CYCLIC 7-EDGE-CUTS IN FULLERENE GRAPHS

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Cyclic 7-edge-cuts in fullerene graphs

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Abstract

A fullerene graph is a planar cubic graph whose all faces are pentagonal and hexagonal. The structure of cyclic edge-cuts of fullerene graphs of sizes at most 6 is known. In the paper we study cyclic 7-edge connectivity of fullerene graphs, distinguishing between degenerated and non-degenerated cyclic edge-cuts, regarding the arrangement of the 12 pentagons. We prove that if there exists a non-degenerated cyclic 7-edge-cut in a fullerene graph, then the graph is a nanotube unless it is one of the two exceptions presented. We determined that there are 57 configurations of degenerated cyclic 7-edge-cuts, and we listed all of them.

Keywords: fullerene, fullerene graph, cyclic edge-connectivity, cyclic edge-cut

1 Introduction

Mathematicians adopted the notion of fullerenes and defined the *fullerene* graphs as the plane cubic 3-connected graphs with only pentagonal and hexagonal faces. *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. Nanotubes with the ends left open, so called *open-ended* nanotubes, are also interesting objects, see e.g. [8].

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 twelve pentagons, thus, there are at least twelve 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*. Kardoš and Škrekovski [4] characterized 5- and 6-edge-cuts, and independently the 5-edge-cuts were characterized by Kutnar and Marušič [6].

An *edge-cut* of a connected graph G is a set of edges $C \subseteq E(G)$ 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 $G - C$ contains 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 cyclic edge-cut C of a fullerene graph G is *non-degenerated*, if both components of $G - C$ contain precisely six pentagons. Otherwise, C is *degenerated*. Obviously, the trivial cyclic edge-cuts are degenerated.

There is a family of fullerene graphs, which have many non-degenerated cyclic edge-cuts – the nanotubes. A fullerene graph is a *nanotube*, if it can be divided into a cylindrical part containing only hexagons, and two caps, each containing six pentagons and maybe some hexagons. Moreover, at least one of the pentagons should have an edge incident to the outer face of a cap. The cylindrical part should have the following structure: It contains a ring of hexagons $h_1, h_2, \ldots, h_p$ such that after unfolding it back into the hexagonal grid, there are two unit vectors a_1 and a_2 forming a 60° angle such that each $h_i - h_{i-1}$ is either a_1 or a_2 for $i = 1, \ldots, p$, where $h_0 = h_p$. (Here the hexagons are identified with their centers.) In this case, the cylindrical part is an open-ended nanotube of type (p_1, p_2), where p_j denotes the number of occurences of a_j, $j = 1, 2$. The pair (p_1, p_2) of coefficients in the equation $r = p_1 a_1 + p_2 a_2$ fully determines the type of the nanotube. It is easy to see that the vectors a_1 and a_2 can always be chosen in such a way that $p_1 \geq p_2$, which we assume in the sequel. See Fig. 1 for an illustration. We say that $p_1 + p_2$ is the *width* of the nanotube.
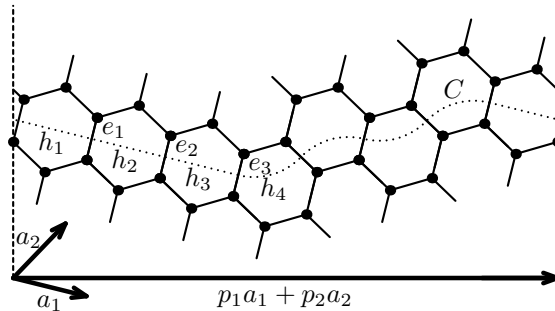

Figure 1: An example of a nanotube of type $(6, 2)$.

The nanotubes of types $(n, 0)$ are called *zigzag*, those of types (n, n) are called *armchair* (both types have mirror symmetry), the others are *chiral* (without mirror symmetry). In the light of this definition, also the buckyball C_{60} can be viewed as the first in the series of nanotubes of type $(5, 5)$ with a single layer of hexagons in the cylindrical part, see Fig. 2.

The nanotubes that are interesting in material science usually have the length-to-diameter ratio very large. But in many other fullerenes the nanotube-like structure can be found. We say that two non-degenerated cyclic edge-cuts are *parallel* if both of them induce the two partitions containing the same six pentagons in each, and the corresponding rings of hexagons do not share a face. Such a ring of hexagons is called a *layer*, and the maximal number of parallel layers is the *lenght* of a nanotube. Thus the cylindrical part of a nanotube is comprised of several face-disjoint layers.

It is easy to see that the ring of hexagons induces a non-degenerated cyclic edge-cut in a nanotube. In [4] it was proven that nanotubes are the only graphs having non-degenerated cyclic 5 and 6-edge-cuts, however, there exist fullerene graphs that are not nanotubes and have non-degenerated cyclic k-edge-cut, for some $k \geq 7$. In the paper we consider non-degenerated cyclic 7-edge-cuts and prove that there exist precisely two
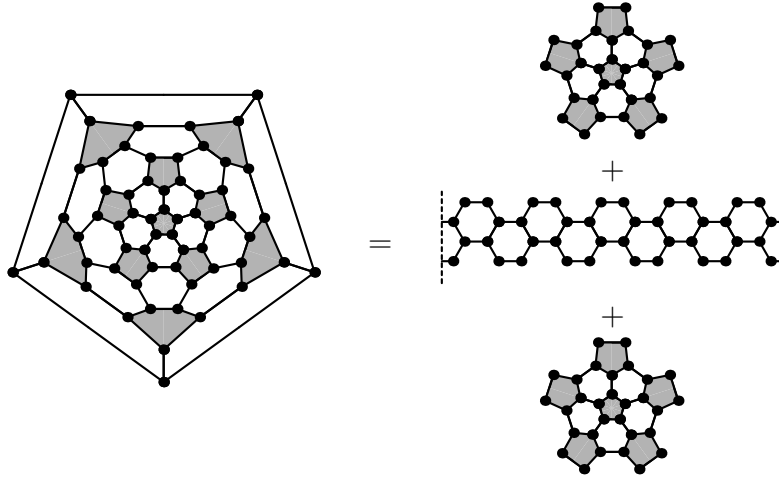
Figure 2: The buckyball is the smallest nanotube of type $(5,5)$.

fullerenes with non-degenerated cyclic 7-edge-cut, which are not nanotubes.

An important notion in this paper is a cut-vector. Let G be a fullerene graph and C a k-edge cut in G, and let H be one of the two components of the graph $G - C$. Let $e_1 = v_1 w_1, e_2 = v_2 w_2, \ldots, e_k = v_k w_k$ be the edges of C enumerated as they appear cyclically around H. We assume that v_i's are in H. Let α_i be the length of the facial subwalk from v_i to v_{i+1} minus 1 (notice that $v_{k+1} = v_1$). Observe that $\alpha_i = -1$ if $v_i = v_{i+1}$.

We name the sequence $[\alpha_1, \alpha_2, \ldots, \alpha_k]$ a *cut-vector* $v(C)$ (*regarding H*). It is easy to see that the coordinates α_i in fullerenes could only have values -1, 0, 1, 2 or 3, since each face of G is of size 5 or 6. For instance, the cut-vector of the configuration $6D02$ from Fig. 4 is $[-1, 1, 0, 0, 0, 1]$.

