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Cyclic edge-cuts in fullerene graphs

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Abstract In this paper, we study cyclic edge-cuts in fullerene graphs. First, we show that the cyclic edge-cuts of a fullerene graph can be constructed from its trivial cyclic 5- and 6-edge-cuts using three basic operations. This result immediatelly implies the fact that fullerene graphs are cyclically 5-edge-connected. Next, we characterize a class of nanotubes as the only fullerene graphs with non-trivial cyclic 5-edge-cuts. A similar result is also given for cyclic 6-edge-cuts of fullerene graphs.

Keywords Fullerene · Fullerene graph · Cyclic edge-cut · Cyclical edge-connectivity

1 Introduction

Since the discovery of the first fullerene molecule [9] in 1985, the fullerenes have been the objects of interest of scientists all over the world. The name *fullerenes* was given to cubic carbon molecules in which the atoms are arranged on a sphere in pentagons and hexagons. A useful and comprehensive overview of the actual development is the book of Fowler and Manolopoulos [6], where the authors bring results from several different topics in mathematics and chemistry concerning fullerenes and their structure.

Many properties of fullerene molecules can be studied using mathematical tools. Thus, mathematicians adopted the notion of fullerenes and defined the *fullerene graphs* as the plane cubic 3-connected graphs with only pentagonal and hexagonal faces.

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Various structural properties of fullerene graphs have been studied. See the papers [1,2,4,8,13] for results on perfect matchings i.e. Kekulé structures of fullerenes. In [7] the independence number of fullerenes is studied. One of the central questions remains hamiltonicity of this class of graphs. See [10] for a list of open problems on fullerene graphs.

Similar problems are studied also for the nanotubes. *Nanotubes* are members of the fullerene structural family. They are cylindrical in shape, with the ends typically capped with a hemisphere of the fullerene structure. See [11] for results on the number of Kekulé structures in nanotubes. Nanotubes with the ends left open (*open-ended* nanotubes) are also interesting objects, see e.g. [12].

Došlić proved that fullerene graphs are cyclically 4-edge connected [2] and cyclically 5-edge connected [3]. The cyclic edge-connectivity of a fullerene graph cannot exceed 5, since it contains 12 pentagons, thus, there are at least 12 cyclic 5-edge-cuts—formed by the edges pointing outwards of each pentagonal face. There are also cyclic 6-edge-cuts formed by the edges pointing outwards of each hexagonal face. These cyclic 5- and 6-edge-cuts will be called *trivial*.

Regarding the edge-cuts, there are some natural questions to ask: Are the 12 trivial cyclic 5-edge-cuts the only cyclic 5-edge-cuts in the fullerene graphs? Or, there are fullerenes with more than 12 cyclic 5-edge-cuts! Similar questions can be posed for the cyclic edge-cuts of bigger size.

In this paper, we study cyclic edge-cuts in fullerene graphs. First, as an auxiliary result, we show that the cyclic edge-cuts of a fullerene graph can be constructed from its trivial cyclic 5- and 6-edge-cuts using three basic operations. This result immediatelly implies the fact that fullerene graphs are cyclically 5-edge-connected. Similar technique is used in [5] to characterize boundary sequences in fullerene-like structures. Next, we characterize a class of nanotubes as the only fullerene graphs with non-trivial cyclic 5-edge-cuts. A similar result is also given for cyclic 6-edge-cuts of fullerene graphs.

An *edge-cut* of a graph G is a set of edges $C \subset E(G)$ such that $G - C$ is disconnected. A graph G is *k-edge-connected* if G cannot be separated into two components by removing less than k edges. An edge-cut C of a graph G is *cyclic* if each component of $G - C$ has a cycle. A graph G is *cyclically k-edge-connected* if G cannot be separated into two components, each containing a cycle, by removing less than k edges.

A graph drawn in the plane such that the edges are not crossing is a *plane* graph. A plane graph has one infinite face, called the *outer* face. All other faces are finite, and they are called *inner* faces.

