ON CYCLIC EDGE-CONNECTIVITY OF FULLERENES

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Abstract

A graph is said to be cyclic \( k \)-edge-connected, if at least \( k \) edges must be removed to disconnect it into two components, each containing a cycle. Such a set of \( k \) edges is called a cyclic-\( k \)-edge cutset and it is called a trivial cyclic-\( k \)-edge cutset if at least one of the resulting two components induces a single \( k \)-cycle.

It is known that fullerenes, that is, 3-connected cubic planar graphs all of whose faces are pentagons and hexagons, are cyclic 5-edge-connected. In this article it is shown that a fullerene \( F \) containing a nontrivial cyclic-5-edge cutset admits two antipodal pentacaps, that is, two antipodal pentagonal faces whose neighboring faces are also pentagonal. Moreover, it is shown that \( F \) has a Hamilton cycle, and as a consequence at least \( 15 \cdot 2^{\frac{n}{20}} \) perfect matchings, where \( n \) is the order of \( F \).

Keywords: graph, fullerene graph, cyclic edge-connectivity, Hamilton cycle, perfect matching.

1 Introduction

A fullerene graph (in short a fullerene) is a 3-connected cubic planar graph, all of whose faces are pentagons and hexagons. By Euler formula the number of pentagons equals 12. From a chemical point of view, fullerenes correspond to carbon 'sphere'-shaped molecules, the important class of molecules which is a basis of thousands of patents for a broad range of commercial applications \cite{23, 25}. Graph-theoretic observations on structural properties of fullerenes are important in this respect \cite{1, 3, 6, 7, 12, 13, 14, 15, 24}.

In this paper cyclic edge-connectivity of fullerenes, that is, the number \( k \) such that a fullerene cannot be separated into two components, each containing a cycle, by deletion of fewer than \( k \) edges, is considered. In general, a graph is said to be cyclically \( k \)-edge-connected, in short cyclically \( k \)-connected, if at least \( k \) edges must be removed to disconnect it into two components, each containing a cycle. Cyclic edge-connectivity was extensively studied (see \cite{2, 15, 19, 20, 22}). A set of \( k \) edges whose elimination disconnects a graph into two components, each containing a cycle, is called a cyclic-\( k \)-edge cutset, in short a cyclic-\( k \)-cutset and moreover, it is called a trivial cyclic-\( k \)-cutset if at least one of the resulting two components induces a single \( k \)-cycle. An edge from a cyclic-\( k \)-cutset is called cyclic-cutedge.

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The concept of cyclic edge-connectivity played an important role in obtaining some structural properties of fullerenes, such as bicriticality and 2-extendability, that further imply certain lower bounds on the number of perfect matchings in fullerenes \[8, 9, 10, 11, 26\]. (Recall that a perfect matching \(M\) in a graph is a set of disjoint edges such that every vertex of the graph is covered by an edge from \(M\).) A perfect matching in a graph coincides, with the so-called Kekulé structure in chemistry, and the number of perfect matchings is an indicator of the stability of a fullerene. However, in any fullerene the cyclic edge-connectivity cannot exceed 5, since by deleting the five edges connecting a pentagonal face, two components each containing a cycle are obtained. In \[10, \text{Theorem 2}\] it was proven that it is in fact precisely 5.

The main object of this paper is to give a more detailed description of cyclic-5-cutsets in fullerenes. We show that, with the exception of a very special family of fullerenes possessing two antipodal pentacaps, that is, two antipodal pentagonal faces whose neighboring faces are also pentagonal, every other fullerene has only trivial cyclic-5-cutsets (see Theorem 2.4).

Furthermore, we prove that fullerenes admitting a nontrivial cyclic-5-cutset contain a Hamilton cycle, that is, a cycle going through all vertices (see Theorem 2.4), thus making a small contribution to the open problem regarding existence of Hamilton cycles in fullerenes \[21\]. (Note that this problem is a special case of the Barnette’s conjecture \[3\] which says that every 3-connected planar graph whose largest faces are hexagons, contains a Hamilton cycle.) As an immediate consequence of this result it is shown that every fullerene of order \(n\) admitting a nontrivial cyclic-5-cutset has at least \(15 \cdot 2^\lfloor \frac{m}{20} \rfloor\) perfect matchings, thus improving (in the case of nontrivially cyclically 5-edge-connected fullerenes) the best known lower bound of \(3(m+2)/4\) for the number of perfect matchings in a general fullerene of order \(m\) (see \[26\]).

