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ORIGINAL PAPER

On decompositions of leapfrog fullerenes

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Abstract It is shown that given a fullerene F with the number of vertices n divisible by 4, and such that no two pentagons in F share an edge, the corresponding leapfrog fullerene Le(F) contains a long cycle of length $3n - 6$ missing out only one hexagon.

Keywords Graph · Fullerene graph · Cyclic edge-connectivity · Perfect matchings · Leapfrog operation

1 Introductory remarks

Fullerenes, discovered in 1985, are all-carbon 'sphere'-shaped molecules with trivalent polyhedral skeletons, having 12 pentagonal faces and all other hexagonal faces. This important class of molecules is a basis of thousands of patents for a broad range of pharmaceutical, electronic and other commercial applications [1,2]. The most stable fullerene is Buckminsterfullerene that consists of 60 carbon atoms. It was obtained for the first time in the graphite vaporization experiment [3] and spectroscopic evidences of his structure are given in [4]. R. F. Curl, H. Kroto and R. E. Smalley received the

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Nobel Prize for this discovery. From a mathematical point of view, fullerenes correspond to 3-regular and 3-edge-connected planar graphs which have, in view of the well known Euler formula, 12 pentagons and the remaining faces are hexagons. (A graph is 3-edge-connected if three edges are needed to be removed in order to disconnect the graph.) It is therefore not surprising that many questions about the chemistry of fullerenes together with the methods used to answer these questions find their natural environment in a graph-theoretic context.

One of the many open problems with regards to fullerenes concerns the number of Kekulé structures in a fullerene, the so called *Kekulé number* [5–15]. Cast in a graph-theoretic language, the Kekulé number corresponds to the number of perfect matchings in a fullerene. In [10] it was shown that a fullerene of order m has at least $(\mathrm{m}+2)/2$ perfect matchings. This result was further improved in [5] to a lower bound $\lceil 3(m+2)/4 \rceil$. Also, it was very recently shown in [9] that for all sufficiently large m there is a fullerene of order m for which the number of perfect matchings is exponential in m.

The leapfrog fullerene Le(F) is obtained from a fullerene F by performing the so called tripling (leapfrog transformation) which consists in the truncation of the dual Du(F)of F. Hence, Le(F) = Trun(Du(F)). We show that given a fullerene F with the number of vertices n divisible by 4, and obeying IPR (isolated pentagon rule, that is, no two pentagons share an edge), the corresponding leapfrog fullerene Le(F) constains at least $2n$ decompositions to a long cycle of length $3n - 6$ and a hexagon, proved in Theorem 3.5, the proof of which relies on a classical result of Payan and Sakarovitch about induced trees in trivalent graphs [16].

In the next section we give some basic graph-theoretic definitions and notations and prove a result about cyclical edge-connectivity in certain graphs obtained by a small modification of fullerenes. This result together with the above mentioned result of Payan and Sakarovitch is vital in the proof of our main result.

2 Graph-theoretic background

Throughout this paper graphs are finite, undirected and connected, unless specified otherwise. For notations and definitions not defined here we refer the reader to [17]. For adjacent vertices x and y in X, we write $x \sim y$ and denote the corresponding edge by xy. Given a graph X we let $V(X)$ and $E(X)$ be the vertex set and the edge set of X, respectively. If $x \in V(X)$ then $N(x)$ denotes the neighbors set of x and $N_i(x)$ denotes the set of vertices that are at distance $i > 1$ from x. If $S \subseteq V(X)$, then $S^c = V(X) \setminus S$ denotes the complement of S and the graph induced on S is denoted by $X[S]$.

Given a graph Xwe let $H(X)$ denote the multigraph obtained from X by suppressing its vertices of degree 2 (that is, by contracting one of the incident edges). Further, if $|V(X)| \geq 10$ and $x \in V(X)$, let $R_x(X)$ denote the graph $H(X[(\{x\} \cup N(x))^c])$. An example is shown in Fig. 1.

