Which fullerenes are stable?

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ABSTRACT. A fullerene is a molecule composed of carbon in the shape of a hollow sphere, ellipsoid, tube, and many other forms. The spherical ones are called buckyballs and they look like the balls used in football game. The first stable cluster of fullerenes was discovered by Kroto and his co-authors who received the Nobel Prize. In this paper, we introduced some classes of stable fullerene graphs.

Keywords: fullerene, leapfrog operation, dual graph, graph eigenvalue.

1. INTRODUCTION

In graph theory a fullerene is a three connected cubic graph whose faces are pentagons and hexagons satisfying in Euler's formula. The first and the most stable fullerene C_{60}, namely is composed of 60 carbon atoms, 90 edges, 12 pentagons and 20 hexagons, see Figure 1. It is discovered in 1985 by Kroto et al. [11,12] who received the Nobel Prize for this discovery. It is not difficult to prove that the other classes of fullerenes have 12 pentagons, too. In other words, by using Euler's theorem, a fullerene on n vertices has exactly 12 pentagons and $n/2 - 10$ hexagons while n is a natural number equal or greater than 20 and $n \neq 22$, for more details about mathematics of fullerene graphs see Refs [2,4,8-10] as well as [13-16]. In the structure of C_{60} fullerene, all pentagons are isolated which introduce a new class of fullerenes called IPR (Isolated Pentagon Rules) fullerene. IPR fullerenes are fullerenes where no two pentagons share an edge. Among all classes of fullerenes, the IPR fullerenes have the special interest as they tend to be more stable [7]. Here, we introduce some conditions that a fullerene is stable.
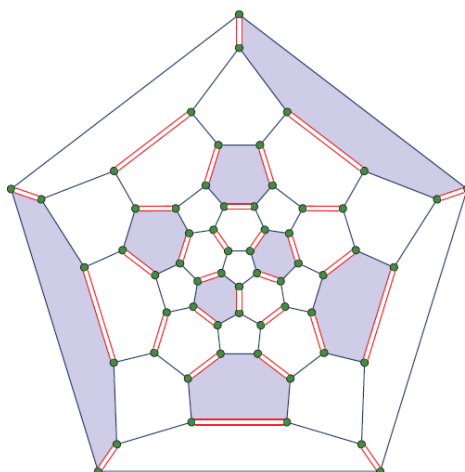
Figure 1. 2-D graph of fullerene C_{60}.

There is a list of groups that can act as a symmetry group of a convex polyhedron [3,6]. They can be divided into icosahedral, octahedral, tetrahedral, dihedral, cyclic and others. Symmetry of fullerenes has been studied deeply. The possible symmetry groups G for fullerenes are 28 point groups [5]. Babić, Klein and Sah in [1] classified all fullerenes up to 70 vertices with respect to their symmetry group. Fowler and Manolopoulos [6] found symmetry groups of all fullerenes with up to 100 vertices. For each symmetry group G they found the smallest G -fullerene and the smallest G - fullerene obeying IPR (isolated pentagon rule). They described how to create a new fullerene with the same symmetry group having more hexagonal faces and obeying IPR once a fullerene is given.

The dual of a fullerene is the plane graph obtained by substituting the roles of vertices and faces: the vertex set of the dual graph is the set of faces of the original graph and two vertices in the dual graph are adjacent if and only if the two faces share an edge in the original graph. The dual of a fullerene with *n* vertices is a plane graph where every face is a triangle. This operation is called triangulation. The triangulation on a fullerene provides one which contains 12 vertices of degree 5 and *n*/2 - 10 vertices of degree 6.

The Stellisation $St(G)$ of the plane graph G, adds a vertex in the center of each face of a planar graph G, and connects the new vertex with each boundary vertex of the corresponding face. Notice that this operation is also a triangulation.

Truncation, $Tr(G)$ of a plane graph G is an operation that adds two new vertices on each edge and then removes the vertices of G. Two vertices are adjacent if they are added to the same edge of G or they belong to two successive edges incident to the same vertex of G. The truncation of a polyhedron cuts off one third of each edge at each of both ends.

