

Cyclic 7-edge-cuts in fullerene graphs

František Kardoš, Matjaž Krnc, Borut Lužar, Riste Škrekovski

▶ To cite this version:

František Kardoš, Matjaž Krnc, Borut Lužar, Riste Škrekovski. Cyclic 7-edge-cuts in fullerene graphs. Journal of Mathematical Chemistry, 2010, 47 (2), pp.771-789. 10.1007/s10910-009-9599-0 . hal-00966751

HAL Id: hal-00966751 https://hal.science/hal-00966751

Submitted on 27 Mar 2014

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Cyclic 7-edge-cuts in fullerene graphs

František Kardoš^{*a*}, Matjaž Krnc^{*b*}, Borut Lužar^{*b*} and Riste Škrekovski^{*b*}

^a Institute of Mathematics, Faculty of Science, P. J. Šafárik University, Jesenná 5, 040 01 Košice, Slovakia frantisek.kardos@upjs.sk

> ^b Department of Mathematics, University of Ljubljana, Jadranska 19, 1111 Ljubljana, Slovenia {matjaz.krnc, borut.luzar}@gmail.com

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 up to 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 also list the configurations of degenerated cyclic 7-edge-cuts.

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 (*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 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 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 edgecuts – 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 some hexagons. 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 $i = 1, \ldots, p, h_0 = h_p$. (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 $r = p_1a_1 + p_2a_2$ 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 $p_1 \ge p_2$.



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 *arm*chair (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.

The nanotubes that are interesting in material science usually have the length-todiameter 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 denoted a *layer*, and the maximal number of parallel layers is the *lenght* of a nanotube.

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 nondegenerated cyclic 5 and 6-edge-cuts, however, there exist graphs that are not nanotubes and have non-degenerated cyclic k-edge-cut, for some $k \ge 7$. In the paper we consider non-degenerated cyclic 7-edge-cuts and prove that there exist precisely two fullerenes with non-degenerated cyclic 7-edge-cut, which are not nanotubes.



Figure 2: The buckyball is the first nanotube of type (5, 5).

Below we pose some known results regarding the non-trivial cyclic 5- and 6-edge-cuts. Let G_k denote a 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 $k \ge 1$.



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.

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 components of graph G - C. We label the vertices of degree one or two in H by v_1, v_2, \ldots, v_k . Let α_i be the number of 3-vertices between v_i and v_{i+1} (notice that $v_{k+1} = v_1$) on the segment on the outer face. Note that each vertex x of degree one in H is treated as two 2-vertices y and w. We define that between y and w there is -1 vertex of degree three.

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 components 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, see Fig. 4 for examples. Observe, that each non-degenerated cyclic edge-cut has two complementary cut-vectors associated with each of

the components of G - C. Here complementary means that knowing one of them is enough, since the sum of components of the same index is in fullerenes always equal to two (only edges of hexagons are elements of non-degenerated cyclic edge-cut). The sum of cut-vector's components 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 number 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. Then

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

Using Euler's formula, we also have that

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

Putting it all together we get

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

and hence

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

Proof of Lemma 1. Let *H* be the component of G - C that corresponds to α . By the choice of *C*, *H* has n_1 1-vertices, n_2 2-vertices, where $2n_1 + n_2 = k$, and 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

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

Hence

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

7

which proves the lemma.

4

The type of a cut-vector α is the vector obtained from α after omitting the components with value 1. For example, the type of the cut-vector [2, 1, 1, 0, 1, 2, 0] is [2, 0, 2, 0]. If no two consecutive components 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 components 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 only two direction vectors.

The notion of cut-vector defined, we can now proceed with cyclic 6-edge-cuts. Unlike cyclic 5-edge-cuts, there exist degenerated cyclic 6-edge-cuts, which are not trivial.

Theorem 2 There are precisely seven non-isomorphic graphs that can be obtained as components of degenerated cyclic 6-edge-cuts with less than six pentagons. Moreover, the graphs with i pentagons are unique for i = 0, 1, 2, 3, 4.



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 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).

- (O₁) If a component H contains a vertex of degree one, then using (O₁) one can modify the k-edge-cut C into a (k-1)-edge-cut C₁.
- (O₂) If a component H contains two adjacent vertices of degree two, then using (O₂) one can modify the k-edge-cut C into a k-edge-cut C_2 .
- (O₃) If the vertices of the outer faces of H are consecutively of degree 2 and 3, then using (O₃) 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. On Fig. 6 an example of constructing a degenerate cyclic 7-edge-cut is presented, and on Fig. 7 we listed the degenerated cyclic 7-edge-cuts.



Figure 6: An example of construction.

On Table 1 for each configuration depicted on 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 an inverse O_2^{-1} .