A graph is said to be *k-connected* if k edges need to be removed to disconnect the graph. A *fullerene graph* (in short a *fullerene*) is a trivalent spherical map, and thus a 2-connected cubic planar graph, all of whose faces are pentagons and hexagons. By Euler formula there are exactly 12 faces of size 5 and all other faces of size 6. Further,

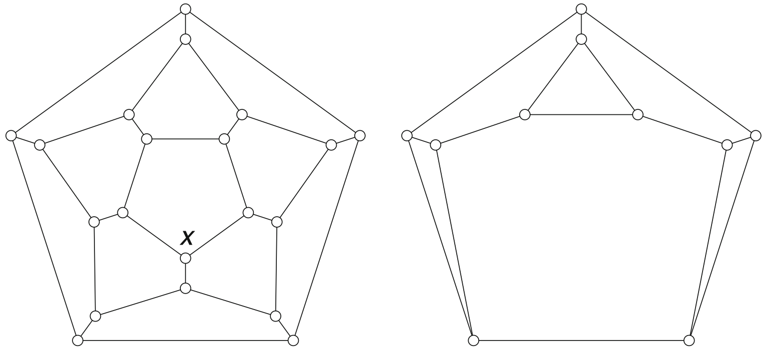


Fig. 1 The dodecahedron X on the left and its $R_x(X)$ on the right

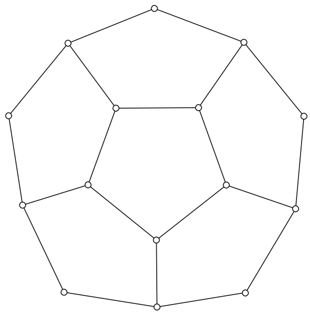


Fig. 2 The pentacap

it is easily seen that a fullerene must necessarily be 3-connected and that its smallest cycle is of length 5 (see [18,19]).

A graph is said to be *cyclically k-edge-connected*, if at least k edges must be removed to disconnect it into two components, each containing a cycle. The set of k edges whose elimination disconnect a graph into two components, each containing a cycle is called a *cyclic-k-edge cutset* and moreover, it is called a *trivial cyclic-k-cutset* if at least one of the resulting two components induces a single k-cycle. An edge from a cyclic-k-cutset is called *cyclic-cutedge*.

Clearly, in any fullerene F the cyclic connectivity cannot exceed 5, since by deleting the five edges connecting a pentagonal face, two components each containing a cycle are obtained. In fact, as was proved by Došlič [19, Theorem 2], the cyclic connectivity of a fullerene is precisely 5. However, a somewhat more detailed information about cyclic-5-cutset in fullerenes, taken from [20, Theorem 1], will be also needed.

The *pentacap* is a planar graph on 15 vertices with 7 faces of which one is a 10-gon and six are pentagons (see Fig. 2). Observe that the dodecahedron is obtained as a union of two pentacaps, by identifying the 10 vertices on the outer ring of the two pentacaps.

Proposition 2.1 [20, Theorem 1] *Let F be a fullerene admitting a nontrivial cyclic-5-cutset. Then F contains a pentacap, more precisely, it contains two disjoint pentacaps.*