Throughout this paper graphs are finite, undirected and connected, unless specified otherwise. For notations and definitions not defined here we refer the reader to \[16\]. For adjacent vertices \(u\) and \(v\) in \(X\), we write \(u \sim v\) and denote the corresponding edge by \(uv\). Given a graph \(X\) we let \(V(X)\) and \(E(X)\) be the vertex set and the edge set of \(X\), respectively. If \(u \in V(X)\) then \(N(u)\) denotes the neighbors set of \(u\) and \(N_i(u)\) denotes the set of vertices at distance \(i > 1\) from \(u\). If \(S \subseteq V(X)\), then \(S^c = V(X) \setminus S\) denotes the complement of \(S\) and the graph induced on \(S\) is denoted by \(X[S]\). Moreover, \(X' = X[S + S']\) denotes the graph with the vertex set \(V(X') = S \cup S'\) and the edge set \(E(X') = E(X[S]) \cup \{uv \mid u \in S, v \in S'\}\).

2 Fullerenes admitting a nontrivial cyclic-5-cutset

An immediate consequence of cyclic 5-edge-connectivity of a fullerene is the following result about the girth of a fullerene, that is, about the length of its smallest cycle.

**Proposition 2.1** The girth of a fullerene is 5.

Let \(C\) be a cycle in a planar embedding of a fullerene \(F\). Then we let the inside \(\text{Ins}(C)\) and the outside \(\text{Out}(C)\) be the set of vertices of \(F\) that lie inside \(C\) and outside \(C\), respectively. The following result is an immediate consequence of the well known Euler’s formula for connected planar graphs. (Euler’s formula states that the number of faces of a connected planar graph \(X\) in its planar embedding is equal to \(|E(X)| + |V(X)| - 2\).)

**Proposition 2.2** Let \(C\) be a cycle of length 10 in a fullerene \(F\) such that there exist exactly five vertices on \(C\) having a neighbor in the interior of \(C\). Then exactly six pentagons exist in the subgraph induced by \(V(C) \cup \text{Ins}(C)\).
In this section we will prove that every fullerene admitting a nontrivial cyclic-5-cutset contains two antipodal pentacaps (see Theorem 2.4), where the pentacap is a planar graph on 15 vertices with 7 faces of which one is a 10-gon and six are pentagons (see Figure 1). Observe that the dodecahedron is obtained as a union of two pentacaps, by identifying the ten vertices on the outer ring of the two pentacaps. The following lemma will be useful in this respect.

![Figure 1: The pentacap.](image)

**Lemma 2.3** Let $F$ be a fullerene containing a ring $R$ of five faces, and let $C$ and $C'$ be the inner cycle and the outer cycle of $R$, respectively. Then either

(i) $C$ or $C'$ is a face, or

(ii) both $C$ and $C'$ are of length 10, and the five faces of $R$ are all hexagonal.

**Proof.** Let $f_0, f_1, f_2, f_3$ and $f_4$ be the faces in the ring $R$ such that $f_i$ is adjacent to $f_{i+1}$, $i \in \mathbb{Z}_5$. Let $T$ be the set of edges between these five faces (depicted in bold in Figure 2). Clearly, $T$ is a cyclic-5-cutset of $F$. Moreover, if $T$ is a trivial cyclic-5-cutset of then either $C$ or $C'$ is a face. We may therefore assume that $T$ is a nontrivial cyclic-5-cutset, and that neither $C$ nor $C'$ is a face.

![Figure 2: The local structure of a fullerene that admits a nontrivial cyclic-5-cutset.](image)

Let $S = \text{Ins}(C)$ and $S' = \text{Out}(C')$, respectively, be the inside of $C$ and the outside of $C'$. Let $l = l(C)$ and $l' = l(C')$ be the corresponding lengths of cycles $C$ and $C'$. With no loss of generality, let $l \leq l'$. Depending on whether the five faces are either all pentagonal at the one extreme or all hexagonal at the other extreme, or possibly some pentagonal and some hexagonal, we have that

$$15 \leq l + l' \leq 20. \quad (1)$$
Since $T$ is a nontrivial cyclic-5-cutset and $C$ is not a face, we must have that $l \geq 6$.