Observe that each cyclic edge-cut has two cut-vectors associated with each of the components of $G - C$. Let $[\alpha_1, \alpha_2, \ldots, \alpha_k]$ and $[\beta_1, \beta_2, \ldots, \beta_k]$ be the two cut-vectors corresponding to a cyclic edge-cut C. If C is non-degenerated, only hexagons are incident with the edges of a cut, hence, $\alpha_i + \beta_i = 2$ for $i = 1, 2, \ldots, k$. Therefore, the second cut-vector is determined by the first one. Moreover, also the sum of cut-vector's coordinates has a nice property, which is given in the following lemma:

Lemma 1 *Let C be a non-degenerated k-cut in a fullerene graph G, and let $\alpha = [\alpha_1, \alpha_2, \ldots, \alpha_k]$ be one of its two cut-vectors. Then, $\alpha_1 + \alpha_2 + \cdots + \alpha_k = k$.*

To prove the lemma above, we use an extension of a result from [4, Lemma 1]:

Lemma 2 *Let C be an edge-cut in a fullerene graph G and H a component of $G - C$. Let n_1 and n_2 be the numbers of vertices of degree one and two, f_5 the number of pentagons, and l the size of the outer face of H. Then, $6 - f_5 = 4n_1 + 2n_2 - l$.*

Proof. Let m be the number of edges, n_3 the number of 3-vertices, and f_6 the number of hexagons of H. Then

$$n_1 + 2n_2 + 3n_3 = 2m = 5f_5 + 6f_6 + l.$$

Using Euler's formula, we also have that

$$n_1 + n_2 + n_3 + f_5 + f_6 + 1 - m - 2 = 0.$$

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Putting these two equations together we infer

$$6(n_1 + n_2 + n_3 + f_5 + f_6 + 1 - m - 2) = 0$$
$$(2n_1 + 4n_2 + 6n_3 - 4m) + (5f_5 + 6f_6 + l - 2m) + 4n_1 + 2n_2 + f_5 - l - 6 = 0$$
$$4n_1 + 2n_2 - f_5 - l - 6 = 0,$$

and finally

$$4n_1 + 2n_2 - l = 6 - f_5.$$

$\square$

Proof of Lemma 1. Let H be the component of $G - C$ that corresponds to α. Then H has n_1 1-vertices and n_2 2-vertices such that $2n_1 + n_2 = k$. It also has six 5-faces. The length of its outer face is

$$l = k + \sum_{i=1}^{k} \alpha_i = 2n_1 + n_2 + \sum_{i=1}^{k} \alpha_i.$$

On the other hand, by Lemma 2 we have

$$l = 4n_1 + 2n_2,$$

and hence

$$\sum_{i=1}^{k} \alpha_i = 2n_1 + n_2 = k,$$

which proves the lemma. $\square$

The *type* of a cut-vector α is the vector obtained from α after omitting the coordinates with value 1. For an example, the type of the cut-vector $[2, 1, 1, 0, 1, 2, 0]$ is $[2, 0, 2, 0]$. If no two consecutive coordinates of the cut-vector's type have the same value, we say that the cut is *nanotubical*. The notion nanotubical derives from the fact, that the two same consecutive coordinates imply that there are all three direction vectors contained in the cut, and we know that the fullerene is a nanotube if and only if there exists a cut containing at most two direction vectors. Moreover, if the cut is nanotubical, each subsequence of the form $2, 1, \ldots, 1, 0$ of the cut-vector containing k 1's corresponds to $k + 1$ times the unit vector a_1, and each subsequence of the form $0, 1, \ldots, 1, 2$ of the cut-vector containing ℓ 1's corresponds to $\ell + 1$ times the unit vector a_2. Therefore, we can use the following characterization:

Proposition 1 *A fullerene graph is a nanotube if and only if it has a nanotubical cut. Moreover, if the nanotube is of type (p_1, p_2), then the cut has size $p_1 + p_2$.*

Below we pose some known results regarding the non-trivial cyclic 5- and 6-edge-cuts. Denote by G_k the fullerene graph comprised of two caps formed by six pentagons, and k layers of hexagons, see Fig. 3.

Theorem 1 *A fullerene graph has non-trivial cyclic 5-edge-cut if and only if it is isomorphic to the graph G_k for some integer $k \geq 1$.*
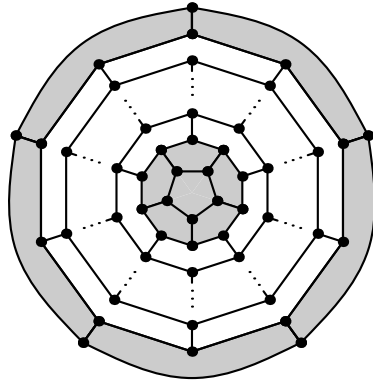
Figure 3: The graphs G_k are the only fullerene graphs with non-trivial cyclic 5-edge-cuts.

As an immediate corollary we obtain that all non-trivial cyclic 5-edge-cuts in fullerene graphs are non-degenerated. Unlike cyclic 5-edge-cuts, there exist degenerated cyclic 6-edge-cuts, which are not trivial.

Theorem 2 *There exist precisely seven non-isomorphic graphs that can be obtained as components of degenerated cyclic 6-edge-cuts with less than six pentagons (see Fig. 4). Moreover, the graphs with i pentagons are unique for $i = 0, 1, 2, 3, 4$. There are exactly two graphs with 5 pentagons on the other hand.*
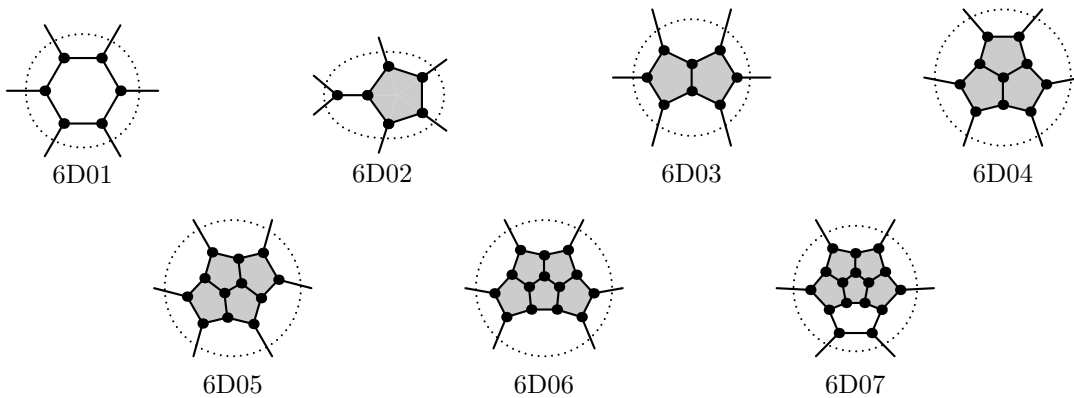

Figure 4: Degenerated cyclic 6-edge-cuts.

Non-degenerated cyclic 6-edge-cuts are, similarly as cyclic 5-edge-cuts, nanotubical. In [4] the following characterization is given:

Theorem 3 *A fullerene graph has non-degenerated cyclic 6-edge-cut if and only if it is a nanotube of type (p_1, p_2), where*

(a) $p_1 + p_2 = 6$; *or*

(b) $p_1 = 5$, $p_2 = 0$, *with at least 2 layers of hexagons.*

2   Degenerated cyclic 7-edge-cuts

In this section we list the degenerated cyclic 7-edge-cuts. There are 57 non-isomorphic graphs that can be obtained as components of degenerate cyclic 7-edge-cuts with less then 6 pentagons. To obtain the configurations we used the reverses of operations O_1, O_2 and O_3 presented in [4]. Each of the three operations O_i, $i \in \{1, 2, 3\}$, modifies the cyclic k-edge-cut C into another cyclic edge-cut C_i. Below a brief description of the operations is given (see also Fig. 5).

(O_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.*

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

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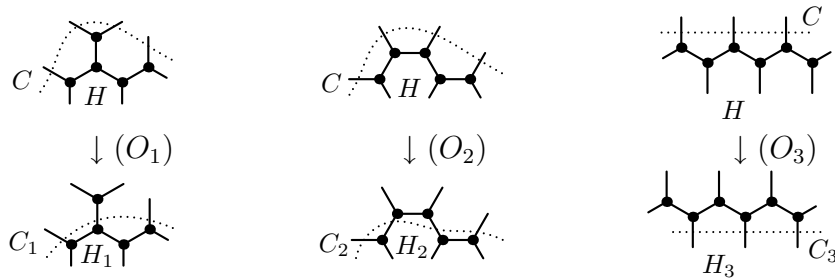

Figure 5: The operations O_1, O_2 and O_3.

Using the three operations, all cyclic edge-cuts in a fullerene could be constructed, see [4, Theorem 1]. Note that the operation O_3 can be applied only if there are six pentagons in the configuration H, therefore when reconstructing degenerated cyclic edge-cuts from the trivial ones, it is never used. In Fig. 6, an example of constructing a degenerate cyclic 7-edge-cut is presented, and in Fig. 7 we listed the degenerated cyclic 7-edge-cuts.
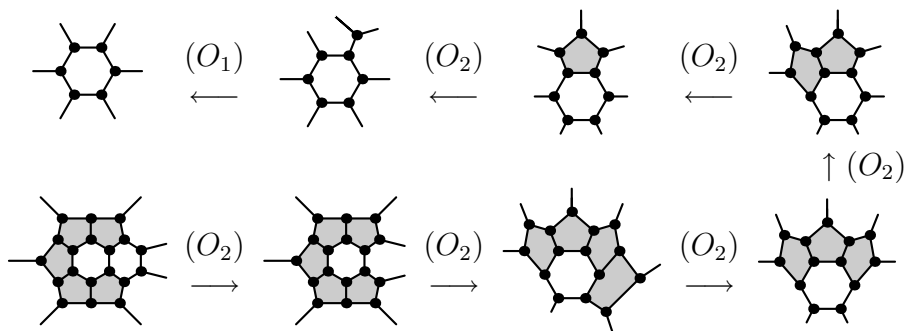

Figure 6: An example of construction.

