7$ | |
| $D_{3d}$ | $\mathcal{E}_{11}$ | |
| $D_{3h}$ | $\mathcal{J}_1$, $\mathcal{M}_1$, $\mathcal{M}_3$, $\mathcal{N}_2$, $\mathcal{O}_1$ | |
| $D_{3h}$ | $\mathcal{K}_1$, $\mathcal{K}_3$ , $\mathcal{E}_8$ | $r \equiv 0 \pmod 3$ |
| $D_{3h}$ | $\mathcal{M}_2$ | $s \equiv 0 \pmod 3$ |
| $D_{3h}$ | $\mathcal{N}_1$, $\mathcal{O}_2$ , $\mathcal{O}_3$ | $r + s \equiv 0 \pmod 3$ |
| $D_{3h}$ | $\mathcal{E}_9$ | |
| $D_{3d}$ | $\mathcal{R}_1$, $\mathcal{R}_2$ | $r \equiv 0 \pmod 3$ |
| $D_{3d}$ | $\mathcal{R}_6$ | $p \equiv 0 \pmod 3$ |

| | | |
|---|---|---|
| $D_{3d}$ | $\mathcal{D}_{14}$ | $r \equiv 0 \pmod 3$ |
| $D_{3h}$ | $\mathcal{J}_2$ | $r \equiv 0 \pmod 3$ |
| $D_{3h}$ | $\mathcal{E}_{10}$ | $s \equiv 0 \pmod 3$ |
| $D_{3d}$ | $\mathcal{E}_{12}$, $\mathcal{P}_4$,$\mathcal{P}_5$,$\mathcal{P}_6$ | $r \equiv 0 \pmod 3$ |
| $D_{3d}$ | $\mathcal{P}_7$ | $p + s \equiv 0 \pmod 3$ |
| $D_{3d}$ | $\mathcal{Q}_1$ | $r \equiv p + s \ (mod 3)$ |

Construction of a TSKS for families $\mathcal{K}_2$ and $\mathcal{L}_1$

Let us denote by $P_1$ and $P_2$ two vertices of $S(\Gamma)$ such that the angle between $CP_1$ and $CP_2$ has value 1. In $S(\Gamma)$, $P_1$ (resp. $P_2$) is connected by an edge direction segment to its image $P_1'$ (resp. $P_2'$) obtained by the planar reflection exchanging the two hexagons with centers $C$ and $C'$ respectively. Let us denote by $A_1$ (resp $A_2$) the middle point of $P_1P_1'$ (resp. $P_2P_2'$). The region $CP_1A_1A_2P_2$ is a fundamental domain for $S(\Gamma)$. Let $S$ be the set of all the edges orthogonal to $A_1A_2$ and which saturates the vertices of this domain. A TSKS for $\Gamma$ is obtained by the orbit of $S$ induced by the action of $D_{3h}$ on the domain. See Figure 3.7 for $\mathcal{K}_2$, a quite similar Figure could be drawn for $\mathcal{L}_1$.

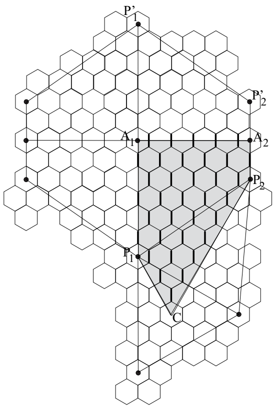


Figure 3.7

Construction of a TSKS for families $\mathcal{P}_1$, $\mathcal{P}_2$,$\mathcal{P}_3$,$\mathcal{R}_3$,$\mathcal{R}_4$,$\mathcal{R}_5$, $\mathcal{R}_7$

Let $P_1$ be a vertex of the central triangular face of $S(\Gamma)$ containing $C$. Let $P_2$ be a vertex of $S(\Gamma)$ such that $CP_2$ is a central direction segment and the angle $P_1CP_2$ has value 1.

Observe that one of the two vertices $P_i$ has the property that there exists another vertex $P_3$ of $S(\Gamma)$ such that the segment $P_iP_3$ is an edge direction segment. It turns out that the region $CP_1P_2P_3$ is a fundamental domain for $S(\Gamma)$. Consider the set $S$ of all the edges parallel to the segment $P_1P_3$ and saturating the vertices of the domain. A TSKS is obtained by the orbit of $S$ induced by the action of $D_{3d}$ on the domain. See Figure 3.8 which refers to $\mathcal{P}_1$, for the other families the situation is similar.