If $l \in \{6, 7\}$ then there either exists one edge or there are two edges having one endvertex in $C$ and the other in $S$ whose deletion disconnects $F$, contradicting 3-connectedness of $F$. Therefore $l \geq 8$.

Suppose first that $l = 8$. Then there exists a set of three edges $\{u_1v_1, u_2v_2, u_3v_3\}$ such that $u_1, u_2, u_3 \in V(C)$, $u_i \neq u_j$ for $i \neq j$ and $v_1, v_2, v_3 \in S$. Since $F$ is cyclically 5-connected it follows that the subgraph of $F$ induced by $S$ is a forest and so $X = F[S + \{u_1, u_2, u_3\}]$ is a forest, too. Let $m = |S \cup \{u_1, u_2, u_3\}|$. Since all of the vertices in $S$ are of valency 3 we have that $2|E(X)| = 3(m - 3) + 3$, whereas on the other hand $2|E(X)| = 2(|V(X)| - p) = 2(m - p)$, where $p$ denotes the number of components of $X$. It follows that

$$m = 6 - 2p.$$ \hspace{1cm} (2)

Then by (2) it follows that $p = 1$ and so $m = 4$. This implies that $|S| = 1$ and therefore $v_1 = v_2 = v_3$. But as $R$ consists of five faces one can easily see that the subgraph induced by $V(C) \cup \text{Ins}(C)$ contains a cycle of length 3 or 4, contradicting Proposition 2.1.

Suppose next that $l = 9$. Then there exists a set of four edges $\{u_1v_1, u_2v_2, u_3v_3, u_4v_4\}$ such that $u_1, u_2, u_3, u_4 \in V(C)$, $u_i \neq u_j$ for $i \neq j$ and $v_1, v_2, v_3, v_4 \in S$. Since $F$ is cyclically 5-connected it follows that the subgraph of $F$ induced by $S$ is a forest and so $X = F[S + \{u_1, u_2, u_3, u_4\}]$ is a forest, too. Let $m = |S \cup \{u_1, u_2, u_3, u_4\}|$. A counting argument similar to the one used in the previous paragraph gives us

$$m = 8 - 2p,$$ \hspace{1cm} (3)

where $p$ is the number of connected components of $X$. Clearly $p \leq 2$. If $p = 1$ then (3) gives us $m = 6$ and so there exist two vertices in $S$, say $v_1 = v_2$ and $v_3 = v_4$. Then $X$ has two vertices of valency 3 and four vertices of valency 1. But since $l = 9$ one can easily see that, as in the case $l = 8$, the subgraph induced by $V(C) \cup \text{Ins}(C)$ contains a cycle of length 3 or 4, contradicting Proposition 2.1. If $p = 2$ then (3) implies that $m = 4$, and so $S = \emptyset$. Then without loss of generality $u_1 \sim u_2$ and $u_3 \sim u_4$. But then again the fact that $l = 9$ implies the existence of a cycle of length less then or equal to 4 in the graph induced by $V(C) \cup \text{Ins}(C)$, a contradiction.

Now (1) implies that $l = l' = 10$ and therefore all of the faces $f_i, i \in \mathbb{Z}_5$, on $R$ are hexagons, completing the proof of Lemma 2.3. 

Given a ring of faces $R$ in a planar embedding of a fullerene $F$ with inner cycle $C$ and outer cycle $C'$ we let a face $f \in R$ be of type $(j) = (j)_C$ if there exist $j$ vertices on $f$ having the third neighbor (the one different form the immediate neighbors on $C$) in $\text{Ins}(C) \cup V(C)$. Clearly $0 \leq j \leq 2$. Further, a ring $R$ of $r$ faces $f_1, f_2, \ldots, f_r$ such that $f_i$ is adjacent to $f_{i+1}$, $i \in \mathbb{Z}_r$, is said to be of type $(j_1 j_2 \ldots j_r) = (j_1 j_2 \ldots j_r)_C$ if $f_i \in R$ is of type $(j_i)$ for every $i \in \mathbb{Z}_r$. For example, a ring in which the inner cycle is a face is of type $(00000)$ if the inner cycle is a pentagon and of type $(000000)$ if the inner cycle is a hexagon.