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 two exceptions. There exist precisely two fullerene graphs, which have non-degenerated cyclic 7-edge-cuts and that are not nanotubical. We also characterize



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]	_	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	D03	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	D09	D18, D20
D15	4	0	13	[-1, 1, 1, 1, 0, 1, 2]	6D05	D09	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]	_	D26, D25	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	С –	2	19	[0, 1, 1, 1, 1, 1, 1]		D28	-
D40	C F	2	19	[0, 1, 0, 1, 2, 0, 2]		D28, D29, D30	D47, D48
D41	G F	2	19	[0, 0, 2, 1, 0, 1, 2]	_	D29, D31	D48 D40
D42	D F	2	19	[0, 0, 2, 0, 1, 1, 2]		D30, D31, D32	D48, D49
D43	\mathbf{O}		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.

the types of nanotubes in which non-degenerate cyclic 7-edge-cuts exist. It is obvious that nanotubes of type (p_1, p_2) , where $p_1 + p_2 \ge 8$, cannot contain such a cut, due to the width of the cylindrical part (of course, degenerate cyclic edge-cuts are not limited by the type).

Regarding nanotube types, where the sum $p_1 + p_2 < 7$, it was already proven in [4] that only graphs G_k contain non-trivial cyclic 5-edge-cuts, in other words, for $p_1 + p_2 = 5$, only nanotubes of type (5,0) exist. On the other hand, there are more possible types for $p_1 + p_2 = 6$. For type (6,0) there exist five different caps, while for types (5,1), (4,2), and (3,3) caps are unique. On Fig. 8 the caps retrieved from nanotubes of specified types are presented. Note that nanotubes with $p_1 + p_2 < 5$ do not exist, due to cyclic 5-edge-connectivity of fullerenes.



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

Now, let us state the main theorem of this article.

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

- (a) $p_1 + p_2 = 7; or$
- (b) $p_1 + p_2 = 6$, and the nanotube is not the smallest nanotube of types (3,3), and (4,2), or it is not of type (6,0) with one layer of hexagons and with both caps isomorphic to the first configuration on Fig. 8; or
- (c) $p_1 + p_2 = 5$, with at least 2 layers of hexagons;

unless it is isomorphic to one of the two graphs depicted in Fig. 9.



Figure 9: The only two non-nanotubical fullerenes with a 7-edge-cut.

Proof. 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, it is obvious that G is a nanotube. Let us firstly consider such cuts.

We prove that all nanotubes, which contain cyclic 7-edge-cuts, are of type (p_1, p_2) , where $p_1 + p_2 = k$, $k \in \{5, 6, 7\}$. Consider cases regarding k. Let k = 5 and let the cylindrical part of the nanotube have only one layer of hexagons. Then, 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 to obtain the cut of greater length.

Now, let k = 6 and 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 hexagon, so all such nanotubes have a configuration on Fig. 10, where exists a non-degenerated cyclic 7-edge-cut.



Figure 10: The cap of a nanotube of type (5, 1) with a non-degenerate cyclic 7-edge-cut.

On the other hand, the unique 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. On Fig. 11 the smallest two nanotubes of each type are presented.



Figure 11: The two smallest nanotubes of types (4, 2) (on the top), and (3, 3) (at the bottom).

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, so the nanotubes with both such caps need at least two layers of hexagons to obtain a nondegenerate 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. In case, when k = 7, simply the edges in cyclindrical part are used to obtain a cyclic 7-edge-cut.

Now, let C be non-nanotubical non-degenerated 7-edge cut. Consider the cut-vector of C. If it contains any 3, the complement must contain -1, since the cut is non-degenerated. If there is a -1, it corresponds to a vertex of degree 1 in one of the components; anytime the cut vector looks like $[\ldots, a, -1, b, \ldots]$, if we remove the vertex from the component, we get a non-degenerate cyclic 6-edge cut, with the cut vector $[\ldots, (a-1), (b-1), \ldots]$, see Fig. 12 for 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.



Figure 12: If the cut-vector of a k-cut contains -1, we can change it into a (k-1)-cut.

Therefore, we deal only with 0s, 1s and 2s. 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.

Now, we will consider each of the cut-vectors separetly and prove that any cut with such a cut-vector is either a part of a nanotube, part of the graphs depicted in Fig. 9,

$\left[2,2,2,0,0,0\right]$	[2, 2, 0, 2, 0, 0]	[2, 2, 0, 0]
$\left[2,2,2,1,0,0,0\right]$	[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.

or a part of a configuration, which is non-realizable. Notice that the cuts are depicted with the dotted lines on figures.

[2,2,2,1,0,0,0]: Consider the configuration of Fig. 13, left. Notice that the face A cannot be pentagonal, otherwise there would be a cyclic 3-edge-cut, which is impossible [3]. 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].



Figure 13: The component associated with the cut-vector [2, 2, 2, 1, 0, 0, 0].

[2,1,2,2,0,0,0]: Consider the configuration of Fig. 14, left. Similarly as in the case above, we may see that face A is of length 6. We obtain a non-degenerated 5-edge-cut with a cut-vector [2,1,0,1,1]. Theorem 1 implies that such a configuration is non-realizable.