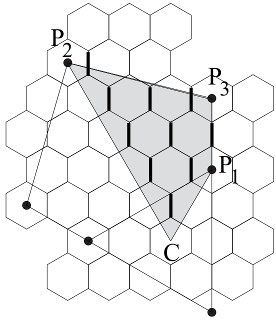


Figure 3.8

Construction of a TSKS for family $\mathcal{E}_{11}$

Let $P_1, P_2, P_3$ be three consecutive vertices of the central hexagonal face of $S(\Gamma)$ containing $C$. Let $Q_1, Q_2$ denote the vertices of $S(\Gamma)$ such that $P_1P_2Q_2Q_1$ is a face of $S(\Gamma)$. Let $A$ (resp. $B$) be the middle point of $P_2P_3$ (resp. $Q_1Q_2$). The region $CAP_2Q_2B$ is a fundamental domain for $S(\Gamma)$. Note that $P_2A$ is in the same orbit as $BQ_2$ under the action of the group. Now consider two central direction lines $L_1, L_2$ through $P_2$ such that their respective intersections $D$ and $E$ with $CA$ and $CB$ are contained in the hexagonal face centered in $C$. Let $S_1$ be the set of edges not perpendicular to $CA$ nor to $CE$ and which saturate all vertices of the region $CDP_2E$, let $S_2$ be the set of edges parallel to $P_2A$ which saturate all vertices of the region $DAP_2$, finally let $S_3$ be the set of edges parallel to $BQ_2$ and which saturate all vertices of $EP_2Q_2B$. The orbit of $S_1 \cup S_2 \cup S_3$ induced by the action of $D_{3d}$ on the domain gives a TSKS (see Figure 3.9).

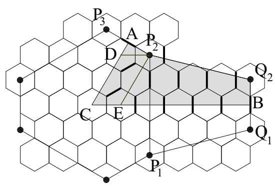


Figure 3.9

Construction of a TSKS for families $\mathcal{J}_1$, $\mathcal{M}_1$, $\mathcal{M}_3$, $\mathcal{N}_2$, $\mathcal{O}_1$

In all these families, if we consider the embedding $S(\Gamma)$ of the signature on the sphere and we draw the geodetic line connecting $C$ and $C'$, then this line gives rise to a central direction segment of $\Lambda$. Denote by $A$ the middle point of this segment. Let $P_1$ be a vertex of $S(\Gamma)$ such that $CP_1$ is a central direction segment and makes an angle of type 1 with $AC$.

Let $\Gamma \in \mathcal{J}_1$. Let $P_2$ a vertex of $S(\Gamma)$ which is linked to $P_1$ and which is not a vertex of the central triangular face of $S(\Gamma)$. The image $P_2'$ of $P_2$ by the planar reflexion exchanging the northern with the southern emisphere, defines a segment $P_2P_2'$ parallel to $CA$. Denote by $B$ the middle point of $P_2P_2'$. It turns out that the region $CP_1P_2BA$ is a fundamental domain for $S(\Gamma)$. From $P_2$ draw the line parallel to $CP_1$ and let $D$ be its intersection with the segment $CA$. Let $S_1$ be the set of all the edges parallel to $AB$ and saturating all the vertices of $DABP_2$. Let $S_2$ be the set of all the edges parallel to $P_1P_2$ and saturating all the vertices of $CP_1P_2D$. A TSKS is obtained by the orbit of $S_1 \cup S_2$ induced by the action of $D_{3h}$ on the domain (see Figure 3.10).

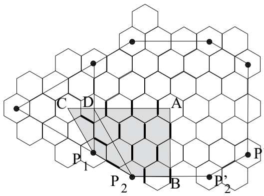


Figure 3.10

In the cases $\mathcal{M}_1$, $\mathcal{M}_3$, $\mathcal{N}_2$ and $\mathcal{O}_1$, let $P_1'$ be the image of $P_1$ by the reflection exchanging the northern and the southern hemisphere and let $B$ be the middle point of $P_1P_1'$. From $B$, in the direction perpendicular to $BP_1$, is located a vertex $P_2$ of $S(\Gamma)$, such that $AP_2$ is perpendicular to $CA$. It turns out that the region $ACP_1BP_2$ is a fundamental domain for $S(\Gamma)$. From $P_2$ draw the line parallel to $CP_1$ and let $D$ be its intersection with the segment $CA$. Let $S_1$ be the set of all the edges parallel to $AP_2$ and saturating the vertices of the region $ADP_2$. Let $S_2$ be the set of all the edges parallel to $P_1B$ and saturating the vertices of the region $CP_1BP_2D$. A TSKS is obtained by the orbit of $S_1 \cup S_2$ induced by the action of $D_{3h}$ on the domain (see Figure 3.11).