2 Generating the cyclic edge-cuts

In this section, we introduce three operations to construct all cyclic edge-cuts of a fullerene graph from the trivial ones. These operations are used in the study of cyclic 5- and 6-edge-cuts in the next sections. In the figures of this paper, the edges of the edge-cuts are marked by dotted lines passing through them. The pentagonal faces are usually in the figures filled with grey color.

Let G be a fullerene graph and $C \subset E(G)$ be a cyclic k-edge-cut. If we remove the edges of C the graph G splits into two components, each containing a cycle. Because there are twelve pentagons in G, at least one of the two components contains at most six pentagons. Denote this component by H. The vertices of degree one and two in H are precisely the endvertices of the cut edges, thus they are all incident with the outer face O of H. We use the following simple property of the edge-cuts in fullerene graphs:

Lemma 1 *Let C be an edge-cut in a fullerene graph G. Suppose that a component H of $G - C$ does not contain any vertices of degree one. Let n_2 be the number of vertices of degree two, f_5 the number of pentagons, and l the size of the outer face of H. Then,*

$$6 - f_5 = 2n_2 - l.$$

Proof Let m be the number of edges, n_3 the number of vertices of degree three, and f_6 the numbers of hexagons of H. Then, obviously

$$2n_2 + 3n_3 \;=\; 2m \;=\; 5f_5 + 6f_6 + l.$$

On the other hand, by Euler's formula, we have

$$n_2 + n_3 + f_5 + f_6 + 1 - m - 2 = 0.$$

Hence,

$$(4n_2 + 6n_3 - 4m) + (5f_5 + 6f_6 + l - 2m) + 2n_2 + f_5 - l - 6 = 0,$$

which finally implies that

$$6 - f_5 = 2n_2 - l.$$

□

Now, we present the three operations. Each of the operations (O_i) modifies the cyclic k-edge-cut C into another cyclic edge-cut C_i. Moreover, $G - C_i$ contains a component H_i which is a proper subgraph of H. Let n denote the number of vertices of H.

- (O_1) Suppose that v is a vertex of degree one in H. Then, exactly two edges incident with v (in G) belong to the cut C, say e_1 and e_2. Let the third edge incident with v be e_3. Then, obviously $C_1 = C \setminus \{e_1, e_2\} \cup \{e_3\}$ is a cyclic $(k-1)$-edge-cut in G with a component $H_1 = H - v$ on $n - 1$ vertices having at most six pentagonal faces. See Fig. 1 for illustration.
- (O_2) Suppose that H contains at least two inner faces and that v_1 and v_2 are two adjacent vertices of degree two in H. Let e be the edge v_1v_2 and $e_i \in C$, $e_i' \notin C$ the other two edges incident with v_i, $i = 1, 2$, see Fig. 2. Then $C_2 = C \setminus \{e_1, e_2\} \cup \{e_1', e_2'\}$ is a k-edge-cut in G with a component $H_2 = H - v_1 - v_2$

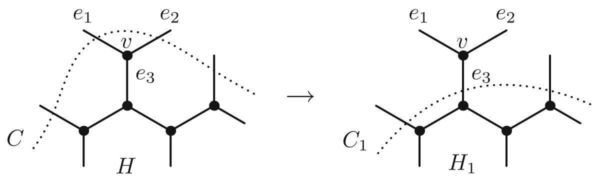

Fig. 1 If a component H contains a vertex of degree one, then using (O_1) one can modify the k-edge-cut C into a $(k-1)$-edge-cut C_1

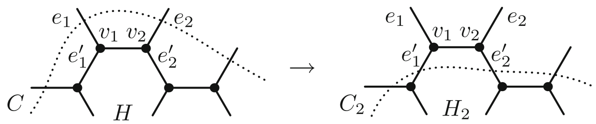

Fig. 2 If a component H contains two adjacent vertices of degree two, then using using (O_2) one can modify the k-edge-cut C into a k-edge-cut C_2

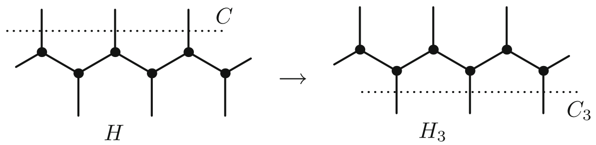

Fig. 3 If the vertices of the outer face of H are consequently of degree 2 and 3, then using (O_3) one can modify the k-edge-cut C into a k-edge-cut C_3

on $n-2$ vertices having at most six pentagonal faces. Notice that the assumption of the number of inner faces of H assures that C_2 is a cyclic edge-cut.