In Table 1 for each configuration depicted in Fig. 7 we list the number of pentagonal and hexagonal faces (denoted by f_5 and f_6), the number of vertices (denoted by v), the cut-vector, and the configurations that arise when applying operations O_1, O_2 and the inverse O_2^{-1}.
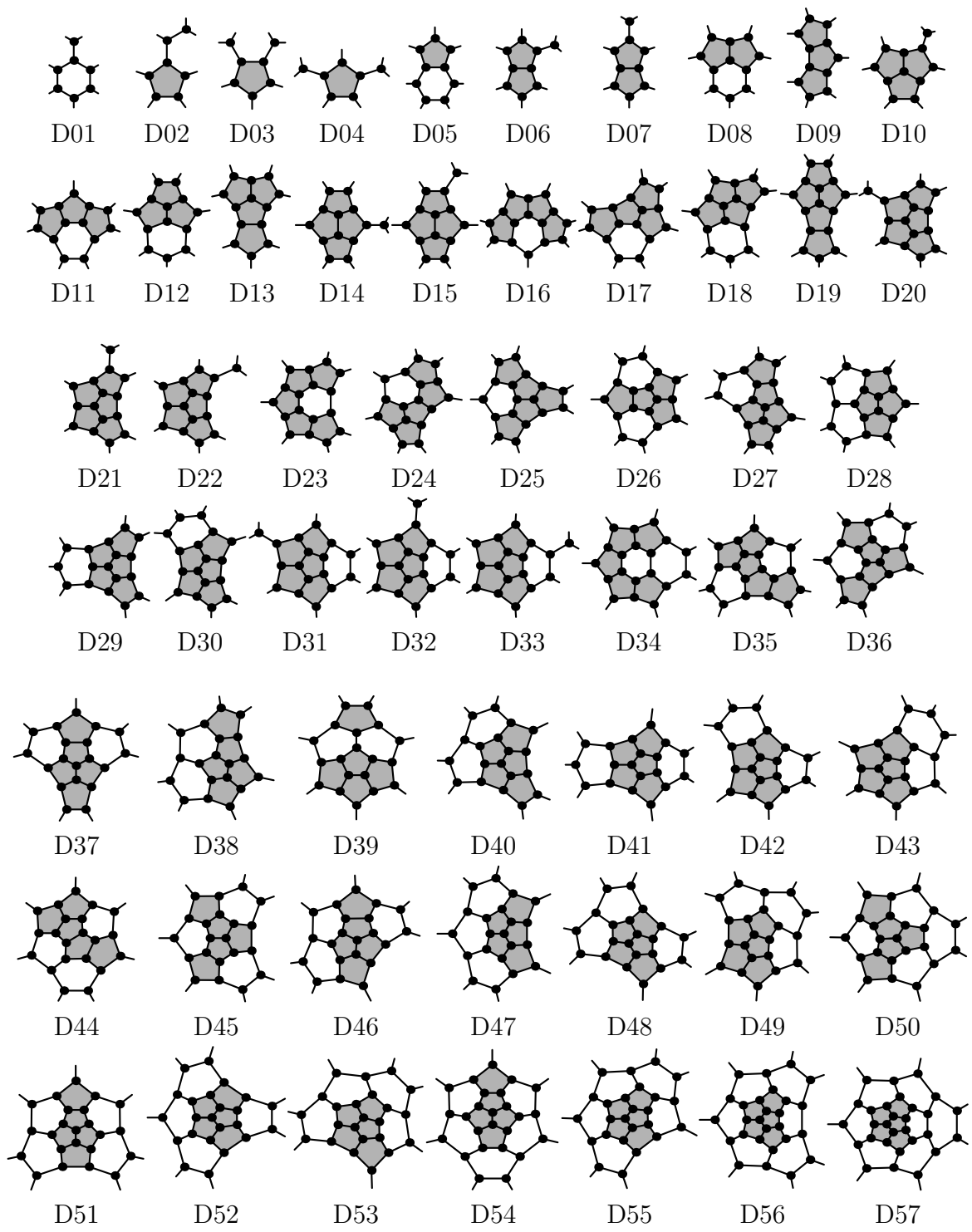
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Figure 7: Degenerated cyclic 7-edge-cuts.

cut	f_5	f_6	v	cut-vector	O_1	O_2	O_2^{-1}
D01	0	1	7	$[-1, 1, 0, 0, 0, 0, 1]$	6D01	–	D05
D02	1	0	7	$[-1, 0, 1, 0, 0, 0, 2]$	6D02	–	D05, D06
D03	1	0	7	$[-1, 1, 0, 0, 1, -1, 2]$	6D02	–	D05, D06
D04	1	0	7	$[-1, 1, 0, 1, -1, 1, 1]$	6D02	–	D06, D07
D05	1	1	9	$[0, 0, 0, 1, 0, 0, 1]$	–	D01, D02, D03	D08
D06	2	0	9	$[-1, 1, 0, 1, 0, 0, 2]$	6D03	D02, D03, D04	D08, D09, D10
D07	2	0	9	$[-1, 1, 1, 0, 0, 1, 1]$	6D03	D04	D09, D10
D08	2	1	11	$[0, 0, 1, 0, 1, 0, 1]$	–	D05, D06	D11, D12
D09	3	0	11	$[0, 0, 1, 1, 0, 0, 2]$	–	D06, D07	D11, D13
D10	3	0	11	$[-1, 1, 1, 0, 1, 0, 2]$	6D04	D06, D07	D12, D13, D14, D15
D11	3	1	13	$[0, 1, 0, 1, 0, 1, 1]$	–	D08, D09	D16, D17
D12	3	1	13	$[0, 0, 1, 1, 0, 1, 1]$	–	D08, D10	D17, D18
D13	4	0	13	$[0, 0, 2, 0, 1, 0, 2]$	–	D09, D10	D17, D19
D14	4	0	13	$[-1, 2, 0, 1, 1, 0, 2]$	6D05	D10	D18, D20
D15	4	0	13	$[-1, 1, 1, 1, 0, 1, 2]$	6D05	D10	D18, D19, D20, D21, D22
D16	4	1	15	$[0, 1, 1, 0, 1, 1, 1]$	–	D11	D23, D24, D25
D17	4	1	15	$[0, 1, 0, 1, 1, 0, 2]$	–	D11, D12, D13	D24, D25, D26, D27
D18	4	1	15	$[0, 0, 1, 1, 1, 0, 2]$	–	D12, D14, D15	D27, D28, D29, D30
D19	5	0	15	$[0, 0, 2, 1, 0, 1, 2]$	–	D13, D15	D27
D20	5	0	15	$[-1, 2, 0, 2, 0, 1, 2]$	6D06	D14, D15	D29, D30, D31
D21	5	0	15	$[-1, 1, 2, 0, 1, 1, 2]$	6D06	D15	D30, D32
D22	5	0	15	$[-1, 1, 1, 1, 1, 0, 3]$	6D06	D15	–
D23	5	1	17	$[0, 1, 1, 1, 1, 0, 2]$	–	D16	D34
D24	5	1	17	$[0, 1, 1, 1, 0, 1, 2]$	–	D16, D17	D35
D25	5	1	17	$[0, 1, 1, 0, 2, 0, 2]$	–	D16, D17	D36
D26	4	2	17	$[0, 1, 1, 0, 1, 1, 1]$	–	D17	D35, D36, D37
D27	5	1	17	$[0, 1, 0, 2, 0, 1, 2]$	–	D17, D18, D19	D37, D38
D28	4	2	17	$[0, 1, 0, 1, 1, 1, 1]$	–	D18	D38, D39, D40
D29	5	1	17	$[0, 0, 2, 0, 2, 0, 2]$	–	D18, D20	D40, D41
D30	5	1	17	$[0, 0, 1, 2, 0, 1, 2]$	–	D18, D20, D21	D40, D42
D31	5	1	17	$[-1, 2, 1, 0, 1, 1, 2]$	6D07	D20	D41, D42
D32	5	1	17	$[-1, 2, 0, 1, 1, 1, 2]$	6D07	D21	D42, D43
D33	5	1	17	$[-1, 1, 1, 1, 1, 1, 2]$	6D07	–	D43
D34	5	2	19	$[0, 1, 1, 1, 1, 1, 1]$	–	D23	–
D35	5	2	19	$[0, 1, 1, 1, 1, 0, 2]$	–	D24, D26	D44
D36	5	2	19	$[0, 1, 1, 1, 0, 1, 2]$	–	D25, D26	D45
D37	5	2	19	$[0, 1, 1, 0, 2, 0, 2]$	–	D26, D27	D46
D38	5	2	19	$[0, 1, 1, 0, 1, 1, 2]$	–	D27, D28	D46
D39	5	2	19	$[0, 1, 1, 1, 1, 1, 1]$	–	D28	–
D40	5	2	19	$[0, 1, 0, 1, 2, 0, 2]$	–	D28, D29, D30	D47, D48
D41	5	2	19	$[0, 0, 2, 1, 0, 1, 2]$	–	D29, D31	D48
D42	5	2	19	$[0, 0, 2, 0, 1, 1, 2]$	–	D30, D31, D32	D48, D49
D43	5	2	19	$[0, 0, 1, 1, 1, 1, 2]$	–	D32, D33	D49