Construction of a TSKS for families $\mathcal{K}_1$, $\mathcal{K}_3$, $\mathcal{E}_8$, $\mathcal{M}_2$, $\mathcal{N}_1$ $\mathcal{O}_2$, $\mathcal{O}_3$, $\mathcal{E}_9$

Let $\Gamma \in \mathcal{K}_1 \cup \mathcal{K}_3 \cup \mathcal{E}_8$. Let $P_1$ and $P_2$ be two vertices of $S(\Gamma)$ such that $CP_1$ and $CP_2$ are edge direction segments and $P_1CP_2$ is an angle of value 1. Without loss in generality, let $P_1$ be the furthest from $C$. Let $P_1'$ and $P_2'$ be respectively the image of $P_1$ and $P_2$

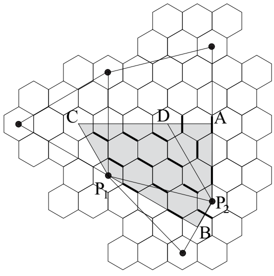


Figure 3.11

by the reflection exchanging the northern and the southern hemisphere, and let $A$ (resp. $B$) be the middle point of $P_1P_1'$ (resp. $P_2P_2'$). The region defined by $CP_1ABP_2$ is a fundamental domain for $S(\Gamma)$. This fundamental domain can be divided into 3 internal disjoint regions. Namely: draw a central direction line, say $s$, through $C$, thus dividing the angle $P_1CP_2$ into two equal parts. Now, consider the central direction line through $P_1$ forming an angle of type 0.5 with the segment $CP_1$ and intersecting the fundamental domain. Let $D$ denote its intersection with the line $s$. Let $E$ be a point on the segment $P_2B$ such that $DE$ is a central direction segment and forms an angle of type 2 with $CD$. Let $S_1$ be the set of all edges parallel to $CP_2$ and saturating all the vertices of the region $CDEP_2$. Let $S_2$ be the set of all edges parallel to $AB$ and saturating all vertices of the region $DEBAP_1$. Let $S_3$ be the set of all edges parallel to $CP_1$ and saturating all vertices of the region $CDP_1$. A TSKS is obtained by the orbit of $S_1 \cup S_2 \cup S_3$ induced by the action of $D_{3h}$ on the domain. See Figure 3.12 for the family $\mathcal{K}_1$, for the other families it is quite similar.

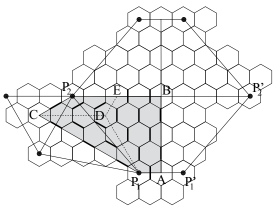


Figure 3.12

Let $\Gamma \in \mathcal{M}_2 \cup \mathcal{N}_1 \cup \mathcal{O}_2 \cup \mathcal{O}_3$. Draw the three edge direction lines from $C$. These lines join $C$ with three points of $S(\Gamma)$ which form a triangle. Let $P_1$ be one of these points. Let $P_2$ be a vertex of $S(\Gamma)$, consecutive to $P_1$, not lying on the triangle, and on

the same hemisphere of $C$ and $P_1$. Draw a line connecting $C$ and $C'$, forming an edge direction segment on $\Lambda$ and forming an angle of type 1 with $CP_1$. Let $A$ be the middle point of this segment. Let $P_1'$ be the image of $P_1$ by the reflection which exchanges the northern and the southern hemisphere. Let $B$ be the middle point of the segment $P_1P_1'$. The region $CP_1BP_2A$ is a fundamental domain for $S(\Gamma)$. This fundamental domain can be divided into 3 regions. Namely: draw a central direction line, say $s$, passing through $C$, and dividing the angle $P_1CA$ into two equal parts. Now, let $A'$ be the center of the hexagon on $AP_2$ that is the nearest to $A$ (with $A = A'$ if $A$ is the center of an hexagon). Take the central direction lines through $A'$ and $P_1$ respectively, which intersect $s$ insight the fundamental domain. Let $D$ denote the intersection that is the furthest from $C$. As in the previous case, $CD$ and the two lines through centers and that form with $CD$ an angle of type 2, define the division into three regions. We call $E$ the intersection between $P_1B$ and a line through $D$. Let $S_1$ be the set of all edges parallel to $BP_2$ and saturating all vertices of the region $DEBP_2A$. Let $S_2$ be the set of all edges parallel to $CA$ and saturating all vertices of the region $DA'AC$. Let $S_3$ be the set of all edges parallel to $CP_1$ and saturating all vertices of the region $CDEP_1$. A TSKS is obtained by the orbit of $S_1 \cup S_2 \cup S_3$ induced by the action of $D_{3h}$ on the domain.
See Figure 3.13 for the family $\mathcal{M}_2$, for the other families it is quite similar.