We may now prove the main theorem of this paper.

**Theorem 2.4** Let $F$ be a fullerene admitting a nontrivial cyclic-5-cutset. Then $F$ contains a pentacap, more precisely, either $F$ is the dodecahedron or it contains two disjoint antipodal pentacaps.
**Proof.** It is clear that the dodecahedron admits a nontrivial cyclic-5-cutset. Therefore, let $F$ be a fullerene admitting a nontrivial cyclic-5-cutset $T$ different from the dodecahedron. Then there exists a ring $R$ of five faces $f_0, f_1, f_2, f_3$ and $f_4$ in $F$ such that $f_i$ is adjacent to $f_{i+1}$, $i \in \mathbb{Z}_5$, via an edge from $T$. Let $C_0$ be the inner cycle of $R$ and $C_1$ be the outer cycle of $R$. Let $S_0 = \text{Ins}(C_0)$ and $S_1 = \text{Out}(C_1)$, respectively, be the inside of $C_0$ and the outside of $C_1$. Let $l_0 = l(C)$ and $l_1 = l(C')$ be the corresponding lengths of cycles $C_0$ and $C_1$. By Lemma 2.3 we have that $l_0 = l_1 = 10$. Hence the five faces of $R$ are all hexagonal and precisely five vertices having a neighbor in $S_0$ exist on $C_0$. Depending on the arrangement of the vertices on $C_0$ having a neighbor in $S_0$ the ring $R$ is of one of the following six types: (01112), (01121), (00212), (00122), (02102) or (11111) (see Figure 3). (Note that these are all possible types since $l_0 = 10$.)

![Figure 3: The six possible types of $R$.](image)

We claim that only type (11111) can occur. Let $C_0 = u_0u_1 \ldots u_9$ and first, Suppose that there exist $i, j \in \mathbb{Z}_9, j \notin \{i - 1, i, i + 1\}$, such that $u_i$ and $u_j$ are adjacent. Since $F$ has girth 5 we have that

$$4 \leq i - j \leq 5.$$ 

Now planarity and 3-connectivity of $F$ combined together imply that either $u_i, u_{i+1}, \ldots, u_{j-1}, u_j$ or $u_j, u_{j+1}, \ldots, u_{i-1}, u_i$ determine a face, say $f$, in $F$ (observe that $u_i$ and $u_j$ lie on nonneighboring faces of $R$). Checking all possible types one can see that $R$ is either of type (00212) or of type
(00122). But then \(ff_i f_{i+1} f_{i+2}\) (where \(f_i, f_{i+1}\) and \(f_{i+2}\), \(i \in \mathbb{Z}_5\), are faces of \(R\) of nonzero type), is a ring of four faces. This is impossible in view of cyclic 5-edge-connectivity of \(F\).

Next, suppose that there exist \(i, j \in \mathbb{Z}_9\), \(j \neq i\), such that \(N(u_i) \cap N(u_j) \cap S_0 \neq \emptyset\). Since \(F\) has girth 5 we have that
\[
3 \leq i - j \leq 5.
\]
Now planarity and 3-connectivity of \(F\) combined together imply that either \(u_i, u_{i+1}, \ldots, u_{j-1}, u_j\) or \(u_j, u_{j+1}, \ldots, u_{i-1}, u_i\) determinate a face, say \(f\), in \(F\), and so \(u_i\) and \(u_j\) lie on nonneighboring faces of \(R\). Clearly, \(f\) is a neighbor of either one or two faces of \(R\) having type (0). If the former case holds then \(f\) is pentagonal, and moreover \(f\) together with the four faces in \(R\) different from the type (0) face adjacent to \(f\), form a ring of five faces, contradicting Lemma 2.3. If the latter holds then \(f\) together with the three nonzero type \((\neq 0)\) faces of \(R\) form a ring of four faces, contradicting cyclic 5-edge-connectivity of \(F\).