cut	f_5	f_6	v	vector	O_1	O_2	O_2^{-1}
D44	5	3	21	[0, 1, 1, 1, 1, 1, 1]	–	D35	–
D45	5	3	21	[0, 1, 1, 1, 1, 0, 2]	–	D36	D50
D46	5	3	21	[0, 1, 1, 1, 0, 1, 2]	–	D37, D38	D51
D47	5	3	21	[0, 1, 1, 0, 1, 2, 1]	–	D40	D52
D48	5	3	21	[0, 1, 0, 2, 0, 1, 2]	–	D40, D41, D42	D52, D53
D49	5	3	21	[0, 1, 0, 1, 1, 1, 2]	–	D42, D43	D53
D50	5	4	23	[0, 1, 1, 1, 1, 1, 1]	–	D45	–
D51	5	4	23	[0, 1, 1, 1, 1, 0, 2]	–	D46	D54
D52	5	4	23	[0, 1, 1, 0, 2, 0, 2]	–	D47, D48	D55
D53	5	4	23	[0, 1, 1, 0, 1, 1, 2]	–	D48, D49	D55
D54	5	5	25	[0, 1, 1, 1, 1, 1, 1]	–	D51	–
D55	5	5	25	[0, 1, 1, 1, 0, 1, 2]	–	D52, D53	D56
D56	5	6	27	[0, 1, 1, 1, 1, 0, 2]	–	D55	D57
D57	5	7	29	[0, 1, 1, 1, 1, 1, 1]	–	D56	–

Table 1: Degenerated cyclic 7-edge cuts.

3 Non-degenerated cyclic 7-edge-cuts

In this section, we consider the non-degenerated cyclic 7-edge-cuts. We prove that all non-degenerated cyclic 7-edge-cuts are contained in fullerene graphs which are nanotubes, with only two exceptions. There exist precisely two fullerene graphs, which have non-degenerated cyclic 7-edge-cuts and that are not nanotubical. We also characterize the types of nanotubes in which non-degenerate cyclic 7-edge-cuts exist.

Note that nanotubes with $p_1 + p_2 < 5$ do not exist due to cyclic 5-edge-connectivity of fullerenes. Regarding nanotubes with $p_1 + p_2 = 5$, it was already proven in [4] that only nanotubes of type $(5, 0)$ exist, moreover, the caps are unique, see Theorem 1.

On the other hand, there are more possible nanotube types for $p_1 + p_2 = 6$. If we look for minimal caps, for type $(6, 0)$ there exist five different caps, while for types $(5, 1)$, $(4, 2)$, and $(3, 3)$ the minimal caps are unique, see Fig. 8. These are the caps which cannot be made smaller without introducing denegerated cuts. This is the shortest list
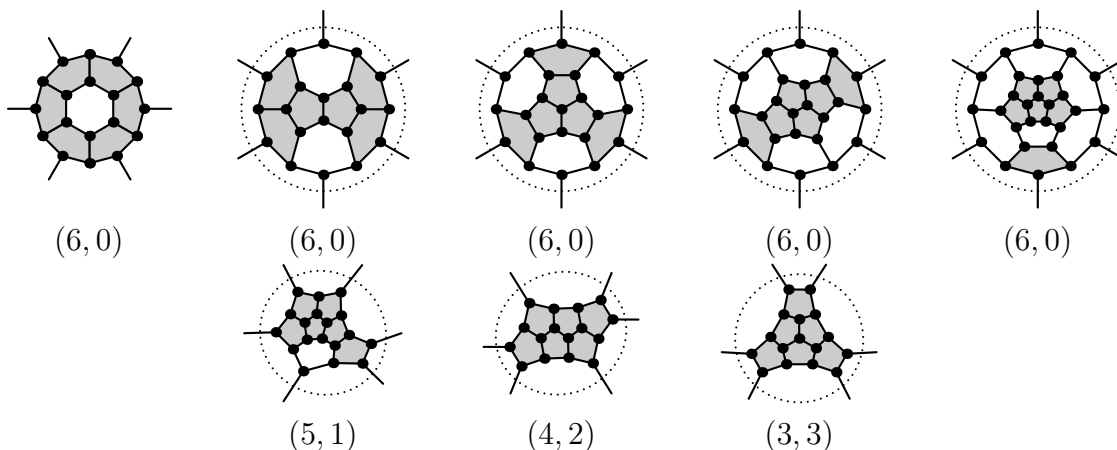

Figure 8: The (minimal) caps of (p_1, p_2)-nanotubes, where $p_1 + p_2 = 6$.

of caps such that every other cap in a nanotube with $p_1 + p_2 = 6$ contains (precisely) one of them as a subgraph. If you want to preserve the size of the cut, the caps for the type $(6, 0)$ can be extended only using O_3^{-1}, meaning adding whole layers of hexagons, since there are no 2's in the corresponding cut-vectors. Therefore, there are no other cups for this type of nanotubes. The three caps of the types where $p_2 > 0$ can be extended only using O_2^{-1}, meaning adding one hexagon in a step, since there is always at least one 2 in the corresponding cut-vector. Applying O_2^{-1} in the described way does not modify the type (p_1, p_2) of nanotubical cap. This way, we can find five more caps for nanotubes of type $(5, 1)$ and seven more caps for nanotubes of types $(4, 2)$ and $(3, 3)$. See Fig. 9 for an illustration. Thus, there are altogether $5 + 6 + 8 + 8 = 27$ caps.
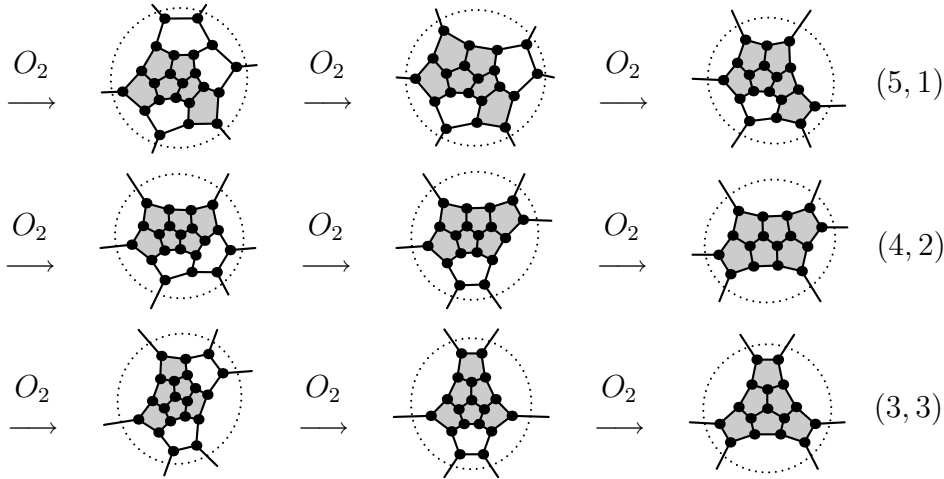
Figure 9: All other caps of the nanotubes with $p_1 + p_2 = 6$ and $p_2 > 0$ are derived from the minimal ones using O_2^{-1}.