(O_3) Suppose that the outer face O is of size $2k$ with k 2-vertices and k 3-vertices alternating on O. Each of the 3-vertices on O is incident with exactly one edge that is not on O.

We claim that C_3 is a k-edge-cut. See Fig. 3 for illustration. Let $v_1, v_2, \ldots, v_k$ be the vertices of degree three on O in a cyclic order. If some v_i and v_{i+1} (where $v_{k+1} = v_1$) were adjacent, there would be a triangular face, what is not possible. If v_i and v_j $(j > i+1)$ were adjacent, then also v_{i+1} and v_{j-1} would be adjacent, otherwise there would be a face of size at least seven. But then also v_{i+2} and v_{j-2} would be adjacent, etc., and after finitely many such steps we get a face of size 3 or 2, what is impossible. Therefore, each v_i is adjacent to a vertex not on O.

Now we prove that C_3 is a cyclic edge-cut. Suppose that the graph H_3 obtained from H by removing the vertices incident with O contains a vertex w of degree at most one in H_3. Then, w is linked to at least two vertices on O, say v_i and v_j, $i < j$. If $j = i+1$, then there would be a face of size four. On the other hand, if $j > i+1$, then there would be a face of size at least eight. Altogether, we conclude that H_3 is of minimum degree two, hence, it contains a cycle.

Notice, that if C is a trivial cyclic edge-cut and the component H is a cycle on 5 or 6 vertices, then the operations (O_1), (O_2), and (O_3) cannot be applied.

Lemma 2 *Let C be a non-trivial cyclic k-edge-cut in a fullerene graph G, and let H be a component of $G - C$ which contains at most six pentagons. Then, one of the operations (O_1), (O_2), and (O_3) can be applied to get another cyclic edge-cut C^* with a component H^* of $G - C^*$ such that it is a proper subgraph of H.*

Proof If the component H contains a vertex of degree one, then the operation (O_1) can be easily applied, and we are done. Thus, in what follows, we assume that H is of minimum degree two.

Notice that H has at least two inner faces; otherwise we infer that H is a trivial cyclic 5- or 6-edge-cut, which is excluded by the assumption of the lemma. Now, if H contains two adjacent vertices of degree two, then the operation (O_2) can be applied to obtain a new edge-cut that satisfies the requirements of the lemma.

Suppose now that there are no vertices of degree two adjacent in H. Lemma 1 gives us the equality

$$6 - f_5 = 2n_2 - l,$$

where f_5 is the number of pentagons in H, n_2 is the number of 2-vertices, and l is the size of the outer face O. Because of the choise of the component H, it holds $6 - f_5 \geq 0$. On the other hand, since there is at least one vertex of degree three between each two vertices of degree two on O, we have $2n_2 - l \leq 0$. Therefore, we conclude that $f_5 = 6$ and $l = 2n_2 = 2k$. Hence, there are k 2-vertices and k 3-vertices alternating on O, so the operation (O_3) can be applied. □

Theorem 1 *The cyclic edge-cuts of a fullerene graph can be constructed from the trivial ones using the reverse operations of (O_1), (O_2), and (O_3).*

Proof Let C be a cyclic edge-cut in a fullerene graph G. If C is not trivial, we apply Lemma 2. As the number of vertices of the component H is decreasing, after finitely many reverse operations of (O_1), (O_2), (O_3) we obtain a trivial cyclic edge-cut. Now, reversing this sequence of operations, one infers C. □

3 Cyclic edge-cuts in nanotubes

Consider the fullerene graphs and the cyclic edge-cuts in them. The number of pentagons in the components of $G - C$ may vary. If one of the components contains less than six pentagons, then the other component can be arbitrarily large. On the other hand, if both components contain at most six pentagons, we can apply the operations introduced in the previous section to both of them.