Hence we have that \(N(u_i) \cap N(u_j) \cap S_0 = \emptyset\) for \(i, j \in \mathbb{Z}_9\), \(j \neq i\), and therefore \(|S_0| \geq 5\). Note also that this implies that \(R\) is of type different from type (0012) and type (0021) (see also Figure 3). If \(F\lceil S_0\rceil\) and so also \(X = F\lceil S_0 + \{u_1, u_2, u_3, u_4, u_5\}\rceil\) is a forest then a simple counting argument shows that
\[
|S_0 \cup \{u_1, u_2, u_3, u_4, u_5\}| = 10 - 2p,
\]
where \(p\) is the number of connected components of \(X\). But since \(|S_0 \cup \{u_1, u_2, u_3, u_4, u_5\}| \geq 10\) and \(p \geq 1\) this is clearly impossible. Therefore \(F\lceil S_0\rceil\) contains a cycle and there exists a ring \(R'\) of five faces whose outer cycle is \(C_0\). By Lemma 2.3 either the inner cycle of \(R'\) is a pentagonal face and all faces of \(R'\) are pentagonal, or all faces of \(R'\) are hexagonal. In the first case we are done. In the second case we replace \(R\) with \(R'\) in our analyze. Continuing with this line of argument and using the fact that \(F\) is finite in some stage we have to reach a ring of five pentagonal faces giving rise to the pentacap. In particular, since a ring adjacent to a ring of type (01112), (01121) or (02102) always contains a hexagonal face this process can stop only if \(R\) is of type (11111). This completes the proof of Theorem 2.4.

We remark that Theorem 2.4 implies that fullerenes admitting a nontrivial cyclic-5-cutset are a special class of the so-called carbon nanotubes (see [17]).

3 Hamilton cycles in fullerenes admitting a nontrivial cyclic-5-cutset

In this section it is proven that the Barnette conjecture is true for fullerenes admitting a nontrivial cyclic-5-cutset (see Theorem 3.1). The key factor in the proof of this result is Theorem 2.4. In particular, by Theorem 2.4 we know that each fullerene admitting a nontrivial cyclic-5-cutset contains two antipodal pentacaps and moreover, from the proof of Theorem 2.4 one may deduce that between these two pentacaps there exist rings of five hexagonal faces (hexagonal rings) such that in each hexagon \(H\) exist two vertices, first of which has a neighbor inside the ring which \(H\) belongs to and second have a neighbor outside the ring which \(H\) belongs to.

Theorem 3.1 Let \(F\) be a fullerene admitting a nontrivial cyclic-5-cutset. Then \(F\) has a Hamilton cycle. Moreover,
(i) if the number of hexagonal faces in $F$ is odd then there exists a path of faces containing precisely two pentagons from each of the two pentacaps in $F$ whose boundary gives rise to a Hamilton cycle in $F$; and

(ii) if the number of hexagonal faces in $F$ is even then there exists a path of faces containing precisely six pentagons, of which two are from the first pentacap and four from the other pentacap, whose boundary gives rise to a Hamilton cycle in $F$.

**Proof.** By Theorem 2.4 the fullerene $F$ contains two antipodal pentacaps. From the proof of Theorem 2.4 we may deduce that between these two pentacaps there exist rings each consisting of five hexagonal faces, in short hexagonal rings, such that for each of these rings the following holds: in each hexagon in the ring there exist a vertex having a neighbor inside this ring, and a vertex having a neighbor outside this ring.

Let $k$ be the number of hexagonal faces in $F$. Observe that $k = 5r$ where $r$ is the number of hexagonal rings in $F$. We proceed the proof by induction on $r$.

If $r = 0$ then $F$ is the dodecahedron in which a path of faces containing precisely six pentagons whose boundary gives rise to a Hamilton cycle clearly exists (see also Figure 4). Further, in Figures 5 and 6 Hamilton cycles in $F$ are shown if $r = 1$ and $r = 2$. Hence, the statement of the theorem holds for $r \leq 2$.