Figure 14: 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. 15. 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 [2,0,1,1,1,0] and [0,1,1,1,1,1]. On the other hand, if A is hexagonal, we obtain a nanotubical cut with the cut vector [1,1,1,2,0,1].



Figure 15: 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. 16, left, is considered again. If it is of size five, the configuration is non-realizable, since a degenerated 6-edgecut 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.



Figure 16: 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. 17, left, is taken in consideration. For A 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 the nanotubical cut with the cut-vector [2,0,1,1,1,1] is obtained.



Figure 17: 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. 18, left, is pentagonal, we once again obtain a non-realizable cut-vector [2,2,0,1,0,0]. If A is hexagonal, a nondegenerate cyclic 6-edge-cut with the cut-vector [2,2,0,1,1,0] is obtained. By Theorem 3 it must be nanotubical.



Figure 18: 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. 19, left, 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-vector [1, 2, 1, 1, 0, 1].



Figure 19: 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. 20, left. 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 is by Theorem 3 nanotubic. (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 [4].)



Figure 20: 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. 21, left. 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].



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

- [2,1,2,1,0,0,1]: Consider the face A from Fig. 22, left. 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 [2, 1, 2, 0, 1, 0], which can only appear in a nanotube.
- [2,1,1,2,1,0,0]: Consider the face A from Fig. 23, left. 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 a nanotubical cut-vector [2,0,1,1,1,1].



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



Figure 23: 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. 24, left. 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 cut-vector. If A is hexagonal, we obtain a nondegenerated 7-edge-cut with the cut vector [2, 1, 2, 0, 2, 0, 0], which has already been considered and leads to nanotubic cuts only.



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

[2,1,1,1,2,0,0]: In this case we consider two sub cases again, starting with the case with A being hexagonal. In that case we obtain a 6-edge-cut with the cut-vector [1, 1, 1, 1, 1, 1] (see Fig. 25), which is nanotubical.



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

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 configuration with such a cut. It is composed by five pentagons and one hexagon, which is by the component with 0 value in the cut. We obtain the left configuration on Fig. 26. Obviously, it is realizable and 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 on Fig 26, left. We distinguish cases regarding their sizes. Notice that in all cases we obtain a cut with the cut-vector, which has two consecutive components 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 the 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 Fig 26, 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 26: 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 cut-vector [0, 1, 1, 1, 1, 1], which is realizable uniquely. We get the middle graph drawn in Fig 26, which is isomorphic to the left graph of Fig. 9. There is no nanotubical cut in it, so this fullerene is not a nanotube.

If the face B is pentagonal, we again obtain a 6-cut with cut-vector [0, 1, 1, 1, 1, 1], which is realizable uniquely. We get the right graph draw in Fig 26. It is a nanotube of type (4, 3).



Figure 27: 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. The configuration is again realizable. We obtain the graph depicted in Fig. 27, which is isomorphic to the right graph of Fig. 9. It is not a nanotube, since there is no nanotubical cut in it.

[2,1,1,2,0,1,0]: Consider the faces A and B on Fig. 28, left. If both of them are hexagonal, we obtain a cut with the cut-vector [1,1,1,1,1,1], therefore it is nanotubical. 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. 28. Therefore, we deal only with configurations already mentioned above.



Figure 28: The components associated with the cut-vector [2, 1, 1, 2, 0, 1, 0].

This proves the theorem.

Acknowledgement. Supported in part by bilateral projects BI-SK/05-07-001 and SK-SI-0007-08 between Slovenia and Slovakia, by Slovak Research and Development Agency under the contract No. APVV-0007-07, by the Slovak VEGA Grant 1/3004/06, and by the Slovenian ARRS Research Grant P1-0297.

References

- T. Došlić, On lower bounds of number of perfect matchings in fullerene graphs, J. Math. Chem. 24 (1998) 359–364.
- [2] T. Došlić, On some structural properties of fullerene graphs, J. Math. Chem. 31 (2002) 187–195.
- [3] T. Došlić, Cyclical edge-connectivity of fullerene graphs and (k, 6)-cages, J. Math. Chem. 33 (2003) 103–112.
- [4] F. Kardoš and R. Škrekovski, Cyclic edge-cuts in fullerene graphs, J. Math. Chem. 22 (2008) 121–132.
- [5] D. J. Klein and X. Liu, *Theorems for carbon cages*, J. Math. Chem. **33** (1992) 199–205.
- [6] K. Kutnar and D. Marušič, On cyclic edge-connectivity of fullerenes, Discrete App. Math. 156(10) (2008) 1661-1669.
- [7] J. Qian and F. Zhang, On the number of Kekulé structures in capped zigzag nanotubes, J. Math. Chem. 38 (2005) 233–246.
- [8] F. Zhang and L. Wang, k-resonance of open-ended carbon nanotubes, J. Math. Chem. 35 (2004) 87–103.