A cyclic edge-cut C of a fullerene graph G is *non-degenerate* if both components of $G - C$ contain precisely six pentagons. Otherwise, C is *degenerate*. Obviously, the trivial cyclic edge-cuts are degenerate.

There is a family of fullerene graphs, which have many non-degenerate cyclic edge-cuts—the nanotubes. Nanotubes are cylindrical in shape, with the ends typically capped with a hemisphere-like structure. The cylindrical part of the nanotube can be

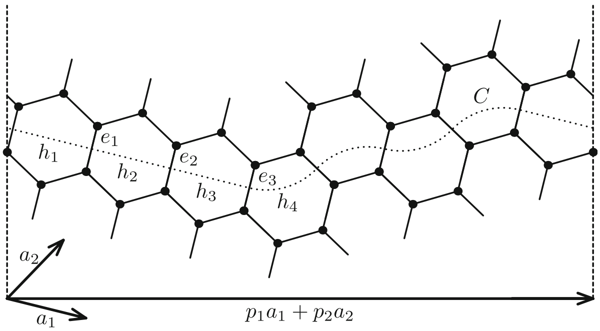

Fig. 4 An example of a nanotube of type (6, 2) and a cyclic edge-cut $C = \{e_1, e_2, e_3, \ldots\}$ cutting through the hexagons $h_1, h_2, h_3, \ldots$ in it

obtained from a planar hexagonal grid by identifying objects lying on two parallel lines. The way the grid is wrapped is represented by a pair of indices (p_1, p_2). The numbers p_1 and p_2 denote the coefficients of the linear combination of the unit vectors a_1 and a_2 such that the vector $p_1a_1 + p_2a_2$ joins pairs of identified points, see Fig. 4. The following result is perhaps known, but for sake of completeness, we include it:

Lemma 3 *There are precisely six pentagons in each of the two caps of a nanotube.*

Proof Let G be a nanotube of type (p_1, p_2) and let $p = p_1 + p_2$. Then, inside the cylindrical part of G, we can find a cyclic sequence of p hexagons $(h_1, h_2, \ldots, h_p)$ such that h_i and h_{i+1} are adjacent (where $h_{p+1} = h_1$). Moreover, if we identify each hexagon with its central point, then the vector $h_{i+1} - h_i$ is either a_1 or a_2, $i = 1, \ldots, p$. Let e_i be the edge incident with both h_i and h_{i+1}, $i = 1, \ldots, p$. Then, $C = \{e_1, \ldots, e_p\}$ is a non-degenerate cyclic p-edge-cut in G. It is easy to see that the length of the outer face of both components H_1 and H_2 of $G - C$ is equal, since the one is the translation of the other for a vector $a_2 - a_1$. In this translation, the 2-vertices on the outer face of H_1 correspond to the 3-vertices on the outer face of H_2 and vice-versa. On the other hand, the number of 2-vertices on both of them is p, thus, the same is the number of 3-vertices. Now, for both components in the equation given by Lemma 1

$$6 - f_5 = 2n_2 - l$$

we have $2k - (k + k) = 0$ on the right side, thus the number f_5 of pentagons is six in both H_1 and H_2. □

Notice that the nanotubes are not the only fullerene graphs having non-degenerate cyclic edge-cuts. The fullerene graph depicted in Fig. 5 has precisely one non-degenerate cyclic edge-cut, and obviously it is not a nanotube, since it needs more than two unit vectors to traverse the hexagons around.

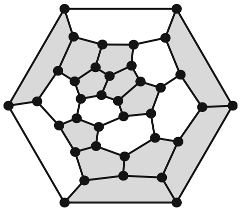

Fig. 5 An example of a fullerene graph with non-degenerate cyclic edge-cut, which is not a nanotube

4 Cyclic 5-edge-cuts

In this short section, we consider the cyclic 5-edge-cuts. Notice that Theorem 1 gives immediately the following facts:

Corollary 1 *Every fullerene graph is cyclically 5-edge-connected.*

Proof Since the size of the cyclic edge-cuts does not increase while using the operations (O_1), (O_2), and (O_3), the size of the cyclic edge-cut cannot be smaller than the size of the trivial ones, therefore, there are no cyclic edge-cuts of size less than five. □

Corollary 2 *There are no nanotubes of types* (p_1, p_2) *with* $p_1 + p_2 \leq 4$.