Let F be a fullerene graph on n vertices. A leapfrog transform F^l of F is a graph on $3n$ vertices obtained by truncating the dual of F. Hence, $F^l = Du(St(F)) = Tr(Du(F))$, where $Du(F)$ denotes the dual of F. It is easy to check that F^l itself is a fullerene graph. We say that F^l is a leapfrog fullerene obtained from F and write $F^l = Le(F)$. In other words, for a given fullerene F_n put an extra vertex into the centre of each face of F_n. Then connect these new vertices with all the vertices surrounding the corresponding face. Then the dual polyhedron is again a fullerene having $3n$ vertices 12 pentagonal and $(3n/2)-10$ hexagonal faces. A sequence of stellation dualization rotates the parent s-gonal faces by π/s. Leapfrog operation is illustrated, for pentagonal and hexagonal faces, in Figures 2,3. The leapfrog operation of a fullerene graph (see Figures 4,5) is usually used for construction of bigger and isolated pentagon fullerenes. It should be noted that for a fullerene graph F, Aut(F) = Aut($Le(F)$).
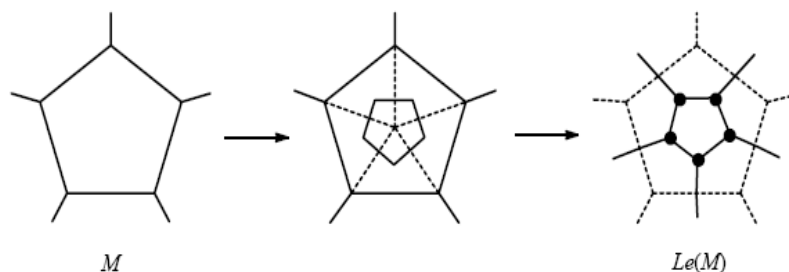

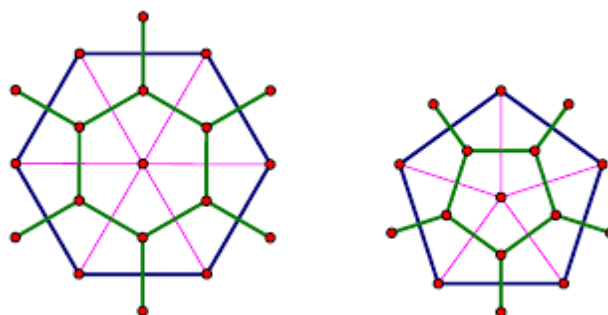**Figure 2**. Leapfrog of a pentagonal face.
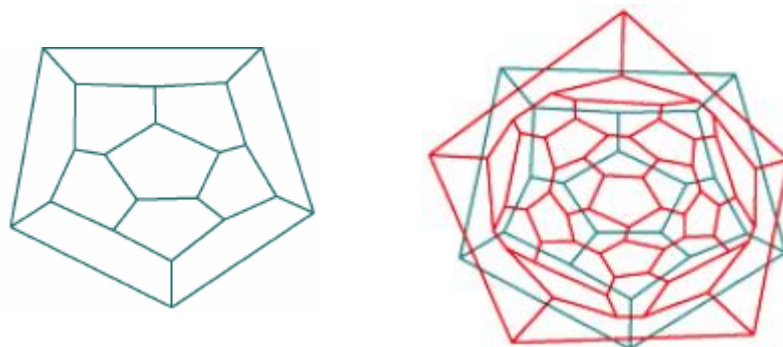

Figure 3. Leapfrog of a hexagonal face.

Figure 4. Leapfrog of fullerene C_{20}.