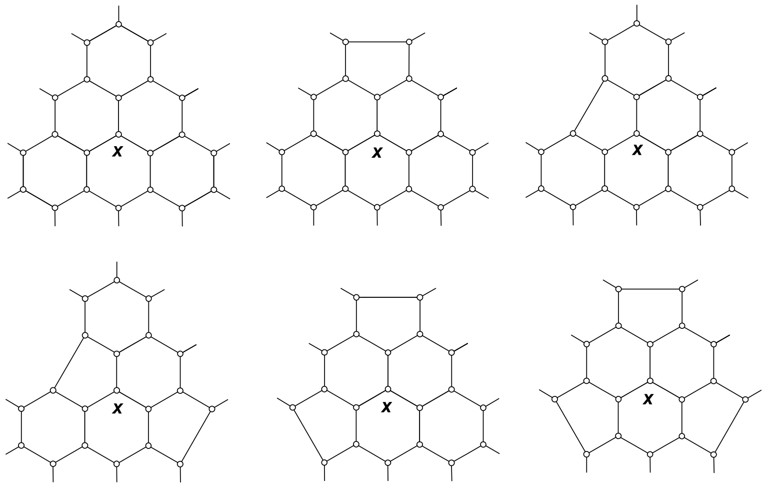


Fig. 3 All possibilities for a local structure of the fullerene F

Note that, since the order of any fullerene F is at least 20, the graph $R_x(F)$ is well defined for every vertex $x \in V(F)$ and that, moreover, $|\mathrm{V}(\mathrm{R_x(F)})| = |\mathrm{V(F)}| - 10 = n - 10$. Further, if the order of F is divisible by 4, the order of $R_x(F)$ is congruent to 2 modulo 4.

The next lemma, showing that with the transformation $F \to R_x(F)$ the cyclic connectivity drops by at most 1, will prove crucial for our main result.

Lemma 2.2 *Let F be a fullerene of order divisible by* 4 *and obeying IPR. Then for every vertex $x \in V(F)$ the graph $R_x(F)$ is cyclically* 4*-connected.*

Proof Let $x \in V(F)$. Clearly, in view of our assumptions, there are precisely six possibilities for the local structure surrounding the vertex x, shown in Fig. 3. Therefore, there are also six possibilities for the local structure of $R_x(F)$, depending on the type of vertex x, again shown in Fig. 4. We shall do the analysis for the case Y_1 in detail, the analysis in the other five cases is done in a similar way.

Therefore, let $x \in V(F)$ be such that the local structure of $R_x(F)$ is Y_1 (see Fig. 4). Let $Q = \{x\} \cup N(x) \cup N_2(x)$ denote the set of vertices that were deleted from F (the black vertices in Fig. 4). Observe that each edge of $R_x(F)$ lies on exactly two faces and that exactly one 11-gonal face C exists in $R_x(F)$. The sizes of other faces of $R_x(F)$ depend on the sizes of the faces of F adjacent to the faces shown in the second picture of Fig. 3. Moreover, as we are assuming that F has no adjacent pentagons, one can easily see that $R_x(F)$ has no triangles and that for any pair of edges on the 11-gonal face C, this face is the only face of $R_x(F)$ containing both of these edges.

Suppose that $R_x(F)$ is not cyclically 4-edge-connected. Then there exists a cyclic-k-cutset T of $E(R_x(F))$ where $k \leq 3$. By deleting the edges in T the graph $R_x(F)$ decomposes into two components, say R and R', each containing a cycle. Since one endvertex of any edge in T belongs to R and the other endvertex belongs to R', one can easily see that there must be an even number of edges from T lying on C. It follows that either no edge or two edges from T lie on C.