Proof Each nanotube of type (p_1, p_2) contains a cyclic $(p_1 + p_2)$-edge-cut. Thus, $p_1 + p_2 \geq 5$. □

Another easy application of the Theorem 1 is the characterization of fullerene graphs with non-trivial cyclic 5-edge cuts.

Let G_k denote the fullerene graph with the structure that two caps formed of six pentagons are joined by k layers of hexagons, see Fig. 6. Notice that for $k \geq 1$ these graph are nanotubes of type $(5, 0)$. Also notice that the graph G_0 is isomorphic to the dodecahedron. It is easy to see that the graph G_k has precisely k non-trivial non-degenerate cyclic 5-edge cuts.

Theorem 2 *A fullerene graph has non-trivial cyclic 5-edge-cuts if and only if it is isomorphic to the graph* G_k *for some integer* $k \geq 1$.

Proof As follows from Theorem 1, for each non-trivial cyclic 5-edge-cut there is a finite sequence of operations which yields a trivial edge-cut. Since there are no cyclic 4-edge-cuts, there cannot be any operation (O_1) in the sequence.

Let us reconstruct the original edge-cut. We start with a pentagon, the only trivial cyclic 5-edge-cut. If the operation (O_2) was used, there would be a quadrangular face. So the operation (O_3) has to be used, and hence a configuration of six pentagons is obtained, see Fig. 7.

In the next steps the operation (O_2) cannot be used again, because there would be more than six pentagons in the component inside the cut, so the only possible operation is (O_3). Therefore, for all non-trivial cyclic 5-edge-cuts C in a fullerene graph G one

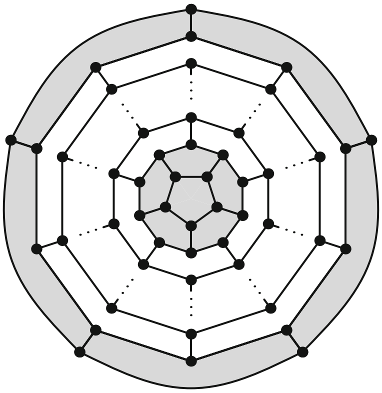

Fig. 6 The graphs G_k are the only fullerene graphs with non-trivial cyclic 5-edge-cuts

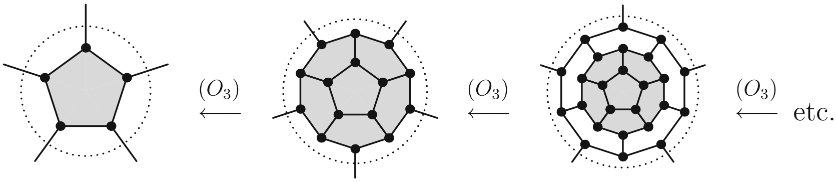

Fig. 7 The only possible way to reconstruct a cyclic 5-edge-cut

of the components of $G - C$ has the following structure: it contains a configuration of six pentagons then surrounded by certain number of rings each contanining five hexagons. Moreover, since the cut is non-trivial, the other component cannot be a pentagon only, thus it also has the structure described above. Altogether, the fullerene graph G is isomorphic to G_k for some $k \geq 1$. □

Corollary 3 *All non-trivial cyclic 5-edge-cuts in fullerene graphs are non-degenerate.*

Proof By Theorem 2, the graphs G_k are the only fullerene graphs with non-trivial cyclic 5-egde-cuts and all non-trivial cyclic 5-edge-cuts of the graphs G_k are non-degenerate. □

Corollary 4 *The graphs G_k, $k \geq 1$, are the only nanotubes of type (p_1, p_2) with $p_1 + p_2 = 5$.*

Proof The claim easily follows from Theorem 2 and the fact that each nanotube of type (p_1, p_2) has a non-degenerate $(p_1 + p_2)$-edge-cut. □

5 Cyclic 6-edge-cuts

Unlike the non-trivial cyclic 5-edge-cuts, not all the non-trivial cyclic 6-edge-cuts of fullerene graphs are non-degenerate. In Fig. 8, a sequence of six degenerate cyclic 6-edge-cuts is depicted.