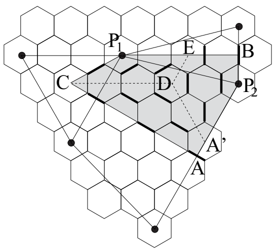


Figure 3.13

The case $\mathcal{E}_9$ is treated as follows. Let $P$ be a vertex of the hexagonal face of $S(\Gamma)$ that contains the point $C$, let $P_1$ and $P_2$ be the two vertices adjacent to $P$ in the face, and let $P_3$ be the vertex adjacent to $P$ not in the face. Now, define $A_i$ as the middle point of $PP_i$ for $i = 1, 2, 3$, $B_j$ as the orthogonal projection of $A_3$ on the line $CA_j$ for $j = 1, 2$. The central direction lines through $P$ meet $CA_i$ at $E_i$ $(i = 1, 2)$ with an angle $PE_iA_i$ of value 1. The fundamental domain is defined as the union of the three regions $CE_1PE_2$,

$PE_1B_1A_3$ and $PE_2B_2A_3$.

Let $S$ be the set of all edges orthogonal neither to $CE_1$ nor to $CE_2$ and saturating all vertices of the region $CE_1PE_2$. For $j \in \{1,2\}$, let $S_j$ be the set of all edges parallel to $A_3B_j$ and saturating all the vertices of the region $PE_jB_jA_3$. A TSKS is obtained by the orbit of $S \cup S_1 \cup S_2$ induced by the action of $D_{3h}$ on the domain.

See Figure 3.14 for the family $\mathcal{E}_9$, for the other families it is quite similar.

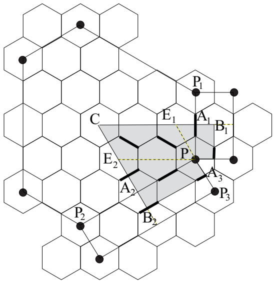


Figure 3.14

Construction of a TSKS for families $\mathcal{R}_1$, $\mathcal{R}_2$, $\mathcal{R}_6$

The center $C$ is the center of a triangle in $S(\Gamma)$. Let $P_1$ and $P_2$ be two vertices of this triangle, and let $A$ be the middle point of $P_1P_2$. Let $P_3$ be the vertex of the triangle $P_1P_2P_3$ of $S(\Gamma)$ which does not contain $C$. From $P_1$, draw the central direction line making a 2.5 angle with $P_1C$ and let $P_4$ be the vertex of $S(\Gamma)$ on this line such that $P_3P_4$ is a segment of $S(\Gamma)$. A fundamental domain for $S(\Gamma)$ is given by the region $CP_1P_4P_3$.

Draw from $C$ the central direction line $l$ which is the bisector of the angle $P_1CP_3$. The line $l$ intersects a central direction line through $P_3$ in the center $D$ of an hexagon of $\Lambda$ in such a way that $CDP_3$ is a 2 angle. Let $E$ be the center of an hexagon on $P_1P_4$ (eventually equal to $P_4$) such that $DE$ is a central direction segment and makes an angle of type 2 with $CD$. Now the fundamental domain is divided into three regions: $CP_1ED$, $CDP_3$, $EP_4P_3D$. Let $S_1$ be the set of all edges parallel to $CP_1$ and saturating all vertices of the region $CP_1ED$, let $S_2$ be the set of all edges parallel to $CP_3$ and saturating all vertices of the region $CDP_3$, let $S_3$ be the set of all edges perpendicular to $EP_4$ and saturating all vertices of the region $DEP_4P_3$. A TSKS is obtained by the orbit of $S_1 \cup S_2 \cup S_3$ induced by the action of $D_{3d}$ on the domain. See Figure 3.15 for family $\mathcal{R}_1$, for the other families it is quite similar.

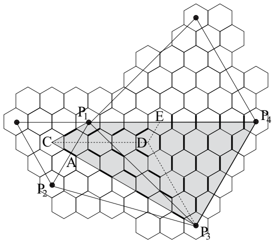


Figure 3.15

Construction of a TSKS for family $\mathcal{D}_{14}$

Consider three consecutive segments of $S(\Gamma)$, say $B'B$, $BA$, $AA'$ in such a way that $B'BA$ is an angle of type 2 and $BAA'$ is an angle of type 3. Let $L_1$, respectively $L_2$, be the middle point of the segment $AA'$, respectively of $BB'$. The region $CL_2BL_1$ is a fundamental domain for $\Gamma$. Let $t$ be the bisector line of the angle $L_2CL_1$ intersecting the segment $L_1B$ in a point $E$. Draw from $A$ the central direction line parallel to $BB'$ and intersecting $CE$ in a point $D$. Let $F$ be the intersection of the axis of $AB$ with the line through $D$ parallel to $AB$. The line from $F$ parallel to $CE$ intersects the segment $AB$ in a point $E'$. Let $S_1$ be the set of edges parallel to $CL_1$ and saturating all vertices of the region $CL_1AD$. Let $S_2$ be the set of edges parallel to $CL_2$ and saturating all vertices of the region $CDFE'BL_2$. Let $S_3$ be the set of edges saturating all vertices of the region $AEFD$ and not parallel neither to $AE$ nor to $AD$. Finally, let $S_4$ be the set of edges orthogonal to $EE'$ and saturating all vertices of the triangle $FEE'$. A TSKS is obtained by the orbit of $S_1 \cup S_2 \cup S_3 \cup S_4$ induced by the action of $D_{3d}$ on the domain (see Figure 3.16).