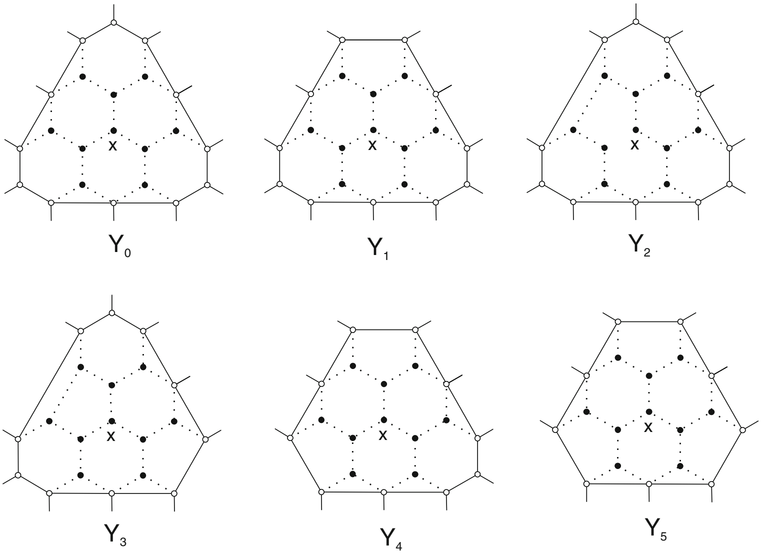


Fig. 4 All possibilities for a local structure of the graph $R_x(F)$

If no of edge in T lies on C, then all the vertices of C belong to the same component, say R. But then the deletion of the edges in T also separates the fullerene F into two components, each containing a cycle, contradicting the fact that F is cyclically 5-edge-connected.

We may now assume that there are exactly two edges in T, say e and e$'$, that lie on C. Two cases need to be considered.

Case 1. Let e and e$'$ have a common vertex.

Therefore, e = yz and e$'$ = y$'$z for some $y, y', z \in V(C)$. Then without loss of generality we may assume that $z \in R$and $y, y' \in R'$. However, depending on whether or not e and e$'$ are also the edges of F three possibilities need to be considered.

Subcase 1.1. Suppose that both e and e$'$ are edges of F. Then y, y$'$ and z are clearly the three bottom left or the three bottom right vertices in the Y_1 local structure of Fig. 4. However, one can easily see that the sets R and $R \cup Q$ are disjoint subsets of F, each containing a cycle, that are seperated with the edges from T, a contradiction as F is cyclically 5-edge connected.

Subcase 1.2. Suppose that neither e nor e$'$ belongs to $E(F)$ and let $w, w' \in N_2(x)$ be such that $w \in N(y) \cap N(z)$ and $w' \in N(y') \cap N(z)$ (black vertices in Fig. 4). Then the sets R and $R \cup Q$ are disjoint subsets of F, each containing a cycle, that are separated by wz, w$'$z and T. But since e and e$'$ are not in $E(F)$, the sets R and $R \cup Q$ are separated with less than five edges, again a contradiction.

Subcase 1.3. Let e = yz be an edge of F and let e$'$ = y$'z \notin$ E(F). Then there exists $w' \in N_2(x)$ such that $w' \in N(y') \cap N(z)$. But then the sets R and $R \cup Q$ are disjoint subsets of F, each containing a cycle, that are separated by $w'z$ and T. But since e$'$ is not in E(F), the sets R and $R \cup Q$ are separated by less then five edges, a contradiction.

Case 2. Let e and e$'$ have no common vertex.

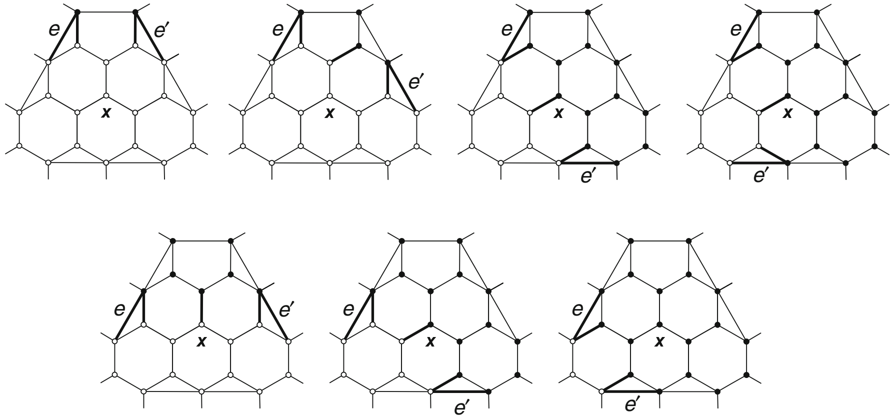


Fig. 5 The possibilities for cyclic-cutedges and e′ in $R_x(F)$ when e and e′ do not share an endvertex and none of them is an edge of F with the corresponding cyclic-cutedges of F