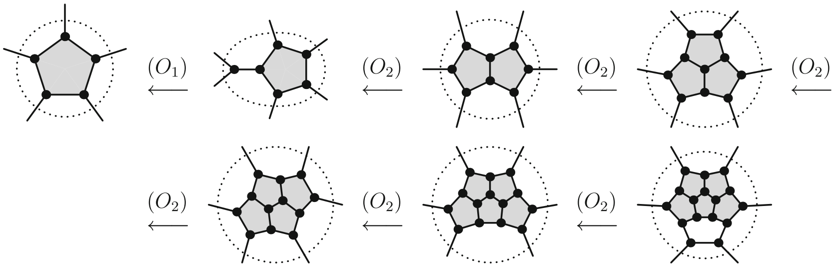

Fig. 8 Degenerate cyclic 6-edge-cuts that can be reconstructed from a pentagon

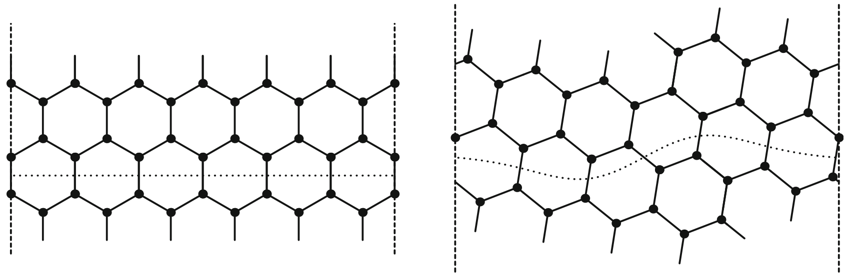

Fig. 9 The nanotubes of types (6, 0) and (5, 1) with examples of cyclic 6-edge-cut in both of them

Theorem 3 *There are precisely seven non-isomorphic graphs that can be obtained as components of degenerate cyclic 6-edge-cuts with less than six pentagons. Moreover, the graphs with i pentagons are unique for* $i = 0, 1, \ldots, 4$.

Proof By Theorem 1 each degenerate cyclic 6-edge-cut can be reconstructed from a trivial one.

If we start with a trivial cyclic 6-edge-cut, which is degenerate, then the operation (O_1) yields a cyclic 7-edge-cut, the operation (O_2) creates a quadrangular face, and the operation (O_3) gives a configuration containing six pentagons.

Let us start with a pentagon. To avoid creating cyclic 7-edge-cuts, quadrangular faces, or too many pentagons, we can only use the operation (O_1) once and then the operation (O_2) several times, see Fig. 8. More precisely, we can use (O_2) consequently at most five times. Using (O_2) once more yields a configuration of six pentagons. This way we get all non-trivial degenerate cyclic 6-edge-cuts. □

In the sequel, we deal with non-degenerate cyclic 6-edge-cuts. In Figs. 9 and 10, the nanotubes of the types (p_1, p_2) with $p_1 + p_2 = 6$ with examples of non-degenerate cyclic 6-edge-cut in them are depicted.

Nanotubes end with caps, each containing six pentagons. For the nanotubes of type (5, 0) there is only such cap possible, see Fig. 7. How can the caps of nanotubes of the types (p_1, p_2) with $p_1 + p_2 = 6$ look like? Is there at least one cap possible for all four types of nanotubes? The answers are consequences of the following characterization:

Theorem 4 *A fullerene graph has a non-degenerate cyclic 6-edge-cut if and only if it a nanotube of type* (p_1, p_2) *with* $p_1 + p_2 = 6$, *or it is a nanotube of type* $(5, 0)$ *with at least two layers of hexagons.*