Theorem 4 *A fullerene graph G has a non-degenerated cyclic 7-edge-cut if and only if it is a nanotube of type (p_1, p_2) such that*

(a) $p_1 + p_2 = 7$; or

(b) $p_1 + p_2 \leq 6$, and G is not isomorphic to one of the four graphs depicted in Fig. 10;

unless G is isomorphic to one of the two graphs depicted in Fig. 11.

Proof. It is easy to see that both graphs shown in Fig. 11 contain non-degenerate cyclic 7-edge-cuts.

Suppose now G is a nanotubical fullerene of type (p_1, p_2). We do not need to consider nanotubes with $p_1 + p_2 \geq 8$ here, since in the second part of the proof we conclude that if a fullerene graph contains a non-degenerated cyclic 7-edge-cut and it is nanotubic, then its width is at most 7.

In nanotubes with $p_1 + p_2 = 7$, simply the edges in the cylindrical part can be used to obtain a cyclic 7-edge-cut.

Let $p_1 + p_2 = 6$. We consider nanotubes of types $(5, 1)$, $(4, 2)$, $(3, 3)$, and $(6, 0)$ separately. The nanotubes of type $(5, 1)$ have uniquely defined caps, which contain a

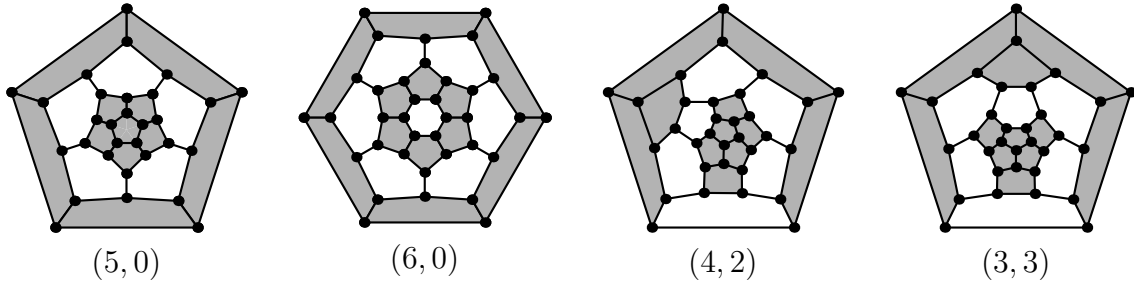(5, 0) (6, 0) (4, 2) (3, 3)

Figure 10: The only four nanotubical fullerenes with $p_1 + p_2 \leq 6$ not having a non-degenerate cyclic 7-edge-cut.
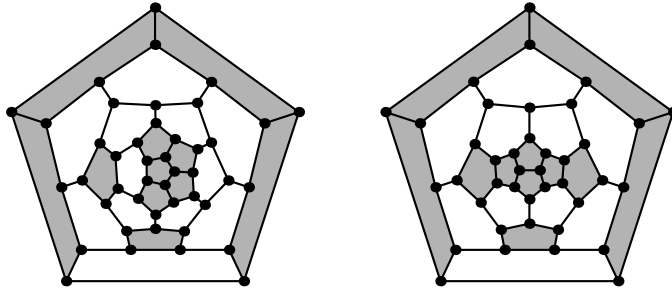

Figure 11: The only two non-nanotubical fullerenes with a non-degenerate cyclic 7-edge-cut.
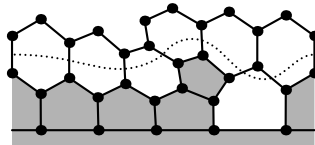

Figure 12: The cap of a nanotube of type $(5, 1)$ with a non-degenerate cyclic 7-edge-cut.

hexagon, so all such nanotubes have a configuration shown in Fig. 12, where a non-degenerated cyclic 7-edge-cut can be found.

On the other hand, the unique minimal caps of nanotubes of types $(4, 2)$ and $(3, 3)$ do not contain any hexagonal faces. So there exist nanotubes of such types that do not have non-degenerate cyclic 7-edge-cut. In fact for each type only the smallest nanotube is such, while all others have it. In Fig. 13, the smallest two nanotubes of each type are presented.

It remains to consider the nanotubes of type $(6, 0)$. There are five possible caps for this type, see Fig. 8. Only the first cap does not contain a hexagonal face incident with edges of the cut, so the nanotubes with both such caps need at least two layers of hexagons to obtain a non-degenerate cyclic 7-edge-cut. In all other configurations there are at least two edges in the cap that are not adjacent to a pentagonal face (the edges of cap's hexagon), and can be elements of the cut.

If $p_1 + p_2 = 5$ then $p_1 = 5$ and $p_2 = 0$. Recall that there is a unique cap for such a nanotube. Now, consider the cylindrical part of the nanotube with only one layer of hexagons. The only edges not adjacent to pentagons are the edges between hexagonal faces. There are only five such edges, thus a cyclic 7-edge-cut could not be obtained. On the other hand, having two or more layers, the edges between layers could be used
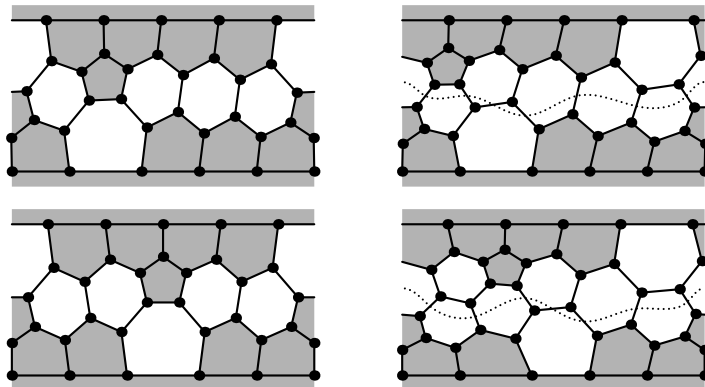
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Figure 13: The two smallest nanotubes of types $(4, 2)$ (on the top), and $(3, 3)$ (at the bottom).

to obtain the cut of size 7.

Now, we will prove the other direction. Let G be a fullerene graph and C a non-degenerated cyclic 7-edge-cut in G. Let H be one of the components of graph $G - C$. If C is nanotubical, then by the definition G is a nanotube with $p_1 + p_2 = 7$.

fSuppose that C is a non-nanotubical non-degenerated 7-edge cut. Consider the cut-vector of C. If there is a -1, it corresponds to a vertex of degree 1 in one of the components; anytime the cut-vector looks like $[\dots, a, -1, b, \dots]$, if we remove the vertex from the component, we get a non-degenerate cyclic 6-edge cut with the cut-vector $[\dots, a-1, b-1, \dots]$, see Fig. 14 for an illustration. By Theorem 3, it is contained in a nanotube, moreover, if we insert the removed vertex back, we get a non-degenerated 7-edge-cut in the nanotube. If the cut-vector contains any 3 as a coordinate, the complement must contain -1, since the cut is non-degenerated. So we apply the previous argument on the other component.
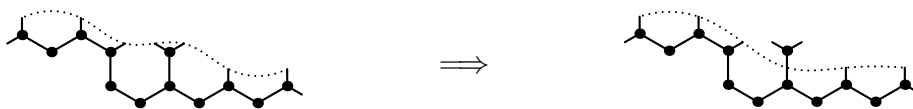
Figure 14: If the cut-vector of a k-cut contains -1, we can change it into a $(k-1)$-cut.

Therefore, we deal only with cut-vectors whose coordinates are 0's, 1's and 2's. Then, due to the definition, we have at least two consecutive 0's or 2's. So, the type of the cut-vector is one of the following three: $[2, 2, 2, 0, 0, 0]$, $[2, 2, 0, 2, 0, 0]$ or $[2, 2, 0, 0]$. Table 2 lists all possible cut-vectors (up to symmetry) which could arise from these types.