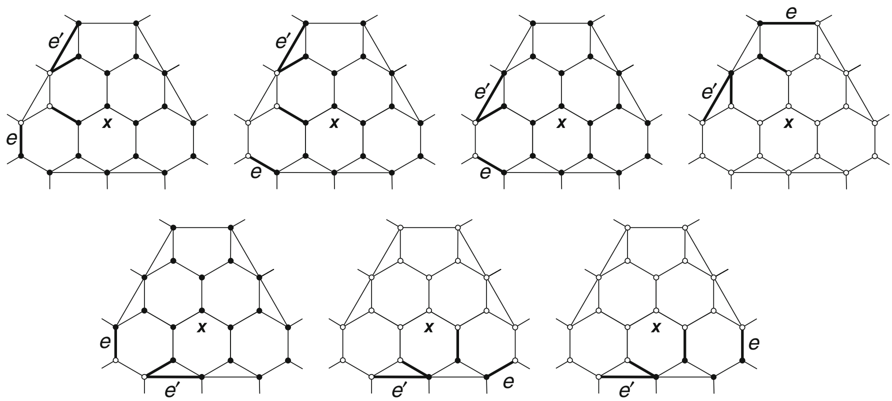


Fig. 6 The possibilities for cyclic-cutedges e and e′ in $R_x(F)$ if $e \in E(F), e' \notin E(F)$ and the distance between endvertices of e and e′ on C is 2 or 3 with the corresponding cyclic-cutedges of F

Also in this case, depending on whether or not e and e′ belong to F, three possibilities need to be considered.

Subcase 2.1. Suppose that neither e nor e′ is an edge of F. Then it is clearly sufficient to consider the seven possibilities shown in Fig. 5 where vertices from one of the two sets R and R' are colored white and vertices from the other set are colored black. Moreover, adding vertices of Q to R and R' as shown in Fig. 5, we deduce that in all these possibilities there exists a cyclic-k-cutset of cardinality less then 5 in F (since e and e′ are not in E(F)), a contradiction.

Subcase 2.2. Let e be an edge of F and let $e' \notin E(F)$. If the endvertices of e and e′ on 11-gonal face C are at most distance 3 apart, then it is clearly sufficient to consider the seven possibilities shown in Fig. 6. Similarly as above one can see that in all these local structures there exists a cyclic-k-cutset in F of cardinality less than 5, a contradiction.

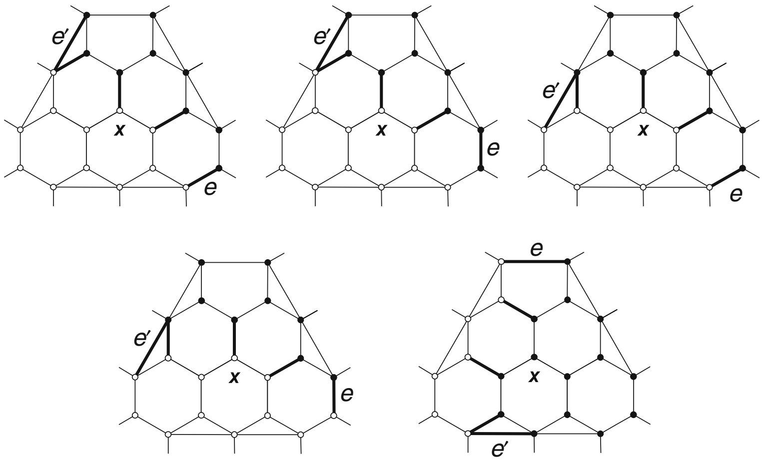


Fig. 7 The possibilities for cyclic-cutedges e and e′ in $R_x(F)$ if $e \in E(F)$, $e' \notin E(F)$ and the endvertices of e and e′ are at least distance 4 apart on C with the corresponding cyclic-cutedges of F