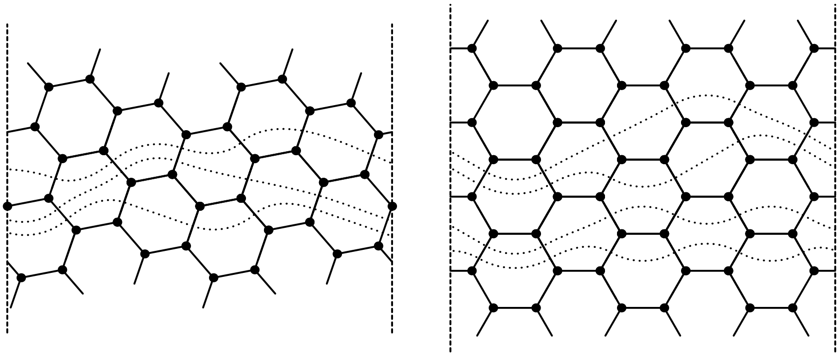

Fig. 10 The nanotubes of types (4, 2) and (3, 3) with examples of cyclic 6-edge-cuts in them

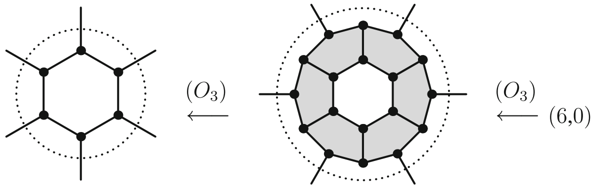

Fig. 11 The cyclic 6-edge-cuts reconstructed from a hexagon

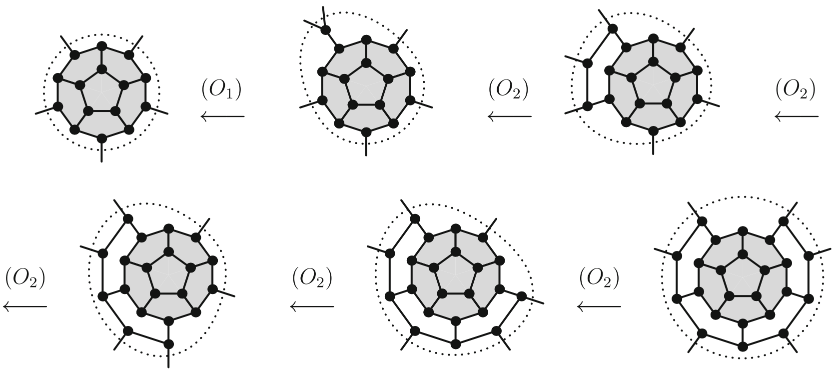

Fig. 12 The cyclic 6-edge-cuts reconstructed from a non-trivial cyclic 5-edge-cut

Proof It is easy to see that all the nanotubes of type (p_1, p_2) with $p_1 + p_2 = 6$ have non-degenerate cyclic 6-edge-cuts, e.g. those illustrated in Figs. 9 and 10. Notice that the nanotube G_1 of type $(5, 0)$ has only one non-degenerate cyclic edge-cut of size five. The nanotubes G_k, $k \geq 2$ of type $(5, 0)$ have non-degenerate cyclic 6-edge-cuts, e.g. those depicted in Fig. 12.

Suppose a fullerene graph G has a non-degenerate cyclic 6-edge-cut C, separating the graph into the components H_1 and H_2. Then we can reconstruct the cut C from the trivial ones with respect to H_1 and also with respect to H_2.

To reconstruct a cyclic 6-edge-cut, one can start with a trivial 5-edge-cut or a trivial 6-edge-cut.

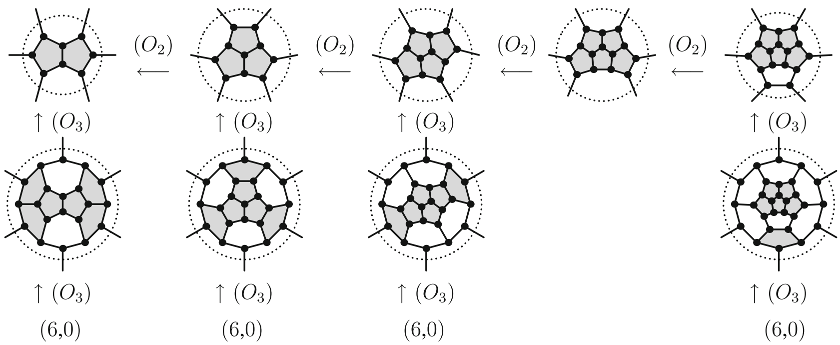

Fig. 13 The cyclic 6-edge cuts reconstructed from a trivial cyclic 5-edge-cut (first part). These cuts lead to nanotubes of type (6, 0)

If we start with a hexagon, the operation (O_1) cannot be used. If the operation (O_2) was used, there would be a quadrangular face. So the operation (O_3) has to be used and a configuration containing six pentagons is obtained, see Fig. 11. In the next steps only the operation (O_3) can be used again, otherwise there are more than six pentagons inside the cut. This way we get a cap of the nanotube of type (6, 0).