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C_{34} fullerene   Le(C_{34}) = C_{102}
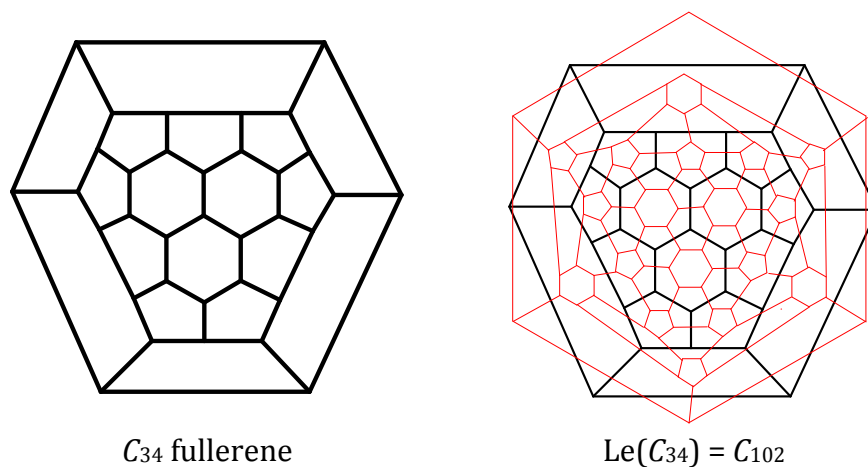
Figure 5. The fullerene C_{34} and Le(C_{102})**.**

This means that the leapfrog of an icosahedral fullerene is also icosahedral. It is a well-known fact that among all fullerene graphs, icosahedral fullerenes are more stable. Hence, if we have an icosahedral fullerene, then we can construct an infinite family of stable fullerenes by using leapfrog operation. We can also apply our method to construct big stable fullerenes with icosahedral symmetries. For example, $Le^2(C_{60})$ is a stable fullerene with 540 vertices and with an icosahedral symmetry, see Figure 6.
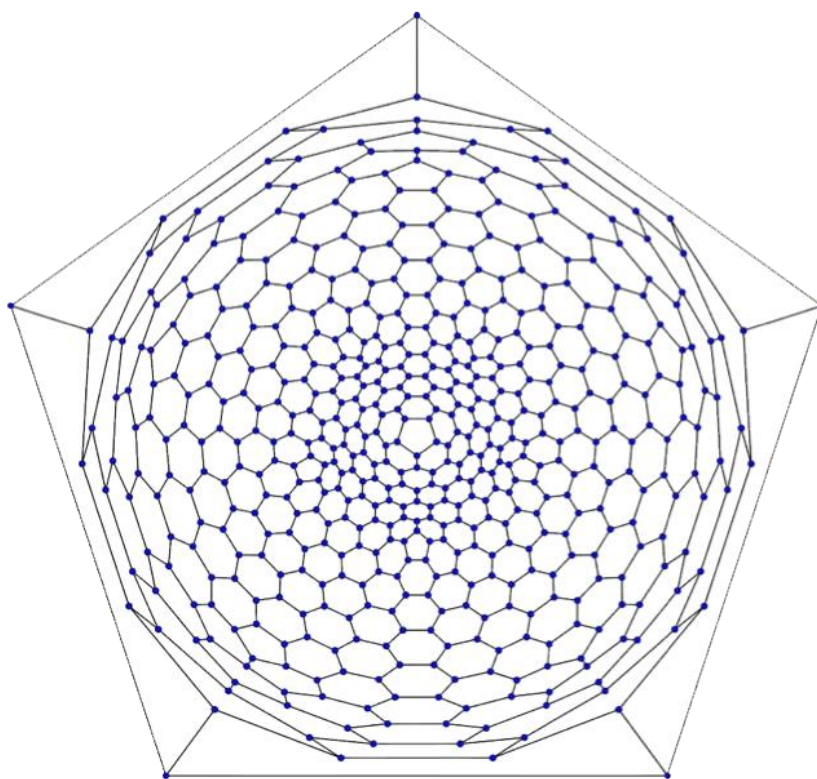
Figure 6. Fullerene C_{540} with icosahedral symmetry.