![Figure 4: A Hamilton cycle in the dodecahedron (r = 0).](image)

![Figure 5: A Hamilton cycle in F if r = 1.](image)

![Figure 6: A Hamilton cycle in F if r = 2.](image)

Assume now that the statement of the theorem holds for fullerenes with $r > 2$ hexagonal rings and let $F$ be a fullerene admitting a nontrivial cyclic-5-cutset with $r + 1$ hexagonal rings. Denote by $R$ the hexagonal ring in $F$ adjacent to one of the two pentacaps, and denote by $R'$ the hexagonal ring adjacent to $R$. Furthermore, let $C_0$ and $C_1$ be the inner and the outer cycle of $R$, respectively. Clearly $C_1$ is the inner cycle of $R'$. Let $C_2$ be the outer cycle of $R'$. Further, let
\(v_i^j \in V(C_i), i \in \{0, 1, 2\} \) and \(j \in \mathbb{Z}_{10}\), be such that \(v_0^{2j} \sim v_1^{2j} \) and \(v_1^{2j+1} \sim v_2^{2j+1}\). Now we construct a fullerene admitting a nontrivial cyclic-5-cutset with \(r\) hexagonal rings as follows. By deleting of all the vertices on the cycle \(C_1\), that is vertices \(v_i^j, j \in \mathbb{Z}_{10}\) (with the incident edges), and by adding edges \(v_0^{2j} v_2^{2j-1}, j \in \mathbb{Z}_{10}\), we obtain a fullerene admitting a nontrivial cyclic-5-cutset with \(r\) hexagonal rings. Denote this fullerene by \(\tilde{F}\) (see Figures 7 and 8).

If \(r + 1\) is even then \(r\) is odd. Hence, by the induction hypothesis a path of faces containing precisely two pentagons from each of the two pentacaps whose boundary gives rise to a Hamilton cycle exists in \(\tilde{F}\). But then one can construct a path of faces in \(F\) containing precisely six pentagons whose boundary gives rise to a Hamilton cycle, as illustrated in Figure 7.

Suppose now that \(r + 1\) odd, \(\tilde{F}\) has an even number of hexagons. Therefore, by induction hypothesis there exists a path of faces containing precisely six pentagons, of which two are from the first pentacap and four from the other pentacap, whose boundary gives rise to a Hamilton cycle in \(\tilde{F}\). Again, one can construct a path of faces in \(F\) containing precisely two pentagons from each of the two pentacaps whose boundary gives rise to a Hamilton cycle in \(F\) as illustrated in Figure 8. This completes the proof Theorem 3.1.

![Figure 7: A local structure of a Hamilton cycle in \(\tilde{F}\) on the left-hand side picture and a local structure of a Hamilton cycle in \(F\) on the right-hand side picture for \(r + 1\) even.](image)

Observe that a path of faces in a fullerene admitting a nontrivial cyclic-5-cutset \(F\) whose boundary gives rise to a Hamilton cycle in \(F\) that was constructed in the proof of Theorem 3.1 is not unique. As illustrated in Figure 9 one can see that the following proposition holds.

**Proposition 3.2** Let \(F\) be a fullerene of order \(n\) admitting a nontrivial cyclic-5-cutset and let \(r\) be the number of hexagonal rings in \(F\). Then

(i) if \(r\) is even then \(F\) has at least \(5 \cdot 2^{r+1}\) different Hamilton cycles; and

(ii) if \(r\) is odd then \(F\) has at least \(5 \cdot 2^{r+1}\) different Hamilton cycles.

Since every Hamilton cycle in a fullerene \(F\) gives rise to three perfect matchings in \(F\), Proposition 3.2 gives a lower bound of the number on perfect matchings in a fullerene admitting a nontrivial cyclic-5-cutset. Since the number of hexagonal rings in a fullerene admitting a nontrivial cyclic-5-cutset is \(r = \frac{n}{10} - 2\) the following corollary holds.
Figure 8: A local structure of a Hamilton cycle in $\tilde{F}$ on the left-hand side picture and a local structure of a Hamilton cycle in $F$ on the right-hand side picture for $r + 1$ odd.

Figure 9: Four different paths of faces in a fullerene $F$ admitting a nontrivial cyclic-5-cutset with $r = 2$ whose boundary gives rise to a Hamilton cycle in $F$ for a chosen pentagon adjacent to the central pentagon in a pentacap. Since the pentagon adjacent to the central pentagon in the pentacap can be chosen in five different ways this fullerene has at least $5 \cdot 2^{\frac{r}{2} + 1} = 20$ different Hamilton cycles.

**Corollary 3.3** Let $F$ be a fullerene of order $n$ admitting a nontrivial cyclic-5-cutset. Then the number of perfect matchings in $F$ is at least $15 \cdot 2^{\lfloor \frac{n}{5} \rfloor}$. 
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