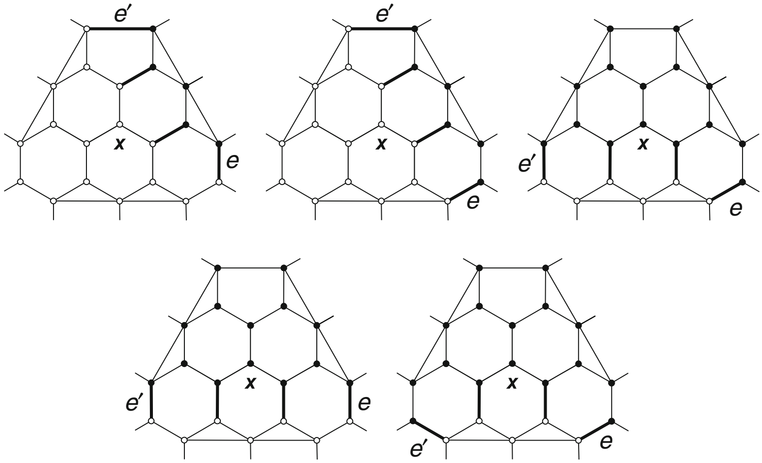


Fig. 8 The possibilities for cyclic-cutedges e and e′ in $R_x(F)$ if $e, e' \in E(F)$ and they do not share an endvertex with the corresponding cyclic-cutedges of F

Let now e and e′ on 11-gonal face C be at least distance 4 apart. Clearly, there exist two different faces $B$and B′ of $R_x(F)$ adjacent to C of which the first contains e and the second contains e′. If these two faces are disjoint (they do not have a common edge) then in view of the fact that each cycle in $R_x(F)$ contains an even number of edges from T, beside the edges e and e′, there exist at least two more edges in T, and so $|T| \geq 4$, a contradiction. Therefore we may assume that B and B′ share an edge, say e''. Clearly it is sufficient to consider the five possibilities shown in Fig. 7. Moreover, in all these possibilities (see Fig. 7) there exists a cyclic-5-cutset in F. Therefore, Proposition 2.1 implies that either this cyclic-5-cutset is trivial or F contains the pen-

tacap. Furthermore, as e and e′ are at least distance 4 apart on C, one can easily see that the cyclic-cutedges in Fig. 7 together with e'' cannot separate a pentagon of F. Therefore, F contains the pentacap, a contradiction.
Subcase 2.3. Let both e and e′ be edges of F. Observe, that it is sufficient to consider the five possibilities shown in Fig. 8. One can easily see that in all of these possibilities for the local structure there exists a cyclic-5-cutset of F. As in Subcase 2.2, Proposition 2.1 implies that in all these cases F contains the pentacap, a contradiction. This completes the proof of Lemma 2.2 □

Remark Note that for a fullerene F in which there exist adjacent pentagons the graph $R_x(F)$ may not be cyclically 4-edge-connected (see also Fig. 1).

3 The leapfrog fullerenes

A few additional graph-theoretic concepts are needed before we can embark on the proof of our main theorem. We say that, given a graph (or more generally a loopless multigraph) X, a subset S of V(X) is *cyclically stable* if the induced subgraph X[S] is acyclic (a forest). The following two results are due to Payan and Sakarovitch [16]. The first one may be deduced from [16, Théoreme 5] whereas the second one is a rephrasing of [16, Théoreme 6]. They will be used in the proof of Lemma 3.3 below.