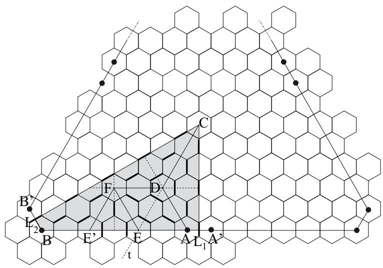


Figure 3.16

Construction of a TSKS for families $\mathcal{J}_2$ and $\mathcal{E}_{10}$

Let $\Gamma \in \mathcal{J}_2$. Consider the triangle of $\Lambda$ whose vertices are vertices of the central triangular face of $S(\Gamma)$ (obviously its center is $C$). Let $P_1$ be one of the vertices of this triangle, and $P_2$ be the vertex adjacent to $P_1$ in $S(\Gamma)$ not included in the triangular face. The vertex $P_2$ is adjacent in $S(\Gamma)$ to its image $P_2'$ by the reflection which exchanges the northern with the southern hemisphere. Let denote by $A$ the middle point of $P_2P_2'$, and $B$ the intersection of the line containing $A$ and orthogonal to $P_2A$ and that containing $C$, parallel to $P_2A$ and making a 1 angle with $CP_1$. The region $CP_1P_2AB$ is a fundamental domain for $\Gamma$.

The set of edges selected to generate a TSKS is constructed as follows: let $S_1$ be the set of all edges lying on the segment $CP_1$. Let $S_2$ be the set of all edges parallel to $CB$, with at least one vertex in the domain, except for those which have a vertex on $CP_1$. The edges of $S_1 \cup S_2$ do not saturate all vertices of the domain and to each vertex $v_i$ which is not covered, we associate an edge $e_i$, orthogonal to $AB$, in this manner: if the orthogonal projection $v_i'$ of $v_i$ on $AB$ is the middle of an edge, we associate this edge to $v_i$. Else, if not, $v_i'$ is exactly at the middle point between two edges crossing $AB$, and we associate $v_i$ to the one of these that is closest from $B$. For each $i$, take a path starting from $e_i$ and ending with an edge disjoint from $CP_1$ and with vertex $v_i$. It is always possible to choose these paths mutually disjoint. Delete from $S_2$ all the edges on these paths and substitute them with the remaining edges of the paths, thus obtaining a new set $S_2'$. The set $S = S_1 \cup S_2'$ saturates all vertices of the domain and the orbit of $S$ under the action of $D_{3h}$ gives rise to a TSKS for $\Gamma$ (see Figure 3.17).

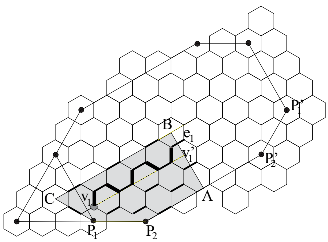


Figure 3.17

Let $\Gamma \in \mathcal{E}_{10}$. Consider the hexagon on $\Lambda$ whose vertices are the vertices of the central hexagonal face of $S(\Gamma)$ (obviously its center is $C$). Let $P_2P_1P_3$ be three consecutive vertices of this hexagon, with $P_2P_1$ longer than $P_1P_3$. Let denote by $D$ the middle point of $P_1P_2$ and by $E$ the middle point of $P_1P_3$. Let $D'$, $P_1'$ and $E'$ be the respective images of $D$, $P_1$ and $E$ by the reflection exchanging the northern and the southern hemisphere. The middle point $B$ of $DD'$ and the middle point $F$ of $EE'$ defines a line $BF$ that contains the middle point $A$ of $P_1P_1'$. The region $CFB$ is a fundamental domain for $\Gamma$. Take the center $Q$ internal to the segment $CE$ and such that the line containing $P_1Q$ is a central direction line. Consider the set $S_1$ of all edges parallel to $QE$ and saturating all vertices of the region $P_1AFQ$. Since the region $CQP_1AB$ is equal to the fundamental domain of $J_2$ considered in the previous construction above, we select a set $S$ of edges saturating all vertices of $CQP_1AB$ exactly as we did for $J_2$. Let $S' = S_1 \cup S$. The orbit of $S'$ under the action of $D_{3h}$ gives rise to a TSKS for $\Gamma$ (see Figure 3.18).