$[2, 2, 2, 0, 0, 0]$	$[2, 2, 0, 2, 0, 0]$	$[2, 2, 0, 0]$
$[2, 2, 2, 1, 0, 0, 0]$	$[2, 1, 2, 0, 2, 0, 0]$	$[2, 2, 1, 1, 1, 0, 0]$, $[2, 2, 1, 1, 0, 0, 1]$
$[2, 1, 2, 2, 0, 0, 0]$	$[2, 2, 1, 0, 2, 0, 0]$	$[2, 1, 2, 1, 1, 0, 0]$, $[2, 1, 2, 1, 0, 0, 1]$
	$[2, 2, 0, 1, 2, 0, 0]$	$[2, 1, 1, 2, 1, 0, 0]$, $[2, 1, 2, 1, 0, 1, 0]$
	$[2, 2, 0, 2, 0, 0, 1]$	$[2, 1, 1, 1, 2, 0, 0]$, $[2, 1, 1, 2, 0, 1, 0]$

Table 2: All possible cut-vectors that arise from non-nanotubical cut types.

Now, we will consider each of the cut-vectors separately and prove that any cut with such a cut-vector is either:

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- a part of a nanotube with $p_1 + p_2 \leq 7$; or

- a part of the graphs depicted in Fig. 11; or

- a part of a configuration which is non-realizable.

This analysis will establish the theorem. Notice that the cuts are depicted with the dotted lines in figures that follow.

[2,2,2,1,0,0,0]: Consider the configuration shown in Fig. 15. Notice that the face A cannot be pentagonal. Thus it is of length 6, and we obtain a non-degenerated 5-edge-cut with a cut-vector $[2, 2, 0, 0, 1]$. But by Theorem 1 it follows that such a configuration is non-realizable, since the only cut-vector of non-degenerated 5-edge-cut is $[1, 1, 1, 1, 1]$.

$[2, 2, 2, 1, 0, 0, 0]$-cut $\qquad$ $[2, 2, 0, 0, 1]$-cut
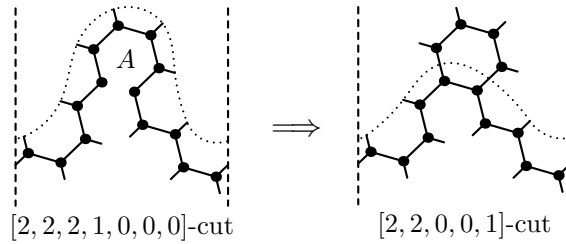
Figure 15: The component associated with the cut-vector $[2, 2, 2, 1, 0, 0, 0]$.

[2,1,2,2,0,0,0]: Consider the configuration shown in Fig. 16. Similarly as in the case above, A must be of length 6. We obtain a non-degenerated 5-edge-cut with a cut-vector $[2, 1, 0, 1, 1]$ and Theorem 1 implies that such a configuration is non-realizable.

$[2, 1, 2, 2, 0, 0, 0]$-cut $\qquad$ $[2, 1, 0, 1, 1]$-cut
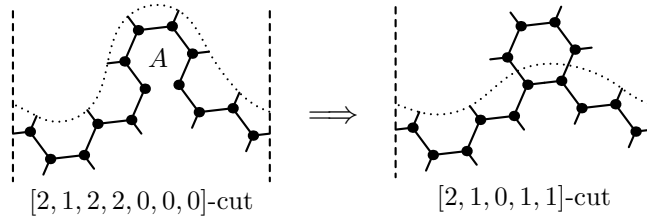
Figure 16: The component associated with the cut-vector $[2, 1, 2, 2, 0, 0, 0]$.

[2,1,2,0,2,0,0]: Consider the size of the face A from Fig. 17. If A is pentagonal, we obtain a degenerated 6-edge-cut with the cut-vector $[2, 0, 1, 0, 1, 1]$. Such a configuration is non-realizable by Theorem 2, since the cut-vectors of degenerated 6-edge-cuts with a component containing five pentagons are only $[2, 0, 1, 1, 1, 0]$ and $[0, 1, 1, 1, 1, 1]$. On the other hand, if A is hexagonal, we obtain a non-degenerated 6-edge-cut with the cut-vector $[2, 0, 1, 1, 1, 1]$, which is nanotubical; by Theorem 3 it occures in a nanotube with $p_1 + p_2 \leq 6$. It is easy to see that it is contained in a nanotube of type $(5, 1)$.
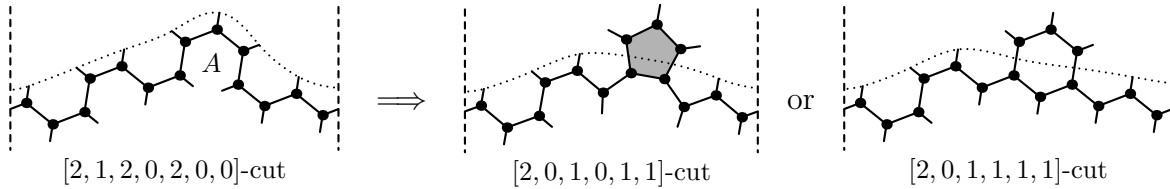
13

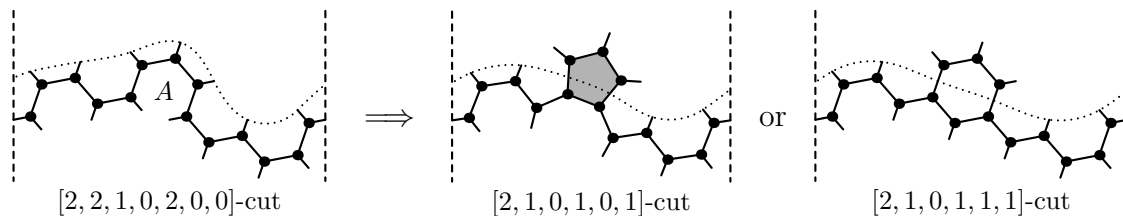Figure 17: The component associated with the cut-vector $[2, 1, 2, 0, 2, 0, 0]$.

[2,2,1,0,2,0,0]: In this case the size of the face A from Fig. 18, is considered. If it is of size five, the configuration is non-realizable, since a degenerated 6-edge-cut with the cut-vector $[2, 1, 0, 1, 0, 1]$ is obtained. There is no such a degenerated cut according to Theorem 2. If A is hexagonal, we obtain a cut with the cut-vector $[2, 1, 0, 1, 1, 1]$, which is nanotubical; it is contained in a nanotube of type $(4, 2)$. Since the original cut is non-degenerate, the six hexagons cut by the new 6-edge-cut are not surrounded by pentagons only. Therefore, the graph is not the exceptional one shown in Fig. 10.

Figure 18: The component associated with the cut-vector $[2, 2, 1, 0, 2, 0, 0]$.

[2,2,0,1,2,0,0]: Similarly as in the two cases above the size of the face A from Fig. 19 is taken in consideration. For A being pentagonal we once again obtain a non-realizable configuration, due to a cut with the cut-vector $[2, 0, 1, 1, 0, 1]$. For A hexagonal a nanotubical cut with the cut-vector $[2, 0, 1, 1, 1, 1]$ is obtained; it is contained in a nanotube of type $(5, 1)$.
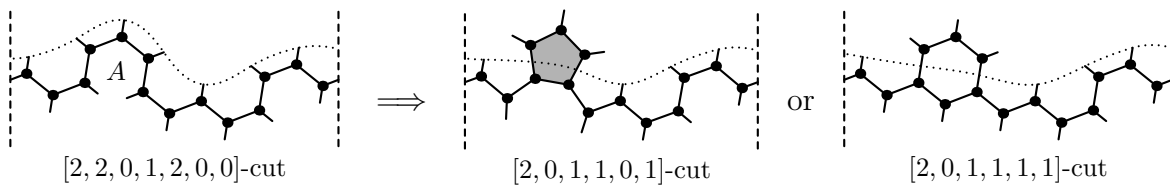

Figure 19: The component associated with the cut-vector $[2, 2, 0, 1, 2, 0, 0]$.