In Quantum Chemistry, the early Hückel theory calculates the levels of π-electron energy of the molecular orbitals, in conjugated hydrocarbons, as roots of the characteristic polynomial:

$$P(G,x) = \det[x\mathbf{I} - \mathrm{A}(G)].$$

In the above, I is the idendity matrix of a pertinent order and A the adjacency matrix of the graph G. The characteristic polynomial is involved in the evaluation of topological resonance energy TRE, the topological effect on molecular orbitals TEMO, the aromatic sextet theory, the Kekulé structure count, etc. The nullity of a molecular graph is the number of zeros of the characteristic polynomial.

Since the fullerene graphs are not bipartite, the smallest eigenvalue is greater than -3. Some chemists believe that a necessary condition for the physical existence of a fullerene is that the graph should have exactly half its eigenvalues positive.

Lemma 1 [7]. If X is a cubic planar graph with leapfrog graph $Le(X)$, then $Le(X)$ has at most half of its eigenvalues positive and at most half of its eigenvalues negative.

Theorem 2 [7]. If X is a cubic planar graph, then its leapfrog $Le(\mathrm{X})$ has exactly half of its eigenvalues negative. If, in addition, X has a face of length not divisible by three, then its leapfrog $Le(X)$ also has exactly half of its eigenvalues positive.

Let F be a fullerene graph. According to Theorem 2, the leapfrog graph $Le(F)$ has exactly half of its eigenvalues negative. Further, since F has a face of length not divisible by three (it has 12 pentagons), then its leapfrog $Le(F)$ also has exactly half of its eigenvalues positive. This means that leapfrog fullerenes are more stable.

Corollary 3. Let F be a fullerene graph, then the nullity of $Le(F)$ is an even integer number.

Proof. Let the number of positive eigenvalues of F be k ($k \leq n/2$), then according to Theorem 2, $Le(F)$ has $2k$ non-zero eigenvalues. This means that the nullity of $Le(F)$ is n-$2k$ and the proof is completed.

It is well-known that a molecular graph with nullity zero is more stable. In other words, leapfrog fullerenes with nullity zero are more stable.

Example 1. Consider the polyhedral graph C$_{32}$ depicted in Figure 7. By a direct computation, one can see that the spectrum of F is as follows:

$$Spec(F) = \begin{pmatrix} -3 & 2.56 & 2 & 1.56 & -1 & 0 & 1 & 1.56 & 2 & 2.56 & 3 \\ 1 & 3 & 2 & 3 & 4 & 6 & 4 & 3 & 2 & 3 & 1 \end{pmatrix}.$$

The nullity of this polyhedral graph is 6.

4. Conclusions

Fullerenes are spherical carbon molecules that can be modeled as cubic plane graphs where all faces are pentagons or hexagons. Euler's formula implies that a fullerene with *n* vertices contains exactly 12 pentagons and $n/2 - 10$ hexagons. A rich mathematics of cubic planar graphs and fullerene graphs has developed since they were considered by Goldberg, Coxeter, and others and many mathematical properties of fullerenes have established simple and beautiful solutions. Yet many remarkable chemical and mathematical problems in the field remain unsolved. The stability of fullerenes is very important factor that in this paper, we introduced some mathematical properties for it.
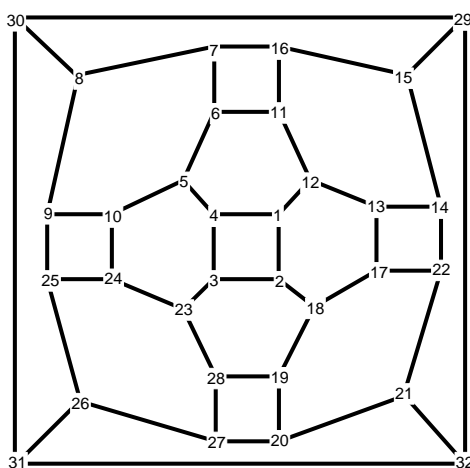

Figure 7. Fullerene graph C_{32}.

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