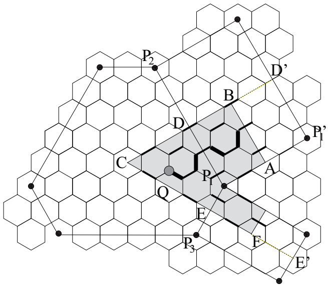


Figure 3.18

Construction of a TSKS for family $\mathcal{E}_{12}$

Let $\Gamma \in \mathcal{E}_{12}$. Consider the hexagon on $\Lambda$ whose vertices are the vertices of the central hexagonal face of $S(\Gamma)$ (obviously its center is $C$). Let $P_2P_1P_3$ be three consecutive vertices of this hexagon, with $P_3P_1$ longer than $P_1P_2$. Let $P_1', P_2', P_3'$ be vertices of $S(\Gamma)$ such that $P_1'$ is adjacent to $P_1$ but is not on the central hexagonal face, and such that $P_1P_1'P_2'P_2$ and $P_1P_1'P_3'P_3$ are two faces of $S(\Gamma)$.

Let $Q$, $R$ , $Q'$, $R'$ be the middle points of the segments $P_1P_3$, $P_1P_2$,$P_1'P_3'$ and $P_1'P_2'$ respectively. Consider the embedding of $S(\Gamma)$ on the sphere and let $A$ (respectively $B$) be the middle point of the segment $QQ'$ (resp. $RR'$). Let $F$ be the middle point of $AB$. The region defined by $ABC$ (or, more precisely, by $ABRP_1RC$) is a fundamental domain for $\Gamma$.

Let $E$ be a center internal to the segment $CR$ and such that the line containing $EP_1$

is a central direction line. Let $S_1$ be the set of all edges parallel to $ER$ and saturating all vertices of the region $EP_1FB$. Let $S_2$ be the set of all edges parallel to $CA$, saturating all vertices of the region $CEP_1FA$, but with no vertices on $CE$.

If $\frac{r}{3}$ is even, $F$ is at the center of an hexagon or in the middle of an edge parallel to $AC$. Choose $\frac{r}{6}$ edges crossing $AF$ and their respective images by a central symmetry through $F$. For each non-selected vertex, choose an alternating path from the vertex to an edge and reverse the selection of the edges along this path. The resulting selection gives a saturating set with edges parallel of perpendicular to the border of the fundamental domain, agreing with the group action.

If $\frac{r}{3}$ is odd, $F$ is in the middle of an edge. The set of not-covered vertices is divided into three parts, with $\frac{r}{6} - \frac{1}{2}$ vertices at each side of one vertex. Define an alternated path from the central uncovered vertex to $F$, and choose $\frac{r}{6} - \frac{1}{2}$ non-adjacent edges crossing $AF$, and their respective images by the central symmetry through $F$. Then choose alternating paths linking each not covered vertex to one of the edges, and reverse the selection along the alternating paths (see Figure 3.19).

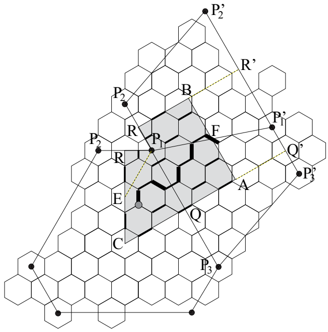


Figure 3.19

Construction of a TSKS for families $\mathcal{P}_4$, $\mathcal{P}_5$,$\mathcal{P}_6$,$\mathcal{P}_7$, $\mathcal{Q}_1$

Let $C$ be the center of an hexagon fixed by the rotation of order 3. Except for $\mathcal{Q}_1$, the point $C$ is included in a triangle in $S(\Gamma)$ whose segments are central direction segments. Let denote by $P_1$ a vertex of this triangle. For $\mathcal{Q}_1$, consider the triangle formed by the vertex of degree one which are insight the hexagonal face of the signature with center $C$. Also in this case, let denote by $P_1$ a vertex of this triangle. On the central direction line through $P_1$, making a $2,5$ angle with $P_1C$ lies a vertex $P_2$ of $S(\Gamma)$. Note that $P_1P_2$ is a segment of $S(\Gamma)$. An edge direction line through $C$, making a 1 angle with $P_1C$ meets a vertex $P_3$ of $S(\Gamma)$. Let $A$ denote the orthogonal projection of $P_2$ on the line $CP_3$, $B$ the middle point of $AP_3$ and $D$ the orthogonal projection of $B$ on the line parallel to $CP_3$ containing $P_2$. The fundamental domain is defined as $CBDP_2P_1$.