[2,2,0,2,0,0,1]: Analogously, if the face A from Fig. 20, is pentagonal, we once again obtain a non-realizable cut-vector $[2, 2, 0, 1, 0, 0]$. If A is hexagonal, a non-degenerate cyclic 6-edge-cut with the cut-vector $[2, 2, 0, 1, 1, 0]$ is obtained. This cut is not nanotubical, however, by Theorem 3 it is contained in a nanotube with $p_1 + p_2 \leq 6$. It is easy to see that it occurs in nanotubes of type $(5, 0)$ with at least two layers of hexagons.
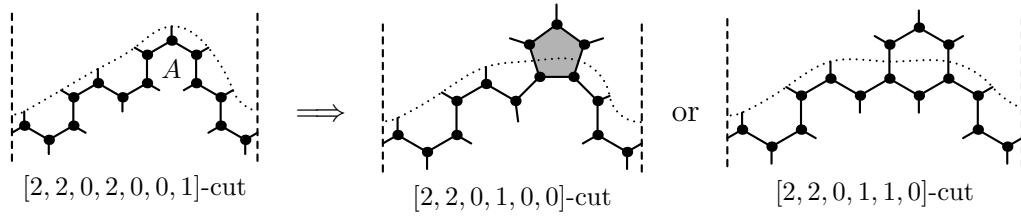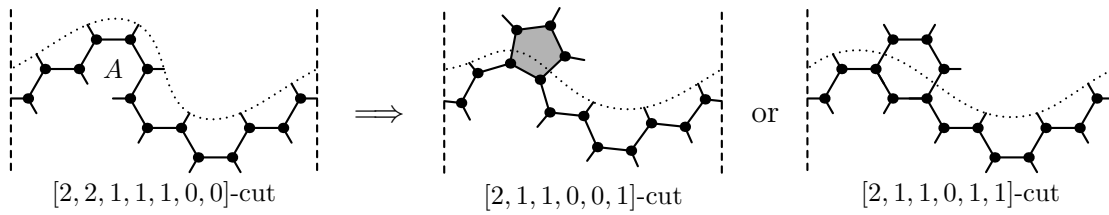
Figure 20: The component associated with the cut-vector $[2, 2, 0, 2, 0, 0, 1]$.

[2,2,1,1,1,0,0]: If the face A from Fig. 21, is pentagonal, we obtain a degenerated cyclic 6-edge-cut with a cut-vector $[2, 1, 1, 0, 0, 1]$ which is non-realizable. If A is hexagonal, we obtain a nanotubical cut with a cut-vector $[2, 1, 1, 0, 1, 1]$. It is contained in a nanotube of type $(3, 3)$. Since the original cut is non-degenerate, the six hexagons cut by the new 6-edge-cut are not surrounded by pentagons only. Therefore, the graph is not the exceptional one shown in Fig. 10.

Figure 21: The component associated with the cut-vector $[2, 2, 1, 1, 1, 0, 0]$.

[2,2,1,1,0,0,1]: Consider the face A from Fig. 22. If A is pentagonal, we obtain a degenerated 6-edge-cut with the cut-vector $[2, 2, 1, 0, 0, 0]$, which is non-realizable. If A is hexagonal, we obtain a non-degenerated 6-edge-cut, which by Theorem 3 can only occur in nanotubes. However, it can be easily checked that it is non-realizable, too, since it leads to a nanotube of type $(4, 1)$, which does not exist.
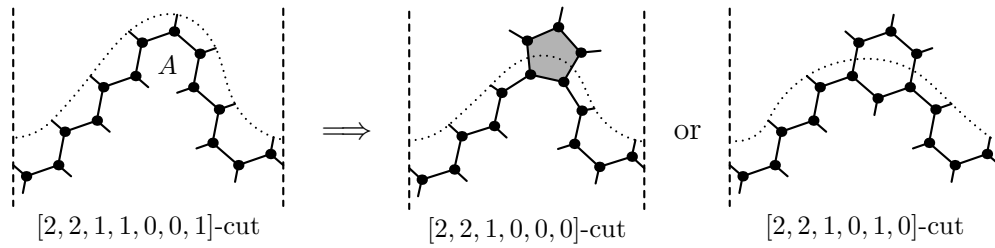

Figure 22: The component associated with the cut-vector $[2, 2, 1, 1, 0, 0, 1]$.

[2,1,2,1,1,0,0]: Consider the face A from Fig. 23. If it is pentagonal, we obtain a cut with the cut-vector $[2, 1, 0, 0, 1, 1]$, which is non-realizable by Theorem 2. If the face A is hexagonal, we obtain a cut with a nanotubical cut-vector $[2, 1, 0, 1, 1, 1]$; it occurs in nanotubes of type $(4, 2)$.

[2,1,2,1,0,0,1]: Consider the face A from Fig. 24. If A is pentagonal, we obtain a degenerated 6-edge-cut with the cut-vector $[2, 1, 2, 0, 0, 0]$, which is non-realizable. If A is hexagonal, we obtain a non-degenerated 6-edge-cut with the cut-vector
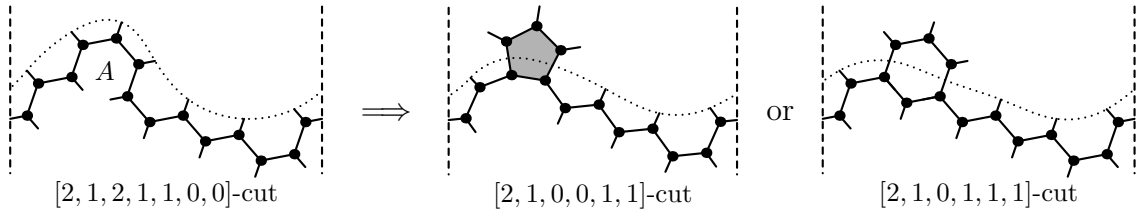
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Figure 23: The components associated with the cut-vector $[2, 1, 2, 1, 1, 0, 0]$.

$[2, 1, 2, 0, 1, 0]$, which must be contained in a nanotube. However, it can only appear in a nanotube of type $(5, 0)$ with at least two layers of hexagons.
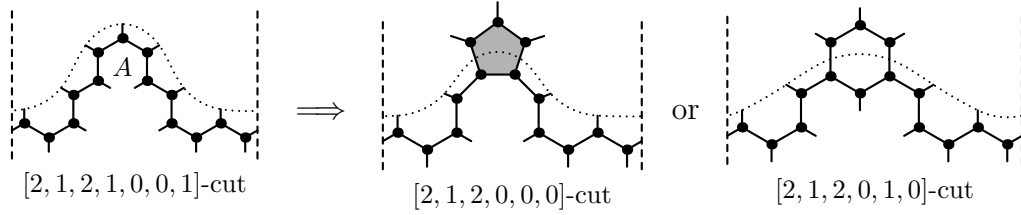

Figure 24: The component associated with the cut-vector $[2, 1, 2, 1, 0, 0, 1]$.

[2,1,1,2,1,0,0]: Consider the face A from Fig. 25. If it is pentagonal, we obtain a cut with the cut-vector $[2, 0, 0, 1, 1, 1]$, which is non-realizable by Theorem 2. If the face A is hexagonal, we obtain a cut with the cut-vector $[2, 0, 1, 1, 1, 1]$ appearing only in nanotubes of type $(5, 1)$.
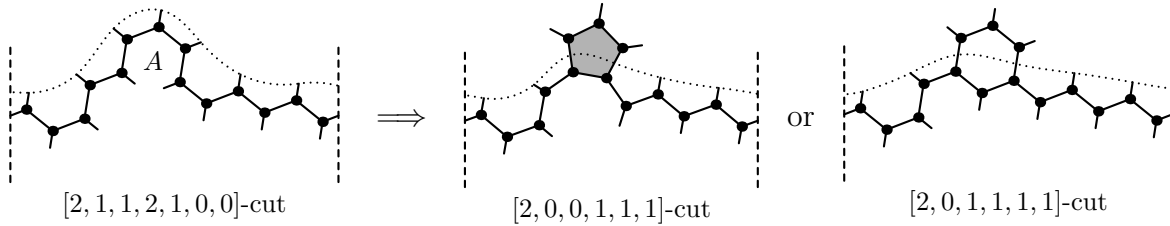

Figure 25: The components associated with the cut-vector $[2, 1, 1, 2, 1, 0, 0]$.

[2,1,2,1,0,1,0]: Consider the face A from Fig. 26. If A is pentagonal, we obtain a degenerated 7-edge-cut with a component of five pentagons and some hexagons, with the cut-vector $[2, 1, 2, 0, 1, 0, 0]$, which is non-realizable, since no degenerated 7-edge-cut in Table 1 has such a cut-vector. If A is hexagonal, we obtain a non-degenerated 7-edge-cut with the cut-vector $[2, 1, 2, 0, 2, 0, 0]$, which has already been considered and leads to nanotubes of type $(5, 1)$.

[2,1,1,1,2,0,0]: Here we consider two subcases, starting with the case that A is hexagonal. In this case we obtain a 6-edge-cut with the cut-vector $[1, 1, 1, 1, 1, 1]$ (see Fig. 27), which occurs on nanotubes of type $(6, 0)$. Since the original cut is non-degenerate, the six hexagons cut by the new 6-edge-cut are not surrounded only by pentagons on both sides. Therefore, the graph G is not in Fig. 10.