Proposition 3.1 [16, Théoreme 5] *Let X be a cyclically 4-connected cubic graph of order n, and let S be a maximum cyclically stable subset of V(X). Then the following hold.*

1. *If* $n \equiv 2 (\mathrm{mod} 4)$ *then* $|S| =$ *(3n-2)/4, and X[S] is a tree and* S^c *is an independent set of vertices;*
2. *If* $n \equiv 0 (\mathrm{mod} 4)$ *then* $|S| =$ *(3n-4)/4, and either X[S] is a tree and* S^c *induces a graph with a single edge, or X[S] has two components and* S^c *is an independent set of vertices.*

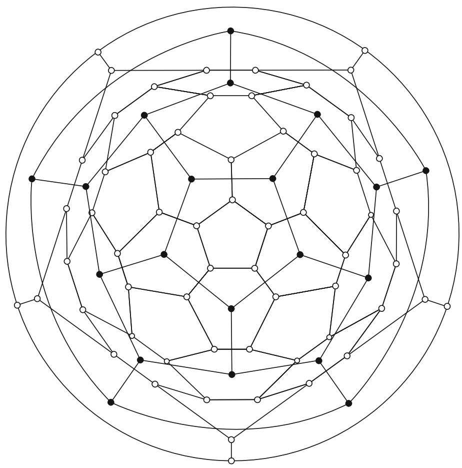
Proposition 3.2 [16, Théoreme] *Let X be a cyclically 4-edge-connected cubic graph and let* $x \in V(X)$*. Then there exists a maximum cyclically stable subset S of V(X) such that* $x \notin S$*.*

Lemma 3.3 *Let F be a fullerene of order divisible by 4 obeying IPR and let* $x \in V(X)$*. Then there exists a decomposition of V(F) into two subsets, the first of which induces a tree and an isolated vertex x, and the second of which is an independent set of vertices. Furthermore, for every vertex of F there exist at least two such decompositions.*

Proof Since the order of F is divisible by 4, the graph $R_x(F)$ is of order $n - 10 \equiv 2(\mathrm{mod} 4)$.

Let $N(x) = \{x_i | i \in \mathbb{Z}_3\}$ be the neighborhood of x and let $N(x_i) = \{x, y_i^j | j \in \mathbb{Z}_2\}$ for $i \in \mathbb{Z}_3$. Since, by Lemma 2.2, $R_x(F)$ is cyclically 4-edge connected, Proposition 3.1 implies that there exists a maximum cyclically stable subset S of $V(R_x(F))$ such that $R_x(F)[S]$ is a tree and S^c is an independent set of vertices. But then one can easily see that the complement of the set $\overline{S} = S \cup \{y_i^j | i \in \mathbb{Z}_3, j \in \mathbb{Z}_2\} \cup \{x\}$ in F is an

Fig. 9 The fullerene C_{20} is a retro-leapfrog fullerene of C_{60}



independent set of vertices and that $F[\bar{S}]$ is a union of a tree and an isolated vertex x. Namely, if the graph $F[S \cup \{y_i^j\}]$, for some $i \in Z_3$ and $j \in Z_2$, contains a cycle then it follows that $R_x(F)[S]$ contains a cycle.

By Proposition 3.1 the set S is of cardinality $|S| = (3n - 32)/4$ and so there clearly exists a vertex v of $R_x(F)$ contained in S. Moreover, Proposition 3.2 implies that there also exists a maximum cyclically stable subset S$'$of $V(R_x(F))$ such that v is not contained in S$'$. Using the some arguments as above, we see that the subgraph of F induced by the set $\bar{S}' = S' \cup \{y_i^j | i \in Z_3, j \in Z_2\} \cup \{x\}$ is a union of a tree and an isolated vertex x and that the complement of $\bar{S}'$ is an independent set of vertices. This completes the proof of Lemma 3.3. □

In the proof of the next theorem we will use the following observation, first made in [21]. Let X = Le(F) be a leapfrog fullerene of a fullerene F. Then F, the so called retro-leapfrog fullerene of X [22,23], is precisely the graph whose vertex set consists of all non-cap hexagons of X (the new hexagons added to the faces of F), with two hexagons adjacent if they share an edge in X. For example, with the leapfrog operation the dodecahedron fullerene C_{20} gives rise to the fullerene C_{60}. Conversely, if we form the graph whose vertex set consists of all hexagons of C_{60} with two hexagons adjacent if they share an edge in C_{60} we get the fullerene C_{20} (see also Fig. 9).