For all cases except $\mathcal{P}_4$, $r = 3$, $s = 1$, $p$ even and $\mathcal{P}_5$, $r = 3$, $s = 1$, we proceed as follows.

The automorphism group of $S(\Gamma)$ contains an involution exchanging the points $B$ and $D$ and fixing the middle point $E$ of $BD$. Let define $S$ as the union of the set of edges of $\Gamma$ that lies along the $CP_1$ line and all edges contained in the fundamental domain that are parallel to $CP_3$, but not adjacent to any vertex of $CP_1$. Some vertices of $\Gamma$ inside $CP_1P_2P_3$ are not incident with any edge of $S$. If the number $v$ of such vertices is even, we choose $\frac{v}{2}$ independent edges crossing $ED$ and their respective images under the central symmetry through $E$. For each uncovered vertex, path in $\Gamma$ joining the vertex to one of the $v$ edges in such a way that all paths are disjoint and are alternating on edges of $S$ and edges not in $S$. Along each path, reverse the selection of edges in $S$ with edges not in $S$. After this operation, we obtain a new set $\bar{S}$ of disjoint edges which saturates all vertices of the domain.

If $v$ is odd, consider the edge $e_1$ of $\Gamma$ that crosses $P_1P_2$ and that is the nearest from $P_2$. Then proceed as in the previous case: choose $v + 1$ independent edges crossing $BD$, symmetric through the point $E$. The edge $e_1$ has the same role of a not covered vertex in the previous case: except for the cases $\mathcal{P}_4$, $r = 3$, $s = 1$, $p$ even and $\mathcal{P}_5$, $r = 3$, $s = 1$, it is possible to define $v + 1$ disjoint alternating paths joining the $v$ vertices plus the edge $e_1$ to the $v + 1$ chosen edges crossing $BD$. Then the selection of edges in $S$ is reversed along each path, thus obtaining a new set $\bar{S}$ of disjoint edges saturating all vertices of the domain.

In both cases, a TSKS for $\Gamma$ is obtained by the orbit of $\bar{S}$ induced by the action of $D_{3d}$ on the domain. See Figure 3.20 for family $\mathcal{P}_5$, for the other families figures are quite similar.

As already remarked, this approch doesn't work in some cases. We prove in the next paragraph the non-existence of a TSKS for all these cases, thus completing the proof of Proposition 3.7.

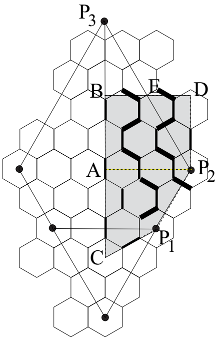


Figure 3.20

### 3.3.1 A non-existence case

In this last paragraph we prove the non-existence of a TSKS for the cases $\mathcal{P}_4$, $r = 3$, $s = 1$, $p$ even and $\mathcal{P}_5$, $r = 3$, $s = 1$. We preserve exactly the same notation used previously for the fundamental domain, that is $CBDP_2P_1$, and we denote by $e_1$ the unique edge of $\Gamma$ that crosses $P_1P_2$, as shown in Figure 3.21 for family $\mathcal{P}_5$.

Suppose that a TSKS does exist in these cases. The set of edges of $\Gamma$ which lie along the $CP_1$ line, the $CB$ line and the $DP_2$ line must be selected in the TSKS since they lie on an axis of symmetry of the graph. For the values of the parameters considered here, there remains an odd number of uncovered vertices inside the fundamental domain, in particular: 9 vertices in the case $\mathcal{P}_5$ and $9 + 3p$ in the case $\mathcal{P}_4$. In order to saturate all vertices of the domain one must select an odd number of edges crossing the border of the fundamental domain. If one select the unique edge crossing $EB$ then it must be selected also the unique edge crossing $ED$, since it is its image under the central symmetry through $E$. So the unique remained possibility is that $e_1$ is an edge of the TSKS. Now, consider the hexagon containing the two edges $e_2$ and $e_3$ of $\Gamma$ inside the fundamental domain and both incident $e_1$. The other two edges of this hexagon incident $e_2$ and $e_3$ must be in the TSKS. This leads to a contradiction since it remains a unique vertex of the hexagon still uncovered with all its neighbourhoods already covered by an edge of the TSKS.

Note that this argument does not work for $\mathcal{P}_4$ and $\mathcal{P}_5$ with different values of the Coxeter coordinates. In fact the length of $DB$ is larger in all that cases.