In the latter case A is pentagonal. We obtain a degenerated 6-edge-cut with the cut-vector $[0, 1, 1, 1, 1, 1]$. By Theorem 2, we know that there exists precisely one
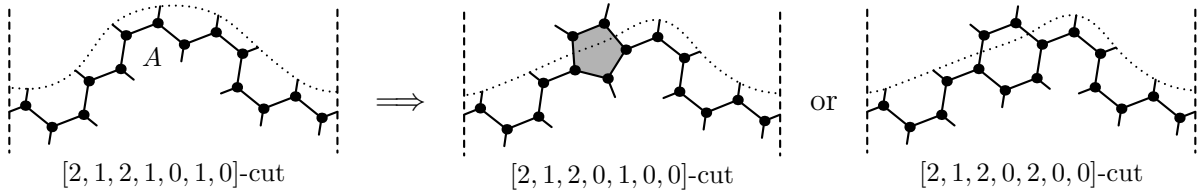
16

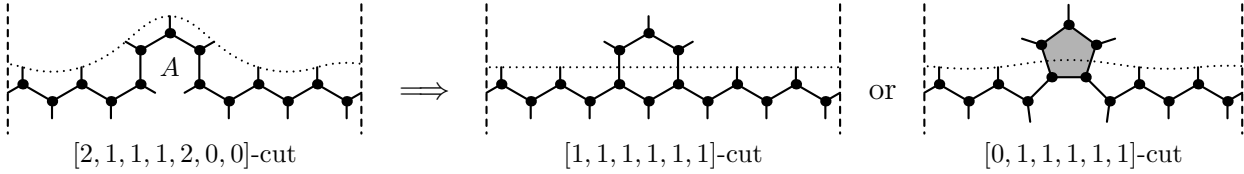Figure 26: The component associated with the cut-vector $[2, 1, 2, 1, 0, 1, 0]$.

Figure 27: The component associated with the cut-vector $[2, 1, 1, 1, 2, 0, 0]$.

configuration with such a cut. It is composed of five pentagons and one hexagon, which is by the component with 0 value in the cut. We obtain the left configuration from Fig. 28. Obviously, it is realizable and it does not have to be nanotubical, so we have to consider the other part of the graph, the complement of the original cut-vector – $[0, 1, 1, 1, 0, 2, 2]$.

Consider the faces A, B, C and D in Fig. 28. We distinguish cases regarding their sizes. Notice that in all cases we obtain a cut whose cut-vector has two consecutive coordinates with value 1. When all four faces are hexagonal, we obtain a nanotubical 6-edge-cut with the cut-vector $[1, 1, 1, 1, 1, 1]$. When at least one of them is pentagonal, a degenerated cut is obtained. By Theorem 2 and the fact that there are two consecutive 1's in the cut-vector of the cut passing the faces A, B, C, D, and the two topmost hexagons drawn in the same figure it follows that either one or two faces are pentagonal. When only one of the faces is pentagonal, we consider two subcases, due to the symmetry, either A is pentagonal or B is pentagonal.
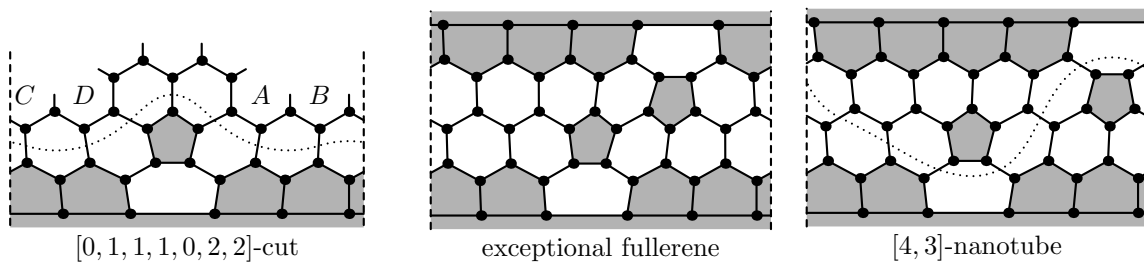

Figure 28: The components associated with the cut-vector $[0, 1, 1, 1, 0, 2, 2]$: the general situation and the cases when only A or B is pentagonal.

If the face A is pentagonal, we obtain a 6-cut with the cut-vector $[0, 1, 1, 1, 1, 1]$, which is uniquely realizable by configuration 6D07 of Fig. 4. We obtain the middle graph drawn in Fig. 28, which is isomorphic to the left graph of Fig. 11. It has no nanotubical cut, so this fullerene is not a nanotube.

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Similarly, if the face B is pentagonal, we again obtain a 6-cut with the cut-vector $[0,1,1,1,1,1]$, which is uniquely realizable. We get the right graph drawn in Fig. 28, where its nanotubical cut is presented. It is a nanotube of type $(4,3)$.
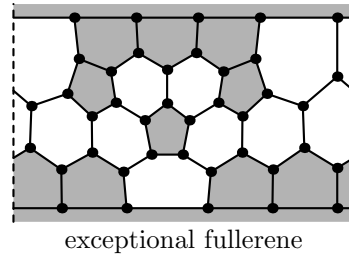

exceptional fullerene

Figure 29: The graph obtained from the cut-vector $[0,1,1,1,0,2,2]$ in the case two of the faces A, B, C, D are pentagonal.

In the latter case precisely two of the faces A, B, C and D are pentagonal. We obtain a degenerated cut with four 5-faces in the interior. The only such configuration has the cut-vector $[1,1,0,1,1,0]$. Notice that between the 0 components are two 1's. That infers the pentagonal faces are A and D, since there must be exactly two hexagons between the pentagons. This configuration is also realizable. We obtain the graph depicted in Fig. 29, which is isomorphic to the right graph of Fig. 11. It is not a nanotube, as it has no nanotubical cut.

[2,1,1,2,0,1,0]: Consider the faces A and B of Fig. 30. If both of them are hexagonal, we obtain a nanotubical cut with the cut-vector $[1,1,1,1,1,1]$. If at least one of them is pentagonal, we obtain a degenerated cut with the cut-vector having three consecutive 1's. The only degenerated cut with the cut-vector having three consecutive 1's has five pentagons in the interior, so exactly one of the faces A and B is pentagonal. In that case, we can always find a cut with the cut-vector $[2,1,1,1,2,0,0]$, see Fig. 30. Therefore, we deal only with configurations considered in the previous case.

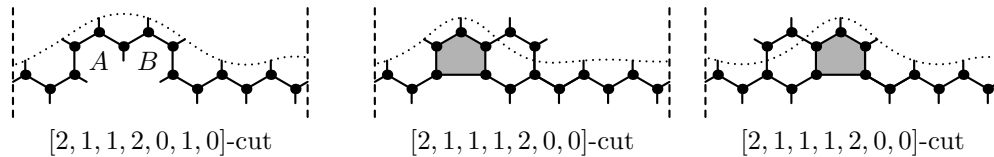$[2,1,1,2,0,1,0]$-cut $[2,1,1,1,2,0,0]$-cut $[2,1,1,1,2,0,0]$-cut

Figure 30: The components associated with the cut-vector $[2,1,1,2,0,1,0]$.

This proves the theorem. $\qquad\square$

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References

[1] T. Došlić, *On lower bounds of number of perfect matchings in fullerene graphs*, J. Math. Chem. **24** (1998) 359.

[2] T. Došlić, *On some structural properties of fullerene graphs*, J. Math. Chem. **31** (2002) 187.

[3] T. Došlić, *Cyclical edge-connectivity of fullerene graphs and $(k,6)$-cages*, J. Math. Chem. **33** (2003) 103.

[4] F. Kardoš and R. Škrekovski, *Cyclic edge-cuts in fullerene graphs*, J. Math. Chem. **22** (2008) 121.

[5] D. J. Klein and X. Liu, *Theorems for carbon cages*, J. Math. Chem. **33** (1992) 199.

[6] K. Kutnar and D. Marušič, *On cyclic edge-connectivity of fullerenes*, Discrete App. Math. **156**(10) (2008) 1661.

[7] J. Qian and F. Zhang, *On the number of Kekulé structures in capped zigzag nanotubes*, J. Math. Chem. **38** (2005) 233.

[8] F. Zhang and L. Wang, *k-resonance of open-ended carbon nanotubes*, J. Math. Chem. **35** (2004) 87.