In the following example we illustrate the method of the proof of Theorem 3.5

Example 3.4 In the right-hand side picture of Fig. 10 we show a disjoint union of a tree of hexagons and a hexagonal face in the leapfrog fullerene X of the fullerene C_{60}, whose boundary is a union of a 174-cycle and a 6-cycle. The left-hand side picture shows this same tree in the retro-leapfrog fullerene of X.

Theorem 3.5 *Let F be a fullerene of order n divisible by* 4 *and obeying IPR, and let Le(F) be the corresponding leapfrog fullerene of order 3n. Then there exist at least 2n decompositions of V(Le(F)) into two disjoint sets C and C$'$ such that |C| = 6, |C$'$| = 3n-6, Le(F)[C] is a* 6*-cycle and Le(F)[C$'$] contains a (3n-6)-cycle.*

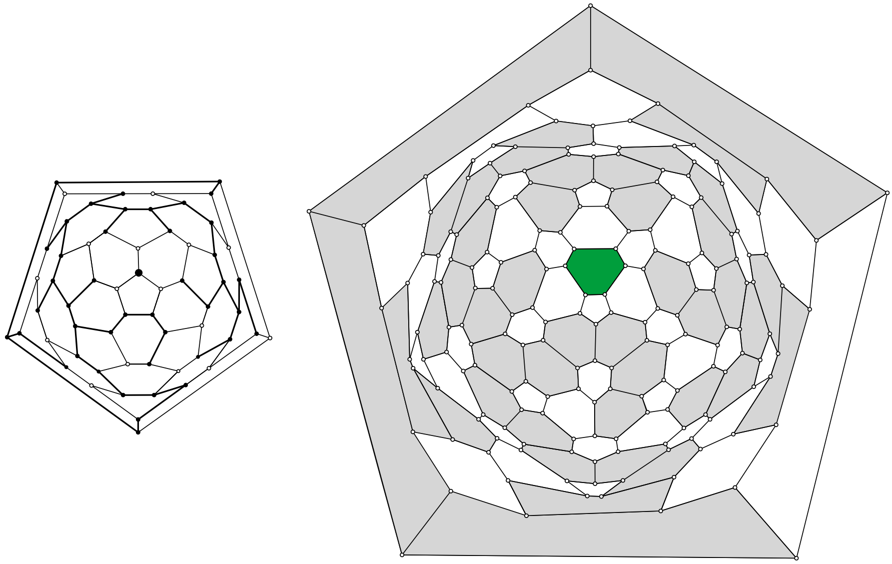


Fig. 10 A disjoint union of a tree of faces and a hexagonal face in the leapfrog fullerene of C_{60}

Proof Let $x \in V(F)$. Since F is a fullerene of order $n \equiv 0(\text{mod} 4)$ such that no two pentagons are adjacent, Lemma 3.3 implies that there exist at least two decompositions of V(F) into two subsets, the first of which induces a union of a tree T and an isolated vertex x, and the second of which is an independent set of vertices. As demonstrated in Example 3.4, the vertex $x \in V(F)$ corresponds to unique hexagon in Le(F) and so it gives rise to a 6-cycle of Le(F). Moreover, the tree T gives rise to a topological disk in Le(F), the boundary of which is a (simple) cycle passing through all but the six vertices which correspond to x. Since there exist n vertices in F, the result follows. □

4 Concluding remarks

It is shown that given a fullerene F with the number of vertices n divisible by 4 and obeying IPR the corresponding leapfrog fullerene Le(F) of F contains 2-factor consisting of a hexagon, resulting from the leapfrog operation, and a long cycle of length $3n - 6$, which is the boundary of a tree of faces all of which are hexagons resulting from the leapfrog operation. It would be interesting to see if the methods applied here could also be used for other types of 2-factors in Le(F) as well as for fullerenes arising from other types of operations performed on fullerenes, such as for example the quadrupling and the septupline operations.

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