To resume our results, the table below gives the list of all fullerenes admitting a TSKS. This list is exhaustive: for each family we point out the Coxeter coordinate values for

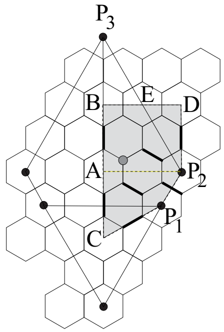


Figure 3.21

which a TSKS exists. For all fullerenes corresponding to the other admissible values a TSKS doesn't exist. Fullerenes in the list are exactly those satisfying the request of our main Theorem 1.1.

| Values for Coxeter Coordinates | Families |
|---|---|
| *All* | $\mathcal{A}_2, \mathcal{C}_2, \mathcal{D}_1, \mathcal{E}_1, \mathcal{E}_2, \mathcal{F}_4, \mathcal{F}_5, \mathcal{F}_1, \mathcal{F}_2,$ $\mathcal{D}_2, \mathcal{D}_3, \mathcal{D}_4, \mathcal{F}_6, \mathcal{F}_7, \mathcal{F}_3, \mathcal{E}_3, \mathcal{E}_4, \mathcal{E}_5, \mathcal{E}_6$ $\mathcal{E}_7, \mathcal{D}_5, \mathcal{D}_6, \mathcal{D}_7, \mathcal{D}_8, \mathcal{D}_9, \mathcal{D}_{10}, \mathcal{D}_{11}, \mathcal{D}_{12}$ $\mathcal{D}_{13}, \mathcal{G}_1, \mathcal{H}_1, \mathcal{H}_2, \mathcal{A}_4, \mathcal{A}_5, \mathcal{I}_1, \mathcal{I}_2, \mathcal{I}_3$ $\mathcal{A}_6, \mathcal{A}_7, \mathcal{H}_3, \mathcal{H}_4, \mathcal{H}_5, \mathcal{H}_6, \mathcal{H}_7, \mathcal{I}_4, \mathcal{I}_5$ $\mathcal{I}_6, \mathcal{I}_7, \mathcal{I}_8, \mathcal{I}_9, \mathcal{I}_{10}, \mathcal{I}_{11}, \mathcal{I}_{12}, \mathcal{I}_{13}, \mathcal{J}_1$ $\mathcal{K}_2, \mathcal{K}_4, \mathcal{L}_1, \mathcal{M}_1, \mathcal{M}_3, \mathcal{N}_2, \mathcal{O}_1, \mathcal{E}_9, \mathcal{E}_{11}$ $\mathcal{P}_1, \mathcal{P}_2, \mathcal{P}_3, \mathcal{R}_3, \mathcal{R}_4, \mathcal{R}_5, \mathcal{R}_7$ |
| $r \equiv 0\ (mod\ 3)$ | $\mathcal{A}_1, \mathcal{A}_3, \mathcal{A}_8, \mathcal{A}_9, \mathcal{B}_1, \mathcal{B}_2, \mathcal{A}_{10}, \mathcal{A}_{11}, \mathcal{J}_2$ $\mathcal{K}_1, \mathcal{K}_3, \mathcal{E}_8, \mathcal{D}_{14}, \mathcal{P}_4^*, \mathcal{P}_5^{**}, \mathcal{P}_6, \mathcal{R}_1, \mathcal{R}_2, \mathcal{E}_{12}$ |
| $p + s \equiv 0\ (mod\ 3)$ | $\mathcal{P}_7$ |
| $r \equiv s \equiv 0\ (mod\ 3)$ | $\mathcal{C}_1, \mathcal{C}_6, \mathcal{C}_8, \mathcal{C}_{10}, \mathcal{C}_{11}, \mathcal{B}_5, \mathcal{B}_6$ |
| $r \equiv s\ (mod\ 3)\ \&\ q \equiv 0 (mod\ 3)$ | $\mathcal{C}_3$ |
| $s \equiv 0\ (mod\ 3)$ | $\mathcal{C}_4, \mathcal{M}_2, \mathcal{E}_{10}$ |
| $p \equiv 0\ (mod\ 3)$ | $\mathcal{R}_6$ |
| $r + s \equiv 0\ (mod\ 3)$ | $\mathcal{N}_1, \mathcal{O}_2, \mathcal{O}_3$ |
| $r \equiv p + s\ (mod\ 3)$ | $\mathcal{Q}_1$ |
| $p \equiv q \equiv -r\ (mod\ 3)$ | $\mathcal{C}_5, \mathcal{C}_7,$ |
| $p - q \equiv -r \equiv s\ (mod\ 3)$ | $\mathcal{C}_9$ |
| $p + q \equiv 0\ \&\ r \equiv s\ (mod\ 3)$ | $\mathcal{B}_3$ |
| $r \equiv s\ (mod\ 3)$ | $\mathcal{B}_4$ |

$*$: except $r = 3$ , $s = 1$, p even. $**$: except $r = 3$ , $s = 1$.

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