If we start with a pentagon, the operation (O_1) has to be used exactly once, since the operations (O_2) and (O_3) do not change the size of the edge-cut. If (O_1) is not used as a first operation, we first get some non-trivial cyclic 5-edge-cut, thus the fullerene is the nanotube of type (5, 0). Starting with some nontrivial 5-edge-cut, after applying the operation (O_1), the operation (O_2) can be used at most four times, see Fig. 12. If there was only one layer of hexagons, all these cyclic 6-edge-cuts would be degenerate, therefore there are at least two layers of hexagons in the nanotube.

If we start with a pentagon and first apply the operation (O_1), as a second step we have to use (O_2). In the next steps we get the cyclic 6-edge-cuts depicted in Figs. 13 and 14. In some steps both (O_2) and (O_3) can be applied, in some steps only (O_2) or only (O_3) is applicable. Once there are six pentagons in the component and only one of the operations can be used, we do not continue in listing more edge-cuts, because the structure of the corresponding components is determined by the configuration of the six pentagons. In all such cases we get the caps of the nanotubes of type (p_1, p_2) with $p_1 + p_2 = 6$. □

Corollary 5 *There are five possible caps for the natotubes of type* (6, 0). *On the other hand, the configurations of the six pentagons in the caps of the nanotubes of types* (5, 1), (4, 2), *and* (3, 3) *are unique.*

Proof In the proof of Theorem 4, we listed all possible configuration of at most six pentagons in components of cyclic 6-edge-cuts. The configurations of the six pentagons in the caps of the nanotube (6, 0) can be seen in Fig. 11, right, and in Fig. 13, the second row. The configuration of the six pentagons for the nanotubes of types (5, 1), (4, 2), and (3, 3) are determined uniquely, see Fig. 14. □

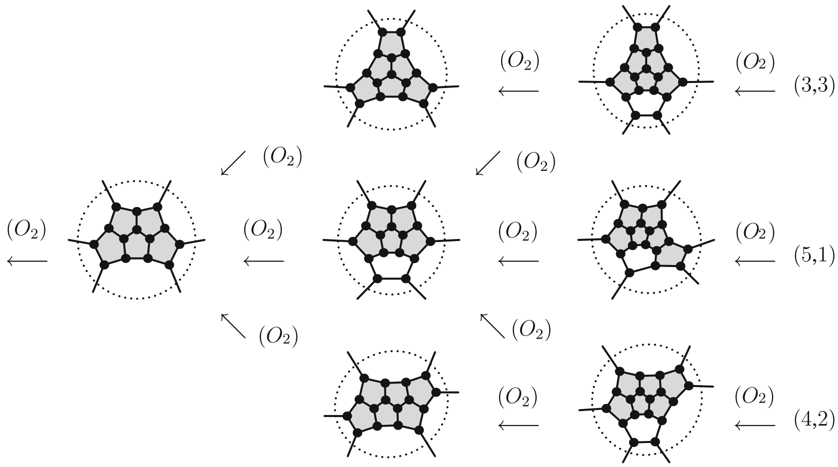

Fig. 14 The cyclic 6-edge cuts reconstructed from a trivial cyclic 5-edge-cut (second part). These cuts lead to the nanotubes of other types

Corollary 6 *A fullerene graph has a non-trivial cyclic 6-edge-cut different from a pentagon with a pending edge if and only if it contains at least one pair of adjacent pentagons.*

Proof The claim immediately follows from the proof of the Theorem 4, since all non-trivial cyclic 6-edge-cuts different from a pentagon with a pending edge contain at least one pair of adjacent pentagons. □

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